



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:04 AM GMT

PDB ID : 3KO1
Title : Crystal structure of thermosome from *Acidianus tengchongensis* strain S5
Authors : Huo, Y.; Zhang, K.; Hu, Z.; Wang, L.; Zhai, Y.; Zhou, Q.; Lander, G.; He, Y.;
Zhu, J.; Xu, W.; Dong, Z.; Sun, F.
Deposited on : 2009-11-12
Resolution : 3.70 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

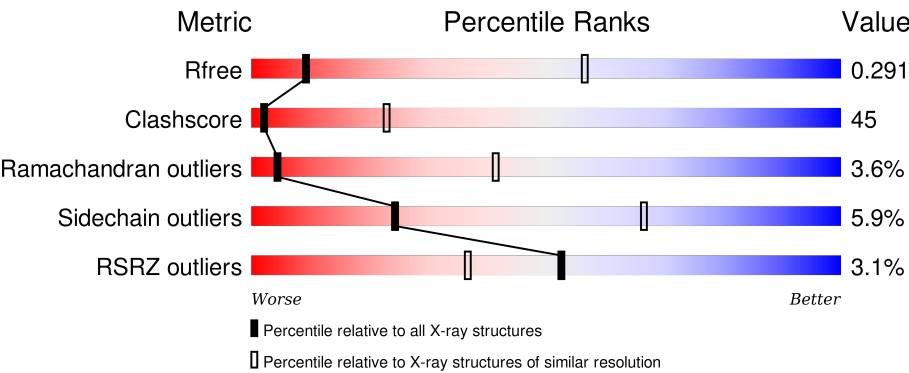
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	553	<div><div>2%</div><div>36%</div><div>50%</div><div>5%</div><div>9%</div></div>
1	B	553	<div><div>3%</div><div>36%</div><div>50%</div><div>5%</div><div>9%</div></div>
1	C	553	<div><div>3%</div><div>37%</div><div>49%</div><div>5%</div><div>9%</div></div>
1	D	553	<div><div>3%</div><div>36%</div><div>50%</div><div>5%</div><div>9%</div></div>
1	E	553	<div><div>5%</div><div>36%</div><div>50%</div><div>5%</div><div>9%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	553	
1	G	553	
1	H	553	
1	I	553	

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	ADP	D	800	-	-	-	X
2	ADP	G	800	-	-	-	X
2	ADP	H	800	-	-	-	X
2	ADP	I	800	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34884 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 Chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	0	0
			3849	2423	658	757	11			
1	B	505	Total	C	N	O	S	0	0	0
			3849	2423	658	757	11			
1	C	505	Total	C	N	O	S	0	0	0
			3849	2423	658	757	11			
1	D	505	Total	C	N	O	S	0	0	0
			3849	2423	658	757	11			
1	E	505	Total	C	N	O	S	0	0	0
			3849	2423	658	757	11			
1	F	505	Total	C	N	O	S	0	0	0
			3849	2423	658	757	11			
1	G	505	Total	C	N	O	S	0	0	0
			3849	2423	658	757	11			
1	H	505	Total	C	N	O	S	0	0	0
			3849	2423	658	757	11			
1	I	505	Total	C	N	O	S	0	0	0
			3849	2423	658	757	11			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

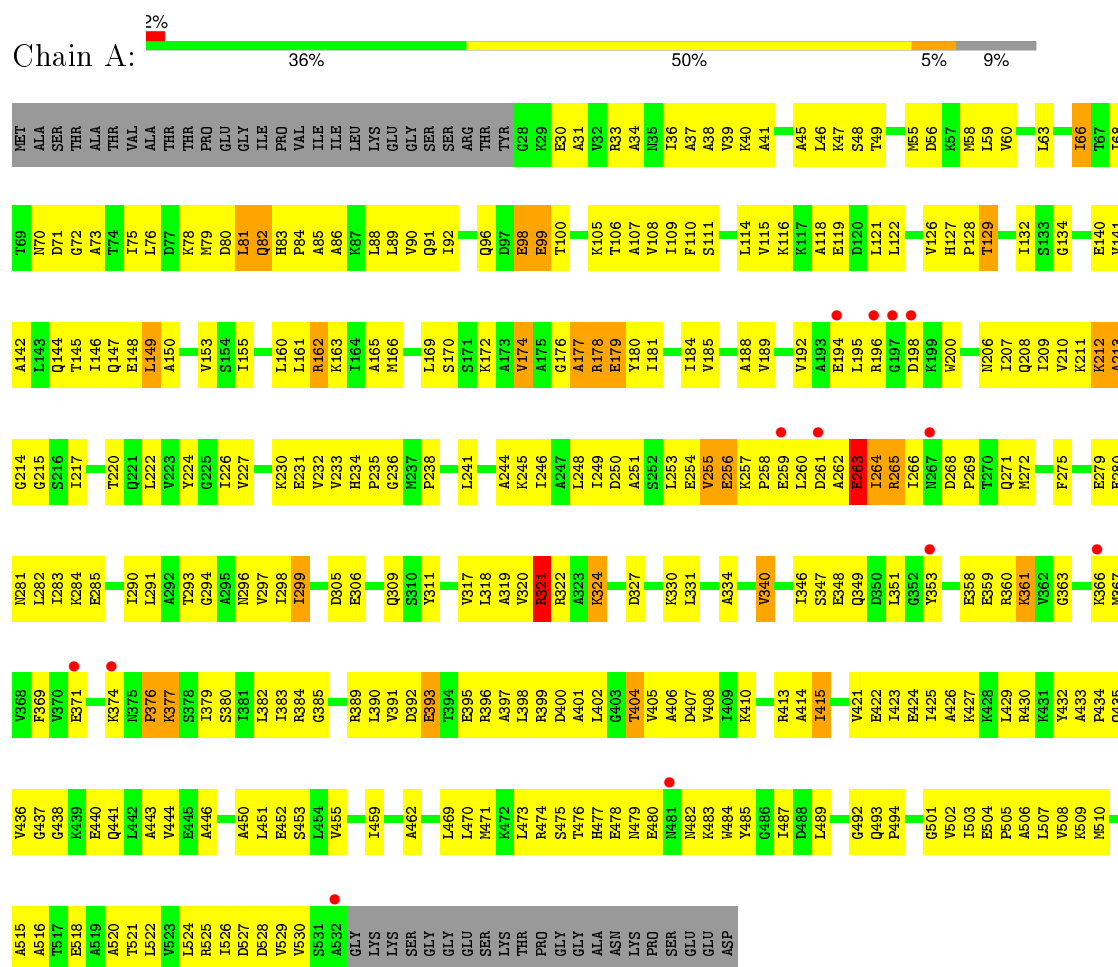


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	7	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	7	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	7	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	7	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	7	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	7	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	7	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	7	0
			27	10	5	10	2		
2	I	1	Total	C	N	O	P	7	0
			27	10	5	10	2		

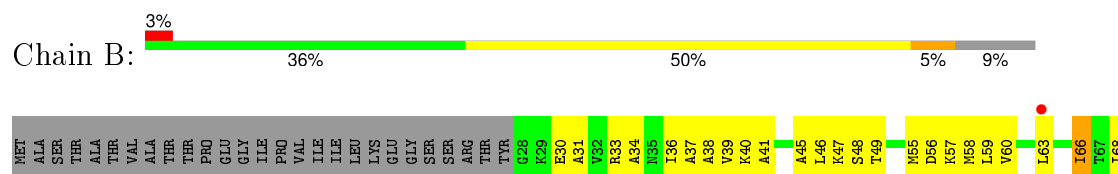
3 Residue-property plots

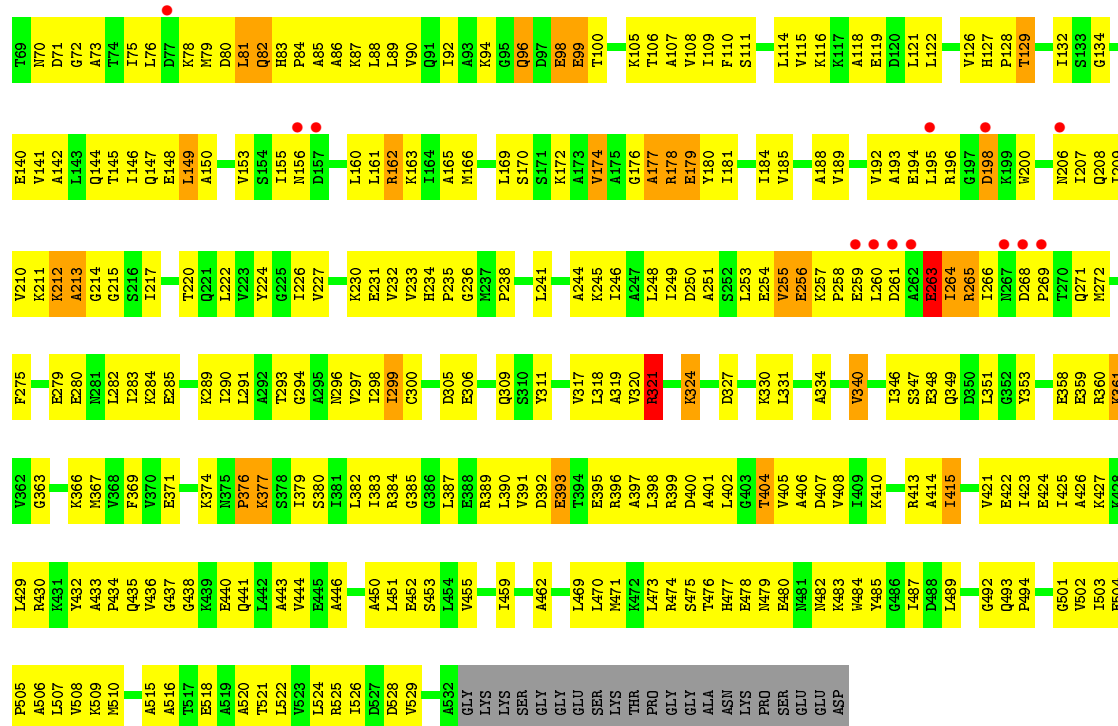
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Chaperonin

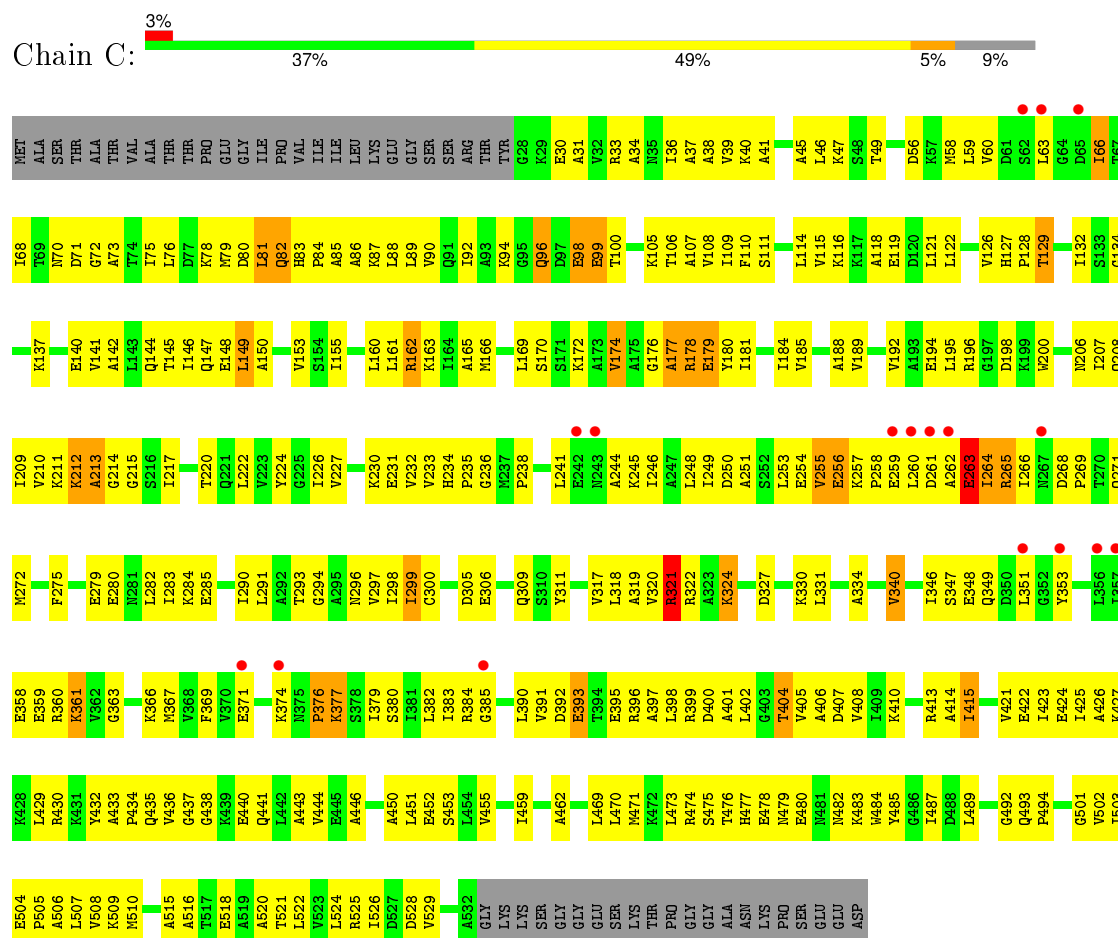


• Molecule 1: Chaperonin

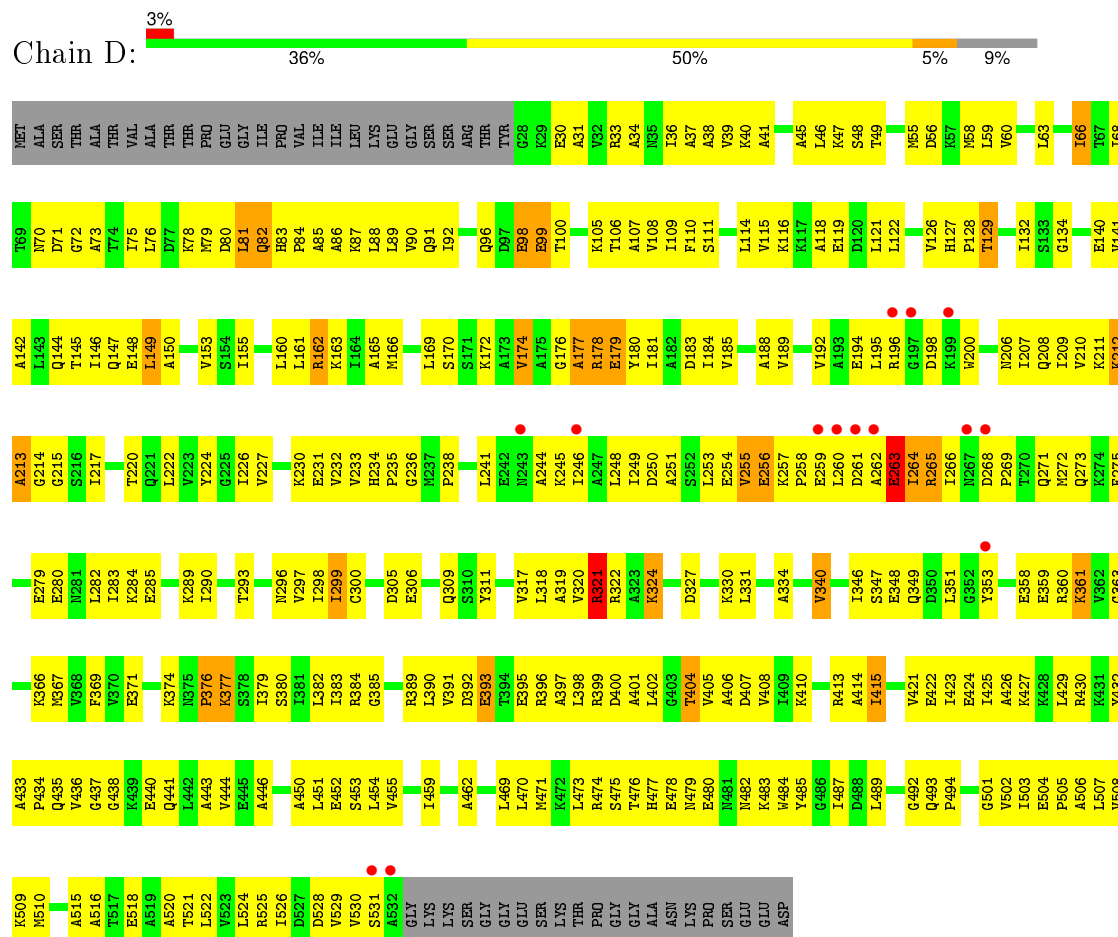




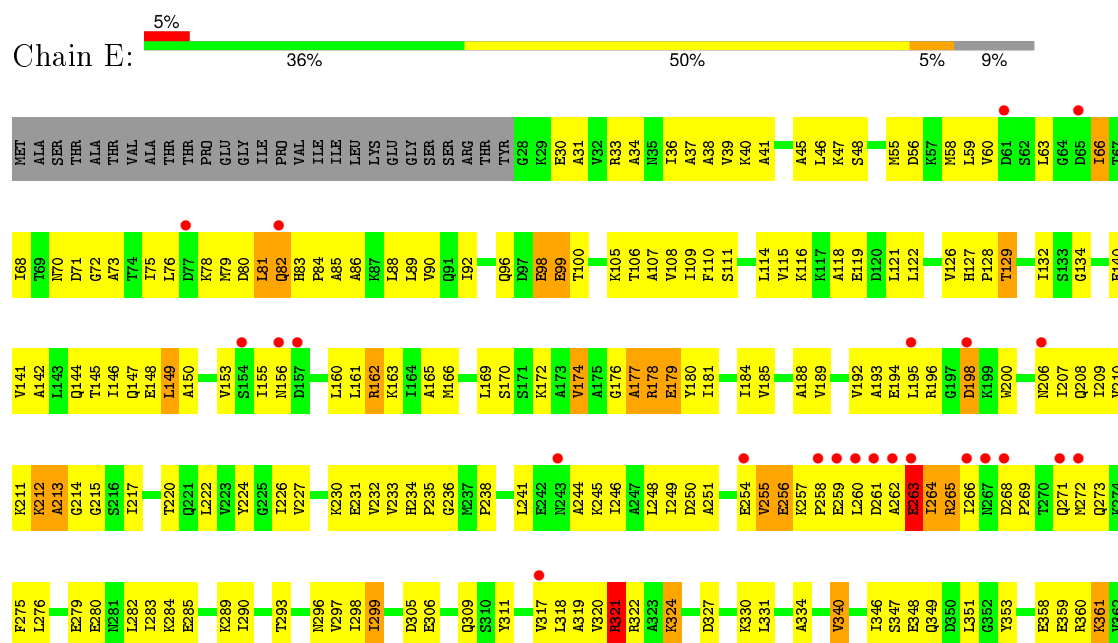
• Molecule 1: Chaperonin

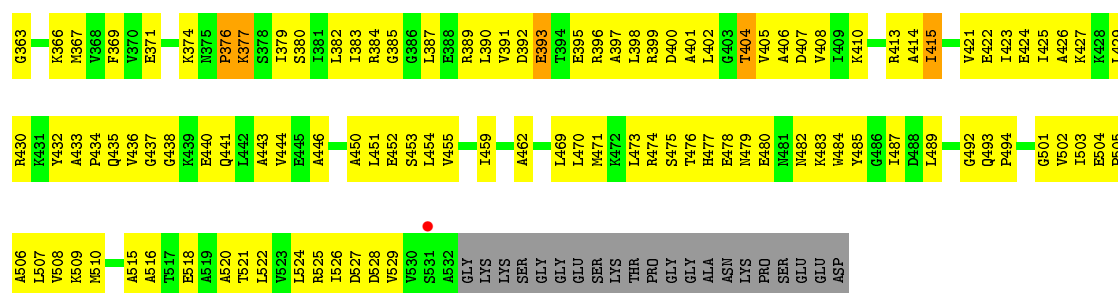


● Molecule 1: Chaperonin

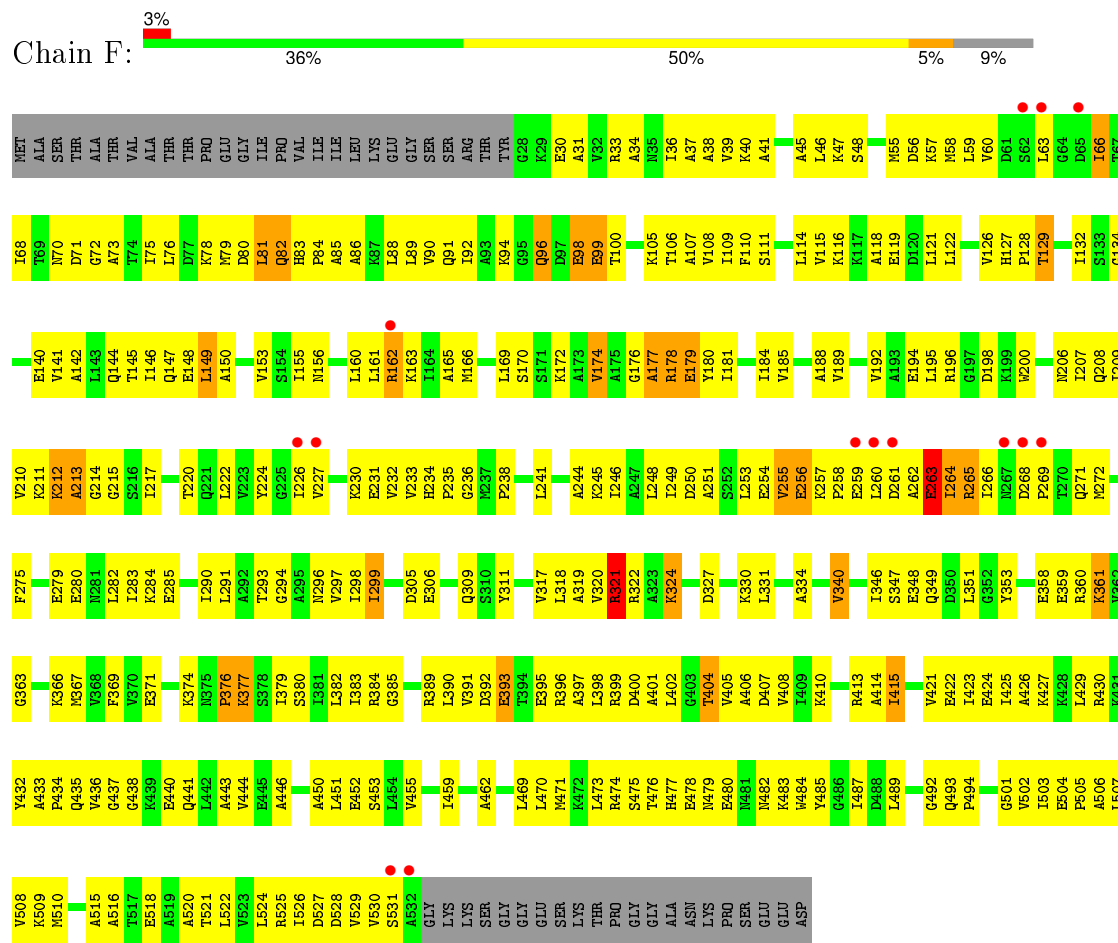


● Molecule 1: Chaperonin

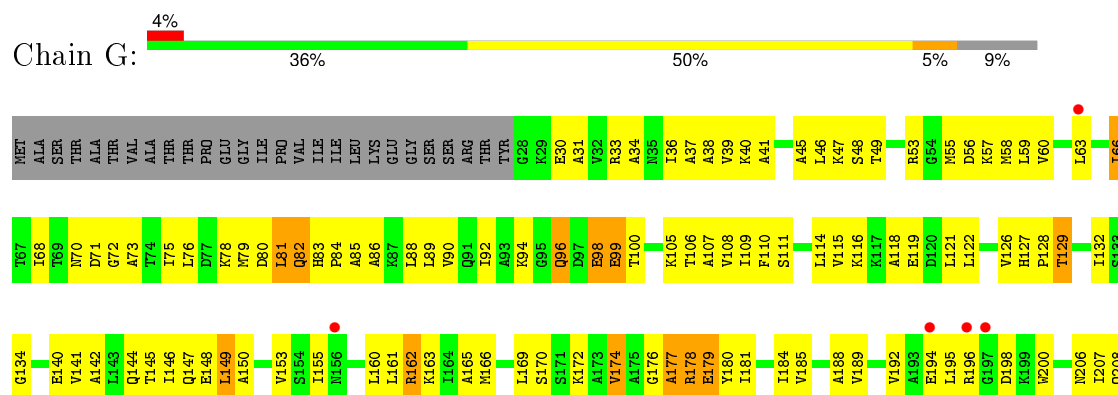


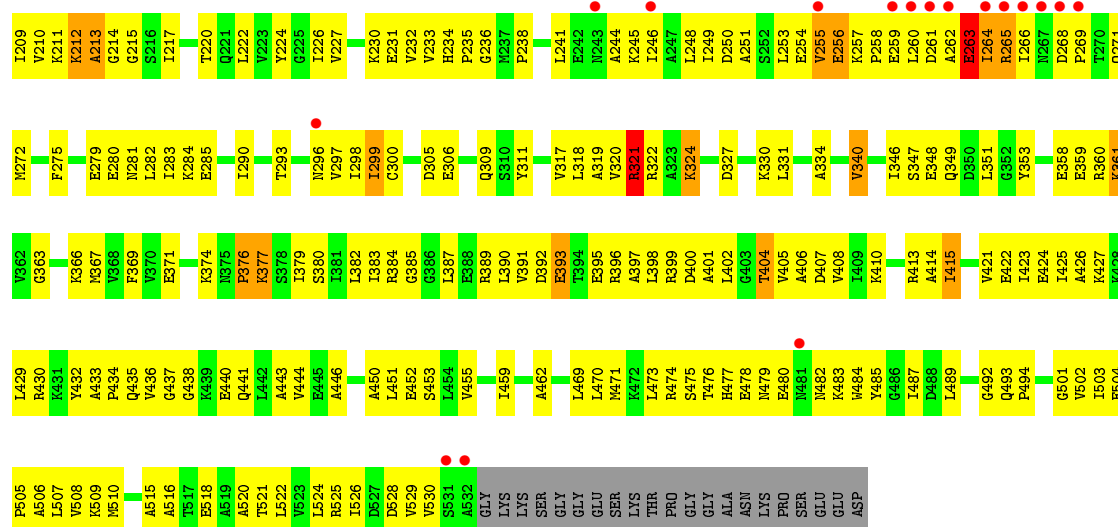


• Molecule 1: Chaperonin

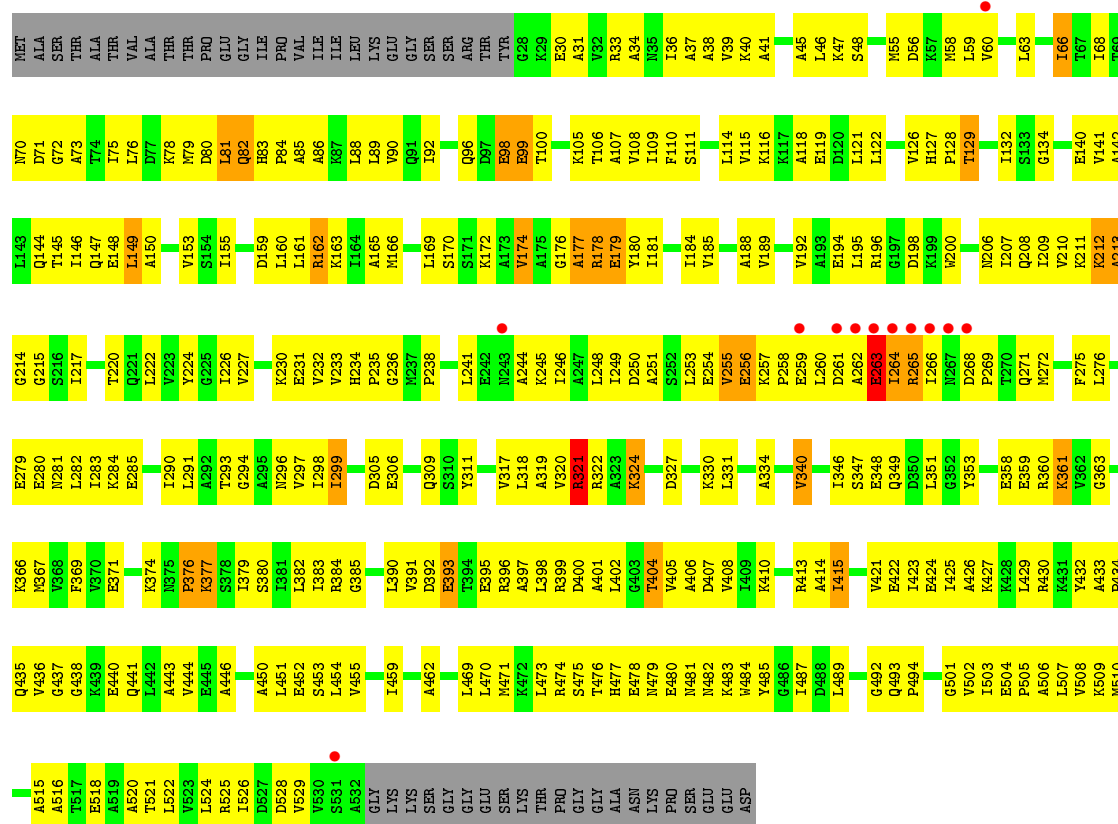


• Molecule 1: Chaperonin





• Molecule 1: Chaperonin



• Molecule 1: Chaperonin



A515	A516	T517	E518	A519	A520	T521	L522	V523	L524	R525	I526	D527	D528	V529	V530	S531	A532	GLY	LYS	LYS	SER	GLY	GLY	GLU	SER	LYS	THR	PRO	GLY	GLY	ALA	ASN	LYS	PRO	SER	GLU	GLU	ASP																	
V436	G437	G438	K439	E440	Q441	L442	A443	P444	E445	A446	A450	L451	E452	S453	L454	V455	L459	L469	L470	M471	K472	L473	R474	S475	T476	H477	E478	M479	E480	M481	K482	K483	M484	G486	L487	D488	L489	G492	Q493	P494	G501	V502	I503	E504	P505	A506	L507	V508	R509	M510					
M367	V368	F369	V370	E371	K374	R375	P376	K377	S378	I379	S380	I381	L382	I383	R384	G385	L390	V391	D392	E393	T394	E395	R396	A397	L398	R399	D400	A401	L402	G403	T404	V405	A406	D407	V408	I409	K410	R413	A414	I415	V421	E422	I423	E424	I425	A426	K427	L428	L429	R430	K431	Y432	A433	P434	Q435
E279	E280	N281	L282	L283	K284	E285	L290	T293	N296	V297	L298	I299	D305	E306	D309	S310	Y311	V317	L318	A319	V320	R321	R322	K323	K324	D327	K330	L331	A334	V340	T346	S347	E348	Q349	D350	L351	G352	Y353	E358	E359	R360	K361	V362	G363	K366										
A142	L143	Q144	T145	I146	Q147	E148	L149	A150	V153	G154	L155	M156	L160	L161	R162	K163	I164	M166	L169	S170	S171	K172	A173	V174	A175	G176	A177	R178	E179	V180	I181	I184	V185	A188	V189	V192	A193	E194	L195	R196	G197	D198	K199	W200	N206	I207	Q208	L209	V210	E140	K211				
T69	N70	D71	G72	A73	T74	L75	D77	K78	M79	D80	L81	Q82	H83	P84	A85	A86	K87	L88	L89	V90	Q91	I92	Q96	D97	E98	E99	T100	K105	T106	A107	V108	I109	F110	S111	L114	V115	K116	K117	A118	E119	D120	L121	L122	V126	H127	P128	T129	I132	S133	G134	E140	V141			
A213	G214	G215	S216	I217	T220	Q221	L222	Y224	G225	I226	V227	K230	E231	V232	V233	H234	P235	G236	M237	P238	L241	E242	I243	A244	K245	I246	A247	L248	I249	D250	A251	S252	L253	E254	V255	E256	K257	P258	E259	L260	D261	A262	E263	I264	R265	L266	E267	D268	P269	T270	Q271	M272	F275	L276	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	223.67Å 283.04Å 160.75Å 90.00° 133.90° 90.00°	Depositor
Resolution (Å)	48.39 – 3.70 48.39 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.39-3.70) 99.5 (48.39-3.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 3.67Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.277 , 0.283 0.286 , 0.291	Depositor DCC
R_{free} test set	3825 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	98.4	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 72.6	EDS
Estimated twinning fraction	0.080 for h+2*k,-h-l 0.099 for -h-2*k,-k,l 0.089 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	1 of 76142 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	34884	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ADP

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	0.46	0/3886	0.67	3/5245 (0.1%)
1	B	0.46	0/3886	0.67	3/5245 (0.1%)
1	C	0.46	0/3886	0.67	3/5245 (0.1%)
1	D	0.46	0/3886	0.67	3/5245 (0.1%)
1	E	0.46	0/3886	0.67	3/5245 (0.1%)
1	F	0.46	0/3886	0.67	3/5245 (0.1%)
1	G	0.46	0/3886	0.67	3/5245 (0.1%)
1	H	0.46	0/3886	0.67	3/5245 (0.1%)
1	I	0.46	0/3886	0.67	3/5245 (0.1%)
All	All	0.46	0/34974	0.67	27/47205 (0.1%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	257	LYS	C-N-CD	-7.18	104.80	120.60
1	B	257	LYS	C-N-CD	-7.18	104.81	120.60
1	F	257	LYS	C-N-CD	-7.18	104.81	120.60
1	H	257	LYS	C-N-CD	-7.17	104.81	120.60
1	A	257	LYS	C-N-CD	-7.17	104.83	120.60
1	D	257	LYS	C-N-CD	-7.16	104.85	120.60
1	I	257	LYS	C-N-CD	-7.16	104.86	120.60
1	C	257	LYS	C-N-CD	-7.15	104.86	120.60
1	G	257	LYS	C-N-CD	-7.15	104.87	120.60
1	D	263	GLU	N-CA-C	-6.08	94.59	111.00
1	G	263	GLU	N-CA-C	-6.06	94.63	111.00
1	A	263	GLU	N-CA-C	-6.06	94.64	111.00
1	F	263	GLU	N-CA-C	-6.06	94.64	111.00
1	B	263	GLU	N-CA-C	-6.06	94.64	111.00
1	C	263	GLU	N-CA-C	-6.06	94.64	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	263	GLU	N-CA-C	-6.06	94.64	111.00
1	I	263	GLU	N-CA-C	-6.06	94.65	111.00
1	H	263	GLU	N-CA-C	-6.04	94.69	111.00
1	C	257	LYS	N-CA-C	-5.29	96.71	111.00
1	E	257	LYS	N-CA-C	-5.29	96.71	111.00
1	A	257	LYS	N-CA-C	-5.29	96.72	111.00
1	D	257	LYS	N-CA-C	-5.29	96.72	111.00
1	G	257	LYS	N-CA-C	-5.29	96.72	111.00
1	I	257	LYS	N-CA-C	-5.29	96.73	111.00
1	F	257	LYS	N-CA-C	-5.28	96.74	111.00
1	B	257	LYS	N-CA-C	-5.28	96.74	111.00
1	H	257	LYS	N-CA-C	-5.27	96.76	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3849	0	3995	360	2
1	B	3849	0	3995	358	11
1	C	3849	0	3995	346	5
1	D	3849	0	3995	363	6
1	E	3849	0	3995	378	12
1	F	3849	0	3995	389	1
1	G	3849	0	3995	374	2
1	H	3849	0	3995	348	11
1	I	3849	0	3995	351	3
2	A	27	0	12	1	0
2	B	27	0	12	1	0
2	C	27	0	12	1	0
2	D	27	0	12	1	0
2	E	27	0	12	1	0
2	F	27	0	12	1	0
2	G	27	0	12	1	0
2	H	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	27	0	12	1	0
All	All	34884	0	36063	3175	28

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 45.

