



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:42 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

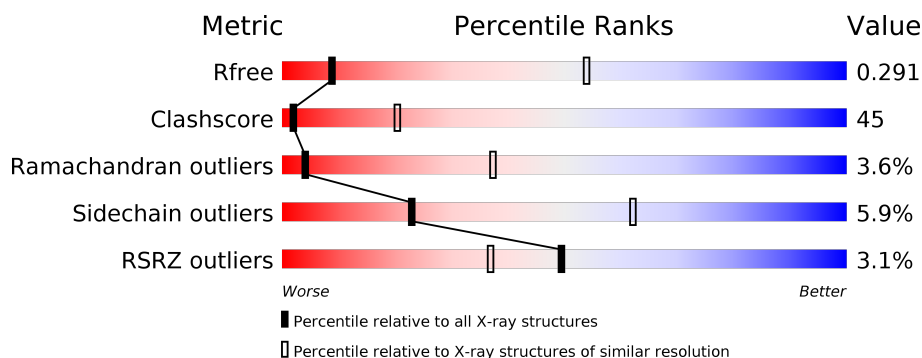
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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}	100719	1234 (3.90-3.50)
Clashscore	112137	1377 (3.90-3.50)
Ramachandran outliers	110173	1323 (3.90-3.50)
Sidechain outliers	110143	1320 (3.90-3.50)
RSRZ outliers	101464	1262 (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	
1	B	553	
1	C	553	
1	D	553	
1	E	553	
1	F	553	

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Mol	Chain	Length	Quality of chain
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.

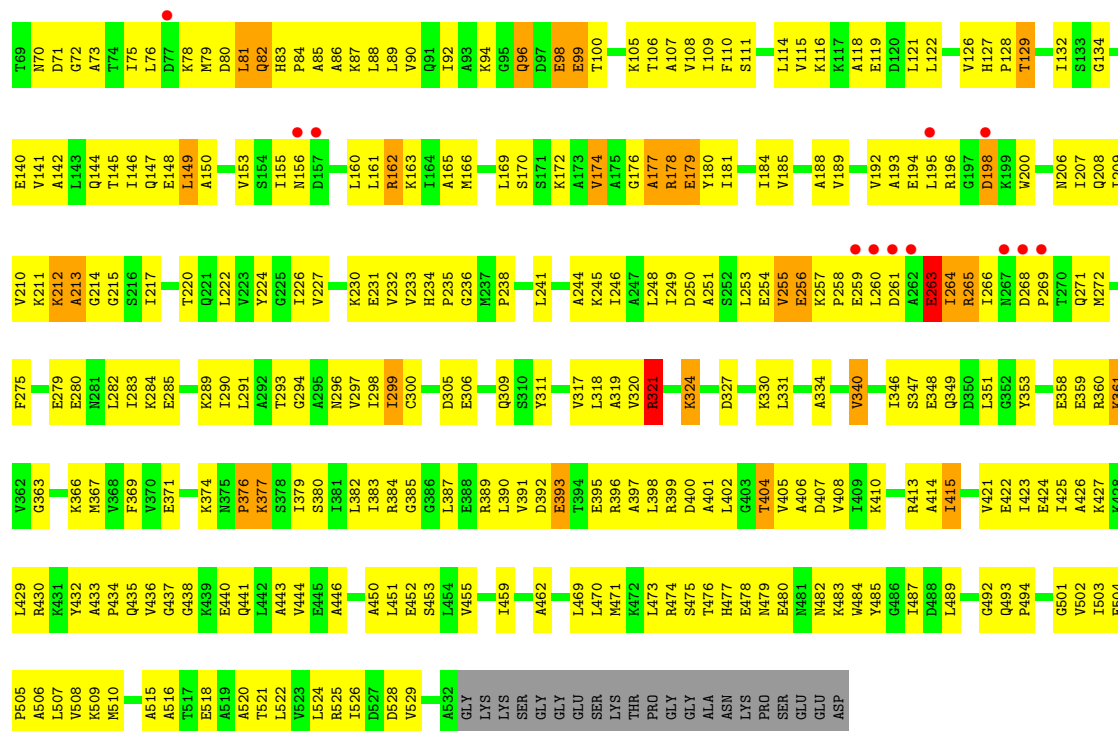
- Molecule 1 is a protein called Chaperonin.

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			

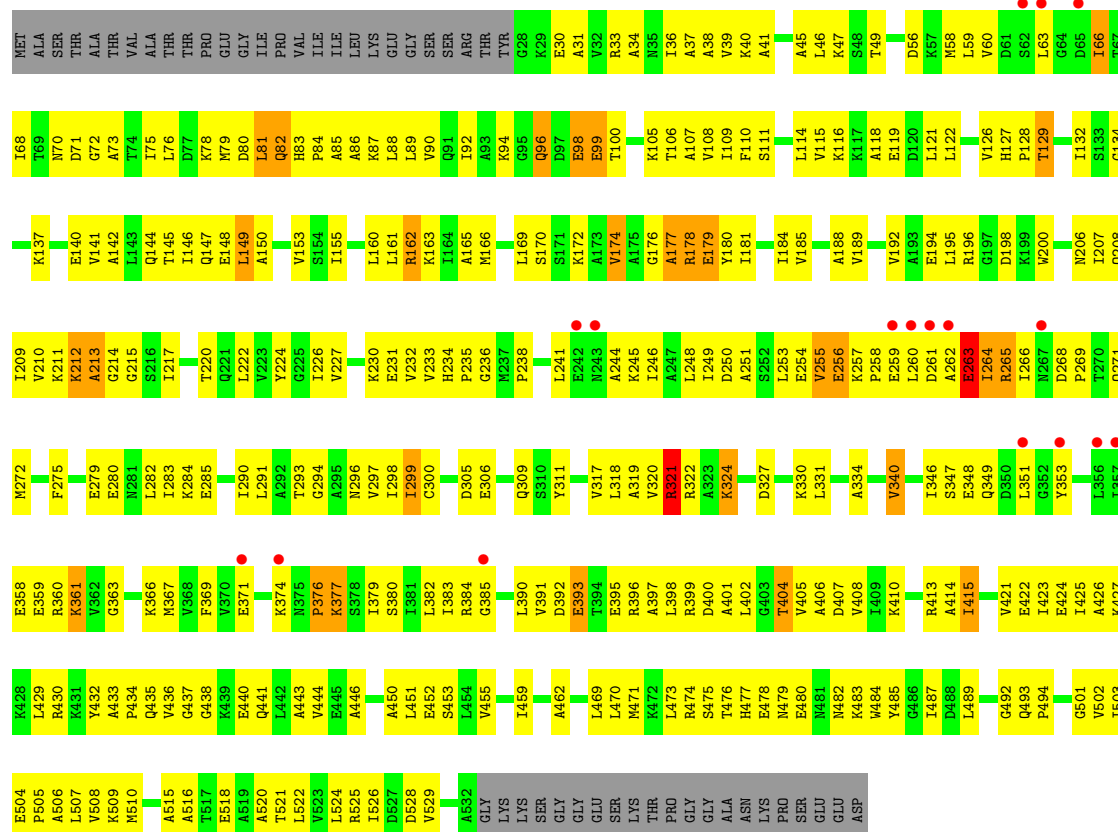
- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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		



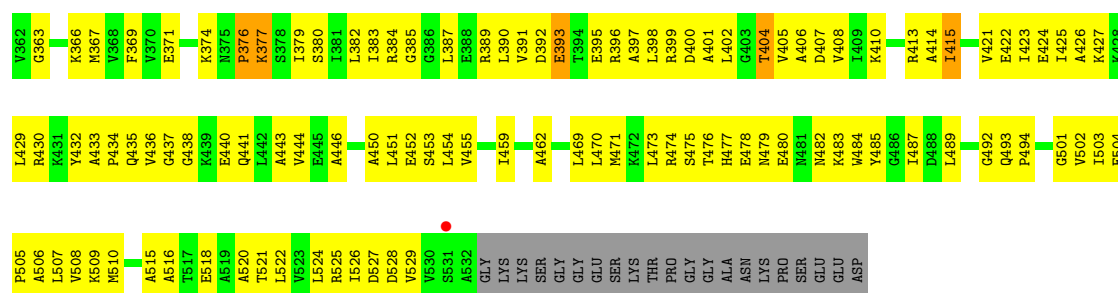
• Molecule 1: Chaperonin



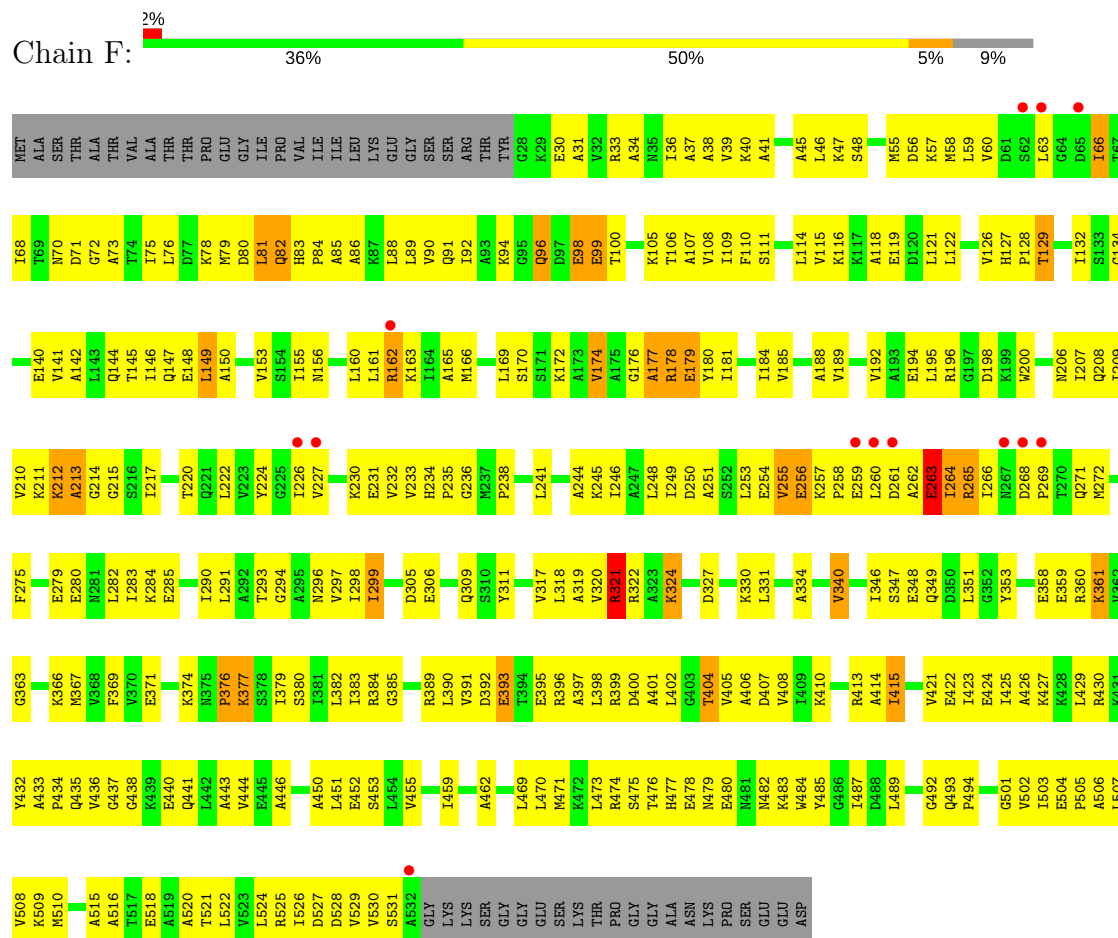
Chain D: 3% 36% 50% 5% 9%

Residue	Amino Acid	Residue	Amino Acid	Residue	Amino Acid	Residue	Amino Acid	Residue	Amino Acid
166	MET	167	LEU	168	LEU	169	LEU	170	LEU
171	ALA	172	ALA	173	ALA	174	ALA	175	ALA
176	THR	177	THR	178	THR	179	THR	180	THR
181	ALA	182	ALA	183	ALA	184	ALA	185	ALA
186	THR	187	THR	188	THR	189	THR	190	THR
191	ALA	192	ALA	193	ALA	194	ALA	195	ALA
196	THR	197	THR	198	THR	199	THR	200	THR
201	ALA	202	ALA	203	ALA	204	ALA	205	ALA
206	THR	207	THR	208	THR	209	THR	210	THR
211	ALA	212	ALA	213	ALA	214	ALA	215	ALA
216	THR	217	THR	218	THR	219	THR	220	THR
221	ALA	222	ALA	223	ALA	224	ALA	225	ALA
226	THR	227	THR	228	THR	229	THR	230	THR
231	ALA	232	ALA	233	ALA	234	ALA	235	ALA
236	THR	237	THR	238	THR	239	THR	240	THR
241	ALA	242	ALA	243	ALA	244	ALA	245	ALA
246	THR	247	THR	248	THR	249	THR	250	THR
251	ALA	252	ALA	253	ALA	254	ALA	255	ALA
256	THR	257	THR	258	THR	259	THR	260	THR
261	ALA	262	ALA	263	ALA	264	ALA	265	ALA
266	THR	267	THR	268	THR	269	THR	270	THR
271	ALA	272	ALA	273	ALA	274	ALA	275	ALA
276	THR	277	THR	278	THR	279	THR	280	THR
281	ALA	282	ALA	283	ALA	284	ALA	285	ALA
286	THR	287	THR	288	THR	289	THR	290	THR
291	ALA	292	ALA	293	ALA	294	ALA	295	ALA
296	THR	297	THR	298	THR	299	THR	300	THR
301	ALA	302	ALA	303	ALA	304	ALA	305	ALA
306	THR	307	THR	308	THR	309	THR	310	THR
311	ALA	312	ALA	313	ALA	314	ALA	315	ALA
316	THR	317	THR	318	THR	319	THR	320	THR
321	ALA	322	ALA	323	ALA	324	ALA	325	ALA
326	THR	327	THR	328	THR	329	THR	330	THR
331	ALA	332	ALA	333	ALA	334	ALA	335	ALA
336	THR	337	THR	338	THR	339	THR	340	THR
341	ALA	342	ALA	343	ALA	344	ALA	345	ALA
346	THR	347	THR	348	THR	349	THR	350	THR
351	ALA	352	ALA	353	ALA	354	ALA	355	ALA
356	THR	357	THR	358	THR	359	THR	360	THR
361	ALA	362	ALA	363	ALA	364	ALA	365	ALA
366	THR	367	THR	368	THR	369	THR	370	THR
371	ALA	372	ALA	373	ALA	374	ALA	375	ALA
376	THR	377	THR	378	THR	379	THR	380	THR
381	ALA	382	ALA	383	ALA	384	ALA	385	ALA
386	THR	387	THR	388	THR	389	THR	390	THR
391	ALA	392	ALA	393	ALA	394	ALA	395	ALA
396	THR	397	THR	398	THR	399	THR	400	THR
401	ALA	402	ALA	403	ALA	404	ALA	405	ALA
406	THR	407	THR	408	THR	409	THR	410	THR
411	ALA	412	ALA	413	ALA	414	ALA	415	ALA
416	THR	417	THR	418	THR	419			

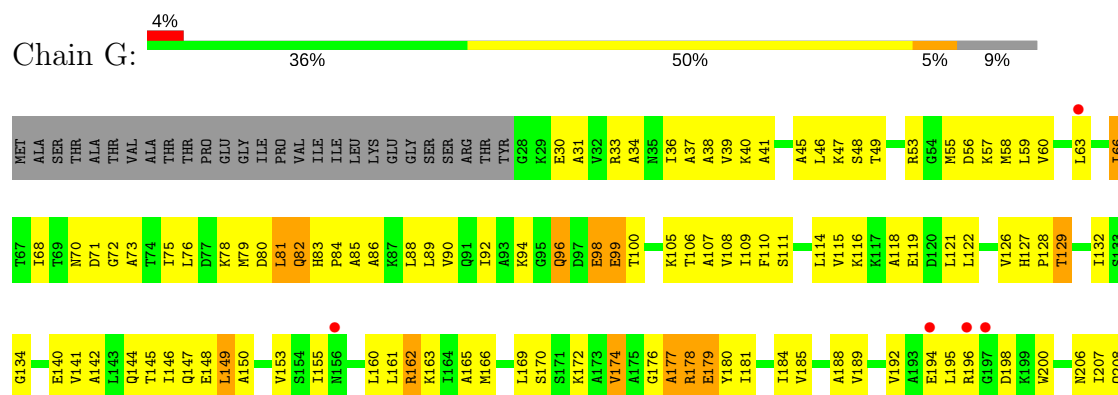
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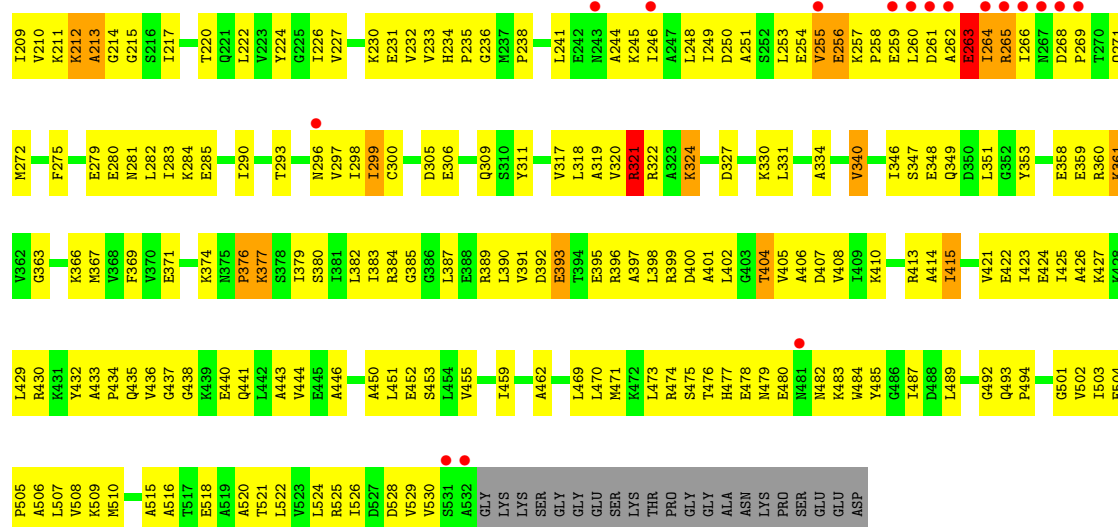


• Molecule 1: Chaperonin

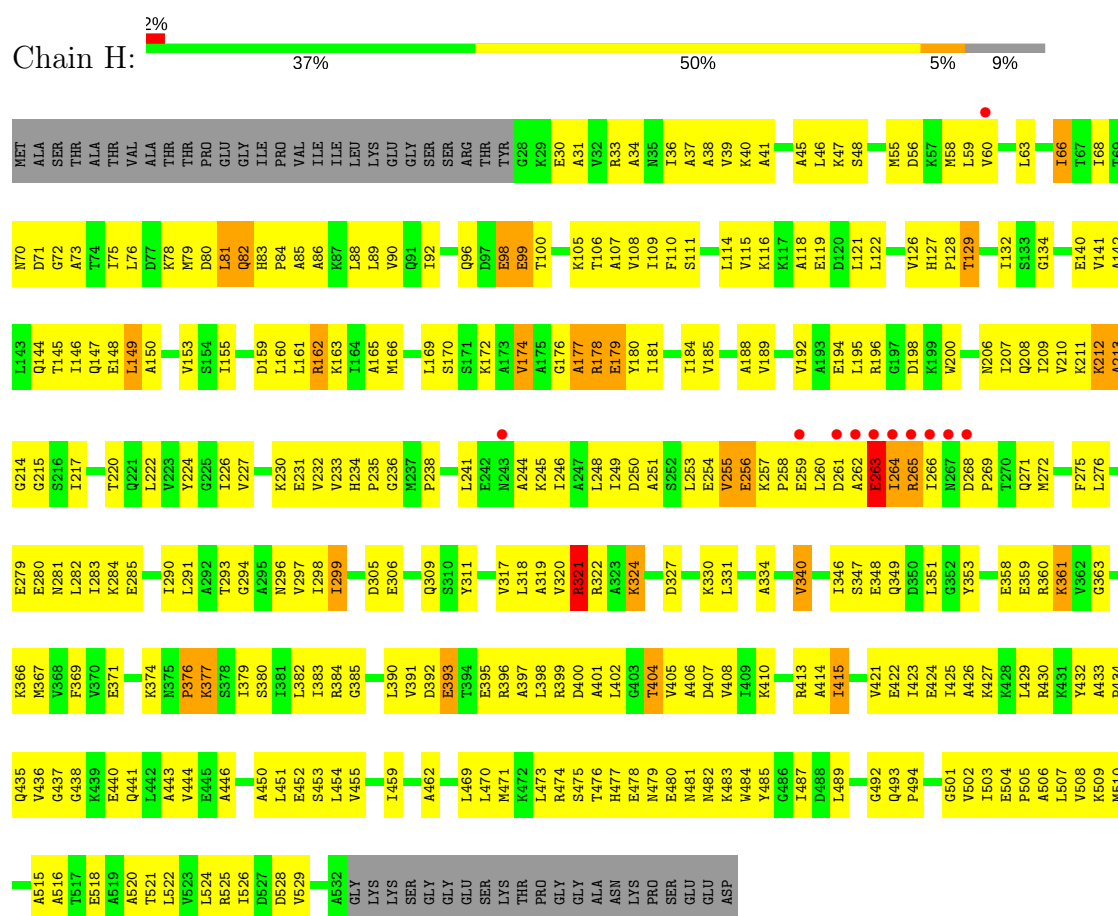


• Molecule 1: Chaperonin

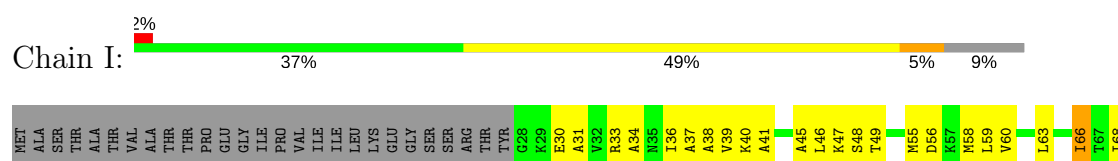




• Molecule 1: Chaperonin



• Molecule 1: Chaperonin



A515	A516	T517	E518	A519	A520	T521	L522	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	V444	E445	A446	A450	L451	E452	S453	L454	V455	L459	A462	L469	L470	M471	K472	L473	R474	S475	T476	H477	E478	M479	E480	M481	K482	K483	W484	Y485	G486	I487	D488	L489																
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	R429	P430	K431	Y432	A433	P434	Q435
E279	E280	N281	L282	I283	K284	E285	L290	T293	N296	V297	L298	I299	D305	E306	Q309	S310	Y311	V317	L318	A319	V320	R321	R322	A323	K324	D327	K330	L331	A334	V340	T346	S347	E348	Q349	D350	L351	G352	Y353	E358	E359	R360	K361	V362	G363	K366										
A213	G214	G215	S216	I217	T220	Q221	L222	V223	Y224	G225	I226	V227	K230	E231	L232	V233	H234	P235	G236	M237	P238	L241	E242	N243	A244	K245	I246	A247	L248	I249	D250	V251	S252	L253	E254	V255	E256	K257	P258	E259	L260	D261	A262	E263	I264	R265	I266	K267	D268	P269	T270	Q271	M272	F275	L276
L142	L143	Q144	T145	I146	Q147	E148	L149	A150	V153	L154	I155	M156	L160	L161	R162	K163	I164	A165	M166	L169	S170	S171	K172	A173	V174	A175	G176	A177	R178	E179	V180	I181	I184	V185	A188	E189	V192	A193	E194	L195	R196	G197	D198	K199	W200	N206	I207	Q208	I209	V210	K211	E140	K212		
T69	N70	D71	G72	A73	T74	L75	L76	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	K214		

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 , 72.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.080 for h+2*1,k,-h-l 0.099 for -h-2*1,-k,l 0.089 for h,-k,-h-l	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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(°)	Ideal(°)
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(°)	Ideal(°)
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:D:60:VAL:HG22	1:D:66:ILE:HG22	1.23	1.10
1:E:185:VAL:HG13	1:E:402:LEU:HD23	1.32	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:D:529:VAL:HG12	1:E:58:MET:HB3	1.40	1.01
1:F:260:LEU:HD12	1:F:261:ASP:H	1.23	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:D:245:LYS:N	1:D:296:ASN:HD22	1.61	0.99
1:G:245:LYS:N	1:G: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:D:421:VAL:O	1:D:425:ILE:HG12	1.66	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: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:B:423:ILE:HD12	1:B:424:GLU:N	1.82	0.95
1:H:423:ILE:HD12	1:H:424:GLU:N	1.82	0.95
1:C:423:ILE:HD12	1:C:424:GLU:N	1.82	0.94
1:E:66:ILE:H	1:E:66:ILE:HD13	1.32	0.94
1:G:421:VAL:O	1:G:425:ILE:HG12	1.66	0.94
1:D:423:ILE:HD12	1:D:424:GLU:N	1.82	0.94
1:I:66:ILE:HD13	1:I:66:ILE:H	1.32	0.94
1:E:421:VAL:O	1:E:425:ILE:HG12	1.66	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:260:LEU:HD12	1:H:261:ASP:H	1.23	0.94
1:A:66:ILE:HD13	1:A:66:ILE:H	1.32	0.94
1:C:260:LEU:HD12	1:C:261:ASP:H	1.23	0.94
1:G:260:LEU:HD12	1:G: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:HD13	1:H:66:ILE:H	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: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: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: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:C:258:PRO:HG2	1:C:279:GLU:OE2	1.72	0.89
1:F:258:PRO:HG2	1:F: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:A:258:PRO:HG2	1:A:279:GLU:OE2	1.72	0.89
1:B:258:PRO:HG2	1:B: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:D:258:PRO:HG2	1:D:279:GLU:OE2	1.72	0.89
1:G:258:PRO:HG2	1:G:279:GLU:OE2	1.72	0.89
1:F:260:LEU:CD1	1:F:261:ASP:N	2.35	0.89
1:A:212:LYS:HA	1:A:212:LYS:HE2	1.53	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:H:260:LEU:CD1	1:H:261:ASP:N	2.35	0.89
1:D:212:LYS:HE2	1:D:212:LYS:HA	1.53	0.88
1:I:258:PRO:HG2	1:I:279:GLU:OE2	1.72	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:A:217:ILE:HG12	1:A:385:GLY:HA2	1.57	0.87
1:B:260:LEU:CD1	1:B:261:ASP:N	2.35	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:C:217:ILE:HG12	1:C:385:GLY:HA2	1.57	0.85
1:F:269:PRO:HA	1:F:272:MET:HG2	1.57	0.85
1:I:361:LYS:HB3	1:I:366:LYS:HG2	1.59	0.85
1:D:361:LYS:HB3	1:D:366:LYS:HG2	1.59	0.85
1:I:269:PRO:HA	1:I:272:MET:HG2	1.57	0.85
1:E:260:LEU:CD1	1:E:261:ASP:N	2.35	0.85
1:E:217:ILE:HG12	1:E:385:GLY:HA2	1.57	0.84
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: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:C:361:LYS:HB3	1:C:366:LYS:HG2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:361:LYS:HB3	1:H:366:LYS:HG2	1.59	0.84
1:H:76:LEU:HD23	1:H:90:VAL:HG12	1.60	0.84
1:B:361:LYS:HB3	1:B:366:LYS:HG2	1.59	0.84
1:F:529:VAL:CG1	1:G:58:MET:HB3	2.04	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:A:290:ILE:O	1:A:293:THR:HG22	1.82	0.80
1:H:60:VAL:HG22	1:H:66:ILE:CG2	2.10	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: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:G:60:VAL:HG22	1:G:66:ILE:CG2	2.10	0.80
1:B:290:ILE:O	1:B:293:THR:HG22	1.82	0.80
1:C:260:LEU:CD1	1:C:261:ASP:OD1	2.30	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:A:245:LYS:H	1:A:296:ASN:HD22	1.28	0.79
1:B:260:LEU:CD1	1:B:261:ASP:OD1	2.30	0.79
1:F:245:LYS:H	1:F:296:ASN:HD22	1.28	0.79
1:I:260:LEU:CD1	1:I:261:ASP:OD1	2.30	0.79

