



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2024 – 01:10 AM EST

PDB ID : 4G9I  
Title : Crystal structure of T.kodakarensis HypF  
Authors : Tominaga, T.; Watanabe, S.; Matsumi, R.; Atomi, H.; Imanaka, T.; Miki, K.  
Deposited on : 2012-07-24  
Resolution : 4.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

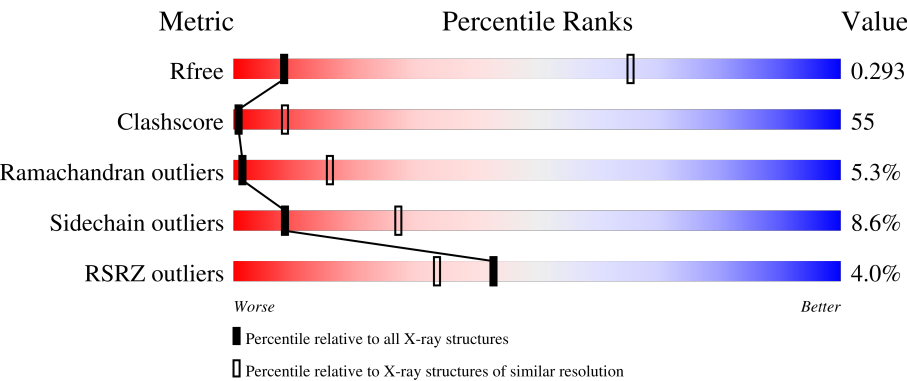
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 4.50 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 <sub>free</sub>	164625	1050 (5.10-3.90)
Clashscore	180529	1106 (5.10-3.90)
Ramachandran outliers	177936	1006 (5.10-3.90)
Sidechain outliers	177891	1008 (5.12-3.88)
RSRZ outliers	164620	1046 (5.10-3.90)

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

Mol	Chain	Length	Quality of chain
1	A	772	<div><div>3%</div><div>25%</div><div>64%</div><div>9%</div><div>..</div></div>
1	B	772	<div><div>5%</div><div>26%</div><div>63%</div><div>9%</div><div>.</div></div>
1	C	772	<div><div>3%</div><div>29%</div><div>60%</div><div>9%</div><div>.</div></div>
1	D	772	<div><div>3%</div><div>28%</div><div>63%</div><div>8%</div><div>.</div></div>
1	E	772	<div><div>4%</div><div>27%</div><div>63%</div><div>8%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
1	F	772	<div><div></div><div>5%</div><div>27%</div><div>64%</div><div>7%</div><div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 36065 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 Hydrogenase maturation protein HypF.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	766	Total	C	N	O	S	Se	0	0	0
			6032	3862	1028	1113	11	18			
1	B	762	Total	C	N	O	S	Se	0	0	0
			6008	3847	1024	1108	11	18			
1	C	756	Total	C	N	O	S	Se	0	0	0
			5964	3819	1017	1100	11	17			
1	D	765	Total	C	N	O	S	Se	0	0	0
			6027	3859	1027	1112	11	18			
1	E	762	Total	C	N	O	S	Se	0	0	0
			6008	3847	1024	1108	11	18			
1	F	762	Total	C	N	O	S	Se	0	0	0
			6008	3847	1024	1108	11	18			

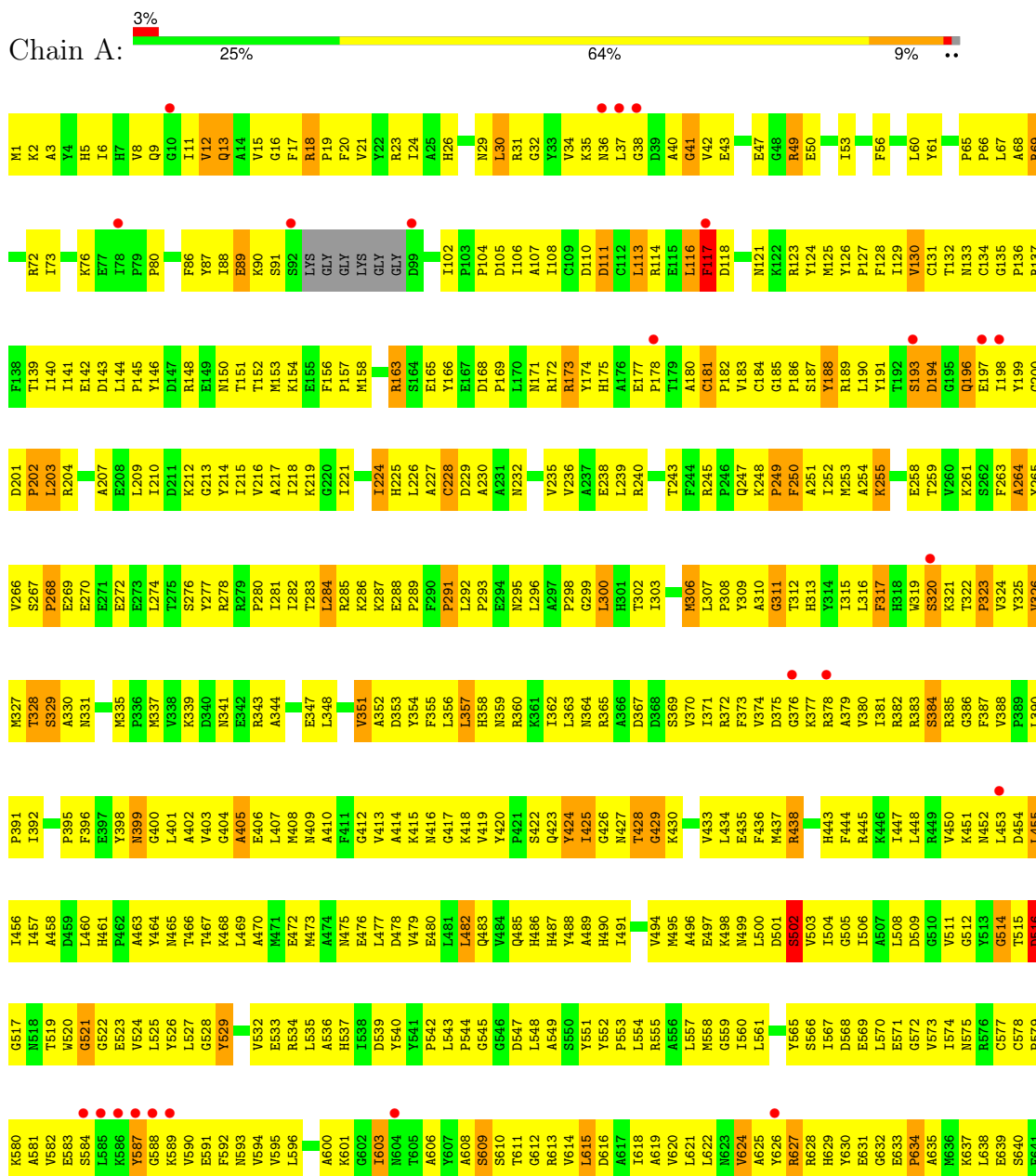
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

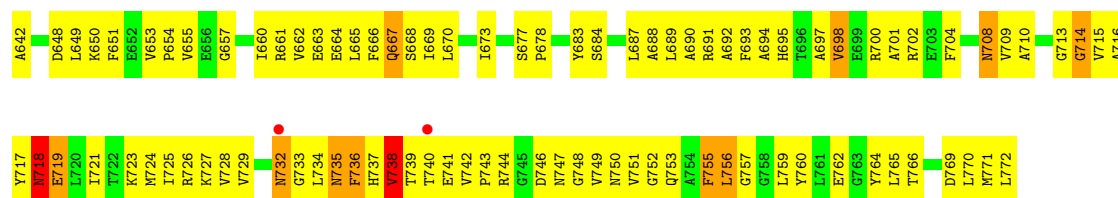
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		
2	C	3	Total	Zn	0	0
			3	3		
2	D	3	Total	Zn	0	0
			3	3		
2	E	3	Total	Zn	0	0
			3	3		
2	F	3	Total	Zn	0	0
			3	3		

### 3 Residue-property plots

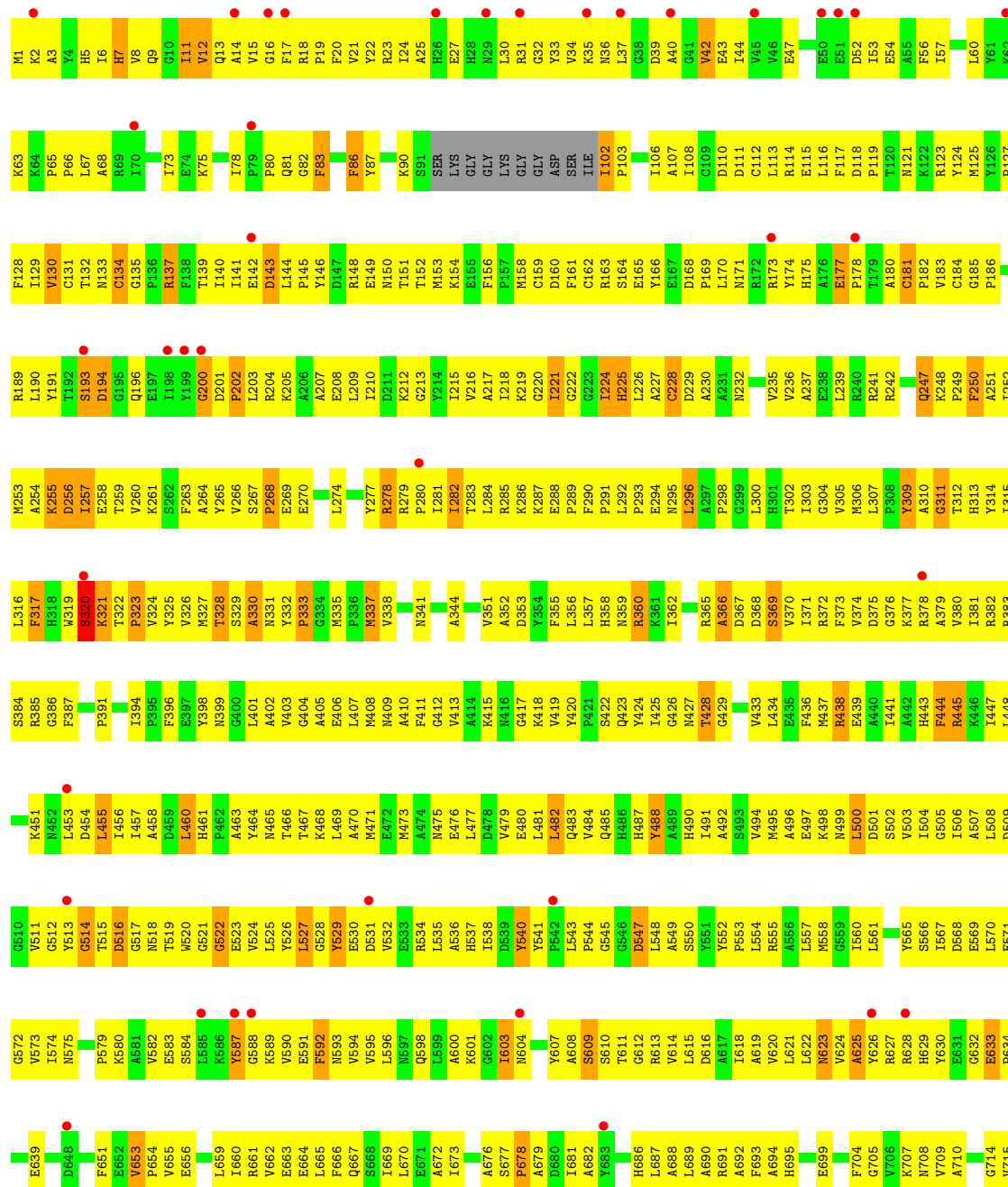
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: Hydrogenase maturation protein HypF