All (3175) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:LEU:HD12	1:D:261:ASP:N	1.43	1.34
1:A:260:LEU:HD12	1:A:261:ASP:N	1.43	1.33
1:G:260:LEU:HD12	1:G:261:ASP:N	1.43	1.32
1:E:260:LEU:HD12	1:E:261:ASP:N	1.43	1.32
1:H:260:LEU:HD12	1:H:261:ASP:N	1.43	1.32
1:F:260:LEU:HD12	1:F:261:ASP:N	1.43	1.32
1:B:260:LEU:HD12	1:B:261:ASP:N	1.43	1.30
1:C:260:LEU:HD12	1:C:261:ASP:N	1.43	1.30
1:I:260:LEU:HD12	1:I:261:ASP:N	1.43	1.30
1:G:256:GLU:O	1:G:258:PRO:HD3	1.38	1.22
1:B:256:GLU:O	1:B:258:PRO:HD3	1.38	1.22
1:F:256:GLU:O	1:F:258:PRO:HD3	1.38	1.21
1:D:256:GLU:O	1:D:258:PRO:HD3	1.38	1.20
1:E:256:GLU:O	1:E:258:PRO:HD3	1.38	1.20
1:I:256:GLU:O	1:I:258:PRO:HD3	1.38	1.19
1:A:256:GLU:O	1:A:258:PRO:HD3	1.38	1.19
1:H:256:GLU:O	1:H:258:PRO:HD3	1.38	1.19
1:B:60:VAL:HG22	1:B:66:ILE:HG22	1.23	1.17
1:I:60:VAL:HG22	1:I:66:ILE:HG22	1.23	1.17
1:C:256:GLU:O	1:C:258:PRO:HD3	1.39	1.17
1:F:185:VAL:HG13	1:F:402:LEU:HD23	1.32	1.12
1:I:185:VAL:HG13	1:I:402:LEU:HD23	1.32	1.12
1:H:60:VAL:HG22	1:H:66:ILE:HG22	1.23	1.12
1:G:60:VAL:HG22	1:G:66:ILE:HG22	1.23	1.11
1:C:60:VAL:HG22	1:C:66:ILE:HG22	1.23	1.10
1:F:60:VAL:HG22	1:F:66:ILE:HG22	1.23	1.10
1:E:185:VAL:HG13	1:E:402:LEU:HD23	1.32	1.10
1:D:60:VAL:HG22	1:D:66:ILE:HG22	1.23	1.10
1:A:60:VAL:HG22	1:A:66:ILE:HG22	1.23	1.10
1:E:60:VAL:HG22	1:E:66:ILE:HG22	1.23	1.10
1:G:185:VAL:HG13	1:G:402:LEU:HD23	1.31	1.08
1:D:185:VAL:HG13	1:D:402:LEU:HD23	1.31	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:VAL:HG13	1:B:402:LEU:HD23	1.31	1.08
1:A:185:VAL:HG13	1:A:402:LEU:HD23	1.32	1.07
1:H:185:VAL:HG13	1:H:402:LEU:HD23	1.31	1.06
1:C:185:VAL:HG13	1:C:402:LEU:HD23	1.31	1.06
1:F:529:VAL:HG12	1:G:58:MET:HB3	1.15	1.06
1:E:522:LEU:HD11	1:F:68:ILE:HD12	1.37	1.04
1:I:260:LEU:HD12	1:I:261:ASP:H	1.23	1.02
1:E:260:LEU:HD12	1:E:261:ASP:H	1.23	1.01
1:A:260:LEU:HD12	1:A:261:ASP:H	1.23	1.01
1:F:260:LEU:HD12	1:F:261:ASP:H	1.23	1.01
1:D:529:VAL:HG12	1:E:58:MET:HB3	1.40	1.01
1:E:522:LEU:HD11	1:F:68:ILE:CD1	1.89	1.00
1:I:245:LYS:N	1:I:296:ASN:HD22	1.61	0.99
1:G:245:LYS:N	1:G:296:ASN:HD22	1.61	0.99
1:D:245:LYS:N	1:D:296:ASN:HD22	1.61	0.99
1:H:245:LYS:N	1:H:296:ASN:HD22	1.61	0.98
1:B:245:LYS:N	1:B:296:ASN:HD22	1.61	0.98
1:E:245:LYS:N	1:E:296:ASN:HD22	1.61	0.97
1:C:245:LYS:N	1:C:296:ASN:HD22	1.61	0.96
1:B:421:VAL:O	1:B:425:ILE:HG12	1.66	0.96
1:F:245:LYS:N	1:F:296:ASN:HD22	1.61	0.96
1:F:529:VAL:HG12	1:G:58:MET:CB	1.94	0.96
1:I:421:VAL:O	1:I:425:ILE:HG12	1.66	0.96
1:D:421:VAL:O	1:D:425:ILE:HG12	1.66	0.96
1:C:421:VAL:O	1:C:425:ILE:HG12	1.66	0.96
1:H:421:VAL:O	1:H:425:ILE:HG12	1.66	0.96
1:A:245:LYS:N	1:A:296:ASN:HD22	1.61	0.95
1:F:421:VAL:O	1:F:425:ILE:HG12	1.66	0.95
1:E:423:ILE:HD12	1:E:424:GLU:N	1.82	0.95
1:A:423:ILE:HD12	1:A:424:GLU:N	1.82	0.95
1:F:423:ILE:HD12	1:F:424:GLU:N	1.82	0.95
1:G:423:ILE:HD12	1:G:424:GLU:N	1.82	0.95
1:I:423:ILE:HD12	1:I:424:GLU:N	1.82	0.95
1:H:423:ILE:HD12	1:H:424:GLU:N	1.82	0.95
1:B:423:ILE:HD12	1:B:424:GLU:N	1.82	0.95
1:E:66:ILE:HD13	1:E:66:ILE:H	1.32	0.94
1:C:423:ILE:HD12	1:C:424:GLU:N	1.82	0.94
1:G:421:VAL:O	1:G:425:ILE:HG12	1.66	0.94
1:I:66:ILE:HD13	1:I:66:ILE:H	1.32	0.94
1:D:423:ILE:HD12	1:D:424:GLU:N	1.82	0.94
1:H:260:LEU:HD12	1:H:261:ASP:H	1.23	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:421:VAL:O	1:E:425:ILE:HG12	1.66	0.94
1:A:66:ILE:HD13	1:A:66:ILE:H	1.32	0.94
1:G:260:LEU:HD12	1:G:261:ASP:H	1.23	0.94
1:C:260:LEU:HD12	1:C:261:ASP:H	1.23	0.94
1:A:421:VAL:O	1:A:425:ILE:HG12	1.66	0.93
1:D:66:ILE:HD13	1:D:66:ILE:H	1.32	0.93
1:B:66:ILE:HD13	1:B:66:ILE:H	1.32	0.93
1:C:66:ILE:HD13	1:C:66:ILE:H	1.32	0.93
1:H:66:ILE:H	1:H:66:ILE:HD13	1.32	0.92
1:B:260:LEU:HD12	1:B:261:ASP:H	1.23	0.91
1:D:400:ASP:O	1:D:404:THR:HG22	1.71	0.91
1:G:256:GLU:O	1:G:258:PRO:CD	2.19	0.91
1:I:212:LYS:HA	1:I:212:LYS:HE2	1.53	0.91
1:C:212:LYS:HA	1:C:212:LYS:HE2	1.53	0.91
1:E:212:LYS:HE2	1:E:212:LYS:HA	1.53	0.91
1:D:256:GLU:O	1:D:258:PRO:CD	2.19	0.90
1:G:400:ASP:O	1:G:404:THR:HG22	1.71	0.90
1:A:400:ASP:O	1:A:404:THR:HG22	1.71	0.90
1:D:260:LEU:HD12	1:D:261:ASP:H	1.23	0.90
1:G:212:LYS:HE2	1:G:212:LYS:HA	1.53	0.90
1:A:256:GLU:O	1:A:258:PRO:CD	2.19	0.90
1:G:66:ILE:H	1:G:66:ILE:HD13	1.32	0.90
1:E:256:GLU:O	1:E:258:PRO:CD	2.19	0.90
1:E:258:PRO:HG2	1:E:279:GLU:OE2	1.72	0.90
1:F:66:ILE:HD13	1:F:66:ILE:H	1.32	0.90
1:H:256:GLU:O	1:H:258:PRO:CD	2.19	0.90
1:B:400:ASP:O	1:B:404:THR:HG22	1.71	0.89
1:F:258:PRO:HG2	1:F:279:GLU:OE2	1.72	0.89
1:C:258:PRO:HG2	1:C:279:GLU:OE2	1.72	0.89
1:B:212:LYS:HA	1:B:212:LYS:HE2	1.53	0.89
1:F:400:ASP:O	1:F:404:THR:HG22	1.71	0.89
1:B:258:PRO:HG2	1:B:279:GLU:OE2	1.72	0.89
1:A:258:PRO:HG2	1:A:279:GLU:OE2	1.72	0.89
1:C:256:GLU:O	1:C:258:PRO:CD	2.19	0.89
1:I:400:ASP:O	1:I:404:THR:HG22	1.71	0.89
1:G:258:PRO:HG2	1:G:279:GLU:OE2	1.72	0.89
1:D:258:PRO:HG2	1:D:279:GLU:OE2	1.72	0.89
1:F:260:LEU:CD1	1:F:261:ASP:N	2.35	0.89
1:H:260:LEU:CD1	1:H:261:ASP:N	2.35	0.89
1:F:256:GLU:O	1:F:258:PRO:CD	2.19	0.89
1:E:88:LEU:HD11	1:F:389:ARG:HH12	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:212:LYS:HA	1:H:212:LYS:HE2	1.53	0.89
1:A:212:LYS:HA	1:A:212:LYS:HE2	1.53	0.89
1:I:258:PRO:HG2	1:I:279:GLU:OE2	1.72	0.88
1:D:212:LYS:HE2	1:D:212:LYS:HA	1.53	0.88
1:H:400:ASP:O	1:H:404:THR:HG22	1.71	0.88
1:E:400:ASP:O	1:E:404:THR:HG22	1.71	0.88
1:B:256:GLU:O	1:B:258:PRO:CD	2.19	0.88
1:C:400:ASP:O	1:C:404:THR:HG22	1.71	0.88
1:F:212:LYS:HA	1:F:212:LYS:HE2	1.53	0.88
1:F:88:LEU:HD11	1:G:389:ARG:HH12	1.36	0.88
1:H:258:PRO:HG2	1:H:279:GLU:OE2	1.72	0.88
1:I:256:GLU:O	1:I:258:PRO:CD	2.19	0.87
1:A:58:MET:HB3	1:I:529:VAL:HG12	1.57	0.87
1:G:260:LEU:CD1	1:G:261:ASP:N	2.35	0.87
1:B:260:LEU:CD1	1:B:261:ASP:N	2.35	0.87
1:A:217:ILE:HG12	1:A:385:GLY:HA2	1.57	0.87
1:D:269:PRO:HA	1:D:272:MET:HG2	1.57	0.87
1:F:217:ILE:HG12	1:F:385:GLY:HA2	1.57	0.87
1:B:269:PRO:HA	1:B:272:MET:HG2	1.57	0.86
1:A:530:VAL:O	1:B:59:LEU:HD23	1.75	0.86
1:G:217:ILE:HG12	1:G:385:GLY:HA2	1.57	0.86
1:A:269:PRO:HA	1:A:272:MET:HG2	1.57	0.86
1:D:217:ILE:HG12	1:D:385:GLY:HA2	1.57	0.86
1:B:217:ILE:HG12	1:B:385:GLY:HA2	1.57	0.86
1:E:269:PRO:HA	1:E:272:MET:HG2	1.57	0.86
1:C:260:LEU:CD1	1:C:261:ASP:N	2.35	0.86
1:C:269:PRO:HA	1:C:272:MET:HG2	1.57	0.86
1:H:269:PRO:HA	1:H:272:MET:HG2	1.57	0.85
1:I:217:ILE:HG12	1:I:385:GLY:HA2	1.57	0.85
1:F:269:PRO:HA	1:F:272:MET:HG2	1.57	0.85
1:C:217:ILE:HG12	1:C:385:GLY:HA2	1.57	0.85
1:I:361:LYS:HB3	1:I:366:LYS:HG2	1.59	0.85
1:I:269:PRO:HA	1:I:272:MET:HG2	1.57	0.85
1:D:361:LYS:HB3	1:D:366:LYS:HG2	1.59	0.85
1:E:260:LEU:CD1	1:E:261:ASP:N	2.35	0.85
1:F:361:LYS:HB3	1:F:366:LYS:HG2	1.59	0.84
1:G:269:PRO:HA	1:G:272:MET:HG2	1.57	0.84
1:E:217:ILE:HG12	1:E:385:GLY:HA2	1.57	0.84
1:A:260:LEU:CD1	1:A:261:ASP:N	2.35	0.84
1:C:76:LEU:HD23	1:C:90:VAL:HG12	1.60	0.84
1:H:361:LYS:HB3	1:H:366:LYS:HG2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:LYS:HB3	1:C:366:LYS:HG2	1.59	0.84
1:H:76:LEU:HD23	1:H:90:VAL:HG12	1.60	0.84
1:F:529:VAL:CG1	1:G:58:MET:HB3	2.04	0.84
1:B:361:LYS:HB3	1:B:366:LYS:HG2	1.59	0.84
1:H:217:ILE:HG12	1:H:385:GLY:HA2	1.57	0.84
1:D:260:LEU:CD1	1:D:261:ASP:N	2.35	0.83
1:B:76:LEU:HD23	1:B:90:VAL:HG12	1.60	0.83
1:E:361:LYS:HB3	1:E:366:LYS:HG2	1.59	0.83
1:D:76:LEU:HD23	1:D:90:VAL:HG12	1.60	0.83
1:E:76:LEU:HD23	1:E:90:VAL:HG12	1.60	0.83
1:I:76:LEU:HD23	1:I:90:VAL:HG12	1.60	0.83
1:A:361:LYS:HB3	1:A:366:LYS:HG2	1.59	0.83
1:G:76:LEU:HD23	1:G:90:VAL:HG12	1.60	0.82
1:D:245:LYS:H	1:D:296:ASN:HD22	1.28	0.82
1:F:76:LEU:HD23	1:F:90:VAL:HG12	1.60	0.82
1:A:76:LEU:HD23	1:A:90:VAL:HG12	1.60	0.82
1:I:260:LEU:CD1	1:I:261:ASP:N	2.35	0.81
1:C:245:LYS:H	1:C:296:ASN:HD22	1.28	0.81
1:F:530:VAL:O	1:G:59:LEU:HD23	1.80	0.81
1:G:361:LYS:HB3	1:G:366:LYS:HG2	1.59	0.81
1:F:88:LEU:CD1	1:G:389:ARG:HH12	1.93	0.81
1:C:290:ILE:O	1:C:293:THR:HG22	1.82	0.80
1:H:60:VAL:HG22	1:H:66:ILE:CG2	2.10	0.80
1:A:290:ILE:O	1:A:293:THR:HG22	1.82	0.80
1:B:245:LYS:H	1:B:296:ASN:HD22	1.28	0.80
1:H:260:LEU:CD1	1:H:261:ASP:OD1	2.30	0.80
1:A:260:LEU:CD1	1:A:261:ASP:OD1	2.30	0.80
1:D:290:ILE:O	1:D:293:THR:HG22	1.82	0.80
1:I:245:LYS:H	1:I:296:ASN:HD22	1.28	0.80
1:E:260:LEU:CD1	1:E:261:ASP:OD1	2.30	0.80
1:G:60:VAL:HG22	1:G:66:ILE:CG2	2.10	0.80
1:G:245:LYS:H	1:G:296:ASN:HD22	1.28	0.80
1:G:290:ILE:O	1:G:293:THR:HG22	1.81	0.80
1:C:260:LEU:CD1	1:C:261:ASP:OD1	2.30	0.80
1:B:290:ILE:O	1:B:293:THR:HG22	1.82	0.80
1:H:290:ILE:O	1:H:293:THR:HG22	1.82	0.80
1:C:351:LEU:HD23	1:C:351:LEU:H	1.48	0.79
1:B:260:LEU:CD1	1:B:261:ASP:OD1	2.30	0.79
1:I:260:LEU:CD1	1:I:261:ASP:OD1	2.30	0.79
1:F:245:LYS:H	1:F:296:ASN:HD22	1.28	0.79
1:A:245:LYS:H	1:A:296:ASN:HD22	1.28	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:351:LEU:HD23	1:G:351:LEU:H	1.47	0.79
1:A:529:VAL:HG12	1:B:58:MET:HB3	1.63	0.79
1:D:260:LEU:CD1	1:D:261:ASP:OD1	2.30	0.79
1:E:60:VAL:HG22	1:E:66:ILE:CG2	2.10	0.79
1:G:260:LEU:CD1	1:G:261:ASP:OD1	2.30	0.79
1:F:351:LEU:HD23	1:F:351:LEU:H	1.48	0.79
1:I:290:ILE:O	1:I:293:THR:HG22	1.82	0.79
1:F:290:ILE:O	1:F:293:THR:HG22	1.81	0.79
1:E:290:ILE:O	1:E:293:THR:HG22	1.82	0.79
1:H:351:LEU:HD23	1:H:351:LEU:H	1.48	0.79
1:B:351:LEU:H	1:B:351:LEU:HD23	1.48	0.79
1:F:260:LEU:CD1	1:F:261:ASP:OD1	2.30	0.79
1:E:351:LEU:HD23	1:E:351:LEU:H	1.48	0.79
1:D:60:VAL:HG22	1:D:66:ILE:CG2	2.10	0.78
1:E:245:LYS:H	1:E:296:ASN:HD22	1.28	0.78
1:I:351:LEU:HD23	1:I:351:LEU:H	1.48	0.78
1:H:60:VAL:CG2	1:H:66:ILE:HG22	2.12	0.78
1:G:141:VAL:HG21	1:G:432:TYR:CD1	2.19	0.78
1:F:290:ILE:HG21	1:F:298:ILE:HD12	1.66	0.78
1:I:141:VAL:HG21	1:I:432:TYR:CD1	2.19	0.78
1:A:129:THR:HG21	1:B:462:ALA:O	1.83	0.78
1:F:91:GLN:HE21	1:G:387:LEU:HD21	1.49	0.78
1:A:60:VAL:HG22	1:A:66:ILE:CG2	2.10	0.78
1:I:290:ILE:HG21	1:I:298:ILE:HD12	1.66	0.78
1:B:141:VAL:HG21	1:B:432:TYR:CD1	2.19	0.78
1:A:351:LEU:H	1:A:351:LEU:HD23	1.47	0.78
1:D:60:VAL:CG2	1:D:66:ILE:HG22	2.12	0.77
1:G:290:ILE:HG21	1:G:298:ILE:HD12	1.66	0.77
1:E:290:ILE:HG21	1:E:298:ILE:HD12	1.66	0.77
1:D:351:LEU:H	1:D:351:LEU:HD23	1.47	0.77
1:D:141:VAL:HG21	1:D:432:TYR:CD1	2.19	0.77
1:F:141:VAL:HG21	1:F:432:TYR:CD1	2.19	0.77
1:H:141:VAL:HG21	1:H:432:TYR:CD1	2.19	0.77
1:A:290:ILE:HG21	1:A:298:ILE:HD12	1.66	0.77
1:I:60:VAL:HG22	1:I:66:ILE:CG2	2.10	0.77
1:F:91:GLN:NE2	1:G:387:LEU:HD21	2.00	0.77
1:D:433:ALA:O	1:D:436:VAL:HG22	1.85	0.77
1:C:141:VAL:HG21	1:C:432:TYR:CD1	2.19	0.76
1:E:433:ALA:O	1:E:436:VAL:HG22	1.85	0.76
1:F:60:VAL:HG22	1:F:66:ILE:CG2	2.10	0.76
1:A:60:VAL:CG2	1:A:66:ILE:HG22	2.12	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:ILE:HG21	1:D:298:ILE:HD12	1.66	0.76
1:C:60:VAL:HG22	1:C:66:ILE:CG2	2.10	0.76
1:E:141:VAL:HG21	1:E:432:TYR:CD1	2.19	0.76
1:A:141:VAL:HG21	1:A:432:TYR:CD1	2.19	0.76
1:C:60:VAL:CG2	1:C:66:ILE:HG22	2.12	0.76
1:F:60:VAL:CG2	1:F:66:ILE:HG22	2.12	0.76
1:B:220:THR:HG22	1:B:384:ARG:N	2.01	0.76
1:H:290:ILE:HG21	1:H:298:ILE:HD12	1.66	0.76
1:G:433:ALA:O	1:G:436:VAL:HG22	1.85	0.76
1:B:433:ALA:O	1:B:436:VAL:HG22	1.85	0.76
1:H:433:ALA:O	1:H:436:VAL:HG22	1.85	0.76
1:D:88:LEU:HD11	1:E:389:ARG:HH12	1.50	0.76
1:B:290:ILE:HG21	1:B:298:ILE:HD12	1.66	0.76
1:H:220:THR:HG22	1:H:384:ARG:N	2.01	0.76
1:C:290:ILE:HG21	1:C:298:ILE:HD12	1.66	0.76
1:D:220:THR:HG22	1:D:384:ARG:N	2.01	0.76
1:I:433:ALA:O	1:I:436:VAL:HG22	1.85	0.76
1:A:433:ALA:O	1:A:436:VAL:HG22	1.85	0.76
1:H:254:GLU:HA	1:H:305:ASP:HB2	1.68	0.76
1:H:89:LEU:HD21	1:H:108:VAL:HG23	1.68	0.76
1:G:254:GLU:HA	1:G:305:ASP:HB2	1.68	0.75
1:E:89:LEU:HD21	1:E:108:VAL:HG23	1.68	0.75
1:I:220:THR:HG22	1:I:384:ARG:N	2.01	0.75
1:H:245:LYS:H	1:H:296:ASN:HD22	1.28	0.75
1:E:141:VAL:HG21	1:E:432:TYR:CE1	2.21	0.75
1:D:141:VAL:HG21	1:D:432:TYR:CE1	2.21	0.75
1:C:433:ALA:O	1:C:436:VAL:HG22	1.85	0.75
1:C:220:THR:HG22	1:C:384:ARG:N	2.01	0.75
1:F:433:ALA:O	1:F:436:VAL:HG22	1.85	0.75
1:E:526:ILE:HD12	1:F:58:MET:HB2	1.68	0.75
1:E:220:THR:HG22	1:E:384:ARG:N	2.01	0.75
1:F:527:ASP:HB2	1:G:55:MET:HB3	1.69	0.75
1:E:254:GLU:HA	1:E:305:ASP:HB2	1.68	0.75
1:G:424:GLU:OE2	1:G:477:HIS:CD2	2.40	0.75
1:C:424:GLU:OE2	1:C:477:HIS:CD2	2.40	0.75
1:I:141:VAL:HG21	1:I:432:TYR:CE1	2.21	0.75
1:I:432:TYR:CE2	1:I:436:VAL:HG12	2.22	0.75
1:H:141:VAL:HG21	1:H:432:TYR:CE1	2.21	0.75
1:A:141:VAL:HG21	1:A:432:TYR:CE1	2.21	0.75
1:H:424:GLU:OE2	1:H:477:HIS:CD2	2.40	0.75
1:D:89:LEU:HD21	1:D:108:VAL:HG23	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:254:GLU:HA	1:I:305:ASP:HB2	1.68	0.75
1:B:424:GLU:OE2	1:B:477:HIS:CD2	2.40	0.75
1:D:424:GLU:OE2	1:D:477:HIS:CD2	2.40	0.75
1:G:141:VAL:HG21	1:G:432:TYR:CE1	2.21	0.75
1:B:141:VAL:HG21	1:B:432:TYR:CE1	2.21	0.75
1:A:254:GLU:HA	1:A:305:ASP:HB2	1.68	0.75
1:B:81:LEU:HD12	1:B:81:LEU:H	1.52	0.75
1:E:248:LEU:HD11	1:E:331:LEU:HD22	1.69	0.75
1:E:424:GLU:OE2	1:E:477:HIS:CD2	2.40	0.74
1:A:424:GLU:OE2	1:A:477:HIS:CD2	2.40	0.74
1:D:432:TYR:CE2	1:D:436:VAL:HG12	2.22	0.74
1:F:141:VAL:HG21	1:F:432:TYR:CE1	2.21	0.74
1:E:81:LEU:H	1:E:81:LEU:HD12	1.52	0.74
1:C:141:VAL:HG21	1:C:432:TYR:CE1	2.21	0.74
1:G:220:THR:HG22	1:G:384:ARG:N	2.01	0.74
1:B:89:LEU:HD21	1:B:108:VAL:HG23	1.68	0.74
1:A:220:THR:HG22	1:A:384:ARG:N	2.01	0.74
1:F:424:GLU:OE2	1:F:477:HIS:CD2	2.40	0.74
1:I:424:GLU:OE2	1:I:477:HIS:CD2	2.40	0.74
1:C:432:TYR:CE2	1:C:436:VAL:HG12	2.22	0.74
1:C:248:LEU:HD11	1:C:331:LEU:HD22	1.69	0.74
1:E:432:TYR:CE2	1:E:436:VAL:HG12	2.22	0.74
1:H:81:LEU:H	1:H:81:LEU:HD12	1.52	0.74
1:A:280:GLU:HG2	1:A:284:LYS:HE3	1.69	0.74
1:F:220:THR:HG22	1:F:384:ARG:N	2.01	0.74
1:D:81:LEU:H	1:D:81:LEU:HD12	1.52	0.74
1:A:248:LEU:HD11	1:A:331:LEU:HD22	1.69	0.74
1:F:432:TYR:CE2	1:F:436:VAL:HG12	2.22	0.74
1:A:299:ILE:H	1:A:299:ILE:HD13	1.53	0.74
1:F:280:GLU:HG2	1:F:284:LYS:HE3	1.69	0.74
1:B:60:VAL:HG22	1:B:66:ILE:CG2	2.10	0.74
1:F:530:VAL:O	1:G:59:LEU:CD2	2.35	0.74
1:B:254:GLU:HA	1:B:305:ASP:HB2	1.68	0.74
1:G:89:LEU:HD21	1:G:108:VAL:HG23	1.68	0.74
1:A:89:LEU:HD21	1:A:108:VAL:HG23	1.68	0.74
1:G:299:ILE:H	1:G:299:ILE:HD13	1.53	0.74
1:F:89:LEU:HD21	1:F:108:VAL:HG23	1.68	0.74
1:B:248:LEU:HD11	1:B:331:LEU:HD22	1.69	0.74
1:F:299:ILE:H	1:F:299:ILE:HD13	1.53	0.74
1:I:280:GLU:HG2	1:I:284:LYS:HE3	1.69	0.74
1:G:424:GLU:OE2	1:G:477:HIS:HD2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:424:GLU:OE2	1:I:477:HIS:HD2	1.71	0.73
1:H:432:TYR:CE2	1:H:436:VAL:HG12	2.22	0.73
1:C:254:GLU:HA	1:C:305:ASP:HB2	1.68	0.73
1:E:525:ARG:CG	1:F:56:ASP:OD2	2.36	0.73
1:A:432:TYR:CE2	1:A:436:VAL:HG12	2.22	0.73
1:G:248:LEU:HD11	1:G:331:LEU:HD22	1.69	0.73
1:G:280:GLU:HG2	1:G:284:LYS:HE3	1.69	0.73
1:A:401:ALA:O	1:A:405:VAL:HG23	1.89	0.73
1:B:432:TYR:CE2	1:B:436:VAL:HG12	2.22	0.73
1:D:280:GLU:HG2	1:D:284:LYS:HE3	1.69	0.73
1:G:81:LEU:HD12	1:G:81:LEU:H	1.52	0.73
1:D:209:ILE:HB	1:D:399:ARG:HH22	1.53	0.73
1:E:60:VAL:CG2	1:E:66:ILE:HG22	2.12	0.73
1:F:153:VAL:HG23	1:F:160:LEU:HD23	1.70	0.73
1:E:424:GLU:OE2	1:E:477:HIS:HD2	1.71	0.73
1:F:424:GLU:OE2	1:F:477:HIS:HD2	1.71	0.73
1:C:424:GLU:OE2	1:C:477:HIS:HD2	1.71	0.73
1:G:432:TYR:CE2	1:G:436:VAL:HG12	2.22	0.73
1:D:299:ILE:H	1:D:299:ILE:HD13	1.53	0.73
1:I:401:ALA:O	1:I:405:VAL:HG23	1.88	0.73
1:C:81:LEU:H	1:C:81:LEU:HD12	1.53	0.73
1:C:264:ILE:HG13	1:C:265:ARG:N	2.02	0.73
1:D:248:LEU:HD11	1:D:331:LEU:HD22	1.69	0.73
1:F:254:GLU:HA	1:F:305:ASP:HB2	1.68	0.73
1:I:248:LEU:HD11	1:I:331:LEU:HD22	1.69	0.73
1:E:153:VAL:HG23	1:E:160:LEU:HD23	1.70	0.73
1:B:424:GLU:OE2	1:B:477:HIS:HD2	1.71	0.73
1:D:424:GLU:OE2	1:D:477:HIS:HD2	1.72	0.73
1:H:401:ALA:O	1:H:405:VAL:HG23	1.88	0.73
1:E:280:GLU:HG2	1:E:284:LYS:HE3	1.69	0.73
1:C:280:GLU:HG2	1:C:284:LYS:HE3	1.69	0.73
1:E:209:ILE:HB	1:E:399:ARG:HH22	1.53	0.73
1:F:209:ILE:HB	1:F:399:ARG:HH22	1.53	0.73
1:G:401:ALA:O	1:G:405:VAL:HG23	1.88	0.73
1:I:81:LEU:HD12	1:I:81:LEU:H	1.52	0.73
1:D:254:GLU:HA	1:D:305:ASP:HB2	1.68	0.73
1:C:153:VAL:HG23	1:C:160:LEU:HD23	1.70	0.73
1:F:452:GLU:O	1:F:455:VAL:HG22	1.89	0.73
1:B:452:GLU:O	1:B:455:VAL:HG22	1.89	0.73
1:I:89:LEU:HD21	1:I:108:VAL:HG23	1.68	0.73
1:A:81:LEU:H	1:A:81:LEU:HD12	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:209:ILE:HB	1:G:399:ARG:HH22	1.54	0.73
1:C:299:ILE:HD13	1:C:299:ILE:H	1.53	0.72
1:I:299:ILE:HD13	1:I:299:ILE:H	1.53	0.72
1:D:401:ALA:O	1:D:405:VAL:HG23	1.89	0.72
1:H:209:ILE:HB	1:H:399:ARG:HH22	1.54	0.72
1:C:89:LEU:HD21	1:C:108:VAL:HG23	1.68	0.72
1:G:153:VAL:HG23	1:G:160:LEU:HD23	1.70	0.72
1:E:527:ASP:HB3	1:F:57:LYS:HZ2	1.53	0.72
1:H:415:ILE:HD12	1:H:506:ALA:HA	1.72	0.72
1:E:299:ILE:H	1:E:299:ILE:HD13	1.53	0.72
1:B:280:GLU:HG2	1:B:284:LYS:HE3	1.69	0.72
1:C:209:ILE:HB	1:C:399:ARG:HH22	1.53	0.72
1:C:415:ILE:HD12	1:C:506:ALA:HA	1.72	0.72
1:H:452:GLU:O	1:H:455:VAL:HG22	1.89	0.72
1:I:452:GLU:O	1:I:455:VAL:HG22	1.89	0.72
1:A:424:GLU:OE2	1:A:477:HIS:HD2	1.72	0.72
1:A:452:GLU:O	1:A:455:VAL:HG22	1.89	0.72
1:F:81:LEU:H	1:F:81:LEU:HD12	1.52	0.72
1:F:401:ALA:O	1:F:405:VAL:HG23	1.88	0.72
1:A:153:VAL:HG23	1:A:160:LEU:HD23	1.70	0.72
1:B:153:VAL:HG23	1:B:160:LEU:HD23	1.70	0.72
1:H:299:ILE:HD13	1:H:299:ILE:H	1.53	0.72
1:H:248:LEU:HD11	1:H:331:LEU:HD22	1.69	0.72
1:F:531:SER:HB2	1:G:60:VAL:O	1.90	0.72
1:F:248:LEU:HD11	1:F:331:LEU:HD22	1.69	0.72
1:B:209:ILE:HB	1:B:399:ARG:HH22	1.54	0.72
1:I:60:VAL:CG2	1:I:66:ILE:HG22	2.12	0.72
1:I:209:ILE:HB	1:I:399:ARG:HH22	1.54	0.72
1:C:401:ALA:O	1:C:405:VAL:HG23	1.88	0.72
1:H:153:VAL:HG23	1:H:160:LEU:HD23	1.70	0.72
1:H:280:GLU:HG2	1:H:284:LYS:HE3	1.69	0.72
1:H:38:ALA:O	1:H:41:ALA:HB3	1.90	0.72
1:D:415:ILE:HD12	1:D:506:ALA:HA	1.72	0.72
1:E:401:ALA:O	1:E:405:VAL:HG23	1.89	0.72
1:C:38:ALA:O	1:C:41:ALA:HB3	1.90	0.72
1:F:415:ILE:HD12	1:F:506:ALA:HA	1.72	0.71
1:H:264:ILE:HG13	1:H:265:ARG:N	2.03	0.71
1:G:415:ILE:HD12	1:G:506:ALA:HA	1.72	0.71
1:B:401:ALA:O	1:B:405:VAL:HG23	1.88	0.71
1:A:38:ALA:O	1:A:41:ALA:HB3	1.90	0.71
1:I:153:VAL:HG23	1:I:160:LEU:HD23	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ALA:O	1:B:41:ALA:HB3	1.90	0.71
1:D:153:VAL:HG23	1:D:160:LEU:HD23	1.70	0.71
1:B:299:ILE:H	1:B:299:ILE:HD13	1.53	0.71
1:B:415:ILE:HD12	1:B:506:ALA:HA	1.72	0.71
1:A:209:ILE:HB	1:A:399:ARG:HH22	1.54	0.71
1:D:452:GLU:O	1:D:455:VAL:HG22	1.89	0.71
1:E:38:ALA:O	1:E:41:ALA:HB3	1.90	0.71
1:G:38:ALA:O	1:G:41:ALA:HB3	1.90	0.71
1:E:529:VAL:HG12	1:F:58:MET:HB3	1.72	0.71
1:I:38:ALA:O	1:I:41:ALA:HB3	1.90	0.71
1:D:38:ALA:O	1:D:41:ALA:HB3	1.90	0.71
1:G:60:VAL:CG2	1:G:66:ILE:HG22	2.12	0.71
1:I:415:ILE:HD12	1:I:506:ALA:HA	1.72	0.71
1:E:415:ILE:HD12	1:E:506:ALA:HA	1.72	0.71
1:D:264:ILE:HG13	1:D:265:ARG:N	2.02	0.71
1:G:452:GLU:O	1:G:455:VAL:HG22	1.89	0.71
1:F:264:ILE:HG13	1:F:265:ARG:N	2.03	0.71
1:C:452:GLU:O	1:C:455:VAL:HG22	1.89	0.71
1:E:452:GLU:O	1:E:455:VAL:HG22	1.89	0.71
1:D:529:VAL:HG12	1:E:58:MET:CB	2.19	0.71
1:F:469:LEU:HB3	1:F:487:ILE:HD13	1.73	0.70
1:B:60:VAL:CG2	1:B:66:ILE:HG22	2.12	0.70
1:F:38:ALA:O	1:F:41:ALA:HB3	1.90	0.70
1:D:259:GLU:C	1:D:259:GLU:OE1	2.30	0.70
1:B:264:ILE:HG13	1:B:265:ARG:N	2.03	0.70
1:G:469:LEU:HB3	1:G:487:ILE:HD13	1.73	0.70
1:H:259:GLU:OE1	1:H:259:GLU:C	2.30	0.70
1:B:259:GLU:OE1	1:B:259:GLU:C	2.30	0.70
1:A:415:ILE:HD12	1:A:506:ALA:HA	1.72	0.70
1:C:469:LEU:HB3	1:C:487:ILE:HD13	1.73	0.70
1:A:259:GLU:OE1	1:A:259:GLU:C	2.30	0.70
1:F:259:GLU:C	1:F:259:GLU:OE1	2.30	0.70
1:E:264:ILE:HG13	1:E:265:ARG:N	2.02	0.70
1:H:424:GLU:OE2	1:H:477:HIS:HD2	1.71	0.70
1:E:259:GLU:C	1:E:259:GLU:OE1	2.30	0.70
1:C:259:GLU:OE1	1:C:259:GLU:C	2.30	0.70
1:A:425:ILE:O	1:A:429:LEU:HB2	1.92	0.70
1:I:107:ALA:O	1:I:111:SER:HB2	1.92	0.70
1:D:398:LEU:O	1:D:402:LEU:HG	1.92	0.70
1:B:425:ILE:O	1:B:429:LEU:HB2	1.92	0.70
1:A:469:LEU:HB3	1:A:487:ILE:HD13	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107:ALA:O	1:F:111:SER:HB2	1.92	0.69
1:H:469:LEU:HB3	1:H:487:ILE:HD13	1.73	0.69
1:G:83:HIS:CG	1:G:84:PRO:HD2	2.27	0.69
1:H:475:SER:O	1:H:478:GLU:HG2	1.92	0.69
1:B:398:LEU:O	1:B:402:LEU:HG	1.92	0.69
1:F:83:HIS:CG	1:F:84:PRO:HD2	2.27	0.69
1:A:264:ILE:HG13	1:A:265:ARG:N	2.03	0.69
1:E:264:ILE:HG13	1:E:265:ARG:O	1.92	0.69
1:E:469:LEU:HB3	1:E:487:ILE:HD13	1.73	0.69
1:B:83:HIS:CG	1:B:84:PRO:HD2	2.27	0.69
1:F:398:LEU:O	1:F:402:LEU:HG	1.92	0.69
1:B:475:SER:O	1:B:478:GLU:HG2	1.93	0.69
1:H:107:ALA:O	1:H:111:SER:HB2	1.92	0.69
1:I:259:GLU:OE1	1:I:259:GLU:C	2.30	0.69
1:G:220:THR:CG2	1:G:384:ARG:H	2.05	0.69
1:B:107:ALA:O	1:B:111:SER:HB2	1.92	0.69
1:D:475:SER:O	1:D:478:GLU:HG2	1.92	0.69
1:G:66:ILE:H	1:G:66:ILE:CD1	2.06	0.69
1:D:425:ILE:O	1:D:429:LEU:HB2	1.92	0.69
1:E:220:THR:CG2	1:E:384:ARG:H	2.05	0.69
1:H:83:HIS:CG	1:H:84:PRO:HD2	2.27	0.69
1:E:470:LEU:O	1:E:474:ARG:HG2	1.93	0.69
1:F:475:SER:O	1:F:478:GLU:HG2	1.92	0.69
1:A:475:SER:O	1:A:478:GLU:HG2	1.92	0.69
1:C:475:SER:O	1:C:478:GLU:HG2	1.92	0.69
1:H:398:LEU:O	1:H:402:LEU:HG	1.92	0.69
1:H:425:ILE:O	1:H:429:LEU:HB2	1.92	0.69
1:B:220:THR:CG2	1:B:384:ARG:H	2.05	0.69
1:D:83:HIS:CG	1:D:84:PRO:HD2	2.27	0.69
1:D:470:LEU:O	1:D:474:ARG:HG2	1.93	0.69
1:G:259:GLU:OE1	1:G:259:GLU:C	2.30	0.69
1:I:398:LEU:O	1:I:402:LEU:HG	1.92	0.69
1:E:398:LEU:O	1:E:402:LEU:HG	1.92	0.69
1:C:398:LEU:O	1:C:402:LEU:HG	1.92	0.69
1:C:425:ILE:O	1:C:429:LEU:HB2	1.92	0.69
1:E:425:ILE:O	1:E:429:LEU:HB2	1.92	0.69
1:B:264:ILE:HG13	1:B:265:ARG:O	1.92	0.69
1:C:220:THR:CG2	1:C:384:ARG:H	2.05	0.69
1:F:470:LEU:O	1:F:474:ARG:HG2	1.93	0.69
1:A:398:LEU:O	1:A:402:LEU:HG	1.92	0.69
1:G:475:SER:O	1:G:478:GLU:HG2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:ILE:HG13	1:D:265:ARG:O	1.92	0.69
1:G:264:ILE:HG13	1:G:265:ARG:O	1.92	0.69
1:B:469:LEU:HB3	1:B:487:ILE:HD13	1.73	0.69
1:H:220:THR:CG2	1:H:384:ARG:H	2.05	0.69
1:E:107:ALA:O	1:E:111:SER:HB2	1.92	0.69
1:I:220:THR:CG2	1:I:384:ARG:H	2.05	0.69
1:D:107:ALA:O	1:D:111:SER:HB2	1.92	0.69
1:A:107:ALA:O	1:A:111:SER:HB2	1.92	0.69
1:C:107:ALA:O	1:C:111:SER:HB2	1.91	0.69
1:D:469:LEU:HB3	1:D:487:ILE:HD13	1.73	0.69
1:C:83:HIS:CG	1:C:84:PRO:HD2	2.27	0.69
1:E:475:SER:O	1:E:478:GLU:HG2	1.92	0.69
1:G:470:LEU:O	1:G:474:ARG:HG2	1.93	0.69
1:I:470:LEU:O	1:I:474:ARG:HG2	1.93	0.69
1:F:66:ILE:CD1	1:F:66:ILE:H	2.06	0.69
1:E:83:HIS:CG	1:E:84:PRO:HD2	2.27	0.69
1:I:475:SER:O	1:I:478:GLU:HG2	1.92	0.69
1:G:264:ILE:HG13	1:G:265:ARG:N	2.02	0.69
1:A:220:THR:CG2	1:A:384:ARG:H	2.05	0.69
1:F:220:THR:CG2	1:F:384:ARG:H	2.05	0.69
1:G:425:ILE:O	1:G:429:LEU:HB2	1.92	0.69
1:H:184:ILE:HD12	1:H:222:LEU:HD22	1.75	0.69
1:F:184:ILE:HD12	1:F:222:LEU:HD22	1.75	0.69
1:I:264:ILE:HG13	1:I:265:ARG:N	2.02	0.68
1:I:469:LEU:HB3	1:I:487:ILE:HD13	1.73	0.68
1:E:184:ILE:HD12	1:E:222:LEU:HD22	1.75	0.68
1:I:83:HIS:CG	1:I:84:PRO:HD2	2.28	0.68
1:C:264:ILE:HG13	1:C:265:ARG:O	1.92	0.68
1:A:144:GLN:O	1:A:148:GLU:HG2	1.94	0.68
1:C:144:GLN:O	1:C:148:GLU:HG2	1.94	0.68
1:I:184:ILE:HD12	1:I:222:LEU:HD22	1.75	0.68
1:G:184:ILE:HD12	1:G:222:LEU:HD22	1.75	0.68
1:I:425:ILE:O	1:I:429:LEU:HB2	1.92	0.68
1:A:83:HIS:CG	1:A:84:PRO:HD2	2.27	0.68
1:G:107:ALA:O	1:G:111:SER:HB2	1.92	0.68
1:B:144:GLN:O	1:B:148:GLU:HG2	1.94	0.68
1:D:184:ILE:HD12	1:D:222:LEU:HD22	1.75	0.68
1:A:264:ILE:HG13	1:A:265:ARG:O	1.92	0.68
1:A:184:ILE:HD12	1:A:222:LEU:HD22	1.75	0.68
1:B:184:ILE:HD12	1:B:222:LEU:HD22	1.75	0.68
1:B:470:LEU:O	1:B:474:ARG:HG2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:425:ILE:O	1:F:429:LEU:HB2	1.92	0.68
1:F:264:ILE:HG13	1:F:265:ARG:O	1.92	0.68
1:D:91:GLN:NE2	1:E:387:LEU:HD21	2.09	0.68
1:D:144:GLN:O	1:D:148:GLU:HG2	1.94	0.68
1:A:470:LEU:O	1:A:474:ARG:HG2	1.93	0.68
1:E:162:ARG:NH1	1:E:162:ARG:HB2	2.09	0.68
1:A:66:ILE:CD1	1:A:66:ILE:H	2.06	0.68
1:D:217:ILE:HD11	1:D:390:LEU:HD21	1.76	0.68
1:I:264:ILE:HG13	1:I:265:ARG:O	1.93	0.68
1:D:220:THR:CG2	1:D:384:ARG:H	2.05	0.68
1:G:144:GLN:O	1:G:148:GLU:HG2	1.94	0.68
1:H:470:LEU:O	1:H:474:ARG:HG2	1.93	0.68
1:C:470:LEU:O	1:C:474:ARG:HG2	1.93	0.68
1:H:264:ILE:HG13	1:H:265:ARG:O	1.92	0.68
1:A:162:ARG:HB2	1:A:162:ARG:NH1	2.09	0.68
1:G:398:LEU:O	1:G:402:LEU:HG	1.92	0.68
1:F:76:LEU:HD23	1:F:90:VAL:CG1	2.24	0.68
1:G:248:LEU:HD13	1:G:299:ILE:HD11	1.76	0.68
1:I:144:GLN:O	1:I:148:GLU:HG2	1.94	0.68
1:C:184:ILE:HD12	1:C:222:LEU:HD22	1.75	0.68
1:E:255:VAL:HA	1:E:283:ILE:HD11	1.76	0.68
1:B:255:VAL:HA	1:B:283:ILE:HD11	1.76	0.68
1:C:529:VAL:HG12	1:D:58:MET:HB3	1.74	0.68
1:G:245:LYS:N	1:G:296:ASN:ND2	2.41	0.67
1:I:217:ILE:HD11	1:I:390:LEU:HD21	1.76	0.67
1:H:255:VAL:HA	1:H:283:ILE:HD11	1.76	0.67
1:A:248:LEU:HD13	1:A:299:ILE:HD11	1.76	0.67
1:I:208:GLN:HB3	1:I:380:SER:OG	1.94	0.67
1:A:208:GLN:HB3	1:A:380:SER:OG	1.94	0.67
1:F:144:GLN:O	1:F:148:GLU:HG2	1.94	0.67
1:C:162:ARG:NH1	1:C:162:ARG:HB2	2.09	0.67
1:C:76:LEU:HD23	1:C:90:VAL:CG1	2.24	0.67
1:H:76:LEU:HD23	1:H:90:VAL:CG1	2.24	0.67
1:E:208:GLN:HB3	1:E:380:SER:OG	1.94	0.67
1:G:208:GLN:HB3	1:G:380:SER:OG	1.94	0.67
1:E:144:GLN:O	1:E:148:GLU:HG2	1.94	0.67
1:I:162:ARG:HB2	1:I:162:ARG:NH1	2.09	0.67
1:B:76:LEU:HD23	1:B:90:VAL:CG1	2.24	0.67
1:E:76:LEU:HD23	1:E:90:VAL:CG1	2.24	0.67
1:E:525:ARG:HG3	1:F:56:ASP:HB2	1.76	0.67
1:I:269:PRO:HA	1:I:272:MET:CG	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:VAL:HG13	1:G:359:GLU:OE2	1.95	0.67
1:I:255:VAL:HA	1:I:283:ILE:HD11	1.76	0.67
1:B:208:GLN:HB3	1:B:380:SER:OG	1.94	0.67
1:H:144:GLN:O	1:H:148:GLU:HG2	1.94	0.67
1:F:162:ARG:HB2	1:F:162:ARG:NH1	2.09	0.67
1:G:162:ARG:HB2	1:G:162:ARG:NH1	2.09	0.67
1:D:66:ILE:H	1:D:66:ILE:CD1	2.06	0.67
1:E:305:ASP:O	1:E:309:GLN:HG3	1.95	0.67
1:B:305:ASP:O	1:B:309:GLN:HG3	1.95	0.67
1:F:208:GLN:HB3	1:F:380:SER:OG	1.94	0.67
1:C:208:GLN:HB3	1:C:380:SER:OG	1.94	0.67
1:H:471:MET:SD	1:H:474:ARG:HD3	2.35	0.67
1:I:66:ILE:H	1:I:66:ILE:CD1	2.06	0.67
1:F:217:ILE:HD11	1:F:390:LEU:HD21	1.76	0.67
1:D:76:LEU:HD23	1:D:90:VAL:CG1	2.24	0.67
1:A:76:LEU:HD23	1:A:90:VAL:CG1	2.24	0.67
1:H:248:LEU:HD13	1:H:299:ILE:HD11	1.76	0.67
1:D:162:ARG:NH1	1:D:162:ARG:HB2	2.09	0.67
1:E:269:PRO:HA	1:E:272:MET:CG	2.25	0.67
1:G:305:ASP:O	1:G:309:GLN:HG3	1.95	0.67
1:I:305:ASP:O	1:I:309:GLN:HG3	1.95	0.67
1:E:248:LEU:HD13	1:E:299:ILE:HD11	1.76	0.67
1:D:208:GLN:HB3	1:D:380:SER:OG	1.94	0.67
1:D:248:LEU:HD13	1:D:299:ILE:HD11	1.76	0.67
1:C:471:MET:SD	1:C:474:ARG:HD3	2.35	0.67
1:B:162:ARG:HB2	1:B:162:ARG:NH1	2.09	0.67
1:E:232:VAL:HG13	1:E:359:GLU:OE2	1.95	0.67
1:D:232:VAL:HG13	1:D:359:GLU:OE2	1.95	0.67
1:H:305:ASP:O	1:H:309:GLN:HG3	1.95	0.67
1:C:305:ASP:O	1:C:309:GLN:HG3	1.95	0.67
1:I:471:MET:SD	1:I:474:ARG:HD3	2.35	0.67
1:G:217:ILE:HD11	1:G:390:LEU:HD21	1.76	0.67
1:B:217:ILE:HD11	1:B:390:LEU:HD21	1.76	0.67
1:H:217:ILE:HD11	1:H:390:LEU:HD21	1.76	0.67
1:A:232:VAL:HG13	1:A:359:GLU:OE2	1.95	0.67
1:D:255:VAL:HA	1:D:283:ILE:HD11	1.76	0.67
1:G:471:MET:SD	1:G:474:ARG:HD3	2.35	0.67
1:B:471:MET:SD	1:B:474:ARG:HD3	2.35	0.67
1:H:162:ARG:NH1	1:H:162:ARG:HB2	2.09	0.67
1:D:525:ARG:HH11	1:D:525:ARG:HG2	1.60	0.67
1:E:66:ILE:CD1	1:E:66:ILE:H	2.06	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:PRO:HA	1:B:272:MET:CG	2.25	0.66
1:F:232:VAL:HG13	1:F:359:GLU:OE2	1.95	0.66
1:I:232:VAL:HG13	1:I:359:GLU:OE2	1.95	0.66
1:F:255:VAL:HA	1:F:283:ILE:HD11	1.76	0.66
1:F:471:MET:SD	1:F:474:ARG:HD3	2.35	0.66
1:A:479:ASN:HB2	1:A:482:ASN:OD1	1.96	0.66
1:B:232:VAL:HG13	1:B:359:GLU:OE2	1.95	0.66
1:B:331:LEU:HD23	1:B:331:LEU:O	1.96	0.66
1:H:331:LEU:HD23	1:H:331:LEU:O	1.96	0.66
1:C:479:ASN:HB2	1:C:482:ASN:OD1	1.96	0.66
1:E:217:ILE:HD11	1:E:390:LEU:HD21	1.76	0.66
1:E:331:LEU:O	1:E:331:LEU:HD23	1.96	0.66
1:F:305:ASP:O	1:F:309:GLN:HG3	1.95	0.66
1:D:479:ASN:HB2	1:D:482:ASN:OD1	1.96	0.66
1:A:525:ARG:HG2	1:A:525:ARG:HH11	1.61	0.66
1:H:232:VAL:HG13	1:H:359:GLU:OE2	1.95	0.66
1:B:248:LEU:HD13	1:B:299:ILE:HD11	1.76	0.66
1:A:471:MET:SD	1:A:474:ARG:HD3	2.35	0.66
1:F:479:ASN:HB2	1:F:482:ASN:OD1	1.96	0.66
1:H:423:ILE:HG21	1:H:473:LEU:HD12	1.78	0.66
1:A:269:PRO:HA	1:A:272:MET:CG	2.25	0.66
1:C:255:VAL:HA	1:C:283:ILE:HD11	1.76	0.66
1:E:471:MET:SD	1:E:474:ARG:HD3	2.35	0.66
1:A:245:LYS:N	1:A:296:ASN:ND2	2.41	0.66
1:F:423:ILE:HG21	1:F:473:LEU:HD12	1.78	0.66
1:G:415:ILE:HG13	1:G:421:VAL:HG21	1.78	0.66
1:I:76:LEU:HD23	1:I:90:VAL:CG1	2.24	0.66
1:C:232:VAL:HG13	1:C:359:GLU:OE2	1.95	0.66
1:A:305:ASP:O	1:A:309:GLN:HG3	1.95	0.66
1:H:208:GLN:HB3	1:H:380:SER:OG	1.94	0.66
1:E:525:ARG:HG2	1:F:56:ASP:OD2	1.95	0.66
1:E:526:ILE:HA	1:F:56:ASP:O	1.96	0.66
1:B:415:ILE:HG13	1:B:421:VAL:HG21	1.78	0.66
1:F:231:GLU:HG3	1:F:366:LYS:HZ2	1.60	0.66
1:G:76:LEU:HD23	1:G:90:VAL:CG1	2.24	0.66
1:I:210:VAL:HG23	1:I:382:LEU:CD1	2.26	0.66
1:G:210:VAL:HG23	1:G:382:LEU:CD1	2.26	0.66
1:B:88:LEU:HD22	1:C:58:MET:HE1	1.78	0.66
1:D:471:MET:SD	1:D:474:ARG:HD3	2.35	0.66
1:I:525:ARG:HG2	1:I:525:ARG:HH11	1.60	0.66
1:I:415:ILE:HG13	1:I:421:VAL:HG21	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ILE:HD11	1:A:390:LEU:HD21	1.76	0.66
1:H:269:PRO:HA	1:H:272:MET:CG	2.25	0.66
1:H:220:THR:HG22	1:H:384:ARG:H	1.61	0.66
1:A:255:VAL:HA	1:A:283:ILE:HD11	1.76	0.66
1:C:248:LEU:HD13	1:C:299:ILE:HD11	1.76	0.66
1:I:331:LEU:HD23	1:I:331:LEU:O	1.96	0.66
1:B:220:THR:HG22	1:B:384:ARG:H	1.61	0.66
1:G:479:ASN:HB2	1:G:482:ASN:OD1	1.96	0.66
1:F:127:HIS:CD2	1:F:129:THR:HB	2.31	0.66
1:B:479:ASN:HB2	1:B:482:ASN:OD1	1.96	0.66
1:E:415:ILE:HG13	1:E:421:VAL:HG21	1.78	0.66
1:C:210:VAL:HG23	1:C:382:LEU:CD1	2.26	0.66
1:E:525:ARG:HG2	1:E:525:ARG:HH11	1.61	0.65
1:E:245:LYS:N	1:E:296:ASN:ND2	2.41	0.65
1:I:423:ILE:HG21	1:I:473:LEU:HD12	1.78	0.65
1:C:423:ILE:HG21	1:C:473:LEU:HD12	1.78	0.65
1:F:269:PRO:HA	1:F:272:MET:CG	2.25	0.65
1:H:210:VAL:HG23	1:H:382:LEU:CD1	2.26	0.65
1:D:210:VAL:HG23	1:D:382:LEU:CD1	2.26	0.65
1:E:46:LEU:N	1:E:46:LEU:HD12	2.12	0.65
1:H:127:HIS:CD2	1:H:129:THR:HB	2.31	0.65
1:G:525:ARG:HG2	1:G:525:ARG:HH11	1.60	0.65
1:H:415:ILE:HG13	1:H:421:VAL:HG21	1.78	0.65
1:D:473:LEU:O	1:D:476:THR:HG22	1.97	0.65
1:A:415:ILE:HG13	1:A:421:VAL:HG21	1.78	0.65
1:D:269:PRO:HA	1:D:272:MET:CG	2.25	0.65
1:C:217:ILE:HD11	1:C:390:LEU:HD21	1.76	0.65
1:F:248:LEU:HD13	1:F:299:ILE:HD11	1.76	0.65
1:D:331:LEU:HD23	1:D:331:LEU:O	1.96	0.65
1:D:305:ASP:O	1:D:309:GLN:HG3	1.95	0.65
1:B:128:PRO:O	1:B:132:ILE:HG12	1.96	0.65
1:B:127:HIS:CD2	1:B:129:THR:HB	2.31	0.65
1:I:127:HIS:CD2	1:I:129:THR:HB	2.31	0.65
1:C:127:HIS:CD2	1:C:129:THR:HB	2.31	0.65
1:D:127:HIS:CD2	1:D:129:THR:HB	2.31	0.65
1:F:473:LEU:O	1:F:476:THR:HG22	1.97	0.65
1:D:423:ILE:HG21	1:D:473:LEU:HD12	1.78	0.65
1:G:269:PRO:HA	1:G:272:MET:CG	2.25	0.65
1:G:255:VAL:HA	1:G:283:ILE:HD11	1.76	0.65
1:A:220:THR:HG22	1:A:384:ARG:H	1.61	0.65
1:I:248:LEU:HD13	1:I:299:ILE:HD11	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:VAL:O	1:A:459:ILE:HG12	1.97	0.65
1:D:455:VAL:O	1:D:459:ILE:HG12	1.96	0.65
1:E:479:ASN:HB2	1:E:482:ASN:OD1	1.96	0.65
1:H:455:VAL:O	1:H:459:ILE:HG12	1.97	0.65
1:I:455:VAL:O	1:I:459:ILE:HG12	1.97	0.65
1:I:128:PRO:O	1:I:132:ILE:HG12	1.96	0.65
1:C:128:PRO:O	1:C:132:ILE:HG12	1.96	0.65
1:H:169:LEU:HD12	1:H:170:SER:N	2.12	0.65
1:G:46:LEU:N	1:G:46:LEU:HD12	2.12	0.65
1:H:46:LEU:N	1:H:46:LEU:HD12	2.12	0.65
1:B:210:VAL:HG23	1:B:382:LEU:CD1	2.26	0.65
1:E:210:VAL:HG23	1:E:382:LEU:CD1	2.26	0.65
1:G:331:LEU:O	1:G:331:LEU:HD23	1.96	0.65
1:I:46:LEU:N	1:I:46:LEU:HD12	2.12	0.65
1:B:525:ARG:HH11	1:B:525:ARG:HG2	1.61	0.65
1:B:259:GLU:OE1	1:B:260:LEU:N	2.30	0.65
1:A:423:ILE:HG21	1:A:473:LEU:HD12	1.78	0.65
1:F:220:THR:HG22	1:F:384:ARG:H	1.61	0.65
1:D:128:PRO:O	1:D:132:ILE:HG12	1.97	0.65
1:C:46:LEU:HD12	1:C:46:LEU:N	2.12	0.65
1:E:128:PRO:O	1:E:132:ILE:HG12	1.97	0.65
1:I:169:LEU:HD12	1:I:170:SER:N	2.12	0.65
1:B:46:LEU:N	1:B:46:LEU:HD12	2.12	0.65
1:D:245:LYS:N	1:D:296:ASN:ND2	2.41	0.65
1:A:473:LEU:O	1:A:476:THR:HG22	1.97	0.65
1:B:231:GLU:HG3	1:B:366:LYS:HZ2	1.62	0.65
1:A:127:HIS:CD2	1:A:129:THR:HB	2.31	0.65
1:F:455:VAL:O	1:F:459:ILE:HG12	1.97	0.65
1:D:46:LEU:N	1:D:46:LEU:HD12	2.12	0.65
1:A:121:LEU:O	1:A:126:VAL:HG22	1.97	0.65
1:C:66:ILE:CD1	1:C:66:ILE:H	2.06	0.65
1:F:415:ILE:HG13	1:F:421:VAL:HG21	1.78	0.65
1:I:473:LEU:O	1:I:476:THR:HG22	1.97	0.65
1:B:473:LEU:O	1:B:476:THR:HG22	1.97	0.65
1:D:88:LEU:CD1	1:E:389:ARG:HH12	2.09	0.65
1:A:210:VAL:HG23	1:A:382:LEU:CD1	2.26	0.65
1:F:331:LEU:O	1:F:331:LEU:HD23	1.96	0.65
1:G:455:VAL:O	1:G:459:ILE:HG12	1.97	0.65
1:C:455:VAL:O	1:C:459:ILE:HG12	1.96	0.65
1:D:91:GLN:HE21	1:E:387:LEU:HD21	1.62	0.65
1:H:128:PRO:O	1:H:132:ILE:HG12	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:121:LEU:O	1:I:126:VAL:HG22	1.97	0.65
1:H:479:ASN:HB2	1:H:482:ASN:OD1	1.96	0.65
1:E:423:ILE:HG21	1:E:473:LEU:HD12	1.78	0.65
1:G:423:ILE:HG21	1:G:473:LEU:HD12	1.78	0.65
1:C:220:THR:HG22	1:C:384:ARG:H	1.61	0.65
1:C:331:LEU:HD23	1:C:331:LEU:O	1.96	0.65
1:F:210:VAL:HG23	1:F:382:LEU:CD1	2.26	0.65
1:A:331:LEU:O	1:A:331:LEU:HD23	1.96	0.65
1:E:121:LEU:O	1:E:126:VAL:HG22	1.97	0.65
1:G:260:LEU:C	1:G:260:LEU:HD12	2.17	0.65
1:G:473:LEU:O	1:G:476:THR:HG22	1.97	0.65
1:A:128:PRO:O	1:A:132:ILE:HG12	1.96	0.65
1:E:127:HIS:CD2	1:E:129:THR:HB	2.31	0.65
1:G:169:LEU:HD12	1:G:170:SER:N	2.12	0.65
1:D:121:LEU:O	1:D:126:VAL:HG22	1.97	0.65
1:D:259:GLU:OE1	1:D:260:LEU:N	2.30	0.64
1:C:415:ILE:HG13	1:C:421:VAL:HG21	1.78	0.64
1:C:473:LEU:O	1:C:476:THR:HG22	1.97	0.64
1:B:455:VAL:O	1:B:459:ILE:HG12	1.97	0.64
1:F:128:PRO:O	1:F:132:ILE:HG12	1.96	0.64
1:I:479:ASN:HB2	1:I:482:ASN:OD1	1.96	0.64
1:H:121:LEU:O	1:H:126:VAL:HG22	1.97	0.64
1:B:121:LEU:O	1:B:126:VAL:HG22	1.97	0.64
1:F:169:LEU:HD12	1:F:170:SER:N	2.12	0.64
1:I:259:GLU:OE1	1:I:260:LEU:N	2.30	0.64
1:C:269:PRO:HA	1:C:272:MET:CG	2.25	0.64
1:A:149:LEU:O	1:A:149:LEU:HD23	1.98	0.64
1:A:169:LEU:HD12	1:A:170:SER:N	2.12	0.64
1:D:169:LEU:HD12	1:D:170:SER:N	2.12	0.64
1:E:259:GLU:OE1	1:E:260:LEU:N	2.30	0.64
1:C:260:LEU:C	1:C:260:LEU:HD12	2.17	0.64
1:B:245:LYS:N	1:B:296:ASN:ND2	2.41	0.64
1:H:473:LEU:O	1:H:476:THR:HG22	1.97	0.64
1:G:128:PRO:O	1:G:132:ILE:HG12	1.96	0.64
1:F:525:ARG:HG2	1:F:525:ARG:HH11	1.61	0.64
1:C:525:ARG:HH11	1:C:525:ARG:HG2	1.60	0.64
1:E:473:LEU:O	1:E:476:THR:HG22	1.97	0.64
1:B:149:LEU:O	1:B:149:LEU:HD23	1.98	0.64
1:F:46:LEU:HD12	1:F:46:LEU:N	2.12	0.64
1:A:46:LEU:N	1:A:46:LEU:HD12	2.12	0.64
1:E:169:LEU:HD12	1:E:170:SER:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:525:ARG:HG2	1:H:525:ARG:HH11	1.61	0.64
1:A:259:GLU:OE1	1:A:260:LEU:N	2.30	0.64
1:F:245:LYS:N	1:F:296:ASN:ND2	2.41	0.64
1:B:423:ILE:HG21	1:B:473:LEU:HD12	1.78	0.64
1:C:121:LEU:O	1:C:126:VAL:HG22	1.97	0.64
1:C:169:LEU:HD12	1:C:170:SER:N	2.12	0.64
1:F:259:GLU:OE1	1:F:260:LEU:N	2.30	0.64
1:C:259:GLU:OE1	1:C:260:LEU:N	2.30	0.64
1:I:220:THR:HG22	1:I:384:ARG:H	1.61	0.64
1:G:127:HIS:CD2	1:G:129:THR:HB	2.31	0.64
1:D:149:LEU:HD23	1:D:149:LEU:O	1.98	0.64
1:E:149:LEU:HD23	1:E:149:LEU:O	1.98	0.64
1:G:259:GLU:OE1	1:G:260:LEU:N	2.30	0.64
1:F:260:LEU:HD12	1:F:260:LEU:C	2.17	0.64
1:A:231:GLU:HG3	1:A:366:LYS:HZ2	1.63	0.64
1:B:66:ILE:H	1:B:66:ILE:CD1	2.06	0.64
1:H:66:ILE:H	1:H:66:ILE:CD1	2.06	0.64
1:G:110:PHE:CE2	1:G:451:LEU:HG	2.33	0.64
1:G:220:THR:HG22	1:G:384:ARG:H	1.61	0.64
1:C:110:PHE:CE2	1:C:451:LEU:HG	2.33	0.64
1:B:169:LEU:HD12	1:B:170:SER:N	2.12	0.64
1:E:455:VAL:O	1:E:459:ILE:HG12	1.97	0.64
1:F:121:LEU:O	1:F:126:VAL:HG22	1.97	0.64
1:G:155:ILE:HG21	1:G:200:TRP:CH2	2.34	0.63
1:A:527:ASP:HB2	1:B:55:MET:HG3	1.80	0.63
1:E:527:ASP:HB3	1:F:57:LYS:NZ	2.13	0.63
1:D:415:ILE:HG13	1:D:421:VAL:HG21	1.78	0.63
1:D:284:LYS:HD3	1:D:311:TYR:HE2	1.64	0.63
1:G:149:LEU:HD23	1:G:149:LEU:O	1.98	0.63
1:C:245:LYS:N	1:C:296:ASN:ND2	2.41	0.63
1:F:266:ILE:HG21	1:F:272:MET:SD	2.39	0.63
1:C:284:LYS:HD3	1:C:311:TYR:HE2	1.64	0.63
1:I:155:ILE:HG21	1:I:200:TRP:CH2	2.34	0.63
1:H:408:VAL:HG22	1:H:505:PRO:HG3	1.81	0.63
1:F:110:PHE:CE2	1:F:451:LEU:HG	2.33	0.63
1:C:149:LEU:O	1:C:149:LEU:HD23	1.98	0.63
1:F:149:LEU:HD23	1:F:149:LEU:O	1.98	0.63
1:H:259:GLU:OE1	1:H:260:LEU:N	2.30	0.63
1:A:389:ARG:HH12	1:I:88:LEU:HD11	1.63	0.63
1:D:220:THR:HG22	1:D:384:ARG:H	1.61	0.63
1:I:110:PHE:CE2	1:I:451:LEU:HG	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:ILE:HG21	1:C:272:MET:SD	2.39	0.63
1:G:210:VAL:HG23	1:G:382:LEU:HD13	1.81	0.63
1:A:284:LYS:HD3	1:A:311:TYR:HE2	1.64	0.63
1:I:110:PHE:HE2	1:I:451:LEU:HG	1.64	0.63
1:G:121:LEU:O	1:G:126:VAL:HG22	1.97	0.63
1:F:155:ILE:HG21	1:F:200:TRP:CH2	2.34	0.63
1:H:149:LEU:O	1:H:149:LEU:HD23	1.98	0.63
1:I:149:LEU:O	1:I:149:LEU:HD23	1.98	0.63
1:I:266:ILE:HG21	1:I:272:MET:SD	2.39	0.63
1:B:430:ARG:HG2	1:B:430:ARG:HH11	1.64	0.63
1:G:408:VAL:HG22	1:G:505:PRO:HG3	1.81	0.63
1:D:110:PHE:CE2	1:D:451:LEU:HG	2.33	0.63
1:E:110:PHE:CE2	1:E:451:LEU:HG	2.33	0.63
1:H:110:PHE:HE2	1:H:451:LEU:HG	1.64	0.63
1:B:110:PHE:CE2	1:B:451:LEU:HG	2.33	0.63
1:B:266:ILE:HG21	1:B:272:MET:SD	2.39	0.63
1:H:210:VAL:HG23	1:H:382:LEU:HD13	1.81	0.63
1:G:284:LYS:HD3	1:G:311:TYR:HE2	1.64	0.63
1:E:110:PHE:HE2	1:E:451:LEU:HG	1.64	0.63
1:I:408:VAL:HG22	1:I:505:PRO:HG3	1.81	0.63
1:B:260:LEU:HD12	1:B:260:LEU:C	2.17	0.63
1:D:210:VAL:HG23	1:D:382:LEU:HD13	1.81	0.63
1:C:210:VAL:HG23	1:C:382:LEU:HD13	1.81	0.63
1:A:408:VAL:HG22	1:A:505:PRO:HG3	1.81	0.63
1:B:155:ILE:HG21	1:B:200:TRP:CH2	2.34	0.63
1:E:266:ILE:HG21	1:E:272:MET:SD	2.39	0.62
1:G:266:ILE:HG21	1:G:272:MET:SD	2.39	0.62
1:D:155:ILE:HG21	1:D:200:TRP:CH2	2.34	0.62
1:E:155:ILE:HG21	1:E:200:TRP:CH2	2.34	0.62
1:A:110:PHE:CE2	1:A:451:LEU:HG	2.33	0.62
1:H:245:LYS:N	1:H:296:ASN:ND2	2.41	0.62
1:D:231:GLU:HG3	1:D:366:LYS:HZ2	1.64	0.62
1:H:430:ARG:HG2	1:H:430:ARG:HH11	1.64	0.62
1:I:210:VAL:HG23	1:I:382:LEU:HD13	1.81	0.62
1:F:129:THR:HG23	1:G:53:ARG:HH12	1.63	0.62
1:D:110:PHE:HE2	1:D:451:LEU:HG	1.64	0.62
1:C:155:ILE:HG21	1:C:200:TRP:CH2	2.34	0.62
1:D:408:VAL:HG22	1:D:505:PRO:HG3	1.81	0.62
1:A:266:ILE:HG21	1:A:272:MET:SD	2.39	0.62
1:G:231:GLU:HG3	1:G:366:LYS:HZ2	1.64	0.62
1:I:430:ARG:HH11	1:I:430:ARG:HG2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:430:ARG:HH11	1:F:430:ARG:HG2	1.64	0.62
1:I:284:LYS:HD3	1:I:311:TYR:HE2	1.64	0.62
1:H:110:PHE:CE2	1:H:451:LEU:HG	2.33	0.62
1:D:260:LEU:HD11	1:D:261:ASP:OD1	2.00	0.62
1:B:260:LEU:HD11	1:B:261:ASP:OD1	2.00	0.62
1:B:260:LEU:HD12	1:B:261:ASP:CA	2.29	0.62
1:B:408:VAL:HG22	1:B:505:PRO:HG3	1.81	0.62
1:D:266:ILE:HG21	1:D:272:MET:SD	2.39	0.62
1:B:210:VAL:HG23	1:B:382:LEU:HD13	1.81	0.62
1:H:266:ILE:HG21	1:H:272:MET:SD	2.39	0.62
1:A:230:LYS:NZ	1:A:321:ARG:NH1	2.48	0.62
1:D:531:SER:HB2	1:E:60:VAL:O	2.00	0.62
1:E:430:ARG:HH11	1:E:430:ARG:HG2	1.64	0.62
1:A:430:ARG:HG2	1:A:430:ARG:HH11	1.64	0.62
1:F:230:LYS:NZ	1:F:321:ARG:NH1	2.48	0.62
1:H:155:ILE:HG21	1:H:200:TRP:CH2	2.34	0.62
1:H:260:LEU:HD11	1:H:261:ASP:OD1	2.00	0.62
1:C:260:LEU:HD11	1:C:261:ASP:OD1	2.00	0.62
1:H:231:GLU:HG3	1:H:366:LYS:HZ2	1.65	0.62
1:C:231:GLU:HG3	1:C:366:LYS:HZ2	1.64	0.62
1:G:110:PHE:HE2	1:G:451:LEU:HG	1.64	0.62
1:C:110:PHE:HE2	1:C:451:LEU:HG	1.64	0.62
1:G:230:LYS:NZ	1:G:321:ARG:NH1	2.48	0.62
1:A:155:ILE:HG21	1:A:200:TRP:CH2	2.34	0.62
1:G:260:LEU:HD11	1:G:261:ASP:OD1	2.00	0.62
1:I:260:LEU:HD11	1:I:261:ASP:OD1	2.00	0.62
1:E:220:THR:HG22	1:E:384:ARG:H	1.61	0.62
1:B:110:PHE:HE2	1:B:451:LEU:HG	1.64	0.62
1:G:297:VAL:HG23	1:G:318:LEU:O	2.00	0.62
1:A:110:PHE:HE2	1:A:451:LEU:HG	1.64	0.62
1:F:210:VAL:HG23	1:F:382:LEU:HD13	1.81	0.62
1:E:284:LYS:HD3	1:E:311:TYR:HE2	1.64	0.62
1:A:238:PRO:HB2	1:A:241:LEU:HD21	1.82	0.62
1:C:230:LYS:NZ	1:C:321:ARG:NH1	2.48	0.62
1:D:230:LYS:NZ	1:D:321:ARG:NH1	2.48	0.62
1:C:260:LEU:HD12	1:C:261:ASP:CA	2.29	0.61
1:E:427:LYS:NZ	1:E:477:HIS:O	2.33	0.61
1:C:427:LYS:NZ	1:C:477:HIS:O	2.33	0.61
1:B:297:VAL:HG23	1:B:318:LEU:O	2.00	0.61
1:C:430:ARG:HG2	1:C:430:ARG:HH11	1.64	0.61
1:H:284:LYS:HD3	1:H:311:TYR:HE2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:408:VAL:HG22	1:F:505:PRO:HG3	1.81	0.61
1:C:408:VAL:HG22	1:C:505:PRO:HG3	1.81	0.61
1:I:231:GLU:HG3	1:I:366:LYS:HZ2	1.65	0.61
1:G:238:PRO:HB2	1:G:241:LEU:HD21	1.82	0.61
1:D:430:ARG:HH11	1:D:430:ARG:HG2	1.64	0.61
1:G:105:LYS:O	1:G:109:ILE:HG12	2.00	0.61
1:A:297:VAL:HG23	1:A:318:LEU:O	2.00	0.61
1:I:105:LYS:O	1:I:109:ILE:HG12	2.00	0.61
1:H:105:LYS:O	1:H:109:ILE:HG12	2.00	0.61
1:F:105:LYS:O	1:F:109:ILE:HG12	2.00	0.61
1:E:230:LYS:NZ	1:E:321:ARG:NH1	2.48	0.61
1:D:427:LYS:NZ	1:D:477:HIS:O	2.33	0.61
1:C:297:VAL:HG23	1:C:318:LEU:O	2.00	0.61
1:F:284:LYS:HD3	1:F:311:TYR:HE2	1.64	0.61
1:B:88:LEU:HD22	1:C:58:MET:CE	2.31	0.61
1:F:110:PHE:HE2	1:F:451:LEU:HG	1.64	0.61
1:H:230:LYS:NZ	1:H:321:ARG:NH1	2.48	0.61
1:I:230:LYS:NZ	1:I:321:ARG:NH1	2.48	0.61
1:D:238:PRO:HB2	1:D:241:LEU:HD21	1.82	0.61
1:A:105:LYS:O	1:A:109:ILE:HG12	2.00	0.61
1:E:260:LEU:HD11	1:E:261:ASP:OD1	2.00	0.61
1:D:297:VAL:HG23	1:D:318:LEU:O	2.00	0.61
1:G:427:LYS:NZ	1:G:477:HIS:O	2.33	0.61
1:E:408:VAL:HG22	1:E:505:PRO:HG3	1.81	0.61
1:A:530:VAL:O	1:B:59:LEU:CD2	2.48	0.61
1:H:297:VAL:HG23	1:H:318:LEU:O	2.00	0.61
1:B:284:LYS:HD3	1:B:311:TYR:HE2	1.64	0.61
1:D:260:LEU:HD12	1:D:261:ASP:CA	2.29	0.61
1:I:427:LYS:NZ	1:I:477:HIS:O	2.33	0.61
1:B:230:LYS:NZ	1:B:321:ARG:NH1	2.48	0.61
1:E:88:LEU:CD2	1:F:58:MET:CE	2.79	0.61
1:A:427:LYS:NZ	1:A:477:HIS:O	2.33	0.61
1:B:427:LYS:NZ	1:B:477:HIS:O	2.33	0.61
1:G:430:ARG:HG2	1:G:430:ARG:HH11	1.64	0.61
1:I:238:PRO:HB2	1:I:241:LEU:HD21	1.82	0.61
1:I:245:LYS:N	1:I:296:ASN:ND2	2.41	0.61
1:F:297:VAL:HG23	1:F:318:LEU:O	2.00	0.61
1:E:105:LYS:O	1:E:109:ILE:HG12	2.00	0.61
1:I:260:LEU:HD12	1:I:260:LEU:C	2.17	0.60
1:I:297:VAL:HG23	1:I:318:LEU:O	2.00	0.60
1:A:260:LEU:HD11	1:A:261:ASP:OD1	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:260:LEU:HD12	1:I:261:ASP:CA	2.29	0.60
1:H:427:LYS:NZ	1:H:477:HIS:O	2.33	0.60
1:A:207:ILE:HA	1:A:379:ILE:O	2.02	0.60
1:G:260:LEU:HD12	1:G:261:ASP:CA	2.29	0.60
1:D:105:LYS:O	1:D:109:ILE:HG12	2.00	0.60
1:I:207:ILE:HA	1:I:379:ILE:O	2.02	0.60
1:E:502:VAL:O	1:E:502:VAL:HG12	2.02	0.60
1:C:415:ILE:HG23	1:C:506:ALA:HB2	1.84	0.60
1:E:210:VAL:HG23	1:E:382:LEU:HD13	1.81	0.60
1:H:238:PRO:HB2	1:H:241:LEU:HD21	1.82	0.60
1:C:238:PRO:HB2	1:C:241:LEU:HD21	1.82	0.60
1:B:358:GLU:HG3	1:B:360:ARG:HH22	1.67	0.60
1:F:427:LYS:NZ	1:F:477:HIS:O	2.33	0.60
1:C:105:LYS:O	1:C:109:ILE:HG12	2.00	0.60
1:G:502:VAL:O	1:G:502:VAL:HG12	2.02	0.60
1:A:415:ILE:HG23	1:A:506:ALA:HB2	1.84	0.60
1:D:207:ILE:HA	1:D:379:ILE:O	2.02	0.60
1:B:238:PRO:HB2	1:B:241:LEU:HD21	1.82	0.60
1:D:119:GLU:HA	1:D:122:LEU:HD23	1.84	0.60
1:G:529:VAL:HG12	1:H:58:MET:HB3	1.84	0.60
1:E:260:LEU:C	1:E:260:LEU:HD12	2.17	0.60
1:G:415:ILE:HG23	1:G:506:ALA:HB2	1.84	0.60
1:E:231:GLU:HG3	1:E:366:LYS:HZ2	1.66	0.60
1:B:105:LYS:O	1:B:109:ILE:HG12	2.00	0.60
1:E:238:PRO:HB2	1:E:241:LEU:HD21	1.82	0.60
1:H:260:LEU:HD12	1:H:260:LEU:C	2.17	0.60
1:F:260:LEU:HD11	1:F:261:ASP:OD1	2.00	0.60
1:A:210:VAL:HG23	1:A:382:LEU:HD13	1.81	0.60
1:G:119:GLU:HA	1:G:122:LEU:HD23	1.84	0.60
1:F:238:PRO:HB2	1:F:241:LEU:HD21	1.82	0.60
1:H:358:GLU:HG3	1:H:360:ARG:HH22	1.67	0.60
1:A:119:GLU:HA	1:A:122:LEU:HD23	1.84	0.60
1:A:502:VAL:O	1:A:502:VAL:HG12	2.02	0.60
1:B:161:LEU:HD12	1:B:161:LEU:N	2.17	0.60
1:E:119:GLU:HA	1:E:122:LEU:HD23	1.84	0.60
1:G:207:ILE:HA	1:G:379:ILE:O	2.02	0.60
1:H:502:VAL:HG12	1:H:502:VAL:O	2.02	0.60
1:I:415:ILE:HG23	1:I:506:ALA:HB2	1.84	0.59
1:B:432:TYR:O	1:B:435:GLN:HG2	2.02	0.59
1:C:432:TYR:O	1:C:435:GLN:HG2	2.02	0.59
1:B:207:ILE:HA	1:B:379:ILE:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:358:GLU:HG3	1:I:360:ARG:HH22	1.67	0.59
1:B:502:VAL:HG12	1:B:502:VAL:O	2.02	0.59
1:B:415:ILE:HG23	1:B:506:ALA:HB2	1.84	0.59
1:D:358:GLU:HG3	1:D:360:ARG:HH22	1.67	0.59
1:H:119:GLU:HA	1:H:122:LEU:HD23	1.84	0.59
1:E:415:ILE:HG23	1:E:506:ALA:HB2	1.84	0.59
1:E:297:VAL:HG23	1:E:318:LEU:O	2.00	0.59
1:G:324:LYS:O	1:G:327:ASP:OD2	2.21	0.59
1:B:119:GLU:HA	1:B:122:LEU:HD23	1.84	0.59
1:C:207:ILE:HA	1:C:379:ILE:O	2.02	0.59
1:F:119:GLU:HA	1:F:122:LEU:HD23	1.84	0.59
1:I:166:MET:HE1	1:I:179:GLU:HG2	1.85	0.59
1:E:324:LYS:O	1:E:327:ASP:OD2	2.21	0.59
1:H:415:ILE:HG23	1:H:506:ALA:HB2	1.84	0.59
1:F:358:GLU:HG3	1:F:360:ARG:HH22	1.67	0.59
1:H:324:LYS:O	1:H:327:ASP:OD2	2.21	0.59
1:E:161:LEU:N	1:E:161:LEU:HD12	2.17	0.59
1:F:161:LEU:HD12	1:F:161:LEU:N	2.17	0.59
1:A:161:LEU:HD12	1:A:161:LEU:N	2.17	0.59
1:I:502:VAL:O	1:I:502:VAL:HG12	2.02	0.59
1:C:502:VAL:HG12	1:C:502:VAL:O	2.02	0.59
1:C:161:LEU:HD12	1:C:161:LEU:N	2.17	0.59
1:F:527:ASP:N	1:G:56:ASP:O	2.26	0.59
1:I:324:LYS:O	1:I:327:ASP:OD2	2.21	0.59
1:E:207:ILE:HA	1:E:379:ILE:O	2.02	0.59
1:E:358:GLU:HG3	1:E:360:ARG:HH22	1.67	0.59
1:B:324:LYS:O	1:B:327:ASP:OD2	2.21	0.59
1:F:207:ILE:HA	1:F:379:ILE:O	2.02	0.59
1:A:358:GLU:HG3	1:A:360:ARG:HH22	1.67	0.59
1:C:358:GLU:HG3	1:C:360:ARG:HH22	1.67	0.59
1:D:502:VAL:HG12	1:D:502:VAL:O	2.02	0.59
1:I:432:TYR:O	1:I:435:GLN:HG2	2.03	0.59
1:A:432:TYR:O	1:A:435:GLN:HG2	2.02	0.59
1:D:161:LEU:HD12	1:D:161:LEU:N	2.17	0.59
1:C:119:GLU:HA	1:C:122:LEU:HD23	1.84	0.59
1:H:174:VAL:HG12	1:H:174:VAL:O	2.03	0.59
1:I:161:LEU:N	1:I:161:LEU:HD12	2.17	0.59
1:E:88:LEU:HD22	1:F:58:MET:HE2	1.84	0.59
1:G:358:GLU:HG3	1:G:360:ARG:HH22	1.67	0.59
1:A:260:LEU:C	1:A:260:LEU:HD12	2.17	0.58
1:G:432:TYR:O	1:G:435:GLN:HG2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:TYR:O	1:D:435:GLN:HG2	2.03	0.58
1:H:432:TYR:O	1:H:435:GLN:HG2	2.03	0.58
1:E:432:TYR:O	1:E:435:GLN:HG2	2.02	0.58
1:F:174:VAL:HG12	1:F:174:VAL:O	2.03	0.58
1:G:161:LEU:HD12	1:G:161:LEU:N	2.17	0.58
1:H:161:LEU:HD12	1:H:161:LEU:N	2.17	0.58
1:F:256:GLU:C	1:F:258:PRO:HD3	2.22	0.58
1:B:153:VAL:CG2	1:B:160:LEU:HD23	2.33	0.58
1:I:153:VAL:CG2	1:I:160:LEU:HD23	2.33	0.58
1:F:127:HIS:HD2	1:F:129:THR:HB	1.68	0.58
1:F:502:VAL:O	1:F:502:VAL:HG12	2.02	0.58
1:G:153:VAL:CG2	1:G:160:LEU:HD23	2.33	0.58
1:H:127:HIS:HD2	1:H:129:THR:HB	1.69	0.58
1:E:450:ALA:O	1:E:453:SER:HB2	2.04	0.58
1:F:432:TYR:O	1:F:435:GLN:HG2	2.03	0.58
1:H:153:VAL:CG2	1:H:160:LEU:HD23	2.34	0.58
1:G:127:HIS:HD2	1:G:129:THR:HB	1.69	0.58
1:I:119:GLU:HA	1:I:122:LEU:HD23	1.84	0.58
1:A:450:ALA:O	1:A:453:SER:HB2	2.04	0.58
1:I:450:ALA:O	1:I:453:SER:HB2	2.04	0.58
1:B:142:ALA:HA	1:B:425:ILE:HG23	1.86	0.58
1:F:415:ILE:HG23	1:F:506:ALA:HB2	1.84	0.58
1:B:450:ALA:O	1:B:453:SER:HB2	2.04	0.58
1:C:450:ALA:O	1:C:453:SER:HB2	2.04	0.58
1:D:450:ALA:O	1:D:453:SER:HB2	2.04	0.58
1:I:142:ALA:HA	1:I:425:ILE:HG23	1.86	0.58
1:D:324:LYS:O	1:D:327:ASP:OD2	2.21	0.58
1:D:415:ILE:HD13	1:D:415:ILE:H	1.69	0.58
1:D:415:ILE:HG23	1:D:506:ALA:HB2	1.84	0.58
1:C:142:ALA:HA	1:C:425:ILE:HG23	1.86	0.58
1:A:127:HIS:HD2	1:A:129:THR:HB	1.69	0.58