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:VAL:HG22	1:F:66:ILE:CG2	2.10	0.76
1:A:141:VAL:HG21	1:A:432:TYR:CD1	2.19	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:B:220:THR:HG22	1:B:384:ARG:N	2.01	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:433:ALA:O	1:B:436:VAL:HG22	1.85	0.76
1:D:88:LEU:HD11	1:E:389:ARG:HH12	1.50	0.76
1:G:433:ALA:O	1:G:436:VAL:HG22	1.85	0.76
1:H:290:ILE:HG21	1:H:298:ILE:HD12	1.66	0.76
1:H:433:ALA:O	1:H:436:VAL:HG22	1.85	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: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:I:433:ALA:O	1:I:436:VAL:HG22	1.85	0.76
1:H:89:LEU:HD21	1:H:108:VAL:HG23	1.68	0.76
1:E:89:LEU:HD21	1:E:108:VAL:HG23	1.68	0.75
1:G:254:GLU:HA	1:G:305:ASP:HB2	1.68	0.75
1:I:220:THR:HG22	1:I:384:ARG:N	2.01	0.75
1:E:141:VAL:HG21	1:E:432:TYR:CE1	2.21	0.75
1:H:245:LYS:H	1:H:296:ASN:HD22	1.28	0.75
1:C:220:THR:HG22	1:C:384:ARG:N	2.01	0.75
1:C:433:ALA:O	1:C:436:VAL:HG22	1.85	0.75
1:D:141:VAL:HG21	1:D:432:TYR:CE1	2.21	0.75
1:F:433:ALA:O	1:F:436:VAL:HG22	1.85	0.75
1:E:220:THR:HG22	1:E:384:ARG:N	2.01	0.75
1:E:254:GLU:HA	1:E:305:ASP:HB2	1.68	0.75
1:E:526:ILE:HD12	1:F:58:MET:HB2	1.68	0.75
1:F:527:ASP:HB2	1:G:55:MET:HB3	1.69	0.75
1:A:141:VAL:HG21	1:A:432:TYR:CE1	2.21	0.75
1:C:424:GLU:OE2	1:C:477:HIS:CD2	2.40	0.75
1:G:424:GLU:OE2	1:G:477:HIS:CD2	2.40	0.75
1:H:141:VAL:HG21	1:H:432:TYR:CE1	2.21	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:D:89:LEU:HD21	1:D:108:VAL:HG23	1.68	0.75
1:H:424:GLU:OE2	1:H:477:HIS:CD2	2.40	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:A:254:GLU:HA	1:A:305:ASP:HB2	1.68	0.75
1:B:141:VAL:HG21	1:B:432:TYR:CE1	2.21	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: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: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:E:424:GLU:OE2	1:E:477:HIS:CD2	2.40	0.74
1:E:81:LEU:H	1:E:81:LEU:HD12	1.52	0.74
1:F:141:VAL:HG21	1:F:432:TYR:CE1	2.21	0.74
1:A:220:THR:HG22	1:A:384:ARG:N	2.01	0.74
1:B:89:LEU:HD21	1:B:108:VAL:HG23	1.68	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:C:248:LEU:HD11	1:C:331:LEU:HD22	1.69	0.74
1:C:432:TYR:CE2	1:C:436:VAL:HG12	2.22	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: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:A:248:LEU:HD11	1:A:331:LEU:HD22	1.69	0.74
1:D:81:LEU:H	1:D:81:LEU:HD12	1.52	0.74
1:F:220:THR:HG22	1:F:384:ARG:N	2.01	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:F:432:TYR:CE2	1:F:436:VAL:HG12	2.22	0.74
1:A:89:LEU:HD21	1:A:108:VAL:HG23	1.68	0.74
1:B:254:GLU:HA	1:B:305:ASP:HB2	1.68	0.74
1:B:60:VAL:HG22	1:B:66:ILE:CG2	2.10	0.74
1:G:89:LEU:HD21	1:G:108:VAL:HG23	1.68	0.74
1:F:530:VAL:O	1:G:59:LEU:CD2	2.35	0.74
1:F:89:LEU:HD21	1:F:108:VAL:HG23	1.68	0.74
1:G:299:ILE:H	1:G:299:ILE:HD13	1.53	0.74
1:B:248:LEU:HD11	1:B:331:LEU:HD22	1.69	0.74
1:F:299:ILE:HD13	1:F:299:ILE:H	1.53	0.74
1:I:280:GLU:HG2	1:I:284:LYS:HE3	1.69	0.74
1:C:254:GLU:HA	1:C:305:ASP:HB2	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:424:GLU:OE2	1:G:477:HIS:HD2	1.71	0.73
1:H:432:TYR:CE2	1:H:436:VAL:HG12	2.22	0.73
1:I:424:GLU:OE2	1:I:477:HIS:HD2	1.71	0.73
1:A:432:TYR:CE2	1:A:436:VAL:HG12	2.22	0.73
1:E:525:ARG:CG	1:F:56:ASP:OD2	2.36	0.73
1:G:280:GLU:HG2	1:G:284:LYS:HE3	1.69	0.73
1:G:248:LEU:HD11	1:G:331:LEU:HD22	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:D:209:ILE:HB	1:D:399:ARG:HH22	1.53	0.73
1:G:81:LEU:HD12	1:G:81:LEU:H	1.52	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:C:424:GLU:OE2	1:C:477:HIS:HD2	1.71	0.73
1:C:81:LEU:HD12	1:C:81:LEU:H	1.53	0.73
1:D:299:ILE:H	1:D:299:ILE:HD13	1.53	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:G:432:TYR:CE2	1:G:436:VAL:HG12	2.22	0.73
1:I:401:ALA:O	1:I:405:VAL:HG23	1.88	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:E:153:VAL:HG23	1:E:160:LEU:HD23	1.70	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:B:424:GLU:OE2	1:B:477:HIS:HD2	1.71	0.73
1:C:280:GLU:HG2	1:C:284:LYS:HE3	1.69	0.73
1:D:424:GLU:OE2	1:D:477:HIS:HD2	1.72	0.73
1:E:280:GLU:HG2	1:E: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:H:401:ALA:O	1:H:405:VAL:HG23	1.88	0.73
1:C:153:VAL:HG23	1:C:160:LEU:HD23	1.70	0.73
1:D:254:GLU:HA	1:D:305:ASP:HB2	1.68	0.73
1:F:452:GLU:O	1:F:455:VAL:HG22	1.89	0.73
1:I:81:LEU:HD12	1:I:81:LEU:H	1.52	0.73
1:A:81:LEU:H	1:A:81:LEU:HD12	1.52	0.73
1:B:452:GLU:O	1:B:455:VAL:HG22	1.89	0.73
1:G:209:ILE:HB	1:G:399:ARG:HH22	1.54	0.73

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:VAL:HG23	1:D:160:LEU:HD23	1.70	0.71
1:I:153:VAL:HG23	1:I:160:LEU:HD23	1.70	0.71
1:B:299:ILE:H	1:B:299:ILE:HD13	1.53	0.71
1:A:209:ILE:HB	1:A:399:ARG:HH22	1.54	0.71
1:B:415:ILE:HD12	1:B:506:ALA:HA	1.72	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:D:38:ALA:O	1:D: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:264:ILE:HG13	1:D:265:ARG:N	2.02	0.71
1:E:415:ILE:HD12	1:E:506:ALA:HA	1.72	0.71
1:G:452:GLU:O	1:G:455:VAL:HG22	1.89	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: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:F:264:ILE:HG13	1:F:265:ARG:N	2.03	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:B:264:ILE:HG13	1:B:265:ARG:N	2.03	0.70
1:D:259:GLU:C	1:D:259:GLU:OE1	2.30	0.70
1:G:469:LEU:HB3	1:G:487:ILE:HD13	1.73	0.70
1:A:415:ILE:HD12	1:A:506:ALA:HA	1.72	0.70
1:B:259:GLU:OE1	1:B:259:GLU:C	2.30	0.70
1:C:469:LEU:HB3	1:C:487:ILE:HD13	1.73	0.70
1:H:259:GLU:OE1	1:H:259:GLU:C	2.30	0.70
1:A:259:GLU:OE1	1:A:259:GLU:C	2.30	0.70
1:E:264:ILE:HG13	1:E:265:ARG:N	2.02	0.70
1:F:259:GLU:C	1:F:259:GLU:OE1	2.30	0.70
1:H:424:GLU:OE2	1:H:477:HIS:HD2	1.71	0.70
1:A:425:ILE:O	1:A:429:LEU:HB2	1.92	0.70
1:C:259:GLU:OE1	1:C:259:GLU:C	2.30	0.70
1:E:259:GLU:OE1	1:E:259:GLU:C	2.30	0.70
1:I:107:ALA:O	1:I:111:SER:HB2	1.92	0.70
1:A:469:LEU:HB3	1:A:487:ILE:HD13	1.73	0.70
1:B:425:ILE:O	1:B:429:LEU:HB2	1.92	0.70
1:D:398:LEU:O	1:D:402:LEU:HG	1.92	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: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:H:469:LEU:HB3	1:H:487:ILE:HD13	1.73	0.69
1:A:264:ILE:HG13	1:A:265:ARG:N	2.03	0.69
1:B:398:LEU:O	1:B:402:LEU:HG	1.92	0.69
1:B:83:HIS:CG	1:B:84:PRO:HD2	2.27	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:F:83:HIS:CG	1:F:84:PRO:HD2	2.27	0.69
1:B:475:SER:O	1:B:478:GLU:HG2	1.93	0.69
1:F:398:LEU:O	1:F:402:LEU:HG	1.92	0.69
1:H:107:ALA:O	1:H:111:SER:HB2	1.92	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:220:THR:CG2	1:G:384:ARG:H	2.05	0.69
1:I:259:GLU:OE1	1:I:259:GLU:C	2.30	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: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: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:G:66:ILE:H	1:G:66:ILE:CD1	2.06	0.69
1:H:83:HIS:CG	1:H:84:PRO:HD2	2.27	0.69
1:B:220:THR:CG2	1:B:384:ARG:H	2.05	0.69
1:D:470:LEU:O	1:D:474:ARG:HG2	1.93	0.69
1:D:83:HIS:CG	1:D:84:PRO:HD2	2.27	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: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: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:398:LEU:O	1:E:402:LEU:HG	1.92	0.69
1:E:425:ILE:O	1:E:429:LEU:HB2	1.92	0.69
1:F:470:LEU:O	1:F: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:A:107:ALA:O	1:A:111:SER:HB2	1.92	0.69
1:B:469:LEU:HB3	1:B:487:ILE:HD13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:HIS:CG	1:C:84:PRO:HD2	2.27	0.69
1:D:107:ALA:O	1:D:111:SER:HB2	1.92	0.69
1:D:264:ILE:HG13	1:D:265:ARG:O	1.92	0.69
1:E:107:ALA:O	1:E:111:SER:HB2	1.92	0.69
1:E:475:SER:O	1:E:478:GLU:HG2	1.92	0.69
1:G:264:ILE:HG13	1:G:265:ARG:O	1.92	0.69
1:G:470:LEU:O	1:G:474:ARG:HG2	1.93	0.69
1:G:475:SER:O	1:G:478:GLU:HG2	1.92	0.69
1:I:220:THR:CG2	1:I:384:ARG:H	2.05	0.69
1:I:470:LEU:O	1:I:474:ARG:HG2	1.93	0.69
1:A:398:LEU:O	1:A:402:LEU:HG	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:H:220:THR:CG2	1:H:384:ARG:H	2.05	0.69
1:A:220:THR:CG2	1:A:384:ARG:H	2.05	0.69
1:E:83:HIS:CG	1:E:84:PRO:HD2	2.27	0.69
1:F:220:THR:CG2	1:F:384:ARG:H	2.05	0.69
1:F:66:ILE:CD1	1:F:66:ILE:H	2.06	0.69
1:G:264:ILE:HG13	1:G:265:ARG:N	2.02	0.69
1:I:475:SER:O	1:I:478:GLU:HG2	1.92	0.69
1:F:184:ILE:HD12	1:F:222:LEU:HD22	1.75	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:E:184:ILE:HD12	1:E:222:LEU:HD22	1.75	0.68
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: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:C:264:ILE:HG13	1:C:265:ARG:O	1.92	0.68
1:G:184:ILE:HD12	1:G:222:LEU:HD22	1.75	0.68
1:I:184:ILE:HD12	1:I:222:LEU:HD22	1.75	0.68
1:I:83:HIS:CG	1:I:84:PRO:HD2	2.28	0.68
1:A:83:HIS:CG	1:A:84:PRO:HD2	2.27	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:G:107:ALA:O	1:G:111:SER:HB2	1.92	0.68
1:I:425:ILE:O	1:I:429:LEU:HB2	1.92	0.68
1:A:184:ILE:HD12	1:A:222:LEU:HD22	1.75	0.68
1:A:264:ILE:HG13	1:A:265:ARG:O	1.92	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:A:470:LEU:O	1:A:474:ARG:HG2	1.93	0.68
1:D:144:GLN:O	1:D:148:GLU:HG2	1.94	0.68
1:D:91:GLN:NE2	1:E:387:LEU:HD21	2.09	0.68
1:E:162:ARG:NH1	1:E:162:ARG:HB2	2.09	0.68
1:F:264:ILE:HG13	1:F:265:ARG:O	1.92	0.68
1:F:425:ILE:O	1:F:429:LEU:HB2	1.92	0.68
1:A:66:ILE:CD1	1:A:66:ILE:H	2.06	0.68
1:C:470:LEU:O	1:C:474:ARG:HG2	1.93	0.68
1:D:217:ILE:HD11	1:D:390:LEU:HD21	1.76	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:I:264:ILE:HG13	1:I:265:ARG:O	1.93	0.68
1:A:162:ARG:HB2	1:A:162:ARG:NH1	2.09	0.68
1:H:264:ILE:HG13	1:H:265:ARG:O	1.92	0.68
1:C:184:ILE:HD12	1:C:222:LEU:HD22	1.75	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:G:398:LEU:O	1:G:402:LEU:HG	1.92	0.68
1:I:144:GLN:O	1:I:148:GLU:HG2	1.94	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:A:248:LEU:HD13	1:A:299:ILE:HD11	1.76	0.67
1:G:245:LYS:N	1:G:296:ASN:ND2	2.41	0.67
1:H:255:VAL:HA	1:H:283:ILE:HD11	1.76	0.67
1:I:217:ILE:HD11	1:I:390:LEU:HD21	1.76	0.67
1:A:208:GLN:HB3	1:A:380:SER:OG	1.94	0.67
1:C:162:ARG:NH1	1:C:162:ARG:HB2	2.09	0.67
1:F:144:GLN:O	1:F:148:GLU:HG2	1.94	0.67
1:I:208:GLN:HB3	1:I:380:SER:OG	1.94	0.67
1:C:76:LEU:HD23	1:C:90:VAL:CG1	2.24	0.67
1:E:144:GLN:O	1:E:148:GLU:HG2	1.94	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:H:76:LEU:HD23	1:H:90:VAL:CG1	2.24	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:B:208:GLN:HB3	1:B:380:SER:OG	1.94	0.67
1:E:525:ARG:HG3	1:F:56:ASP:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:232:VAL:HG13	1:G:359:GLU:OE2	1.95	0.67
1:H:144:GLN:O	1:H:148:GLU:HG2	1.94	0.67
1:I:269:PRO:HA	1:I:272:MET:CG	2.25	0.67
1:I:255:VAL:HA	1:I:283:ILE:HD11	1.76	0.67
1:B:305:ASP:O	1:B:309:GLN:HG3	1.95	0.67
1:C:208:GLN:HB3	1:C:380:SER:OG	1.94	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:F:208:GLN:HB3	1:F:380:SER:OG	1.94	0.67
1:H:471:MET:SD	1:H:474:ARG:HD3	2.35	0.67
1:A:76:LEU:HD23	1:A:90:VAL:CG1	2.24	0.67
1:D:162:ARG:NH1	1:D:162:ARG:HB2	2.09	0.67
1:D:76:LEU:HD23	1:D:90:VAL:CG1	2.24	0.67
1:F:217:ILE:HD11	1:F:390:LEU:HD21	1.76	0.67
1:H:248:LEU:HD13	1:H:299:ILE:HD11	1.76	0.67
1:I:66:ILE:H	1:I:66:ILE:CD1	2.06	0.67
1:B:162:ARG:HB2	1:B:162:ARG:NH1	2.09	0.67
1:C:471:MET:SD	1:C:474:ARG:HD3	2.35	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:E:248:LEU:HD13	1:E:299:ILE:HD11	1.76	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:C:305:ASP:O	1:C:309:GLN:HG3	1.95	0.67
1:D:232:VAL:HG13	1:D:359:GLU:OE2	1.95	0.67
1:E:232:VAL:HG13	1:E:359:GLU:OE2	1.95	0.67
1:H:305:ASP:O	1:H:309:GLN:HG3	1.95	0.67
1:I:471:MET:SD	1:I:474:ARG:HD3	2.35	0.67
1:A:232:VAL:HG13	1:A:359:GLU:OE2	1.95	0.67
1:B:217:ILE:HD11	1:B:390:LEU:HD21	1.76	0.67
1:B:471:MET:SD	1:B:474:ARG:HD3	2.35	0.67
1:D:255:VAL:HA	1:D:283:ILE:HD11	1.76	0.67
1:D:525:ARG:HH11	1:D:525:ARG:HG2	1.60	0.67
1:G:217:ILE:HD11	1:G:390:LEU:HD21	1.76	0.67
1:G:471:MET:SD	1:G:474:ARG:HD3	2.35	0.67
1:H:162:ARG:NH1	1:H:162:ARG:HB2	2.09	0.67
1:H:217:ILE:HD11	1:H:390:LEU:HD21	1.76	0.67
1:A:479:ASN:HB2	1:A:482:ASN:OD1	1.96	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:E:66:ILE:CD1	1:E:66:ILE:H	2.06	0.66
1:F:255:VAL:HA	1:F:283:ILE:HD11	1.76	0.66
1:F:232:VAL:HG13	1:F:359:GLU:OE2	1.95	0.66
1:F:471:MET:SD	1:F:474:ARG:HD3	2.35	0.66
1:I:232:VAL:HG13	1:I:359:GLU:OE2	1.95	0.66
1:B:331:LEU:HD23	1:B:331:LEU:O	1.96	0.66
1:B:232:VAL:HG13	1:B:359:GLU:OE2	1.95	0.66
1:C:479:ASN:HB2	1:C:482:ASN:OD1	1.96	0.66
1:H:331:LEU:HD23	1:H:331:LEU:O	1.96	0.66
1:A:525:ARG:HG2	1:A:525:ARG:HH11	1.61	0.66
1:D:479:ASN:HB2	1:D: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:A:471:MET:SD	1:A:474:ARG:HD3	2.35	0.66
1:B:248:LEU:HD13	1:B:299:ILE:HD11	1.76	0.66
1:F:479:ASN:HB2	1:F:482:ASN:OD1	1.96	0.66
1:H:232:VAL:HG13	1:H:359:GLU:OE2	1.95	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:H:423:ILE:HG21	1:H:473:LEU:HD12	1.78	0.66
1:A:245:LYS:N	1:A:296:ASN:ND2	2.41	0.66
1:A:305:ASP:O	1:A:309:GLN:HG3	1.95	0.66
1:C:232:VAL:HG13	1:C:359:GLU:OE2	1.95	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:H:208:GLN:HB3	1:H:380:SER:OG	1.94	0.66
1:I:76:LEU:HD23	1:I:90:VAL:CG1	2.24	0.66
1:B:415:ILE:HG13	1:B:421:VAL:HG21	1.78	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:F:231:GLU:HG3	1:F:366:LYS:HZ2	1.60	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:G:210:VAL:HG23	1:G:382:LEU:CD1	2.26	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:I:525:ARG:HG2	1:I:525:ARG:HH11	1.60	0.66
1:A:255:VAL:HA	1:A:283:ILE:HD11	1.76	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:C:248:LEU:HD13	1:C:299:ILE:HD11	1.76	0.66
1:H:220:THR:HG22	1:H:384:ARG:H	1.61	0.66
1:H:269:PRO:HA	1:H:272:MET:CG	2.25	0.66
1:I:331:LEU:HD23	1:I:331:LEU:O	1.96	0.66
1:I:415:ILE:HG13	1:I:421:VAL:HG21	1.78	0.66
1:B:220:THR:HG22	1:B:384:ARG:H	1.61	0.66
1:B:479:ASN:HB2	1:B:482:ASN:OD1	1.96	0.66
1:F:127:HIS:CD2	1:F:129:THR:HB	2.31	0.66
1:G:479:ASN:HB2	1:G:482:ASN:OD1	1.96	0.66
1:C:210:VAL:HG23	1:C:382:LEU:CD1	2.26	0.66
1:E:415:ILE:HG13	1:E:421:VAL:HG21	1.78	0.66
1:C:423:ILE:HG21	1:C:473:LEU:HD12	1.78	0.65
1:D:210:VAL:HG23	1:D:382:LEU:CD1	2.26	0.65
1:E:245:LYS:N	1:E:296:ASN:ND2	2.41	0.65
1:E:46:LEU:N	1:E:46:LEU:HD12	2.12	0.65
1:E:525:ARG:HH11	1:E:525:ARG:HG2	1.61	0.65
1:F:269:PRO:HA	1:F:272:MET:CG	2.25	0.65
1:G:525:ARG:HG2	1:G:525:ARG:HH11	1.60	0.65
1:H:127:HIS:CD2	1:H:129:THR:HB	2.31	0.65
1:H:210:VAL:HG23	1:H:382:LEU:CD1	2.26	0.65
1:I:423:ILE:HG21	1:I:473:LEU:HD12	1.78	0.65
1:A:415:ILE:HG13	1:A:421:VAL:HG21	1.78	0.65
1:B:127:HIS:CD2	1:B:129:THR:HB	2.31	0.65
1:B:128:PRO:O	1:B:132:ILE:HG12	1.96	0.65
1:C:127:HIS:CD2	1:C:129:THR:HB	2.31	0.65
1:C:217:ILE:HD11	1:C:390:LEU:HD21	1.76	0.65
1:D:127:HIS:CD2	1:D:129:THR:HB	2.31	0.65
1:D:269:PRO:HA	1:D:272:MET:CG	2.25	0.65
1:D:305:ASP:O	1:D:309:GLN:HG3	1.95	0.65
1:D:331:LEU:HD23	1:D:331:LEU:O	1.96	0.65
1:D:473:LEU:O	1:D:476:THR:HG22	1.97	0.65
1:F:248:LEU:HD13	1:F:299:ILE:HD11	1.76	0.65
1:H:415:ILE:HG13	1:H:421:VAL:HG21	1.78	0.65
1:I:127:HIS:CD2	1:I:129:THR:HB	2.31	0.65
1:A:220:THR:HG22	1:A:384:ARG:H	1.61	0.65
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:D:423:ILE:HG21	1:D:473:LEU:HD12	1.78	0.65
1:E:479:ASN:HB2	1:E:482:ASN:OD1	1.96	0.65
1:F:473:LEU:O	1:F:476:THR:HG22	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:255:VAL:HA	1:G:283:ILE:HD11	1.76	0.65
1:G:269:PRO:HA	1:G:272:MET:CG	2.25	0.65
1:I:248:LEU:HD13	1:I:299:ILE:HD11	1.76	0.65
1:C:128:PRO:O	1:C:132:ILE:HG12	1.96	0.65
1:G:46:LEU:N	1:G:46:LEU:HD12	2.12	0.65
1:H:169:LEU:HD12	1:H:170:SER:N	2.12	0.65
1:H:455:VAL:O	1:H:459:ILE:HG12	1.97	0.65
1:H:46:LEU:N	1:H:46:LEU:HD12	2.12	0.65
1:I:128:PRO:O	1:I:132:ILE:HG12	1.96	0.65
1:I:455:VAL:O	1:I:459:ILE:HG12	1.97	0.65
1:B:210:VAL:HG23	1:B:382:LEU:CD1	2.26	0.65
1:B:525:ARG:HG2	1:B:525:ARG:HH11	1.61	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:A:423:ILE:HG21	1:A:473:LEU:HD12	1.78	0.65
1:B:259:GLU:OE1	1:B:260:LEU:N	2.30	0.65
1:B:46:LEU:N	1:B:46:LEU:HD12	2.12	0.65
1:C:46:LEU:HD12	1:C:46:LEU:N	2.12	0.65
1:D:128:PRO:O	1:D:132:ILE:HG12	1.97	0.65
1:E:128:PRO:O	1:E:132:ILE:HG12	1.97	0.65
1:F:220:THR:HG22	1:F:384:ARG:H	1.61	0.65
1:I:169:LEU:HD12	1:I:170:SER:N	2.12	0.65
1:A:121:LEU:O	1:A:126:VAL:HG22	1.97	0.65
1:A:127:HIS:CD2	1:A:129:THR:HB	2.31	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:D:245:LYS:N	1:D:296:ASN:ND2	2.41	0.65
1:D:46:LEU:N	1:D:46:LEU:HD12	2.12	0.65
1:F:455:VAL:O	1:F:459:ILE:HG12	1.97	0.65
1:A:210:VAL:HG23	1:A:382:LEU:CD1	2.26	0.65
1:B:473:LEU:O	1:B:476:THR:HG22	1.97	0.65
1:C:455:VAL:O	1:C:459:ILE:HG12	1.96	0.65
1:C:66:ILE:H	1:C:66:ILE:CD1	2.06	0.65
1:D:91:GLN:HE21	1:E:387:LEU:HD21	1.62	0.65
1:D:88:LEU:CD1	1:E:389:ARG:HH12	2.09	0.65
1:F:331:LEU:O	1:F:331:LEU:HD23	1.96	0.65
1:F:415:ILE:HG13	1:F:421:VAL:HG21	1.78	0.65
1:G:455:VAL:O	1:G:459:ILE:HG12	1.97	0.65
1:H:128:PRO:O	1:H:132:ILE:HG12	1.96	0.65
1:H:479:ASN:HB2	1:H:482:ASN:OD1	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:I:473:LEU:O	1:I:476:THR:HG22	1.97	0.65
1:A:331:LEU:O	1:A:331:LEU:HD23	1.96	0.65
1:C:331:LEU:HD23	1:C:331:LEU:O	1.96	0.65
1:C:220:THR:HG22	1:C:384:ARG:H	1.61	0.65
1:E:121:LEU:O	1:E:126:VAL:HG22	1.97	0.65
1:E:423:ILE:HG21	1:E:473:LEU:HD12	1.78	0.65
1:F:210:VAL:HG23	1:F:382:LEU:CD1	2.26	0.65
1:G:423:ILE:HG21	1:G:473:LEU:HD12	1.78	0.65
1:A:128:PRO:O	1:A:132:ILE:HG12	1.96	0.65
1:D:121:LEU:O	1:D:126:VAL:HG22	1.97	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: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:B:121:LEU:O	1:B:126:VAL:HG22	1.97	0.64
1:B:455:VAL:O	1:B:459:ILE:HG12	1.97	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:D:259:GLU:OE1	1:D:260:LEU:N	2.30	0.64
1:F:128:PRO:O	1:F:132:ILE:HG12	1.96	0.64
1:F:169:LEU:HD12	1:F:170:SER:N	2.12	0.64
1:H:121:LEU:O	1:H:126:VAL:HG22	1.97	0.64
1:I:479:ASN:HB2	1:I:482:ASN:OD1	1.96	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:C:269:PRO:HA	1:C:272:MET:CG	2.25	0.64
1:D:169:LEU:HD12	1:D:170:SER:N	2.12	0.64
1:I:259:GLU:OE1	1:I:260:LEU:N	2.30	0.64
1:B:245:LYS:N	1:B:296:ASN:ND2	2.41	0.64
1:C:260:LEU:C	1:C:260:LEU:HD12	2.17	0.64
1:C:525:ARG:HH11	1:C:525:ARG:HG2	1.60	0.64
1:E:259:GLU:OE1	1:E:260:LEU:N	2.30	0.64
1:F:525:ARG:HG2	1:F:525:ARG:HH11	1.61	0.64
1:G:128:PRO:O	1:G:132:ILE:HG12	1.96	0.64
1:H:473:LEU:O	1:H:476:THR:HG22	1.97	0.64
1:A:46:LEU:N	1:A:46:LEU:HD12	2.12	0.64
1:B:149:LEU:HD23	1:B:149:LEU:O	1.98	0.64
1:E:169:LEU:HD12	1:E:170:SER:N	2.12	0.64
1:E:473:LEU:O	1:E:476:THR:HG22	1.97	0.64
1:F:46:LEU:HD12	1:F:46:LEU:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:525:ARG:HH11	1:H:525:ARG:HG2	1.61	0.64
1:A:259:GLU:OE1	1:A:260:LEU:N	2.30	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:245:LYS:N	1:F:296:ASN:ND2	2.41	0.64
1:C:259:GLU:OE1	1:C:260:LEU:N	2.30	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:F:259:GLU:OE1	1:F:260:LEU:N	2.30	0.64
1:G:127:HIS:CD2	1:G:129:THR:HB	2.31	0.64
1:I:220:THR:HG22	1:I:384:ARG:H	1.61	0.64
1:A:231:GLU:HG3	1:A:366:LYS:HZ2	1.63	0.64
1:F:260:LEU:HD12	1:F:260:LEU:C	2.17	0.64
1:G:259:GLU:OE1	1:G:260:LEU:N	2.30	0.64
1:B:66:ILE:H	1:B:66:ILE:CD1	2.06	0.64
1:G:110:PHE:CE2	1:G:451:LEU:HG	2.33	0.64
1:H:66:ILE:H	1:H:66:ILE:CD1	2.06	0.64
1:B:169:LEU:HD12	1:B:170:SER:N	2.12	0.64
1:C:110:PHE:CE2	1:C:451:LEU:HG	2.33	0.64
1:G:220:THR:HG22	1:G:384:ARG:H	1.61	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:A:527:ASP:HB2	1:B:55:MET:HG3	1.80	0.63
1:G:155:ILE:HG21	1:G:200:TRP:CH2	2.34	0.63
1:D:284:LYS:HD3	1:D:311:TYR:HE2	1.64	0.63
1:D:415:ILE:HG13	1:D:421:VAL:HG21	1.78	0.63
1:E:527:ASP:HB3	1:F:57:LYS:NZ	2.13	0.63
1:G:149:LEU:HD23	1:G:149:LEU:O	1.98	0.63
1:C:149:LEU:O	1:C:149:LEU:HD23	1.98	0.63
1:C:245:LYS:N	1:C:296:ASN:ND2	2.41	0.63
1:C:284:LYS:HD3	1:C:311:TYR:HE2	1.64	0.63
1:F:266:ILE:HG21	1:F:272:MET:SD	2.39	0.63
1:F:110:PHE:CE2	1:F:451:LEU:HG	2.33	0.63
1:H:408:VAL:HG22	1:H:505:PRO:HG3	1.81	0.63
1:I:155:ILE:HG21	1:I:200:TRP:CH2	2.34	0.63
1:F:149:LEU:HD23	1:F:149:LEU:O	1.98	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:H:259:GLU:OE1	1:H:260:LEU:N	2.30	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:A:284:LYS:HD3	1:A:311:TYR:HE2	1.64	0.63
1:C:266:ILE:HG21	1:C:272:MET:SD	2.39	0.63
1:F:155:ILE:HG21	1:F:200:TRP:CH2	2.34	0.63
1:G:121:LEU:O	1:G:126:VAL:HG22	1.97	0.63
1:G:210:VAL:HG23	1:G:382:LEU:HD13	1.81	0.63
1:H:149:LEU:O	1:H:149:LEU:HD23	1.98	0.63
1:I:110:PHE:HE2	1:I:451:LEU:HG	1.64	0.63
1:I:149:LEU:O	1:I:149:LEU:HD23	1.98	0.63
1:B:110:PHE:CE2	1:B:451:LEU:HG	2.33	0.63
1:B:430:ARG:HG2	1:B:430:ARG:HH11	1.64	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:G:408:VAL:HG22	1:G:505:PRO:HG3	1.81	0.63
1:H:110:PHE:HE2	1:H:451:LEU:HG	1.64	0.63
1:I:266:ILE:HG21	1:I:272:MET:SD	2.39	0.63
1:B:266:ILE:HG21	1:B:272:MET:SD	2.39	0.63
1:E:110:PHE:HE2	1:E:451:LEU:HG	1.64	0.63
1:G:284:LYS:HD3	1:G:311:TYR:HE2	1.64	0.63
1:H:210:VAL:HG23	1:H:382:LEU:HD13	1.81	0.63
1:I:408:VAL:HG22	1:I:505:PRO:HG3	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:B:260:LEU:HD12	1:B:260:LEU:C	2.17	0.63
1:C:210:VAL:HG23	1:C:382:LEU:HD13	1.81	0.63
1:D:210:VAL:HG23	1:D:382:LEU:HD13	1.81	0.63
1:A:110:PHE:CE2	1:A:451:LEU:HG	2.33	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: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:C:155:ILE:HG21	1:C:200:TRP:CH2	2.34	0.62
1:D:110:PHE:HE2	1:D:451:LEU:HG	1.64	0.62
1:D:231:GLU:HG3	1:D:366:LYS:HZ2	1.64	0.62
1:D:408:VAL:HG22	1:D:505:PRO:HG3	1.81	0.62
1:F:129:THR:HG23	1:G:53:ARG:HH12	1.63	0.62
1:H:245:LYS:N	1:H:296:ASN:ND2	2.41	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:A:266:ILE:HG21	1:A:272:MET:SD	2.39	0.62
1:F:430:ARG:HH11	1:F:430:ARG:HG2	1.64	0.62
1:G:231:GLU:HG3	1:G:366:LYS:HZ2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:110:PHE:CE2	1:H:451:LEU:HG	2.33	0.62
1:I:284:LYS:HD3	1:I:311:TYR:HE2	1.64	0.62
1:I:430:ARG:HG2	1:I:430:ARG:HH11	1.64	0.62
1:B:210:VAL:HG23	1:B:382:LEU:HD13	1.81	0.62
1:B:260:LEU:HD12	1:B:261:ASP:CA	2.29	0.62
1:B:260:LEU:HD11	1:B:261:ASP:OD1	2.00	0.62
1:B:408:VAL:HG22	1:B:505:PRO:HG3	1.81	0.62
1:D:260:LEU:HD11	1:D:261:ASP:OD1	2.00	0.62
1:D:266:ILE:HG21	1:D:272:MET:SD	2.39	0.62
1:A:230:LYS:NZ	1:A:321:ARG:NH1	2.48	0.62
1:H:266:ILE:HG21	1:H:272:MET:SD	2.39	0.62
1:A:430:ARG:HG2	1:A:430:ARG:HH11	1.64	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: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:A:155:ILE:HG21	1:A:200:TRP:CH2	2.34	0.62
1:C:110:PHE:HE2	1:C:451:LEU:HG	1.64	0.62
1:C:260:LEU:HD11	1:C:261:ASP:OD1	2.00	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:G:230:LYS:NZ	1:G:321:ARG:NH1	2.48	0.62
1:H:260:LEU:HD11	1:H:261:ASP:OD1	2.00	0.62
1:H:231:GLU:HG3	1:H:366:LYS:HZ2	1.65	0.62
1:B:110:PHE:HE2	1:B:451:LEU:HG	1.64	0.62
1:E:220:THR:HG22	1:E:384:ARG:H	1.61	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:A:110:PHE:HE2	1:A:451:LEU:HG	1.64	0.62
1:G:297:VAL:HG23	1:G:318:LEU:O	2.00	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:E:284:LYS:HD3	1:E:311:TYR:HE2	1.64	0.62
1:F:210:VAL:HG23	1:F:382:LEU:HD13	1.81	0.62
1:B:297:VAL:HG23	1:B:318:LEU:O	2.00	0.61
1:C:260:LEU:HD12	1:C:261:ASP:CA	2.29	0.61
1:C:408:VAL:HG22	1:C:505:PRO:HG3	1.81	0.61
1:C:430:ARG:HG2	1:C:430:ARG:HH11	1.64	0.61
1:C:427:LYS:NZ	1:C:477:HIS:O	2.33	0.61
1:E:427:LYS:NZ	1:E:477:HIS:O	2.33	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:H:284:LYS:HD3	1:H:311:TYR:HE2	1.64	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:G:238:PRO:HB2	1:G:241:LEU:HD21	1.82	0.61
1:I:231:GLU:HG3	1:I:366:LYS:HZ2	1.65	0.61
1:A:297:VAL:HG23	1:A:318:LEU:O	2.00	0.61
1:E:230:LYS:NZ	1:E:321:ARG:NH1	2.48	0.61
1:F:105:LYS:O	1:F:109:ILE:HG12	2.00	0.61
1:H:105:LYS:O	1:H:109:ILE:HG12	2.00	0.61
1:I:105:LYS:O	1:I:109:ILE:HG12	2.00	0.61
1:A:105:LYS:O	1:A:109:ILE:HG12	2.00	0.61
1:C:297:VAL:HG23	1:C:318:LEU:O	2.00	0.61
1:B:88:LEU:HD22	1:C:58:MET:CE	2.31	0.61
1:D:238:PRO:HB2	1:D:241:LEU:HD21	1.82	0.61
1:D:427:LYS:NZ	1:D:477:HIS:O	2.33	0.61
1:F:110:PHE:HE2	1:F:451:LEU:HG	1.64	0.61
1:F:284:LYS:HD3	1:F:311:TYR:HE2	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:297:VAL:HG23	1:D:318:LEU:O	2.00	0.61
1:E:260:LEU:HD11	1:E:261:ASP:OD1	2.00	0.61
1:E:408:VAL:HG22	1:E:505:PRO:HG3	1.81	0.61
1:G:427:LYS:NZ	1:G:477:HIS:O	2.33	0.61
1:B:284:LYS:HD3	1:B:311:TYR:HE2	1.64	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:230:LYS:NZ	1:B:321:ARG:NH1	2.48	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: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:E:88:LEU:CD2	1:F:58:MET:CE	2.79	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:E:105:LYS:O	1:E:109:ILE:HG12	2.00	0.61
1:F:297:VAL:HG23	1:F:318:LEU:O	2.00	0.61
1:I:245:LYS:N	1:I:296:ASN:ND2	2.41	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:A:207:ILE:HA	1:A:379:ILE:O	2.02	0.60
1:H:427:LYS:NZ	1:H:477:HIS:O	2.33	0.60
1:I:260:LEU:HD12	1:I:261:ASP:CA	2.29	0.60
1:D:105:LYS:O	1:D:109:ILE:HG12	2.00	0.60
1:E:502:VAL:O	1:E:502:VAL:HG12	2.02	0.60
1:G:260:LEU:HD12	1:G:261:ASP:CA	2.29	0.60
1:I:207:ILE:HA	1:I:379:ILE:O	2.02	0.60
1:B:358:GLU:HG3	1:B:360:ARG:HH22	1.67	0.60
1:C:238:PRO:HB2	1:C:241:LEU:HD21	1.82	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:105:LYS:O	1:C:109:ILE:HG12	2.00	0.60
1:F:427:LYS:NZ	1:F:477:HIS:O	2.33	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: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:D:207:ILE:HA	1:D:379:ILE:O	2.02	0.60
1:G:529:VAL:HG12	1:H:58:MET:HB3	1.84	0.60
1:B:105:LYS:O	1:B:109:ILE:HG12	2.00	0.60
1:E:231:GLU:HG3	1:E:366:LYS:HZ2	1.66	0.60
1:E:238:PRO:HB2	1:E:241:LEU:HD21	1.82	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:A:119:GLU:HA	1:A:122:LEU:HD23	1.84	0.60
1:A:210:VAL:HG23	1:A:382:LEU:HD13	1.81	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:F:238:PRO:HB2	1:F:241:LEU:HD21	1.82	0.60
1:F:260:LEU:HD11	1:F:261:ASP:OD1	2.00	0.60
1:G:119:GLU:HA	1:G:122:LEU:HD23	1.84	0.60
1:H:260:LEU:HD12	1:H:260:LEU:C	2.17	0.60
1:H:358:GLU:HG3	1:H:360:ARG:HH22	1.67	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:O	1:H:502:VAL:HG12	2.02	0.60
1:B:207:ILE:HA	1:B:379:ILE:O	2.02	0.59
1:B:432:TYR:O	1:B:435:GLN:HG2	2.02	0.59
1:B:502:VAL:HG12	1:B:502:VAL:O	2.02	0.59
1:C:432:TYR:O	1:C:435:GLN:HG2	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:I:415:ILE:HG23	1:I:506:ALA:HB2	1.84	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:B:119:GLU:HA	1:B:122:LEU:HD23	1.84	0.59
1:E:297:VAL:HG23	1:E:318:LEU:O	2.00	0.59
1:E:415:ILE:HG23	1:E:506:ALA:HB2	1.84	0.59
1:G:324:LYS:O	1:G:327:ASP:OD2	2.21	0.59
1:C:207:ILE:HA	1:C:379:ILE:O	2.02	0.59
1:E:324:LYS:O	1:E:327:ASP:OD2	2.21	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:A:161:LEU:HD12	1:A:161:LEU:N	2.17	0.59
1:C:161:LEU:N	1:C:161:LEU:HD12	2.17	0.59
1:C:502:VAL:HG12	1:C:502:VAL:O	2.02	0.59
1:E:161:LEU:HD12	1:E:161:LEU:N	2.17	0.59
1:F:161:LEU:HD12	1:F:161:LEU:N	2.17	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:H:415:ILE:HG23	1:H:506:ALA:HB2	1.84	0.59
1:I:502:VAL:O	1:I:502:VAL:HG12	2.02	0.59
1:E:207:ILE:HA	1:E:379:ILE:O	2.02	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:A:358:GLU:HG3	1:A:360:ARG:HH22	1.67	0.59
1:B:324:LYS:O	1:B:327:ASP:OD2	2.21	0.59
1:C:358:GLU:HG3	1:C:360:ARG:HH22	1.67	0.59
1:D:502:VAL:O	1:D:502:VAL:HG12	2.02	0.59
1:E:358:GLU:HG3	1:E:360:ARG:HH22	1.67	0.59
1:F:207:ILE:HA	1:F:379:ILE:O	2.02	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:I:432:TYR:O	1:I:435:GLN:HG2	2.03	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:D:432:TYR:O	1:D:435:GLN:HG2	2.03	0.58