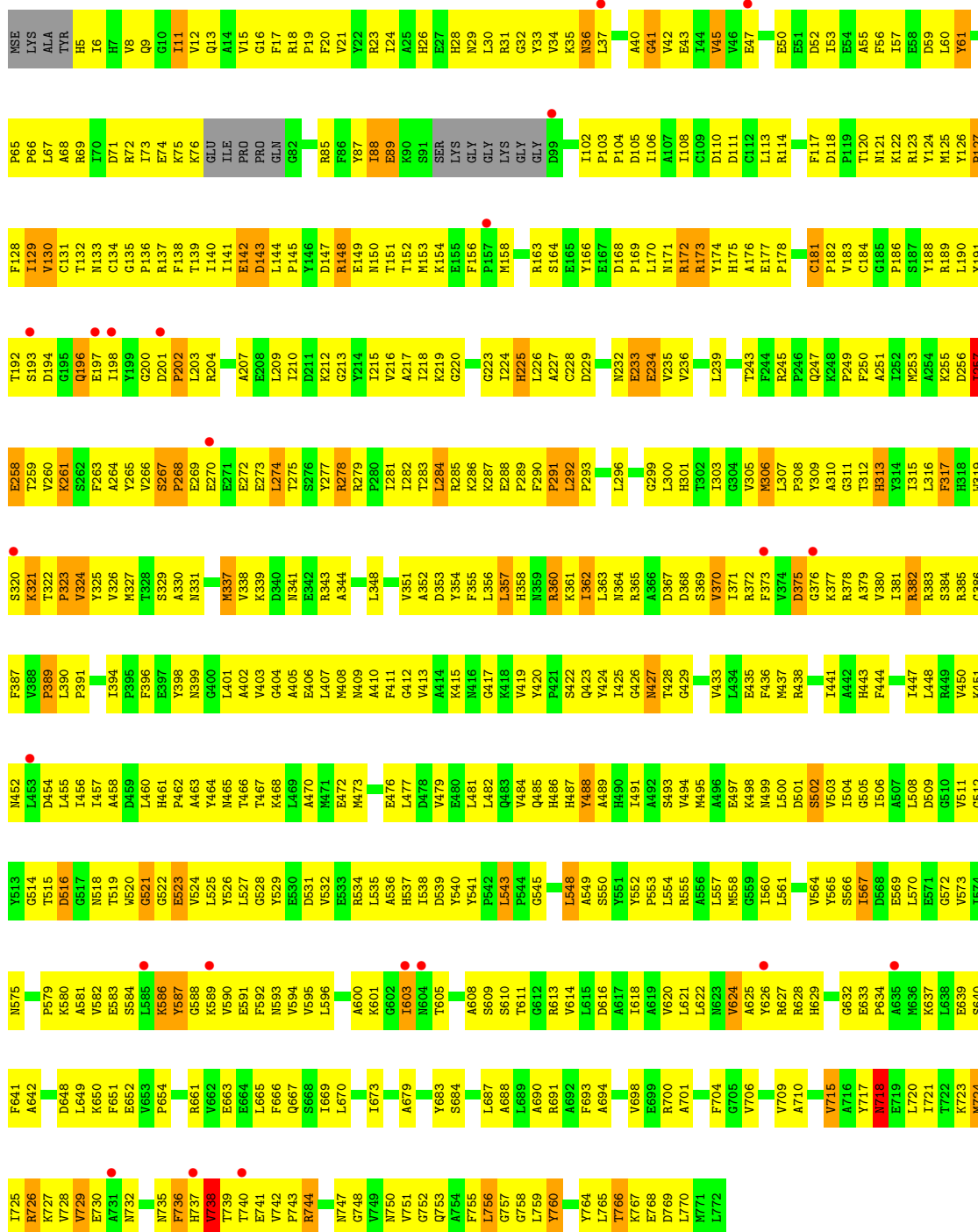


● Molecule 1: Hydrogenase maturation protein HypF

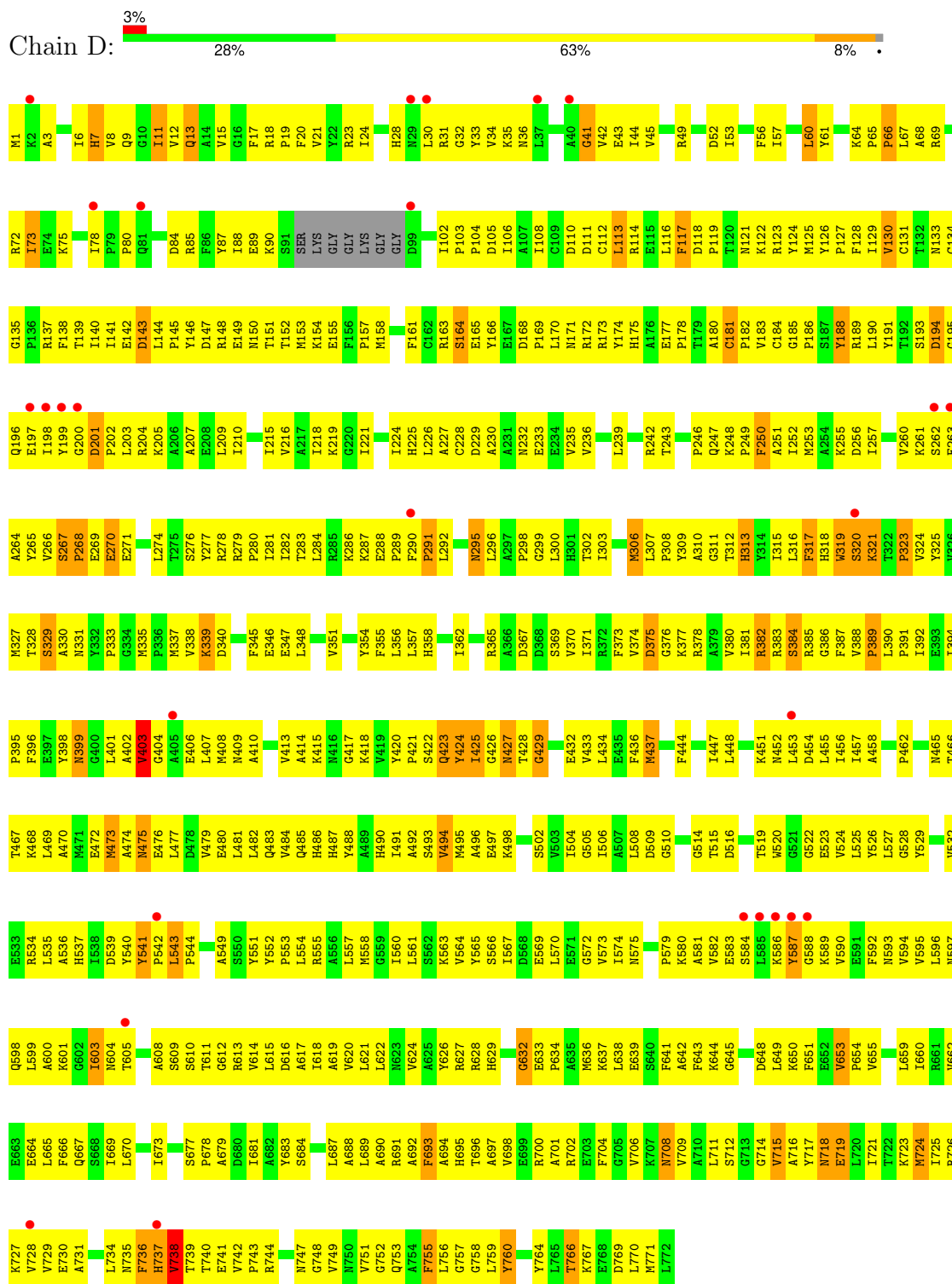




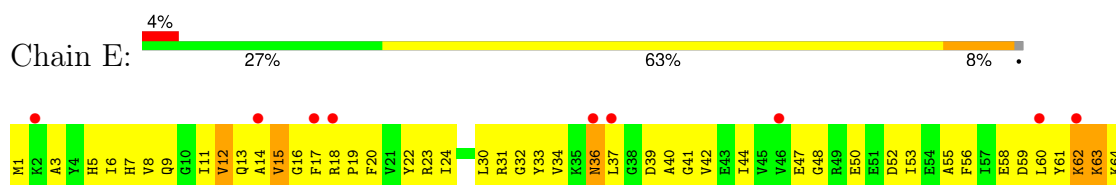
• Molecule 1: Hydrogenase maturation protein HypF