1:H:433:ALA:HB3	1:H:434:PRO:HD3	1.86	0.58
1:G:222:LEU:H	1:G:222:LEU:HD23	1.69	0.58
1:H:207:ILE:HA	1:H:379:ILE:O	2.02	0.58
1:G:174:VAL:O	1:G:174:VAL:HG12	2.03	0.58
1:I:415:ILE:HD13	1:I:415:ILE:H	1.69	0.58
1:A:222:LEU:HD23	1:A:222:LEU:H	1.69	0.58
1:C:222:LEU:HD23	1:C:222:LEU:H	1.69	0.58
1:F:324:LYS:O	1:F:327:ASP:OD2	2.21	0.58
1:C:324:LYS:O	1:C:327:ASP:OD2	2.21	0.58
1:C:174:VAL:HG12	1:C:174:VAL:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:528:ASP:HB3	1:G:57:LYS:CD	2.34	0.58
1:B:415:ILE:H	1:B:415:ILE:HD13	1.69	0.58
1:A:415:ILE:H	1:A:415:ILE:HD13	1.69	0.58
1:H:450:ALA:O	1:H:453:SER:HB2	2.04	0.58
1:F:415:ILE:H	1:F:415:ILE:HD13	1.69	0.58
1:D:226:ILE:HG13	1:D:331:LEU:HA	1.86	0.58
1:E:222:LEU:H	1:E:222:LEU:HD23	1.69	0.58
1:A:260:LEU:HD12	1:A:261:ASP:CA	2.29	0.57
1:G:142:ALA:HA	1:G:425:ILE:HG23	1.86	0.57
1:A:142:ALA:HA	1:A:425:ILE:HG23	1.86	0.57
1:C:232:VAL:CG1	1:C:318:LEU:HD11	2.34	0.57
1:G:232:VAL:CG1	1:G:318:LEU:HD11	2.34	0.57
1:I:433:ALA:HB3	1:I:434:PRO:HD3	1.86	0.57
1:F:527:ASP:HB2	1:G:55:MET:CB	2.33	0.57
1:E:226:ILE:HG13	1:E:331:LEU:HA	1.86	0.57
1:B:222:LEU:HD23	1:B:222:LEU:H	1.69	0.57
1:C:415:ILE:HD13	1:C:415:ILE:H	1.69	0.57
1:H:265:ARG:O	1:H:266:ILE:HG12	2.04	0.57
1:I:265:ARG:O	1:I:266:ILE:HG12	2.04	0.57
1:B:433:ALA:HB3	1:B:434:PRO:HD3	1.86	0.57
1:F:433:ALA:HB3	1:F:434:PRO:HD3	1.86	0.57
1:C:433:ALA:HB3	1:C:434:PRO:HD3	1.86	0.57
1:E:433:ALA:HB3	1:E:434:PRO:HD3	1.86	0.57
1:H:226:ILE:HG13	1:H:331:LEU:HA	1.86	0.57
1:D:153:VAL:CG2	1:D:160:LEU:HD23	2.33	0.57
1:A:324:LYS:O	1:A:327:ASP:OD2	2.21	0.57
1:F:260:LEU:HD12	1:F:261:ASP:CA	2.29	0.57
1:C:265:ARG:O	1:C:266:ILE:HG12	2.04	0.57
1:A:153:VAL:CG2	1:A:160:LEU:HD23	2.33	0.57
1:I:222:LEU:HD23	1:I:222:LEU:H	1.69	0.57
1:E:127:HIS:HD2	1:E:129:THR:HB	1.68	0.57
1:B:174:VAL:HG12	1:B:174:VAL:O	2.03	0.57
1:D:142:ALA:HA	1:D:425:ILE:HG23	1.86	0.57
1:A:245:LYS:HG2	1:A:353:TYR:CD1	2.40	0.57
1:F:232:VAL:CG1	1:F:318:LEU:HD11	2.35	0.57
1:I:232:VAL:CG1	1:I:318:LEU:HD11	2.34	0.57
1:I:226:ILE:HG13	1:I:331:LEU:HA	1.86	0.57
1:E:153:VAL:CG2	1:E:160:LEU:HD23	2.33	0.57
1:C:127:HIS:HD2	1:C:129:THR:HB	1.68	0.57
1:C:98:GLU:HG3	1:C:99:GLU:H	1.69	0.57
1:D:174:VAL:HG12	1:D:174:VAL:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:174:VAL:O	1:I:174:VAL:HG12	2.03	0.57
1:B:245:LYS:HG2	1:B:353:TYR:CD1	2.40	0.57
1:E:245:LYS:HG2	1:E:353:TYR:CD1	2.40	0.57
1:E:174:VAL:O	1:E:174:VAL:HG12	2.03	0.57
1:D:260:LEU:HD12	1:D:260:LEU:C	2.17	0.57
1:G:245:LYS:HG2	1:G:353:TYR:CD1	2.40	0.57
1:C:245:LYS:HG2	1:C:353:TYR:CD1	2.40	0.57
1:F:226:ILE:HG13	1:F:331:LEU:HA	1.86	0.57
1:H:222:LEU:HD23	1:H:222:LEU:H	1.69	0.57
1:I:127:HIS:HD2	1:I:129:THR:HB	1.68	0.57
1:G:450:ALA:O	1:G:453:SER:HB2	2.04	0.57
1:G:351:LEU:H	1:G:351:LEU:CD2	2.17	0.57
1:A:232:VAL:CG1	1:A:318:LEU:HD11	2.35	0.57
1:A:433:ALA:HB3	1:A:434:PRO:HD3	1.86	0.57
1:C:153:VAL:CG2	1:C:160:LEU:HD23	2.33	0.57
1:F:222:LEU:HD23	1:F:222:LEU:H	1.69	0.57
1:D:147:GLN:HE21	1:D:413:ARG:HH22	1.53	0.57
1:H:98:GLU:HG3	1:H:99:GLU:H	1.69	0.57
1:I:245:LYS:HG2	1:I:353:TYR:CD1	2.40	0.57
1:D:265:ARG:O	1:D:266:ILE:HG12	2.04	0.57
1:E:265:ARG:O	1:E:266:ILE:HG12	2.04	0.57
1:G:265:ARG:O	1:G:266:ILE:HG12	2.04	0.57
1:H:299:ILE:HD13	1:H:299:ILE:N	2.20	0.57
1:F:162:ARG:HB2	1:F:162:ARG:HH11	1.70	0.57
1:H:383:ILE:HG22	1:H:391:VAL:HG23	1.87	0.57
1:A:383:ILE:HG22	1:A:391:VAL:HG23	1.87	0.57
1:H:245:LYS:HG2	1:H:353:TYR:CD1	2.40	0.57
1:F:245:LYS:HG2	1:F:353:TYR:CD1	2.40	0.57
1:B:232:VAL:CG1	1:B:318:LEU:HD11	2.35	0.57
1:D:433:ALA:HB3	1:D:434:PRO:HD3	1.86	0.57
1:G:147:GLN:HE21	1:G:413:ARG:HH22	1.53	0.57
1:B:98:GLU:HG3	1:B:99:GLU:H	1.69	0.57
1:D:98:GLU:HG3	1:D:99:GLU:H	1.69	0.57
1:D:520:ALA:O	1:D:524:LEU:HD13	2.05	0.57
1:A:174:VAL:O	1:A:174:VAL:HG12	2.03	0.57
1:D:256:GLU:C	1:D:258:PRO:HD3	2.22	0.57
1:E:88:LEU:CD2	1:F:58:MET:HE1	2.35	0.57
1:H:415:ILE:HD13	1:H:415:ILE:H	1.69	0.57
1:H:142:ALA:HA	1:H:425:ILE:HG23	1.86	0.57
1:E:415:ILE:H	1:E:415:ILE:HD13	1.69	0.57
1:F:265:ARG:O	1:F:266:ILE:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:ILE:N	1:F:299:ILE:HD13	2.20	0.57
1:D:222:LEU:H	1:D:222:LEU:HD23	1.69	0.57
1:F:166:MET:HE1	1:F:179:GLU:HG2	1.87	0.57
1:C:147:GLN:HE21	1:C:413:ARG:HH22	1.53	0.57
1:B:383:ILE:HG22	1:B:391:VAL:HG23	1.87	0.57
1:F:147:GLN:HE21	1:F:413:ARG:HH22	1.53	0.57
1:H:260:LEU:HD12	1:H:261:ASP:CA	2.29	0.56
1:A:351:LEU:H	1:A:351:LEU:CD2	2.17	0.56
1:E:462:ALA:HB2	1:E:489:LEU:HD12	1.87	0.56
1:A:162:ARG:HH11	1:A:162:ARG:HB2	1.70	0.56
1:H:147:GLN:HE21	1:H:413:ARG:HH22	1.53	0.56
1:D:245:LYS:HG2	1:D:353:TYR:CD1	2.40	0.56
1:H:244:ALA:HA	1:H:296:ASN:ND2	2.21	0.56
1:E:244:ALA:HA	1:E:296:ASN:ND2	2.21	0.56
1:I:462:ALA:HB2	1:I:489:LEU:HD12	1.87	0.56
1:A:147:GLN:HE21	1:A:413:ARG:HH22	1.53	0.56
1:D:508:VAL:HG13	1:D:509:LYS:N	2.20	0.56
1:G:256:GLU:C	1:G:258:PRO:HD3	2.22	0.56
1:E:88:LEU:HD23	1:F:58:MET:HE1	1.86	0.56
1:F:244:ALA:HA	1:F:296:ASN:ND2	2.21	0.56
1:E:142:ALA:HA	1:E:425:ILE:HG23	1.86	0.56
1:A:265:ARG:O	1:A:266:ILE:HG12	2.04	0.56
1:D:232:VAL:CG1	1:D:318:LEU:HD11	2.34	0.56
1:A:226:ILE:HG13	1:A:331:LEU:HA	1.86	0.56
1:B:226:ILE:HG13	1:B:331:LEU:HA	1.86	0.56
1:H:462:ALA:HB2	1:H:489:LEU:HD12	1.87	0.56
1:D:462:ALA:HB2	1:D:489:LEU:HD12	1.87	0.56
1:G:162:ARG:HB2	1:G:162:ARG:HH11	1.70	0.56
1:H:162:ARG:HH11	1:H:162:ARG:HB2	1.70	0.56
1:B:147:GLN:HE21	1:B:413:ARG:HH22	1.53	0.56
1:F:508:VAL:HG13	1:F:509:LYS:N	2.20	0.56
1:C:99:GLU:HG3	1:C:407:ASP:OD2	2.06	0.56
1:C:520:ALA:O	1:C:524:LEU:HD13	2.05	0.56
1:E:98:GLU:HG3	1:E:99:GLU:H	1.69	0.56
1:F:520:ALA:O	1:F:524:LEU:HD13	2.05	0.56
1:F:98:GLU:HG3	1:F:99:GLU:H	1.69	0.56
1:A:520:ALA:O	1:A:524:LEU:HD13	2.05	0.56
1:I:98:GLU:HG3	1:I:99:GLU:H	1.69	0.56
1:I:147:GLN:HE21	1:I:413:ARG:HH22	1.53	0.56
1:I:88:LEU:O	1:I:92:ILE:HG13	2.06	0.56
1:D:180:TYR:O	1:D:184:ILE:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:VAL:HG13	1:A:509:LYS:N	2.20	0.56
1:A:244:ALA:HA	1:A:296:ASN:ND2	2.21	0.56
1:G:415:ILE:H	1:G:415:ILE:HD13	1.69	0.56
1:G:433:ALA:HB3	1:G:434:PRO:HD3	1.86	0.56
1:C:226:ILE:HG13	1:C:331:LEU:HA	1.86	0.56
1:D:299:ILE:N	1:D:299:ILE:HD13	2.20	0.56
1:B:88:LEU:O	1:B:92:ILE:HG13	2.06	0.56
1:C:180:TYR:O	1:C:184:ILE:HG12	2.06	0.56
1:I:508:VAL:HG13	1:I:509:LYS:N	2.20	0.56
1:G:520:ALA:O	1:G:524:LEU:HD13	2.05	0.56
1:I:520:ALA:O	1:I:524:LEU:HD13	2.05	0.56
1:I:244:ALA:HA	1:I:296:ASN:ND2	2.20	0.56
1:A:88:LEU:O	1:A:92:ILE:HG13	2.06	0.56
1:B:180:TYR:O	1:B:184:ILE:HG12	2.06	0.56
1:D:127:HIS:HD2	1:D:129:THR:HB	1.69	0.56
1:F:450:ALA:O	1:F:453:SER:HB2	2.04	0.56
1:I:443:ALA:O	1:I:446:ALA:HB3	2.06	0.56
1:H:520:ALA:O	1:H:524:LEU:HD13	2.05	0.56
1:B:520:ALA:O	1:B:524:LEU:HD13	2.05	0.56
1:E:260:LEU:HD12	1:E:261:ASP:CA	2.29	0.56
1:B:265:ARG:O	1:B:266:ILE:HG12	2.04	0.56
1:E:232:VAL:CG1	1:E:318:LEU:HD11	2.35	0.56
1:G:226:ILE:HG13	1:G:331:LEU:HA	1.86	0.56
1:H:126:VAL:O	1:H:126:VAL:HG23	2.06	0.56
1:E:99:GLU:HG3	1:E:407:ASP:OD2	2.06	0.56
1:A:99:GLU:HG3	1:A:407:ASP:OD2	2.06	0.56
1:E:88:LEU:O	1:E:92:ILE:HG13	2.05	0.56
1:B:244:ALA:HA	1:B:296:ASN:ND2	2.20	0.56
1:H:180:TYR:O	1:H:184:ILE:HG12	2.06	0.56
1:B:127:HIS:HD2	1:B:129:THR:HB	1.69	0.56
1:B:99:GLU:HG3	1:B:407:ASP:OD2	2.06	0.56
1:D:99:GLU:HG3	1:D:407:ASP:OD2	2.06	0.56
1:G:443:ALA:O	1:G:446:ALA:HB3	2.06	0.56
1:E:88:LEU:HD22	1:F:58:MET:CE	2.36	0.56
1:F:88:LEU:O	1:F:92:ILE:HG13	2.06	0.56
1:H:232:VAL:CG1	1:H:318:LEU:HD11	2.34	0.56
1:B:462:ALA:HB2	1:B:489:LEU:HD12	1.87	0.56
1:H:430:ARG:O	1:H:434:PRO:HD3	2.06	0.56
1:D:88:LEU:O	1:D:92:ILE:HG13	2.06	0.56
1:G:88:LEU:O	1:G:92:ILE:HG13	2.06	0.56
1:F:180:TYR:O	1:F:184:ILE:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLU:HG3	1:A:99:GLU:H	1.69	0.56
1:A:443:ALA:O	1:A:446:ALA:HB3	2.06	0.56
1:G:98:GLU:HG3	1:G:99:GLU:H	1.69	0.56
1:E:383:ILE:HG22	1:E:391:VAL:HG23	1.87	0.56
1:C:443:ALA:O	1:C:446:ALA:HB3	2.06	0.56
1:D:244:ALA:HA	1:D:296:ASN:ND2	2.21	0.56
1:F:142:ALA:HA	1:F:425:ILE:HG23	1.86	0.56
1:E:39:VAL:HG13	1:E:89:LEU:HD22	1.88	0.56
1:C:299:ILE:HD13	1:C:299:ILE:N	2.20	0.56
1:F:153:VAL:CG2	1:F:160:LEU:HD23	2.33	0.56
1:F:462:ALA:HB2	1:F:489:LEU:HD12	1.87	0.56
1:A:126:VAL:O	1:A:126:VAL:HG23	2.06	0.56
1:F:126:VAL:O	1:F:126:VAL:HG23	2.06	0.56
1:H:99:GLU:HG3	1:H:407:ASP:OD2	2.06	0.56
1:F:99:GLU:HG3	1:F:407:ASP:OD2	2.06	0.56
1:C:192:VAL:HG11	1:C:206:ASN:HB2	1.88	0.56
1:D:443:ALA:O	1:D:446:ALA:HB3	2.06	0.56
1:H:443:ALA:O	1:H:446:ALA:HB3	2.06	0.56
1:G:244:ALA:HA	1:G:296:ASN:ND2	2.20	0.55
1:B:39:VAL:HG13	1:B:89:LEU:HD22	1.88	0.55
1:D:470:LEU:CD2	1:D:474:ARG:HD2	2.37	0.55
1:I:180:TYR:O	1:I:184:ILE:HG12	2.06	0.55
1:H:470:LEU:CD2	1:H:474:ARG:HD2	2.37	0.55
1:C:470:LEU:CD2	1:C:474:ARG:HD2	2.37	0.55
1:I:162:ARG:HB2	1:I:162:ARG:HH11	1.70	0.55
1:D:383:ILE:HG22	1:D:391:VAL:HG23	1.87	0.55
1:D:430:ARG:O	1:D:434:PRO:HD3	2.06	0.55
1:I:363:GLY:HA2	1:I:384:ARG:NH2	2.21	0.55
1:A:363:GLY:HA2	1:A:384:ARG:NH2	2.21	0.55
1:B:299:ILE:N	1:B:299:ILE:HD13	2.20	0.55
1:C:462:ALA:HB2	1:C:489:LEU:HD12	1.87	0.55
1:E:470:LEU:CD2	1:E:474:ARG:HD2	2.37	0.55
1:C:88:LEU:O	1:C:92:ILE:HG13	2.06	0.55
1:B:470:LEU:CD2	1:B:474:ARG:HD2	2.37	0.55
1:I:126:VAL:O	1:I:126:VAL:HG23	2.06	0.55
1:C:508:VAL:HG13	1:C:509:LYS:N	2.20	0.55
1:E:508:VAL:HG13	1:E:509:LYS:N	2.20	0.55
1:G:383:ILE:HG22	1:G:391:VAL:HG23	1.87	0.55
1:C:244:ALA:HA	1:C:296:ASN:ND2	2.21	0.55
1:B:508:VAL:HG13	1:B:509:LYS:N	2.21	0.55
1:G:212:LYS:HA	1:G:212:LYS:CE	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:430:ARG:O	1:I:434:PRO:HD3	2.06	0.55
1:A:430:ARG:O	1:A:434:PRO:HD3	2.06	0.55
1:D:363:GLY:HA2	1:D:384:ARG:NH2	2.21	0.55
1:B:88:LEU:CD2	1:C:58:MET:HE1	2.35	0.55
1:H:63:LEU:HD23	1:H:63:LEU:O	2.06	0.55
1:I:383:ILE:HG22	1:I:391:VAL:HG23	1.87	0.55
1:B:192:VAL:HG11	1:B:206:ASN:HB2	1.88	0.55
1:I:351:LEU:CD2	1:I:351:LEU:H	2.17	0.55
1:C:430:ARG:O	1:C:434:PRO:HD3	2.06	0.55
1:H:255:VAL:HG13	1:H:305:ASP:OD1	2.07	0.55
1:C:363:GLY:HA2	1:C:384:ARG:NH2	2.21	0.55
1:G:299:ILE:HD13	1:G:299:ILE:N	2.20	0.55
1:I:39:VAL:HG13	1:I:89:LEU:HD22	1.88	0.55
1:A:180:TYR:O	1:A:184:ILE:HG12	2.06	0.55
1:E:126:VAL:HG23	1:E:126:VAL:O	2.06	0.55
1:F:230:LYS:HZ1	1:F:321:ARG:NH1	2.04	0.55
1:D:192:VAL:HG11	1:D:206:ASN:HB2	1.88	0.55
1:F:192:VAL:HG11	1:F:206:ASN:HB2	1.88	0.55
1:F:383:ILE:HG22	1:F:391:VAL:HG23	1.87	0.55
1:E:63:LEU:HD23	1:E:63:LEU:O	2.06	0.55
1:F:63:LEU:HD23	1:F:63:LEU:O	2.06	0.55
1:E:430:ARG:O	1:E:434:PRO:HD3	2.06	0.55
1:H:363:GLY:HA2	1:H:384:ARG:NH2	2.21	0.55
1:G:255:VAL:HG13	1:G:305:ASP:OD1	2.07	0.55
1:D:39:VAL:HG13	1:D:89:LEU:HD22	1.88	0.55
1:F:363:GLY:HA2	1:F:384:ARG:NH2	2.21	0.55
1:A:462:ALA:HB2	1:A:489:LEU:HD12	1.87	0.55
1:F:470:LEU:CD2	1:F:474:ARG:HD2	2.37	0.55
1:I:470:LEU:CD2	1:I:474:ARG:HD2	2.37	0.55
1:D:162:ARG:HB2	1:D:162:ARG:HH11	1.70	0.55
1:D:126:VAL:O	1:D:126:VAL:HG23	2.06	0.55
1:G:508:VAL:HG13	1:G:509:LYS:N	2.20	0.55
1:F:443:ALA:O	1:F:446:ALA:HB3	2.06	0.55
1:G:192:VAL:HG11	1:G:206:ASN:HB2	1.88	0.55
1:I:63:LEU:HD23	1:I:63:LEU:O	2.06	0.55
1:A:63:LEU:O	1:A:63:LEU:HD23	2.06	0.55
1:C:256:GLU:C	1:C:258:PRO:HD3	2.22	0.55
1:B:363:GLY:HA2	1:B:384:ARG:NH2	2.21	0.55
1:A:39:VAL:HG13	1:A:89:LEU:HD22	1.88	0.55
1:D:255:VAL:HG13	1:D:305:ASP:OD1	2.07	0.55
1:E:180:TYR:O	1:E:184:ILE:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:LEU:CD2	1:A:474:ARG:HD2	2.37	0.55
1:B:162:ARG:HB2	1:B:162:ARG:HH11	1.70	0.55
1:D:232:VAL:HG22	1:D:359:GLU:OE2	2.07	0.55
1:F:430:ARG:O	1:F:434:PRO:HD3	2.06	0.55
1:E:363:GLY:HA2	1:E:384:ARG:NH2	2.21	0.55
1:H:88:LEU:O	1:H:92:ILE:HG13	2.06	0.55
1:C:162:ARG:HH11	1:C:162:ARG:HB2	1.70	0.55
1:I:230:LYS:HZ2	1:I:321:ARG:NH1	2.05	0.55
1:I:99:GLU:HG3	1:I:407:ASP:OD2	2.06	0.55
1:I:383:ILE:N	1:I:383:ILE:HD12	2.22	0.55
1:A:178:ARG:H	1:A:178:ARG:HE	1.55	0.55
1:B:443:ALA:O	1:B:446:ALA:HB3	2.06	0.55
1:E:520:ALA:O	1:E:524:LEU:HD13	2.05	0.55
1:E:147:GLN:HE21	1:E:413:ARG:HH22	1.53	0.55
1:E:256:GLU:C	1:E:258:PRO:HD3	2.22	0.55
1:E:212:LYS:CE	1:E:212:LYS:HA	2.33	0.55
1:H:351:LEU:H	1:H:351:LEU:CD2	2.17	0.55
1:E:351:LEU:H	1:E:351:LEU:CD2	2.17	0.55
1:G:462:ALA:HB2	1:G:489:LEU:HD12	1.87	0.55
1:G:470:LEU:CD2	1:G:474:ARG:HD2	2.37	0.55
1:G:180:TYR:O	1:G:184:ILE:HG12	2.06	0.55
1:H:508:VAL:HG13	1:H:509:LYS:N	2.20	0.55
1:G:99:GLU:HG3	1:G:407:ASP:OD2	2.06	0.55
1:H:423:ILE:HD12	1:H:424:GLU:HG2	1.89	0.55
1:G:430:ARG:O	1:G:434:PRO:HD3	2.06	0.55
1:B:126:VAL:O	1:B:126:VAL:HG23	2.06	0.55
1:C:383:ILE:HG22	1:C:391:VAL:HG23	1.87	0.55
1:C:383:ILE:N	1:C:383:ILE:HD12	2.22	0.55
1:E:443:ALA:O	1:E:446:ALA:HB3	2.06	0.55
1:A:76:LEU:CD2	1:A:90:VAL:HG12	2.36	0.55
1:F:351:LEU:H	1:F:351:LEU:CD2	2.17	0.55
1:A:232:VAL:HG22	1:A:359:GLU:OE2	2.07	0.55
1:F:255:VAL:HG13	1:F:305:ASP:OD1	2.07	0.55
1:E:383:ILE:HD12	1:E:383:ILE:N	2.22	0.55
1:D:383:ILE:N	1:D:383:ILE:HD12	2.22	0.55
1:G:63:LEU:O	1:G:63:LEU:HD23	2.06	0.55
1:G:423:ILE:HD12	1:G:424:GLU:HG2	1.89	0.54
1:G:232:VAL:HG22	1:G:359:GLU:OE2	2.07	0.54
1:B:430:ARG:O	1:B:434:PRO:HD3	2.06	0.54
1:A:299:ILE:HD13	1:A:299:ILE:N	2.20	0.54
1:C:255:VAL:HG13	1:C:305:ASP:OD1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:VAL:O	1:C:126:VAL:HG23	2.06	0.54
1:G:126:VAL:O	1:G:126:VAL:HG23	2.06	0.54
1:H:383:ILE:HD12	1:H:383:ILE:N	2.22	0.54
1:B:232:VAL:HG22	1:B:359:GLU:OE2	2.07	0.54
1:E:111:SER:O	1:E:115:VAL:HG23	2.08	0.54
1:C:39:VAL:HG13	1:C:89:LEU:HD22	1.88	0.54
1:E:487:ILE:O	1:E:489:LEU:HD22	2.08	0.54
1:I:192:VAL:HG11	1:I:206:ASN:HB2	1.88	0.54
1:E:347:SER:C	1:E:349:GLN:H	2.11	0.54
1:C:178:ARG:H	1:C:178:ARG:HE	1.55	0.54
1:B:63:LEU:O	1:B:63:LEU:HD23	2.06	0.54
1:B:256:GLU:C	1:B:258:PRO:HD3	2.22	0.54
1:C:232:VAL:HG22	1:C:359:GLU:OE2	2.07	0.54
1:F:232:VAL:HG22	1:F:359:GLU:OE2	2.07	0.54
1:G:363:GLY:HA2	1:G:384:ARG:NH2	2.21	0.54
1:I:487:ILE:O	1:I:489:LEU:HD22	2.08	0.54
1:C:63:LEU:O	1:C:63:LEU:HD23	2.06	0.54
1:D:63:LEU:O	1:D:63:LEU:HD23	2.06	0.54
1:B:255:VAL:HG13	1:B:305:ASP:OD1	2.07	0.54
1:I:178:ARG:HE	1:I:178:ARG:H	1.55	0.54
1:A:347:SER:C	1:A:349:GLN:H	2.11	0.54
1:B:178:ARG:H	1:B:178:ARG:HE	1.55	0.54
1:H:256:GLU:C	1:H:258:PRO:HD3	2.22	0.54
1:H:232:VAL:HG22	1:H:359:GLU:OE2	2.07	0.54
1:B:487:ILE:O	1:B:489:LEU:HD22	2.08	0.54
1:B:111:SER:O	1:B:115:VAL:HG23	2.08	0.54
1:I:299:ILE:HD13	1:I:299:ILE:N	2.20	0.54
1:H:230:LYS:HZ1	1:H:321:ARG:NH1	2.05	0.54
1:F:178:ARG:HE	1:F:178:ARG:H	1.55	0.54
1:F:347:SER:C	1:F:349:GLN:H	2.11	0.54
1:A:192:VAL:HG11	1:A:206:ASN:HB2	1.88	0.54
1:H:192:VAL:HG11	1:H:206:ASN:HB2	1.88	0.54
1:H:39:VAL:HG13	1:H:89:LEU:HD22	1.88	0.54
1:G:39:VAL:HG13	1:G:89:LEU:HD22	1.88	0.54
1:F:39:VAL:HG13	1:F:89:LEU:HD22	1.88	0.54
1:C:487:ILE:O	1:C:489:LEU:HD22	2.08	0.54
1:B:118:ALA:O	1:B:122:LEU:HD22	2.08	0.54
1:B:166:MET:HE1	1:B:179:GLU:HG2	1.89	0.54
1:G:347:SER:C	1:G:349:GLN:H	2.11	0.54
1:D:178:ARG:HE	1:D:178:ARG:H	1.55	0.54
1:I:255:VAL:HG13	1:I:305:ASP:OD1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:VAL:HG13	1:A:305:ASP:OD1	2.07	0.54
1:E:299:ILE:N	1:E:299:ILE:HD13	2.20	0.54
1:I:256:GLU:C	1:I:258:PRO:HD3	2.22	0.54
1:B:181:ILE:O	1:B:185:VAL:HG23	2.08	0.54
1:D:529:VAL:HG12	1:E:58:MET:SD	2.48	0.54
1:I:232:VAL:HG22	1:I:359:GLU:OE2	2.07	0.54
1:D:351:LEU:H	1:D:351:LEU:CD2	2.17	0.54
1:A:111:SER:O	1:A:115:VAL:HG23	2.08	0.54
1:F:487:ILE:O	1:F:489:LEU:HD22	2.08	0.54
1:G:118:ALA:O	1:G:122:LEU:HD22	2.08	0.54
1:A:383:ILE:N	1:A:383:ILE:HD12	2.22	0.54
1:B:383:ILE:HD12	1:B:383:ILE:N	2.22	0.54
1:F:383:ILE:N	1:F:383:ILE:HD12	2.22	0.54
1:C:265:ARG:HD2	1:C:266:ILE:N	2.23	0.54
1:E:255:VAL:HG13	1:E:305:ASP:OD1	2.07	0.54
1:C:284:LYS:HD3	1:C:311:TYR:CE2	2.43	0.54
1:H:284:LYS:HD3	1:H:311:TYR:CE2	2.43	0.54
1:G:470:LEU:HD22	1:G:474:ARG:HD2	1.90	0.54
1:C:470:LEU:HD22	1:C:474:ARG:HD2	1.90	0.54
1:H:482:ASN:O	1:H:483:LYS:C	2.47	0.54
1:B:347:SER:C	1:B:349:GLN:H	2.11	0.54
1:C:347:SER:C	1:C:349:GLN:H	2.11	0.54
1:F:423:ILE:HD12	1:F:424:GLU:HG2	1.89	0.54
1:H:76:LEU:CD2	1:H:90:VAL:HG12	2.36	0.54
1:D:284:LYS:HD3	1:D:311:TYR:CE2	2.43	0.54
1:E:284:LYS:HD3	1:E:311:TYR:CE2	2.43	0.54
1:D:118:ALA:O	1:D:122:LEU:HD22	2.08	0.54
1:D:504:GLU:OE1	2:D:800:ADP:H2'	2.09	0.53
1:E:423:ILE:HD12	1:E:424:GLU:HG2	1.90	0.53
1:D:423:ILE:HD12	1:D:424:GLU:HG2	1.90	0.53
1:B:76:LEU:CD2	1:B:90:VAL:HG12	2.36	0.53
1:B:351:LEU:H	1:B:351:LEU:CD2	2.17	0.53
1:G:111:SER:O	1:G:115:VAL:HG23	2.08	0.53
1:C:233:VAL:HG22	1:C:309:GLN:OE1	2.08	0.53
1:G:482:ASN:O	1:G:483:LYS:C	2.47	0.53
1:E:192:VAL:HG11	1:E:206:ASN:HB2	1.88	0.53
1:D:530:VAL:O	1:E:59:LEU:HD23	2.07	0.53
1:C:423:ILE:HD12	1:C:424:GLU:HG2	1.90	0.53
1:A:265:ARG:HD2	1:A:266:ILE:N	2.23	0.53
1:E:232:VAL:HG22	1:E:359:GLU:OE2	2.07	0.53
1:E:233:VAL:HG22	1:E:309:GLN:OE1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:SER:O	1:F:115:VAL:HG23	2.08	0.53
1:H:487:ILE:O	1:H:489:LEU:HD22	2.08	0.53
1:E:470:LEU:HD22	1:E:474:ARG:HD2	1.90	0.53
1:F:470:LEU:HD22	1:F:474:ARG:HD2	1.90	0.53
1:E:118:ALA:O	1:E:122:LEU:HD22	2.08	0.53
1:G:383:ILE:N	1:G:383:ILE:HD12	2.22	0.53
1:I:347:SER:C	1:I:349:GLN:H	2.11	0.53
1:F:529:VAL:HG12	1:G:58:MET:SD	2.47	0.53
1:I:504:GLU:OE1	2:I:800:ADP:H2'	2.09	0.53
1:G:361:LYS:CB	1:G:366:LYS:HG2	2.36	0.53
1:D:111:SER:O	1:D:115:VAL:HG23	2.08	0.53
1:B:284:LYS:HD3	1:B:311:TYR:CE2	2.43	0.53
1:G:524:LEU:N	1:G:524:LEU:HD12	2.24	0.53
1:G:178:ARG:HE	1:G:178:ARG:H	1.55	0.53
1:G:265:ARG:HD2	1:G:266:ILE:N	2.23	0.53
1:H:111:SER:O	1:H:115:VAL:HG23	2.08	0.53
1:F:284:LYS:HD3	1:F:311:TYR:CE2	2.43	0.53
1:A:487:ILE:O	1:A:489:LEU:HD22	2.08	0.53
1:D:487:ILE:O	1:D:489:LEU:HD22	2.08	0.53
1:I:181:ILE:O	1:I:185:VAL:HG23	2.08	0.53
1:B:185:VAL:O	1:B:189:VAL:HG23	2.09	0.53
1:A:423:ILE:HD12	1:A:424:GLU:HG2	1.90	0.53
1:I:423:ILE:HD12	1:I:424:GLU:HG2	1.90	0.53
1:I:265:ARG:HD2	1:I:266:ILE:N	2.23	0.53
1:C:111:SER:O	1:C:115:VAL:HG23	2.08	0.53
1:G:487:ILE:O	1:G:489:LEU:HD22	2.08	0.53
1:D:470:LEU:HD22	1:D:474:ARG:HD2	1.90	0.53
1:I:470:LEU:HD22	1:I:474:ARG:HD2	1.90	0.53
1:F:118:ALA:O	1:F:122:LEU:HD22	2.08	0.53
1:F:524:LEU:HD12	1:F:524:LEU:N	2.24	0.53
1:H:347:SER:C	1:H:349:GLN:H	2.11	0.53
1:F:185:VAL:O	1:F:189:VAL:HG23	2.09	0.53
1:D:66:ILE:HD13	1:D:66:ILE:N	2.13	0.53
1:F:58:MET:HG3	1:F:68:ILE:HG22	1.91	0.53
1:B:423:ILE:HD12	1:B:424:GLU:HG2	1.90	0.53
1:B:265:ARG:HD2	1:B:266:ILE:N	2.23	0.53
1:E:265:ARG:HD2	1:E:266:ILE:N	2.23	0.53
1:C:351:LEU:CD2	1:C:351:LEU:H	2.17	0.53
1:I:111:SER:O	1:I:115:VAL:HG23	2.08	0.53
1:E:162:ARG:HH11	1:E:162:ARG:HB2	1.70	0.53
1:C:118:ALA:O	1:C:122:LEU:HD22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:118:ALA:O	1:I:122:LEU:HD22	2.08	0.53
1:C:524:LEU:N	1:C:524:LEU:HD12	2.24	0.53
1:E:524:LEU:HD12	1:E:524:LEU:N	2.24	0.53
1:E:178:ARG:H	1:E:178:ARG:HE	1.55	0.53
1:F:181:ILE:O	1:F:185:VAL:HG23	2.08	0.53
1:E:181:ILE:O	1:E:185:VAL:HG23	2.08	0.53
1:G:181:ILE:O	1:G:185:VAL:HG23	2.08	0.53
1:G:185:VAL:O	1:G:189:VAL:HG23	2.09	0.53
1:H:181:ILE:O	1:H:185:VAL:HG23	2.08	0.53
1:G:504:GLU:OE1	2:G:800:ADP:H2'	2.09	0.53
1:D:265:ARG:HD2	1:D:266:ILE:N	2.23	0.53
1:I:231:GLU:HG3	1:I:366:LYS:NZ	2.24	0.53
1:D:58:MET:HG3	1:D:68:ILE:HG22	1.91	0.53
1:B:482:ASN:O	1:B:483:LYS:C	2.47	0.53
1:I:185:VAL:O	1:I:189:VAL:HG23	2.09	0.53
1:D:181:ILE:O	1:D:185:VAL:HG23	2.08	0.53
1:C:185:VAL:O	1:C:189:VAL:HG23	2.09	0.53
1:H:423:ILE:CD1	1:H:424:GLU:HG2	2.39	0.53
1:A:504:GLU:OE1	2:A:800:ADP:H2'	2.09	0.53
1:F:212:LYS:CE	1:F:212:LYS:HA	2.33	0.53
1:H:265:ARG:HD2	1:H:266:ILE:N	2.23	0.53
1:F:265:ARG:HD2	1:F:266:ILE:N	2.23	0.53
1:F:530:VAL:HG21	1:G:79:MET:CE	2.39	0.53
1:H:233:VAL:HG22	1:H:309:GLN:OE1	2.09	0.53
1:A:284:LYS:HD3	1:A:311:TYR:CE2	2.43	0.53
1:C:230:LYS:HZ1	1:C:321:ARG:NH1	2.05	0.53
1:G:530:VAL:O	1:H:59:LEU:HD23	2.08	0.53
1:H:178:ARG:HE	1:H:178:ARG:H	1.55	0.53
1:E:185:VAL:O	1:E:189:VAL:HG23	2.09	0.53
1:E:504:GLU:OE1	2:E:800:ADP:H2'	2.09	0.53
1:C:361:LYS:CB	1:C:366:LYS:HG2	2.36	0.53
1:E:361:LYS:CB	1:E:366:LYS:HG2	2.36	0.53
1:B:233:VAL:HG22	1:B:309:GLN:OE1	2.08	0.53
1:G:284:LYS:HD3	1:G:311:TYR:CE2	2.43	0.53
1:C:58:MET:HG3	1:C:68:ILE:HG22	1.91	0.53
1:E:482:ASN:O	1:E:483:LYS:C	2.47	0.53
1:H:244:ALA:C	1:H:296:ASN:HD22	2.12	0.53
1:F:504:GLU:OE1	2:F:800:ADP:H2'	2.09	0.53
1:A:423:ILE:CD1	1:A:424:GLU:HG2	2.39	0.53
1:G:423:ILE:CD1	1:G:424:GLU:HG2	2.39	0.53
1:I:212:LYS:HA	1:I:212:LYS:CE	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:VAL:HG22	1:D:309:GLN:OE1	2.09	0.53
1:B:470:LEU:HD22	1:B:474:ARG:HD2	1.90	0.53
1:D:482:ASN:O	1:D:483:LYS:C	2.47	0.53
1:F:230:LYS:HZ1	1:F:321:ARG:HH12	1.57	0.53
1:H:58:MET:HG3	1:H:68:ILE:HG22	1.91	0.53
1:A:118:ALA:O	1:A:122:LEU:HD22	2.08	0.53
1:D:347:SER:C	1:D:349:GLN:H	2.11	0.53
1:C:181:ILE:O	1:C:185:VAL:HG23	2.08	0.52
1:G:244:ALA:C	1:G:296:ASN:HD22	2.12	0.52
1:A:482:ASN:O	1:A:483:LYS:C	2.47	0.52
1:H:118:ALA:O	1:H:122:LEU:HD22	2.08	0.52
1:E:58:MET:HG3	1:E:68:ILE:HG22	1.91	0.52
1:B:423:ILE:CD1	1:B:424:GLU:HG2	2.39	0.52
1:E:231:GLU:HG3	1:E:366:LYS:NZ	2.24	0.52
1:I:233:VAL:HG22	1:I:309:GLN:OE1	2.09	0.52
1:C:482:ASN:O	1:C:483:LYS:C	2.47	0.52
1:B:230:LYS:HZ2	1:B:321:ARG:NH1	2.07	0.52
1:H:185:VAL:O	1:H:189:VAL:HG23	2.09	0.52
1:A:423:ILE:C	1:A:423:ILE:HD12	2.30	0.52
1:B:423:ILE:C	1:B:423:ILE:HD12	2.30	0.52
1:E:272:MET:O	1:E:275:PHE:HB3	2.10	0.52
1:H:363:GLY:HA2	1:H:384:ARG:HH22	1.74	0.52
1:G:233:VAL:HG22	1:G:309:GLN:OE1	2.08	0.52
1:A:233:VAL:HG22	1:A:309:GLN:OE1	2.09	0.52
1:F:363:GLY:HA2	1:F:384:ARG:HH22	1.75	0.52
1:A:185:VAL:O	1:A:189:VAL:HG23	2.09	0.52
1:G:58:MET:HG3	1:G:68:ILE:HG22	1.91	0.52
1:D:244:ALA:C	1:D:296:ASN:HD22	2.12	0.52
1:I:423:ILE:CD1	1:I:424:GLU:HG2	2.39	0.52
1:D:423:ILE:HD12	1:D:423:ILE:C	2.30	0.52
1:H:272:MET:O	1:H:275:PHE:HB3	2.10	0.52
1:H:231:GLU:HG3	1:H:366:LYS:NZ	2.24	0.52
1:C:231:GLU:HG3	1:C:366:LYS:NZ	2.24	0.52
1:D:524:LEU:HD12	1:D:524:LEU:N	2.24	0.52
1:B:524:LEU:N	1:B:524:LEU:HD12	2.24	0.52
1:H:166:MET:HE1	1:H:179:GLU:HG2	1.92	0.52
1:A:181:ILE:O	1:A:185:VAL:HG23	2.08	0.52
1:H:504:GLU:OE1	2:H:800:ADP:H2'	2.09	0.52
1:B:272:MET:O	1:B:275:PHE:HB3	2.10	0.52
1:A:272:MET:O	1:A:275:PHE:HB3	2.10	0.52
1:F:272:MET:O	1:F:275:PHE:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:272:MET:O	1:G:275:PHE:HB3	2.10	0.52
1:A:231:GLU:HG3	1:A:366:LYS:NZ	2.24	0.52
1:G:306:GLU:HA	1:G:309:GLN:NE2	2.25	0.52
1:F:233:VAL:HG22	1:F:309:GLN:OE1	2.08	0.52
1:D:306:GLU:HA	1:D:309:GLN:NE2	2.25	0.52
1:H:524:LEU:N	1:H:524:LEU:HD12	2.24	0.52
1:I:234:HIS:CD2	1:I:236:GLY:H	2.28	0.52
1:F:234:HIS:CD2	1:F:236:GLY:H	2.28	0.52
1:E:234:HIS:CD2	1:E:236:GLY:H	2.28	0.52
1:D:185:VAL:O	1:D:189:VAL:HG23	2.09	0.52
1:F:423:ILE:CD1	1:F:424:GLU:HG2	2.39	0.52
1:C:423:ILE:CD1	1:C:424:GLU:HG2	2.39	0.52
1:H:361:LYS:CB	1:H:366:LYS:HG2	2.36	0.52
1:A:470:LEU:HD22	1:A:474:ARG:HD2	1.90	0.52
1:E:162:ARG:HH11	1:E:162:ARG:CB	2.23	0.52
1:I:482:ASN:O	1:I:483:LYS:C	2.47	0.52
1:I:524:LEU:N	1:I:524:LEU:HD12	2.24	0.52
1:D:234:HIS:CD2	1:D:236:GLY:H	2.28	0.52
1:A:58:MET:HG3	1:A:68:ILE:HG22	1.91	0.52
1:C:363:GLY:HA2	1:C:384:ARG:HH22	1.74	0.52
1:G:363:GLY:HA2	1:G:384:ARG:HH22	1.74	0.52
1:G:127:HIS:ND1	1:G:128:PRO:HD2	2.25	0.52
1:A:524:LEU:N	1:A:524:LEU:HD12	2.24	0.52
1:G:166:MET:HE1	1:G:179:GLU:HG2	1.91	0.52
1:G:234:HIS:CD2	1:G:236:GLY:H	2.28	0.52
1:A:256:GLU:C	1:A:258:PRO:HD3	2.22	0.52
1:B:504:GLU:OE1	2:B:800:ADP:H2'	2.09	0.52
1:F:244:ALA:C	1:F:296:ASN:HD22	2.12	0.52
1:D:423:ILE:CD1	1:D:424:GLU:HG2	2.39	0.52
1:D:361:LYS:CB	1:D:366:LYS:HG2	2.36	0.52
1:F:231:GLU:HG3	1:F:366:LYS:NZ	2.24	0.52
1:B:361:LYS:CB	1:B:366:LYS:HG2	2.36	0.52
1:I:76:LEU:CD2	1:I:90:VAL:HG12	2.36	0.52
1:F:360:ARG:NH1	1:F:371:GLU:OE2	2.43	0.52
1:E:360:ARG:NH1	1:E:371:GLU:OE2	2.43	0.52
1:C:234:HIS:CD2	1:C:236:GLY:H	2.28	0.52
1:C:423:ILE:HD12	1:C:423:ILE:C	2.30	0.52
1:A:68:ILE:HG13	1:A:68:ILE:O	2.10	0.52
1:B:58:MET:HG3	1:B:68:ILE:HG22	1.91	0.52
1:D:363:GLY:HA2	1:D:384:ARG:HH22	1.74	0.52
1:H:306:GLU:HA	1:H:309:GLN:NE2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:HIS:ND1	1:F:128:PRO:HD2	2.25	0.52
1:H:127:HIS:ND1	1:H:128:PRO:HD2	2.25	0.52
1:C:230:LYS:HZ1	1:C:321:ARG:HH12	1.58	0.52
1:G:68:ILE:HG13	1:G:68:ILE:O	2.10	0.52
1:C:504:GLU:OE1	2:C:800:ADP:H2'	2.09	0.52
1:B:68:ILE:HG13	1:B:68:ILE:O	2.10	0.52
1:C:162:ARG:HH11	1:C:162:ARG:CB	2.23	0.52
1:G:162:ARG:HH11	1:G:162:ARG:CB	2.23	0.52
1:E:423:ILE:HD11	1:E:477:HIS:NE2	2.26	0.51
1:D:272:MET:O	1:D:275:PHE:HB3	2.10	0.51
1:C:272:MET:O	1:C:275:PHE:HB3	2.10	0.51
1:A:127:HIS:ND1	1:A:128:PRO:HD2	2.25	0.51
1:E:306:GLU:HA	1:E:309:GLN:NE2	2.25	0.51
1:C:68:ILE:O	1:C:68:ILE:HG13	2.10	0.51
1:B:234:HIS:CD2	1:B:236:GLY:H	2.28	0.51
1:G:66:ILE:N	1:G:66:ILE:HD13	2.14	0.51
1:H:423:ILE:C	1:H:423:ILE:HD12	2.30	0.51
1:I:306:GLU:HA	1:I:309:GLN:NE2	2.25	0.51
1:A:363:GLY:HA2	1:A:384:ARG:HH22	1.75	0.51
1:H:470:LEU:HD22	1:H:474:ARG:HD2	1.90	0.51
1:E:127:HIS:ND1	1:E:128:PRO:HD2	2.25	0.51
1:G:360:ARG:NH1	1:G:371:GLU:OE2	2.43	0.51
1:H:234:HIS:CD2	1:H:236:GLY:H	2.28	0.51
1:I:58:MET:HG3	1:I:68:ILE:HG22	1.91	0.51
1:H:423:ILE:HD11	1:H:477:HIS:NE2	2.26	0.51
1:H:212:LYS:HA	1:H:212:LYS:CE	2.33	0.51
1:I:363:GLY:HA2	1:I:384:ARG:HH22	1.75	0.51
1:E:363:GLY:HA2	1:E:384:ARG:HH22	1.75	0.51
1:I:127:HIS:ND1	1:I:128:PRO:HD2	2.25	0.51
1:B:423:ILE:HD11	1:B:477:HIS:NE2	2.26	0.51
1:B:363:GLY:HA2	1:B:384:ARG:HH22	1.75	0.51
1:D:68:ILE:O	1:D:68:ILE:HG13	2.10	0.51
1:H:162:ARG:HH11	1:H:162:ARG:CB	2.23	0.51
1:H:230:LYS:HZ1	1:H:321:ARG:HH12	1.58	0.51
1:E:68:ILE:HG13	1:E:68:ILE:O	2.10	0.51
1:D:423:ILE:HD11	1:D:477:HIS:NE2	2.26	0.51
1:I:272:MET:O	1:I:275:PHE:HB3	2.10	0.51
1:B:306:GLU:HA	1:B:309:GLN:NE2	2.25	0.51
1:D:162:ARG:CB	1:D:162:ARG:HH11	2.23	0.51
1:A:360:ARG:NH1	1:A:371:GLU:OE2	2.43	0.51
1:F:68:ILE:HG13	1:F:68:ILE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:ALA:C	1:B:296:ASN:HD22	2.12	0.51
1:I:415:ILE:O	1:I:503:ILE:HG23	2.11	0.51
1:A:423:ILE:HD11	1:A:477:HIS:NE2	2.26	0.51
1:I:423:ILE:HD12	1:I:424:GLU:H	1.73	0.51
1:A:162:ARG:HH11	1:A:162:ARG:CB	2.23	0.51
1:F:129:THR:HG23	1:G:53:ARG:NH1	2.25	0.51
1:E:230:LYS:HZ2	1:E:321:ARG:NH1	2.08	0.51
1:H:68:ILE:O	1:H:68:ILE:HG13	2.10	0.51
1:H:360:ARG:NH1	1:H:371:GLU:OE2	2.43	0.51
1:I:360:ARG:NH1	1:I:371:GLU:OE2	2.43	0.51
1:E:423:ILE:CD1	1:E:424:GLU:HG2	2.39	0.51
1:G:423:ILE:C	1:G:423:ILE:HD12	2.30	0.51
1:I:423:ILE:HD11	1:I:477:HIS:NE2	2.26	0.51
1:A:415:ILE:O	1:A:503:ILE:HG23	2.11	0.51
1:C:306:GLU:HA	1:C:309:GLN:NE2	2.25	0.51
1:F:162:ARG:CB	1:F:162:ARG:HH11	2.23	0.51
1:B:360:ARG:NH1	1:B:371:GLU:OE2	2.43	0.51
1:D:360:ARG:NH1	1:D:371:GLU:OE2	2.43	0.51
1:B:245:LYS:HG2	1:B:353:TYR:HD1	1.76	0.51
1:F:423:ILE:HD11	1:F:477:HIS:NE2	2.26	0.51
1:F:361:LYS:CB	1:F:366:LYS:HG2	2.36	0.51
1:F:76:LEU:CD2	1:F:90:VAL:HG12	2.36	0.51
1:E:255:VAL:HA	1:E:283:ILE:CD1	2.41	0.51
1:I:162:ARG:HH11	1:I:162:ARG:CB	2.23	0.51
1:C:360:ARG:NH1	1:C:371:GLU:OE2	2.43	0.51
1:E:244:ALA:C	1:E:296:ASN:HD22	2.12	0.51
1:D:415:ILE:O	1:D:503:ILE:HG23	2.11	0.51
1:E:423:ILE:HD12	1:E:423:ILE:C	2.30	0.51
1:G:423:ILE:HD11	1:G:477:HIS:NE2	2.26	0.51
1:B:290:ILE:HG21	1:B:298:ILE:CD1	2.40	0.51
1:A:127:HIS:HD2	1:A:129:THR:CG2	2.24	0.51
1:C:108:VAL:O	1:C:111:SER:HB3	2.11	0.51
1:B:127:HIS:ND1	1:B:128:PRO:HD2	2.25	0.51
1:C:127:HIS:ND1	1:C:128:PRO:HD2	2.25	0.51
1:B:71:ASP:O	1:B:75:ILE:HG12	2.11	0.51
1:I:245:LYS:HG2	1:I:353:TYR:HD1	1.76	0.51
1:C:415:ILE:O	1:C:503:ILE:HG23	2.11	0.51
1:H:255:VAL:HA	1:H:283:ILE:CD1	2.41	0.51
1:A:108:VAL:O	1:A:111:SER:HB3	2.11	0.51
1:F:482:ASN:O	1:F:483:LYS:C	2.47	0.51
1:B:127:HIS:HD2	1:B:129:THR:CG2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:HIS:HD2	1:C:129:THR:CG2	2.24	0.51
1:C:163:LYS:HD3	1:C:501:GLY:HA2	1.93	0.51
1:C:244:ALA:C	1:C:296:ASN:HD22	2.12	0.50
1:C:245:LYS:HG2	1:C:353:TYR:HD1	1.76	0.50
1:F:415:ILE:O	1:F:503:ILE:HG23	2.11	0.50
1:G:415:ILE:O	1:G:503:ILE:HG23	2.11	0.50
1:D:231:GLU:HG3	1:D:366:LYS:NZ	2.24	0.50
1:G:231:GLU:HG3	1:G:366:LYS:NZ	2.24	0.50
1:I:280:GLU:O	1:I:284:LYS:HG3	2.12	0.50
1:I:108:VAL:O	1:I:111:SER:HB3	2.11	0.50
1:D:127:HIS:ND1	1:D:128:PRO:HD2	2.25	0.50
1:D:230:LYS:HZ1	1:D:321:ARG:NH1	2.09	0.50
1:C:505:PRO:O	1:C:508:VAL:HG12	2.12	0.50
1:B:161:LEU:HD12	1:B:161:LEU:H	1.77	0.50
1:C:166:MET:HE1	1:C:179:GLU:HG2	1.93	0.50
1:A:234:HIS:CD2	1:A:236:GLY:H	2.28	0.50
1:D:71:ASP:O	1:D:75:ILE:HG12	2.11	0.50
1:B:163:LYS:HD3	1:B:501:GLY:HA2	1.93	0.50
1:H:415:ILE:O	1:H:503:ILE:HG23	2.11	0.50
1:G:76:LEU:CD2	1:G:90:VAL:HG12	2.36	0.50
1:G:71:ASP:O	1:G:75:ILE:HG12	2.11	0.50
1:E:108:VAL:O	1:E:111:SER:HB3	2.11	0.50
1:F:108:VAL:O	1:F:111:SER:HB3	2.11	0.50
1:C:255:VAL:HA	1:C:283:ILE:CD1	2.41	0.50
1:F:306:GLU:HA	1:F:309:GLN:NE2	2.25	0.50
1:F:208:GLN:HE22	1:F:227:VAL:H	1.60	0.50
1:H:280:GLU:O	1:H:284:LYS:HG3	2.12	0.50
1:I:505:PRO:O	1:I:508:VAL:HG12	2.11	0.50
1:D:34:ALA:O	1:D:37:ALA:HB3	2.12	0.50
1:G:245:LYS:HG2	1:G:353:TYR:HD1	1.76	0.50
1:B:231:GLU:HG3	1:B:366:LYS:NZ	2.24	0.50
1:D:76:LEU:CD2	1:D:90:VAL:HG12	2.36	0.50
1:A:306:GLU:HA	1:A:309:GLN:NE2	2.25	0.50
1:A:280:GLU:O	1:A:284:LYS:HG3	2.12	0.50
1:G:208:GLN:HE22	1:G:227:VAL:H	1.60	0.50
1:A:479:ASN:CB	1:A:482:ASN:OD1	2.59	0.50
1:H:479:ASN:CB	1:H:482:ASN:OD1	2.59	0.50
1:G:230:LYS:HZ2	1:G:321:ARG:NH1	2.10	0.50
1:A:71:ASP:O	1:A:75:ILE:HG12	2.11	0.50
1:I:244:ALA:C	1:I:296:ASN:HD22	2.12	0.50
1:D:245:LYS:HG2	1:D:353:TYR:HD1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:ILE:HD11	1:C:477:HIS:NE2	2.26	0.50
1:I:85:ALA:O	1:I:88:LEU:HB3	2.12	0.50
1:E:290:ILE:HG21	1:E:298:ILE:CD1	2.40	0.50
1:H:108:VAL:O	1:H:111:SER:HB3	2.11	0.50
1:F:127:HIS:HD2	1:F:129:THR:CG2	2.24	0.50
1:D:127:HIS:HD2	1:D:129:THR:CG2	2.24	0.50
1:E:505:PRO:O	1:E:508:VAL:HG12	2.12	0.50
1:H:245:LYS:HG2	1:H:353:TYR:HD1	1.76	0.50
1:F:280:GLU:O	1:F:284:LYS:HG3	2.12	0.50
1:I:284:LYS:HD3	1:I:311:TYR:CE2	2.43	0.50
1:C:85:ALA:O	1:C:88:LEU:HB3	2.12	0.50
1:I:479:ASN:CB	1:I:482:ASN:OD1	2.59	0.50
1:A:230:LYS:HZ2	1:A:321:ARG:NH1	2.08	0.50
1:I:68:ILE:HG13	1:I:68:ILE:O	2.10	0.50
1:F:393:GLU:HG3	1:F:396:ARG:HH21	1.77	0.50
1:C:34:ALA:O	1:C:37:ALA:HB3	2.12	0.50
1:A:422:GLU:N	1:A:422:GLU:OE1	2.45	0.50
1:E:88:LEU:HD11	1:F:389:ARG:NH1	2.18	0.50
1:G:423:ILE:HG21	1:G:473:LEU:CD1	2.42	0.50
1:I:423:ILE:HG21	1:I:473:LEU:CD1	2.42	0.50
1:A:85:ALA:O	1:A:88:LEU:HB3	2.12	0.50
1:I:255:VAL:HA	1:I:283:ILE:CD1	2.41	0.50
1:H:470:LEU:O	1:H:470:LEU:HD23	2.12	0.50
1:E:127:HIS:HD2	1:E:129:THR:CG2	2.24	0.50
1:H:393:GLU:HG3	1:H:396:ARG:HH21	1.77	0.50
1:G:34:ALA:O	1:G:37:ALA:HB3	2.12	0.50
1:B:422:GLU:N	1:B:422:GLU:OE1	2.45	0.50
1:I:422:GLU:OE1	1:I:422:GLU:N	2.45	0.50
1:G:108:VAL:O	1:G:111:SER:HB3	2.11	0.50
1:I:209:ILE:HD12	1:I:209:ILE:N	2.27	0.50
1:D:470:LEU:O	1:D:470:LEU:HD23	2.12	0.50
1:F:470:LEU:O	1:F:470:LEU:HD23	2.12	0.50
1:B:162:ARG:HH11	1:B:162:ARG:CB	2.23	0.50
1:G:479:ASN:CB	1:G:482:ASN:OD1	2.59	0.50
1:H:71:ASP:O	1:H:75:ILE:HG12	2.11	0.50
1:A:91:GLN:NE2	1:B:387:LEU:HD21	2.26	0.50
1:F:71:ASP:O	1:F:75:ILE:HG12	2.11	0.50
1:B:505:PRO:O	1:B:508:VAL:HG12	2.12	0.50
1:H:423:ILE:HG21	1:H:473:LEU:CD1	2.42	0.50
1:B:212:LYS:CE	1:B:212:LYS:HA	2.33	0.50
1:A:437:GLY:O	1:A:441:GLN:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:THR:HB	1:B:382:LEU:O	2.12	0.50
1:G:209:ILE:HD12	1:G:209:ILE:N	2.27	0.50
1:H:208:GLN:HE22	1:H:227:VAL:H	1.60	0.50
1:G:470:LEU:O	1:G:470:LEU:HD23	2.12	0.50
1:A:470:LEU:O	1:A:470:LEU:HD23	2.12	0.50
1:H:163:LYS:HD3	1:H:501:GLY:HA2	1.93	0.50
1:E:393:GLU:HG3	1:E:396:ARG:HH21	1.77	0.50
1:I:376:PRO:HG2	1:I:377:LYS:H	1.77	0.50
1:F:245:LYS:HG2	1:F:353:TYR:HD1	1.76	0.50
1:D:423:ILE:HG21	1:D:473:LEU:CD1	2.42	0.50
1:A:290:ILE:HG21	1:A:298:ILE:CD1	2.40	0.50
1:B:108:VAL:O	1:B:111:SER:HB3	2.11	0.50
1:F:220:THR:HB	1:F:382:LEU:O	2.12	0.50
1:I:470:LEU:HD23	1:I:470:LEU:O	2.12	0.50
1:B:470:LEU:O	1:B:470:LEU:HD23	2.12	0.50
1:F:505:PRO:O	1:F:508:VAL:HG12	2.11	0.50
1:F:163:LYS:HD3	1:F:501:GLY:HA2	1.93	0.50
1:H:376:PRO:HG2	1:H:377:LYS:H	1.77	0.50
1:G:393:GLU:HG3	1:G:396:ARG:HH21	1.77	0.50
1:E:85:ALA:O	1:E:88:LEU:HB3	2.12	0.49
1:E:245:LYS:HG2	1:E:353:TYR:HD1	1.76	0.49
1:B:415:ILE:O	1:B:503:ILE:HG23	2.11	0.49
1:B:426:ALA:O	1:B:429:LEU:N	2.46	0.49
1:F:85:ALA:O	1:F:88:LEU:HB3	2.12	0.49
1:C:437:GLY:O	1:C:441:GLN:HB2	2.12	0.49
1:D:85:ALA:O	1:D:88:LEU:HB3	2.12	0.49
1:E:36:ILE:HG23	1:E:115:VAL:HG12	1.94	0.49
1:E:220:THR:HB	1:E:382:LEU:O	2.12	0.49
1:E:208:GLN:HE22	1:E:227:VAL:H	1.60	0.49
1:H:209:ILE:N	1:H:209:ILE:HD12	2.27	0.49
1:C:208:GLN:HE22	1:C:227:VAL:H	1.59	0.49
1:H:127:HIS:HD2	1:H:129:THR:CG2	2.24	0.49
1:D:230:LYS:HZ2	1:D:321:ARG:NH1	2.09	0.49
1:I:71:ASP:O	1:I:75:ILE:HG12	2.11	0.49
1:C:422:GLU:N	1:C:422:GLU:OE1	2.45	0.49
1:E:422:GLU:OE1	1:E:422:GLU:N	2.45	0.49
1:F:426:ALA:O	1:F:429:LEU:N	2.45	0.49
1:F:423:ILE:HG21	1:F:473:LEU:CD1	2.42	0.49
1:B:423:ILE:HG21	1:B:473:LEU:CD1	2.42	0.49
1:H:437:GLY:O	1:H:441:GLN:HB2	2.12	0.49
1:A:255:VAL:HA	1:A:283:ILE:CD1	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:ILE:N	1:D:209:ILE:HD12	2.27	0.49
1:C:280:GLU:O	1:C:284:LYS:HG3	2.12	0.49
1:B:280:GLU:O	1:B:284:LYS:HG3	2.12	0.49
1:B:208:GLN:HE22	1:B:227:VAL:H	1.60	0.49
1:A:208:GLN:HE22	1:A:227:VAL:H	1.60	0.49
1:I:127:HIS:HD2	1:I:129:THR:CG2	2.24	0.49
1:G:127:HIS:HD2	1:G:129:THR:CG2	2.24	0.49
1:G:505:PRO:O	1:G:508:VAL:HG12	2.11	0.49
1:I:393:GLU:HG3	1:I:396:ARG:HH21	1.77	0.49
1:A:163:LYS:HD3	1:A:501:GLY:HA2	1.93	0.49
1:A:34:ALA:O	1:A:37:ALA:HB3	2.12	0.49
1:D:163:LYS:HD3	1:D:501:GLY:HA2	1.93	0.49
1:D:422:GLU:OE1	1:D:422:GLU:N	2.45	0.49
1:B:437:GLY:O	1:B:441:GLN:HB2	2.12	0.49
1:E:437:GLY:O	1:E:441:GLN:HB2	2.12	0.49
1:D:280:GLU:O	1:D:284:LYS:HG3	2.12	0.49
1:A:209:ILE:N	1:A:209:ILE:HD12	2.27	0.49
1:B:85:ALA:O	1:B:88:LEU:HB3	2.12	0.49
1:D:479:ASN:CB	1:D:482:ASN:OD1	2.59	0.49
1:G:230:LYS:HZ1	1:G:321:ARG:HH12	1.60	0.49
1:C:393:GLU:HG3	1:C:396:ARG:HH21	1.77	0.49
1:E:34:ALA:O	1:E:37:ALA:HB3	2.12	0.49
1:C:71:ASP:O	1:C:75:ILE:HG12	2.11	0.49
1:C:376:PRO:HG2	1:C:377:LYS:H	1.77	0.49
1:E:71:ASP:O	1:E:75:ILE:HG12	2.11	0.49
1:A:393:GLU:HG3	1:A:396:ARG:HH21	1.77	0.49
1:G:422:GLU:N	1:G:422:GLU:OE1	2.45	0.49
1:F:423:ILE:C	1:F:423:ILE:HD12	2.30	0.49
1:C:246:ILE:HA	1:C:297:VAL:HG13	1.94	0.49
1:A:246:ILE:HA	1:A:297:VAL:HG13	1.94	0.49
1:D:108:VAL:O	1:D:111:SER:HB3	2.11	0.49
1:C:470:LEU:HD23	1:C:470:LEU:O	2.12	0.49
1:A:505:PRO:O	1:A:508:VAL:HG12	2.11	0.49
1:I:163:LYS:HD3	1:I:501:GLY:HA2	1.93	0.49
1:E:423:ILE:HG21	1:E:473:LEU:CD1	2.42	0.49
1:E:415:ILE:O	1:E:503:ILE:HG23	2.11	0.49
1:F:530:VAL:O	1:G:59:LEU:HA	2.12	0.49
1:B:210:VAL:HG23	1:B:382:LEU:HD12	1.95	0.49
1:H:36:ILE:HG23	1:H:115:VAL:HG12	1.95	0.49
1:G:280:GLU:O	1:G:284:LYS:HG3	2.12	0.49
1:E:280:GLU:O	1:E:284:LYS:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ILE:HD12	1:B:209:ILE:N	2.27	0.49
1:E:230:LYS:HZ1	1:E:321:ARG:NH1	2.10	0.49
1:A:161:LEU:HD12	1:A:161:LEU:H	1.77	0.49
1:F:34:ALA:O	1:F:37:ALA:HB3	2.12	0.49
1:I:34:ALA:O	1:I:37:ALA:HB3	2.12	0.49
1:F:422:GLU:N	1:F:422:GLU:OE1	2.45	0.49
1:I:503:ILE:N	1:I:503:ILE:HD12	2.28	0.49
1:C:503:ILE:HG22	1:C:504:GLU:N	2.28	0.49
1:C:423:ILE:HG21	1:C:473:LEU:CD1	2.42	0.49
1:I:220:THR:HB	1:I:382:LEU:O	2.12	0.49
1:C:220:THR:HB	1:C:382:LEU:O	2.12	0.49
1:G:36:ILE:HG23	1:G:115:VAL:HG12	1.94	0.49
1:E:209:ILE:HD12	1:E:209:ILE:N	2.27	0.49
1:H:85:ALA:O	1:H:88:LEU:HB3	2.12	0.49
1:D:505:PRO:O	1:D:508:VAL:HG12	2.11	0.49
1:E:161:LEU:H	1:E:161:LEU:HD12	1.77	0.49
1:G:163:LYS:HD3	1:G:501:GLY:HA2	1.93	0.49
1:G:376:PRO:HG2	1:G:377:LYS:H	1.77	0.49
1:H:34:ALA:O	1:H:37:ALA:HB3	2.12	0.49
1:B:503:ILE:HG22	1:B:504:GLU:N	2.28	0.49
1:C:503:ILE:N	1:C:503:ILE:HD12	2.28	0.49
1:E:503:ILE:HG22	1:E:504:GLU:N	2.28	0.49
1:A:212:LYS:CE	1:A:212:LYS:HA	2.33	0.49
1:F:246:ILE:HA	1:F:297:VAL:HG13	1.94	0.49
1:D:437:GLY:O	1:D:441:GLN:HB2	2.12	0.49
1:B:36:ILE:HG23	1:B:115:VAL:HG12	1.95	0.49
1:A:220:THR:HB	1:A:382:LEU:O	2.12	0.49
1:B:255:VAL:HA	1:B:283:ILE:CD1	2.41	0.49
1:F:36:ILE:HG23	1:F:115:VAL:HG12	1.94	0.49
1:I:36:ILE:HG23	1:I:115:VAL:HG12	1.95	0.49
1:C:36:ILE:HG23	1:C:115:VAL:HG12	1.94	0.49
1:G:85:ALA:O	1:G:88:LEU:HB3	2.12	0.49
1:E:470:LEU:HD23	1:E:470:LEU:O	2.12	0.49
1:D:393:GLU:HG3	1:D:396:ARG:HH21	1.77	0.49
1:B:34:ALA:O	1:B:37:ALA:HB3	2.12	0.49
1:A:426:ALA:O	1:A:429:LEU:N	2.45	0.49
1:G:246:ILE:HA	1:G:297:VAL:HG13	1.95	0.49
1:G:437:GLY:O	1:G:441:GLN:HB2	2.12	0.49
1:D:220:THR:HB	1:D:382:LEU:O	2.12	0.49
1:G:220:THR:HB	1:G:382:LEU:O	2.12	0.49
1:D:208:GLN:HE22	1:D:227:VAL:H	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:209:ILE:N	1:F:209:ILE:HD12	2.27	0.49
1:C:209:ILE:N	1:C:209:ILE:HD12	2.27	0.49
1:H:505:PRO:O	1:H:508:VAL:HG12	2.11	0.49
1:F:376:PRO:HG2	1:F:377:LYS:H	1.77	0.49
1:B:393:GLU:HG3	1:B:396:ARG:HH21	1.77	0.49
1:E:163:LYS:HD3	1:E:501:GLY:HA2	1.93	0.49
1:C:426:ALA:O	1:C:429:LEU:N	2.45	0.49
1:H:503:ILE:HG22	1:H:504:GLU:N	2.28	0.49
1:H:423:ILE:HD12	1:H:424:GLU:H	1.73	0.49
1:E:76:LEU:CD2	1:E:90:VAL:HG12	2.36	0.49
1:I:290:ILE:HG21	1:I:298:ILE:CD1	2.40	0.49
1:F:290:ILE:HG21	1:F:298:ILE:CD1	2.40	0.49
1:E:479:ASN:CB	1:E:482:ASN:OD1	2.59	0.49
1:D:230:LYS:HZ1	1:D:321:ARG:HH12	1.60	0.49
1:D:161:LEU:HD12	1:D:161:LEU:H	1.77	0.49
1:I:161:LEU:HD12	1:I:161:LEU:H	1.76	0.49
1:G:161:LEU:HD12	1:G:161:LEU:H	1.77	0.49
1:E:376:PRO:HG2	1:E:377:LYS:H	1.77	0.49
1:H:422:GLU:N	1:H:422:GLU:OE1	2.45	0.49
1:D:503:ILE:HD12	1:D:503:ILE:N	2.28	0.49
1:D:503:ILE:HG22	1:D:504:GLU:N	2.28	0.49
1:A:245:LYS:HG2	1:A:353:TYR:HD1	1.76	0.49
1:H:127:HIS:HD2	1:H:129:THR:CB	2.26	0.49
1:C:127:HIS:HD2	1:C:129:THR:CB	2.26	0.49
1:D:66:ILE:N	1:D:66:ILE:CD1	2.76	0.48
1:I:503:ILE:HG22	1:I:504:GLU:N	2.28	0.48
1:A:423:ILE:HG21	1:A:473:LEU:CD1	2.42	0.48
1:F:423:ILE:HD12	1:F:424:GLU:H	1.73	0.48
1:I:423:ILE:C	1:I:423:ILE:HD12	2.30	0.48
1:E:426:ALA:O	1:E:429:LEU:N	2.45	0.48
1:A:503:ILE:HG22	1:A:504:GLU:N	2.28	0.48
1:F:263:GLU:C	1:F:264:ILE:HG22	2.34	0.48
1:H:246:ILE:HA	1:H:297:VAL:HG13	1.94	0.48
1:A:127:HIS:HD2	1:A:129:THR:CB	2.26	0.48
1:I:210:VAL:HG23	1:I:382:LEU:HD12	1.95	0.48
1:F:255:VAL:HA	1:F:283:ILE:CD1	2.41	0.48
1:C:58:MET:HG3	1:C:68:ILE:CG2	2.43	0.48
1:C:479:ASN:CB	1:C:482:ASN:OD1	2.59	0.48
1:B:110:PHE:O	1:B:114:LEU:HD13	2.13	0.48
1:G:230:LYS:HZ1	1:G:321:ARG:NH1	2.09	0.48
1:F:58:MET:HG3	1:F:68:ILE:CG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:GLU:C	1:E:264:ILE:HG22	2.34	0.48
1:H:217:ILE:HD11	1:H:390:LEU:CD2	2.44	0.48
1:H:220:THR:HB	1:H:382:LEU:O	2.12	0.48
1:F:210:VAL:HG23	1:F:382:LEU:HD12	1.95	0.48
1:A:36:ILE:HG23	1:A:115:VAL:HG12	1.95	0.48
1:D:255:VAL:HA	1:D:283:ILE:CD1	2.41	0.48
1:I:208:GLN:HE22	1:I:227:VAL:H	1.60	0.48
1:D:482:ASN:O	1:D:485:TYR:N	2.40	0.48
1:G:110:PHE:O	1:G:114:LEU:HD13	2.13	0.48
1:D:110:PHE:O	1:D:114:LEU:HD13	2.13	0.48
1:H:110:PHE:O	1:H:114:LEU:HD13	2.13	0.48
1:H:522:LEU:HD11	1:I:68:ILE:CD1	2.43	0.48
1:H:426:ALA:O	1:H:429:LEU:N	2.45	0.48
1:B:217:ILE:HD11	1:B:390:LEU:CD2	2.44	0.48
1:H:263:GLU:C	1:H:264:ILE:HG22	2.34	0.48
1:H:232:VAL:HG12	1:H:318:LEU:HD11	1.95	0.48
1:I:246:ILE:HA	1:I:297:VAL:HG13	1.94	0.48
1:I:437:GLY:O	1:I:441:GLN:HB2	2.12	0.48
1:B:127:HIS:HD2	1:B:129:THR:CB	2.26	0.48
1:E:127:HIS:HD2	1:E:129:THR:CB	2.26	0.48
1:I:482:ASN:O	1:I:485:TYR:N	2.40	0.48
1:B:358:GLU:CG	1:B:360:ARG:HH22	2.27	0.48
1:H:58:MET:HG3	1:H:68:ILE:CG2	2.44	0.48
1:F:161:LEU:HD12	1:F:161:LEU:H	1.77	0.48
1:B:376:PRO:HG2	1:B:377:LYS:H	1.77	0.48
1:G:66:ILE:CD1	1:G:66:ILE:N	2.76	0.48
1:I:426:ALA:O	1:I:429:LEU:N	2.45	0.48
1:A:423:ILE:HD12	1:A:424:GLU:H	1.73	0.48
1:G:232:VAL:HG12	1:G:318:LEU:HD11	1.95	0.48
1:I:232:VAL:HG12	1:I:318:LEU:HD11	1.95	0.48
1:F:437:GLY:O	1:F:441:GLN:HB2	2.12	0.48
1:E:255:VAL:HG13	1:E:305:ASP:CG	2.34	0.48
1:A:110:PHE:O	1:A:114:LEU:HD13	2.13	0.48
1:E:330:LYS:O	1:E:334:ALA:HB2	2.14	0.48
1:A:244:ALA:C	1:A:296:ASN:HD22	2.12	0.48
1:G:426:ALA:O	1:G:429:LEU:N	2.45	0.48
1:G:503:ILE:HG22	1:G:504:GLU:N	2.28	0.48
1:B:263:GLU:C	1:B:264:ILE:HG22	2.34	0.48
1:E:246:ILE:HA	1:E:297:VAL:HG13	1.94	0.48
1:D:232:VAL:HG11	1:D:318:LEU:HD11	1.95	0.48
1:D:210:VAL:HG23	1:D:382:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:255:VAL:HG13	1:H:305:ASP:CG	2.34	0.48
1:D:36:ILE:HG23	1:D:115:VAL:HG12	1.94	0.48
1:B:255:VAL:HG13	1:B:305:ASP:CG	2.34	0.48
1:C:469:LEU:HB3	1:C:487:ILE:CD1	2.43	0.48
1:D:127:HIS:HD2	1:D:129:THR:CB	2.26	0.48
1:I:358:GLU:CG	1:I:360:ARG:HH22	2.27	0.48
1:D:376:PRO:HG2	1:D:377:LYS:H	1.77	0.48
1:B:66:ILE:N	1:B:66:ILE:CD1	2.76	0.48
1:G:58:MET:HG3	1:G:68:ILE:CG2	2.44	0.48
1:F:503:ILE:N	1:F:503:ILE:HD12	2.28	0.48
1:D:263:GLU:C	1:D:264:ILE:HG22	2.34	0.48
1:C:263:GLU:C	1:C:264:ILE:HG22	2.34	0.48
1:A:361:LYS:CB	1:A:366:LYS:HG2	2.36	0.48
1:C:232:VAL:HG12	1:C:318:LEU:HD11	1.95	0.48
1:B:58:MET:HG3	1:B:68:ILE:CG2	2.44	0.48
1:D:246:ILE:HA	1:D:297:VAL:HG13	1.94	0.48
1:G:255:VAL:HG13	1:G:305:ASP:CG	2.34	0.48
1:D:58:MET:HG3	1:D:68:ILE:CG2	2.44	0.48
1:F:110:PHE:O	1:F:114:LEU:HD13	2.13	0.48
1:C:161:LEU:H	1:C:161:LEU:HD12	1.77	0.48
1:D:166:MET:HE1	1:D:179:GLU:HG2	1.96	0.48
1:E:58:MET:HG3	1:E:68:ILE:CG2	2.44	0.48
1:H:503:ILE:N	1:H:503:ILE:HD12	2.28	0.48
1:E:473:LEU:C	1:E:473:LEU:HD13	2.34	0.48
1:G:503:ILE:N	1:G:503:ILE:HD12	2.28	0.48
1:G:232:VAL:HG11	1:G:318:LEU:HD11	1.95	0.48
1:C:210:VAL:HG23	1:C:382:LEU:HD12	1.95	0.48
1:D:255:VAL:HG13	1:D:305:ASP:CG	2.34	0.48
1:G:227:VAL:HG22	1:G:369:PHE:HD1	1.79	0.48
1:A:227:VAL:HG22	1:A:369:PHE:HD1	1.79	0.48
1:F:479:ASN:CB	1:F:482:ASN:OD1	2.59	0.48
1:I:127:HIS:HD2	1:I:129:THR:CB	2.26	0.48
1:G:127:HIS:HD2	1:G:129:THR:CB	2.26	0.48
1:I:110:PHE:O	1:I:114:LEU:HD13	2.13	0.48
1:E:358:GLU:CG	1:E:360:ARG:HH22	2.27	0.48
1:G:358:GLU:CG	1:G:360:ARG:HH22	2.27	0.48
1:H:529:VAL:HG12	1:I:58:MET:HB3	1.95	0.48
1:H:260:LEU:CD1	1:H:260:LEU:C	2.81	0.48
1:A:473:LEU:C	1:A:473:LEU:HD13	2.34	0.48
1:A:58:MET:HG3	1:A:68:ILE:CG2	2.44	0.48
1:D:263:GLU:C	1:D:264:ILE:CG2	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:263:GLU:C	1:I:264:ILE:HG22	2.34	0.48
1:B:479:ASN:CB	1:B:482:ASN:OD1	2.59	0.48
1:C:358:GLU:CG	1:C:360:ARG:HH22	2.27	0.48
1:B:503:ILE:HD12	1:B:503:ILE:N	2.28	0.48
1:F:503:ILE:HG22	1:F:504:GLU:N	2.28	0.48
1:C:423:ILE:HD12	1:C:424:GLU:H	1.73	0.48
1:A:503:ILE:N	1:A:503:ILE:HD12	2.28	0.48
1:D:212:LYS:CE	1:D:212:LYS:HA	2.33	0.48
1:C:232:VAL:HG11	1:C:318:LEU:HD11	1.95	0.48
1:F:232:VAL:HG12	1:F:318:LEU:HD11	1.95	0.48
1:F:246:ILE:O	1:F:351:LEU:HB2	2.14	0.48
1:H:246:ILE:O	1:H:351:LEU:HB2	2.14	0.48
1:A:255:VAL:HG13	1:A:305:ASP:CG	2.34	0.48
1:A:299:ILE:HG22	1:A:320:VAL:HG23	1.96	0.48
1:F:299:ILE:HG22	1:F:320:VAL:HG23	1.96	0.48
1:F:358:GLU:CG	1:F:360:ARG:HH22	2.27	0.48
1:B:330:LYS:O	1:B:334:ALA:HB2	2.14	0.48
1:F:217:ILE:HD11	1:F:390:LEU:CD2	2.44	0.48
1:A:263:GLU:C	1:A:264:ILE:HG22	2.34	0.48
1:B:469:LEU:HB3	1:B:487:ILE:CD1	2.43	0.48
1:C:110:PHE:O	1:C:114:LEU:HD13	2.13	0.48
1:G:330:LYS:O	1:G:334:ALA:HB2	2.14	0.48
1:A:376:PRO:HG2	1:A:377:LYS:H	1.77	0.48
1:B:473:LEU:HD13	1:B:473:LEU:C	2.34	0.47
1:H:263:GLU:C	1:H:264:ILE:CG2	2.82	0.47
1:G:263:GLU:C	1:G:264:ILE:CG2	2.82	0.47
1:C:290:ILE:HG21	1:C:298:ILE:CD1	2.40	0.47
1:A:210:VAL:HG23	1:A:382:LEU:HD12	1.95	0.47
1:D:227:VAL:HG22	1:D:369:PHE:HD1	1.79	0.47
1:F:255:VAL:HG13	1:F:305:ASP:CG	2.34	0.47
1:D:469:LEU:HB3	1:D:487:ILE:CD1	2.43	0.47
1:I:178:ARG:NE	1:I:178:ARG:H	2.12	0.47
1:I:58:MET:HG3	1:I:68:ILE:CG2	2.44	0.47
1:H:330:LYS:O	1:H:334:ALA:HB2	2.14	0.47
1:C:260:LEU:CD1	1:C:260:LEU:C	2.81	0.47
1:E:503:ILE:N	1:E:503:ILE:HD12	2.28	0.47
1:G:217:ILE:HD11	1:G:390:LEU:CD2	2.44	0.47
1:C:217:ILE:HD11	1:C:390:LEU:CD2	2.44	0.47
1:G:263:GLU:C	1:G:264:ILE:HG22	2.34	0.47
1:I:436:VAL:HG23	1:I:437:GLY:N	2.30	0.47
1:A:232:VAL:HG11	1:A:318:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:214:GLY:HA3	1:H:384:ARG:HH21	1.79	0.47
1:G:210:VAL:HG23	1:G:382:LEU:HD12	1.95	0.47
1:H:227:VAL:HG22	1:H:369:PHE:HD1	1.79	0.47
1:E:110:PHE:O	1:E:114:LEU:HD13	2.13	0.47
1:B:230:LYS:HZ1	1:B:321:ARG:HH12	1.62	0.47
1:A:178:ARG:NE	1:A:178:ARG:H	2.12	0.47
1:C:76:LEU:CD2	1:C:90:VAL:HG12	2.36	0.47
1:D:249:ILE:HD12	1:D:346:ILE:HD11	1.96	0.47
1:I:249:ILE:HD12	1:I:346:ILE:HD11	1.96	0.47
1:B:232:VAL:HG12	1:B:318:LEU:HD11	1.95	0.47
1:B:246:ILE:O	1:B:351:LEU:HB2	2.14	0.47
1:E:232:VAL:HG11	1:E:318:LEU:HD11	1.96	0.47
1:A:246:ILE:O	1:A:351:LEU:HB2	2.14	0.47
1:D:214:GLY:HA3	1:D:384:ARG:HH21	1.79	0.47
1:F:214:GLY:HA3	1:F:384:ARG:HH21	1.79	0.47
1:D:299:ILE:HG22	1:D:320:VAL:HG23	1.96	0.47
1:C:227:VAL:HG22	1:C:369:PHE:HD1	1.79	0.47
1:F:482:ASN:O	1:F:485:TYR:N	2.40	0.47
1:F:127:HIS:HD2	1:F:129:THR:CB	2.26	0.47
1:G:178:ARG:H	1:G:178:ARG:NE	2.12	0.47
1:D:258:PRO:CG	1:D:279:GLU:OE2	2.56	0.47
1:E:423:ILE:HD12	1:E:424:GLU:H	1.73	0.47
1:B:249:ILE:HD12	1:B:346:ILE:HD11	1.96	0.47
1:A:528:ASP:OD2	1:A:529:VAL:N	2.48	0.47
1:B:246:ILE:HA	1:B:297:VAL:HG13	1.94	0.47
1:I:246:ILE:O	1:I:351:LEU:HB2	2.14	0.47
1:D:246:ILE:O	1:D:351:LEU:HB2	2.14	0.47
1:H:436:VAL:HG23	1:H:437:GLY:N	2.30	0.47
1:E:210:VAL:HG23	1:E:382:LEU:HD12	1.95	0.47
1:A:214:GLY:HA3	1:A:384:ARG:HH21	1.79	0.47
1:H:299:ILE:HG22	1:H:320:VAL:HG23	1.96	0.47
1:B:227:VAL:HG22	1:B:369:PHE:HD1	1.79	0.47
1:A:121:LEU:HB3	1:A:126:VAL:CG2	2.44	0.47
1:D:121:LEU:HB3	1:D:126:VAL:CG2	2.44	0.47
1:H:211:LYS:HE3	1:H:395:GLU:OE2	2.14	0.47
1:F:211:LYS:HE3	1:F:395:GLU:OE2	2.14	0.47
1:C:211:LYS:HE3	1:C:395:GLU:OE2	2.14	0.47
1:F:473:LEU:C	1:F:473:LEU:HD13	2.34	0.47
1:G:473:LEU:C	1:G:473:LEU:HD13	2.34	0.47
1:H:473:LEU:C	1:H:473:LEU:HD13	2.34	0.47
1:I:528:ASP:OD2	1:I:529:VAL:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:361:LYS:CB	1:I:366:LYS:HG2	2.36	0.47
1:F:232:VAL:HG11	1:F:318:LEU:HD11	1.95	0.47
1:C:141:VAL:CG2	1:C:432:TYR:CE1	2.97	0.47
1:G:299:ILE:HG22	1:G:320:VAL:HG23	1.96	0.47
1:E:230:LYS:HZ1	1:E:321:ARG:HH12	1.61	0.47
1:D:358:GLU:CG	1:D:360:ARG:HH22	2.27	0.47
1:H:178:ARG:H	1:H:178:ARG:NE	2.12	0.47
1:A:330:LYS:O	1:A:334:ALA:HB2	2.14	0.47
1:B:528:ASP:OD2	1:B:529:VAL:N	2.48	0.47
1:B:436:VAL:HG23	1:B:437:GLY:N	2.30	0.47
1:H:46:LEU:O	1:H:47:LYS:C	2.53	0.47
1:G:121:LEU:HB3	1:G:126:VAL:CG2	2.44	0.47
1:G:211:LYS:HE3	1:G:395:GLU:OE2	2.14	0.47
1:C:330:LYS:O	1:C:334:ALA:HB2	2.14	0.47
1:G:258:PRO:CG	1:G:279:GLU:OE2	2.56	0.47
1:I:473:LEU:C	1:I:473:LEU:HD13	2.35	0.47
1:A:263:GLU:C	1:A:264:ILE:CG2	2.82	0.47
1:A:249:ILE:HD12	1:A:346:ILE:HD11	1.96	0.47
1:G:290:ILE:HG21	1:G:298:ILE:CD1	2.40	0.47
1:E:246:ILE:O	1:E:351:LEU:HB2	2.14	0.47