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:GLN:HE21	1:F:413:ARG:HH22	1.53	0.57
1:F:166:MET:HE1	1:F:179:GLU:HG2	1.87	0.57
1:F:265:ARG:O	1:F:266:ILE:HG12	2.04	0.57
1:F:299:ILE:HD13	1:F:299:ILE:N	2.20	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:A:162:ARG:HH11	1:A:162:ARG:HB2	1.70	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:H:147:GLN:HE21	1:H:413:ARG:HH22	1.53	0.56
1:H:260:LEU:HD12	1:H:261:ASP:CA	2.29	0.56
1:A:147:GLN:HE21	1:A:413:ARG:HH22	1.53	0.56
1:D:245:LYS:HG2	1:D:353:TYR:CD1	2.40	0.56
1:D:508:VAL:HG13	1:D:509:LYS:N	2.20	0.56
1:E:244:ALA:HA	1:E:296:ASN:ND2	2.21	0.56
1:H:244:ALA:HA	1:H:296:ASN:ND2	2.21	0.56
1:I:462:ALA:HB2	1:I:489:LEU:HD12	1.87	0.56
1:A:226:ILE:HG13	1:A:331:LEU:HA	1.86	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:D:462:ALA:HB2	1:D:489:LEU:HD12	1.87	0.56
1:E:142:ALA:HA	1:E:425:ILE:HG23	1.86	0.56
1:E:98:GLU:HG3	1:E:99:GLU:H	1.69	0.56
1:G:256:GLU:C	1:G:258:PRO:HD3	2.22	0.56
1:H:462:ALA:HB2	1:H:489:LEU:HD12	1.87	0.56
1:A:265:ARG:O	1:A:266:ILE:HG12	2.04	0.56
1:A:520:ALA:O	1:A:524:LEU:HD13	2.05	0.56
1:B:147:GLN:HE21	1:B:413:ARG:HH22	1.53	0.56
1:B:226:ILE:HG13	1:B:331:LEU:HA	1.86	0.56
1:D:232:VAL:CG1	1:D:318:LEU:HD11	2.34	0.56
1:F:244:ALA:HA	1:F:296:ASN:ND2	2.21	0.56
1:F:508:VAL:HG13	1:F:509:LYS:N	2.20	0.56
1:F:520:ALA:O	1:F:524:LEU:HD13	2.05	0.56
1:E:88:LEU:HD23	1:F:58:MET:HE1	1.86	0.56
1:F:98:GLU:HG3	1:F:99:GLU:H	1.69	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:I:147:GLN:HE21	1:I:413:ARG:HH22	1.53	0.56
1:I:98:GLU:HG3	1:I:99:GLU:H	1.69	0.56
1:A:508:VAL:HG13	1:A:509:LYS:N	2.20	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:I:88:LEU:O	1:I:92:ILE:HG13	2.06	0.56
1:A:244:ALA:HA	1:A:296:ASN:ND2	2.21	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: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: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:G:520:ALA:O	1:G:524:LEU:HD13	2.05	0.56
1:I:508:VAL:HG13	1:I:509:LYS:N	2.20	0.56
1:I:520:ALA:O	1:I:524:LEU:HD13	2.05	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:B:520:ALA:O	1:B:524:LEU:HD13	2.05	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:H:520:ALA:O	1:H:524:LEU:HD13	2.05	0.56
1:I:244:ALA:HA	1:I:296:ASN:ND2	2.20	0.56
1:I:443:ALA:O	1:I:446:ALA:HB3	2.06	0.56
1:A:99:GLU:HG3	1:A:407:ASP:OD2	2.06	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:E:260:LEU:HD12	1:E:261:ASP:CA	2.29	0.56
1:E:99:GLU:HG3	1:E:407:ASP:OD2	2.06	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:B:127:HIS:HD2	1:B:129:THR:HB	1.69	0.56
1:B:244:ALA:HA	1:B:296:ASN:ND2	2.20	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:E:88:LEU:O	1:E:92:ILE:HG13	2.05	0.56
1:G:443:ALA:O	1:G:446:ALA:HB3	2.06	0.56
1:H:180:TYR:O	1:H:184:ILE:HG12	2.06	0.56
1:A:443:ALA:O	1:A:446:ALA:HB3	2.06	0.56
1:A:98:GLU:HG3	1:A:99:GLU:H	1.69	0.56
1:B:462:ALA:HB2	1:B:489:LEU:HD12	1.87	0.56
1:C:443:ALA:O	1:C:446:ALA:HB3	2.06	0.56
1:D:88:LEU:O	1:D:92:ILE:HG13	2.06	0.56
1:E:383:ILE:HG22	1:E:391:VAL:HG23	1.87	0.56
1:E:88:LEU:HD22	1:F:58:MET:CE	2.36	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:F:88:LEU:O	1:F:92:ILE:HG13	2.06	0.56
1:G:88:LEU:O	1:G:92:ILE:HG13	2.06	0.56
1:G:98:GLU:HG3	1:G:99:GLU:H	1.69	0.56
1:H:232:VAL:CG1	1:H:318:LEU:HD11	2.34	0.56
1:H:430:ARG:O	1:H:434:PRO:HD3	2.06	0.56
1:A:126:VAL:HG23	1:A:126:VAL:O	2.06	0.56
1:C:192:VAL:HG11	1:C:206:ASN:HB2	1.88	0.56
1:C:299:ILE:HD13	1:C:299:ILE:N	2.20	0.56
1:D:244:ALA:HA	1:D:296:ASN:ND2	2.21	0.56
1:D:443:ALA:O	1:D:446:ALA:HB3	2.06	0.56
1:E:39:VAL:HG13	1:E:89:LEU:HD22	1.88	0.56
1:F:126:VAL:O	1:F:126:VAL:HG23	2.06	0.56
1:F:153:VAL:CG2	1:F:160:LEU:HD23	2.33	0.56
1:F:99:GLU:HG3	1:F:407:ASP:OD2	2.06	0.56
1:F:142:ALA:HA	1:F:425:ILE:HG23	1.86	0.56
1:F:462:ALA:HB2	1:F:489:LEU:HD12	1.87	0.56
1:H:99:GLU:HG3	1:H:407:ASP:OD2	2.06	0.56
1:H:443:ALA:O	1:H:446:ALA:HB3	2.06	0.56
1:B:39:VAL:HG13	1:B:89:LEU:HD22	1.88	0.55
1:C:470:LEU:CD2	1:C:474:ARG:HD2	2.37	0.55
1:D:383:ILE:HG22	1:D:391:VAL:HG23	1.87	0.55
1:D:470:LEU:CD2	1:D:474:ARG:HD2	2.37	0.55
1:G:244:ALA:HA	1:G:296:ASN:ND2	2.20	0.55
1:H:470:LEU:CD2	1:H:474:ARG:HD2	2.37	0.55
1:I:162:ARG:HH11	1:I:162:ARG:HB2	1.70	0.55
1:I:180:TYR:O	1:I:184:ILE:HG12	2.06	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:B:470:LEU:CD2	1:B:474:ARG:HD2	2.37	0.55
1:C:462:ALA:HB2	1:C:489:LEU:HD12	1.87	0.55
1:C:508:VAL:HG13	1:C:509:LYS:N	2.20	0.55
1:C:88:LEU:O	1:C:92:ILE:HG13	2.06	0.55
1:D:430:ARG:O	1:D:434:PRO:HD3	2.06	0.55
1:E:470:LEU:CD2	1:E:474:ARG:HD2	2.37	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:I:126:VAL:O	1:I:126:VAL:HG23	2.06	0.55
1:I:363:GLY:HA2	1:I:384:ARG:NH2	2.21	0.55
1:A:430:ARG:O	1:A:434:PRO:HD3	2.06	0.55
1:B:192:VAL:HG11	1:B:206:ASN:HB2	1.88	0.55
1:B:508:VAL:HG13	1:B:509:LYS:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:ALA:HA	1:C:296:ASN:ND2	2.21	0.55
1:B:88:LEU:CD2	1:C:58:MET:HE1	2.35	0.55
1:D:363:GLY:HA2	1:D:384:ARG:NH2	2.21	0.55
1:G:212:LYS:HA	1:G:212:LYS:CE	2.33	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:I:430:ARG:O	1:I:434:PRO:HD3	2.06	0.55
1:A:180:TYR:O	1:A:184:ILE:HG12	2.06	0.55
1:C:363:GLY:HA2	1:C:384:ARG:NH2	2.21	0.55
1:C:430:ARG:O	1:C:434:PRO:HD3	2.06	0.55
1:D:192:VAL:HG11	1:D:206:ASN:HB2	1.88	0.55
1:E:126:VAL:HG23	1:E:126:VAL:O	2.06	0.55
1:E:63:LEU:HD23	1:E:63:LEU:O	2.06	0.55
1:F:192:VAL:HG11	1:F:206:ASN:HB2	1.88	0.55
1:F:230:LYS:HZ1	1:F:321:ARG:NH1	2.04	0.55
1:F:383:ILE:HG22	1:F:391:VAL:HG23	1.87	0.55
1:F:63:LEU:HD23	1:F:63:LEU:O	2.06	0.55
1:G:299:ILE:HD13	1:G:299:ILE:N	2.20	0.55
1:H:255:VAL:HG13	1:H:305:ASP:OD1	2.07	0.55
1:I:351:LEU:CD2	1:I:351:LEU:H	2.17	0.55
1:I:39:VAL:HG13	1:I:89:LEU:HD22	1.88	0.55
1:A:462:ALA:HB2	1:A:489:LEU:HD12	1.87	0.55
1:A:63:LEU:O	1:A:63:LEU:HD23	2.06	0.55
1:D:126:VAL:HG23	1:D:126:VAL:O	2.06	0.55
1:D:162:ARG:HB2	1:D:162:ARG:HH11	1.70	0.55
1:D:39:VAL:HG13	1:D:89:LEU:HD22	1.88	0.55
1:E:430:ARG:O	1:E:434:PRO:HD3	2.06	0.55
1:F:363:GLY:HA2	1:F:384:ARG:NH2	2.21	0.55
1:F:443:ALA:O	1:F:446:ALA:HB3	2.06	0.55
1:F:470:LEU:CD2	1:F:474:ARG:HD2	2.37	0.55
1:G:192:VAL:HG11	1:G:206:ASN:HB2	1.88	0.55
1:G:255:VAL:HG13	1:G:305:ASP:OD1	2.07	0.55
1:G:508:VAL:HG13	1:G:509:LYS:N	2.20	0.55
1:H:363:GLY:HA2	1:H:384:ARG:NH2	2.21	0.55
1:I:470:LEU:CD2	1:I:474:ARG:HD2	2.37	0.55
1:I:63:LEU:HD23	1:I:63:LEU:O	2.06	0.55
1:A:470:LEU:CD2	1:A:474:ARG:HD2	2.37	0.55
1:A:39:VAL:HG13	1:A:89:LEU:HD22	1.88	0.55
1:B:162:ARG:HB2	1:B:162:ARG:HH11	1.70	0.55
1:B:363:GLY:HA2	1:B:384:ARG:NH2	2.21	0.55
1:C:256:GLU:C	1:C:258:PRO:HD3	2.22	0.55