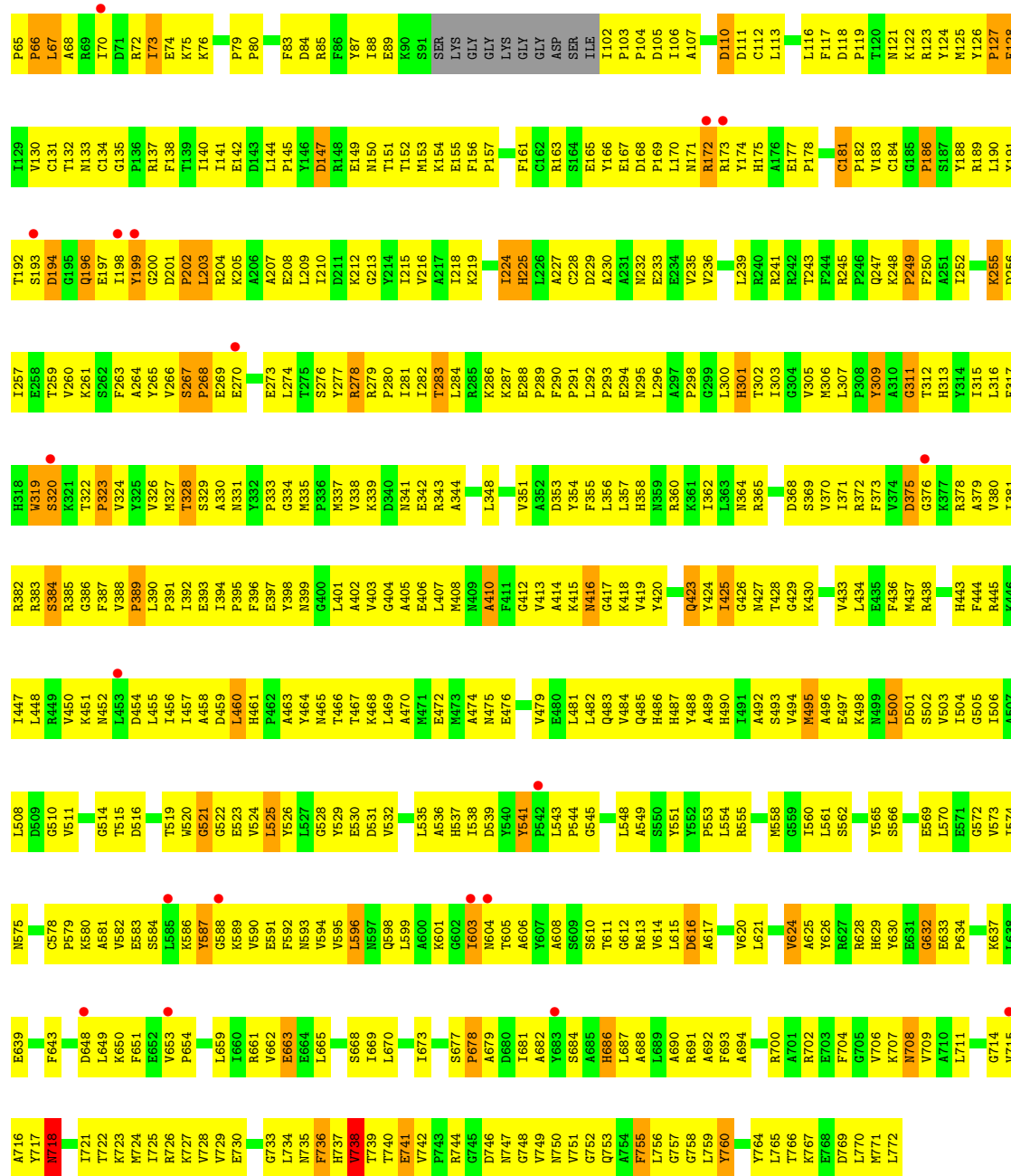


• Molecule 1: Hydrogenase maturation protein HypF

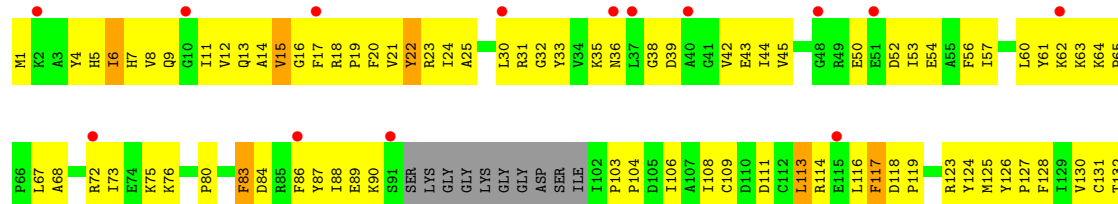


• Molecule 1: Hydrogenase maturation protein HypF





• Molecule 1: Hydrogenase maturation protein HypF



G733	L734	N735	F736	H737	V738	T739	T740	E741	P742	P743	R744	G748	V749	N750	G751	G752	G753	A754	F755	L756	G757	G758	L759	Y760	Y764	L765	T766	K767	E768	D769	L770	M771	L772	G196	E197	I198	Y199	D200	G201	P202	L203	K204	K205	A206	E207	A208	L209	D210	D211	P280	K212	K213	T214	I215	V216	A217	L218	F219	M219	T215	M215	T215	M215	E215	F216	P217	M218	R217	R217	Y174	H175	A176	E177	P178	T179	A180	C181	P182	V183	C184	G185	P186	S187	Y188	R189	L190	A254	Y191	T192	S193	D194	G195
S262	F263	A264	Y265	V266	S267	P268	E269	E270	L274	Y277	R278	R279	D280	E281	K282	T283	L284	R285	K286	K287	E288	P289	F290	P291	L292	P293	E294	N295	P298	G299	L300	H301	N302	T303	G304	V305	K306	L307	P308	Y309	A310	G311	T312	H313	L314	L315	F317	S384	R385	G386	F387	S320	K321	T322	P323	V324	Y325																																			
V326	M327	T328	S329	A330	N331	Y332	P333	G334	M335	P336	M337	V338	K339	D340	N341	E342	R343	A344	L348	D353	Y354	F355	L356	L357	H358	N359	R360	L363	N364	R365	D368	S369	V370	I371	R372	F373	V374	D375	G376	K377	R378	A379	V380	I381	R382	R383	S384	R385	G386	F387	S320	K321	T322	P323	V324	Y325																																				
E393	I394	P395	F396	E397	Y398	N399	G400	L401	A402	V403	G404	A405	E406	L407	M408	V409	G412	V413	A414	K415	M416	G417	K418	V419	P420	L421	S422	K423	Y424	I425	G426	M427	T428	G429	K430	V433	L434	H443	F444	R445	K446	I447	L448	K451	M452	L453	D454	L455	V456	I457	A458	D459	L460	H461	P462																																					
A463	Y464	N465	T466	K467	K468	L469	A470	M471	E472	M473	A474	M475	E476	L477	D478	V479	L481	L482	Q485	H486	H487	Y488	A489	H490	I491	A492	S493	Y494	M495	A496	E497	K498	N499	L500	D501	S502	V503	I504	G505	I506	A507	L508	D509	G510	V511	G512	Y513	G514	T515	S516	L518	L519	W520	G521	G522	E523	V524																																			
L525	Y526	L527	V532	E533	L534	R534	L535	A536	H537	Y540	Y541	P542	L543	P544	G545	L548	A549	S550	Y551	Y552	P553	L554	R555	A556	L557	M558	G559	I560	L561	S562	K563	V564	Y565	S566	I567	D568	E569	L570	V573	L574	C577	G578	P579	K580	A581	V582	E583	S584	L585	L586	Y587	G588	K589	V590	E591																																					
F592	N593	V594	Y595	L596	N597	O598	L599	A600	K601	G602	L603	N604	T605	A608	S609	S610	T611	G612	R613	V614	L615	D616	A617	L618	A619	V620	L621	L622	A625	V626	R627	R628	H629	V630	E631	G632	E633	P634	A635	M636	K637	L638	E639	S640	F641	A642	F643	D648	L649	K650	P651	G652	V653	E658	L659																																					
V662	E663	E664	L665	F666	O667	S668	L669	P678	Y683	S684	A685	H686	L687	A688	G752	G753	A754	F755	L756	G757	G758	L759	Y760	Y764	L765	T766	K767	E768	D769	L770	M771	L772	G713	G714	V715	A716	Y717	N718	L720	I721	T722	K723	M724	I725	R726	K727	V728	W729	E730	A731	N732																																									

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	265.81Å 265.81Å 693.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 4.50 15.00 – 4.50	Depositor EDS
% Data completeness (in resolution range)	90.5 (15.00-4.50) 92.0 (15.00-4.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.46 (at 4.45Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.279 , 0.300 0.298 , 0.293	Depositor DCC
$R_{free}$ test set	4204 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	143.9	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 121.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	36065	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	186.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN

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	0.25	0/6151	0.49	0/8308
1	B	0.25	0/6127	0.49	1/8275 (0.0%)
1	C	0.25	0/6080	0.49	0/8208
1	D	0.25	0/6146	0.49	0/8301
1	E	0.25	0/6127	0.49	0/8275
1	F	0.25	0/6127	0.50	0/8275
All	All	0.25	0/36758	0.49	1/49642 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	GLY	N-CA-C	5.11	125.88	113.10

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	6032	0	5969	684	1
1	B	6008	0	5954	671	0
1	C	5964	0	5909	669	0
1	D	6027	0	5970	674	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	6008	0	5954	616	0
1	F	6008	0	5955	667	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
All	All	36065	0	35711	3925	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 55.