1:A:232:VAL:HG12	1:A:318:LEU:HD11	1.95	0.47
1:A:359:GLU:HG2	1:A:359:GLU:O	2.15	0.47
1:D:430:ARG:NH1	1:D:430:ARG:HG2	2.29	0.47
1:D:436:VAL:HG23	1:D:437:GLY:N	2.30	0.47
1:F:436:VAL:HG23	1:F:437:GLY:N	2.30	0.47
1:C:430:ARG:NH1	1:C:430:ARG:HG2	2.29	0.47
1:C:436:VAL:HG23	1:C:437:GLY:N	2.30	0.47
1:E:436:VAL:HG23	1:E:437:GLY:N	2.30	0.47
1:I:214:GLY:HA3	1:I:384:ARG:HH21	1.80	0.47
1:I:255:VAL:HG13	1:I:305:ASP:CG	2.34	0.47
1:C:255:VAL:HG13	1:C:305:ASP:CG	2.34	0.47
1:A:469:LEU:HB3	1:A:487:ILE:CD1	2.43	0.47
1:C:46:LEU:O	1:C:47:LYS:C	2.53	0.47
1:D:46:LEU:O	1:D:47:LYS:C	2.53	0.47
1:I:121:LEU:HB3	1:I:126:VAL:CG2	2.44	0.47
1:B:121:LEU:HB3	1:B:126:VAL:CG2	2.44	0.47
1:A:46:LEU:O	1:A:47:LYS:C	2.53	0.47
1:A:230:LYS:HZ1	1:A:321:ARG:NH1	2.10	0.47
1:B:230:LYS:HZ1	1:B:321:ARG:NH1	2.12	0.47
1:A:358:GLU:CG	1:A:360:ARG:HH22	2.27	0.47
1:E:211:LYS:HE3	1:E:395:GLU:OE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:LYS:HE3	1:D:395:GLU:OE2	2.14	0.47
1:I:211:LYS:HE3	1:I:395:GLU:OE2	2.15	0.47
1:G:234:HIS:ND1	1:G:235:PRO:HD2	2.30	0.47
1:C:234:HIS:ND1	1:C:235:PRO:HD2	2.30	0.47
1:B:75:ILE:O	1:B:79:MET:HB3	2.15	0.47
1:D:75:ILE:O	1:D:79:MET:HB3	2.15	0.47
1:C:75:ILE:O	1:C:79:MET:HB3	2.15	0.47
1:F:330:LYS:O	1:F:334:ALA:HB2	2.14	0.47
1:C:56:ASP:OD1	1:C:70:ASN:HB3	2.15	0.47
1:D:282:LEU:O	1:D:285:GLU:HB3	2.15	0.47
1:I:330:LYS:O	1:I:334:ALA:HB2	2.14	0.47
1:A:271:GLN:OE1	1:A:271:GLN:HA	2.15	0.47
1:F:528:ASP:OD2	1:F:529:VAL:N	2.48	0.47
1:D:528:ASP:OD2	1:D:529:VAL:N	2.48	0.47
1:C:473:LEU:HD13	1:C:473:LEU:C	2.34	0.47
1:D:473:LEU:C	1:D:473:LEU:HD13	2.34	0.47
1:D:217:ILE:HD11	1:D:390:LEU:CD2	2.43	0.47
1:H:290:ILE:HG21	1:H:298:ILE:CD1	2.40	0.47
1:G:359:GLU:HG2	1:G:359:GLU:O	2.15	0.47
1:B:232:VAL:HG11	1:B:318:LEU:HD11	1.95	0.47
1:H:210:VAL:HG23	1:H:382:LEU:HD12	1.95	0.47
1:C:214:GLY:HA3	1:C:384:ARG:HH21	1.79	0.47
1:F:227:VAL:HG22	1:F:369:PHE:HD1	1.79	0.47
1:F:469:LEU:HB3	1:F:487:ILE:CD1	2.43	0.47
1:C:482:ASN:O	1:C:485:TYR:N	2.40	0.47
1:H:161:LEU:HD12	1:H:161:LEU:H	1.77	0.47
1:F:234:HIS:ND1	1:F:235:PRO:HD2	2.30	0.47
1:D:234:HIS:ND1	1:D:235:PRO:HD2	2.30	0.47
1:A:234:HIS:ND1	1:A:235:PRO:HD2	2.30	0.47
1:F:75:ILE:O	1:F:79:MET:HB3	2.15	0.47
1:H:271:GLN:OE1	1:H:271:GLN:HA	2.15	0.47
1:F:529:VAL:CG1	1:G:58:MET:SD	3.03	0.47
1:F:263:GLU:C	1:F:264:ILE:CG2	2.82	0.47
1:F:530:VAL:O	1:G:59:LEU:HD22	2.13	0.47
1:B:214:GLY:HA3	1:B:384:ARG:HH21	1.79	0.47
1:G:255:VAL:HA	1:G:283:ILE:CD1	2.41	0.47
1:E:299:ILE:HG22	1:E:320:VAL:HG23	1.96	0.47
1:B:299:ILE:HG22	1:B:320:VAL:HG23	1.96	0.47
1:E:227:VAL:HG22	1:E:369:PHE:HD1	1.79	0.47
1:B:46:LEU:O	1:B:47:LYS:C	2.53	0.47
1:H:121:LEU:HB3	1:H:126:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:528:ASP:OD2	1:G:529:VAL:N	2.48	0.47
1:A:166:MET:HE1	1:A:179:GLU:HG2	1.96	0.47
1:E:75:ILE:O	1:E:79:MET:HB3	2.15	0.47
1:H:406:ALA:O	1:H:410:LYS:HG3	2.15	0.47
1:G:271:GLN:HA	1:G:271:GLN:OE1	2.15	0.47
1:B:271:GLN:OE1	1:B:271:GLN:HA	2.15	0.47
1:A:259:GLU:CD	1:A:259:GLU:C	2.74	0.47
1:I:259:GLU:CD	1:I:259:GLU:C	2.74	0.47
1:I:66:ILE:N	1:I:66:ILE:CD1	2.76	0.47
1:A:150:ALA:HA	1:A:415:ILE:HG22	1.97	0.47
1:C:249:ILE:HD12	1:C:346:ILE:HD11	1.96	0.47
1:D:290:ILE:HG21	1:D:298:ILE:CD1	2.40	0.47
1:G:249:ILE:HD12	1:G:346:ILE:HD11	1.96	0.47
1:G:246:ILE:O	1:G:351:LEU:HB2	2.14	0.47
1:H:232:VAL:HG11	1:H:318:LEU:HD11	1.95	0.47
1:D:359:GLU:HG2	1:D:359:GLU:O	2.15	0.47
1:H:83:HIS:CD2	1:H:84:PRO:HD2	2.50	0.47
1:C:84:PRO:HG2	1:C:85:ALA:H	1.80	0.47
1:E:121:LEU:HB3	1:E:126:VAL:HG21	1.97	0.47
1:F:121:LEU:HB3	1:F:126:VAL:CG2	2.44	0.47
1:A:230:LYS:HZ1	1:A:321:ARG:HH12	1.61	0.47
1:C:178:ARG:H	1:C:178:ARG:NE	2.12	0.47
1:H:528:ASP:OD2	1:H:529:VAL:N	2.48	0.47
1:G:282:LEU:O	1:G:285:GLU:HB3	2.15	0.47
1:I:271:GLN:OE1	1:I:271:GLN:HA	2.15	0.47
1:C:259:GLU:CD	1:C:259:GLU:C	2.74	0.46
1:H:66:ILE:CD1	1:H:66:ILE:N	2.76	0.46
1:E:526:ILE:HD11	1:F:68:ILE:HG21	1.96	0.46
1:F:56:ASP:OD1	1:F:70:ASN:HB3	2.15	0.46
1:B:505:PRO:C	1:B:507:LEU:N	2.69	0.46
1:F:249:ILE:HD12	1:F:346:ILE:HD11	1.96	0.46
1:E:232:VAL:HG12	1:E:318:LEU:HD11	1.95	0.46
1:A:436:VAL:HG23	1:A:437:GLY:N	2.30	0.46
1:I:299:ILE:HG22	1:I:320:VAL:HG23	1.96	0.46
1:I:227:VAL:HG22	1:I:369:PHE:HD1	1.79	0.46
1:B:121:LEU:HB3	1:B:126:VAL:HG21	1.97	0.46
1:I:194:GLU:C	1:I:195:LEU:HD12	2.36	0.46
1:D:178:ARG:NE	1:D:178:ARG:H	2.12	0.46
1:H:56:ASP:OD1	1:H:70:ASN:HB3	2.15	0.46
1:D:330:LYS:O	1:D:334:ALA:HB2	2.14	0.46
1:E:406:ALA:O	1:E:410:LYS:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:C	1:A:260:LEU:CD1	2.81	0.46
1:F:259:GLU:C	1:F:259:GLU:CD	2.74	0.46
1:I:212:LYS:O	1:I:213:ALA:O	2.33	0.46
1:I:359:GLU:O	1:I:359:GLU:HG2	2.15	0.46
1:C:45:ALA:C	1:C:46:LEU:HD12	2.36	0.46
1:C:121:LEU:HB3	1:C:126:VAL:CG2	2.44	0.46
1:D:194:GLU:C	1:D:195:LEU:HD12	2.36	0.46
1:E:194:GLU:C	1:E:195:LEU:HD12	2.36	0.46
1:H:75:ILE:O	1:H:79:MET:HB3	2.15	0.46
1:I:75:ILE:O	1:I:79:MET:HB3	2.15	0.46
1:A:406:ALA:O	1:A:410:LYS:HG3	2.16	0.46
1:B:56:ASP:OD1	1:B:70:ASN:HB3	2.15	0.46
1:C:271:GLN:OE1	1:C:271:GLN:HA	2.15	0.46
1:C:212:LYS:HA	1:C:212:LYS:CE	2.33	0.46
1:B:263:GLU:C	1:B:264:ILE:CG2	2.82	0.46
1:E:217:ILE:HD11	1:E:390:LEU:CD2	2.43	0.46
1:H:249:ILE:HD12	1:H:346:ILE:HD11	1.96	0.46
1:A:84:PRO:HG2	1:A:85:ALA:H	1.80	0.46
1:D:232:VAL:HG12	1:D:318:LEU:HD11	1.95	0.46
1:H:141:VAL:CG2	1:H:432:TYR:CE1	2.97	0.46
1:E:141:VAL:CG2	1:E:432:TYR:CE1	2.97	0.46
1:D:208:GLN:C	1:D:209:ILE:HD12	2.36	0.46
1:B:84:PRO:HG2	1:B:85:ALA:H	1.80	0.46
1:C:528:ASP:OD2	1:C:529:VAL:N	2.48	0.46
1:A:121:LEU:HB3	1:A:126:VAL:HG21	1.97	0.46
1:E:121:LEU:HB3	1:E:126:VAL:CG2	2.44	0.46
1:A:194:GLU:C	1:A:195:LEU:HD12	2.36	0.46
1:C:230:LYS:HZ2	1:C:321:ARG:NH1	2.13	0.46
1:C:505:PRO:C	1:C:507:LEU:N	2.69	0.46
1:E:505:PRO:C	1:E:507:LEU:N	2.69	0.46
1:B:188:ALA:HA	1:B:379:ILE:HD11	1.97	0.46
1:B:211:LYS:HE3	1:B:395:GLU:OE2	2.14	0.46
1:G:406:ALA:O	1:G:410:LYS:HG3	2.16	0.46
1:I:282:LEU:O	1:I:285:GLU:HB3	2.15	0.46
1:B:406:ALA:O	1:B:410:LYS:HG3	2.15	0.46
1:A:282:LEU:O	1:A:285:GLU:HB3	2.15	0.46
1:F:406:ALA:O	1:F:410:LYS:HG3	2.16	0.46
1:E:271:GLN:OE1	1:E:271:GLN:HA	2.15	0.46
1:I:56:ASP:OD1	1:I:70:ASN:HB3	2.15	0.46
1:F:528:ASP:HB3	1:G:57:LYS:HD3	1.97	0.46
1:E:525:ARG:HG3	1:F:56:ASP:OD2	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:ALA:HA	1:C:415:ILE:HG22	1.97	0.46
1:G:150:ALA:HA	1:G:415:ILE:HG22	1.97	0.46
1:G:212:LYS:O	1:G:213:ALA:O	2.33	0.46
1:A:212:LYS:O	1:A:213:ALA:O	2.34	0.46
1:I:84:PRO:HG2	1:I:85:ALA:H	1.80	0.46
1:E:263:GLU:C	1:E:264:ILE:CG2	2.82	0.46
1:I:263:GLU:C	1:I:264:ILE:CG2	2.82	0.46
1:H:290:ILE:HG12	1:H:346:ILE:CD1	2.46	0.46
1:C:246:ILE:O	1:C:351:LEU:HB2	2.14	0.46
1:H:359:GLU:HG2	1:H:359:GLU:O	2.15	0.46
1:I:232:VAL:HG11	1:I:318:LEU:HD11	1.95	0.46
1:D:84:PRO:HG2	1:D:85:ALA:H	1.80	0.46
1:A:208:GLN:C	1:A:209:ILE:HD12	2.36	0.46
1:G:45:ALA:C	1:G:46:LEU:HD12	2.36	0.46
1:I:45:ALA:C	1:I:46:LEU:HD12	2.36	0.46
1:I:121:LEU:HB3	1:I:126:VAL:HG21	1.97	0.46
1:F:46:LEU:O	1:F:47:LYS:C	2.53	0.46
1:C:121:LEU:HB3	1:C:126:VAL:HG21	1.97	0.46
1:G:194:GLU:C	1:G:195:LEU:HD12	2.36	0.46
1:B:194:GLU:C	1:B:195:LEU:HD12	2.36	0.46
1:A:224:TYR:HA	1:A:379:ILE:HG22	1.98	0.46
1:E:234:HIS:ND1	1:E:235:PRO:HD2	2.30	0.46
1:E:282:LEU:O	1:E:285:GLU:HB3	2.15	0.46
1:C:282:LEU:O	1:C:285:GLU:HB3	2.15	0.46
1:E:56:ASP:OD1	1:E:70:ASN:HB3	2.15	0.46
1:H:282:LEU:O	1:H:285:GLU:HB3	2.15	0.46
1:B:259:GLU:CD	1:B:259:GLU:C	2.74	0.46
1:D:423:ILE:HD12	1:D:424:GLU:H	1.73	0.46
1:D:212:LYS:O	1:D:213:ALA:O	2.34	0.46
1:F:212:LYS:O	1:F:213:ALA:O	2.34	0.46
1:F:83:HIS:CD2	1:F:84:PRO:HD2	2.50	0.46
1:A:528:ASP:HB3	1:B:57:LYS:HE3	1.97	0.46
1:G:436:VAL:HG23	1:G:437:GLY:N	2.30	0.46
1:E:208:GLN:C	1:E:209:ILE:HD12	2.36	0.46
1:G:153:VAL:O	1:G:153:VAL:HG13	2.16	0.46
1:I:469:LEU:HB3	1:I:487:ILE:CD1	2.43	0.46
1:F:121:LEU:HB3	1:F:126:VAL:HG21	1.97	0.46
1:H:234:HIS:ND1	1:H:235:PRO:HD2	2.30	0.46
1:D:56:ASP:OD1	1:D:70:ASN:HB3	2.15	0.46
1:D:271:GLN:OE1	1:D:271:GLN:HA	2.15	0.46
1:G:423:ILE:HD12	1:G:424:GLU:H	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:83:HIS:CD2	1:I:84:PRO:HD2	2.50	0.46
1:F:359:GLU:O	1:F:359:GLU:HG2	2.15	0.46
1:A:210:VAL:O	1:A:382:LEU:HD12	2.16	0.46
1:B:153:VAL:O	1:B:153:VAL:HG13	2.16	0.46
1:B:83:HIS:CD2	1:B:84:PRO:HD2	2.50	0.46
1:H:84:PRO:HG2	1:H:85:ALA:H	1.80	0.46
1:I:46:LEU:O	1:I:47:LYS:C	2.53	0.46
1:D:188:ALA:HA	1:D:379:ILE:HD11	1.98	0.46
1:A:211:LYS:HE3	1:A:395:GLU:OE2	2.15	0.46
1:D:211:LYS:HD2	1:D:391:VAL:HG22	1.98	0.46
1:I:234:HIS:ND1	1:I:235:PRO:HD2	2.30	0.46
1:B:234:HIS:ND1	1:B:235:PRO:HD2	2.30	0.46
1:A:56:ASP:OD1	1:A:70:ASN:HB3	2.15	0.46
1:F:528:ASP:O	1:G:58:MET:N	2.41	0.46
1:B:212:LYS:O	1:B:213:ALA:O	2.34	0.46
1:A:290:ILE:HG12	1:A:346:ILE:CD1	2.46	0.46
1:I:290:ILE:HG12	1:I:346:ILE:CD1	2.46	0.46
1:B:359:GLU:HG2	1:B:359:GLU:O	2.15	0.46
1:I:141:VAL:CG2	1:I:432:TYR:CE1	2.97	0.46
1:H:210:VAL:O	1:H:382:LEU:HD12	2.16	0.46
1:E:214:GLY:HA3	1:E:384:ARG:HH21	1.79	0.46
1:G:56:ASP:OD1	1:G:70:ASN:HB3	2.15	0.46
1:G:214:GLY:HA3	1:G:384:ARG:HH21	1.79	0.46
1:G:210:VAL:O	1:G:382:LEU:HD12	2.16	0.46
1:G:208:GLN:C	1:G:209:ILE:HD12	2.36	0.46
1:C:208:GLN:C	1:C:209:ILE:HD12	2.36	0.46
1:I:208:GLN:C	1:I:209:ILE:HD12	2.36	0.46
1:E:46:LEU:O	1:E:47:LYS:C	2.53	0.46
1:H:194:GLU:C	1:H:195:LEU:HD12	2.36	0.46
1:C:224:TYR:HA	1:C:379:ILE:HG22	1.98	0.46
1:F:224:TYR:HA	1:F:379:ILE:HG22	1.98	0.46
1:F:178:ARG:NE	1:F:178:ARG:H	2.12	0.46
1:B:178:ARG:H	1:B:178:ARG:NE	2.12	0.46
1:A:75:ILE:O	1:A:79:MET:HB3	2.15	0.46
1:F:271:GLN:OE1	1:F:271:GLN:HA	2.15	0.46
1:H:259:GLU:C	1:H:259:GLU:CD	2.74	0.46
1:D:150:ALA:HA	1:D:415:ILE:HG22	1.97	0.46
1:H:150:ALA:HA	1:H:415:ILE:HG22	1.98	0.46
1:E:359:GLU:O	1:E:359:GLU:HG2	2.15	0.46
1:E:430:ARG:NH1	1:E:430:ARG:HG2	2.29	0.46
1:A:430:ARG:NH1	1:A:430:ARG:HG2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:ILE:HG22	1:C:320:VAL:HG23	1.96	0.46
1:F:153:VAL:HG13	1:F:153:VAL:O	2.16	0.46
1:H:208:GLN:C	1:H:209:ILE:HD12	2.36	0.46
1:A:45:ALA:C	1:A:46:LEU:HD12	2.36	0.46
1:G:505:PRO:C	1:G:507:LEU:N	2.69	0.46
1:A:505:PRO:C	1:A:507:LEU:N	2.69	0.46
1:C:194:GLU:C	1:C:195:LEU:HD12	2.36	0.46
1:G:522:LEU:O	1:G:526:ILE:HG12	2.16	0.46
1:F:282:LEU:O	1:F:285:GLU:HB3	2.15	0.46
1:E:259:GLU:C	1:E:259:GLU:CD	2.74	0.46
1:E:528:ASP:OD2	1:E:529:VAL:N	2.48	0.46
1:F:150:ALA:HA	1:F:415:ILE:HG22	1.98	0.46
1:C:263:GLU:C	1:C:264:ILE:CG2	2.82	0.46
1:B:290:ILE:HG12	1:B:346:ILE:CD1	2.46	0.46
1:G:430:ARG:HG2	1:G:430:ARG:NH1	2.29	0.46
1:G:84:PRO:HG2	1:G:85:ALA:H	1.80	0.46
1:G:46:LEU:O	1:G:47:LYS:C	2.53	0.46
1:D:121:LEU:HB3	1:D:126:VAL:HG21	1.97	0.46
1:I:230:LYS:HZ1	1:I:321:ARG:HH12	1.64	0.46
1:B:224:TYR:HA	1:B:379:ILE:HG22	1.98	0.46
1:H:211:LYS:HD2	1:H:391:VAL:HG22	1.98	0.46
1:E:492:GLY:O	1:E:493:GLN:HB2	2.16	0.46
1:C:522:LEU:O	1:C:526:ILE:HG12	2.16	0.46
1:G:259:GLU:CD	1:G:259:GLU:C	2.74	0.46
1:E:522:LEU:O	1:E:526:ILE:HG12	2.16	0.46
1:F:84:PRO:HG2	1:F:85:ALA:H	1.80	0.46
1:I:217:ILE:HD11	1:I:390:LEU:CD2	2.44	0.46
1:C:290:ILE:HG12	1:C:346:ILE:CD1	2.46	0.46
1:C:359:GLU:HG2	1:C:359:GLU:O	2.15	0.46
1:F:141:VAL:CG2	1:F:432:TYR:CE1	2.97	0.46
1:H:153:VAL:O	1:H:153:VAL:HG13	2.16	0.46
1:C:127:HIS:CG	1:C:128:PRO:HD2	2.51	0.46
1:E:127:HIS:CG	1:E:128:PRO:HD2	2.51	0.46
1:G:127:HIS:CG	1:G:128:PRO:HD2	2.51	0.46
1:H:230:LYS:HZ2	1:H:321:ARG:NH1	2.13	0.46
1:E:178:ARG:H	1:E:178:ARG:NE	2.13	0.46
1:H:522:LEU:O	1:H:526:ILE:HG12	2.16	0.46
1:I:406:ALA:O	1:I:410:LYS:HG3	2.15	0.46
1:B:260:LEU:CD1	1:B:261:ASP:CG	2.85	0.45
1:I:258:PRO:CG	1:I:279:GLU:OE2	2.56	0.45
1:D:83:HIS:CD2	1:D:84:PRO:HD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:210:VAL:O	1:F:382:LEU:HD12	2.16	0.45
1:D:153:VAL:HG13	1:D:153:VAL:O	2.16	0.45
1:E:469:LEU:HB3	1:E:487:ILE:CD1	2.43	0.45
1:G:83:HIS:CD2	1:G:84:PRO:HD2	2.50	0.45
1:H:45:ALA:C	1:H:46:LEU:HD12	2.36	0.45
1:H:121:LEU:HB3	1:H:126:VAL:CG2	2.44	0.45
1:G:121:LEU:HB3	1:G:126:VAL:HG21	1.97	0.45
1:I:166:MET:CE	1:I:178:ARG:HG2	2.47	0.45
1:B:211:LYS:HD2	1:B:391:VAL:HG22	1.98	0.45
1:B:166:MET:CE	1:B:178:ARG:HG2	2.47	0.45
1:D:31:ALA:O	1:D:34:ALA:N	2.49	0.45
1:A:522:LEU:O	1:A:526:ILE:HG12	2.16	0.45
1:D:40:LYS:HD3	1:D:116:LYS:HG2	1.99	0.45
1:B:282:LEU:O	1:B:285:GLU:HB3	2.15	0.45
1:E:527:ASP:N	1:F:56:ASP:O	2.46	0.45
1:I:150:ALA:HA	1:I:415:ILE:HG22	1.98	0.45
1:I:522:LEU:O	1:I:526:ILE:HG12	2.16	0.45
1:G:75:ILE:O	1:G:79:MET:HB3	2.15	0.45
1:G:290:ILE:HG12	1:G:346:ILE:CD1	2.46	0.45
1:F:290:ILE:HG12	1:F:346:ILE:CD1	2.46	0.45
1:I:432:TYR:CZ	1:I:436:VAL:HG12	2.52	0.45
1:E:432:TYR:CZ	1:E:436:VAL:HG12	2.52	0.45
1:A:141:VAL:CG2	1:A:432:TYR:CE1	2.97	0.45
1:B:208:GLN:C	1:B:209:ILE:HD12	2.36	0.45
1:I:153:VAL:O	1:I:153:VAL:HG13	2.16	0.45
1:E:45:ALA:C	1:E:46:LEU:HD12	2.36	0.45
1:I:127:HIS:CG	1:I:128:PRO:HD2	2.51	0.45
1:H:505:PRO:C	1:H:507:LEU:N	2.69	0.45
1:F:194:GLU:C	1:F:195:LEU:HD12	2.36	0.45
1:A:188:ALA:HA	1:A:379:ILE:HD11	1.98	0.45
1:I:224:TYR:HA	1:I:379:ILE:HG22	1.98	0.45
1:D:224:TYR:HA	1:D:379:ILE:HG22	1.98	0.45
1:H:358:GLU:CG	1:H:360:ARG:HH22	2.27	0.45
1:H:224:TYR:HA	1:H:379:ILE:HG22	1.98	0.45
1:E:31:ALA:O	1:E:34:ALA:N	2.49	0.45
1:C:40:LYS:HD3	1:C:116:LYS:HG2	1.99	0.45
1:D:406:ALA:O	1:D:410:LYS:HG3	2.16	0.45
1:H:260:LEU:CD1	1:H:261:ASP:CG	2.85	0.45
1:E:66:ILE:CD1	1:E:66:ILE:N	2.76	0.45
1:E:84:PRO:HG2	1:E:85:ALA:H	1.80	0.45
1:D:426:ALA:O	1:D:429:LEU:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:492:GLY:O	1:G:493:GLN:HB2	2.16	0.45
1:A:83:HIS:CD2	1:A:84:PRO:HD2	2.50	0.45
1:B:432:TYR:CZ	1:B:436:VAL:HG12	2.52	0.45
1:D:210:VAL:O	1:D:382:LEU:HD12	2.16	0.45
1:B:45:ALA:C	1:B:46:LEU:HD12	2.36	0.45
1:A:527:ASP:HB2	1:B:55:MET:CG	2.45	0.45
1:E:188:ALA:HA	1:E:379:ILE:HD11	1.98	0.45
1:F:188:ALA:HA	1:F:379:ILE:HD11	1.98	0.45
1:C:211:LYS:HD2	1:C:391:VAL:HG22	1.98	0.45
1:E:166:MET:CE	1:E:178:ARG:HG2	2.47	0.45
1:F:31:ALA:O	1:F:34:ALA:N	2.49	0.45
1:I:31:ALA:O	1:I:34:ALA:N	2.49	0.45
1:F:250:ASP:O	1:F:251:ALA:HB2	2.17	0.45
1:B:522:LEU:O	1:B:526:ILE:HG12	2.16	0.45
1:F:40:LYS:HD3	1:F:116:LYS:HG2	1.99	0.45
1:D:522:LEU:O	1:D:526:ILE:HG12	2.16	0.45
1:A:492:GLY:O	1:A:493:GLN:HB2	2.16	0.45
1:H:492:GLY:O	1:H:493:GLN:HB2	2.16	0.45
1:E:150:ALA:HA	1:E:415:ILE:HG22	1.98	0.45
1:C:212:LYS:O	1:C:213:ALA:O	2.34	0.45
1:C:210:VAL:O	1:C:382:LEU:HD12	2.16	0.45
1:F:166:MET:CE	1:F:178:ARG:HG2	2.47	0.45
1:F:211:LYS:HD2	1:F:391:VAL:HG22	1.98	0.45
1:D:166:MET:CE	1:D:178:ARG:HG2	2.47	0.45
1:G:166:MET:CE	1:G:178:ARG:HG2	2.47	0.45
1:H:166:MET:CE	1:H:178:ARG:HG2	2.47	0.45
1:B:31:ALA:O	1:B:34:ALA:N	2.49	0.45
1:I:250:ASP:O	1:I:251:ALA:HB2	2.17	0.45
1:E:250:ASP:O	1:E:251:ALA:HB2	2.17	0.45
1:E:260:LEU:CD1	1:E:261:ASP:CG	2.85	0.45
1:I:260:LEU:CD1	1:I:260:LEU:C	2.81	0.45
1:E:83:HIS:CD2	1:E:84:PRO:HD2	2.50	0.45
1:I:244:ALA:HA	1:I:296:ASN:HD22	1.82	0.45
1:B:492:GLY:O	1:B:493:GLN:HB2	2.16	0.45
1:B:430:ARG:HG2	1:B:430:ARG:NH1	2.29	0.45
1:F:430:ARG:HG2	1:F:430:ARG:NH1	2.29	0.45
1:H:436:VAL:HG21	1:H:441:GLN:HA	1.99	0.45
1:E:436:VAL:HG21	1:E:441:GLN:HA	1.99	0.45
1:B:210:VAL:O	1:B:382:LEU:HD12	2.16	0.45
1:C:83:HIS:CD2	1:C:84:PRO:HD2	2.50	0.45
1:B:127:HIS:CG	1:B:128:PRO:HD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:HIS:CG	1:D:128:PRO:HD2	2.51	0.45
1:I:505:PRO:C	1:I:507:LEU:N	2.69	0.45
1:D:505:PRO:C	1:D:507:LEU:N	2.69	0.45
1:E:321:ARG:HB3	1:E:322:ARG:H	1.56	0.45
1:G:224:TYR:HA	1:G:379:ILE:HG22	1.98	0.45
1:C:406:ALA:O	1:C:410:LYS:HG3	2.15	0.45
1:B:40:LYS:HD3	1:B:116:LYS:HG2	1.99	0.45
1:I:260:LEU:CD1	1:I:261:ASP:CG	2.85	0.45
1:B:150:ALA:HA	1:B:415:ILE:HG22	1.98	0.45
1:B:423:ILE:HD12	1:B:424:GLU:H	1.73	0.45
1:E:212:LYS:O	1:E:213:ALA:O	2.34	0.45
1:E:290:ILE:HG12	1:E:346:ILE:CD1	2.46	0.45
1:E:249:ILE:HD12	1:E:346:ILE:HD11	1.97	0.45
1:F:208:GLN:C	1:F:209:ILE:HD12	2.36	0.45
1:C:153:VAL:O	1:C:153:VAL:HG13	2.16	0.45
1:A:153:VAL:HG13	1:A:153:VAL:O	2.16	0.45
1:D:45:ALA:C	1:D:46:LEU:HD12	2.36	0.45
1:F:45:ALA:C	1:F:46:LEU:HD12	2.36	0.45
1:F:230:LYS:HZ2	1:F:321:ARG:NH1	2.15	0.45
1:A:161:LEU:CD1	1:A:161:LEU:H	2.30	0.45
1:E:224:TYR:HA	1:E:379:ILE:HG22	1.98	0.45
1:G:211:LYS:HD2	1:G:391:VAL:HG22	1.98	0.45
1:E:166:MET:HE1	1:E:179:GLU:HG2	1.99	0.45
1:G:31:ALA:O	1:G:34:ALA:N	2.49	0.45
1:B:250:ASP:O	1:B:251:ALA:HB2	2.17	0.45
1:E:40:LYS:HD3	1:E:116:LYS:HG2	1.99	0.45
1:H:40:LYS:HD3	1:H:116:LYS:HG2	1.99	0.45
1:F:529:VAL:HG12	1:G:58:MET:CG	2.46	0.45
1:C:244:ALA:HA	1:C:296:ASN:HD22	1.82	0.45
1:C:142:ALA:O	1:C:425:ILE:HD12	2.17	0.45
1:B:476:THR:HG21	1:B:494:PRO:HB3	1.99	0.45
1:E:142:ALA:O	1:E:425:ILE:HD12	2.17	0.45
1:D:290:ILE:HG12	1:D:346:ILE:CD1	2.46	0.45
1:D:436:VAL:HG21	1:D:441:GLN:HA	1.99	0.45
1:C:432:TYR:CZ	1:C:436:VAL:HG12	2.52	0.45
1:F:209:ILE:CB	1:F:399:ARG:HH22	2.28	0.45
1:F:127:HIS:CG	1:F:128:PRO:HD2	2.51	0.45
1:H:127:HIS:CG	1:H:128:PRO:HD2	2.51	0.45
1:G:188:ALA:HA	1:G:379:ILE:HD11	1.98	0.45
1:D:492:GLY:O	1:D:493:GLN:HB2	2.16	0.45
1:F:172:LYS:HG3	1:F:397:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:ASP:O	1:D:251:ALA:HB2	2.17	0.45
1:G:432:TYR:CZ	1:G:436:VAL:HG12	2.52	0.45
1:G:436:VAL:HG21	1:G:441:GLN:HA	1.99	0.45
1:I:210:VAL:O	1:I:382:LEU:HD12	2.16	0.45
1:E:153:VAL:HG23	1:E:160:LEU:CD2	2.45	0.45
1:H:321:ARG:HB3	1:H:322:ARG:H	1.56	0.45
1:C:188:ALA:HA	1:C:379:ILE:HD11	1.98	0.45
1:E:211:LYS:HD2	1:E:391:VAL:HG22	1.98	0.45
1:H:172:LYS:HG3	1:H:397:ALA:HB2	1.99	0.45
1:G:172:LYS:HG3	1:G:397:ALA:HB2	1.99	0.45
1:C:146:ILE:HB	1:C:510:MET:HE3	1.99	0.45
1:A:146:ILE:HB	1:A:510:MET:HE2	1.99	0.45
1:A:68:ILE:HD12	1:I:522:LEU:HD11	1.98	0.45
1:E:210:VAL:O	1:E:382:LEU:HD12	2.16	0.45
1:C:166:MET:CE	1:C:178:ARG:HG2	2.46	0.45
1:C:31:ALA:O	1:C:34:ALA:N	2.49	0.45
1:H:31:ALA:O	1:H:34:ALA:N	2.49	0.45
1:C:172:LYS:HG3	1:C:397:ALA:HB2	1.99	0.45
1:A:172:LYS:HG3	1:A:397:ALA:HB2	1.99	0.45
1:D:260:LEU:CD1	1:D:261:ASP:CG	2.85	0.45
1:D:142:ALA:O	1:D:425:ILE:HD12	2.17	0.45
1:F:142:ALA:O	1:F:425:ILE:HD12	2.17	0.45
1:H:432:TYR:CZ	1:H:436:VAL:HG12	2.52	0.45
1:E:153:VAL:HG13	1:E:153:VAL:O	2.16	0.45
1:I:188:ALA:HA	1:I:379:ILE:HD11	1.98	0.45
1:G:161:LEU:CD1	1:G:161:LEU:H	2.30	0.45
1:I:40:LYS:HD3	1:I:116:LYS:HG2	1.99	0.45
1:A:40:LYS:HD3	1:A:116:LYS:HG2	1.99	0.45
1:A:142:ALA:O	1:A:425:ILE:HD12	2.17	0.44
1:F:432:TYR:CZ	1:F:436:VAL:HG12	2.52	0.44
1:I:89:LEU:CD2	1:I:108:VAL:HG23	2.44	0.44
1:H:165:ALA:O	1:H:169:LEU:HG	2.17	0.44
1:E:165:ALA:O	1:E:169:LEU:HG	2.18	0.44
1:I:161:LEU:CD1	1:I:161:LEU:H	2.30	0.44
1:A:98:GLU:OE1	1:A:98:GLU:HA	2.17	0.44
1:G:98:GLU:OE1	1:G:98:GLU:HA	2.17	0.44
1:A:31:ALA:O	1:A:34:ALA:N	2.49	0.44
1:E:244:ALA:HA	1:E:296:ASN:HD22	1.82	0.44
1:F:265:ARG:HD2	1:F:265:ARG:C	2.38	0.44
1:A:153:VAL:HG23	1:A:160:LEU:CD2	2.45	0.44
1:F:165:ALA:O	1:F:169:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ALA:O	1:B:169:LEU:HG	2.18	0.44
1:G:321:ARG:HB3	1:G:322:ARG:H	1.56	0.44
1:F:161:LEU:CD1	1:F:161:LEU:H	2.30	0.44
1:I:211:LYS:HD2	1:I:391:VAL:HG22	1.98	0.44
1:A:166:MET:CE	1:A:178:ARG:HG2	2.47	0.44
1:F:492:GLY:O	1:F:493:GLN:HB2	2.16	0.44
1:H:212:LYS:O	1:H:213:ALA:O	2.34	0.44
1:C:436:VAL:HG21	1:C:441:GLN:HA	1.99	0.44
1:D:82:GLN:O	1:D:83:HIS:C	2.56	0.44
1:F:522:LEU:O	1:F:526:ILE:HG12	2.16	0.44
1:I:492:GLY:O	1:I:493:GLN:HB2	2.16	0.44
1:C:492:GLY:O	1:C:493:GLN:HB2	2.16	0.44
1:D:259:GLU:C	1:D:259:GLU:CD	2.74	0.44
1:A:260:LEU:CD1	1:A:261:ASP:CG	2.85	0.44
1:G:260:LEU:CD1	1:G:261:ASP:CG	2.85	0.44
1:B:260:LEU:C	1:B:260:LEU:CD1	2.81	0.44
1:I:142:ALA:O	1:I:425:ILE:HD12	2.17	0.44
1:I:414:ALA:HA	1:I:506:ALA:H	1.83	0.44
1:C:414:ALA:HA	1:C:506:ALA:H	1.83	0.44
1:I:82:GLN:O	1:I:83:HIS:C	2.56	0.44
1:E:265:ARG:HD2	1:E:265:ARG:C	2.38	0.44
1:I:265:ARG:HD2	1:I:265:ARG:C	2.38	0.44
1:G:59:LEU:HD13	1:G:78:LYS:HB2	2.00	0.44
1:A:82:GLN:O	1:A:83:HIS:C	2.56	0.44
1:A:127:HIS:CG	1:A:128:PRO:HD2	2.51	0.44
1:G:469:LEU:HB3	1:G:487:ILE:CD1	2.43	0.44
1:G:82:GLN:O	1:G:83:HIS:C	2.56	0.44
1:H:529:VAL:HG12	1:I:58:MET:SD	2.57	0.44
1:E:260:LEU:C	1:E:260:LEU:CD1	2.81	0.44
1:A:66:ILE:CD1	1:A:66:ILE:N	2.76	0.44
1:E:82:GLN:O	1:E:83:HIS:C	2.56	0.44
1:B:142:ALA:O	1:B:425:ILE:HD12	2.17	0.44
1:C:476:THR:HG21	1:C:494:PRO:HB3	1.99	0.44
1:G:141:VAL:CG2	1:G:432:TYR:CE1	2.97	0.44
1:A:39:VAL:HG11	1:A:115:VAL:HG21	2.00	0.44
1:C:39:VAL:HG11	1:C:115:VAL:HG21	2.00	0.44
1:C:529:VAL:HG12	1:D:58:MET:SD	2.57	0.44
1:G:165:ALA:O	1:G:169:LEU:HG	2.17	0.44
1:A:165:ALA:O	1:A:169:LEU:HG	2.17	0.44
1:E:161:LEU:H	1:E:161:LEU:CD1	2.30	0.44
1:D:530:VAL:O	1:E:59:LEU:CD2	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:172:LYS:HG3	1:I:397:ALA:HB2	1.99	0.44
1:C:515:ALA:O	1:C:518:GLU:HB3	2.18	0.44
1:F:145:THR:O	1:F:145:THR:HG22	2.18	0.44
1:D:260:LEU:CD1	1:D:260:LEU:C	2.81	0.44
1:B:414:ALA:HA	1:B:506:ALA:H	1.83	0.44
1:I:146:ILE:HB	1:I:510:MET:HE3	1.98	0.44
1:H:265:ARG:C	1:H:265:ARG:HD2	2.38	0.44
1:H:249:ILE:HD13	1:H:340:VAL:HB	2.00	0.44
1:I:430:ARG:NH1	1:I:430:ARG:HG2	2.29	0.44
1:A:432:TYR:CZ	1:A:436:VAL:HG12	2.52	0.44
1:C:82:GLN:O	1:C:83:HIS:C	2.56	0.44
1:C:110:PHE:CZ	1:C:114:LEU:HD11	2.53	0.44
1:F:110:PHE:HD1	1:F:516:ALA:CB	2.31	0.44
1:H:110:PHE:CZ	1:H:114:LEU:HD11	2.53	0.44
1:F:505:PRO:C	1:F:507:LEU:N	2.69	0.44
1:D:98:GLU:HA	1:D:98:GLU:OE1	2.17	0.44
1:B:391:VAL:HG13	1:B:392:ASP:N	2.33	0.44
1:F:98:GLU:OE1	1:F:98:GLU:HA	2.17	0.44
1:I:98:GLU:OE1	1:I:98:GLU:HA	2.17	0.44
1:E:391:VAL:HG13	1:E:392:ASP:N	2.33	0.44
1:F:391:VAL:HG13	1:F:392:ASP:N	2.33	0.44
1:H:59:LEU:HD13	1:H:78:LYS:HB2	2.00	0.44
1:A:250:ASP:O	1:A:251:ALA:HB2	2.17	0.44
1:H:515:ALA:O	1:H:518:GLU:HB3	2.18	0.44
1:G:440:GLU:O	1:G:444:VAL:HG23	2.18	0.44
1:B:440:GLU:O	1:B:444:VAL:HG23	2.18	0.44
1:D:515:ALA:O	1:D:518:GLU:HB3	2.18	0.44
1:A:476:THR:HG21	1:A:494:PRO:HB3	1.99	0.44
1:G:414:ALA:HA	1:G:506:ALA:H	1.83	0.44
1:A:217:ILE:HD11	1:A:390:LEU:CD2	2.43	0.44
1:B:265:ARG:HD2	1:B:265:ARG:C	2.38	0.44
1:C:265:ARG:HD2	1:C:265:ARG:C	2.38	0.44
1:C:249:ILE:HD13	1:C:340:VAL:HB	2.00	0.44
1:A:436:VAL:HG21	1:A:441:GLN:HA	1.99	0.44
1:H:89:LEU:CD2	1:H:108:VAL:HG23	2.44	0.44
1:B:89:LEU:CD2	1:B:108:VAL:HG23	2.44	0.44
1:F:153:VAL:HG23	1:F:160:LEU:CD2	2.45	0.44
1:H:469:LEU:HB3	1:H:487:ILE:CD1	2.43	0.44
1:I:165:ALA:O	1:I:169:LEU:HG	2.18	0.44
1:G:110:PHE:CZ	1:G:114:LEU:HD11	2.53	0.44
1:I:110:PHE:CZ	1:I:114:LEU:HD11	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:PHE:CZ	1:E:114:LEU:HD11	2.53	0.44
1:E:110:PHE:HD1	1:E:516:ALA:CB	2.31	0.44
1:A:110:PHE:CZ	1:A:114:LEU:HD11	2.53	0.44
1:D:391:VAL:HG13	1:D:392:ASP:N	2.33	0.44
1:E:59:LEU:HD13	1:E:78:LYS:HB2	2.00	0.44
1:E:172:LYS:HG3	1:E:397:ALA:HB2	1.99	0.44
1:G:250:ASP:O	1:G:251:ALA:HB2	2.17	0.44
1:D:440:GLU:O	1:D:444:VAL:HG23	2.18	0.44
1:G:145:THR:O	1:G:145:THR:HG22	2.18	0.44
1:D:146:ILE:HB	1:D:510:MET:HE3	2.00	0.44
1:H:142:ALA:O	1:H:425:ILE:HD12	2.17	0.44
1:I:476:THR:HG21	1:I:494:PRO:HB3	1.99	0.44
1:H:476:THR:HG21	1:H:494:PRO:HB3	1.99	0.44
1:D:265:ARG:C	1:D:265:ARG:HD2	2.38	0.44
1:A:265:ARG:HD2	1:A:265:ARG:C	2.38	0.44
1:D:209:ILE:CB	1:D:399:ARG:HH22	2.28	0.44
1:D:165:ALA:O	1:D:169:LEU:HG	2.17	0.44
1:C:165:ALA:O	1:C:169:LEU:HG	2.17	0.44
1:C:110:PHE:HD1	1:C:516:ALA:CB	2.31	0.44
1:B:110:PHE:HD1	1:B:516:ALA:CB	2.31	0.44
1:D:172:LYS:HG3	1:D:397:ALA:HB2	1.99	0.44
1:I:515:ALA:O	1:I:518:GLU:HB3	2.18	0.44
1:I:440:GLU:O	1:I:444:VAL:HG23	2.18	0.44
1:E:515:ALA:O	1:E:518:GLU:HB3	2.18	0.44
1:D:145:THR:HG22	1:D:145:THR:O	2.18	0.44
1:E:145:THR:HG22	1:E:145:THR:O	2.18	0.44
1:B:244:ALA:HA	1:B:296:ASN:HD22	1.82	0.44
1:B:146:ILE:HB	1:B:510:MET:HE3	1.99	0.44
1:D:414:ALA:HA	1:D:506:ALA:H	1.83	0.44
1:H:146:ILE:HB	1:H:510:MET:HE3	1.99	0.44
1:B:59:LEU:HD13	1:B:78:LYS:HB2	2.00	0.44
1:B:249:ILE:HD13	1:B:340:VAL:HB	2.00	0.44
1:H:81:LEU:N	1:H:81:LEU:HD12	2.28	0.44
1:G:89:LEU:CD2	1:G:108:VAL:HG23	2.44	0.44
1:E:505:PRO:C	1:E:507:LEU:H	2.22	0.44
1:H:161:LEU:CD1	1:H:161:LEU:H	2.30	0.44
1:A:211:LYS:HD2	1:A:391:VAL:HG22	1.98	0.44
1:H:250:ASP:O	1:H:251:ALA:HB2	2.17	0.44
1:C:250:ASP:O	1:C:251:ALA:HB2	2.17	0.44
1:F:258:PRO:CG	1:F:279:GLU:OE2	2.56	0.43
1:A:66:ILE:HD13	1:A:66:ILE:N	2.13	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:244:ALA:HA	1:G:296:ASN:HD22	1.82	0.43
1:G:142:ALA:O	1:G:425:ILE:HD12	2.17	0.43
1:E:414:ALA:HA	1:E:506:ALA:H	1.83	0.43
1:I:436:VAL:HG21	1:I:441:GLN:HA	1.99	0.43
1:F:436:VAL:HG21	1:F:441:GLN:HA	1.99	0.43
1:G:233:VAL:HG22	1:G:309:GLN:CD	2.39	0.43
1:F:233:VAL:HG22	1:F:309:GLN:CD	2.39	0.43
1:H:82:GLN:O	1:H:83:HIS:C	2.56	0.43
1:I:110:PHE:HD1	1:I:516:ALA:CB	2.31	0.43
1:I:58:MET:CB	1:I:68:ILE:HG22	2.48	0.43
1:A:440:GLU:O	1:A:444:VAL:HG23	2.18	0.43
1:A:59:LEU:HD13	1:A:78:LYS:HB2	2.00	0.43
1:H:145:THR:O	1:H:145:THR:HG22	2.18	0.43
1:I:145:THR:HG22	1:I:145:THR:O	2.18	0.43
1:C:145:THR:HG22	1:C:145:THR:O	2.18	0.43
1:F:260:LEU:CD1	1:F:261:ASP:CG	2.85	0.43
1:C:260:LEU:CD1	1:C:261:ASP:CG	2.85	0.43
1:A:244:ALA:HA	1:A:296:ASN:HD22	1.82	0.43
1:D:476:THR:HG21	1:D:494:PRO:HB3	1.99	0.43
1:H:298:ILE:O	1:H:319:ALA:HA	2.19	0.43
1:A:233:VAL:HG22	1:A:309:GLN:CD	2.39	0.43
1:B:233:VAL:HG22	1:B:309:GLN:CD	2.39	0.43
1:C:88:LEU:HD11	1:D:389:ARG:HH12	1.83	0.43
1:G:525:ARG:HG2	1:G:525:ARG:NH1	2.31	0.43
1:G:110:PHE:HD1	1:G:516:ALA:CB	2.31	0.43
1:B:110:PHE:CZ	1:B:114:LEU:HD11	2.53	0.43
1:C:161:LEU:CD1	1:C:161:LEU:H	2.30	0.43
1:H:188:ALA:HA	1:H:379:ILE:HD11	1.98	0.43
1:C:98:GLU:HA	1:C:98:GLU:OE1	2.17	0.43
1:G:391:VAL:HG13	1:G:392:ASP:N	2.33	0.43
1:C:391:VAL:HG13	1:C:392:ASP:N	2.33	0.43
1:F:515:ALA:O	1:F:518:GLU:HB3	2.18	0.43
1:I:72:GLY:O	1:I:73:ALA:C	2.57	0.43
1:C:72:GLY:O	1:C:73:ALA:C	2.57	0.43
1:D:484:TRP:HA	1:D:484:TRP:CE3	2.53	0.43
1:G:58:MET:CB	1:G:68:ILE:HG22	2.48	0.43
1:G:249:ILE:HD13	1:G:340:VAL:HB	2.00	0.43
1:F:249:ILE:HD13	1:F:340:VAL:HB	2.00	0.43
1:D:432:TYR:CZ	1:D:436:VAL:HG12	2.52	0.43
1:E:233:VAL:HG22	1:E:309:GLN:CD	2.39	0.43
1:C:233:VAL:HG22	1:C:309:GLN:CD	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:MET:CB	1:C:68:ILE:HG22	2.48	0.43
1:G:482:ASN:O	1:G:485:TYR:N	2.40	0.43
1:H:482:ASN:O	1:H:485:TYR:N	2.40	0.43
1:D:505:PRO:C	1:D:507:LEU:H	2.22	0.43
1:F:505:PRO:C	1:F:507:LEU:H	2.22	0.43
1:D:161:LEU:CD1	1:D:161:LEU:H	2.30	0.43
1:H:98:GLU:HA	1:H:98:GLU:OE1	2.17	0.43
1:B:98:GLU:HA	1:B:98:GLU:OE1	2.17	0.43
1:F:440:GLU:O	1:F:444:VAL:HG23	2.18	0.43
1:F:59:LEU:HD13	1:F:78:LYS:HB2	2.00	0.43
1:B:258:PRO:CG	1:B:279:GLU:OE2	2.56	0.43
1:F:476:THR:HG21	1:F:494:PRO:HB3	1.99	0.43
1:A:414:ALA:HA	1:A:506:ALA:H	1.83	0.43
1:B:58:MET:CB	1:B:68:ILE:HG22	2.48	0.43
1:I:249:ILE:HD13	1:I:340:VAL:HB	2.00	0.43
1:H:39:VAL:HG11	1:H:115:VAL:HG21	2.00	0.43
1:D:58:MET:CB	1:D:68:ILE:HG22	2.48	0.43
1:D:110:PHE:HD1	1:D:516:ALA:CB	2.31	0.43
1:I:505:PRO:C	1:I:507:LEU:H	2.22	0.43
1:I:391:VAL:HG13	1:I:392:ASP:N	2.33	0.43
1:A:515:ALA:O	1:A:518:GLU:HB3	2.18	0.43
1:B:415:ILE:HG23	1:B:506:ALA:CB	2.48	0.43
1:I:415:ILE:HG23	1:I:506:ALA:CB	2.48	0.43
1:H:414:ALA:HA	1:H:506:ALA:H	1.83	0.43
1:G:476:THR:HG21	1:G:494:PRO:HB3	1.99	0.43
1:G:265:ARG:HD2	1:G:265:ARG:C	2.38	0.43
1:B:436:VAL:HG21	1:B:441:GLN:HA	1.99	0.43
1:E:39:VAL:HG11	1:E:115:VAL:HG21	2.00	0.43
1:B:81:LEU:HD22	1:B:86:ALA:HB1	2.01	0.43
1:H:110:PHE:HD1	1:H:516:ALA:CB	2.31	0.43
1:A:110:PHE:HD1	1:A:516:ALA:CB	2.31	0.43
1:B:161:LEU:CD1	1:B:161:LEU:H	2.30	0.43
1:E:98:GLU:OE1	1:E:98:GLU:HA	2.17	0.43
1:B:515:ALA:O	1:B:518:GLU:HB3	2.18	0.43
1:G:484:TRP:HA	1:G:484:TRP:CE3	2.54	0.43
1:F:58:MET:CB	1:F:68:ILE:HG22	2.48	0.43
1:H:244:ALA:HA	1:H:296:ASN:HD22	1.82	0.43
1:B:505:PRO:C	1:B:507:LEU:H	2.22	0.43
1:F:244:ALA:HA	1:F:296:ASN:HD22	1.82	0.43
1:G:146:ILE:HB	1:G:510:MET:HE3	2.01	0.43
1:H:233:VAL:HG22	1:H:309:GLN:CD	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:LEU:HD22	1:E:86:ALA:HB1	2.01	0.43
1:B:482:ASN:O	1:B:485:TYR:N	2.40	0.43
1:G:46:LEU:O	1:G:49:THR:N	2.43	0.43
1:E:128:PRO:HG3	1:F:55:MET:CE	2.48	0.43
1:H:505:PRO:C	1:H:507:LEU:H	2.22	0.43
1:A:59:LEU:HD23	1:I:530:VAL:O	2.19	0.43
1:G:515:ALA:O	1:G:518:GLU:HB3	2.18	0.43
1:B:94:LYS:O	1:B:96:GLN:N	2.48	0.43
1:D:59:LEU:HD13	1:D:78:LYS:HB2	2.00	0.43
1:H:440:GLU:O	1:H:444:VAL:HG23	2.18	0.43
1:G:40:LYS:HD3	1:G:116:LYS:HG2	1.99	0.43
1:B:484:TRP:HA	1:B:484:TRP:CE3	2.53	0.43
1:A:145:THR:O	1:A:145:THR:HG22	2.18	0.43
1:E:484:TRP:HA	1:E:484:TRP:CE3	2.54	0.43
1:F:415:ILE:HG23	1:F:506:ALA:CB	2.48	0.43
1:E:146:ILE:HB	1:E:510:MET:HE3	2.01	0.43
1:D:298:ILE:O	1:D:319:ALA:HA	2.19	0.43
1:A:88:LEU:CD1	1:B:389:ARG:HH12	2.32	0.43
1:E:298:ILE:O	1:E:319:ALA:HA	2.19	0.43
1:A:132:ILE:HD12	1:A:521:THR:HB	2.01	0.43
1:G:81:LEU:HD22	1:G:86:ALA:HB1	2.01	0.43
1:C:81:LEU:HD22	1:C:86:ALA:HB1	2.01	0.43
1:F:110:PHE:CZ	1:F:114:LEU:HD11	2.53	0.43
1:H:58:MET:CB	1:H:68:ILE:HG22	2.48	0.43
1:H:118:ALA:O	1:H:122:LEU:CD2	2.67	0.43
1:H:391:VAL:HG13	1:H:392:ASP:N	2.33	0.43
1:G:72:GLY:O	1:G:73:ALA:C	2.57	0.43
1:C:484:TRP:HA	1:C:484:TRP:CE3	2.54	0.43
1:F:414:ALA:HA	1:F:506:ALA:H	1.83	0.43
1:H:264:ILE:HD12	1:H:265:ARG:HH22	1.84	0.43
1:F:264:ILE:HD12	1:F:265:ARG:HH22	1.84	0.43
1:A:298:ILE:O	1:A:319:ALA:HA	2.19	0.43
1:F:298:ILE:O	1:F:319:ALA:HA	2.18	0.43
1:B:141:VAL:CG2	1:B:432:TYR:CE1	2.97	0.43
1:H:430:ARG:HG2	1:H:430:ARG:NH1	2.29	0.43
1:D:233:VAL:HG22	1:D:309:GLN:CD	2.39	0.43
1:I:39:VAL:HG11	1:I:115:VAL:HG21	2.00	0.43
1:G:155:ILE:O	1:G:155:ILE:HG12	2.19	0.43
1:D:110:PHE:CZ	1:D:114:LEU:HD11	2.53	0.43
1:G:118:ALA:O	1:G:122:LEU:CD2	2.67	0.43
1:F:161:LEU:N	1:F:161:LEU:CD1	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:161:LEU:N	1:H:161:LEU:CD1	2.82	0.43
1:C:94:LYS:O	1:C:96:GLN:N	2.48	0.43
1:B:172:LYS:HG3	1:B:397:ALA:HB2	1.99	0.43
1:H:484:TRP:CE3	1:H:484:TRP:HA	2.54	0.43
1:B:145:THR:O	1:B:145:THR:HG22	2.18	0.43
1:E:58:MET:CB	1:E:68:ILE:HG22	2.48	0.43
1:A:415:ILE:HG23	1:A:506:ALA:CB	2.48	0.43
1:C:298:ILE:O	1:C:319:ALA:HA	2.19	0.43
1:B:298:ILE:O	1:B:319:ALA:HA	2.19	0.43
1:I:298:ILE:O	1:I:319:ALA:HA	2.19	0.43
1:E:249:ILE:HD13	1:E:340:VAL:HB	2.00	0.43
1:I:233:VAL:HG22	1:I:309:GLN:CD	2.39	0.43
1:A:284:LYS:HB3	1:A:311:TYR:CE2	2.54	0.43
1:C:209:ILE:CB	1:C:399:ARG:HH22	2.28	0.43
1:H:155:ILE:O	1:H:155:ILE:HG12	2.19	0.43
1:I:230:LYS:HZ1	1:I:321:ARG:NH1	2.14	0.43
1:G:161:LEU:CD1	1:G:161:LEU:N	2.82	0.43
1:I:134:GLY:HA3	1:I:443:ALA:CB	2.49	0.43
1:B:134:GLY:HA3	1:B:443:ALA:CB	2.49	0.43
1:B:72:GLY:O	1:B:73:ALA:C	2.57	0.43
1:E:72:GLY:O	1:E:73:ALA:C	2.57	0.43
1:F:484:TRP:CE3	1:F:484:TRP:HA	2.53	0.43
1:E:476:THR:HG21	1:E:494:PRO:HB3	1.99	0.43
1:A:58:MET:CB	1:A:68:ILE:HG22	2.48	0.43
1:I:264:ILE:HD12	1:I:265:ARG:HH22	1.84	0.43
1:D:81:LEU:HD22	1:D:86:ALA:HB1	2.01	0.43
1:H:459:ILE:O	1:H:462:ALA:HB3	2.19	0.43
1:F:155:ILE:HG12	1:F:155:ILE:O	2.19	0.43
1:A:505:PRO:C	1:A:507:LEU:H	2.22	0.43
1:E:118:ALA:O	1:E:122:LEU:CD2	2.67	0.43
1:A:134:GLY:HA3	1:A:443:ALA:CB	2.49	0.43
1:E:440:GLU:O	1:E:444:VAL:HG23	2.18	0.43
1:C:440:GLU:O	1:C:444:VAL:HG23	2.18	0.43
1:H:258:PRO:CG	1:H:279:GLU:OE2	2.56	0.42
1:C:415:ILE:HG23	1:C:506:ALA:CB	2.48	0.42
1:D:249:ILE:HD13	1:D:340:VAL:HB	2.00	0.42
1:G:39:VAL:HG11	1:G:115:VAL:HG21	2.00	0.42
1:F:89:LEU:CD2	1:F:108:VAL:HG23	2.44	0.42
1:H:284:LYS:HB3	1:H:311:TYR:CE2	2.54	0.42
1:D:459:ILE:O	1:D:462:ALA:HB3	2.19	0.42
1:A:482:ASN:O	1:A:485:TYR:N	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:LEU:N	1:D:46:LEU:CD1	2.82	0.42
1:D:46:LEU:O	1:D:49:THR:N	2.43	0.42
1:H:525:ARG:HG2	1:H:525:ARG:NH1	2.31	0.42
1:G:505:PRO:C	1:G:507:LEU:H	2.22	0.42
1:D:321:ARG:HB3	1:D:322:ARG:H	1.56	0.42
1:E:505:PRO:O	1:E:507:LEU:N	2.52	0.42
1:G:134:GLY:HA3	1:G:443:ALA:CB	2.49	0.42
1:C:134:GLY:HA3	1:C:443:ALA:CB	2.49	0.42
1:E:134:GLY:HA3	1:E:443:ALA:CB	2.49	0.42
1:A:484:TRP:HA	1:A:484:TRP:CE3	2.54	0.42
1:D:244:ALA:HA	1:D:296:ASN:HD22	1.82	0.42
1:C:298:ILE:O	1:C:298:ILE:HG23	2.19	0.42
1:B:459:ILE:O	1:B:462:ALA:HB3	2.19	0.42
1:B:39:VAL:HG11	1:B:115:VAL:HG21	2.00	0.42
1:C:284:LYS:HB3	1:C:311:TYR:CE2	2.54	0.42
1:D:153:VAL:HG23	1:D:160:LEU:CD2	2.45	0.42
1:F:46:LEU:CD1	1:F:46:LEU:N	2.82	0.42
1:A:505:PRO:O	1:A:507:LEU:N	2.52	0.42
1:F:508:VAL:CG1	1:F:509:LYS:N	2.83	0.42
1:E:508:VAL:CG1	1:E:509:LYS:N	2.83	0.42
1:B:118:ALA:O	1:B:122:LEU:CD2	2.67	0.42
1:A:391:VAL:HG13	1:A:392:ASP:N	2.33	0.42
1:D:134:GLY:HA3	1:D:443:ALA:CB	2.49	0.42
1:I:484:TRP:CE3	1:I:484:TRP:HA	2.54	0.42
1:D:245:LYS:H	1:D:296:ASN:ND2	2.07	0.42
1:F:82:GLN:O	1:F:83:HIS:C	2.56	0.42
1:I:268:ASP:HB3	1:I:269:PRO:HD2	2.02	0.42
1:A:298:ILE:O	1:A:298:ILE:HG23	2.20	0.42
1:H:298:ILE:HG23	1:H:298:ILE:O	2.20	0.42
1:I:298:ILE:O	1:I:298:ILE:HG23	2.20	0.42
1:D:39:VAL:HG11	1:D:115:VAL:HG21	2.00	0.42
1:B:82:GLN:O	1:B:83:HIS:C	2.56	0.42
1:F:321:ARG:HB3	1:F:322:ARG:H	1.56	0.42
1:A:155:ILE:HG12	1:A:155:ILE:O	2.19	0.42
1:C:505:PRO:C	1:C:507:LEU:H	2.22	0.42
1:A:72:GLY:O	1:A:73:ALA:C	2.57	0.42
1:C:398:LEU:HD12	1:C:398:LEU:HA	1.88	0.42
1:A:264:ILE:HD12	1:A:265:ARG:HH22	1.84	0.42
1:A:89:LEU:CD2	1:A:108:VAL:HG23	2.44	0.42
1:E:284:LYS:HB3	1:E:311:TYR:CE2	2.54	0.42
1:A:459:ILE:O	1:A:462:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:459:ILE:O	1:G:462:ALA:HB3	2.19	0.42
1:C:459:ILE:O	1:C:462:ALA:HB3	2.19	0.42
1:I:132:ILE:HD12	1:I:521:THR:HB	2.01	0.42
1:E:132:ILE:HD12	1:E:521:THR:HB	2.01	0.42
1:H:505:PRO:O	1:H:507:LEU:N	2.52	0.42
1:H:508:VAL:CG1	1:H:509:LYS:N	2.83	0.42
1:G:505:PRO:O	1:G:507:LEU:N	2.52	0.42
1:B:155:ILE:O	1:B:155:ILE:HG12	2.19	0.42
1:E:155:ILE:HG12	1:E:155:ILE:O	2.19	0.42
1:F:118:ALA:O	1:F:122:LEU:CD2	2.67	0.42
1:E:161:LEU:CD1	1:E:161:LEU:N	2.82	0.42
1:C:118:ALA:O	1:C:122:LEU:CD2	2.67	0.42
1:C:59:LEU:HD13	1:C:78:LYS:HB2	2.00	0.42
1:D:529:VAL:CG1	1:E:58:MET:HB3	2.29	0.42
1:C:268:ASP:HB3	1:C:269:PRO:HD2	2.02	0.42
1:A:249:ILE:HD13	1:A:340:VAL:HB	2.00	0.42
1:G:298:ILE:O	1:G:319:ALA:HA	2.19	0.42
1:F:351:LEU:HD23	1:F:351:LEU:N	2.26	0.42
1:A:433:ALA:O	1:A:434:PRO:C	2.58	0.42
1:H:106:THR:O	1:H:107:ALA:C	2.58	0.42
1:I:284:LYS:HB3	1:I:311:TYR:CE2	2.54	0.42
1:I:81:LEU:HD22	1:I:86:ALA:HB1	2.01	0.42
1:A:81:LEU:HD22	1:A:86:ALA:HB1	2.01	0.42
1:H:209:ILE:CB	1:H:399:ARG:HH22	2.28	0.42
1:E:482:ASN:O	1:E:485:TYR:N	2.40	0.42
1:C:46:LEU:O	1:C:49:THR:N	2.43	0.42
1:I:155:ILE:O	1:I:155:ILE:HG12	2.19	0.42
1:D:505:PRO:O	1:D:507:LEU:N	2.52	0.42
1:D:508:VAL:CG1	1:D:509:LYS:N	2.83	0.42
1:I:161:LEU:CD1	1:I:161:LEU:N	2.82	0.42
1:F:260:LEU:CD1	1:F:260:LEU:C	2.81	0.42
1:C:258:PRO:CG	1:C:279:GLU:OE2	2.56	0.42
1:E:264:ILE:HD12	1:E:265:ARG:HH22	1.84	0.42
1:G:433:ALA:O	1:G:434:PRO:C	2.58	0.42
1:D:141:VAL:CG2	1:D:432:TYR:CE1	2.97	0.42
1:H:433:ALA:O	1:H:434:PRO:C	2.58	0.42
1:D:106:THR:O	1:D:107:ALA:C	2.58	0.42
1:C:153:VAL:HG23	1:C:160:LEU:CD2	2.45	0.42
1:C:106:THR:O	1:C:107:ALA:C	2.58	0.42
1:G:153:VAL:HG23	1:G:160:LEU:CD2	2.45	0.42
1:B:284:LYS:HB3	1:B:311:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:ILE:HD12	1:F:521:THR:HB	2.01	0.42
1:C:46:LEU:CD1	1:C:46:LEU:N	2.82	0.42
1:G:508:VAL:CG1	1:G:509:LYS:N	2.83	0.42
1:D:118:ALA:O	1:D:122:LEU:CD2	2.67	0.42
1:D:72:GLY:O	1:D:73:ALA:C	2.57	0.42
1:I:256:GLU:O	1:I:258:PRO:CG	2.68	0.42
1:E:88:LEU:CD2	1:F:58:MET:HE2	2.47	0.42
1:F:284:LYS:HB3	1:F:311:TYR:CE2	2.54	0.42
1:F:195:LEU:HD11	1:F:200:TRP:CH2	2.55	0.42
1:G:529:VAL:HG12	1:H:58:MET:SD	2.60	0.42
1:B:161:LEU:CD1	1:B:161:LEU:N	2.82	0.42
1:A:161:LEU:CD1	1:A:161:LEU:N	2.82	0.42
1:F:72:GLY:O	1:F:73:ALA:C	2.57	0.42
1:F:528:ASP:O	1:G:57:LYS:HA	2.19	0.42
1:B:505:PRO:O	1:B:507:LEU:N	2.52	0.42
1:D:268:ASP:HB3	1:D:269:PRO:HD2	2.02	0.42
1:E:264:ILE:CG1	1:E:265:ARG:O	2.66	0.42
1:F:298:ILE:HG23	1:F:298:ILE:O	2.20	0.42
1:B:106:THR:O	1:B:107:ALA:C	2.58	0.42
1:A:106:THR:O	1:A:107:ALA:C	2.58	0.42
1:E:46:LEU:N	1:E:46:LEU:CD1	2.82	0.42
1:H:132:ILE:HD12	1:H:521:THR:HB	2.01	0.42
1:B:132:ILE:HD12	1:B:521:THR:HB	2.01	0.42
1:C:505:PRO:O	1:C:507:LEU:N	2.52	0.42
1:E:484:TRP:HE3	1:E:484:TRP:HA	1.85	0.42
1:H:140:GLU:HA	1:H:140:GLU:OE2	2.20	0.42
1:B:289:LYS:HE3	1:B:289:LYS:HB2	1.86	0.42
1:C:291:LEU:O	1:C:294:GLY:N	2.53	0.42
1:I:506:ALA:O	1:I:510:MET:HB2	2.20	0.42
1:C:264:ILE:HD12	1:C:265:ARG:HH22	1.84	0.42
1:I:249:ILE:CD1	1:I:346:ILE:HD11	2.50	0.42
1:I:459:ILE:O	1:I:462:ALA:HB3	2.19	0.42
1:E:459:ILE:O	1:E:462:ALA:HB3	2.19	0.42
1:E:128:PRO:CG	1:F:55:MET:HE1	2.48	0.42
1:B:46:LEU:O	1:B:49:THR:N	2.43	0.42
1:G:132:ILE:HD12	1:G:521:THR:HB	2.01	0.42
1:I:505:PRO:O	1:I:507:LEU:N	2.52	0.42
1:D:155:ILE:HG12	1:D:155:ILE:O	2.19	0.42
1:E:195:LEU:HD11	1:E:200:TRP:CH2	2.55	0.42
1:A:118:ALA:O	1:A:122:LEU:CD2	2.67	0.42
1:H:134:GLY:HA3	1:H:443:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:TRP:HE3	1:B:484:TRP:HA	1.85	0.42
1:I:59:LEU:HD13	1:I:78:LYS:HB2	2.00	0.42
1:C:506:ALA:O	1:C:510:MET:HB2	2.20	0.42
1:F:506:ALA:O	1:F:510:MET:HB2	2.20	0.42
1:B:264:ILE:HD12	1:B:265:ARG:HH22	1.84	0.42
1:A:268:ASP:HB3	1:A:269:PRO:HD2	2.02	0.42
1:G:268:ASP:HB3	1:G:269:PRO:HD2	2.02	0.42
1:B:298:ILE:HG23	1:B:298:ILE:O	2.19	0.42
1:B:433:ALA:O	1:B:434:PRO:C	2.58	0.42
1:D:433:ALA:O	1:D:434:PRO:C	2.58	0.42
1:F:39:VAL:HG11	1:F:115:VAL:HG21	2.00	0.42
1:D:132:ILE:HD12	1:D:521:THR:HB	2.01	0.42
1:D:195:LEU:HD11	1:D:200:TRP:CH2	2.55	0.42
1:A:321:ARG:HB3	1:A:322:ARG:H	1.56	0.42
1:A:195:LEU:HD11	1:A:200:TRP:CH2	2.55	0.42
1:D:161:LEU:CD1	1:D:161:LEU:N	2.82	0.42
1:I:118:ALA:O	1:I:122:LEU:CD2	2.67	0.42
1:G:176:GLY:O	1:G:177:ALA:C	2.59	0.42
1:D:256:GLU:O	1:D:258:PRO:CG	2.68	0.41
1:B:506:ALA:O	1:B:510:MET:HB2	2.20	0.41
1:D:415:ILE:HG23	1:D:506:ALA:CB	2.48	0.41
1:F:146:ILE:HB	1:F:510:MET:HE3	2.00	0.41
1:G:493:GLN:HA	1:G:494:PRO:HD3	1.90	0.41
1:D:298:ILE:O	1:D:298:ILE:HG23	2.20	0.41
1:A:317:VAL:HG12	1:A:318:LEU:N	2.35	0.41
1:F:433:ALA:O	1:F:434:PRO:C	2.58	0.41
1:D:284:LYS:HB3	1:D:311:TYR:CE2	2.54	0.41
1:B:209:ILE:CB	1:B:399:ARG:HH22	2.28	0.41
1:G:195:LEU:HD11	1:G:200:TRP:CH2	2.55	0.41
1:H:195:LEU:HD11	1:H:200:TRP:CH2	2.55	0.41
1:F:505:PRO:O	1:F:507:LEU:N	2.53	0.41
1:A:484:TRP:HA	1:A:484:TRP:HE3	1.85	0.41
1:H:72:GLY:O	1:H:73:ALA:C	2.57	0.41
1:H:176:GLY:O	1:H:177:ALA:C	2.59	0.41
1:B:140:GLU:HA	1:B:140:GLU:OE2	2.20	0.41
1:E:525:ARG:NH1	1:E:525:ARG:HG2	2.31	0.41
1:B:268:ASP:HB3	1:B:269:PRO:HD2	2.02	0.41
1:G:264:ILE:HD12	1:G:265:ARG:HH22	1.84	0.41
1:E:249:ILE:CD1	1:E:346:ILE:HD11	2.50	0.41
1:E:317:VAL:HG12	1:E:318:LEU:N	2.35	0.41
1:I:433:ALA:O	1:I:434:PRO:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:GLU:HA	1:D:367:MET:O	2.20	0.41
1:G:284:LYS:HB3	1:G:311:TYR:CE2	2.54	0.41
1:F:459:ILE:O	1:F:462:ALA:HB3	2.19	0.41
1:H:484:TRP:HE3	1:H:484:TRP:HA	1.85	0.41
1:A:176:GLY:O	1:A:177:ALA:C	2.59	0.41
1:B:176:GLY:O	1:B:177:ALA:C	2.59	0.41
1:I:176:GLY:O	1:I:177:ALA:C	2.59	0.41
1:E:525:ARG:HG3	1:F:56:ASP:CB	2.46	0.41
1:E:506:ALA:O	1:E:510:MET:HB2	2.20	0.41
1:E:268:ASP:HB3	1:E:269:PRO:HD2	2.02	0.41
1:G:298:ILE:O	1:G:298:ILE:HG23	2.20	0.41
1:E:298:ILE:HG23	1:E:298:ILE:O	2.20	0.41
1:I:106:THR:O	1:I:107:ALA:C	2.58	0.41
1:E:140:GLU:OE2	1:E:140:GLU:HA	2.20	0.41
1:G:260:LEU:C	1:G:260:LEU:CD1	2.81	0.41
1:D:264:ILE:HD12	1:D:265:ARG:HH22	1.84	0.41
1:H:268:ASP:HB3	1:H:269:PRO:HD2	2.01	0.41
1:A:249:ILE:CD1	1:A:346:ILE:HD11	2.50	0.41
1:G:359:GLU:HA	1:G:367:MET:O	2.20	0.41
1:F:359:GLU:HA	1:F:367:MET:O	2.20	0.41
1:F:249:ILE:CD1	1:F:346:ILE:HD11	2.50	0.41
1:I:359:GLU:HA	1:I:367:MET:O	2.20	0.41
1:A:359:GLU:HA	1:A:367:MET:O	2.20	0.41
1:E:89:LEU:CD2	1:E:108:VAL:HG23	2.44	0.41
1:G:106:THR:O	1:G:107:ALA:C	2.58	0.41
1:F:81:LEU:HD22	1:F:86:ALA:HB1	2.01	0.41
1:C:132:ILE:HD12	1:C:521:THR:HB	2.01	0.41
1:H:46:LEU:N	1:H:46:LEU:CD1	2.82	0.41
1:I:508:VAL:CG1	1:I:509:LYS:N	2.83	0.41
1:D:176:GLY:O	1:D:177:ALA:C	2.59	0.41
1:E:48:SER:O	1:E:55:MET:HB2	2.20	0.41
1:A:48:SER:O	1:A:55:MET:HB2	2.21	0.41
1:C:140:GLU:OE2	1:C:140:GLU:HA	2.20	0.41
1:I:454:LEU:HD12	1:I:454:LEU:HA	1.91	0.41
1:G:415:ILE:HG23	1:G:506:ALA:CB	2.48	0.41
1:A:58:MET:CE	1:I:88:LEU:HD22	2.50	0.41
1:C:249:ILE:CD1	1:C:346:ILE:HD11	2.50	0.41
1:C:359:GLU:HA	1:C:367:MET:O	2.20	0.41
1:G:48:SER:O	1:G:55:MET:HB2	2.21	0.41
1:F:106:THR:O	1:F:107:ALA:C	2.58	0.41
1:I:46:LEU:N	1:I:46:LEU:CD1	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LEU:N	1:A:46:LEU:CD1	2.82	0.41
1:I:195:LEU:HD11	1:I:200:TRP:CH2	2.55	0.41
1:A:194:GLU:O	1:A:200:TRP:HA	2.21	0.41
1:F:134:GLY:HA3	1:F:443:ALA:CB	2.49	0.41
1:D:530:VAL:O	1:E:59:LEU:HA	2.19	0.41
1:C:256:GLU:O	1:C:258:PRO:CG	2.68	0.41
1:B:504:GLU:HA	1:B:505:PRO:HD3	1.90	0.41
1:H:506:ALA:O	1:H:510:MET:HB2	2.20	0.41
1:E:415:ILE:HG23	1:E:506:ALA:CB	2.48	0.41
1:A:264:ILE:CG1	1:A:265:ARG:O	2.66	0.41
1:G:194:GLU:O	1:G:200:TRP:HA	2.21	0.41
1:E:194:GLU:O	1:E:200:TRP:HA	2.21	0.41
1:E:230:LYS:NZ	1:E:321:ARG:HH12	2.18	0.41
1:H:522:LEU:HD11	1:I:68:ILE:HD12	2.03	0.41
1:B:291:LEU:O	1:B:294:GLY:N	2.53	0.41
1:D:454:LEU:HD12	1:D:454:LEU:HA	1.91	0.41
1:B:493:GLN:HA	1:B:494:PRO:HD3	1.90	0.41
1:C:317:VAL:HG12	1:C:318:LEU:N	2.35	0.41
1:C:81:LEU:HD13	1:C:87:LYS:HG2	2.03	0.41
1:I:46:LEU:O	1:I:49:THR:N	2.43	0.41
1:A:508:VAL:CG1	1:A:509:LYS:N	2.83	0.41
1:C:321:ARG:HB3	1:C:322:ARG:H	1.56	0.41
1:D:48:SER:O	1:D:55:MET:HB2	2.21	0.41
1:F:291:LEU:O	1:F:294:GLY:N	2.53	0.41
1:H:259:GLU:O	1:H:262:ALA:O	2.39	0.41
1:A:506:ALA:O	1:A:510:MET:HB2	2.20	0.41
1:B:249:ILE:O	1:B:300:CYS:HB2	2.21	0.41
1:A:88:LEU:HD22	1:B:58:MET:CE	2.51	0.41
1:B:317:VAL:HG12	1:B:318:LEU:N	2.35	0.41
1:I:317:VAL:HG12	1:I:318:LEU:N	2.35	0.41
1:D:317:VAL:HG12	1:D:318:LEU:N	2.35	0.41
1:B:81:LEU:HD12	1:B:81:LEU:N	2.28	0.41
1:H:81:LEU:HD22	1:H:86:ALA:HB1	2.01	0.41
1:I:81:LEU:HD13	1:I:87:LYS:HG2	2.03	0.41
1:A:291:LEU:O	1:A:294:GLY:N	2.53	0.41
1:E:454:LEU:HD12	1:E:454:LEU:HA	1.91	0.41
1:A:253:LEU:HG	1:A:253:LEU:O	2.21	0.41
1:I:140:GLU:OE2	1:I:140:GLU:HA	2.20	0.41
1:C:253:LEU:O	1:C:253:LEU:HG	2.21	0.41
1:I:48:SER:O	1:I:55:MET:HB2	2.21	0.41
1:D:506:ALA:O	1:D:510:MET:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:506:ALA:O	1:G:510:MET:HB2	2.20	0.41
1:A:389:ARG:HH12	1:I:88:LEU:CD1	2.31	0.41
1:F:268:ASP:HB3	1:F:269:PRO:HD2	2.02	0.41
1:G:249:ILE:CD1	1:G:346:ILE:HD11	2.50	0.41
1:H:249:ILE:CD1	1:H:346:ILE:HD11	2.50	0.41
1:F:317:VAL:HG12	1:F:318:LEU:N	2.35	0.41
1:H:359:GLU:HA	1:H:367:MET:O	2.20	0.41
1:E:359:GLU:HA	1:E:367:MET:O	2.20	0.41
1:D:436:VAL:CG2	1:D:441:GLN:HA	2.51	0.41
1:C:433:ALA:O	1:C:434:PRO:C	2.58	0.41
1:E:433:ALA:O	1:E:434:PRO:C	2.58	0.41
1:D:81:LEU:HD13	1:D:87:LYS:HG2	2.03	0.41
1:A:525:ARG:NH1	1:A:525:ARG:HG2	2.31	0.41
1:B:46:LEU:N	1:B:46:LEU:CD1	2.82	0.41
1:A:46:LEU:O	1:A:49:THR:N	2.43	0.41
1:B:48:SER:O	1:B:55:MET:HB2	2.21	0.41
1:B:195:LEU:HD11	1:B:200:TRP:CH2	2.55	0.41
1:C:195:LEU:HD11	1:C:200:TRP:CH2	2.55	0.41
1:I:484:TRP:HA	1:I:484:TRP:HE3	1.85	0.41
1:G:140:GLU:OE2	1:G:140:GLU:HA	2.20	0.41
1:F:253:LEU:HG	1:F:253:LEU:O	2.21	0.41
1:D:253:LEU:HG	1:D:253:LEU:O	2.21	0.41
1:G:94:LYS:O	1:G:96:GLN:N	2.48	0.41
1:E:176:GLY:O	1:E:177:ALA:C	2.59	0.41
1:F:176:GLY:O	1:F:177:ALA:C	2.59	0.41
1:C:176:GLY:O	1:C:177:ALA:C	2.59	0.41
1:H:291:LEU:O	1:H:294:GLY:N	2.53	0.41
1:C:259:GLU:O	1:C:262:ALA:O	2.39	0.41
1:I:245:LYS:H	1:I:296:ASN:ND2	2.07	0.41
1:G:249:ILE:O	1:G:300:CYS:HB2	2.21	0.41
1:F:246:ILE:HA	1:F:297:VAL:CG1	2.51	0.41
1:I:436:VAL:CG2	1:I:441:GLN:HA	2.51	0.41
1:A:246:ILE:HA	1:A:297:VAL:CG1	2.51	0.41
1:E:436:VAL:CG2	1:E:441:GLN:HA	2.51	0.41
1:F:194:GLU:O	1:F:200:TRP:HA	2.21	0.41
1:B:194:GLU:O	1:B:200:TRP:HA	2.21	0.41
1:C:155:ILE:O	1:C:155:ILE:HG12	2.19	0.41
1:H:194:GLU:O	1:H:200:TRP:HA	2.21	0.41
1:I:321:ARG:HB3	1:I:322:ARG:H	1.56	0.41
1:A:166:MET:CE	1:A:179:GLU:HG2	2.51	0.41
1:D:484:TRP:HA	1:D:484:TRP:HE3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:GLU:OE2	1:A:140:GLU:HA	2.20	0.41
1:I:253:LEU:HG	1:I:253:LEU:O	2.21	0.41
1:C:66:ILE:N	1:C:66:ILE:CD1	2.76	0.40
1:D:531:SER:HB3	1:E:60:VAL:HB	2.04	0.40
1:D:249:ILE:CD1	1:D:346:ILE:HD11	2.50	0.40
1:H:351:LEU:HD23	1:H:351:LEU:N	2.26	0.40
1:G:436:VAL:CG2	1:G:441:GLN:HA	2.52	0.40
1:H:436:VAL:CG2	1:H:441:GLN:HA	2.51	0.40
1:A:147:GLN:C	1:A:149:LEU:H	2.25	0.40
1:I:194:GLU:O	1:I:200:TRP:HA	2.21	0.40
1:G:253:LEU:HG	1:G:253:LEU:O	2.21	0.40
1:H:253:LEU:HG	1:H:253:LEU:O	2.21	0.40
1:B:253:LEU:HG	1:B:253:LEU:O	2.21	0.40
1:E:259:GLU:O	1:E:262:ALA:O	2.39	0.40
1:H:256:GLU:O	1:H:258:PRO:CG	2.68	0.40
1:F:423:ILE:HG12	1:F:473:LEU:HD11	2.03	0.40
1:I:473:LEU:C	1:I:475:SER:N	2.75	0.40
1:I:264:ILE:CG1	1:I:265:ARG:O	2.67	0.40
1:G:317:VAL:HG12	1:G:318:LEU:N	2.35	0.40
1:H:246:ILE:HA	1:H:297:VAL:CG1	2.51	0.40
1:B:81:LEU:HD13	1:B:87:LYS:HG2	2.03	0.40
1:B:153:VAL:HG23	1:B:160:LEU:CD2	2.45	0.40
1:F:48:SER:O	1:F:55:MET:HB2	2.21	0.40
1:B:147:GLN:C	1:B:149:LEU:H	2.25	0.40
1:D:194:GLU:O	1:D:200:TRP:HA	2.21	0.40
1:C:230:LYS:NZ	1:C:321:ARG:HH12	2.18	0.40
1:C:508:VAL:CG1	1:C:509:LYS:N	2.83	0.40
1:F:166:MET:CE	1:F:179:GLU:HG2	2.51	0.40
1:E:166:MET:CE	1:E:179:GLU:HG2	2.51	0.40
1:C:410:LYS:HE2	1:C:410:LYS:HB3	1.89	0.40
1:F:140:GLU:HA	1:F:140:GLU:OE2	2.20	0.40
1:A:259:GLU:O	1:A:262:ALA:O	2.39	0.40
1:F:259:GLU:O	1:F:262:ALA:O	2.39	0.40
1:E:258:PRO:CG	1:E:279:GLU:OE2	2.56	0.40
1:B:508:VAL:CG1	1:B:509:LYS:N	2.83	0.40
1:G:264:ILE:CG1	1:G:265:ARG:O	2.66	0.40
1:C:249:ILE:O	1:C:300:CYS:HB2	2.21	0.40
1:G:246:ILE:HA	1:G:297:VAL:CG1	2.52	0.40
1:A:84:PRO:HB2	1:B:58:MET:SD	2.61	0.40
1:B:246:ILE:HA	1:B:297:VAL:CG1	2.51	0.40
1:D:246:ILE:HA	1:D:297:VAL:CG1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:GLN:C	1:D:149:LEU:H	2.25	0.40
1:D:166:MET:CE	1:D:179:GLU:HG2	2.51	0.40
1:E:166:MET:HE2	1:E:178:ARG:HG2	2.03	0.40
1:A:410:LYS:HE2	1:A:410:LYS:HB3	1.89	0.40
1:G:484:TRP:HA	1:G:484:TRP:HE3	1.85	0.40
1:H:48:SER:O	1:H:55:MET:HB2	2.21	0.40
1:A:258:PRO:CG	1:A:279:GLU:OE2	2.56	0.40
1:D:423:ILE:HG12	1:D:473:LEU:HD11	2.03	0.40
1:E:246:ILE:HA	1:E:297:VAL:CG1	2.51	0.40
1:F:436:VAL:CG2	1:F:441:GLN:HA	2.51	0.40
1:E:106:THR:O	1:E:107:ALA:C	2.58	0.40
1:G:209:ILE:CB	1:G:399:ARG:HH22	2.28	0.40
1:I:153:VAL:HG23	1:I:160:LEU:CD2	2.45	0.40
1:F:94:LYS:O	1:F:96:GLN:N	2.48	0.40
1:D:140:GLU:OE2	1:D:140:GLU:HA	2.20	0.40
1:H:454:LEU:HD12	1:H:454:LEU:HA	1.91	0.40
1:D:259:GLU:O	1:D:262:ALA:O	2.39	0.40
1:G:259:GLU:O	1:G:262:ALA:O	2.39	0.40
1:G:473:LEU:C	1:G:475:SER:N	2.75	0.40
1:G:423:ILE:HG12	1:G:473:LEU:HD11	2.03	0.40
1:B:473:LEU:C	1:B:475:SER:N	2.75	0.40
1:D:249:ILE:O	1:D:300:CYS:HB2	2.21	0.40
1:G:238:PRO:O	1:G:318:LEU:HD13	2.22	0.40
1:H:317:VAL:HG12	1:H:318:LEU:N	2.35	0.40
1:B:359:GLU:HA	1:B:367:MET:O	2.20	0.40
1:C:89:LEU:CD2	1:C:108:VAL:HG23	2.44	0.40
1:D:347:SER:C	1:D:349:GLN:N	2.75	0.40