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:VAL:HG22	1:G:359:GLU:OE2	2.07	0.54
1:G:423:ILE:HD12	1:G:424:GLU:HG2	1.89	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:B:63:LEU:O	1:B:63:LEU:HD23	2.06	0.54
1:C:178:ARG:H	1:C:178:ARG:HE	1.55	0.54
1:C:39:VAL:HG13	1:C:89:LEU:HD22	1.88	0.54
1:E:111:SER:O	1:E:115:VAL:HG23	2.08	0.54
1:E:347:SER:C	1:E:349:GLN:H	2.11	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: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:C:63:LEU:HD23	1:C:63:LEU:O	2.06	0.54
1:D:63:LEU:HD23	1:D:63:LEU:O	2.06	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: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: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:192:VAL:HG11	1:A:206:ASN:HB2	1.88	0.54
1:B:111:SER:O	1:B:115:VAL:HG23	2.08	0.54
1:B:487:ILE:O	1:B:489:LEU:HD22	2.08	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:H:192:VAL:HG11	1:H:206:ASN:HB2	1.88	0.54
1:H:230:LYS:HZ1	1:H:321:ARG:NH1	2.05	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:I:299:ILE:HD13	1:I:299:ILE:N	2.20	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:C:487:ILE:O	1:C:489:LEU:HD22	2.08	0.54
1:D:178:ARG:HE	1:D:178:ARG:H	1.55	0.54
1:F:39:VAL:HG13	1:F:89:LEU:HD22	1.88	0.54
1:G:347:SER:C	1:G:349:GLN:H	2.11	0.54
1:G:39:VAL:HG13	1:G:89:LEU:HD22	1.88	0.54
1:H:39:VAL:HG13	1:H:89:LEU:HD22	1.88	0.54
1:A:255:VAL:HG13	1:A:305:ASP:OD1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:299:ILE:N	1:E:299:ILE:HD13	2.20	0.54
1:I:255:VAL:HG13	1:I:305:ASP:OD1	2.07	0.54
1:A:111:SER:O	1:A:115:VAL:HG23	2.08	0.54
1:A:383:ILE:N	1:A:383:ILE:HD12	2.22	0.54
1:B:181:ILE:O	1:B:185:VAL:HG23	2.08	0.54
1:B:383:ILE:N	1:B:383:ILE:HD12	2.22	0.54
1:D:351:LEU:H	1:D:351:LEU:CD2	2.17	0.54
1:D:529:VAL:HG12	1:E:58:MET:SD	2.48	0.54
1:F:383:ILE:N	1:F:383:ILE:HD12	2.22	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:I:256:GLU:C	1:I:258:PRO:HD3	2.22	0.54
1:I:232:VAL:HG22	1:I:359:GLU:OE2	2.07	0.54
1:B:347:SER:C	1:B:349:GLN:H	2.11	0.54
1:C:265:ARG:HD2	1:C:266:ILE:N	2.23	0.54
1:C:284:LYS:HD3	1:C:311:TYR:CE2	2.43	0.54
1:C:347:SER:C	1:C:349:GLN:H	2.11	0.54
1:C:470:LEU:HD22	1:C:474:ARG:HD2	1.90	0.54
1:E:255:VAL:HG13	1:E:305:ASP:OD1	2.07	0.54
1:G:470:LEU:HD22	1:G:474:ARG:HD2	1.90	0.54
1:H:284:LYS:HD3	1:H:311:TYR:CE2	2.43	0.54
1:H:482:ASN:O	1:H:483:LYS:C	2.47	0.54
1:D:118:ALA:O	1:D:122:LEU:HD22	2.08	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: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:B:351:LEU:CD2	1:B:351:LEU:H	2.17	0.53
1:B:76:LEU:CD2	1:B:90:VAL:HG12	2.36	0.53
1:C:233:VAL:HG22	1:C:309:GLN:OE1	2.08	0.53
1:D:423:ILE:HD12	1:D:424:GLU:HG2	1.90	0.53
1:D:504:GLU:OE1	2:D:800:ADP:H2'	2.09	0.53
1:E:192:VAL:HG11	1:E:206:ASN:HB2	1.88	0.53
1:E:423:ILE:HD12	1:E:424:GLU:HG2	1.90	0.53
1:D:530:VAL:O	1:E:59:LEU:HD23	2.07	0.53
1:G:111:SER:O	1:G:115:VAL:HG23	2.08	0.53
1:G:482:ASN:O	1:G:483:LYS:C	2.47	0.53
1:A:265:ARG:HD2	1:A:266:ILE:N	2.23	0.53
1:C:423:ILE:HD12	1:C:424:GLU:HG2	1.90	0.53
1:E:118:ALA:O	1:E:122:LEU:HD22	2.08	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:E:232:VAL:HG22	1:E:359:GLU:OE2	2.07	0.53
1:E:470:LEU:HD22	1:E:474:ARG:HD2	1.90	0.53
1:F:111:SER:O	1:F:115:VAL:HG23	2.08	0.53
1:F:470:LEU:HD22	1:F:474:ARG:HD2	1.90	0.53
1:G:383:ILE:N	1:G:383:ILE:HD12	2.22	0.53
1:H:487:ILE:O	1:H:489:LEU:HD22	2.08	0.53
1:I:347:SER:C	1:I:349:GLN:H	2.11	0.53
1:B:284:LYS:HD3	1:B:311:TYR:CE2	2.43	0.53
1:D:111:SER:O	1:D:115:VAL:HG23	2.08	0.53
1:F:529:VAL:HG12	1:G:58:MET:SD	2.47	0.53
1:G:178:ARG:H	1:G:178:ARG:HE	1.55	0.53
1:G:361:LYS:CB	1:G:366:LYS:HG2	2.36	0.53
1:G:524:LEU:HD12	1:G:524:LEU:N	2.24	0.53
1:I:504:GLU:OE1	2:I:800:ADP:H2'	2.09	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:F:284:LYS:HD3	1:F:311:TYR:CE2	2.43	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:A:423:ILE:HD12	1:A:424:GLU:HG2	1.90	0.53
1:B:185:VAL:O	1:B:189:VAL:HG23	2.09	0.53
1:C:111:SER:O	1:C:115:VAL:HG23	2.08	0.53
1:D:470:LEU:HD22	1:D: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:N	1:F:524:LEU:HD12	2.24	0.53
1:G:487:ILE:O	1:G:489:LEU:HD22	2.08	0.53
1:H:347:SER:C	1:H:349:GLN:H	2.11	0.53
1:I:181:ILE:O	1:I:185:VAL:HG23	2.08	0.53
1:I:265:ARG:HD2	1:I:266:ILE:N	2.23	0.53
1:I:423:ILE:HD12	1:I:424:GLU:HG2	1.90	0.53
1:I:470:LEU:HD22	1:I:474:ARG:HD2	1.90	0.53
1:B:265:ARG:HD2	1:B:266:ILE:N	2.23	0.53
1:B:423:ILE:HD12	1:B:424:GLU:HG2	1.90	0.53
1:C:118:ALA:O	1:C:122:LEU:HD22	2.08	0.53
1:C:351:LEU:CD2	1:C:351:LEU:H	2.17	0.53
1:C:524:LEU:HD12	1:C:524:LEU:N	2.24	0.53
1:D:66:ILE:HD13	1:D:66:ILE:N	2.13	0.53
1:E:162:ARG:HH11	1:E:162:ARG:HB2	1.70	0.53
1:E:178:ARG:H	1:E:178:ARG:HE	1.55	0.53
1:E:265:ARG:HD2	1:E:266:ILE:N	2.23	0.53
1:E:524:LEU:HD12	1:E:524:LEU:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:VAL:O	1:F:189:VAL:HG23	2.09	0.53
1:F:58:MET:HG3	1:F:68:ILE:HG22	1.91	0.53
1:I:111:SER:O	1:I:115:VAL:HG23	2.08	0.53
1:I:118:ALA:O	1:I:122:LEU:HD22	2.08	0.53
1:B:482:ASN:O	1:B:483:LYS:C	2.47	0.53
1:D:265:ARG:HD2	1:D:266:ILE:N	2.23	0.53
1:D:58:MET:HG3	1:D:68:ILE:HG22	1.91	0.53
1:E:181:ILE:O	1:E:185:VAL:HG23	2.08	0.53
1:F:181:ILE:O	1:F: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:G:504:GLU:OE1	2:G:800:ADP:H2'	2.09	0.53
1:H:181:ILE:O	1:H:185:VAL:HG23	2.08	0.53
1:I:231:GLU:HG3	1:I:366:LYS:NZ	2.24	0.53
1:A:284:LYS:HD3	1:A:311:TYR:CE2	2.43	0.53
1:A:504:GLU:OE1	2:A:800:ADP:H2'	2.09	0.53
1:C:185:VAL:O	1:C:189:VAL:HG23	2.09	0.53
1:C:230:LYS:HZ1	1:C:321:ARG:NH1	2.05	0.53
1:D:181:ILE:O	1:D:185:VAL:HG23	2.08	0.53
1:F:212:LYS:CE	1:F:212:LYS:HA	2.33	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:178:ARG:HE	1:H:178:ARG:H	1.55	0.53
1:H:233:VAL:HG22	1:H:309:GLN:OE1	2.09	0.53
1:H:265:ARG:HD2	1:H:266:ILE:N	2.23	0.53
1:H:423:ILE:CD1	1:H:424:GLU:HG2	2.39	0.53
1:G:530:VAL:O	1:H:59:LEU:HD23	2.08	0.53
1:I:185:VAL:O	1:I:189:VAL:HG23	2.09	0.53
1:B:233:VAL:HG22	1:B:309:GLN:OE1	2.08	0.53
1:C:361:LYS:CB	1:C:366:LYS:HG2	2.36	0.53
1:C:58:MET:HG3	1:C:68:ILE:HG22	1.91	0.53
1:E:185:VAL:O	1:E:189:VAL:HG23	2.09	0.53
1:E:361:LYS:CB	1:E:366:LYS:HG2	2.36	0.53
1:E:482:ASN:O	1:E:483:LYS:C	2.47	0.53
1:E:504:GLU:OE1	2:E:800:ADP:H2'	2.09	0.53
1:G:284:LYS:HD3	1:G:311:TYR:CE2	2.43	0.53
1:A:118:ALA:O	1:A:122:LEU:HD22	2.08	0.53
1:A:423:ILE:CD1	1:A:424:GLU:HG2	2.39	0.53
1:B:470:LEU:HD22	1:B:474:ARG:HD2	1.90	0.53
1:D:233:VAL:HG22	1:D:309:GLN:OE1	2.09	0.53
1:D:347:SER:C	1:D:349:GLN:H	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:504:GLU:OE1	2:F:800:ADP:H2'	2.09	0.53
1:G:423:ILE:CD1	1:G:424:GLU:HG2	2.39	0.53
1:H:244:ALA:C	1:H:296:ASN:HD22	2.12	0.53
1:H:58:MET:HG3	1:H:68:ILE:HG22	1.91	0.53
1:I:212:LYS:HA	1:I:212:LYS:CE	2.33	0.53
1:A:482:ASN:O	1:A:483:LYS:C	2.47	0.52
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:H:118:ALA:O	1:H:122:LEU:HD22	2.08	0.52
1:B:230:LYS:HZ2	1:B:321:ARG:NH1	2.07	0.52
1:B:423:ILE:CD1	1:B:424:GLU:HG2	2.39	0.52
1:C:482:ASN:O	1:C:483:LYS:C	2.47	0.52
1:E:231:GLU:HG3	1:E:366:LYS:NZ	2.24	0.52
1:E:58:MET:HG3	1:E:68:ILE:HG22	1.91	0.52
1:I:233:VAL:HG22	1:I:309:GLN:OE1	2.09	0.52
1:A:233:VAL:HG22	1:A:309:GLN:OE1	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:F:363:GLY:HA2	1:F:384:ARG:HH22	1.75	0.52
1:G:233:VAL:HG22	1:G:309:GLN:OE1	2.08	0.52
1:H:185:VAL:O	1:H:189:VAL:HG23	2.09	0.52
1:H:363:GLY:HA2	1:H:384:ARG:HH22	1.74	0.52
1:A:185:VAL:O	1:A:189:VAL:HG23	2.09	0.52
1:B:524:LEU:HD12	1:B:524:LEU:N	2.24	0.52
1:C:231:GLU:HG3	1:C:366:LYS:NZ	2.24	0.52
1:D:244:ALA:C	1:D:296:ASN:HD22	2.12	0.52
1:D:423:ILE:HD12	1:D:423:ILE:C	2.30	0.52
1:D:524:LEU:N	1:D:524:LEU:HD12	2.24	0.52
1:G:58:MET:HG3	1:G:68:ILE:HG22	1.91	0.52
1:H:166:MET:HE1	1:H:179:GLU:HG2	1.92	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:I:423:ILE:CD1	1:I:424:GLU:HG2	2.39	0.52
1:A:181:ILE:O	1:A:185:VAL:HG23	2.08	0.52
1:A:231:GLU:HG3	1:A:366:LYS:NZ	2.24	0.52
1:A:272:MET:O	1:A:275:PHE:HB3	2.10	0.52
1:B:272:MET:O	1:B:275:PHE:HB3	2.10	0.52
1:D:306:GLU:HA	1:D:309:GLN:NE2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:234:HIS:CD2	1:E:236:GLY:H	2.28	0.52
1:F:234:HIS:CD2	1:F:236:GLY:H	2.28	0.52
1:F:272:MET:O	1:F:275:PHE:HB3	2.10	0.52
1:F:233:VAL:HG22	1:F:309:GLN:OE1	2.08	0.52
1:G:272:MET:O	1:G:275:PHE:HB3	2.10	0.52
1:G:306:GLU:HA	1:G:309:GLN:NE2	2.25	0.52
1:H:504:GLU:OE1	2:H:800:ADP:H2'	2.09	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:A:470:LEU:HD22	1:A:474:ARG:HD2	1.90	0.52
1:C:423:ILE:CD1	1:C:424:GLU:HG2	2.39	0.52
1:D:185:VAL:O	1:D:189:VAL:HG23	2.09	0.52
1:D:234:HIS:CD2	1:D:236:GLY:H	2.28	0.52
1:E:162:ARG:HH11	1:E:162:ARG:CB	2.23	0.52
1:F:423:ILE:CD1	1:F:424:GLU:HG2	2.39	0.52
1:H:361:LYS:CB	1:H:366:LYS:HG2	2.36	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:A:524:LEU:N	1:A:524:LEU:HD12	2.24	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:127:HIS:ND1	1:G:128:PRO:HD2	2.25	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:G:363:GLY:HA2	1:G:384:ARG:HH22	1.74	0.52
1:A:256:GLU:C	1:A:258:PRO:HD3	2.22	0.52
1:B:361:LYS:CB	1:B:366:LYS:HG2	2.36	0.52
1:B:504:GLU:OE1	2:B:800:ADP:H2'	2.09	0.52
1:C:234:HIS:CD2	1:C:236:GLY:H	2.28	0.52
1:D:361:LYS:CB	1:D:366:LYS:HG2	2.36	0.52
1:D:423:ILE:CD1	1:D:424:GLU:HG2	2.39	0.52
1:E:360:ARG:NH1	1:E:371:GLU:OE2	2.43	0.52
1:F:244:ALA:C	1:F:296:ASN:HD22	2.12	0.52
1:F:231:GLU:HG3	1:F:366:LYS:NZ	2.24	0.52
1:F:360:ARG:NH1	1:F:371:GLU:OE2	2.43	0.52
1:I:76:LEU:CD2	1:I:90:VAL:HG12	2.36	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:C:230:LYS:HZ1	1:C:321:ARG:HH12	1.58	0.52
1:C:423:ILE:HD12	1:C:423:ILE:C	2.30	0.52
1:D:363:GLY:HA2	1:D:384:ARG:HH22	1.74	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:H:306:GLU:HA	1:H:309:GLN:NE2	2.25	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:C:504:GLU:OE1	2:C:800:ADP:H2'	2.09	0.52
1:G:162:ARG:HH11	1:G:162:ARG:CB	2.23	0.52
1:G:68:ILE:HG13	1:G:68:ILE:O	2.10	0.52
1:A:127:HIS:ND1	1:A:128:PRO:HD2	2.25	0.51
1:B:234:HIS:CD2	1:B:236:GLY:H	2.28	0.51
1:C:272:MET:O	1:C:275:PHE:HB3	2.10	0.51
1:C:68:ILE:HG13	1:C:68:ILE:O	2.10	0.51
1:D:272:MET:O	1:D:275:PHE:HB3	2.10	0.51
1:E:306:GLU:HA	1:E:309:GLN:NE2	2.25	0.51
1:E:423:ILE:HD11	1:E:477:HIS:NE2	2.26	0.51
1:A:363:GLY:HA2	1:A:384:ARG:HH22	1.75	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:G:66:ILE:N	1:G:66:ILE:HD13	2.14	0.51
1:H:234:HIS:CD2	1:H:236:GLY:H	2.28	0.51
1:H:423:ILE:C	1:H:423:ILE:HD12	2.30	0.51
1:H:470:LEU:HD22	1:H:474:ARG:HD2	1.90	0.51
1:I:306:GLU:HA	1:I:309:GLN:NE2	2.25	0.51
1:I:58:MET:HG3	1:I:68:ILE:HG22	1.91	0.51
1:E:363:GLY:HA2	1:E:384:ARG:HH22	1.75	0.51
1:H:212:LYS:HA	1:H:212:LYS:CE	2.33	0.51
1:H:423:ILE:HD11	1:H:477:HIS:NE2	2.26	0.51
1:I:127:HIS:ND1	1:I:128:PRO:HD2	2.25	0.51
1:I:363:GLY:HA2	1:I:384:ARG:HH22	1.75	0.51
1:B:363:GLY:HA2	1:B:384:ARG:HH22	1.75	0.51
1:B:423:ILE:HD11	1:B:477:HIS:NE2	2.26	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:A:360:ARG:NH1	1:A:371:GLU:OE2	2.43	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:D:423:ILE:HD11	1:D:477:HIS:NE2	2.26	0.51
1:E:68:ILE:HG13	1:E:68:ILE:O	2.10	0.51
1:I:272:MET:O	1:I:275:PHE:HB3	2.10	0.51
1:A:162:ARG:HH11	1:A:162:ARG:CB	2.23	0.51