All (3925) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ILE:HG21	1:A:69:ARG:H	1.24	1.02
1:D:9:GLN:HE21	1:D:41:GLY:HA2	1.17	1.02
1:D:485:GLN:HE21	1:D:487:HIS:H	1.04	1.01
1:D:451:LYS:HA	1:D:477:LEU:HD21	1.41	0.99
1:F:394:ILE:HD11	1:F:419:VAL:HB	1.41	0.99
1:D:288:GLU:HB3	1:D:289:PRO:HD3	1.45	0.98
1:C:198:ILE:HG13	1:D:122:LYS:HD3	1.39	0.98
1:B:485:GLN:HE21	1:B:487:HIS:H	1.04	0.98
1:B:57:ILE:HG13	1:B:75:LYS:HZ3	1.28	0.98
1:B:456:ILE:HG22	1:B:457:ILE:H	1.26	0.98
1:A:268:PRO:HG2	1:A:378:ARG:HH22	1.28	0.97
1:A:485:GLN:HE21	1:A:487:HIS:H	1.10	0.97
1:B:225:HIS:HA	1:B:330:ALA:HB2	1.44	0.97
1:D:369:SER:H	1:D:385:ARG:HB2	1.28	0.97
1:E:39:ASP:HB3	1:E:144:LEU:HD13	1.45	0.97
1:F:485:GLN:HE21	1:F:487:HIS:H	1.01	0.97
1:F:288:GLU:HB3	1:F:289:PRO:HD3	1.46	0.96
1:D:88:ILE:HG22	1:D:89:GLU:H	1.31	0.96
1:E:127:PRO:HB3	1:E:312:THR:HG22	1.47	0.96
1:C:127:PRO:HB3	1:C:312:THR:HG22	1.46	0.96
1:B:288:GLU:HB3	1:B:289:PRO:HD3	1.47	0.95
1:A:587:TYR:HD1	1:A:588:GLY:H	1.14	0.95
1:A:557:LEU:HD21	1:A:621:LEU:HD13	1.49	0.95
1:C:191:TYR:HB2	1:C:355:PHE:HB2	1.47	0.95
1:A:475:ASN:HD22	1:B:591:GLU:HG2	1.32	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:CYS:SG	1:A:183:VAL:HG22	2.07	0.94
1:E:485:GLN:HE21	1:E:487:HIS:H	0.96	0.94
1:A:11:ILE:HG12	1:A:68:ALA:HA	1.49	0.94
1:E:369:SER:H	1:E:385:ARG:HB2	1.31	0.94
1:B:394:ILE:HD11	1:B:419:VAL:HB	1.47	0.94
1:F:216:VAL:HB	1:F:354:TYR:HB2	1.50	0.94
1:A:379:ALA:HB3	1:A:744:ARG:HH11	1.31	0.94
1:E:169:PRO:HG2	1:E:170:LEU:HD12	1.48	0.94
1:C:288:GLU:HB2	1:C:289:PRO:HD3	1.47	0.93
1:A:287:LYS:HG3	1:A:289:PRO:HD2	1.49	0.93
1:D:127:PRO:HB3	1:D:312:THR:HG22	1.48	0.93
1:B:268:PRO:HG2	1:B:378:ARG:HH22	1.31	0.93
1:C:519:THR:HB	1:C:608:ALA:HA	1.51	0.93
1:D:111:ASP:HB2	1:D:172:ARG:HH22	1.34	0.93
1:E:394:ILE:HD11	1:E:419:VAL:HB	1.51	0.93
1:B:612:GLY:HA2	1:B:615:LEU:HD12	1.51	0.93
1:C:504:ILE:HB	1:C:709:VAL:HG12	1.51	0.93
1:A:288:GLU:HB3	1:A:289:PRO:HD3	1.48	0.92
1:F:207:ALA:HB1	1:F:320:SER:HB2	1.49	0.92
1:A:553:PRO:HB2	1:A:620:VAL:HG21	1.50	0.92
1:F:190:LEU:HD21	1:F:206:ALA:HB2	1.50	0.92
1:D:11:ILE:HG12	1:D:68:ALA:HA	1.51	0.92
1:C:286:LYS:HD2	1:C:303:ILE:HD11	1.51	0.92
1:F:219:LYS:HD3	1:F:358:HIS:H	1.33	0.92
1:A:108:ILE:HG12	1:A:310:ALA:HA	1.52	0.92
1:E:738:VAL:HG23	1:E:744:ARG:HG2	1.51	0.92
1:A:380:VAL:HG12	1:A:381:ILE:H	1.34	0.91
1:E:149:GLU:HA	1:E:154:LYS:HG2	1.49	0.91
1:B:232:ASN:HB3	1:B:235:VAL:HG22	1.52	0.91
1:B:14:ALA:HB3	1:B:103:PRO:HG3	1.53	0.90
1:B:39:ASP:HB3	1:B:144:LEU:HD13	1.52	0.90
1:D:111:ASP:HB3	1:D:172:ARG:HH12	1.33	0.90
1:E:288:GLU:HB3	1:E:289:PRO:HD3	1.52	0.90
1:F:369:SER:H	1:F:385:ARG:HB2	1.35	0.90
1:F:508:LEU:HD22	1:F:611:THR:HG21	1.51	0.90
1:E:191:TYR:HB2	1:E:355:PHE:HB2	1.54	0.89
1:A:628:ARG:NH2	1:A:632:GLY:H	1.69	0.89
1:F:19:PRO:HG2	1:F:132:THR:HG21	1.53	0.89
1:E:287:LYS:HG3	1:E:289:PRO:HD2	1.51	0.89
1:B:149:GLU:HA	1:B:154:LYS:HG2	1.54	0.89
1:E:494:VAL:HG22	1:E:738:VAL:HG22	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ILE:HG23	1:B:277:TYR:HB2	1.54	0.89
1:A:230:ALA:HB2	1:A:326:VAL:HG23	1.55	0.89
1:B:615:LEU:HA	1:B:618:ILE:HD12	1.55	0.89
1:D:331:ASN:HD22	1:D:337:MSE:HA	1.36	0.89
1:D:543:LEU:HD23	1:D:543:LEU:H	1.37	0.89
1:C:281:ILE:HB	1:C:370:VAL:HG12	1.52	0.89
1:A:219:LYS:HD3	1:A:358:HIS:H	1.37	0.88
1:D:281:ILE:HB	1:D:370:VAL:HG12	1.54	0.88
1:D:458:ALA:HB1	1:D:467:THR:HG22	1.55	0.88
1:F:190:LEU:HG	1:F:202:PRO:HB3	1.55	0.88
1:E:153:MSE:HE1	1:E:360:ARG:HD2	1.55	0.88
1:E:765:LEU:HD21	1:E:770:LEU:HD21	1.55	0.88
1:C:369:SER:H	1:C:385:ARG:HB2	1.38	0.88
1:F:282:ILE:HD12	1:F:371:ILE:HG23	1.53	0.87
1:D:106:ILE:HG23	1:D:277:TYR:HB2	1.56	0.87
1:F:261:LYS:NZ	1:F:266:VAL:HB	1.90	0.87
1:F:219:LYS:HA	1:F:224:ILE:HG12	1.56	0.87
1:F:281:ILE:HB	1:F:370:VAL:HG12	1.56	0.87
1:C:371:ILE:HD12	1:C:380:VAL:HG22	1.57	0.87
1:E:690:ALA:HB1	1:E:725:ILE:HG13	1.55	0.87
1:F:653:VAL:HG13	1:F:692:ALA:HB3	1.54	0.87
1:D:566:SER:H	1:D:569:GLU:HB2	1.39	0.86
1:E:485:GLN:NE2	1:E:487:HIS:H	1.73	0.86
1:F:380:VAL:HG23	1:F:740:THR:HA	1.57	0.86
1:A:456:ILE:HG22	1:A:457:ILE:H	1.40	0.86
1:C:207:ALA:HB1	1:C:320:SER:HB2	1.54	0.86
1:C:331:ASN:HD22	1:C:337:MSE:HA	1.41	0.86
1:D:9:GLN:HB2	1:D:72:ARG:HD2	1.56	0.86
1:D:370:VAL:HG22	1:D:382:ARG:HD2	1.57	0.86
1:B:128:PHE:HB3	1:B:360:ARG:HH22	1.38	0.86
1:E:485:GLN:HE21	1:E:487:HIS:N	1.73	0.86
1:A:371:ILE:HB	1:A:380:VAL:HG13	1.56	0.86
1:B:249:PRO:HG3	1:B:300:LEU:HD13	1.58	0.86
1:F:615:LEU:HD12	1:F:638:LEU:HD23	1.56	0.86
1:C:502:SER:HB3	1:C:528:GLY:HA2	1.58	0.86
1:C:485:GLN:HG3	1:C:488:TYR:H	1.41	0.85
1:D:102:ILE:HD11	1:D:144:LEU:HG	1.58	0.85
1:A:201:ASP:N	1:A:202:PRO:HD2	1.91	0.85
1:A:281:ILE:HG12	1:A:306:MSE:HG3	1.55	0.85
1:E:543:LEU:HD23	1:E:543:LEU:H	1.40	0.85
1:C:219:LYS:HA	1:C:224:ILE:HB	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ALA:HB1	1:A:467:THR:HG22	1.58	0.85
1:B:544:PRO:HB2	1:B:555:ARG:HH21	1.42	0.85
1:D:687:LEU:HB3	1:D:724:MSE:HE2	1.56	0.85
1:C:153:MSE:HE1	1:C:360:ARG:HD3	1.57	0.85
1:F:149:GLU:HA	1:F:154:LYS:HG2	1.57	0.85
1:B:765:LEU:HD21	1:B:770:LEU:HD21	1.59	0.85
1:B:369:SER:H	1:B:385:ARG:HB2	1.41	0.85
1:C:543:LEU:HD23	1:C:543:LEU:H	1.41	0.85
1:D:374:VAL:HG21	1:D:744:ARG:HH22	1.41	0.85
1:F:5:HIS:HB3	1:F:76:LYS:HB2	1.59	0.84
1:E:281:ILE:HB	1:E:370:VAL:HG12	1.58	0.84
1:F:589:LYS:HG3	1:F:590:VAL:H	1.42	0.84
1:C:485:GLN:HE22	1:C:514:GLY:HA2	1.42	0.84
1:D:181:CYS:SG	1:D:183:VAL:HG22	2.16	0.84
1:B:191:TYR:HB2	1:B:355:PHE:HB2	1.57	0.84
1:A:404:GLY:HA2	1:A:753:GLN:HE22	1.42	0.84
1:A:589:LYS:HG3	1:A:590:VAL:H	1.40	0.84
1:C:282:ILE:HD12	1:C:371:ILE:HG23	1.59	0.84
1:C:261:LYS:NZ	1:C:266:VAL:HB	1.93	0.84
1:D:247:GLN:HG3	1:D:298:PRO:HG2	1.59	0.84
1:A:425:ILE:HD12	1:A:437:MSE:HE2	1.59	0.84
1:A:524:VAL:HG22	1:A:536:ALA:HB3	1.60	0.84
1:E:270:GLU:HB2	1:E:373:PHE:HE2	1.42	0.84
1:A:163:ARG:HB2	1:A:163:ARG:HH11	1.42	0.83
1:C:258:GLU:HG3	1:C:259:THR:N	1.93	0.83
1:D:233:GLU:HB2	1:D:295:ASN:HD21	1.40	0.83
1:F:265:TYR:HE2	1:F:287:LYS:HD2	1.42	0.83
1:C:457:ILE:HG21	1:C:753:GLN:HB3	1.60	0.83
1:A:491:ILE:HG23	1:A:527:LEU:HD11	1.60	0.83
1:B:281:ILE:HB	1:B:370:VAL:HG12	1.60	0.83
1:C:409:ASN:HD22	1:C:425:ILE:HD11	1.43	0.83
1:A:267:SER:HB2	1:A:270:GLU:HB2	1.59	0.83
1:D:225:HIS:HA	1:D:330:ALA:HB2	1.60	0.83
1:E:425:ILE:HD12	1:E:437:MSE:HE2	1.60	0.83
1:F:57:ILE:HG13	1:F:75:LYS:NZ	1.94	0.83
1:E:18:ARG:HB2	1:E:19:PRO:HD3	1.61	0.83
1:D:506:ILE:HD11	1:D:694:ALA:HA	1.61	0.82
1:A:404:GLY:HA2	1:A:753:GLN:NE2	1.94	0.82
1:B:587:TYR:HD1	1:B:588:GLY:H	1.27	0.82
1:F:225:HIS:HA	1:F:330:ALA:HB2	1.59	0.82
1:E:210:ILE:HD11	1:E:228:CYS:HA	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:VAL:HG22	1:B:738:VAL:HG22	1.59	0.82
1:D:1:MSE:HB3	1:D:80:PRO:HD2	1.61	0.82
1:D:519:THR:HB	1:D:608:ALA:HA	1.60	0.82
1:E:20:PHE:HD2	1:E:23:ARG:HH21	1.26	0.82
1:F:711:LEU:HD13	1:F:725:ILE:HG21	1.61	0.82
1:B:451:LYS:HA	1:B:477:LEU:HD21	1.61	0.82
1:E:380:VAL:HG23	1:E:740:THR:HA	1.61	0.82
1:C:470:ALA:HB1	1:C:481:LEU:HD11	1.61	0.82
1:E:181:CYS:SG	1:E:183:VAL:HG22	2.19	0.82
1:E:249:PRO:HG3	1:E:300:LEU:HD13	1.60	0.82
1:A:281:ILE:HB	1:A:370:VAL:HG12	1.60	0.82
1:B:380:VAL:HG23	1:B:740:THR:HA	1.61	0.82
1:E:201:ASP:N	1:E:202:PRO:HD2	1.94	0.82
1:A:495:MSE:SE	1:A:527:LEU:HD13	2.30	0.81
1:B:331:ASN:HD22	1:B:337:MSE:HA	1.45	0.81
1:C:215:ILE:HD12	1:C:226:LEU:HD23	1.62	0.81
1:E:331:ASN:HD22	1:E:337:MSE:HA	1.45	0.81
1:C:587:TYR:HD1	1:C:588:GLY:H	1.27	0.81