All (28) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:MET:CE	1:B:275:PHE:CD1[2_656]	1.14	1.06
1:E:273:GLN:NE2	1:H:276:LEU:CD1[2_656]	1.28	0.92
1:C:435:GLN:NE2	1:H:478:GLU:O[1_556]	1.36	0.84
1:B:264:ILE:O	1:B:266:ILE:O[2_656]	1.37	0.83
1:D:183:ASP:OD2	1:H:159:ASP:OD1[1_556]	1.39	0.81
1:B:156:ASN:ND2	1:E:193:ALA:CB[4_546]	1.41	0.79
1:D:183:ASP:OD2	1:H:159:ASP:CG[1_556]	1.49	0.71
1:E:266:ILE:O	1:H:264:ILE:O[2_656]	1.56	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:289:LYS:NZ	1:G:281:ASN:OD1[2_656]	1.67	0.53
1:B:193:ALA:CB	1:E:156:ASN:ND2[4_546]	1.71	0.49
1:B:198:ASP:O	1:E:198:ASP:CB[4_546]	1.73	0.47
1:F:156:ASN:ND2	1:I:156:ASN:ND2[4_555]	1.79	0.41
1:E:276:LEU:CD1	1:H:272:MET:CB[2_656]	1.84	0.36
1:C:435:GLN:NE2	1:H:478:GLU:C[1_556]	1.87	0.33
1:B:198:ASP:CB	1:E:198:ASP:O[4_546]	2.00	0.20
1:B:198:ASP:OD1	1:E:198:ASP:OD1[4_546]	2.02	0.18
1:A:281:ASN:OD1	1:B:289:LYS:NZ[2_656]	2.05	0.15
1:E:285:GLU:OE2	1:G:281:ASN:O[2_656]	2.05	0.15
1:B:156:ASN:ND2	1:E:193:ALA:CA[4_546]	2.06	0.14
1:D:266:ILE:O	1:I:264:ILE:O[2_656]	2.07	0.13
1:B:200:TRP:CZ2	1:E:200:TRP:CZ2[4_546]	2.08	0.12
1:D:183:ASP:OD2	1:H:159:ASP:CB[1_556]	2.10	0.10
1:D:289:LYS:NZ	1:H:281:ASN:OD1[2_656]	2.11	0.09
1:D:273:GLN:NE2	1:I:276:LEU:CD1[2_656]	2.12	0.08
1:A:266:ILE:O	1:C:264:ILE:O[2_656]	2.12	0.08
1:B:272:MET:CE	1:B:275:PHE:CE1[2_656]	2.14	0.06
1:C:137:LYS:CD	1:H:481:ASN:OD1[1_556]	2.18	0.02
1:C:137:LYS:CG	1:H:481:ASN:OD1[1_556]	2.19	0.01