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:255:VAL:HA	1:H:283:ILE:CD1	2.41	0.51
1:I:245:LYS:HG2	1:I:353:TYR:HD1	1.76	0.51
1:A:234:HIS:CD2	1:A:236:GLY:H	2.28	0.50
1:B:161:LEU:HD12	1:B:161:LEU:H	1.77	0.50
1:B:163:LYS:HD3	1:B:501:GLY:HA2	1.93	0.50
1:C:166:MET:HE1	1:C:179:GLU:HG2	1.93	0.50
1:C:245:LYS:HG2	1:C:353:TYR:HD1	1.76	0.50
1:C:244:ALA:C	1:C:296:ASN:HD22	2.12	0.50
1:C:505:PRO:O	1:C:508:VAL:HG12	2.12	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:D:231:GLU:HG3	1:D:366:LYS:NZ	2.24	0.50
1:D:71:ASP:O	1:D:75:ILE:HG12	2.11	0.50
1:F:415:ILE:O	1:F:503:ILE:HG23	2.11	0.50
1:G:231:GLU:HG3	1:G:366:LYS:NZ	2.24	0.50
1:G:415:ILE:O	1:G:503:ILE:HG23	2.11	0.50
1:I:108:VAL:O	1:I:111:SER:HB3	2.11	0.50
1:I:280:GLU:O	1:I:284:LYS:HG3	2.12	0.50
1:C:255:VAL:HA	1:C:283:ILE:CD1	2.41	0.50
1:D:34:ALA:O	1:D:37:ALA:HB3	2.12	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:F:208:GLN:HE22	1:F:227:VAL:H	1.60	0.50
1:F:306:GLU:HA	1:F:309:GLN:NE2	2.25	0.50
1:G:71:ASP:O	1:G:75:ILE:HG12	2.11	0.50
1:G:76:LEU:CD2	1:G:90:VAL:HG12	2.36	0.50
1:H:280:GLU:O	1:H:284:LYS:HG3	2.12	0.50
1:H:415:ILE:O	1:H:503:ILE:HG23	2.11	0.50
1:I:505:PRO:O	1:I:508:VAL:HG12	2.11	0.50
1:A:280:GLU:O	1:A:284:LYS:HG3	2.12	0.50
1:A:306:GLU:HA	1:A:309:GLN:NE2	2.25	0.50
1:A:479:ASN:CB	1:A:482:ASN:OD1	2.59	0.50
1:A:71:ASP:O	1:A:75:ILE:HG12	2.11	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:G:208:GLN:HE22	1:G:227:VAL:H	1.60	0.50
1:G:245:LYS:HG2	1:G:353:TYR:HD1	1.76	0.50
1:G:230:LYS:HZ2	1:G:321:ARG:NH1	2.10	0.50
1:H:479:ASN:CB	1:H:482:ASN:OD1	2.59	0.50
1:C:423:ILE:HD11	1:C:477:HIS:NE2	2.26	0.50
1:D:127:HIS:HD2	1:D:129:THR:CG2	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:LYS:HG2	1:D:353:TYR:HD1	1.76	0.50
1:E:290:ILE:HG21	1:E:298:ILE:CD1	2.40	0.50
1:E:505:PRO:O	1:E:508:VAL:HG12	2.12	0.50
1:F:127:HIS:HD2	1:F:129:THR:CG2	2.24	0.50
1:H:108:VAL:O	1:H:111:SER:HB3	2.11	0.50
1:I:244:ALA:C	1:I:296:ASN:HD22	2.12	0.50
1:I:85:ALA:O	1:I:88:LEU:HB3	2.12	0.50
1:A:230:LYS:HZ2	1:A:321:ARG:NH1	2.08	0.50
1:A:422:GLU:N	1:A:422:GLU:OE1	2.45	0.50
1:C:34:ALA:O	1:C:37:ALA:HB3	2.12	0.50
1:C:85:ALA:O	1:C:88:LEU:HB3	2.12	0.50
1:F:280:GLU:O	1:F:284:LYS:HG3	2.12	0.50
1:F:393:GLU:HG3	1:F:396:ARG:HH21	1.77	0.50
1:H:245:LYS:HG2	1:H:353:TYR:HD1	1.76	0.50
1:I:284:LYS:HD3	1:I:311:TYR:CE2	2.43	0.50
1:I:479:ASN:CB	1:I:482:ASN:OD1	2.59	0.50
1:I:68:ILE:O	1:I:68:ILE:HG13	2.10	0.50
1:A:85:ALA:O	1:A:88:LEU:HB3	2.12	0.50
1:B:422:GLU:N	1:B:422:GLU:OE1	2.45	0.50
1:E:127:HIS:HD2	1:E:129:THR:CG2	2.24	0.50
1:E:88:LEU:HD11	1:F:389:ARG:NH1	2.18	0.50
1:G:34:ALA:O	1:G:37:ALA:HB3	2.12	0.50
1:G:423:ILE:HG21	1:G:473:LEU:CD1	2.42	0.50
1:H:393:GLU:HG3	1:H:396:ARG:HH21	1.77	0.50
1:H:470:LEU:O	1:H:470:LEU:HD23	2.12	0.50
1:I:255:VAL:HA	1:I:283:ILE:CD1	2.41	0.50
1:I:422:GLU:N	1:I:422:GLU:OE1	2.45	0.50
1:I:423:ILE:HG21	1:I:473:LEU:CD1	2.42	0.50
1:A:91:GLN:NE2	1:B:387:LEU:HD21	2.26	0.50
1:B:162:ARG:HH11	1:B:162:ARG:CB	2.23	0.50
1:D:470:LEU:O	1:D:470:LEU:HD23	2.12	0.50
1:F:470:LEU:HD23	1:F:470:LEU:O	2.12	0.50
1:F:71:ASP:O	1:F:75:ILE:HG12	2.11	0.50
1:G:108:VAL:O	1:G:111:SER:HB3	2.11	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:I:209:ILE:N	1:I:209:ILE:HD12	2.27	0.50
1:A:437:GLY:O	1:A:441:GLN:HB2	2.12	0.50
1:A:470:LEU:O	1:A:470:LEU:HD23	2.12	0.50
1:B:212:LYS:CE	1:B:212:LYS:HA	2.33	0.50
1:B:220:THR:HB	1:B:382:LEU:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:PRO:O	1:B:508:VAL:HG12	2.12	0.50
1:E:393:GLU:HG3	1:E:396:ARG:HH21	1.77	0.50
1:G:209:ILE:HD12	1:G:209:ILE:N	2.27	0.50
1:G:470:LEU:O	1:G:470:LEU:HD23	2.12	0.50
1:H:208:GLN:HE22	1:H:227:VAL:H	1.60	0.50
1:H:423:ILE:HG21	1:H:473:LEU:CD1	2.42	0.50
1:H:163:LYS:HD3	1:H:501:GLY:HA2	1.93	0.50
1:I:376:PRO:HG2	1:I:377:LYS:H	1.77	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:B:470:LEU:O	1:B:470:LEU:HD23	2.12	0.50
1:D:423:ILE:HG21	1:D:473:LEU:CD1	2.42	0.50
1:F:163:LYS:HD3	1:F:501:GLY:HA2	1.93	0.50
1:F:220:THR:HB	1:F:382:LEU:O	2.12	0.50
1:F:245:LYS:HG2	1:F:353:TYR:HD1	1.76	0.50
1:F:505:PRO:O	1:F:508:VAL:HG12	2.11	0.50
1:G:393:GLU:HG3	1:G:396:ARG:HH21	1.77	0.50
1:H:376:PRO:HG2	1:H:377:LYS:H	1.77	0.50
1:I:470:LEU:HD23	1:I:470:LEU:O	2.12	0.50
1:B:426:ALA:O	1:B:429:LEU:N	2.46	0.49
1:B:415:ILE:O	1:B:503:ILE:HG23	2.11	0.49
1:C:208:GLN:HE22	1:C:227:VAL:H	1.59	0.49
1:C:422:GLU:N	1:C:422:GLU:OE1	2.45	0.49
1:C:437:GLY:O	1:C:441:GLN:HB2	2.12	0.49
1:D:230:LYS:HZ2	1:D:321:ARG:NH1	2.09	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:208:GLN:HE22	1:E:227:VAL:H	1.60	0.49
1:E:245:LYS:HG2	1:E:353:TYR:HD1	1.76	0.49
1:E:220:THR:HB	1:E:382:LEU:O	2.12	0.49
1:E:422:GLU:N	1:E:422:GLU:OE1	2.45	0.49
1:E:85:ALA:O	1:E:88:LEU:HB3	2.12	0.49
1:F:85:ALA:O	1:F:88:LEU:HB3	2.12	0.49
1:H:127:HIS:HD2	1:H:129:THR:CG2	2.24	0.49
1:H:209:ILE:N	1:H:209:ILE:HD12	2.27	0.49
1:I:71:ASP:O	1:I:75:ILE:HG12	2.11	0.49
1:A:163:LYS:HD3	1:A:501:GLY:HA2	1.93	0.49
1:A:208:GLN:HE22	1:A:227:VAL:H	1.60	0.49
1:A:255:VAL:HA	1:A:283:ILE:CD1	2.41	0.49
1:A:34:ALA:O	1:A:37:ALA:HB3	2.12	0.49
1:B:208:GLN:HE22	1:B:227:VAL:H	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:GLU:O	1:B:284:LYS:HG3	2.12	0.49
1:B:423:ILE:HG21	1:B:473:LEU:CD1	2.42	0.49
1:C:280:GLU:O	1:C:284:LYS:HG3	2.12	0.49
1:D:163:LYS:HD3	1:D:501:GLY:HA2	1.93	0.49
1:D:209:ILE:N	1:D:209:ILE:HD12	2.27	0.49
1:D:422:GLU:OE1	1:D: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: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:H:437:GLY:O	1:H:441:GLN:HB2	2.12	0.49
1:I:127:HIS:HD2	1:I:129:THR:CG2	2.24	0.49
1:I:393:GLU:HG3	1:I:396:ARG:HH21	1.77	0.49
1:A:209:ILE:N	1:A:209:ILE:HD12	2.27	0.49
1:A:393:GLU:HG3	1:A:396:ARG:HH21	1.77	0.49
1:B:437:GLY:O	1:B:441:GLN:HB2	2.12	0.49
1:B:85:ALA:O	1:B:88:LEU:HB3	2.12	0.49
1:C:376:PRO:HG2	1:C:377:LYS:H	1.77	0.49
1:C:393:GLU:HG3	1:C:396:ARG:HH21	1.77	0.49
1:C:71:ASP:O	1:C:75:ILE:HG12	2.11	0.49
1:D:280:GLU:O	1:D:284:LYS:HG3	2.12	0.49
1:D:479:ASN:CB	1:D:482:ASN:OD1	2.59	0.49
1:E:34:ALA:O	1:E:37:ALA:HB3	2.12	0.49
1:E:437:GLY:O	1:E:441:GLN:HB2	2.12	0.49
1:E:71:ASP:O	1:E:75:ILE:HG12	2.11	0.49
1:G:230:LYS:HZ1	1:G:321:ARG:HH12	1.60	0.49
1:G:422:GLU:OE1	1:G:422:GLU:N	2.45	0.49
1:A:246:ILE:HA	1:A:297:VAL:HG13	1.94	0.49
1:A:505:PRO:O	1:A:508:VAL:HG12	2.11	0.49
1:C:246:ILE:HA	1:C:297:VAL:HG13	1.94	0.49
1:C:470:LEU:HD23	1:C:470:LEU:O	2.12	0.49
1:D:108:VAL:O	1:D:111:SER:HB3	2.11	0.49
1:F:423:ILE:HD12	1:F:423:ILE:C	2.30	0.49
1:I:163:LYS:HD3	1:I:501:GLY:HA2	1.93	0.49
1:A:161:LEU:HD12	1:A:161:LEU:H	1.77	0.49
1:B:209:ILE:HD12	1:B:209:ILE:N	2.27	0.49
1:B:210:VAL:HG23	1:B:382:LEU:HD12	1.95	0.49
1:E:230:LYS:HZ1	1:E:321:ARG:NH1	2.10	0.49
1:E:280:GLU:O	1:E:284:LYS:HG3	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:ALA:O	1:F:37:ALA:HB3	2.12	0.49
1:F:422:GLU:N	1:F:422:GLU:OE1	2.45	0.49
1:F:530:VAL:O	1:G:59:LEU:HA	2.12	0.49
1:G:280:GLU:O	1:G:284:LYS:HG3	2.12	0.49
1:H:36:ILE:HG23	1:H:115:VAL:HG12	1.95	0.49
1:I:34:ALA:O	1:I:37:ALA:HB3	2.12	0.49
1:C:220:THR:HB	1:C:382:LEU:O	2.12	0.49
1:C:423:ILE:HG21	1:C:473:LEU:CD1	2.42	0.49
1:C:503:ILE:HG22	1:C:504:GLU:N	2.28	0.49
1:D:505:PRO:O	1:D:508:VAL:HG12	2.11	0.49
1:E:161:LEU:HD12	1:E:161:LEU:H	1.77	0.49
1:E:209:ILE:HD12	1:E:209:ILE:N	2.27	0.49
1:G:36:ILE:HG23	1:G:115:VAL:HG12	1.94	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:H:85:ALA:O	1:H:88:LEU:HB3	2.12	0.49
1:I:220:THR:HB	1:I:382:LEU:O	2.12	0.49
1:I:503:ILE:N	1:I:503:ILE:HD12	2.28	0.49
1:A:212:LYS:CE	1:A:212:LYS:HA	2.33	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:B:36:ILE:HG23	1:B:115:VAL:HG12	1.95	0.49
1:B:34:ALA:O	1:B:37:ALA:HB3	2.12	0.49
1:B:503:ILE:HG22	1:B:504:GLU:N	2.28	0.49
1:C:36:ILE:HG23	1:C:115:VAL:HG12	1.94	0.49
1:C:503:ILE:HD12	1:C:503:ILE:N	2.28	0.49
1:D:393:GLU:HG3	1:D:396:ARG:HH21	1.77	0.49
1:D:437:GLY:O	1:D:441:GLN:HB2	2.12	0.49
1:E:470:LEU:HD23	1:E:470:LEU:O	2.12	0.49
1:E:503:ILE:HG22	1:E:504:GLU:N	2.28	0.49
1:F:36:ILE:HG23	1:F:115:VAL:HG12	1.94	0.49
1:F:246:ILE:HA	1:F:297:VAL:HG13	1.94	0.49
1:G:85:ALA:O	1:G:88:LEU:HB3	2.12	0.49
1:I:36:ILE:HG23	1:I:115:VAL:HG12	1.95	0.49
1:A:426:ALA:O	1:A:429:LEU:N	2.45	0.49
1:B:393:GLU:HG3	1:B:396:ARG:HH21	1.77	0.49
1:C:209:ILE:N	1:C:209:ILE:HD12	2.27	0.49
1:D:208:GLN:HE22	1:D:227:VAL:H	1.59	0.49
1:D:220:THR:HB	1:D:382:LEU:O	2.12	0.49
1:E:163:LYS:HD3	1:E:501:GLY:HA2	1.93	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:F:376:PRO:HG2	1:F:377:LYS:H	1.77	0.49
1:G:246:ILE:HA	1:G:297:VAL:HG13	1.95	0.49
1:G:220:THR:HB	1:G:382:LEU:O	2.12	0.49
1:G:437:GLY:O	1:G:441:GLN:HB2	2.12	0.49
1:H:505:PRO:O	1:H:508:VAL:HG12	2.11	0.49
1:C:426:ALA:O	1:C:429:LEU:N	2.45	0.49
1:D:161:LEU:H	1:D:161:LEU:HD12	1.77	0.49
1:D:230:LYS:HZ1	1:D:321:ARG:HH12	1.60	0.49
1:E:376:PRO:HG2	1:E:377:LYS:H	1.77	0.49
1:E:479:ASN:CB	1:E:482:ASN:OD1	2.59	0.49
1:E:76:LEU:CD2	1:E:90:VAL:HG12	2.36	0.49
1:F:290:ILE:HG21	1:F:298:ILE:CD1	2.40	0.49
1:G:161:LEU:HD12	1:G:161:LEU:H	1.77	0.49
1:H:422:GLU:OE1	1:H:422:GLU:N	2.45	0.49
1:H:423:ILE:HD12	1:H:424:GLU:H	1.73	0.49
1:H:503:ILE:HG22	1:H:504:GLU:N	2.28	0.49
1:I:161:LEU:HD12	1:I:161:LEU:H	1.76	0.49
1:I:290:ILE:HG21	1:I:298:ILE:CD1	2.40	0.49
1:A:245:LYS:HG2	1:A:353:TYR:HD1	1.76	0.49
1:C:127:HIS:HD2	1:C:129:THR:CB	2.26	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:H:127:HIS:HD2	1:H:129:THR:CB	2.26	0.49
1:A:127:HIS:HD2	1:A:129:THR:CB	2.26	0.48
1:A:423:ILE:HG21	1:A:473:LEU:CD1	2.42	0.48
1:A:503:ILE:HG22	1:A:504:GLU:N	2.28	0.48
1:B:110:PHE:O	1:B:114:LEU:HD13	2.13	0.48
1:C:479:ASN:CB	1:C:482:ASN:OD1	2.59	0.48
1:C:58:MET:HG3	1:C:68:ILE:CG2	2.43	0.48
1:D:66:ILE:N	1:D:66:ILE:CD1	2.76	0.48
1:E:426:ALA:O	1:E:429:LEU:N	2.45	0.48
1:F:255:VAL:HA	1:F:283:ILE:CD1	2.41	0.48
1:F:263:GLU:C	1:F:264:ILE:HG22	2.34	0.48
1:F:423:ILE:HD12	1:F:424:GLU:H	1.73	0.48
1:G:230:LYS:HZ1	1:G:321:ARG:NH1	2.09	0.48
1:H:246:ILE:HA	1:H:297:VAL:HG13	1.94	0.48
1:I:210:VAL:HG23	1:I:382:LEU:HD12	1.95	0.48
1:I:423:ILE:C	1:I:423:ILE:HD12	2.30	0.48
1:I:503:ILE:HG22	1:I:504:GLU:N	2.28	0.48
1:A:36:ILE:HG23	1:A:115:VAL:HG12	1.95	0.48