1:B:457:ILE:HG21	1:B:753:GLN:HB3	1.61	0.81
1:D:544:PRO:HG2	1:D:555:ARG:HB3	1.62	0.81
1:D:230:ALA:HB1	1:D:296:LEU:HD21	1.62	0.81
1:F:419:VAL:HG11	1:F:751:VAL:HG23	1.62	0.81
1:F:554:LEU:HD11	1:F:579:PRO:HB2	1.60	0.81
1:C:103:PRO:HG2	1:C:137:ARG:HD2	1.60	0.81
1:E:589:LYS:HG3	1:E:590:VAL:H	1.45	0.81
1:A:457:ILE:HG21	1:A:753:GLN:HB3	1.63	0.81
1:A:625:ALA:HB2	1:A:637:LYS:HD3	1.63	0.81
1:B:247:GLN:HE21	1:B:298:PRO:HG2	1.44	0.81
1:F:765:LEU:HD21	1:F:770:LEU:HD21	1.61	0.81
1:B:374:VAL:HG21	1:B:744:ARG:HH22	1.45	0.81
1:B:485:GLN:NE2	1:B:487:HIS:H	1.80	0.81
1:C:6:ILE:HG22	1:C:8:VAL:HG23	1.63	0.81
1:F:247:GLN:HG3	1:F:298:PRO:HG2	1.62	0.81
1:F:504:ILE:HB	1:F:709:VAL:HG12	1.63	0.81
1:B:485:GLN:HG3	1:B:488:TYR:H	1.46	0.80
1:E:484:VAL:HG12	1:E:770:LEU:HD13	1.63	0.80
1:C:225:HIS:HA	1:C:330:ALA:HB2	1.63	0.80
1:A:127:PRO:HB3	1:A:312:THR:HG22	1.62	0.80
1:A:191:TYR:HB2	1:A:355:PHE:HB2	1.64	0.80
1:B:425:ILE:HD12	1:B:437:MSE:HE2	1.61	0.80
1:D:587:TYR:HD1	1:D:588:GLY:H	1.24	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:521:GLY:HA3	1:F:610:SER:HA	1.63	0.80
1:F:580:LYS:HG3	1:F:593:ASN:HD22	1.44	0.80
1:B:519:THR:HB	1:B:608:ALA:HA	1.64	0.80
1:B:451:LYS:HG3	1:B:477:LEU:HD11	1.62	0.80
1:C:181:CYS:SG	1:C:183:VAL:HG22	2.22	0.80
1:C:458:ALA:HB1	1:C:467:THR:HG22	1.63	0.80
1:E:711:LEU:HD13	1:E:725:ILE:HG21	1.64	0.80
1:C:201:ASP:N	1:C:202:PRO:HD2	1.97	0.79
1:D:249:PRO:HG3	1:D:300:LEU:HD13	1.64	0.79
1:F:545:GLY:HA3	1:F:548:LEU:HB2	1.64	0.79
1:F:691:ARG:HD3	1:F:724:MSE:HE3	1.64	0.79
1:C:253:MSE:HG2	1:C:317:PHE:HE1	1.45	0.79
1:C:269:GLU:HB2	1:C:378:ARG:CZ	2.12	0.79
1:C:485:GLN:HB3	1:C:488:TYR:HB2	1.64	0.79
1:B:163:ARG:HH11	1:B:163:ARG:HB2	1.47	0.79
1:F:371:ILE:HD12	1:F:380:VAL:HG22	1.64	0.79
1:E:111:ASP:HB3	1:E:172:ARG:HH22	1.48	0.79
1:F:404:GLY:HA2	1:F:753:GLN:HE22	1.47	0.79
1:B:57:ILE:HG13	1:B:75:LYS:NZ	1.98	0.79
1:B:282:ILE:HD12	1:B:371:ILE:HG23	1.64	0.79
1:B:508:LEU:HD22	1:B:611:THR:HG21	1.65	0.79
1:B:653:VAL:HG13	1:B:692:ALA:HB3	1.64	0.79
1:A:335:MSE:HE1	1:A:430:LYS:HG3	1.63	0.78
1:C:66:PRO:HD2	1:C:133:ASN:HD22	1.48	0.78
1:C:219:LYS:HD3	1:C:358:HIS:H	1.48	0.78
1:E:24:ILE:HD11	1:E:56:PHE:HA	1.65	0.78
1:E:282:ILE:HD12	1:E:371:ILE:HG23	1.65	0.78
1:F:169:PRO:HG2	1:F:170:LEU:HD12	1.64	0.78
1:D:219:LYS:HD3	1:D:358:HIS:H	1.49	0.78
1:E:15:VAL:HG11	1:E:67:LEU:HB2	1.65	0.78
1:E:506:ILE:HB	1:E:711:LEU:HD12	1.65	0.78
1:F:249:PRO:HG3	1:F:300:LEU:HD13	1.65	0.78
1:A:435:GLU:HA	1:A:438:ARG:HD2	1.63	0.78
1:A:225:HIS:HA	1:A:330:ALA:HB2	1.66	0.78
1:A:331:ASN:HD22	1:A:337:MSE:HA	1.48	0.78
1:E:580:LYS:HG3	1:E:593:ASN:HD22	1.48	0.78
1:B:14:ALA:HB3	1:B:103:PRO:CG	2.12	0.78
1:C:690:ALA:HB1	1:C:725:ILE:HG13	1.66	0.78
1:E:268:PRO:HG2	1:E:378:ARG:HH22	1.49	0.78
1:F:269:GLU:HB2	1:F:378:ARG:CZ	2.14	0.78
1:B:337:MSE:HE3	1:B:367:ASP:HA	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:VAL:HG22	1:C:738:VAL:HG22	1.66	0.78
1:E:412:GLY:HA3	1:E:750:ASN:HD22	1.49	0.78
1:A:267:SER:HB2	1:A:270:GLU:CB	2.14	0.78
1:A:412:GLY:HA3	1:A:750:ASN:HD22	1.48	0.78
1:B:526:TYR:O	1:B:532:VAL:HG13	1.83	0.78
1:C:11:ILE:CG2	1:C:69:ARG:H	1.97	0.78
1:C:329:SER:HB2	1:C:331:ASN:HD21	1.49	0.78
1:E:368:ASP:HA	1:E:385:ARG:HD3	1.66	0.78
1:E:30:LEU:HD13	1:E:52:ASP:HB2	1.65	0.77
1:B:412:GLY:HA3	1:B:750:ASN:HD22	1.48	0.77
1:D:553:PRO:HB2	1:D:620:VAL:HG21	1.64	0.77
1:A:106:ILE:HG23	1:A:277:TYR:HB2	1.64	0.77
1:A:183:VAL:HG23	1:A:184:CYS:N	1.99	0.77
1:A:485:GLN:NE2	1:A:487:HIS:H	1.83	0.77
1:D:380:VAL:HG23	1:D:740:THR:HA	1.66	0.77
1:B:282:ILE:HG22	1:B:305:VAL:HB	1.65	0.77
1:C:687:LEU:HB3	1:C:724:MSE:HE2	1.65	0.77
1:D:88:ILE:HG22	1:D:89:GLU:N	1.99	0.77
1:B:371:ILE:HD12	1:B:380:VAL:HG22	1.66	0.77
1:C:207:ALA:O	1:C:210:ILE:HG22	1.85	0.77
1:E:210:ILE:HD13	1:E:216:VAL:HG12	1.65	0.77
1:F:6:ILE:HG23	1:F:73:ILE:HG23	1.67	0.77
1:F:633:GLU:H	1:F:634:PRO:HD2	1.50	0.76
1:C:456:ILE:HG22	1:C:457:ILE:H	1.50	0.76
1:E:729:VAL:HG11	1:E:735:ASN:HB3	1.66	0.76
1:F:373:PHE:CD1	1:F:378:ARG:HB3	2.21	0.76
1:A:11:ILE:HG21	1:A:69:ARG:N	2.00	0.76
1:B:165:GLU:HB3	1:B:171:ASN:ND2	2.01	0.76
1:B:201:ASP:N	1:B:202:PRO:HD2	2.01	0.76
1:C:690:ALA:HB2	1:C:721:ILE:HG23	1.68	0.76
1:F:35:LYS:HG3	1:F:90:LYS:HD2	1.65	0.76
1:B:267:SER:HB2	1:B:270:GLU:HB2	1.67	0.76
1:B:494:VAL:HG11	1:B:710:ALA:HB1	1.68	0.76
1:D:653:VAL:HG13	1:D:692:ALA:HB3	1.67	0.76
1:A:236:VAL:HG13	1:A:295:ASN:HD22	1.50	0.76
1:E:470:ALA:HB1	1:E:481:LEU:HD11	1.68	0.76
1:C:287:LYS:HG3	1:C:289:PRO:HD2	1.68	0.76
1:E:106:ILE:HG23	1:E:277:TYR:HB2	1.66	0.76
1:A:371:ILE:HD12	1:A:380:VAL:HG22	1.68	0.76
1:A:485:GLN:HG3	1:A:488:TYR:H	1.50	0.76
1:D:601:LYS:HD3	1:E:772:LEU:HD11	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:PHE:HB3	1:B:360:ARG:NH2	2.01	0.75
1:C:11:ILE:HG21	1:C:69:ARG:H	1.49	0.75
1:C:110:ASP:O	1:C:113:LEU:HB3	1.86	0.75
1:B:225:HIS:NE2	1:B:327:MSE:HE3	2.01	0.75
1:E:329:SER:HB2	1:E:331:ASN:HD21	1.51	0.75
1:E:371:ILE:HB	1:E:380:VAL:HG13	1.68	0.75
1:F:404:GLY:HA2	1:F:753:GLN:NE2	2.00	0.75
1:A:380:VAL:HG23	1:A:740:THR:HA	1.69	0.75
1:C:198:ILE:HG13	1:D:122:LYS:CD	2.17	0.75
1:E:165:GLU:HB3	1:E:171:ASN:ND2	2.01	0.75
1:A:121:ASN:ND2	1:A:123:ARG:H	1.83	0.75
1:B:557:LEU:HD12	1:B:620:VAL:HB	1.69	0.75
1:D:589:LYS:HG3	1:D:590:VAL:H	1.51	0.75
1:F:111:ASP:HB2	1:F:172:ARG:HH22	1.51	0.75
1:F:255:LYS:HB2	1:F:323:PRO:HB3	1.69	0.75
1:E:215:ILE:HG22	1:E:228:CYS:HB2	1.67	0.75
1:A:190:LEU:O	1:A:196:GLN:HB2	1.87	0.75
1:A:456:ILE:HG22	1:A:457:ILE:N	2.01	0.75
1:A:628:ARG:HH21	1:A:632:GLY:H	1.33	0.75
1:E:633:GLU:H	1:E:634:PRO:HD2	1.52	0.75
1:A:502:SER:HB3	1:A:528:GLY:HA2	1.69	0.74
1:A:765:LEU:HD21	1:A:770:LEU:HD21	1.69	0.74
1:C:249:PRO:HG3	1:C:300:LEU:HD13	1.69	0.74
1:B:52:ASP:O	1:B:56:PHE:HB2	1.87	0.74
1:B:557:LEU:HD21	1:B:621:LEU:HD13	1.69	0.74
1:D:169:PRO:HG2	1:D:170:LEU:HD12	1.67	0.74
1:E:131:CYS:HB2	1:E:172:ARG:HG3	1.67	0.74
1:F:15:VAL:HG12	1:F:16:GLY:H	1.51	0.74
1:F:526:TYR:O	1:F:532:VAL:HG13	1.87	0.74
1:B:456:ILE:HG22	1:B:457:ILE:N	2.02	0.74
1:E:371:ILE:HD12	1:E:380:VAL:HG22	1.69	0.74
1:B:427:ASN:ND2	1:B:429:GLY:H	1.84	0.74
1:E:219:LYS:HG3	1:E:224:ILE:HG22	1.70	0.74
1:B:633:GLU:H	1:B:634:PRO:HD2	1.52	0.74
1:D:121:ASN:ND2	1:D:123:ARG:H	1.84	0.74
1:E:508:LEU:HD22	1:E:611:THR:HG21	1.67	0.74
1:B:108:ILE:HD11	1:B:314:TYR:CD2	2.22	0.74
1:B:287:LYS:HG3	1:B:289:PRO:HD2	1.68	0.74
1:D:371:ILE:HD12	1:D:380:VAL:HG22	1.70	0.74
1:A:521:GLY:HA3	1:A:610:SER:HA	1.69	0.74
1:B:208:GLU:O	1:B:212:LYS:HG2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:GLU:OE1	1:E:284:LEU:HD21	1.87	0.74
1:B:502:SER:HB3	1:B:528:GLY:HA2	1.68	0.74
1:C:190:LEU:HB2	1:C:202:PRO:HB3	1.68	0.74
1:C:273:GLU:HG2	1:C:371:ILE:HD13	1.69	0.74
1:F:330:ALA:HB1	1:F:348:LEU:HD21	1.70	0.74
1:B:35:LYS:HG2	1:B:36:ASN:H	1.53	0.73
1:C:415:LYS:HD3	1:C:448:LEU:HD22	1.70	0.73
1:E:539:ASP:HA	1:E:659:LEU:HD11	1.69	0.73
1:A:461:HIS:CE1	1:A:463:ALA:HB3	2.23	0.73
1:B:236:VAL:HG13	1:B:295:ASN:HD22	1.51	0.73
1:C:373:PHE:CD1	1:C:378:ARG:HB3	2.24	0.73
1:C:650:LYS:HD2	1:C:691:ARG:HH22	1.53	0.73
1:D:35:LYS:HZ3	1:D:90:LYS:HD2	1.53	0.73
1:E:144:LEU:HD12	1:E:447:ILE:HG23	1.69	0.73
1:E:625:ALA:HB2	1:E:637:LYS:HD2	1.70	0.73
1:F:215:ILE:HG22	1:F:228:CYS:HB2	1.69	0.73
1:A:542:PRO:O	1:A:559:GLY:HA3	1.89	0.73
1:B:181:CYS:SG	1:B:183:VAL:HG22	2.28	0.73
1:F:201:ASP:N	1:F:202:PRO:HD2	2.02	0.73
1:A:3:ALA:HB2	1:A:47:GLU:HA	1.70	0.73
1:A:584:SER:HB3	1:A:589:LYS:HB3	1.70	0.73