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	503/553 (91%)	396 (79%)	89 (18%)	18 (4%)	4	41
1	B	503/553 (91%)	397 (79%)	88 (18%)	18 (4%)	4	41
1	C	503/553 (91%)	397 (79%)	88 (18%)	18 (4%)	4	41
1	D	503/553 (91%)	396 (79%)	89 (18%)	18 (4%)	4	41
1	E	503/553 (91%)	397 (79%)	88 (18%)	18 (4%)	4	41
1	F	503/553 (91%)	397 (79%)	88 (18%)	18 (4%)	4	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	503/553 (91%)	396 (79%)	89 (18%)	18 (4%)	4	41
1	H	503/553 (91%)	396 (79%)	89 (18%)	18 (4%)	4	41
1	I	503/553 (91%)	396 (79%)	89 (18%)	18 (4%)	4	41
All	All	4527/4977 (91%)	3568 (79%)	797 (18%)	162 (4%)	4	41

All (162) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	99	GLU
1	A	213	ALA
1	A	321	ARG
1	B	96	GLN
1	B	99	GLU
1	B	213	ALA
1	B	321	ARG
1	C	96	GLN
1	C	99	GLU
1	C	213	ALA
1	C	321	ARG
1	D	96	GLN
1	D	99	GLU
1	D	213	ALA
1	D	321	ARG
1	E	96	GLN
1	E	99	GLU
1	E	213	ALA
1	E	321	ARG
1	F	96	GLN
1	F	99	GLU
1	F	213	ALA
1	F	321	ARG
1	G	96	GLN
1	G	99	GLU
1	G	213	ALA
1	G	321	ARG
1	H	96	GLN
1	H	99	GLU
1	H	213	ALA
1	H	321	ARG
1	I	96	GLN