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:GLU:C	1:D:264:ILE:CG2	2.82	0.48
1:H:260:LEU:CD1	1:H:260:LEU:C	2.81	0.48
1:I:263:GLU:C	1:I:264:ILE:HG22	2.34	0.48
1:A:299:ILE:HG22	1:A:320:VAL:HG23	1.96	0.48
1:A:255:VAL:HG13	1:A:305:ASP:CG	2.34	0.48
1:A:503:ILE:N	1:A:503:ILE:HD12	2.28	0.48
1:B:330:LYS:O	1:B:334:ALA:HB2	2.14	0.48
1:B:503:ILE:HD12	1:B:503:ILE:N	2.28	0.48
1:C:232:VAL:HG11	1:C:318:LEU:HD11	1.95	0.48
1:C:423:ILE:HD12	1:C:424:GLU:H	1.73	0.48
1:D:212:LYS:CE	1:D:212:LYS:HA	2.33	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: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:F:503:ILE:HG22	1:F:504:GLU:N	2.28	0.48
1:H:246:ILE:O	1:H:351:LEU:HB2	2.14	0.48
1:A:263:GLU:C	1:A:264:ILE:HG22	2.34	0.48
1:A:376:PRO:HG2	1:A:377:LYS:H	1.77	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:F:217:ILE:HD11	1:F:390:LEU:CD2	2.44	0.48
1:G:330:LYS:O	1:G:334:ALA:HB2	2.14	0.48
1:A:210:VAL:HG23	1:A:382:LEU:HD12	1.95	0.47
1:B:473:LEU:HD13	1:B:473:LEU:C	2.34	0.47
1:C:290:ILE:HG21	1:C:298:ILE:CD1	2.40	0.47
1:D:227:VAL:HG22	1:D:369:PHE:HD1	1.79	0.47
1:D:469:LEU:HB3	1:D:487:ILE:CD1	2.43	0.47
1:F:255:VAL:HG13	1:F:305:ASP:CG	2.34	0.47
1:G:263:GLU:C	1:G:264:ILE:CG2	2.82	0.47
1:H:263:GLU:C	1:H:264:ILE:CG2	2.82	0.47
1:H:330:LYS:O	1:H:334:ALA:HB2	2.14	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:A:178:ARG:NE	1:A:178:ARG:H	2.12	0.47
1:A:232:VAL:HG11	1:A:318:LEU:HD11	1.95	0.47
1:B:230:LYS:HZ1	1:B:321:ARG:HH12	1.62	0.47
1:C:217:ILE:HD11	1:C:390:LEU:CD2	2.44	0.47
1:C:260:LEU:CD1	1:C:260:LEU:C	2.81	0.47
1:E:110:PHE:O	1:E:114:LEU:HD13	2.13	0.47
1:E:503:ILE:N	1:E:503:ILE:HD12	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:210:VAL:HG23	1:G:382:LEU:HD12	1.95	0.47
1:G:217:ILE:HD11	1:G:390:LEU:CD2	2.44	0.47
1:G:263:GLU:C	1:G:264:ILE:HG22	2.34	0.47
1:H:227:VAL:HG22	1:H:369:PHE:HD1	1.79	0.47
1:H:214:GLY:HA3	1:H:384:ARG:HH21	1.79	0.47
1:I:436:VAL:HG23	1:I:437:GLY:N	2.30	0.47
1:A:246:ILE:O	1:A:351:LEU:HB2	2.14	0.47
1:B:246:ILE:O	1:B:351:LEU:HB2	2.14	0.47
1:B:232:VAL:HG12	1:B:318:LEU:HD11	1.95	0.47
1:C:227:VAL:HG22	1:C:369:PHE:HD1	1.79	0.47
1:C:76:LEU:CD2	1:C:90:VAL:HG12	2.36	0.47
1:D:214:GLY:HA3	1:D:384:ARG:HH21	1.79	0.47
1:D:299:ILE:HG22	1:D:320:VAL:HG23	1.96	0.47
1:D:249:ILE:HD12	1:D:346:ILE:HD11	1.96	0.47
1:E:232:VAL:HG11	1:E:318:LEU:HD11	1.96	0.47
1:F:127:HIS:HD2	1:F:129:THR:CB	2.26	0.47
1:F:214:GLY:HA3	1:F:384:ARG:HH21	1.79	0.47
1:F:482:ASN:O	1:F:485:TYR:N	2.40	0.47
1:G:178:ARG:H	1:G:178:ARG:NE	2.12	0.47
1:I:249:ILE:HD12	1:I:346:ILE:HD11	1.96	0.47
1:A:121:LEU:HB3	1:A:126:VAL:CG2	2.44	0.47
1:A:214:GLY:HA3	1:A:384:ARG:HH21	1.79	0.47
1:A:528:ASP:OD2	1:A:529:VAL:N	2.48	0.47
1:B:227:VAL:HG22	1:B:369:PHE:HD1	1.79	0.47
1:B:246:ILE:HA	1:B:297:VAL:HG13	1.94	0.47
1:B:249:ILE:HD12	1:B:346:ILE:HD11	1.96	0.47
1:C:211:LYS:HE3	1:C:395:GLU:OE2	2.14	0.47
1:D:121:LEU:HB3	1:D:126:VAL:CG2	2.44	0.47
1:D:246:ILE:O	1:D:351:LEU:HB2	2.14	0.47
1:D:258:PRO:CG	1:D:279:GLU:OE2	2.56	0.47
1:E:210:VAL:HG23	1:E:382:LEU:HD12	1.95	0.47
1:E:423:ILE:HD12	1:E:424:GLU:H	1.73	0.47
1:F:211:LYS:HE3	1:F:395:GLU:OE2	2.14	0.47
1:H:299:ILE:HG22	1:H:320:VAL:HG23	1.96	0.47
1:H:211:LYS:HE3	1:H:395:GLU:OE2	2.14	0.47
1:H:436:VAL:HG23	1:H:437:GLY:N	2.30	0.47
1:I:246:ILE:O	1:I:351:LEU:HB2	2.14	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:C:141:VAL:CG2	1:C:432:TYR:CE1	2.97	0.47
1:D:358:GLU:CG	1:D:360:ARG:HH22	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:LYS:HZ1	1:E:321:ARG:HH12	1.61	0.47
1:F:232:VAL:HG11	1:F:318:LEU:HD11	1.95	0.47
1:F:473:LEU:C	1:F:473:LEU:HD13	2.34	0.47
1:G:299:ILE:HG22	1:G:320:VAL:HG23	1.96	0.47
1:G:473:LEU:C	1:G:473:LEU:HD13	2.34	0.47
1:H:178:ARG:H	1:H:178:ARG:NE	2.12	0.47
1:H:473:LEU:C	1:H:473:LEU:HD13	2.34	0.47
1:I:361:LYS:CB	1:I:366:LYS:HG2	2.36	0.47
1:I:528:ASP:OD2	1:I:529:VAL:N	2.48	0.47
1:B:436:VAL:HG23	1:B:437:GLY:N	2.30	0.47
1:C:330:LYS:O	1:C:334:ALA:HB2	2.14	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:H:46:LEU:O	1:H:47:LYS:C	2.53	0.47
1:A:230:LYS:HZ1	1:A:321:ARG:NH1	2.10	0.47
1:A:263:GLU:C	1:A:264:ILE:CG2	2.82	0.47
1:A:46:LEU:O	1:A:47:LYS:C	2.53	0.47
1:B:121:LEU:HB3	1:B:126:VAL:CG2	2.44	0.47
1:B:230:LYS:HZ1	1:B:321:ARG:NH1	2.12	0.47
1:B:75:ILE:O	1:B:79:MET:HB3	2.15	0.47
1:C:255:VAL:HG13	1:C:305:ASP:CG	2.34	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: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:E:246:ILE:O	1:E:351:LEU:HB2	2.14	0.47
1:E:436:VAL:HG23	1:E:437:GLY:N	2.30	0.47
1:F:330:LYS:O	1:F:334:ALA:HB2	2.14	0.47
1:F:436:VAL:HG23	1:F:437:GLY:N	2.30	0.47
1:G:258:PRO:CG	1:G:279:GLU:OE2	2.56	0.47
1:G:290:ILE:HG21	1:G:298:ILE:CD1	2.40	0.47
1:I:214:GLY:HA3	1:I:384:ARG:HH21	1.80	0.47
1:I:211:LYS:HE3	1:I:395:GLU:OE2	2.15	0.47
1:A:232:VAL:HG12	1:A:318:LEU:HD11	1.95	0.47
1:A:271:GLN:OE1	1:A:271:GLN:HA	2.15	0.47
1:A:249:ILE:HD12	1:A:346:ILE:HD11	1.96	0.47
1:A:359:GLU:HG2	1:A:359:GLU:O	2.15	0.47
1:A:358:GLU:CG	1:A:360:ARG:HH22	2.27	0.47
1:A:469:LEU:HB3	1:A:487:ILE:CD1	2.43	0.47
1:C:234:HIS:ND1	1:C:235:PRO:HD2	2.30	0.47
1:C:56:ASP:OD1	1:C:70:ASN:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ILE:O	1:C:79:MET:HB3	2.15	0.47
1:D:282:LEU:O	1:D:285:GLU:HB3	2.15	0.47
1:D:211:LYS:HE3	1:D:395:GLU:OE2	2.14	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:D:75:ILE:O	1:D:79:MET:HB3	2.15	0.47
1:E:211:LYS:HE3	1:E:395:GLU:OE2	2.14	0.47
1:G:234:HIS:ND1	1:G:235:PRO:HD2	2.30	0.47
1:I:121:LEU:HB3	1:I:126:VAL:CG2	2.44	0.47
1:I:255:VAL:HG13	1:I:305:ASP:CG	2.34	0.47
1:I:330:LYS:O	1:I:334:ALA:HB2	2.14	0.47
1:I:473:LEU:C	1:I:473:LEU:HD13	2.35	0.47
1:A:234:HIS:ND1	1:A:235:PRO:HD2	2.30	0.47
1:B:232:VAL:HG11	1:B:318:LEU:HD11	1.95	0.47
1:C:214:GLY:HA3	1:C:384:ARG:HH21	1.79	0.47
1:C:473:LEU:HD13	1:C:473:LEU:C	2.34	0.47
1:C:482:ASN:O	1:C:485:TYR:N	2.40	0.47
1:D:217:ILE:HD11	1:D:390:LEU:CD2	2.43	0.47
1:D:234:HIS:ND1	1:D:235:PRO:HD2	2.30	0.47
1:D:473:LEU:HD13	1:D:473:LEU:C	2.34	0.47
1:D:528:ASP:OD2	1:D:529:VAL:N	2.48	0.47
1:F:227:VAL:HG22	1:F:369:PHE:HD1	1.79	0.47
1:F:234:HIS:ND1	1:F:235:PRO:HD2	2.30	0.47
1:F:469:LEU:HB3	1:F:487:ILE:CD1	2.43	0.47
1:F:528:ASP:OD2	1:F:529:VAL:N	2.48	0.47
1:F:75:ILE:O	1:F:79:MET:HB3	2.15	0.47
1:G:359:GLU:HG2	1:G:359:GLU:O	2.15	0.47
1:H:161:LEU:HD12	1:H:161:LEU:H	1.77	0.47
1:H:271:GLN:OE1	1:H:271:GLN:HA	2.15	0.47
1:H:290:ILE:HG21	1:H:298:ILE:CD1	2.40	0.47
1:H:210:VAL:HG23	1:H:382:LEU:HD12	1.95	0.47
1:A:166:MET:HE1	1:A:179:GLU:HG2	1.96	0.47
1:B:271:GLN:OE1	1:B:271:GLN:HA	2.15	0.47
1:B:299:ILE:HG22	1:B:320:VAL:HG23	1.96	0.47
1:B:214:GLY:HA3	1:B:384:ARG:HH21	1.79	0.47
1:B:46:LEU:O	1:B:47:LYS:C	2.53	0.47
1:E:227:VAL:HG22	1:E:369:PHE:HD1	1.79	0.47
1:E:299:ILE:HG22	1:E:320:VAL:HG23	1.96	0.47
1:E:75:ILE:O	1:E:79:MET:HB3	2.15	0.47
1:F:263:GLU:C	1:F:264:ILE:CG2	2.82	0.47
1:F:529:VAL:CG1	1:G:58:MET:SD	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:530:VAL:O	1:G:59:LEU:HD22	2.13	0.47
1:G:271:GLN:HA	1:G:271:GLN:OE1	2.15	0.47
1:G:255:VAL:HA	1:G:283:ILE:CD1	2.41	0.47
1:G:528:ASP:OD2	1:G:529:VAL:N	2.48	0.47
1:H:121:LEU:HB3	1:H:126:VAL:HG21	1.97	0.47
1:H:406:ALA:O	1:H:410:LYS:HG3	2.15	0.47
1:A:150:ALA:HA	1:A:415:ILE:HG22	1.97	0.47
1:A:230:LYS:HZ1	1:A:321:ARG:HH12	1.61	0.47
1:A:259:GLU:CD	1:A:259:GLU:C	2.74	0.47
1:C:178:ARG:H	1:C:178:ARG:NE	2.12	0.47
1:C:249:ILE:HD12	1:C:346:ILE:HD11	1.96	0.47
1:C:84:PRO:HG2	1:C:85:ALA:H	1.80	0.47
1:D:290:ILE:HG21	1:D:298:ILE:CD1	2.40	0.47
1:D:359:GLU:HG2	1:D:359:GLU:O	2.15	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:G:246:ILE:O	1:G:351:LEU:HB2	2.14	0.47
1:G:282:LEU:O	1:G:285:GLU:HB3	2.15	0.47
1:G:249:ILE:HD12	1:G:346:ILE:HD11	1.96	0.47
1:H:232:VAL:HG11	1:H:318:LEU:HD11	1.95	0.47
1:H:528:ASP:OD2	1:H:529:VAL:N	2.48	0.47
1:H:83:HIS:CD2	1:H:84:PRO:HD2	2.50	0.47
1:I:259:GLU:CD	1:I:259:GLU:C	2.74	0.47
1:I:271:GLN:OE1	1:I:271:GLN:HA	2.15	0.47
1:I:66:ILE:N	1:I:66:ILE:CD1	2.76	0.47
1:A:436:VAL:HG23	1:A:437:GLY:N	2.30	0.46
1:B:121:LEU:HB3	1:B:126:VAL:HG21	1.97	0.46
1:B:505:PRO:C	1:B:507:LEU:N	2.69	0.46
1:C:259:GLU:C	1:C:259:GLU:CD	2.74	0.46
1:D:178:ARG:NE	1:D:178:ARG:H	2.12	0.46
1:D:330:LYS:O	1:D:334:ALA:HB2	2.14	0.46
1:E:232:VAL:HG12	1:E:318:LEU:HD11	1.95	0.46
1:E:406:ALA:O	1:E:410:LYS:HG3	2.16	0.46
1:F:249:ILE:HD12	1:F:346:ILE:HD11	1.96	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:H:56:ASP:OD1	1:H:70:ASN:HB3	2.15	0.46
1:H:66:ILE:CD1	1:H:66:ILE:N	2.76	0.46
1:I:194:GLU:C	1:I:195:LEU:HD12	2.36	0.46
1:I:227:VAL:HG22	1:I:369:PHE:HD1	1.79	0.46
1:I:299:ILE:HG22	1:I:320:VAL:HG23	1.96	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: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:121:LEU:HB3	1:C:126:VAL:CG2	2.44	0.46
1:C:271:GLN:OE1	1:C:271:GLN:HA	2.15	0.46
1:C:45:ALA:C	1:C:46:LEU:HD12	2.36	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:F:259:GLU:C	1:F:259:GLU:CD	2.74	0.46
1:H:75:ILE:O	1:H:79:MET:HB3	2.15	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:I:75:ILE:O	1:I:79:MET:HB3	2.15	0.46
1:A:121:LEU:HB3	1:A:126:VAL:HG21	1.97	0.46
1:A:194:GLU:C	1:A:195:LEU:HD12	2.36	0.46
1:A:282:LEU:O	1:A:285:GLU:HB3	2.15	0.46
1:A:84:PRO:HG2	1:A:85:ALA:H	1.80	0.46
1:B:188:ALA:HA	1:B:379:ILE:HD11	1.97	0.46
1:B:263:GLU:C	1:B:264:ILE:CG2	2.82	0.46
1:B:211:LYS:HE3	1:B:395:GLU:OE2	2.14	0.46
1:B:406:ALA:O	1:B:410:LYS:HG3	2.15	0.46
1:B:84:PRO:HG2	1:B:85:ALA:H	1.80	0.46
1:C:212:LYS:HA	1:C:212:LYS:CE	2.33	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:C:528:ASP:OD2	1:C:529:VAL:N	2.48	0.46
1:D:208:GLN:C	1:D:209:ILE:HD12	2.36	0.46
1:D:232:VAL:HG12	1:D:318:LEU:HD11	1.95	0.46
1:E:121:LEU:HB3	1:E:126:VAL:CG2	2.44	0.46
1:E:217:ILE:HD11	1:E:390:LEU:CD2	2.43	0.46
1:E:271:GLN:OE1	1:E:271:GLN:HA	2.15	0.46
1:E:141:VAL:CG2	1:E:432:TYR:CE1	2.97	0.46
1:E:505:PRO:C	1:E:507:LEU:N	2.69	0.46
1:F:406:ALA:O	1:F:410:LYS:HG3	2.16	0.46
1:G:406:ALA:O	1:G:410:LYS:HG3	2.16	0.46
1:H:249:ILE:HD12	1:H:346:ILE:HD11	1.96	0.46
1:H:141:VAL:CG2	1:H:432:TYR:CE1	2.97	0.46
1:I:282:LEU:O	1:I:285:GLU:HB3	2.15	0.46
1:I:56:ASP:OD1	1:I:70:ASN:HB3	2.15	0.46
1:A:208:GLN:C	1:A:209:ILE:HD12	2.36	0.46
1:A:212:LYS:O	1:A:213:ALA:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:TYR:HA	1:A:379:ILE:HG22	1.98	0.46
1:B:194:GLU:C	1:B:195:LEU:HD12	2.36	0.46
1:C:121:LEU:HB3	1:C:126:VAL:HG21	1.97	0.46
1:C:150:ALA:HA	1:C:415:ILE:HG22	1.97	0.46
1:C:246:ILE:O	1:C:351:LEU:HB2	2.14	0.46
1:C:282:LEU:O	1:C:285:GLU:HB3	2.15	0.46
1:D:84:PRO:HG2	1:D:85:ALA:H	1.80	0.46
1:E:234:HIS:ND1	1:E:235:PRO:HD2	2.30	0.46
1:E:263:GLU:C	1:E:264:ILE:CG2	2.82	0.46
1:E:282:LEU:O	1:E:285:GLU:HB3	2.15	0.46
1:E:56:ASP:OD1	1:E:70:ASN:HB3	2.15	0.46
1:F:46:LEU:O	1:F:47:LYS:C	2.53	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
1:G:150:ALA:HA	1:G:415:ILE:HG22	1.97	0.46
1:G:194:GLU:C	1:G:195:LEU:HD12	2.36	0.46
1:G:212:LYS:O	1:G:213:ALA:O	2.33	0.46
1:G:45:ALA:C	1:G:46:LEU:HD12	2.36	0.46
1:H:282:LEU:O	1:H:285:GLU:HB3	2.15	0.46
1:H:290:ILE:HG12	1:H:346:ILE:CD1	2.46	0.46
1:H:359:GLU:O	1:H:359:GLU:HG2	2.15	0.46
1:I:121:LEU:HB3	1:I:126:VAL:HG21	1.97	0.46
1:I:263:GLU:C	1:I:264:ILE:CG2	2.82	0.46
1:I:232:VAL:HG11	1:I:318:LEU:HD11	1.95	0.46
1:I:45:ALA:C	1:I:46:LEU:HD12	2.36	0.46
1:I:84:PRO:HG2	1:I:85:ALA:H	1.80	0.46
1:B:259:GLU:CD	1:B:259:GLU:C	2.74	0.46
1:A:528:ASP:HB3	1:B:57:LYS:HE3	1.97	0.46
1:D:212:LYS:O	1:D:213:ALA:O	2.34	0.46
1:D:271:GLN:OE1	1:D:271:GLN:HA	2.15	0.46
1:D:423:ILE:HD12	1:D:424:GLU:H	1.73	0.46
1:D:56:ASP:OD1	1:D:70:ASN:HB3	2.15	0.46
1:E:208:GLN:C	1:E:209:ILE:HD12	2.36	0.46
1:F:121:LEU:HB3	1:F:126:VAL:HG21	1.97	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:G:153:VAL:HG13	1:G:153:VAL:O	2.16	0.46
1:G:436:VAL:HG23	1:G:437:GLY:N	2.30	0.46
1:H:234:HIS:ND1	1:H:235:PRO:HD2	2.30	0.46
1:I:469:LEU:HB3	1:I:487:ILE:CD1	2.43	0.46
1:A:210:VAL:O	1:A:382:LEU:HD12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LYS:HE3	1:A:395:GLU:OE2	2.15	0.46
1:A:56:ASP:OD1	1:A:70:ASN:HB3	2.15	0.46
1:B:153:VAL:HG13	1:B:153:VAL:O	2.16	0.46
1:B:234:HIS:ND1	1:B:235:PRO:HD2	2.30	0.46
1:B:83:HIS:CD2	1:B:84:PRO:HD2	2.50	0.46
1:D:188:ALA:HA	1:D:379:ILE:HD11	1.98	0.46
1:D:211:LYS:HD2	1:D:391:VAL:HG22	1.98	0.46
1:F:359:GLU:O	1:F:359:GLU:HG2	2.15	0.46
1:G:423:ILE:HD12	1:G:424:GLU:H	1.73	0.46
1:H:84:PRO:HG2	1:H:85:ALA:H	1.80	0.46
1:I:234:HIS:ND1	1:I:235:PRO:HD2	2.30	0.46
1:I:46:LEU:O	1:I:47:LYS:C	2.53	0.46
1:I:83:HIS:CD2	1:I:84:PRO:HD2	2.50	0.46
1:A:290:ILE:HG12	1:A:346:ILE:CD1	2.46	0.46
1:A:75:ILE:O	1:A:79:MET:HB3	2.15	0.46
1:B:178:ARG:NE	1:B:178:ARG:H	2.12	0.46
1:B:212:LYS:O	1:B:213:ALA:O	2.34	0.46
1:B:359:GLU:HG2	1:B:359:GLU:O	2.15	0.46
1:C:208:GLN:C	1:C:209:ILE:HD12	2.36	0.46
1:C:224:TYR:HA	1:C:379:ILE:HG22	1.98	0.46
1:E:214:GLY:HA3	1:E:384:ARG:HH21	1.79	0.46
1:E:46:LEU:O	1:E:47:LYS:C	2.53	0.46
1:F:178:ARG:NE	1:F:178:ARG:H	2.12	0.46
1:F:224:TYR:HA	1:F:379:ILE:HG22	1.98	0.46
1:F:271:GLN:OE1	1:F:271:GLN:HA	2.15	0.46
1:F:528:ASP:O	1:G:58:MET:N	2.41	0.46
1:G:208:GLN:C	1:G:209:ILE:HD12	2.36	0.46
1:G:210:VAL:O	1:G:382:LEU:HD12	2.16	0.46
1:G:214:GLY:HA3	1:G:384:ARG:HH21	1.79	0.46
1:G:56:ASP:OD1	1:G:70:ASN:HB3	2.15	0.46
1:H:194:GLU:C	1:H:195:LEU:HD12	2.36	0.46
1:H:210:VAL:O	1:H:382:LEU:HD12	2.16	0.46
1:I:208:GLN:C	1:I:209:ILE:HD12	2.36	0.46
1:I:290:ILE:HG12	1:I:346:ILE:CD1	2.46	0.46
1:I:141:VAL:CG2	1:I:432:TYR:CE1	2.97	0.46
1:A:430:ARG:NH1	1:A:430:ARG:HG2	2.29	0.46
1:A:45:ALA:C	1:A:46:LEU:HD12	2.36	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:C:299:ILE:HG22	1:C:320:VAL:HG23	1.96	0.46
1:D:150:ALA:HA	1:D:415:ILE:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:153:VAL:HG13	1:F:153:VAL:O	2.16	0.46
1:F:282:LEU:O	1:F:285:GLU:HB3	2.15	0.46
1:G:505:PRO:C	1:G:507:LEU:N	2.69	0.46
1:G:522:LEU:O	1:G:526:ILE:HG12	2.16	0.46
1:H:150:ALA:HA	1:H:415:ILE:HG22	1.98	0.46
1:H:208:GLN:C	1:H:209:ILE:HD12	2.36	0.46
1:H:259:GLU:C	1:H:259:GLU:CD	2.74	0.46
1:B:290:ILE:HG12	1:B:346:ILE:CD1	2.46	0.46
1:B:224:TYR:HA	1:B:379:ILE:HG22	1.98	0.46
1:C:263:GLU:C	1:C:264:ILE:CG2	2.82	0.46
1:C:522:LEU:O	1:C:526:ILE:HG12	2.16	0.46
1:D:121:LEU:HB3	1:D:126:VAL:HG21	1.97	0.46
1:E:259:GLU:C	1:E:259:GLU:CD	2.74	0.46
1:E:492:GLY:O	1:E:493:GLN:HB2	2.16	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:G:430:ARG:HG2	1:G:430:ARG:NH1	2.29	0.46
1:G:46:LEU:O	1:G:47:LYS:C	2.53	0.46
1:G:84:PRO:HG2	1:G:85:ALA:H	1.80	0.46
1:H:211:LYS:HD2	1:H:391:VAL:HG22	1.98	0.46
1:I:230:LYS:HZ1	1:I:321:ARG:HH12	1.64	0.46
1:C:127:HIS:CG	1:C:128:PRO:HD2	2.51	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:E:127:HIS:CG	1:E:128:PRO:HD2	2.51	0.46
1:E:178:ARG:H	1:E:178:ARG:NE	2.13	0.46
1:E:522:LEU:O	1:E:526:ILE:HG12	2.16	0.46
1:F:141:VAL:CG2	1:F:432:TYR:CE1	2.97	0.46
1:F:84:PRO:HG2	1:F:85:ALA:H	1.80	0.46
1:G:127:HIS:CG	1:G:128:PRO:HD2	2.51	0.46
1:G:259:GLU:CD	1:G:259:GLU:C	2.74	0.46
1:H:153:VAL:O	1:H:153:VAL:HG13	2.16	0.46
1:H:230:LYS:HZ2	1:H:321:ARG:NH1	2.13	0.46
1:H:522:LEU:O	1:H:526:ILE:HG12	2.16	0.46
1:I:217:ILE:HD11	1:I:390:LEU:CD2	2.44	0.46
1:I:406:ALA:O	1:I:410:LYS:HG3	2.15	0.46
1:A:522:LEU:O	1:A:526:ILE:HG12	2.16	0.45
1:B:166:MET:CE	1:B:178:ARG:HG2	2.47	0.45
1:B:211:LYS:HD2	1:B:391:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:LEU:CD1	1:B:261:ASP:CG	2.85	0.45
1:B:282:LEU:O	1:B:285:GLU:HB3	2.15	0.45
1:D:153:VAL:HG13	1:D:153:VAL:O	2.16	0.45
1:D:31:ALA:O	1:D:34:ALA:N	2.49	0.45
1:D:40:LYS:HD3	1:D:116:LYS:HG2	1.99	0.45
1:D:83:HIS:CD2	1:D:84:PRO:HD2	2.50	0.45
1:E:469:LEU:HB3	1:E:487:ILE:CD1	2.43	0.45
1:F:210:VAL:O	1:F:382:LEU:HD12	2.16	0.45
1:G:121:LEU:HB3	1:G:126:VAL:HG21	1.97	0.45
1:G:83:HIS:CD2	1:G:84:PRO:HD2	2.50	0.45
1:H:121:LEU:HB3	1:H:126:VAL:CG2	2.44	0.45
1:H:45:ALA:C	1:H:46:LEU:HD12	2.36	0.45
1:I:166:MET:CE	1:I:178:ARG:HG2	2.47	0.45
1:I:258:PRO:CG	1:I:279:GLU:OE2	2.56	0.45
1:A:188:ALA:HA	1:A:379:ILE:HD11	1.98	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:C:40:LYS:HD3	1:C:116:LYS:HG2	1.99	0.45
1:D:224:TYR:HA	1:D:379:ILE:HG22	1.98	0.45
1:D:406:ALA:O	1:D:410:LYS:HG3	2.16	0.45
1:E:31:ALA:O	1:E:34:ALA:N	2.49	0.45
1:E:432:TYR:CZ	1:E:436:VAL:HG12	2.52	0.45
1:E:45:ALA:C	1:E:46:LEU:HD12	2.36	0.45
1:F:194:GLU:C	1:F:195:LEU:HD12	2.36	0.45
1:F:290:ILE:HG12	1:F:346:ILE:CD1	2.46	0.45
1:E:527:ASP:N	1:F:56:ASP:O	2.46	0.45
1:G:290:ILE:HG12	1:G:346:ILE:CD1	2.46	0.45
1:G:75:ILE:O	1:G:79:MET:HB3	2.15	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:H:505:PRO:C	1:H:507:LEU:N	2.69	0.45
1:I:127:HIS:CG	1:I:128:PRO:HD2	2.51	0.45
1:I:153:VAL:HG13	1:I:153:VAL:O	2.16	0.45
1:I:224:TYR:HA	1:I:379:ILE:HG22	1.98	0.45
1:I:150:ALA:HA	1:I:415:ILE:HG22	1.98	0.45
1:I:432:TYR:CZ	1:I:436:VAL:HG12	2.52	0.45
1:I:522:LEU:O	1:I:526:ILE:HG12	2.16	0.45
1:A:492:GLY:O	1:A: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:B:45:ALA:C	1:B:46:LEU:HD12	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:LEU:O	1:B:526:ILE:HG12	2.16	0.45
1:A:527:ASP:HB2	1:B:55:MET:CG	2.45	0.45
1:C:211:LYS:HD2	1:C:391:VAL:HG22	1.98	0.45
1:D:210:VAL:O	1:D:382:LEU:HD12	2.16	0.45
1:D:426:ALA:O	1:D:429:LEU:N	2.45	0.45
1:D:522:LEU:O	1:D:526:ILE:HG12	2.16	0.45
1:E:166:MET:CE	1:E:178:ARG:HG2	2.47	0.45
1:E:188:ALA:HA	1:E:379:ILE:HD11	1.98	0.45
1:E:66:ILE:N	1:E:66:ILE:CD1	2.76	0.45
1:E:84:PRO:HG2	1:E:85:ALA:H	1.80	0.45
1:F:188:ALA:HA	1:F:379:ILE:HD11	1.98	0.45
1:F:250:ASP:O	1:F:251:ALA:HB2	2.17	0.45
1:F:31:ALA:O	1:F:34:ALA:N	2.49	0.45
1:F:40:LYS:HD3	1:F:116:LYS:HG2	1.99	0.45
1:G:492:GLY:O	1:G:493:GLN:HB2	2.16	0.45
1:H:260:LEU:CD1	1:H:261:ASP:CG	2.85	0.45
1:H:492:GLY:O	1:H:493:GLN:HB2	2.16	0.45
1:I:31:ALA:O	1:I:34:ALA:N	2.49	0.45
1:B:31:ALA:O	1:B:34:ALA:N	2.49	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:D:166:MET:CE	1:D:178:ARG:HG2	2.47	0.45
1:E:150:ALA:HA	1:E:415:ILE:HG22	1.98	0.45
1:E:250:ASP:O	1:E:251:ALA:HB2	2.17	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: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:I:250:ASP:O	1:I:251:ALA:HB2	2.17	0.45
1:B:40:LYS:HD3	1:B:116:LYS:HG2	1.99	0.45
1:B:127:HIS:CG	1:B:128:PRO:HD2	2.51	0.45
1:B:210:VAL:O	1:B:382:LEU:HD12	2.16	0.45
1:B:430:ARG:HG2	1:B:430:ARG:NH1	2.29	0.45
1:B:492:GLY:O	1:B:493:GLN:HB2	2.16	0.45
1:C:406:ALA:O	1:C:410:LYS:HG3	2.15	0.45
1:C:83:HIS:CD2	1:C:84:PRO:HD2	2.50	0.45
1:D:127:HIS:CG	1:D:128:PRO:HD2	2.51	0.45
1:D:505:PRO:C	1:D:507:LEU:N	2.69	0.45
1:E:260:LEU:CD1	1:E:261:ASP:CG	2.85	0.45
1:E:321:ARG:HB3	1:E:322:ARG:H	1.56	0.45
1:E:436:VAL:HG21	1:E:441:GLN:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:HIS:CD2	1:E:84:PRO:HD2	2.50	0.45
1:F:430:ARG:NH1	1:F:430:ARG:HG2	2.29	0.45
1:G:224:TYR:HA	1:G:379:ILE:HG22	1.98	0.45
1:H:436:VAL:HG21	1:H:441:GLN:HA	1.99	0.45
1:I:244:ALA:HA	1:I:296:ASN:HD22	1.82	0.45
1:I:260:LEU:C	1:I:260:LEU:CD1	2.81	0.45
1:I:505:PRO:C	1:I:507:LEU:N	2.69	0.45
1:A:153:VAL:HG13	1:A:153:VAL:O	2.16	0.45
1:A:161:LEU:CD1	1:A:161:LEU:H	2.30	0.45
1:B:150:ALA:HA	1:B:415:ILE:HG22	1.98	0.45
1:B:250:ASP:O	1:B:251:ALA:HB2	2.17	0.45
1:B:423:ILE:HD12	1:B:424:GLU:H	1.73	0.45
1:C:153:VAL:HG13	1:C:153:VAL:O	2.16	0.45
1:D:45:ALA:C	1:D:46:LEU:HD12	2.36	0.45
1:E:40:LYS:HD3	1:E:116:LYS:HG2	1.99	0.45
1:E:166:MET:HE1	1:E:179:GLU:HG2	1.99	0.45
1:E:212:LYS:O	1:E:213:ALA:O	2.34	0.45
1:E:249:ILE:HD12	1:E:346:ILE:HD11	1.97	0.45
1:E:290:ILE:HG12	1:E:346:ILE:CD1	2.46	0.45
1:E:224:TYR:HA	1:E:379:ILE:HG22	1.98	0.45
1:F:208:GLN:C	1:F:209:ILE:HD12	2.36	0.45
1:F:230:LYS:HZ2	1:F:321:ARG:NH1	2.15	0.45
1:F:45:ALA:C	1:F:46:LEU:HD12	2.36	0.45
1:G:31:ALA:O	1:G:34:ALA:N	2.49	0.45
1:G:211:LYS:HD2	1:G:391:VAL:HG22	1.98	0.45
1:H:40:LYS:HD3	1:H:116:LYS:HG2	1.99	0.45
1:I:260:LEU:CD1	1:I:261:ASP:CG	2.85	0.45
1:B:476:THR:HG21	1:B:494:PRO:HB3	1.99	0.45
1:C:142:ALA:O	1:C:425:ILE:HD12	2.17	0.45
1:C:244:ALA:HA	1:C:296:ASN:HD22	1.82	0.45
1:C:432:TYR:CZ	1:C:436:VAL:HG12	2.52	0.45
1:D:250:ASP:O	1:D:251:ALA:HB2	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:D:492:GLY:O	1:D:493:GLN:HB2	2.16	0.45
1:E:142:ALA:O	1:E:425:ILE:HD12	2.17	0.45
1:F:127:HIS:CG	1:F:128:PRO:HD2	2.51	0.45
1:F:172:LYS:HG3	1:F:397:ALA:HB2	1.99	0.45
1:F:209:ILE:CB	1:F:399:ARG:HH22	2.28	0.45
1:F:529:VAL:HG12	1:G:58:MET:CG	2.46	0.45
1:G:188:ALA:HA	1:G:379:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:127:HIS:CG	1:H:128:PRO:HD2	2.51	0.45
1:C:188:ALA:HA	1:C:379:ILE:HD11	1.98	0.45
1:E:153:VAL:HG23	1:E:160:LEU:CD2	2.45	0.45
1:E:211:LYS:HD2	1:E:391:VAL:HG22	1.98	0.45
1:G:172:LYS:HG3	1:G:397:ALA:HB2	1.99	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:H:321:ARG:HB3	1:H:322:ARG:H	1.56	0.45
1:H:172:LYS:HG3	1:H:397:ALA:HB2	1.99	0.45
1:I:210:VAL:O	1:I:382:LEU:HD12	2.16	0.45
1:A:146:ILE:HB	1:A:510:MET:HE2	1.99	0.45
1:A:172:LYS:HG3	1:A:397:ALA:HB2	1.99	0.45
1:C:166:MET:CE	1:C:178:ARG:HG2	2.46	0.45
1:C:172:LYS:HG3	1:C:397:ALA:HB2	1.99	0.45
1:C:31:ALA:O	1:C:34:ALA:N	2.49	0.45
1:C:146:ILE:HB	1:C:510:MET:HE3	1.99	0.45
1:E:210:VAL:O	1:E:382:LEU:HD12	2.16	0.45
1:H:31:ALA:O	1:H:34:ALA:N	2.49	0.45
1:A:68:ILE:HD12	1:I:522:LEU:HD11	1.98	0.45
1:A:40:LYS:HD3	1:A:116:LYS:HG2	1.99	0.45
1:D:142:ALA:O	1:D:425:ILE:HD12	2.17	0.45
1:D:260:LEU:CD1	1:D:261:ASP:CG	2.85	0.45
1:E:153:VAL:HG13	1:E:153:VAL:O	2.16	0.45
1:F:142:ALA:O	1:F:425:ILE:HD12	2.17	0.45
1:G:161:LEU:CD1	1:G:161:LEU:H	2.30	0.45
1:H:432:TYR:CZ	1:H:436:VAL:HG12	2.52	0.45
1:I:188:ALA:HA	1:I:379:ILE:HD11	1.98	0.45
1:I:40:LYS:HD3	1:I:116:LYS:HG2	1.99	0.45
1:A:142:ALA:O	1:A:425:ILE:HD12	2.17	0.44
1:A:31:ALA:O	1:A:34:ALA:N	2.49	0.44
1:A:98:GLU:OE1	1:A:98:GLU:HA	2.17	0.44
1:E:165:ALA:O	1:E:169:LEU:HG	2.18	0.44
1:F:432:TYR:CZ	1:F:436:VAL:HG12	2.52	0.44
1:G:98:GLU:OE1	1:G:98:GLU:HA	2.17	0.44
1:H:165:ALA:O	1:H:169:LEU:HG	2.17	0.44
1:I:89:LEU:CD2	1:I:108:VAL:HG23	2.44	0.44
1:I:161:LEU:CD1	1:I:161:LEU:H	2.30	0.44
1:A:153:VAL:HG23	1:A:160:LEU:CD2	2.45	0.44
1:A:166:MET:CE	1:A:178:ARG:HG2	2.47	0.44
1:B:165:ALA:O	1:B:169:LEU:HG	2.18	0.44
1:E:244:ALA:HA	1:E:296:ASN:HD22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:LEU:CD1	1:F:161:LEU:H	2.30	0.44
1:F:165:ALA:O	1:F:169:LEU:HG	2.18	0.44
1:F:265:ARG:HD2	1:F:265:ARG:C	2.38	0.44
1:F:492:GLY:O	1:F:493:GLN:HB2	2.16	0.44
1:G:321:ARG:HB3	1:G:322:ARG:H	1.56	0.44
1:I:211:LYS:HD2	1:I:391:VAL:HG22	1.98	0.44
1:C:436:VAL:HG21	1:C:441:GLN:HA	1.99	0.44
1:C:492:GLY:O	1:C:493:GLN:HB2	2.16	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:H:212:LYS:O	1:H:213:ALA:O	2.34	0.44
1:I:492:GLY:O	1:I:493:GLN:HB2	2.16	0.44
1:A:127:HIS:CG	1:A:128:PRO:HD2	2.51	0.44
1:A:260:LEU:CD1	1:A:261:ASP:CG	2.85	0.44
1:A:82:GLN:O	1:A:83:HIS:C	2.56	0.44
1:B:260:LEU:C	1:B:260:LEU:CD1	2.81	0.44
1:C:414:ALA:HA	1:C:506:ALA:H	1.83	0.44
1:D:259:GLU:C	1:D:259:GLU:CD	2.74	0.44
1:E:265:ARG:C	1:E:265:ARG:HD2	2.38	0.44
1:G:260:LEU:CD1	1:G:261:ASP:CG	2.85	0.44
1:G:469:LEU:HB3	1:G:487:ILE:CD1	2.43	0.44
1:G:59:LEU:HD13	1:G:78:LYS:HB2	2.00	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:I:142:ALA:O	1:I:425:ILE:HD12	2.17	0.44
1:I:265:ARG:HD2	1:I:265:ARG:C	2.38	0.44
1:I:414:ALA:HA	1:I:506:ALA:H	1.83	0.44
1:I:82:GLN:O	1:I:83:HIS:C	2.56	0.44
1:A:39:VAL:HG11	1:A:115:VAL:HG21	2.00	0.44
1:A:165:ALA:O	1:A:169:LEU:HG	2.17	0.44
1:A:66:ILE:CD1	1:A:66:ILE:N	2.76	0.44
1:B:142:ALA:O	1:B:425:ILE:HD12	2.17	0.44
1:C:39:VAL:HG11	1:C:115:VAL:HG21	2.00	0.44
1:C:476:THR:HG21	1:C:494:PRO:HB3	1.99	0.44
1:C:515:ALA:O	1:C:518:GLU:HB3	2.18	0.44
1:C:529:VAL:HG12	1:D:58:MET:SD	2.57	0.44
1:E:161:LEU:CD1	1:E:161:LEU:H	2.30	0.44
1:E:260:LEU:C	1:E:260:LEU:CD1	2.81	0.44
1:D:530:VAL:O	1:E:59:LEU:CD2	2.65	0.44
1:E:82:GLN:O	1:E:83:HIS:C	2.56	0.44
1:F:145:THR:O	1:F:145:THR:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:165:ALA:O	1:G:169:LEU:HG	2.17	0.44
1:G:141:VAL:CG2	1:G:432:TYR:CE1	2.97	0.44
1:I:172:LYS:HG3	1:I:397:ALA:HB2	1.99	0.44
1:A:250:ASP:O	1:A:251:ALA:HB2	2.17	0.44
1:A:432:TYR:CZ	1:A:436:VAL:HG12	2.52	0.44
1:B:391:VAL:HG13	1:B:392:ASP:N	2.33	0.44
1:B:414:ALA:HA	1:B:506:ALA:H	1.83	0.44
1:B:440:GLU:O	1:B:444:VAL:HG23	2.18	0.44
1:C:110:PHE:CZ	1:C:114:LEU:HD11	2.53	0.44
1:C:82:GLN:O	1:C:83:HIS:C	2.56	0.44
1:D:260:LEU:CD1	1:D:260:LEU:C	2.81	0.44
1:D:515:ALA:O	1:D:518:GLU:HB3	2.18	0.44
1:D:98:GLU:HA	1:D:98:GLU:OE1	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:F:505:PRO:C	1:F:507:LEU:N	2.69	0.44
1:F:110:PHE:HD1	1:F:516:ALA:CB	2.31	0.44
1:F:98:GLU:OE1	1:F:98:GLU:HA	2.17	0.44
1:G:440:GLU:O	1:G:444:VAL:HG23	2.18	0.44
1:H:110:PHE:CZ	1:H:114:LEU:HD11	2.53	0.44
1:H:249:ILE:HD13	1:H:340:VAL:HB	2.00	0.44
1:H:265:ARG:HD2	1:H:265:ARG:C	2.38	0.44
1:H:515:ALA:O	1:H:518:GLU:HB3	2.18	0.44
1:H:59:LEU:HD13	1:H:78:LYS:HB2	2.00	0.44
1:I:430:ARG:NH1	1:I:430:ARG:HG2	2.29	0.44
1:I:146:ILE:HB	1:I:510:MET:HE3	1.98	0.44
1:I:98:GLU:OE1	1:I:98:GLU:HA	2.17	0.44
1:A:110:PHE:CZ	1:A:114:LEU:HD11	2.53	0.44
1:A:217:ILE:HD11	1:A:390:LEU:CD2	2.43	0.44
1:A:436:VAL:HG21	1:A:441:GLN:HA	1.99	0.44
1:A:476:THR:HG21	1:A:494:PRO:HB3	1.99	0.44
1:B:89:LEU:CD2	1:B:108:VAL:HG23	2.44	0.44
1:B:265:ARG:HD2	1:B:265:ARG:C	2.38	0.44
1:C:249:ILE:HD13	1:C:340:VAL:HB	2.00	0.44
1:C:265:ARG:HD2	1:C:265:ARG:C	2.38	0.44
1:D:391:VAL:HG13	1:D:392:ASP:N	2.33	0.44
1:D:440:GLU:O	1:D:444:VAL:HG23	2.18	0.44
1:E:110:PHE:CZ	1:E:114:LEU:HD11	2.53	0.44
1:E:172:LYS:HG3	1:E:397:ALA:HB2	1.99	0.44
1:E:110:PHE:HD1	1:E:516:ALA:CB	2.31	0.44
1:E:59:LEU:HD13	1:E:78:LYS:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:153:VAL:HG23	1:F:160:LEU:CD2	2.45	0.44
1:G:110:PHE:CZ	1:G:114:LEU:HD11	2.53	0.44
1:G:145:THR:O	1:G:145:THR:HG22	2.18	0.44
1:G:250:ASP:O	1:G:251:ALA:HB2	2.17	0.44
1:G:414:ALA:HA	1:G:506:ALA:H	1.83	0.44
1:H:89:LEU:CD2	1:H:108:VAL:HG23	2.44	0.44
1:H:469:LEU:HB3	1:H:487:ILE:CD1	2.43	0.44
1:I:110:PHE:CZ	1:I:114:LEU:HD11	2.53	0.44
1:I:165:ALA:O	1:I:169:LEU:HG	2.18	0.44
1:A:265:ARG:C	1:A:265:ARG:HD2	2.38	0.44
1:B:110:PHE:HD1	1:B:516:ALA:CB	2.31	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:D:145:THR:O	1:D:145:THR:HG22	2.18	0.44
1:D:165:ALA:O	1:D:169:LEU:HG	2.17	0.44
1:D:265:ARG:C	1:D:265:ARG:HD2	2.38	0.44
1:D:172:LYS:HG3	1:D:397:ALA:HB2	1.99	0.44
1:D:209:ILE:CB	1:D:399:ARG:HH22	2.28	0.44
1:D:146:ILE:HB	1:D:510:MET:HE3	2.00	0.44
1:E:145:THR:O	1:E:145:THR:HG22	2.18	0.44
1:E:515:ALA:O	1:E:518:GLU:HB3	2.18	0.44
1:H:142:ALA:O	1:H:425:ILE:HD12	2.17	0.44
1:H:476:THR:HG21	1:H:494:PRO:HB3	1.99	0.44
1:I:440:GLU:O	1:I:444:VAL:HG23	2.18	0.44
1:I:476:THR:HG21	1:I:494:PRO:HB3	1.99	0.44
1:I:515:ALA:O	1:I:518:GLU:HB3	2.18	0.44
1:A:211:LYS:HD2	1:A:391:VAL:HG22	1.98	0.44
1:B:146:ILE:HB	1:B:510:MET:HE3	1.99	0.44
1:B:244:ALA:HA	1:B:296:ASN:HD22	1.82	0.44
1:B:249:ILE:HD13	1:B:340:VAL:HB	2.00	0.44
1:B:59:LEU:HD13	1:B:78:LYS:HB2	2.00	0.44
1:C:250:ASP:O	1:C:251:ALA:HB2	2.17	0.44
1:D:414:ALA:HA	1:D:506:ALA:H	1.83	0.44
1:E:505:PRO:C	1:E:507:LEU:H	2.22	0.44
1:G:89:LEU:CD2	1:G:108:VAL:HG23	2.44	0.44
1:H:161:LEU:CD1	1:H:161:LEU:H	2.30	0.44
1:H:250:ASP:O	1:H:251:ALA:HB2	2.17	0.44
1:H:146:ILE:HB	1:H:510:MET:HE3	1.99	0.44
1:H:81:LEU:HD12	1:H:81:LEU:N	2.28	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ILE:HD13	1:A:66:ILE:N	2.13	0.43
1:C:145:THR:HG22	1:C:145:THR:O	2.18	0.43
1:E:414:ALA:HA	1:E:506:ALA:H	1.83	0.43
1:F:233:VAL:HG22	1:F:309:GLN:CD	2.39	0.43
1:F:258:PRO:CG	1:F:279:GLU:OE2	2.56	0.43
1:F:436:VAL:HG21	1:F:441:GLN:HA	1.99	0.43
1:G:142:ALA:O	1:G:425:ILE:HD12	2.17	0.43
1:G:233:VAL:HG22	1:G:309:GLN:CD	2.39	0.43
1:G:244:ALA:HA	1:G:296:ASN:HD22	1.82	0.43
1:H:145:THR:O	1:H:145:THR:HG22	2.18	0.43
1:H:82:GLN:O	1:H:83:HIS:C	2.56	0.43
1:I:145:THR:HG22	1:I:145:THR:O	2.18	0.43
1:I:436:VAL:HG21	1:I:441:GLN:HA	1.99	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:233:VAL:HG22	1:A:309:GLN:CD	2.39	0.43
1:A:244:ALA:HA	1:A:296:ASN:HD22	1.82	0.43
1:B:110:PHE:CZ	1:B:114:LEU:HD11	2.53	0.43
1:B:233:VAL:HG22	1:B:309:GLN:CD	2.39	0.43
1:C:161:LEU:CD1	1:C:161:LEU:H	2.30	0.43
1:C:260:LEU:CD1	1:C:261:ASP:CG	2.85	0.43
1:C:391:VAL:HG13	1:C:392:ASP:N	2.33	0.43
1:C:72:GLY:O	1:C:73:ALA:C	2.57	0.43
1:C:88:LEU:HD11	1:D:389:ARG:HH12	1.83	0.43
1:C:98:GLU:OE1	1:C:98:GLU:HA	2.17	0.43
1:D:484:TRP:HA	1:D:484:TRP:CE3	2.53	0.43
1:D:476:THR:HG21	1:D:494:PRO:HB3	1.99	0.43
1:F:260:LEU:CD1	1:F:261:ASP:CG	2.85	0.43
1:F:515:ALA:O	1:F:518:GLU:HB3	2.18	0.43
1:G:110:PHE:HD1	1:G:516:ALA:CB	2.31	0.43
1:G:391:VAL:HG13	1:G:392:ASP:N	2.33	0.43
1:G:525:ARG:HG2	1:G:525:ARG:NH1	2.31	0.43
1:H:188:ALA:HA	1:H:379:ILE:HD11	1.98	0.43
1:H:298:ILE:O	1:H:319:ALA:HA	2.19	0.43
1:I:72:GLY:O	1:I:73:ALA:C	2.57	0.43
1:B:98:GLU:OE1	1:B:98:GLU:HA	2.17	0.43
1:C:233:VAL:HG22	1:C:309:GLN:CD	2.39	0.43
1:C:58:MET:CB	1:C:68:ILE:HG22	2.48	0.43
1:D:161:LEU:H	1:D:161:LEU:CD1	2.30	0.43
1:D:432:TYR:CZ	1:D:436:VAL:HG12	2.52	0.43
1:D:505:PRO:C	1:D:507:LEU:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:VAL:HG22	1:E:309:GLN:CD	2.39	0.43
1:F:249:ILE:HD13	1:F:340:VAL:HB	2.00	0.43
1:F:440:GLU:O	1:F:444:VAL:HG23	2.18	0.43
1:F:505:PRO:C	1:F:507:LEU:H	2.22	0.43
1:F:59:LEU:HD13	1:F:78:LYS:HB2	2.00	0.43
1:G:249:ILE:HD13	1:G:340:VAL:HB	2.00	0.43
1:G:482:ASN:O	1:G:485:TYR:N	2.40	0.43
1:G:58:MET:CB	1:G:68:ILE:HG22	2.48	0.43
1:H:482:ASN:O	1:H:485:TYR:N	2.40	0.43
1:H:98:GLU:HA	1:H:98:GLU:OE1	2.17	0.43
1:A:414:ALA:HA	1:A:506:ALA:H	1.83	0.43
1:A:515:ALA:O	1:A:518:GLU:HB3	2.18	0.43
1:B:258:PRO:CG	1:B:279:GLU:OE2	2.56	0.43
1:B:58:MET:CB	1:B:68:ILE:HG22	2.48	0.43
1:D:110:PHE:HD1	1:D:516:ALA:CB	2.31	0.43
1:D:58:MET:CB	1:D:68:ILE:HG22	2.48	0.43
1:F:476:THR:HG21	1:F:494:PRO:HB3	1.99	0.43
1:H:39:VAL:HG11	1:H:115:VAL:HG21	2.00	0.43
1:I:249:ILE:HD13	1:I:340:VAL:HB	2.00	0.43
1:I:391:VAL:HG13	1:I:392:ASP:N	2.33	0.43
1:I:505:PRO:C	1:I:507:LEU:H	2.22	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:B:415:ILE:HG23	1:B:506:ALA:CB	2.48	0.43
1:B:436:VAL:HG21	1:B:441:GLN:HA	1.99	0.43
1:B:515:ALA:O	1:B:518:GLU:HB3	2.18	0.43
1:B:81:LEU:HD22	1:B:86:ALA:HB1	2.01	0.43
1:E:39:VAL:HG11	1:E:115:VAL:HG21	2.00	0.43
1:E:98:GLU:OE1	1:E:98:GLU:HA	2.17	0.43
1:G:265:ARG:HD2	1:G:265:ARG:C	2.38	0.43
1:G:484:TRP:HA	1:G:484:TRP:CE3	2.54	0.43
1:G:476:THR:HG21	1:G:494:PRO:HB3	1.99	0.43
1:H:414:ALA:HA	1:H:506:ALA:H	1.83	0.43
1:H:110:PHE:HD1	1:H:516:ALA:CB	2.31	0.43
1:I:415:ILE:HG23	1:I:506:ALA:CB	2.48	0.43
1:A:145:THR:O	1:A:145:THR:HG22	2.18	0.43
1:B:482:ASN:O	1:B:485:TYR:N	2.40	0.43
1:B:484:TRP:HA	1:B:484:TRP:CE3	2.53	0.43
1:B:505:PRO:C	1:B:507:LEU:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:PRO:HG3	1:F:55:MET:CE	2.48	0.43
1:E:484:TRP:CE3	1:E:484:TRP:HA	2.54	0.43
1:E:81:LEU:HD22	1:E:86:ALA:HB1	2.01	0.43
1:F:244:ALA:HA	1:F:296:ASN:HD22	1.82	0.43
1:F:58:MET:CB	1:F:68:ILE:HG22	2.48	0.43
1:G:40:LYS:HD3	1:G:116:LYS:HG2	1.99	0.43
1:G:46:LEU:O	1:G:49:THR:N	2.43	0.43
1:G:146:ILE:HB	1:G:510:MET:HE3	2.01	0.43
1:G:515:ALA:O	1:G:518:GLU:HB3	2.18	0.43
1:H:244:ALA:HA	1:H:296:ASN:HD22	1.82	0.43
1:H:233:VAL:HG22	1:H:309:GLN:CD	2.39	0.43
1:H:440:GLU:O	1:H:444:VAL:HG23	2.18	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:A:132:ILE:HD12	1:A:521:THR:HB	2.01	0.43
1:A:88:LEU:CD1	1:B:389:ARG:HH12	2.32	0.43
1:C:484:TRP:HA	1:C:484:TRP:CE3	2.54	0.43
1:C:81:LEU:HD22	1:C:86:ALA:HB1	2.01	0.43
1:D:298:ILE:O	1:D:319:ALA:HA	2.19	0.43
1:E:146:ILE:HB	1:E:510:MET:HE3	2.01	0.43
1:E:298:ILE:O	1:E:319:ALA:HA	2.19	0.43
1:F:110:PHE:CZ	1:F:114:LEU:HD11	2.53	0.43
1:F:415:ILE:HG23	1:F:506:ALA:CB	2.48	0.43
1:G:72:GLY:O	1:G:73:ALA:C	2.57	0.43
1:G:81:LEU:HD22	1:G:86:ALA:HB1	2.01	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:H:58:MET:CB	1:H:68:ILE:HG22	2.48	0.43
1:A:298:ILE:O	1:A:319:ALA:HA	2.19	0.43
1:B:145:THR:O	1:B:145:THR:HG22	2.18	0.43
1:B:172:LYS:HG3	1:B:397:ALA:HB2	1.99	0.43
1:B:141:VAL:CG2	1:B:432:TYR:CE1	2.97	0.43
1:C:94:LYS:O	1:C:96:GLN:N	2.48	0.43
1:D:110:PHE:CZ	1:D:114:LEU:HD11	2.53	0.43
1:D:233:VAL:HG22	1:D:309:GLN:CD	2.39	0.43
1:F:161:LEU:N	1:F:161:LEU:CD1	2.82	0.43
1:F:264:ILE:HD12	1:F:265:ARG:HH22	1.84	0.43
1:F:298:ILE:O	1:F:319:ALA:HA	2.18	0.43
1:F:414:ALA:HA	1:F:506:ALA:H	1.83	0.43
1:G:118:ALA:O	1:G:122:LEU:CD2	2.67	0.43
1:G:155:ILE:O	1:G:155:ILE:HG12	2.19	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:H:264:ILE:HD12	1:H:265:ARG:HH22	1.84	0.43
1:H:430:ARG:HG2	1:H:430:ARG:NH1	2.29	0.43
1:H:484:TRP:HA	1:H:484:TRP:CE3	2.54	0.43
1:I:39:VAL:HG11	1:I:115:VAL:HG21	2.00	0.43
1:A:284:LYS:HB3	1:A:311:TYR:CE2	2.54	0.43
1:A:415:ILE:HG23	1:A:506:ALA:CB	2.48	0.43
1:B:134:GLY:HA3	1:B:443:ALA:CB	2.49	0.43
1:B:298:ILE:O	1:B:319:ALA:HA	2.19	0.43
1:B:72:GLY:O	1:B:73:ALA:C	2.57	0.43
1:C:298:ILE:O	1:C:319:ALA:HA	2.19	0.43
1:C:209:ILE:CB	1:C:399:ARG:HH22	2.28	0.43
1:E:249:ILE:HD13	1:E:340:VAL:HB	2.00	0.43
1:E:58:MET:CB	1:E:68:ILE:HG22	2.48	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:G:161:LEU:CD1	1:G:161:LEU:N	2.82	0.43
1:H:155:ILE:HG12	1:H:155:ILE:O	2.19	0.43
1:I:230:LYS:HZ1	1:I:321:ARG:NH1	2.14	0.43
1:I:233:VAL:HG22	1:I:309:GLN:CD	2.39	0.43
1:I:298:ILE:O	1:I:319:ALA:HA	2.19	0.43
1:I:134:GLY:HA3	1:I:443:ALA:CB	2.49	0.43
1:A:134:GLY:HA3	1:A:443:ALA:CB	2.49	0.43
1:A:505:PRO:C	1:A:507:LEU:H	2.22	0.43
1:A:58:MET:CB	1:A:68:ILE:HG22	2.48	0.43
1:C:440:GLU:O	1:C:444:VAL:HG23	2.18	0.43
1:D:81:LEU:HD22	1:D:86:ALA:HB1	2.01	0.43
1:E:118:ALA:O	1:E:122:LEU:CD2	2.67	0.43
1:E:440:GLU:O	1:E:444:VAL:HG23	2.18	0.43
1:E:476:THR:HG21	1:E:494:PRO:HB3	1.99	0.43
1:F:155:ILE:HG12	1:F:155:ILE:O	2.19	0.43
1:H:459:ILE:O	1:H:462:ALA:HB3	2.19	0.43
1:I:264:ILE:HD12	1:I:265:ARG:HH22	1.84	0.43
1:A:482:ASN:O	1:A:485:TYR:N	2.40	0.42
1:A:484:TRP:HA	1:A:484:TRP:CE3	2.54	0.42
1:C:134:GLY:HA3	1:C:443:ALA:CB	2.49	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:D:321:ARG:HB3	1:D:322:ARG:H	1.56	0.42
1:D:459:ILE:O	1:D:462:ALA:HB3	2.19	0.42
1:D:46:LEU:N	1:D:46:LEU:CD1	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:LEU:O	1:D:49:THR:N	2.43	0.42
1:E:134:GLY:HA3	1:E:443:ALA:CB	2.49	0.42
1:E:505:PRO:O	1:E:507:LEU:N	2.52	0.42
1:F:89:LEU:CD2	1:F:108:VAL:HG23	2.44	0.42
1:G:134:GLY:HA3	1:G:443:ALA:CB	2.49	0.42
1:G:39:VAL:HG11	1:G:115:VAL:HG21	2.00	0.42
1:G:505:PRO:C	1:G:507:LEU:H	2.22	0.42
1:H:258:PRO:CG	1:H:279:GLU:OE2	2.56	0.42
1:H:284:LYS:HB3	1:H:311:TYR:CE2	2.54	0.42
1:H:525:ARG:HG2	1:H:525:ARG:NH1	2.31	0.42
1:A:391:VAL:HG13	1:A:392:ASP:N	2.33	0.42
1:A:505:PRO:O	1:A:507:LEU:N	2.52	0.42
1:B:118:ALA:O	1:B:122:LEU:CD2	2.67	0.42
1:B:39:VAL:HG11	1:B:115:VAL:HG21	2.00	0.42
1:B:459:ILE:O	1:B:462:ALA:HB3	2.19	0.42
1:C:284:LYS:HB3	1:C:311:TYR:CE2	2.54	0.42
1:C:298:ILE:O	1:C:298:ILE:HG23	2.19	0.42
1:D:153:VAL:HG23	1:D:160:LEU:CD2	2.45	0.42
1:D:244:ALA:HA	1:D:296:ASN:HD22	1.82	0.42
1:D:134:GLY:HA3	1:D:443:ALA:CB	2.49	0.42
1:E:508:VAL:CG1	1:E:509:LYS:N	2.83	0.42
1:F:46:LEU:CD1	1:F:46:LEU:N	2.82	0.42
1:F:508:VAL:CG1	1:F:509:LYS:N	2.83	0.42
1:I:484:TRP:CE3	1:I:484:TRP:HA	2.54	0.42
1:A:155:ILE:O	1:A:155:ILE:HG12	2.19	0.42
1:A:298:ILE:HG23	1:A:298:ILE:O	2.20	0.42
1:A:72:GLY:O	1:A:73:ALA:C	2.57	0.42
1:B:82:GLN:O	1:B:83:HIS:C	2.56	0.42
1:C:505:PRO:C	1:C:507:LEU:H	2.22	0.42
1:D:245:LYS:H	1:D:296:ASN:ND2	2.07	0.42
1:D:39:VAL:HG11	1:D:115:VAL:HG21	2.00	0.42
1:F:321:ARG:HB3	1:F:322:ARG:H	1.56	0.42
1:F:82:GLN:O	1:F:83:HIS:C	2.56	0.42
1:H:298:ILE:O	1:H:298:ILE:HG23	2.20	0.42
1:I:268:ASP:HB3	1:I:269:PRO:HD2	2.02	0.42
1:I:298:ILE:O	1:I:298:ILE:HG23	2.20	0.42
1:A:89:LEU:CD2	1:A:108:VAL:HG23	2.44	0.42
1:A:264:ILE:HD12	1:A:265:ARG:HH22	1.84	0.42
1:A:459:ILE:O	1:A:462:ALA:HB3	2.19	0.42
1:B:155:ILE:O	1:B:155:ILE:HG12	2.19	0.42
1:C:118:ALA:O	1:C:122:LEU:CD2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:LEU:HD12	1:C:398:LEU:HA	1.88	0.42
1:C:459:ILE:O	1:C:462:ALA:HB3	2.19	0.42
1:C:59:LEU:HD13	1:C:78:LYS:HB2	2.00	0.42
1:E:132:ILE:HD12	1:E:521:THR:HB	2.01	0.42
1:E:155:ILE:O	1:E:155:ILE:HG12	2.19	0.42
1:E:161:LEU:CD1	1:E:161:LEU:N	2.82	0.42
1:E:284:LYS:HB3	1:E:311:TYR:CE2	2.54	0.42
1:F:118:ALA:O	1:F:122:LEU:CD2	2.67	0.42
1:G:459:ILE:O	1:G:462:ALA:HB3	2.19	0.42
1:G:505:PRO:O	1:G:507:LEU:N	2.52	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:I:132:ILE:HD12	1:I:521:THR:HB	2.01	0.42
1:A:249:ILE:HD13	1:A:340:VAL:HB	2.00	0.42
1:A:433:ALA:O	1:A:434:PRO:C	2.58	0.42
1:A:81:LEU:HD22	1:A:86:ALA:HB1	2.01	0.42
1:C:268:ASP:HB3	1:C:269:PRO:HD2	2.02	0.42
1:C:46:LEU:O	1:C:49:THR:N	2.43	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:E:482:ASN:O	1:E:485:TYR:N	2.40	0.42
1:D:529:VAL:CG1	1:E:58:MET:HB3	2.29	0.42
1:F:351:LEU:HD23	1:F:351:LEU:N	2.26	0.42
1:G:298:ILE:O	1:G:319:ALA:HA	2.19	0.42
1:H:106:THR:O	1:H:107:ALA:C	2.58	0.42
1:H:209:ILE:CB	1:H:399:ARG:HH22	2.28	0.42
1:I:155:ILE:HG12	1:I:155:ILE:O	2.19	0.42
1:I:161:LEU:N	1:I:161:LEU:CD1	2.82	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:B:284:LYS:HB3	1:B:311:TYR:CE2	2.54	0.42
1:C:106:THR:O	1:C:107:ALA:C	2.58	0.42
1:C:153:VAL:HG23	1:C:160:LEU:CD2	2.45	0.42
1:C:258:PRO:CG	1:C:279:GLU:OE2	2.56	0.42
1:C:46:LEU:N	1:C:46:LEU:CD1	2.82	0.42
1:D:106:THR:O	1:D:107:ALA:C	2.58	0.42
1:D:118:ALA:O	1:D:122:LEU:CD2	2.67	0.42
1:D:141:VAL:CG2	1:D:432:TYR:CE1	2.97	0.42
1:D:72:GLY:O	1:D:73:ALA:C	2.57	0.42
1:E:264:ILE:HD12	1:E:265:ARG:HH22	1.84	0.42
1:F:132:ILE:HD12	1:F:521:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:260:LEU:CD1	1:F:260:LEU:C	2.81	0.42
1:G:153:VAL:HG23	1:G:160:LEU:CD2	2.45	0.42
1:G:433:ALA:O	1:G:434:PRO:C	2.58	0.42
1:G:508:VAL:CG1	1:G:509:LYS:N	2.83	0.42
1:H:433:ALA:O	1:H:434:PRO:C	2.58	0.42
1:A:161:LEU:CD1	1:A:161:LEU:N	2.82	0.42
1:B:161:LEU:CD1	1:B:161:LEU:N	2.82	0.42
1:E:88:LEU:CD2	1:F:58:MET:HE2	2.47	0.42
1:F:195:LEU:HD11	1:F:200:TRP:CH2	2.55	0.42
1:F:284:LYS:HB3	1:F:311:TYR:CE2	2.54	0.42
1:F:72:GLY:O	1:F:73:ALA:C	2.57	0.42
1:G:529:VAL:HG12	1:H:58:MET:SD	2.60	0.42
1:I:256:GLU:O	1:I:258:PRO:CG	2.68	0.42
1:A:106:THR:O	1:A:107:ALA:C	2.58	0.42
1:B:106:THR:O	1:B:107:ALA:C	2.58	0.42
1:B:132:ILE:HD12	1:B:521:THR:HB	2.01	0.42
1:B:289:LYS:HE3	1:B:289:LYS:HB2	1.86	0.42
1:B:505:PRO:O	1:B:507:LEU:N	2.52	0.42
1:C:291:LEU:O	1:C:294:GLY:N	2.53	0.42
1:C:505:PRO:O	1:C: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:E:46:LEU:N	1:E:46:LEU:CD1	2.82	0.42
1:E:484:TRP:HE3	1:E:484:TRP:HA	1.85	0.42
1:F:298:ILE:HG23	1:F:298:ILE:O	2.20	0.42
1:F:528:ASP:O	1:G:57:LYS:HA	2.19	0.42
1:H:132:ILE:HD12	1:H:521:THR:HB	2.01	0.42
1:H:140:GLU:HA	1:H:140:GLU:OE2	2.20	0.42
1:A:118:ALA:O	1:A:122:LEU:CD2	2.67	0.42
1:B:46:LEU:O	1:B:49:THR:N	2.43	0.42
1:B:484:TRP:HE3	1:B:484:TRP:HA	1.85	0.42
1:C:264:ILE:HD12	1:C:265:ARG:HH22	1.84	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: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:G:132:ILE:HD12	1:G:521:THR:HB	2.01	0.42
1:H:134:GLY:HA3	1:H:443:ALA:CB	2.49	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:I:505:PRO:O	1:I:507:LEU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:506:ALA:O	1:I:510:MET:HB2	2.20	0.42
1:I:59:LEU:HD13	1:I:78:LYS:HB2	2.00	0.42
1:A:195:LEU:HD11	1:A:200:TRP:CH2	2.55	0.42
1:A:268:ASP:HB3	1:A:269:PRO:HD2	2.02	0.42
1:A:321:ARG:HB3	1:A:322:ARG:H	1.56	0.42
1:B:264:ILE:HD12	1:B:265:ARG:HH22	1.84	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:C:506:ALA:O	1:C:510:MET:HB2	2.20	0.42
1:D:161:LEU:CD1	1:D:161:LEU:N	2.82	0.42
1:D:195:LEU:HD11	1:D:200:TRP:CH2	2.55	0.42
1:D:433:ALA:O	1:D:434:PRO:C	2.58	0.42
1:D:132:ILE:HD12	1:D:521:THR:HB	2.01	0.42
1:F:39:VAL:HG11	1:F:115:VAL:HG21	2.00	0.42
1:F:506:ALA:O	1:F:510:MET:HB2	2.20	0.42
1:G:176:GLY:O	1:G:177:ALA:C	2.59	0.42
1:G:268:ASP:HB3	1:G:269:PRO:HD2	2.02	0.42
1:I:118:ALA:O	1:I:122:LEU:CD2	2.67	0.42
1:A:317:VAL:HG12	1:A:318:LEU:N	2.35	0.41
1:A:484:TRP:HA	1:A:484:TRP:HE3	1.85	0.41
1:B:140:GLU:HA	1:B:140:GLU:OE2	2.20	0.41
1:B:209:ILE:CB	1:B:399:ARG:HH22	2.28	0.41
1:B:506:ALA:O	1:B:510:MET:HB2	2.20	0.41
1:D:256:GLU:O	1:D:258:PRO:CG	2.68	0.41
1:D:298:ILE:O	1:D:298:ILE:HG23	2.20	0.41
1:D:284:LYS:HB3	1:D:311:TYR:CE2	2.54	0.41
1:D:415:ILE:HG23	1:D:506:ALA:CB	2.48	0.41
1:F:433:ALA:O	1:F:434:PRO:C	2.58	0.41
1:F:505:PRO:O	1:F:507:LEU:N	2.53	0.41
1:F:146:ILE:HB	1:F:510:MET:HE3	2.00	0.41
1:G:195:LEU:HD11	1:G:200:TRP:CH2	2.55	0.41
1:G:493:GLN:HA	1:G:494:PRO:HD3	1.90	0.41
1:H:176:GLY:O	1:H:177:ALA:C	2.59	0.41
1:H:195:LEU:HD11	1:H:200:TRP:CH2	2.55	0.41
1:H:72:GLY:O	1:H:73:ALA:C	2.57	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:B:268:ASP:HB3	1:B:269:PRO:HD2	2.02	0.41
1:D:359:GLU:HA	1:D:367:MET:O	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:525:ARG:NH1	1:E:525:ARG:HG2	2.31	0.41
1:F:459:ILE:O	1:F:462:ALA:HB3	2.19	0.41
1:G:264:ILE:HD12	1:G:265:ARG:HH22	1.84	0.41
1:G:284:LYS:HB3	1:G:311:TYR:CE2	2.54	0.41
1:H:484:TRP:HE3	1:H:484:TRP:HA	1.85	0.41
1:I:176:GLY:O	1:I:177:ALA:C	2.59	0.41
1:I:433:ALA:O	1:I:434:PRO:C	2.58	0.41
1:E:140:GLU:OE2	1:E:140:GLU:HA	2.20	0.41
1:E:268:ASP:HB3	1:E:269:PRO:HD2	2.02	0.41
1:E:298:ILE:O	1:E:298:ILE:HG23	2.20	0.41
1:E:506:ALA:O	1:E:510:MET:HB2	2.20	0.41
1:E:525:ARG:HG3	1:F:56:ASP:CB	2.46	0.41
1:G:298:ILE:HG23	1:G:298:ILE:O	2.20	0.41
1:I:106:THR:O	1:I:107:ALA:C	2.58	0.41
1:A:249:ILE:CD1	1:A:346:ILE:HD11	2.50	0.41
1:A:359:GLU:HA	1:A:367:MET:O	2.20	0.41
1:A:48:SER:O	1:A:55:MET:HB2	2.21	0.41
1:C:132:ILE:HD12	1:C:521:THR:HB	2.01	0.41
1:C:140:GLU:OE2	1:C:140:GLU:HA	2.20	0.41
1:D:176:GLY:O	1:D:177:ALA:C	2.59	0.41
1:D:264:ILE:HD12	1:D:265:ARG:HH22	1.84	0.41
1:E:89:LEU:CD2	1:E:108:VAL:HG23	2.44	0.41
1:E:48:SER:O	1:E:55:MET:HB2	2.20	0.41
1:F:249:ILE:CD1	1:F:346:ILE:HD11	2.50	0.41
1:F:359:GLU:HA	1:F:367:MET:O	2.20	0.41
1:F:81:LEU:HD22	1:F:86:ALA:HB1	2.01	0.41
1:G:106:THR:O	1:G:107:ALA:C	2.58	0.41
1:G:260:LEU:C	1:G:260:LEU:CD1	2.81	0.41
1:G:359:GLU:HA	1:G:367:MET:O	2.20	0.41
1:H:268:ASP:HB3	1:H:269:PRO:HD2	2.01	0.41
1:H:46:LEU:N	1:H:46:LEU:CD1	2.82	0.41
1:I:359:GLU:HA	1:I:367:MET:O	2.20	0.41
1:I:454:LEU:HD12	1:I:454:LEU:HA	1.91	0.41
1:I:508:VAL:CG1	1:I:509:LYS:N	2.83	0.41
1:A:194:GLU:O	1:A:200:TRP:HA	2.21	0.41
1:A:46:LEU:N	1:A:46:LEU:CD1	2.82	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:D:530:VAL:O	1:E:59:LEU:HA	2.19	0.41
1:F:106:THR:O	1:F:107:ALA:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:GLY:HA3	1:F:443:ALA:CB	2.49	0.41
1:G:415:ILE:HG23	1:G:506:ALA:CB	2.48	0.41
1:G:48:SER:O	1:G:55:MET:HB2	2.21	0.41
1:I:195:LEU:HD11	1:I:200:TRP:CH2	2.55	0.41
1:I:46:LEU:N	1:I:46:LEU:CD1	2.82	0.41
1:A:264:ILE:CG1	1:A:265:ARG:O	2.66	0.41
1:B:291:LEU:O	1:B:294:GLY:N	2.53	0.41
1:B:504:GLU:HA	1:B:505:PRO:HD3	1.90	0.41
1:C:256:GLU:O	1:C:258:PRO:CG	2.68	0.41
1:D:454:LEU:HA	1:D:454:LEU:HD12	1.91	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:E:415:ILE:HG23	1:E:506:ALA:CB	2.48	0.41
1:G:194:GLU:O	1:G:200:TRP:HA	2.21	0.41
1:H:506:ALA:O	1:H:510:MET:HB2	2.20	0.41
1:H:522:LEU:HD11	1:I:68:ILE:HD12	2.03	0.41
1:A:508:VAL:CG1	1:A:509:LYS:N	2.83	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:321:ARG:HB3	1:C:322:ARG:H	1.56	0.41
1:C:81:LEU:HD13	1:C:87:LYS:HG2	2.03	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:I:46:LEU:O	1:I:49:THR:N	2.43	0.41
1:A:253:LEU:O	1:A:253:LEU:HG	2.21	0.41
1:A:291:LEU:O	1:A:294:GLY:N	2.53	0.41
1:A:506:ALA:O	1:A:510:MET:HB2	2.20	0.41
1:A:88:LEU:HD22	1:B:58:MET:CE	2.51	0.41
1:B:249:ILE:O	1:B:300:CYS:HB2	2.21	0.41
1:B:317:VAL:HG12	1:B:318:LEU:N	2.35	0.41
1:B:81:LEU:HD12	1:B:81:LEU:N	2.28	0.41
1:C:253:LEU:O	1:C:253:LEU:HG	2.21	0.41
1:D:317:VAL:HG12	1:D:318:LEU:N	2.35	0.41
1:E:454:LEU:HA	1:E:454:LEU:HD12	1.91	0.41
1:H:259:GLU:O	1:H:262:ALA:O	2.39	0.41
1:H:81:LEU:HD22	1:H:86:ALA:HB1	2.01	0.41
1:I:140:GLU:OE2	1:I:140:GLU:HA	2.20	0.41
1:I:317:VAL:HG12	1:I:318:LEU:N	2.35	0.41
1:I:48:SER:O	1:I:55:MET:HB2	2.21	0.41
1:I:81:LEU:HD13	1:I:87:LYS:HG2	2.03	0.41
1:A:389:ARG:HH12	1:I:88:LEU:CD1	2.31	0.41