1:A:729:VAL:HG11	1:A:735:ASN:HB3	1.70	0.73
1:B:485:GLN:HE21	1:B:487:HIS:N	1.84	0.73
1:D:406:GLU:HG3	1:D:407:LEU:HG	1.69	0.73
1:E:225:HIS:HA	1:E:330:ALA:HB2	1.71	0.73
1:F:690:ALA:HB2	1:F:721:ILE:HG23	1.69	0.73
1:B:550:SER:O	1:B:628:ARG:HG3	1.89	0.73
1:E:691:ARG:HE	1:E:724:MSE:HE2	1.52	0.73
1:B:225:HIS:HA	1:B:330:ALA:CB	2.18	0.73
1:C:339:LYS:HG3	1:C:365:ARG:NH1	2.04	0.73
1:D:219:LYS:HG3	1:D:224:ILE:HG22	1.69	0.73
1:E:654:PRO:HG2	1:E:661:ARG:HB3	1.69	0.73
1:A:111:ASP:HB3	1:A:172:ARG:HH12	1.52	0.72
1:A:268:PRO:HG2	1:A:378:ARG:NH2	2.02	0.72
1:C:284:LEU:HD21	1:C:305:VAL:HG21	1.70	0.72
1:C:292:LEU:HD13	1:C:293:PRO:HD2	1.71	0.72
1:C:11:ILE:O	1:C:11:ILE:HG13	1.88	0.72
1:F:181:CYS:SG	1:F:183:VAL:HG22	2.28	0.72
1:C:589:LYS:H	1:F:475:ASN:ND2	1.86	0.72
1:E:544:PRO:HG2	1:E:555:ARG:HB3	1.71	0.72
1:D:557:LEU:HD12	1:D:620:VAL:HB	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:ALA:HB2	1:E:47:GLU:HA	1.70	0.72
1:C:30:LEU:HD13	1:C:52:ASP:HB2	1.70	0.72
1:E:587:TYR:HD1	1:E:588:GLY:H	1.37	0.72
1:C:485:GLN:NE2	1:C:514:GLY:HA2	2.05	0.72
1:D:193:SER:O	1:D:194:ASP:HB2	1.89	0.72
1:F:281:ILE:HG12	1:F:306:MSE:HG2	1.69	0.72
1:B:254:ALA:HB1	1:B:259:THR:HB	1.69	0.72
1:D:485:GLN:NE2	1:D:487:HIS:H	1.85	0.72
1:B:169:PRO:HG2	1:B:170:LEU:HD12	1.71	0.72
1:C:649:LEU:HB3	1:C:684:SER:HB3	1.70	0.72
1:F:587:TYR:HD1	1:F:588:GLY:H	1.38	0.72
1:A:15:VAL:HG12	1:A:16:GLY:H	1.55	0.72
1:A:379:ALA:HB3	1:A:744:ARG:NH1	2.03	0.72
1:D:225:HIS:NE2	1:D:327:MSE:HE3	2.04	0.72
1:E:22:TYR:CD2	1:E:169:PRO:HB3	2.25	0.72
1:E:239:LEU:O	1:E:243:THR:HG22	1.90	0.72
1:E:404:GLY:HA2	1:E:753:GLN:HE22	1.53	0.72
1:F:18:ARG:HB2	1:F:19:PRO:HD3	1.70	0.72
1:F:191:TYR:HB2	1:F:355:PHE:HB2	1.71	0.72
1:A:148:ARG:O	1:A:151:THR:HG22	1.89	0.71
1:A:274:LEU:HB3	1:A:307:LEU:HD11	1.70	0.71
1:C:369:SER:H	1:C:385:ARG:CB	2.03	0.71
1:F:108:ILE:HA	1:F:134:CYS:SG	2.31	0.71
1:F:331:ASN:HD22	1:F:337:MSE:HA	1.55	0.71
1:D:210:ILE:HD13	1:D:216:VAL:HG12	1.73	0.71
1:F:726:ARG:NH2	1:F:727:LYS:HG2	2.05	0.71
1:A:225:HIS:NE2	1:A:327:MSE:HE3	2.05	0.71
1:D:201:ASP:N	1:D:202:PRO:HD2	2.05	0.71
1:F:373:PHE:CE1	1:F:378:ARG:HB3	2.25	0.71
1:F:491:ILE:HG23	1:F:507:ALA:HB2	1.71	0.71
1:B:371:ILE:HB	1:B:380:VAL:HG13	1.72	0.71
1:B:373:PHE:CE1	1:B:378:ARG:HB3	2.26	0.71
1:B:380:VAL:HG12	1:B:381:ILE:H	1.56	0.71
1:E:153:MSE:CE	1:E:360:ARG:HD2	2.20	0.71
1:A:258:GLU:HA	1:A:261:LYS:HD3	1.73	0.71
1:B:20:PHE:CZ	1:B:63:LYS:HB2	2.25	0.71
1:D:11:ILE:HG21	1:D:69:ARG:H	1.56	0.71
1:E:724:MSE:O	1:E:728:VAL:HG23	1.91	0.71
1:D:170:LEU:HD12	1:D:170:LEU:H	1.54	0.71
1:D:330:ALA:HB1	1:D:348:LEU:HD21	1.71	0.71
1:D:539:ASP:HA	1:D:659:LEU:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ILE:HA	1:B:134:CYS:SG	2.31	0.71
1:C:149:GLU:HA	1:C:154:LYS:HG2	1.72	0.71
1:D:274:LEU:HD22	1:D:307:LEU:HG	1.72	0.71
1:E:207:ALA:O	1:E:210:ILE:HG22	1.89	0.71
1:E:633:GLU:N	1:E:634:PRO:HD2	2.04	0.71
1:F:543:LEU:HD12	1:F:549:ALA:HB3	1.73	0.71
1:B:279:ARG:HD3	1:B:307:LEU:HB2	1.72	0.71
1:C:404:GLY:HA2	1:C:753:GLN:NE2	2.06	0.71
1:D:225:HIS:HA	1:D:330:ALA:CB	2.20	0.71
1:F:554:LEU:O	1:F:558:MSE:HG3	1.89	0.71
1:B:495:MSE:HE2	1:B:755:PHE:HZ	1.55	0.70
1:C:136:PRO:HG3	1:C:360:ARG:NH1	2.06	0.70
1:D:142:GLU:HB3	1:D:150:ASN:O	1.91	0.70
1:D:485:GLN:HG3	1:D:488:TYR:H	1.55	0.70
1:E:445:ARG:HH21	1:E:452:ASN:HD22	1.39	0.70
1:E:553:PRO:HB2	1:E:620:VAL:HG21	1.73	0.70
1:E:583:GLU:H	1:E:583:GLU:CD	1.95	0.70
1:F:687:LEU:HD22	1:F:724:MSE:HB2	1.72	0.70
1:F:6:ILE:HG22	1:F:7:HIS:H	1.56	0.70
1:A:26:HIS:HE1	1:A:87:TYR:HB3	1.57	0.70
1:F:413:VAL:HG21	1:F:448:LEU:HD13	1.73	0.70
1:A:526:TYR:O	1:A:532:VAL:HG13	1.91	0.70
1:F:89:GLU:HG3	1:F:175:HIS:HE2	1.56	0.70
1:F:144:LEU:HD12	1:F:447:ILE:HG23	1.73	0.70
1:B:590:VAL:O	1:B:594:VAL:HG23	1.92	0.70
1:E:495:MSE:HE2	1:E:755:PHE:HZ	1.56	0.70
1:F:391:PRO:HB2	1:F:418:LYS:HB2	1.72	0.70
1:A:601:LYS:HD3	1:B:772:LEU:HD11	1.74	0.70
1:B:18:ARG:HB2	1:B:19:PRO:HD3	1.74	0.70
1:C:391:PRO:HB3	1:C:420:TYR:CE1	2.27	0.70
1:D:144:LEU:HD12	1:D:447:ILE:HG23	1.74	0.70
1:D:694:ALA:HB2	1:D:725:ILE:HG23	1.74	0.70
1:A:207:ALA:HB1	1:A:320:SER:HB2	1.73	0.70
1:B:567:ILE:HG12	1:B:600:ALA:HB1	1.74	0.70
1:D:6:ILE:HB	1:D:44:ILE:HB	1.73	0.70
1:D:8:VAL:HA	1:D:72:ARG:HB2	1.74	0.70
1:D:13:GLN:HE21	1:D:42:VAL:HG23	1.56	0.70
1:D:190:LEU:HB2	1:D:202:PRO:HB2	1.72	0.70
1:F:14:ALA:HB3	1:F:103:PRO:HD3	1.73	0.70
1:A:516:ASP:HA	1:B:603:ILE:HG23	1.73	0.70
1:B:144:LEU:HD12	1:B:447:ILE:HG23	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ARG:HB2	1:C:19:PRO:HD3	1.74	0.70
1:D:329:SER:HB2	1:D:331:ASN:HD21	1.56	0.70
1:E:14:ALA:O	1:E:103:PRO:HG3	1.92	0.70
1:E:292:LEU:HD11	1:E:324:VAL:HG21	1.74	0.70
1:E:330:ALA:HB1	1:E:348:LEU:HD21	1.74	0.70
1:F:434:LEU:HD13	1:F:465:ASN:HB3	1.72	0.70
1:D:263:PHE:HZ	1:D:303:ILE:HG21	1.56	0.70
1:F:225:HIS:NE2	1:F:327:MSE:HE3	2.07	0.70
1:E:208:GLU:O	1:E:212:LYS:HG2	1.91	0.69
1:F:409:ASN:HD22	1:F:425:ILE:HD11	1.56	0.69
1:C:506:ILE:HD11	1:C:694:ALA:HA	1.74	0.69
1:A:504:ILE:O	1:A:709:VAL:HA	1.91	0.69
1:A:649:LEU:HD12	1:A:650:LYS:H	1.56	0.69
1:D:207:ALA:O	1:D:210:ILE:HG22	1.91	0.69
1:D:374:VAL:HG21	1:D:744:ARG:NH2	2.07	0.69
1:F:127:PRO:O	1:F:311:GLY:HA3	1.92	0.69
1:A:379:ALA:CB	1:A:744:ARG:HH11	2.04	0.69
1:B:215:ILE:HD11	1:B:352:ALA:HA	1.72	0.69
1:C:281:ILE:HG12	1:C:306:MSE:HG3	1.74	0.69
1:F:495:MSE:HE2	1:F:755:PHE:HZ	1.57	0.69
1:A:207:ALA:O	1:A:210:ILE:HG22	1.92	0.69
1:A:380:VAL:HG12	1:A:381:ILE:N	2.06	0.69
1:B:20:PHE:HZ	1:B:63:LYS:HB2	1.57	0.69
1:D:205:LYS:O	1:D:209:LEU:HD13	1.92	0.69
1:D:287:LYS:HG3	1:D:289:PRO:HD2	1.74	0.69
1:D:582:VAL:HG11	1:D:626:TYR:O	1.92	0.69
1:E:190:LEU:HB2	1:E:202:PRO:HB3	1.74	0.69
1:F:210:ILE:HD11	1:F:227:ALA:C	2.12	0.69
1:A:32:GLY:O	1:A:87:TYR:HA	1.93	0.69
1:A:227:ALA:HA	1:A:326:VAL:O	1.92	0.69
1:A:472:GLU:O	1:A:476:GLU:HG2	1.92	0.69
1:B:589:LYS:HG3	1:B:590:VAL:H	1.58	0.69
1:C:317:PHE:HE2	1:C:323:PRO:HA	1.57	0.69
1:A:329:SER:HA	1:A:337:MSE:HE2	1.73	0.69
1:A:339:LYS:HA	1:A:362:ILE:HD11	1.74	0.69
1:B:729:VAL:HB	1:B:735:ASN:HD22	1.57	0.69
1:D:409:ASN:HD22	1:D:425:ILE:HD11	1.57	0.69
1:B:207:ALA:O	1:B:210:ILE:HG22	1.92	0.69
1:C:329:SER:HB2	1:C:331:ASN:ND2	2.08	0.69
1:D:633:GLU:H	1:D:634:PRO:HD2	1.57	0.69
1:E:193:SER:O	1:E:194:ASP:HB2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:282:ILE:HG22	1:E:305:VAL:HB	1.75	0.69
1:A:662:VAL:O	1:A:665:LEU:HB3	1.93	0.69
1:B:13:GLN:NE2	1:B:18:ARG:HH21	1.90	0.69
1:B:752:GLY:O	1:B:756:LEU:HB2	1.92	0.69
1:C:57:ILE:HG21	1:C:75:LYS:HE3	1.74	0.69
1:C:435:GLU:HA	1:C:438:ARG:HD2	1.74	0.69
1:D:315:ILE:HG12	1:D:319:TRP:HZ3	1.56	0.69
1:F:19:PRO:HA	1:F:174:TYR:CD1	2.28	0.69
1:F:537:HIS:NE2	1:F:659:LEU:HD22	2.07	0.69
1:A:383:ARG:HH21	1:A:392:ILE:HD11	1.57	0.68
1:E:267:SER:O	1:E:270:GLU:HB3	1.91	0.68
1:A:689:LEU:O	1:A:693:PHE:HB2	1.93	0.68
1:A:590:VAL:H	1:B:475:ASN:HD21	1.41	0.68
1:C:385:ARG:HG3	1:C:386:GLY:H	1.58	0.68
1:E:572:GLY:HA2	1:E:575:ASN:HD22	1.57	0.68
1:F:288:GLU:CB	1:F:289:PRO:HD3	2.22	0.68
1:F:760:TYR:HE2	1:F:767:LYS:HG2	1.59	0.68
1:B:369:SER:HB2	1:B:385:ARG:CB	2.24	0.68
1:C:26:HIS:CE1	1:C:87:TYR:HB3	2.28	0.68
1:D:391:PRO:HB3	1:D:420:TYR:CE1	2.29	0.68
1:F:267:SER:HB2	1:F:270:GLU:HB2	1.76	0.68
1:E:6:ILE:HA	1:E:74:GLU:O	1.93	0.68
1:A:215:ILE:HG22	1:A:228:CYS:HB2	1.74	0.68
1:B:514:GLY:HA3	1:B:520:TRP:CD1	2.29	0.68
1:D:369:SER:H	1:D:385:ARG:CB	2.06	0.68
1:E:639:GLU:HB2	1:E:718:ASN:HD21	1.58	0.68
1:F:230:ALA:HB3	1:F:324:VAL:HB	1.75	0.68