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Mol	Chain	Res	Type
1	I	99	GLU
1	I	213	ALA
1	I	321	ARG
1	A	30	GLU
1	A	100	THR
1	A	177	ALA
1	A	198	ASP
1	B	30	GLU
1	B	100	THR
1	B	177	ALA
1	B	198	ASP
1	C	30	GLU
1	C	100	THR
1	C	177	ALA
1	C	198	ASP
1	D	30	GLU
1	D	100	THR
1	D	177	ALA
1	D	198	ASP
1	E	30	GLU
1	E	100	THR
1	E	177	ALA
1	E	198	ASP
1	F	30	GLU
1	F	100	THR
1	F	177	ALA
1	F	198	ASP
1	G	30	GLU
1	G	100	THR
1	G	177	ALA
1	G	198	ASP
1	H	30	GLU
1	H	100	THR
1	H	177	ALA
1	H	198	ASP
1	I	30	GLU
1	I	100	THR
1	I	177	ALA
1	I	198	ASP
1	A	377	LYS
1	A	438	GLY
1	B	377	LYS

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Mol	Chain	Res	Type
1	B	438	GLY
1	C	377	LYS
1	C	438	GLY
1	D	377	LYS
1	D	438	GLY
1	E	377	LYS
1	E	438	GLY
1	F	377	LYS
1	F	438	GLY
1	G	377	LYS
1	G	438	GLY
1	H	377	LYS
1	H	438	GLY
1	I	377	LYS
1	I	438	GLY
1	A	149	LEU
1	A	174	VAL
1	A	196	ARG
1	B	149	LEU
1	B	174	VAL
1	C	149	LEU
1	C	174	VAL
1	C	196	ARG
1	D	149	LEU
1	D	174	VAL
1	E	149	LEU
1	E	174	VAL
1	E	196	ARG
1	F	149	LEU
1	F	174	VAL
1	F	196	ARG
1	G	149	LEU
1	G	174	VAL
1	G	196	ARG
1	H	149	LEU
1	H	174	VAL
1	H	196	ARG
1	I	149	LEU
1	I	174	VAL
1	I	196	ARG
1	A	348	GLU
1	A	376	PRO