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:321:ARG:HB3	1:I:322:ARG:H	1.56	0.41
1:I:436:VAL:CG2	1:I:441:GLN:HA	2.51	0.41
1:A:147:GLN:C	1:A:149:LEU:H	2.25	0.40
1:B:253:LEU:HG	1:B:253:LEU:O	2.21	0.40
1:C:66:ILE:N	1:C:66:ILE:CD1	2.76	0.40
1:D:249:ILE:CD1	1:D:346:ILE:HD11	2.50	0.40
1:D:531:SER:HB3	1:E:60:VAL:HB	2.04	0.40
1:G:253:LEU:HG	1:G:253:LEU:O	2.21	0.40
1:G:436:VAL:CG2	1:G:441:GLN:HA	2.52	0.40
1:H:253:LEU:HG	1:H:253:LEU:O	2.21	0.40
1:H:351:LEU:HD23	1:H:351:LEU:N	2.26	0.40
1:H:436:VAL:CG2	1:H:441:GLN:HA	2.51	0.40
1:I:194:GLU:O	1:I:200:TRP:HA	2.21	0.40
1:B:147:GLN:C	1:B:149:LEU:H	2.25	0.40
1:B:153:VAL:HG23	1:B:160:LEU:CD2	2.45	0.40
1:B:81:LEU:HD13	1:B:87:LYS:HG2	2.03	0.40
1:C:230:LYS:NZ	1:C:321:ARG:HH12	2.18	0.40
1:C:410:LYS:HE2	1:C:410:LYS:HB3	1.89	0.40
1:C:508:VAL:CG1	1:C:509:LYS:N	2.83	0.40
1:D:194:GLU:O	1:D:200:TRP:HA	2.21	0.40
1:E:166:MET:CE	1:E:179:GLU:HG2	2.51	0.40
1:E:259:GLU:O	1:E:262:ALA:O	2.39	0.40
1:F:140:GLU:HA	1:F:140:GLU:OE2	2.20	0.40
1:F:166:MET:CE	1:F:179:GLU:HG2	2.51	0.40
1:F:423:ILE:HG12	1:F:473:LEU:HD11	2.03	0.40
1:F:48:SER:O	1:F:55:MET:HB2	2.21	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:H:256:GLU:O	1:H:258:PRO:CG	2.68	0.40
1:I:264:ILE:CG1	1:I:265:ARG:O	2.67	0.40
1:I:473:LEU:C	1:I:475:SER:N	2.75	0.40
1:A:259:GLU:O	1:A:262:ALA:O	2.39	0.40
1:A:410:LYS:HE2	1:A:410:LYS:HB3	1.89	0.40
1:B:246:ILE:HA	1:B:297:VAL:CG1	2.51	0.40
1:B:508:VAL:CG1	1:B:509:LYS:N	2.83	0.40
1:A:84:PRO:HB2	1:B:58:MET:SD	2.61	0.40
1:C:249:ILE:O	1:C:300:CYS:HB2	2.21	0.40
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:D:246:ILE:HA	1:D:297:VAL:CG1	2.51	0.40
1:E:166:MET:HE2	1:E:178:ARG:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:PRO:CG	1:E:279:GLU:OE2	2.56	0.40
1:F:259:GLU:O	1:F:262:ALA:O	2.39	0.40
1:G:246:ILE:HA	1:G:297:VAL:CG1	2.52	0.40
1:G:264:ILE:CG1	1:G:265:ARG:O	2.66	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:140:GLU:OE2	1:D:140:GLU:HA	2.20	0.40
1:D:423:ILE:HG12	1:D:473:LEU:HD11	2.03	0.40
1:E:106:THR:O	1:E:107:ALA:C	2.58	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:F:94:LYS:O	1:F:96:GLN:N	2.48	0.40
1:G:209:ILE:CB	1:G:399:ARG:HH22	2.28	0.40
1:H:454:LEU:HD12	1:H:454:LEU:HA	1.91	0.40
1:I:153:VAL:HG23	1:I:160:LEU:CD2	2.45	0.40
1:B:359:GLU:HA	1:B:367:MET:O	2.20	0.40
1:B:473:LEU:C	1:B:475:SER:N	2.75	0.40
1:C:89:LEU:CD2	1:C:108:VAL:HG23	2.44	0.40
1:D:249:ILE:O	1:D:300:CYS:HB2	2.21	0.40
1:D:259:GLU:O	1:D:262:ALA:O	2.39	0.40
1:D:347:SER:C	1:D:349:GLN:N	2.75	0.40
1:G:259:GLU:O	1:G:262:ALA:O	2.39	0.40
1:G:238:PRO:O	1:G:318:LEU:HD13	2.22	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:H:317:VAL:HG12	1:H:318:LEU:N	2.35	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	37
1	B	503/553 (91%)	397 (79%)	88 (18%)	18 (4%)	4	37
1	C	503/553 (91%)	397 (79%)	88 (18%)	18 (4%)	4	37
1	D	503/553 (91%)	396 (79%)	89 (18%)	18 (4%)	4	37
1	E	503/553 (91%)	397 (79%)	88 (18%)	18 (4%)	4	37
1	F	503/553 (91%)	397 (79%)	88 (18%)	18 (4%)	4	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	503/553 (91%)	396 (79%)	89 (18%)	18 (4%)	4	37
1	H	503/553 (91%)	396 (79%)	89 (18%)	18 (4%)	4	37
1	I	503/553 (91%)	396 (79%)	89 (18%)	18 (4%)	4	37
All	All	4527/4977 (91%)	3568 (79%)	797 (18%)	162 (4%)	4	37