1:A:247:GLN:HE22	1:A:637:LYS:HE3	1.59	0.68
1:B:534:ARG:HG2	1:B:535:LEU:N	2.08	0.68
1:C:61:TYR:OH	1:C:73:ILE:HG21	1.92	0.68
1:C:88:ILE:HG22	1:C:89:GLU:H	1.57	0.68
1:C:355:PHE:HB3	1:C:357:LEU:HD21	1.75	0.68
1:E:229:ASP:OD1	1:E:322:THR:HG21	1.94	0.68
1:F:394:ILE:CD1	1:F:419:VAL:HB	2.21	0.68
1:D:373:PHE:CD1	1:D:378:ARG:HB3	2.28	0.68
1:E:8:VAL:HB	1:E:42:VAL:HB	1.75	0.68
1:F:208:GLU:O	1:F:212:LYS:HG2	1.94	0.68
1:F:649:LEU:HB3	1:F:684:SER:HB3	1.76	0.68
1:F:653:VAL:HG11	1:F:689:LEU:HA	1.76	0.68
1:A:553:PRO:CB	1:A:620:VAL:HG21	2.24	0.68
1:A:687:LEU:HD22	1:A:724:MSE:HE3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:460:LEU:O	1:C:462:PRO:HD3	1.94	0.68
1:F:341:ASN:HD22	1:F:357:LEU:HB3	1.59	0.68
1:B:286:LYS:HD2	1:B:303:ILE:HD11	1.75	0.67
1:B:460:LEU:HD12	1:B:483:GLN:HB3	1.76	0.67
1:B:469:LEU:HG	1:B:473:MSE:HG3	1.75	0.67
1:B:524:VAL:HG22	1:B:536:ALA:HB3	1.76	0.67
1:C:589:LYS:HG3	1:C:590:VAL:H	1.57	0.67
1:F:165:GLU:HB3	1:F:171:ASN:ND2	2.09	0.67
1:A:15:VAL:HG11	1:A:67:LEU:O	1.94	0.67
1:A:419:VAL:HG11	1:A:751:VAL:HG23	1.76	0.67
1:D:12:VAL:HG13	1:D:17:PHE:CG	2.29	0.67
1:D:219:LYS:HE3	1:D:358:HIS:CE1	2.29	0.67
1:D:504:ILE:HG22	1:D:505:GLY:N	2.10	0.67
1:E:282:ILE:HG13	1:E:283:THR:H	1.60	0.67
1:F:12:VAL:HG13	1:F:42:VAL:HG21	1.76	0.67
1:F:503:VAL:HB	1:F:708:ASN:O	1.94	0.67
1:A:249:PRO:HG3	1:A:300:LEU:HD13	1.76	0.67
1:A:373:PHE:CD1	1:A:378:ARG:HB3	2.29	0.67
1:B:624:VAL:O	1:B:625:ALA:HB2	1.93	0.67
1:C:267:SER:O	1:C:270:GLU:HB3	1.93	0.67
1:D:32:GLY:O	1:D:87:TYR:HA	1.94	0.67
1:E:408:MSE:HG3	1:E:424:TYR:CE1	2.29	0.67
1:A:102:ILE:HD11	1:A:144:LEU:HG	1.77	0.67
1:C:30:LEU:HG	1:C:47:GLU:O	1.94	0.67
1:C:131:CYS:HB2	1:C:172:ARG:HG3	1.76	0.67
1:E:121:ASN:ND2	1:E:123:ARG:H	1.92	0.67
1:E:428:THR:HA	1:E:433:VAL:HG11	1.76	0.67
1:F:544:PRO:HG2	1:F:555:ARG:HB3	1.76	0.67
1:C:369:SER:N	1:C:385:ARG:HB2	2.10	0.67
1:D:491:ILE:HD11	1:D:505:GLY:HA3	1.75	0.67
1:A:6:ILE:HD12	1:A:73:ILE:HG23	1.76	0.67
1:A:391:PRO:HB3	1:A:420:TYR:CE1	2.29	0.67
1:C:148:ARG:O	1:C:151:THR:HG22	1.94	0.67
1:E:183:VAL:HG23	1:E:184:CYS:N	2.09	0.67
1:F:620:VAL:HG13	1:F:626:TYR:CD1	2.29	0.67
1:A:544:PRO:HD2	1:A:555:ARG:O	1.94	0.67
1:C:253:MSE:HE3	1:C:308:PRO:HB3	1.77	0.67
1:D:369:SER:HB2	1:D:385:ARG:HB3	1.75	0.67
1:F:168:ASP:O	1:F:174:TYR:HB2	1.95	0.67
1:A:219:LYS:HA	1:A:224:ILE:HG22	1.76	0.67
1:B:394:ILE:HG23	1:B:755:PHE:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:VAL:HB	1:B:708:ASN:O	1.94	0.67
1:C:13:GLN:HE21	1:C:42:VAL:HG23	1.58	0.67
1:C:170:LEU:H	1:C:170:LEU:HD12	1.60	0.67
1:C:521:GLY:HA3	1:C:610:SER:HA	1.76	0.67
1:E:415:LYS:HD3	1:E:448:LEU:HD22	1.77	0.67
1:A:225:HIS:HA	1:A:330:ALA:CB	2.24	0.67
1:C:102:ILE:HG23	1:C:141:ILE:HD13	1.76	0.67
1:D:526:TYR:O	1:D:532:VAL:HG13	1.95	0.67
1:A:148:ARG:NH2	1:A:158:MSE:HG3	2.08	0.67
1:B:288:GLU:CB	1:B:289:PRO:HD3	2.23	0.67
1:E:394:ILE:HG23	1:E:755:PHE:HB2	1.76	0.67
1:F:250:PHE:HE2	1:F:328:THR:HG1	1.43	0.67
1:B:268:PRO:HG2	1:B:378:ARG:NH2	2.07	0.66
1:D:163:ARG:HB2	1:D:163:ARG:HH11	1.60	0.66
1:D:191:TYR:HB2	1:D:355:PHE:HB2	1.77	0.66
1:D:554:LEU:O	1:D:558:MSE:HG3	1.96	0.66
1:E:738:VAL:HG12	1:E:742:VAL:HB	1.76	0.66
1:F:396:PHE:CZ	1:F:759:LEU:HD13	2.30	0.66
1:C:34:VAL:HB	1:C:87:TYR:OH	1.95	0.66
1:C:508:LEU:HD22	1:C:611:THR:HG21	1.77	0.66
1:C:649:LEU:HB3	1:C:684:SER:CB	2.25	0.66
1:D:269:GLU:HB2	1:D:378:ARG:CZ	2.25	0.66
1:A:261:LYS:HG3	1:A:266:VAL:HG21	1.75	0.66
1:A:616:ASP:OD2	1:A:634:PRO:HG3	1.94	0.66
1:C:738:VAL:HG12	1:C:742:VAL:O	1.95	0.66
1:D:279:ARG:HD2	1:D:308:PRO:O	1.96	0.66
1:E:373:PHE:CD1	1:E:378:ARG:HB3	2.30	0.66
1:F:398:TYR:HB2	1:F:454:ASP:OD2	1.95	0.66
1:F:580:LYS:HZ2	1:F:590:VAL:HG13	1.60	0.66
1:C:461:HIS:CE1	1:C:463:ALA:HB3	2.31	0.66
1:F:89:GLU:HG3	1:F:175:HIS:NE2	2.10	0.66
1:B:156:PHE:HZ	1:B:359:ASN:HB2	1.61	0.66
1:B:394:ILE:HG22	1:B:396:PHE:H	1.59	0.66
1:F:264:ALA:CB	1:F:286:LYS:HA	2.25	0.66
1:F:412:GLY:HA3	1:F:750:ASN:ND2	2.11	0.66
1:B:267:SER:HB2	1:B:270:GLU:CB	2.26	0.66
1:D:215:ILE:HG22	1:D:228:CYS:HB2	1.78	0.66
1:D:508:LEU:HD22	1:D:611:THR:HG21	1.78	0.66
1:E:504:ILE:HB	1:E:709:VAL:HG12	1.77	0.66
1:F:203:LEU:HD12	1:F:319:TRP:HZ3	1.61	0.66
1:B:142:GLU:HG3	1:B:143:ASP:OD1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ALA:HA	1:B:326:VAL:O	1.96	0.66
1:D:137:ARG:NH2	1:D:178:PRO:HG3	2.10	0.66
1:E:267:SER:HB2	1:E:270:GLU:HB2	1.77	0.66
1:F:261:LYS:HZ1	1:F:266:VAL:HB	1.61	0.66
1:B:22:TYR:CD2	1:B:169:PRO:HB3	2.31	0.66
1:C:756:LEU:O	1:C:759:LEU:HB3	1.96	0.66
1:D:580:LYS:HG3	1:D:593:ASN:HD22	1.61	0.66
1:E:286:LYS:HD2	1:E:303:ILE:HD11	1.78	0.66
1:A:589:LYS:HG3	1:A:590:VAL:N	2.11	0.66
1:C:484:VAL:HG12	1:C:770:LEU:HD22	1.77	0.66
1:C:506:ILE:HG12	1:C:524:VAL:HG12	1.78	0.66
1:D:384:SER:HA	1:D:388:VAL:HG23	1.78	0.66
1:D:502:SER:HB3	1:D:528:GLY:HA2	1.77	0.66
1:E:312:THR:HA	1:E:315:ILE:HG22	1.78	0.66
1:A:425:ILE:HA	1:A:436:PHE:HE1	1.59	0.66
1:C:200:GLY:C	1:C:202:PRO:HD2	2.16	0.66
1:C:337:MSE:HG3	1:C:367:ASP:OD2	1.96	0.66
1:C:698:VAL:HG13	1:C:732:ASN:HD22	1.61	0.66
1:D:239:LEU:O	1:D:243:THR:HG22	1.96	0.66
1:E:649:LEU:HB3	1:E:684:SER:HB3	1.78	0.66
1:C:66:PRO:CD	1:C:133:ASN:HD22	2.08	0.65
1:C:103:PRO:CG	1:C:137:ARG:HD2	2.25	0.65
1:D:491:ILE:HG23	1:D:527:LEU:HD21	1.76	0.65
1:E:263:PHE:HZ	1:E:303:ILE:HG21	1.61	0.65
1:F:301:HIS:HD2	1:F:302:THR:H	1.44	0.65
1:A:485:GLN:HE21	1:A:487:HIS:N	1.90	0.65
1:A:490:HIS:HE1	1:A:746:ASP:HA	1.61	0.65
1:C:412:GLY:HA3	1:C:750:ASN:HD22	1.61	0.65
1:C:591:GLU:HG2	1:F:475:ASN:HD22	1.61	0.65
1:D:9:GLN:NE2	1:D:41:GLY:HA2	2.02	0.65
1:D:700:ARG:HH11	1:D:704:PHE:HE2	1.43	0.65
1:F:239:LEU:HD22	1:F:250:PHE:HZ	1.62	0.65
1:F:570:LEU:O	1:F:573:VAL:HG12	1.97	0.65
1:F:649:LEU:HD12	1:F:650:LYS:H	1.61	0.65
1:D:570:LEU:O	1:D:573:VAL:HG12	1.97	0.65
1:F:615:LEU:CD1	1:F:638:LEU:HD23	2.25	0.65
1:F:619:ALA:HB1	1:F:625:ALA:HB3	1.76	0.65
1:A:166:TYR:CE1	1:A:175:HIS:HA	2.31	0.65
1:A:508:LEU:HD22	1:A:611:THR:HG21	1.79	0.65
1:C:743:PRO:HG2	1:C:748:GLY:HA3	1.79	0.65
1:D:181:CYS:SG	1:D:183:VAL:HG13	2.37	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:VAL:HG23	1:E:68:ALA:HB1	1.79	0.65
1:B:425:ILE:HG22	1:B:436:PHE:HE1	1.61	0.65
1:B:456:ILE:HD12	1:B:480:GLU:O	1.97	0.65
1:C:376:GLY:O	1:C:377:LYS:HG3	1.95	0.65
1:E:270:GLU:OE2	1:E:284:LEU:HD11	1.97	0.65
1:E:404:GLY:HA2	1:E:753:GLN:NE2	2.10	0.65
1:F:409:ASN:HB3	1:F:425:ILE:HD11	1.78	0.65
1:F:616:ASP:OD1	1:F:634:PRO:HG2	1.97	0.65
1:F:641:PHE:HZ	1:F:678:PRO:HB2	1.61	0.65
1:C:620:VAL:HG22	1:C:626:TYR:HA	1.79	0.65
1:E:12:VAL:HA	1:E:68:ALA:HB1	1.77	0.65
1:A:317:PHE:HE2	1:A:323:PRO:HA	1.62	0.65
1:C:522:GLY:HA3	1:C:538:ILE:HD12	1.79	0.65
1:D:20:PHE:HA	1:D:23:ARG:HH21	1.60	0.65
1:D:155:GLU:O	1:D:157:PRO:HD3	1.96	0.65
1:F:504:ILE:HG22	1:F:505:GLY:N	2.11	0.65
1:A:337:MSE:HG3	1:A:367:ASP:OD2	1.97	0.65
1:B:279:ARG:HB2	1:B:309:TYR:HB3	1.79	0.65
1:B:481:LEU:HD12	1:B:482:LEU:H	1.62	0.65
1:C:127:PRO:O	1:C:311:GLY:HA3	1.96	0.65
1:D:233:GLU:HB2	1:D:295:ASN:ND2	2.11	0.65
1:F:456:ILE:HG22	1:F:457:ILE:N	2.12	0.65
1:A:165:GLU:HB3	1:A:171:ASN:ND2	2.11	0.65
1:C:371:ILE:HB	1:C:380:VAL:HG13	1.78	0.65
1:D:456:ILE:HG22	1:D:457:ILE:H	1.60	0.65
1:E:590:VAL:O	1:E:594:VAL:HG23	1.96	0.65
1:F:408:MSE:HG3	1:F:424:TYR:CE1	2.32	0.65
1:F:694:ALA:HB2	1:F:725:ILE:HG12	1.79	0.65
1:B:498:LYS:HE3	1:B:736:PHE:HB2	1.79	0.65
1:B:690:ALA:HB1	1:B:725:ILE:HG13	1.79	0.65
1:C:700:ARG:HH11	1:C:704:PHE:HE2	1.43	0.65