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Mol	Chain	Res	Type
1	A	480	GLU
1	B	196	ARG
1	B	348	GLU
1	B	376	PRO
1	B	480	GLU
1	C	348	GLU
1	C	376	PRO
1	C	480	GLU
1	D	196	ARG
1	D	348	GLU
1	D	376	PRO
1	D	480	GLU
1	E	348	GLU
1	E	376	PRO
1	E	480	GLU
1	F	348	GLU
1	F	376	PRO
1	F	480	GLU
1	G	348	GLU
1	G	376	PRO
1	G	480	GLU
1	H	348	GLU
1	H	376	PRO
1	H	480	GLU
1	I	348	GLU
1	I	376	PRO
1	I	480	GLU
1	A	215	GLY
1	B	215	GLY
1	C	215	GLY
1	D	215	GLY
1	E	215	GLY
1	F	215	GLY
1	G	215	GLY
1	H	215	GLY
1	I	215	GLY
1	B	340	VAL
1	I	340	VAL
1	A	340	VAL
1	C	340	VAL
1	D	340	VAL
1	E	340	VAL

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Mol	Chain	Res	Type
1	F	340	VAL
1	G	340	VAL
1	H	340	VAL

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	410/447 (92%)	386 (94%)	24 (6%)	24	66
1	B	410/447 (92%)	386 (94%)	24 (6%)	24	66
1	C	410/447 (92%)	386 (94%)	24 (6%)	24	66
1	D	410/447 (92%)	386 (94%)	24 (6%)	24	66
1	E	410/447 (92%)	386 (94%)	24 (6%)	24	66
1	F	410/447 (92%)	386 (94%)	24 (6%)	24	66
1	G	410/447 (92%)	386 (94%)	24 (6%)	24	66
1	H	410/447 (92%)	386 (94%)	24 (6%)	24	66
1	I	410/447 (92%)	386 (94%)	24 (6%)	24	66
All	All	3690/4023 (92%)	3474 (94%)	216 (6%)	24	66

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	66	ILE
1	A	80	ASP
1	A	81	LEU
1	A	82	GLN
1	A	98	GLU
1	A	129	THR
1	A	162	ARG
1	A	178	ARG
1	A	179	GLU
1	A	212	LYS

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Mol	Chain	Res	Type
1	A	255	VAL
1	A	256	GLU
1	A	263	GLU
1	A	264	ILE
1	A	265	ARG
1	A	299	ILE
1	A	321	ARG
1	A	324	LYS
1	A	361	LYS
1	A	374	LYS
1	A	393	GLU
1	A	404	THR
1	A	415	ILE
1	B	33	ARG
1	B	66	ILE
1	B	80	ASP
1	B	81	LEU
1	B	82	GLN
1	B	98	GLU
1	B	129	THR
1	B	162	ARG
1	B	178	ARG
1	B	179	GLU
1	B	212	LYS
1	B	255	VAL
1	B	256	GLU
1	B	263	GLU
1	B	264	ILE
1	B	265	ARG
1	B	299	ILE
1	B	321	ARG
1	B	324	LYS
1	B	361	LYS
1	B	374	LYS
1	B	393	GLU
1	B	404	THR
1	B	415	ILE
1	C	33	ARG
1	C	66	ILE
1	C	80	ASP
1	C	81	LEU
1	C	82	GLN

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Mol	Chain	Res	Type
1	C	98	GLU
1	C	129	THR
1	C	162	ARG
1	C	178	ARG
1	C	179	GLU
1	C	212	LYS
1	C	255	VAL
1	C	256	GLU
1	C	263	GLU
1	C	264	ILE
1	C	265	ARG
1	C	299	ILE
1	C	321	ARG
1	C	324	LYS
1	C	361	LYS
1	C	374	LYS
1	C	393	GLU
1	C	404	THR
1	C	415	ILE
1	D	33	ARG
1	D	66	ILE
1	D	80	ASP
1	D	81	LEU
1	D	82	GLN
1	D	98	GLU
1	D	129	THR
1	D	162	ARG
1	D	178	ARG
1	D	179	GLU
1	D	212	LYS
1	D	255	VAL
1	D	256	GLU
1	D	263	GLU
1	D	264	ILE
1	D	265	ARG
1	D	299	ILE
1	D	321	ARG
1	D	324	LYS
1	D	361	LYS
1	D	374	LYS
1	D	393	GLU
1	D	404	THR

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Mol	Chain	Res	Type
1	D	415	ILE
1	E	33	ARG
1	E	66	ILE
1	E	80	ASP
1	E	81	LEU
1	E	82	GLN
1	E	98	GLU
1	E	129	THR
1	E	162	ARG
1	E	178	ARG
1	E	179	GLU
1	E	212	LYS
1	E	255	VAL
1	E	256	GLU
1	E	263	GLU
1	E	264	ILE
1	E	265	ARG
1	E	299	ILE
1	E	321	ARG
1	E	324	LYS
1	E	361	LYS
1	E	374	LYS
1	E	393	GLU
1	E	404	THR
1	E	415	ILE
1	F	33	ARG
1	F	66	ILE
1	F	80	ASP
1	F	81	LEU
1	F	82	GLN
1	F	98	GLU
1	F	129	THR
1	F	162	ARG
1	F	178	ARG
1	F	179	GLU
1	F	212	LYS
1	F	255	VAL
1	F	256	GLU
1	F	263	GLU
1	F	264	ILE
1	F	265	ARG
1	F	299	ILE

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Mol	Chain	Res	Type
1	F	321	ARG
1	F	324	LYS
1	F	361	LYS
1	F	374	LYS
1	F	393	GLU
1	F	404	THR
1	F	415	ILE
1	G	33	ARG
1	G	66	ILE
1	G	80	ASP
1	G	81	LEU
1	G	82	GLN
1	G	98	GLU
1	G	129	THR
1	G	162	ARG
1	G	178	ARG
1	G	179	GLU
1	G	212	LYS
1	G	255	VAL
1	G	256	GLU
1	G	263	GLU
1	G	264	ILE
1	G	265	ARG
1	G	299	ILE
1	G	321	ARG
1	G	324	LYS
1	G	361	LYS
1	G	374	LYS
1	G	393	GLU
1	G	404	THR
1	G	415	ILE
1	H	33	ARG
1	H	66	ILE
1	H	80	ASP
1	H	81	LEU
1	H	82	GLN
1	H	98	GLU
1	H	129	THR
1	H	162	ARG
1	H	178	ARG
1	H	179	GLU
1	H	212	LYS

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Mol	Chain	Res	Type
1	H	255	VAL
1	H	256	GLU
1	H	263	GLU
1	H	264	ILE
1	H	265	ARG
1	H	299	ILE
1	H	321	ARG
1	H	324	LYS
1	H	361	LYS
1	H	374	LYS
1	H	393	GLU
1	H	404	THR
1	H	415	ILE
1	I	33	ARG
1	I	66	ILE
1	I	80	ASP
1	I	81	LEU
1	I	82	GLN
1	I	98	GLU
1	I	129	THR
1	I	162	ARG
1	I	178	ARG
1	I	179	GLU
1	I	212	LYS
1	I	255	VAL
1	I	256	GLU
1	I	263	GLU
1	I	264	ILE
1	I	265	ARG
1	I	299	ILE
1	I	321	ARG
1	I	324	LYS
1	I	361	LYS
1	I	374	LYS
1	I	393	GLU
1	I	404	THR
1	I	415	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (141) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN

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Mol	Chain	Res	Type
1	A	83	HIS
1	A	91	GLN
1	A	96	GLN
1	A	127	HIS
1	A	147	GLN
1	A	151	GLN
1	A	208	GLN
1	A	234	HIS
1	A	281	ASN
1	A	296	ASN
1	A	441	GLN
1	A	461	ASN
1	A	477	HIS
1	A	481	ASN
1	A	511	ASN
1	B	82	GLN
1	B	83	HIS
1	B	96	GLN
1	B	127	HIS
1	B	147	GLN
1	B	151	GLN
1	B	208	GLN
1	B	234	HIS
1	B	281	ASN
1	B	296	ASN
1	B	441	GLN
1	B	461	ASN
1	B	477	HIS
1	B	481	ASN
1	B	511	ASN
1	C	82	GLN
1	C	83	HIS
1	C	91	GLN
1	C	96	GLN
1	C	127	HIS
1	C	147	GLN
1	C	151	GLN
1	C	208	GLN
1	C	234	HIS
1	C	281	ASN
1	C	296	ASN
1	C	441	GLN

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Mol	Chain	Res	Type
1	C	461	ASN
1	C	477	HIS
1	C	481	ASN
1	C	511	ASN
1	D	82	GLN
1	D	83	HIS
1	D	91	GLN
1	D	96	GLN
1	D	127	HIS
1	D	147	GLN
1	D	151	GLN
1	D	208	GLN
1	D	234	HIS
1	D	281	ASN
1	D	296	ASN
1	D	441	GLN
1	D	461	ASN
1	D	477	HIS
1	D	481	ASN
1	D	511	ASN
1	E	82	GLN
1	E	83	HIS
1	E	96	GLN
1	E	127	HIS
1	E	147	GLN
1	E	151	GLN
1	E	208	GLN
1	E	234	HIS
1	E	281	ASN
1	E	296	ASN
1	E	441	GLN
1	E	461	ASN
1	E	477	HIS
1	E	481	ASN
1	E	511	ASN
1	F	82	GLN
1	F	83	HIS
1	F	91	GLN
1	F	96	GLN
1	F	127	HIS
1	F	147	GLN
1	F	151	GLN

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Mol	Chain	Res	Type
1	F	208	GLN
1	F	234	HIS
1	F	281	ASN
1	F	296	ASN
1	F	441	GLN
1	F	461	ASN
1	F	477	HIS
1	F	481	ASN
1	F	511	ASN
1	G	82	GLN
1	G	83	HIS
1	G	91	GLN
1	G	96	GLN
1	G	127	HIS
1	G	147	GLN
1	G	151	GLN
1	G	208	GLN
1	G	234	HIS
1	G	281	ASN
1	G	296	ASN
1	G	441	GLN
1	G	461	ASN
1	G	477	HIS
1	G	481	ASN
1	G	511	ASN
1	H	82	GLN
1	H	83	HIS
1	H	96	GLN
1	H	127	HIS
1	H	147	GLN
1	H	151	GLN
1	H	208	GLN
1	H	234	HIS
1	H	281	ASN
1	H	296	ASN
1	H	441	GLN
1	H	461	ASN
1	H	477	HIS
1	H	481	ASN
1	H	511	ASN
1	I	82	GLN
1	I	83	HIS

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Mol	Chain	Res	Type
1	I	91	GLN
1	I	96	GLN
1	I	127	HIS
1	I	147	GLN
1	I	151	GLN
1	I	208	GLN
1	I	234	HIS
1	I	281	ASN
1	I	296	ASN
1	I	441	GLN
1	I	461	ASN
1	I	477	HIS
1	I	481	ASN
1	I	511	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	800	-	22,29,29	1.01	1 (4%)	27,45,45	2.57	6 (22%)
2	ADP	B	800	-	22,29,29	1.01	1 (4%)	27,45,45	2.56	6 (22%)
2	ADP	C	800	-	22,29,29	1.01	1 (4%)	27,45,45	2.57	6 (22%)
2	ADP	D	800	-	22,29,29	1.02	1 (4%)	27,45,45	2.58	6 (22%)
2	ADP	E	800	-	22,29,29	1.01	1 (4%)	27,45,45	2.57	6 (22%)
2	ADP	F	800	-	22,29,29	1.01	1 (4%)	27,45,45	2.57	6 (22%)
2	ADP	G	800	-	22,29,29	1.01	1 (4%)	27,45,45	2.57	6 (22%)
2	ADP	H	800	-	22,29,29	1.02	1 (4%)	27,45,45	2.57	6 (22%)
2	ADP	I	800	-	22,29,29	1.01	1 (4%)	27,45,45	2.57	6 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	800	-	-	0/12/32/32	0/3/3/3
2	ADP	B	800	-	-	0/12/32/32	0/3/3/3
2	ADP	C	800	-	-	0/12/32/32	0/3/3/3
2	ADP	D	800	-	-	0/12/32/32	0/3/3/3
2	ADP	E	800	-	-	0/12/32/32	0/3/3/3
2	ADP	F	800	-	-	0/12/32/32	0/3/3/3
2	ADP	G	800	-	-	0/12/32/32	0/3/3/3
2	ADP	H	800	-	-	0/12/32/32	0/3/3/3
2	ADP	I	800	-	-	0/12/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	800	ADP	C5-C4	3.08	1.47	1.40
2	B	800	ADP	C5-C4	3.08	1.47	1.40
2	F	800	ADP	C5-C4	3.08	1.47	1.40
2	G	800	ADP	C5-C4	3.09	1.47	1.40
2	A	800	ADP	C5-C4	3.09	1.47	1.40
2	H	800	ADP	C5-C4	3.10	1.47	1.40
2	C	800	ADP	C5-C4	3.10	1.47	1.40
2	D	800	ADP	C5-C4	3.11	1.47	1.40
2	I	800	ADP	C5-C4	3.12	1.47	1.40

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	800	ADP	N3-C2-N1	-7.04	123.50	128.89
2	F	800	ADP	N3-C2-N1	-6.97	123.56	128.89
2	I	800	ADP	N3-C2-N1	-6.97	123.56	128.89
2	A	800	ADP	N3-C2-N1	-6.96	123.57	128.89
2	E	800	ADP	N3-C2-N1	-6.95	123.57	128.89
2	G	800	ADP	N3-C2-N1	-6.93	123.58	128.89
2	H	800	ADP	N3-C2-N1	-6.92	123.60	128.89
2	C	800	ADP	N3-C2-N1	-6.90	123.61	128.89
2	B	800	ADP	N3-C2-N1	-6.90	123.61	128.89
2	I	800	ADP	C2'-C1'-N9	-6.73	104.00	114.29
2	B	800	ADP	C2'-C1'-N9	-6.73	104.01	114.29
2	F	800	ADP	C2'-C1'-N9	-6.73	104.02	114.29
2	C	800	ADP	C2'-C1'-N9	-6.72	104.03	114.29
2	G	800	ADP	C2'-C1'-N9	-6.71	104.04	114.29
2	E	800	ADP	C2'-C1'-N9	-6.71	104.04	114.29
2	H	800	ADP	C2'-C1'-N9	-6.71	104.04	114.29
2	A	800	ADP	C2'-C1'-N9	-6.71	104.04	114.29
2	D	800	ADP	C2'-C1'-N9	-6.69	104.07	114.29
2	C	800	ADP	O3'-C3'-C4'	-4.38	97.92	111.05
2	H	800	ADP	O3'-C3'-C4'	-4.37	97.94	111.05
2	E	800	ADP	O3'-C3'-C4'	-4.37	97.94	111.05
2	G	800	ADP	O3'-C3'-C4'	-4.37	97.94	111.05
2	A	800	ADP	O3'-C3'-C4'	-4.37	97.95	111.05
2	I	800	ADP	O3'-C3'-C4'	-4.36	97.97	111.05
2	B	800	ADP	O3'-C3'-C4'	-4.36	97.98	111.05
2	F	800	ADP	O3'-C3'-C4'	-4.36	97.98	111.05
2	D	800	ADP	O3'-C3'-C4'	-4.35	98.00	111.05
2	C	800	ADP	C4-C5-N7	-3.35	106.40	109.48
2	I	800	ADP	C4-C5-N7	-3.34	106.41	109.48
2	H	800	ADP	C4-C5-N7	-3.34	106.41	109.48
2	D	800	ADP	C4-C5-N7	-3.32	106.43	109.48
2	A	800	ADP	C4-C5-N7	-3.31	106.44	109.48
2	G	800	ADP	C4-C5-N7	-3.31	106.44	109.48
2	B	800	ADP	C4-C5-N7	-3.29	106.45	109.48
2	E	800	ADP	C4-C5-N7	-3.29	106.45	109.48
2	F	800	ADP	C4-C5-N7	-3.29	106.45	109.48
2	D	800	ADP	PA-O3A-PB	-2.78	123.34	132.67
2	I	800	ADP	PA-O3A-PB	-2.78	123.36	132.67
2	H	800	ADP	PA-O3A-PB	-2.78	123.36	132.67
2	G	800	ADP	PA-O3A-PB	-2.77	123.37	132.67
2	A	800	ADP	PA-O3A-PB	-2.77	123.38	132.67
2	B	800	ADP	PA-O3A-PB	-2.77	123.39	132.67
2	F	800	ADP	PA-O3A-PB	-2.76	123.40	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	800	ADP	PA-O3A-PB	-2.76	123.41	132.67
2	C	800	ADP	PA-O3A-PB	-2.75	123.46	132.67
2	I	800	ADP	O2'-C2'-C3'	4.62	126.86	111.83
2	G	800	ADP	O2'-C2'-C3'	4.62	126.86	111.83
2	F	800	ADP	O2'-C2'-C3'	4.63	126.88	111.83
2	B	800	ADP	O2'-C2'-C3'	4.63	126.89	111.83
2	H	800	ADP	O2'-C2'-C3'	4.63	126.89	111.83
2	A	800	ADP	O2'-C2'-C3'	4.63	126.89	111.83
2	E	800	ADP	O2'-C2'-C3'	4.63	126.90	111.83
2	C	800	ADP	O2'-C2'-C3'	4.64	126.91	111.83
2	D	800	ADP	O2'-C2'-C3'	4.64	126.92	111.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	ADP	1	0
2	B	800	ADP	1	0
2	C	800	ADP	1	0
2	D	800	ADP	1	0
2	E	800	ADP	1	0
2	F	800	ADP	1	0
2	G	800	ADP	1	0
2	H	800	ADP	1	0
2	I	800	ADP	1	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	505/553 (91%)	0.13	13 (2%)	59	43	64, 126, 150, 150	0
1	B	505/553 (91%)	0.11	14 (2%)	56	41	64, 126, 150, 150	0
1	C	505/553 (91%)	0.18	17 (3%)	49	34	64, 126, 150, 150	0
1	D	505/553 (91%)	0.10	14 (2%)	56	41	64, 126, 150, 150	0
1	E	505/553 (91%)	0.26	25 (4%)	32	21	64, 126, 150, 150	0
1	F	505/553 (91%)	0.18	14 (2%)	56	41	64, 126, 150, 150	0
1	G	505/553 (91%)	0.23	22 (4%)	38	25	64, 126, 150, 150	0
1	H	505/553 (91%)	0.11	12 (2%)	62	46	64, 126, 150, 150	0
1	I	505/553 (91%)	0.08	9 (1%)	71	57	64, 126, 150, 150	0
All	All	4545/4977 (91%)	0.15	140 (3%)	52	37	64, 127, 150, 150	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	261	ASP	6.9
1	E	259	GLU	5.9
1	B	259	GLU	5.2
1	F	259	GLU	5.1
1	H	267	ASN	5.1
1	C	259	GLU	4.9
1	A	259	GLU	4.4
1	F	267	ASN	4.3
1	C	261	ASP	4.2
1	G	259	GLU	4.0
1	F	63	LEU	4.0
1	F	261	ASP	4.0
1	H	262	ALA	3.6
1	D	532	ALA	3.5
1	E	268	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	267	ASN	3.5
1	E	198	ASP	3.5
1	H	265	ARG	3.4
1	B	261	ASP	3.4
1	G	532	ALA	3.4
1	E	267	ASN	3.4
1	E	154	SER	3.4
1	H	264	ILE	3.4
1	I	267	ASN	3.4
1	G	268	ASP	3.3
1	E	157	ASP	3.3
1	E	260	LEU	3.3
1	C	267	ASN	3.3
1	D	260	LEU	3.2
1	E	156	ASN	3.2
1	D	259	GLU	3.2
1	H	259	GLU	3.2
1	B	260	LEU	3.2
1	G	194	GLU	3.2
1	E	262	ALA	3.1
1	E	263	GLU	3.1
1	G	481	ASN	3.0
1	C	374	LYS	3.0
1	F	162	ARG	3.0
1	B	198	ASP	3.0
1	F	260	LEU	2.9
1	E	261	ASP	2.9
1	C	353	TYR	2.9
1	F	65	ASP	2.9
1	B	156	ASN	2.9
1	B	268	ASP	2.9
1	A	261	ASP	2.8
1	G	531	SER	2.8
1	G	260	LEU	2.8
1	C	371	GLU	2.8
1	G	261	ASP	2.7
1	B	157	ASP	2.7
1	C	262	ALA	2.7
1	A	366	LYS	2.7
1	E	195	LEU	2.7
1	G	63	LEU	2.7
1	G	266	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	197	GLY	2.7
1	B	267	ASN	2.7
1	H	266	ILE	2.7
1	D	199	LYS	2.6
1	C	65	ASP	2.6
1	C	243	ASN	2.6
1	F	269	PRO	2.6
1	E	272	MET	2.6
1	D	268	ASP	2.6
1	A	371	GLU	2.6
1	A	198	ASP	2.6
1	G	264	ILE	2.6
1	H	261	ASP	2.6
1	A	197	GLY	2.6
1	G	243	ASN	2.5
1	F	268	ASP	2.5
1	D	353	TYR	2.5
1	B	262	ALA	2.5
1	E	82	GLN	2.5
1	H	243	ASN	2.5
1	I	265	ARG	2.5
1	B	77	ASP	2.5
1	C	63	LEU	2.4
1	G	267	ASN	2.4
1	A	374	LYS	2.4
1	C	260	LEU	2.4
1	F	62	SER	2.4
1	G	197	GLY	2.4
1	H	263	GLU	2.4
1	C	62	SER	2.4
1	I	259	GLU	2.4
1	F	226	ILE	2.4
1	C	385	GLY	2.4
1	E	206	ASN	2.4
1	B	63	LEU	2.3
1	C	357	ILE	2.3
1	D	531	SER	2.3
1	I	242	GLU	2.3
1	G	262	ALA	2.3
1	E	531	SER	2.3
1	F	532	ALA	2.3
1	I	261	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	262	ALA	2.2
1	E	65	ASP	2.2
1	A	532	ALA	2.2
1	D	246	ILE	2.2
1	A	481	ASN	2.2
1	E	317	VAL	2.2
1	E	254	GLU	2.2
1	C	242	GLU	2.2
1	E	271	GLN	2.2
1	I	82	GLN	2.2
1	G	196	ARG	2.2
1	H	60	VAL	2.2
1	A	267	ASN	2.2
1	A	353	TYR	2.2
1	B	195	LEU	2.2
1	G	296	ASN	2.2
1	A	194	GLU	2.2
1	D	196	ARG	2.2
1	D	243	ASN	2.1
1	C	351	LEU	2.1
1	E	61	ASP	2.1
1	E	77	ASP	2.1
1	E	243	ASN	2.1
1	G	156	ASN	2.1
1	G	269	PRO	2.1
1	I	262	ALA	2.1
1	A	196	ARG	2.1
1	G	255	VAL	2.1
1	H	268	ASP	2.1
1	F	227	VAL	2.1
1	G	265	ARG	2.1
1	I	350	ASP	2.1
1	C	356	LEU	2.1
1	B	269	PRO	2.1
1	B	206	ASN	2.0
1	F	531	SER	2.0
1	I	264	ILE	2.0
1	E	258	PRO	2.0
1	G	246	ILE	2.0
1	E	266	ILE	2.0
1	H	531	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	ADP	G	800	27/27	0.78	0.37	3.03	150,150,150,150	7
2	ADP	H	800	27/27	0.81	0.33	2.54	150,150,150,150	7
2	ADP	D	800	27/27	0.76	0.39	2.39	150,150,150,150	7
2	ADP	I	800	27/27	0.82	0.33	2.38	150,150,150,150	7
2	ADP	B	800	27/27	0.80	0.34	1.90	150,150,150,150	7
2	ADP	A	800	27/27	0.79	0.35	1.84	150,150,150,150	7
2	ADP	E	800	27/27	0.77	0.34	1.56	150,150,150,150	7
2	ADP	C	800	27/27	0.79	0.34	1.55	150,150,150,150	7
2	ADP	F	800	27/27	0.83	0.32	1.23	150,150,150,150	7

6.5 Other polymers [i](#)

There are no such residues in this entry.