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%)	23	62
1	B	410/447 (92%)	386 (94%)	24 (6%)	23	62
1	C	410/447 (92%)	386 (94%)	24 (6%)	23	62
1	D	410/447 (92%)	386 (94%)	24 (6%)	23	62
1	E	410/447 (92%)	386 (94%)	24 (6%)	23	62
1	F	410/447 (92%)	386 (94%)	24 (6%)	23	62
1	G	410/447 (92%)	386 (94%)	24 (6%)	23	62
1	H	410/447 (92%)	386 (94%)	24 (6%)	23	62
1	I	410/447 (92%)	386 (94%)	24 (6%)	23	62
All	All	3690/4023 (92%)	3474 (94%)	216 (6%)	23	62

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	-	25,29,29	1.43	2 (8%)	24,45,45	2.16	5 (20%)
2	ADP	B	800	-	25,29,29	1.43	2 (8%)	24,45,45	2.15	5 (20%)
2	ADP	C	800	-	25,29,29	1.42	2 (8%)	24,45,45	2.16	5 (20%)
2	ADP	D	800	-	25,29,29	1.44	2 (8%)	24,45,45	2.17	5 (20%)
2	ADP	E	800	-	25,29,29	1.44	2 (8%)	24,45,45	2.16	5 (20%)
2	ADP	F	800	-	25,29,29	1.43	2 (8%)	24,45,45	2.16	5 (20%)
2	ADP	G	800	-	25,29,29	1.43	2 (8%)	24,45,45	2.16	5 (20%)
2	ADP	H	800	-	25,29,29	1.44	2 (8%)	24,45,45	2.16	5 (20%)
2	ADP	I	800	-	25,29,29	1.43	2 (8%)	24,45,45	2.16	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	800	ADP	C2'-C1'	-5.26	1.45	1.53
2	G	800	ADP	C2'-C1'	-5.26	1.45	1.53
2	D	800	ADP	C2'-C1'	-5.25	1.45	1.53
2	H	800	ADP	C2'-C1'	-5.24	1.45	1.53
2	B	800	ADP	C2'-C1'	-5.24	1.45	1.53
2	A	800	ADP	C2'-C1'	-5.23	1.45	1.53
2	F	800	ADP	C2'-C1'	-5.22	1.45	1.53
2	I	800	ADP	C2'-C1'	-5.21	1.45	1.53
2	C	800	ADP	C2'-C1'	-5.20	1.45	1.53
2	E	800	ADP	C5-C4	3.08	1.47	1.40
2	B	800	ADP	C5-C4	3.08	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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 (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	800	ADP	N3-C2-N1	-6.15	123.50	128.86
2	F	800	ADP	N3-C2-N1	-6.09	123.56	128.86
2	I	800	ADP	N3-C2-N1	-6.08	123.56	128.86
2	A	800	ADP	N3-C2-N1	-6.07	123.57	128.86
2	E	800	ADP	N3-C2-N1	-6.07	123.57	128.86
2	G	800	ADP	N3-C2-N1	-6.05	123.58	128.86
2	H	800	ADP	N3-C2-N1	-6.04	123.60	128.86
2	C	800	ADP	N3-C2-N1	-6.02	123.61	128.86
2	B	800	ADP	N3-C2-N1	-6.02	123.61	128.86
2	C	800	ADP	O3'-C3'-C4'	-4.51	97.92	111.09
2	H	800	ADP	O3'-C3'-C4'	-4.50	97.94	111.09
2	E	800	ADP	O3'-C3'-C4'	-4.50	97.94	111.09
2	G	800	ADP	O3'-C3'-C4'	-4.50	97.94	111.09
2	A	800	ADP	O3'-C3'-C4'	-4.50	97.95	111.09
2	I	800	ADP	O3'-C3'-C4'	-4.49	97.97	111.09
2	B	800	ADP	O3'-C3'-C4'	-4.49	97.98	111.09
2	F	800	ADP	O3'-C3'-C4'	-4.49	97.98	111.09
2	D	800	ADP	O3'-C3'-C4'	-4.48	98.00	111.09
2	C	800	ADP	C4-C5-N7	-3.12	106.40	109.41
2	I	800	ADP	C4-C5-N7	-3.11	106.41	109.41
2	H	800	ADP	C4-C5-N7	-3.11	106.41	109.41
2	D	800	ADP	C4-C5-N7	-3.09	106.43	109.41
2	A	800	ADP	C4-C5-N7	-3.08	106.44	109.41
2	G	800	ADP	C4-C5-N7	-3.08	106.44	109.41
2	B	800	ADP	C4-C5-N7	-3.06	106.45	109.41
2	E	800	ADP	C4-C5-N7	-3.06	106.45	109.41
2	F	800	ADP	C4-C5-N7	-3.06	106.45	109.41
2	G	800	ADP	C4'-O4'-C1'	-2.08	107.56	109.77
2	H	800	ADP	C4'-O4'-C1'	-2.07	107.56	109.77
2	E	800	ADP	C4'-O4'-C1'	-2.06	107.58	109.77
2	I	800	ADP	C4'-O4'-C1'	-2.06	107.58	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	ADP	C4'-O4'-C1'	-2.04	107.60	109.77
2	B	800	ADP	C4'-O4'-C1'	-2.04	107.60	109.77
2	C	800	ADP	C4'-O4'-C1'	-2.03	107.61	109.77
2	D	800	ADP	C4'-O4'-C1'	-2.02	107.62	109.77
2	F	800	ADP	C4'-O4'-C1'	-2.00	107.64	109.77
2	I	800	ADP	O2'-C2'-C3'	4.69	126.86	111.83
2	G	800	ADP	O2'-C2'-C3'	4.69	126.86	111.83
2	F	800	ADP	O2'-C2'-C3'	4.70	126.88	111.83
2	B	800	ADP	O2'-C2'-C3'	4.70	126.89	111.83
2	H	800	ADP	O2'-C2'-C3'	4.70	126.89	111.83
2	A	800	ADP	O2'-C2'-C3'	4.70	126.89	111.83
2	E	800	ADP	O2'-C2'-C3'	4.70	126.90	111.83
2	C	800	ADP	O2'-C2'-C3'	4.71	126.91	111.83
2	D	800	ADP	O2'-C2'-C3'	4.71	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%)	0.10	13 (2%)	56	44	64, 126, 150, 150	0
1	B	505/553 (91%)	0.09	13 (2%)	56	44	64, 126, 150, 150	0
1	C	505/553 (91%)	0.16	17 (3%)	46	34	64, 126, 150, 150	0
1	D	505/553 (91%)	0.07	14 (2%)	53	41	64, 126, 150, 150	0
1	E	505/553 (91%)	0.23	26 (5%)	29	21	64, 126, 150, 150	0
1	F	505/553 (91%)	0.15	13 (2%)	56	44	64, 126, 150, 150	0
1	G	505/553 (91%)	0.20	22 (4%)	35	25	64, 126, 150, 150	0
1	H	505/553 (91%)	0.09	11 (2%)	62	49	64, 126, 150, 150	0
1	I	505/553 (91%)	0.06	10 (1%)	65	53	64, 126, 150, 150	0
All	All	4545/4977 (91%)	0.13	139 (3%)	49	37	64, 127, 150, 150	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	261	ASP	6.9
1	E	259	GLU	5.7
1	B	259	GLU	5.1
1	H	267	ASN	5.1
1	F	259	GLU	5.0
1	C	259	GLU	4.9
1	A	259	GLU	4.3
1	F	267	ASN	4.3
1	C	261	ASP	4.1
1	F	63	LEU	4.1
1	G	259	GLU	4.0
1	F	261	ASP	4.0
1	H	262	ALA	3.6
1	D	532	ALA	3.6
1	H	265	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	268	ASP	3.5
1	D	267	ASN	3.4
1	H	264	ILE	3.4
1	E	198	ASP	3.4
1	G	532	ALA	3.4
1	E	260	LEU	3.4
1	B	261	ASP	3.4
1	E	267	ASN	3.3
1	E	154	SER	3.3
1	I	267	ASN	3.3
1	G	268	ASP	3.3
1	E	157	ASP	3.3
1	D	260	LEU	3.2
1	B	260	LEU	3.2
1	C	267	ASN	3.2
1	E	156	ASN	3.2
1	G	194	GLU	3.1
1	E	262	ALA	3.1
1	D	259	GLU	3.1
1	H	259	GLU	3.1
1	C	374	LYS	3.1
1	G	481	ASN	3.0
1	F	162	ARG	3.0
1	F	260	LEU	3.0
1	E	263	GLU	3.0
1	E	261	ASP	2.9
1	C	353	TYR	2.9
1	B	156	ASN	2.9
1	B	198	ASP	2.9
1	F	65	ASP	2.9
1	B	268	ASP	2.8
1	G	260	LEU	2.8
1	A	366	LYS	2.8
1	G	261	ASP	2.8
1	G	266	ILE	2.7
1	A	261	ASP	2.7
1	G	531	SER	2.7
1	G	63	LEU	2.7
1	E	195	LEU	2.7
1	D	197	GLY	2.7
1	C	262	ALA	2.7
1	D	199	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	266	ILE	2.7
1	B	157	ASP	2.7
1	C	65	ASP	2.7
1	C	371	GLU	2.7
1	F	269	PRO	2.7
1	C	243	ASN	2.6
1	B	267	ASN	2.6
1	G	264	ILE	2.6
1	A	197	GLY	2.6
1	E	272	MET	2.5
1	I	265	ARG	2.5
1	A	371	GLU	2.5
1	D	268	ASP	2.5
1	H	261	ASP	2.5
1	A	374	LYS	2.5
1	A	198	ASP	2.5
1	D	353	TYR	2.5
1	E	82	GLN	2.5
1	F	268	ASP	2.5
1	G	243	ASN	2.5
1	B	262	ALA	2.5
1	C	260	LEU	2.4
1	G	197	GLY	2.4
1	C	63	LEU	2.4
1	H	243	ASN	2.4
1	C	385	GLY	2.4
1	F	226	ILE	2.4
1	H	263	GLU	2.4
1	B	63	LEU	2.4
1	G	267	ASN	2.4
1	C	357	ILE	2.3
1	F	62	SER	2.3
1	C	62	SER	2.3
1	B	77	ASP	2.3
1	I	259	GLU	2.3
1	A	532	ALA	2.3
1	G	262	ALA	2.3
1	F	532	ALA	2.3
1	D	246	ILE	2.3
1	D	531	SER	2.3
1	D	196	ARG	2.3
1	I	242	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	206	ASN	2.2
1	E	65	ASP	2.2
1	D	262	ALA	2.2
1	G	196	ARG	2.2
1	E	317	VAL	2.2
1	A	481	ASN	2.2
1	I	261	ASP	2.2
1	H	60	VAL	2.2
1	B	195	LEU	2.2
1	E	531	SER	2.2
1	E	271	GLN	2.2
1	G	265	ARG	2.2
1	A	194	GLU	2.1
1	C	242	GLU	2.1
1	A	353	TYR	2.1
1	I	82	GLN	2.1
1	A	196	ARG	2.1
1	G	296	ASN	2.1
1	G	255	VAL	2.1
1	D	243	ASN	2.1
1	E	61	ASP	2.1
1	E	254	GLU	2.1
1	G	269	PRO	2.1
1	C	351	LEU	2.1
1	A	267	ASN	2.1
1	G	156	ASN	2.1
1	H	268	ASP	2.1
1	I	264	ILE	2.1
1	B	269	PRO	2.1
1	C	356	LEU	2.1
1	I	262	ALA	2.1
1	F	227	VAL	2.1
1	E	258	PRO	2.1
1	G	246	ILE	2.1
1	E	243	ASN	2.1
1	E	266	ILE	2.0
1	E	240	ARG	2.0
1	E	77	ASP	2.0
1	I	350	ASP	2.0
1	I	260	LEU	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	3.01	150,150,150,150	7
2	ADP	H	800	27/27	0.81	0.33	2.48	150,150,150,150	7
2	ADP	D	800	27/27	0.76	0.39	2.38	150,150,150,150	7
2	ADP	I	800	27/27	0.82	0.33	2.33	150,150,150,150	7
2	ADP	B	800	27/27	0.80	0.34	1.87	150,150,150,150	7
2	ADP	A	800	27/27	0.79	0.35	1.82	150,150,150,150	7
2	ADP	E	800	27/27	0.78	0.34	1.53	150,150,150,150	7
2	ADP	C	800	27/27	0.79	0.34	1.49	150,150,150,150	7
2	ADP	F	800	27/27	0.83	0.32	1.20	150,150,150,150	7

6.5 Other polymers [i](#)

There are no such residues in this entry.