1:E:30:LEU:CD1	1:E:52:ASP:HB2	2.27	0.65
1:E:232:ASN:HB3	1:E:235:VAL:HG22	1.79	0.65
1:F:743:PRO:HG2	1:F:748:GLY:HA3	1.79	0.65
1:A:26:HIS:CE1	1:A:87:TYR:HB3	2.31	0.64
1:A:589:LYS:H	1:B:475:ASN:ND2	1.95	0.64
1:A:619:ALA:O	1:A:624:VAL:HB	1.97	0.64
1:B:215:ILE:O	1:B:353:ASP:HB2	1.97	0.64
1:B:374:VAL:HG21	1:B:744:ARG:NH2	2.12	0.64
1:C:281:ILE:HG12	1:C:306:MSE:CG	2.27	0.64
1:C:385:ARG:HG3	1:C:386:GLY:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:649:LEU:HD12	1:E:650:LYS:H	1.60	0.64
1:B:263:PHE:HZ	1:B:303:ILE:HG21	1.62	0.64
1:D:690:ALA:HB1	1:D:725:ILE:HG13	1.79	0.64
1:E:103:PRO:HG2	1:E:137:ARG:HD2	1.78	0.64
1:E:137:ARG:O	1:E:141:ILE:HG13	1.97	0.64
1:E:281:ILE:HG12	1:E:306:MSE:CG	2.27	0.64
1:E:329:SER:HA	1:E:337:MSE:HE2	1.80	0.64
1:E:570:LEU:O	1:E:573:VAL:HG12	1.97	0.64
1:E:601:LYS:HB2	1:E:603:ILE:HG13	1.79	0.64
1:E:651:PHE:HB2	1:E:688:ALA:CB	2.27	0.64
1:E:749:VAL:O	1:E:753:GLN:HG3	1.97	0.64
1:F:729:VAL:HG11	1:F:735:ASN:HB3	1.78	0.64
1:A:200:GLY:C	1:A:202:PRO:HD2	2.18	0.64
1:B:219:LYS:HA	1:B:224:ILE:HB	1.77	0.64
1:B:456:ILE:HD11	1:B:479:VAL:HB	1.79	0.64
1:C:292:LEU:HD12	1:C:296:LEU:HD21	1.79	0.64
1:C:405:ALA:O	1:C:466:THR:HG21	1.97	0.64
1:E:224:ILE:HG13	1:E:338:VAL:HG13	1.78	0.64
1:B:491:ILE:HD12	1:B:525:LEU:HD12	1.78	0.64
1:C:37:LEU:HD23	1:C:40:ALA:O	1.98	0.64
1:C:50:GLU:O	1:C:53:ILE:HG22	1.97	0.64
1:D:564:VAL:HG13	1:D:667:GLN:HE21	1.62	0.64
1:E:18:ARG:HH22	1:E:36:ASN:ND2	1.96	0.64
1:F:687:LEU:CD2	1:F:724:MSE:HB2	2.27	0.64
1:A:475:ASN:ND2	1:B:591:GLU:HG2	2.10	0.64
1:A:653:VAL:HG13	1:A:692:ALA:HB3	1.80	0.64
1:C:312:THR:O	1:C:315:ILE:HG22	1.98	0.64
1:D:491:ILE:HG23	1:D:527:LEU:HD11	1.80	0.64
1:D:690:ALA:O	1:D:725:ILE:HG12	1.97	0.64
1:F:456:ILE:HG22	1:F:457:ILE:H	1.61	0.64
1:A:232:ASN:HB3	1:A:235:VAL:HG22	1.79	0.64
1:A:292:LEU:HD11	1:A:324:VAL:HG21	1.80	0.64
1:A:451:LYS:HA	1:A:477:LEU:HD21	1.79	0.64
1:C:409:ASN:ND2	1:C:425:ILE:HD11	2.12	0.64
1:C:601:LYS:NZ	1:F:771:MSE:HE3	2.13	0.64
1:E:519:THR:HB	1:E:608:ALA:HA	1.79	0.64
1:E:521:GLY:HA3	1:E:610:SER:HA	1.79	0.64
1:C:188:TYR:CZ	1:C:312:THR:HG21	2.32	0.64
1:F:581:ALA:HA	1:F:584:SER:HB3	1.80	0.64
1:A:183:VAL:CG2	1:A:184:CYS:N	2.61	0.64
1:C:192:THR:C	1:C:194:ASP:H	1.99	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:MSE:O	1:C:441:ILE:HG13	1.98	0.64
1:F:32:GLY:H	1:F:87:TYR:HD2	1.44	0.64
1:F:380:VAL:HG12	1:F:381:ILE:N	2.12	0.64
1:B:163:ARG:HB2	1:B:163:ARG:NH1	2.12	0.64
1:B:549:ALA:HA	1:B:555:ARG:HB2	1.78	0.64
1:C:583:GLU:H	1:C:583:GLU:CD	2.01	0.64
1:F:142:GLU:HB3	1:F:150:ASN:O	1.98	0.64
1:A:282:ILE:HG13	1:A:283:THR:H	1.63	0.64
1:B:6:ILE:HG23	1:B:73:ILE:HG23	1.80	0.64
1:B:544:PRO:HB2	1:B:555:ARG:NH2	2.13	0.64
1:C:394:ILE:HD11	1:C:419:VAL:HB	1.80	0.64
1:D:216:VAL:HG23	1:D:354:TYR:C	2.18	0.64
1:F:57:ILE:HG13	1:F:75:LYS:HZ3	1.61	0.64
1:F:651:PHE:HB2	1:F:688:ALA:CB	2.28	0.64
1:A:49:ARG:CD	1:A:49:ARG:H	2.09	0.63
1:A:633:GLU:N	1:A:634:PRO:HD2	2.14	0.63
1:A:757:GLY:O	1:A:760:TYR:HB3	1.98	0.63
1:A:759:LEU:HD22	1:A:765:LEU:HB2	1.79	0.63
1:D:524:VAL:HG23	1:D:536:ALA:H	1.62	0.63
1:F:427:ASN:O	1:F:433:VAL:HG21	1.98	0.63
1:A:615:LEU:HD11	1:A:635:ALA:HA	1.81	0.63
1:C:12:VAL:HG13	1:C:13:GLN:H	1.61	0.63
1:C:338:VAL:HG23	1:C:343:ARG:HB2	1.79	0.63
1:D:232:ASN:HB3	1:D:235:VAL:HG22	1.80	0.63
1:E:127:PRO:HB3	1:E:312:THR:CG2	2.27	0.63
1:E:502:SER:HB3	1:E:528:GLY:HA2	1.80	0.63
1:A:752:GLY:O	1:A:756:LEU:HB2	1.97	0.63
1:B:369:SER:HB2	1:B:385:ARG:HB2	1.81	0.63
1:D:161:PHE:O	1:D:164:SER:HB2	1.97	0.63
1:D:529:TYR:HD1	1:D:764:TYR:HB3	1.63	0.63
1:F:373:PHE:CE2	1:F:378:ARG:HD3	2.34	0.63
1:F:549:ALA:HA	1:F:555:ARG:HB2	1.80	0.63
1:B:270:GLU:HB2	1:B:373:PHE:HE2	1.64	0.63
1:B:584:SER:HB3	1:B:589:LYS:HB3	1.80	0.63
1:E:380:VAL:HG12	1:E:381:ILE:H	1.63	0.63
1:A:17:PHE:O	1:A:21:VAL:HG23	1.97	0.63
1:A:485:GLN:OE1	1:A:514:GLY:HA2	1.99	0.63
1:D:653:VAL:HG11	1:D:689:LEU:HD12	1.79	0.63
1:F:221:ILE:HA	1:F:360:ARG:HH22	1.64	0.63
1:F:263:PHE:HZ	1:F:303:ILE:HG21	1.62	0.63
1:F:589:LYS:HG3	1:F:590:VAL:N	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ASP:N	1:A:202:PRO:CD	2.61	0.63
1:B:215:ILE:HG22	1:B:228:CYS:HB2	1.81	0.63
1:B:566:SER:H	1:B:569:GLU:HB2	1.63	0.63
1:B:580:LYS:HE2	1:B:593:ASN:ND2	2.13	0.63
1:D:219:LYS:HG2	1:D:358:HIS:NE2	2.13	0.63
1:F:126:TYR:CZ	1:F:128:PHE:HB2	2.34	0.63
1:A:108:ILE:HG13	1:A:311:GLY:H	1.63	0.63
1:B:265:TYR:O	1:B:284:LEU:HD22	1.98	0.63
1:F:396:PHE:CE2	1:F:759:LEU:HB2	2.34	0.63
1:E:760:TYR:HE2	1:E:767:LYS:HG2	1.64	0.63
1:F:224:ILE:HD13	1:F:357:LEU:HD22	1.81	0.63
1:A:114:ARG:O	1:A:118:ASP:HB2	1.98	0.63
1:A:369:SER:H	1:A:385:ARG:HB2	1.64	0.63
1:A:590:VAL:N	1:B:475:ASN:HD21	1.96	0.63
1:A:629:HIS:HB2	1:A:633:GLU:OE1	1.98	0.63
1:B:501:ASP:O	1:B:503:VAL:HG13	1.99	0.63
1:C:13:GLN:NE2	1:C:42:VAL:HG23	2.13	0.63
1:D:88:ILE:CG2	1:D:89:GLU:H	2.09	0.63
1:D:434:LEU:HD13	1:D:465:ASN:HB3	1.81	0.63
1:D:742:VAL:HG11	1:D:751:VAL:HG11	1.81	0.63
1:F:239:LEU:O	1:F:239:LEU:HD23	1.98	0.63
1:F:613:ARG:HA	1:F:613:ARG:HE	1.64	0.63
1:A:5:HIS:HB3	1:A:76:LYS:HB2	1.80	0.62
1:B:210:ILE:HD11	1:B:228:CYS:N	2.13	0.62
1:B:566:SER:N	1:B:569:GLU:HB2	2.14	0.62
1:C:253:MSE:O	1:C:324:VAL:HA	1.98	0.62
1:F:137:ARG:HH22	1:F:178:PRO:HG3	1.62	0.62
1:A:148:ARG:CZ	1:A:158:MSE:HG3	2.28	0.62
1:B:374:VAL:HG11	1:B:744:ARG:HH22	1.64	0.62
1:B:651:PHE:HE2	1:B:669:ILE:HA	1.63	0.62
1:C:261:LYS:HZ3	1:C:266:VAL:HB	1.63	0.62
1:F:430:LYS:HB2	1:F:433:VAL:HG23	1.80	0.62
1:F:697:ALA:HB1	1:F:709:VAL:HG11	1.80	0.62
1:C:239:LEU:O	1:C:243:THR:HG22	1.98	0.62
1:F:264:ALA:HB2	1:F:286:LYS:HA	1.80	0.62
1:F:620:VAL:HG13	1:F:626:TYR:HD1	1.64	0.62
1:F:665:LEU:HD22	1:F:689:LEU:HD13	1.81	0.62
1:A:20:PHE:O	1:A:24:ILE:HG22	1.99	0.62
1:A:329:SER:HB2	1:A:331:ASN:HD21	1.64	0.62
1:A:494:VAL:HG22	1:A:738:VAL:HG22	1.80	0.62
1:B:8:VAL:HG11	1:B:12:VAL:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:PHE:CD1	1:B:378:ARG:HB3	2.35	0.62
1:A:497:GLU:OE2	1:A:741:GLU:HB3	2.00	0.62
1:A:708:ASN:HB3	1:A:734:LEU:O	1.99	0.62
1:C:104:PRO:HD3	1:C:390:LEU:HD21	1.82	0.62
1:C:281:ILE:HB	1:C:370:VAL:CG1	2.25	0.62
1:D:226:LEU:HD11	1:D:348:LEU:HD23	1.81	0.62
1:D:385:ARG:HG3	1:D:386:GLY:N	2.14	0.62
1:D:408:MSE:HG3	1:D:424:TYR:CE1	2.34	0.62
1:D:553:PRO:CD	1:D:627:ARG:HA	2.30	0.62
1:D:649:LEU:HD12	1:D:650:LYS:H	1.64	0.62
1:E:5:HIS:HB3	1:E:76:LYS:HB2	1.80	0.62
1:E:66:PRO:HD2	1:E:133:ASN:ND2	2.15	0.62
1:F:329:SER:HB2	1:F:331:ASN:HD21	1.65	0.62
1:A:116:LEU:HB3	1:A:129:ILE:HD12	1.80	0.62
1:A:325:TYR:O	1:A:326:VAL:HG23	2.00	0.62
1:B:281:ILE:HG12	1:B:306:MSE:HG2	1.80	0.62
1:C:219:LYS:HE3	1:C:358:HIS:CE1	2.35	0.62
1:D:282:ILE:HD12	1:D:371:ILE:O	1.99	0.62
1:D:373:PHE:CE1	1:D:378:ARG:HB3	2.34	0.62
1:E:370:VAL:H	1:E:382:ARG:HB3	1.64	0.62
1:F:729:VAL:HB	1:F:735:ASN:HD22	1.65	0.62
1:A:534:ARG:HG2	1:A:535:LEU:N	2.14	0.62
1:B:225:HIS:HB2	1:B:328:THR:O	2.00	0.62
1:C:258:GLU:HG3	1:C:259:THR:H	1.61	0.62
1:C:534:ARG:HD3	1:C:537:HIS:HD2	1.65	0.62
1:D:105:ASP:OD1	1:D:139:THR:HG23	1.99	0.62
1:F:193:SER:O	1:F:194:ASP:HB2	2.00	0.62
1:F:464:TYR:HB2	1:F:467:THR:HG23	1.80	0.62
1:F:590:VAL:O	1:F:594:VAL:HG23	2.00	0.62
1:A:475:ASN:ND2	1:B:589:LYS:H	1.98	0.62
1:C:570:LEU:O	1:C:573:VAL:HG12	2.00	0.62
1:C:649:LEU:HD12	1:C:650:LYS:H	1.64	0.62
1:D:408:MSE:HG3	1:D:424:TYR:HE1	1.64	0.62
1:E:111:ASP:HB3	1:E:172:ARG:NH2	2.15	0.62
1:E:142:GLU:HB3	1:E:150:ASN:O	1.99	0.62
1:E:168:ASP:O	1:E:174:TYR:HB2	2.00	0.62
1:A:65:PRO:HG2	1:A:68:ALA:HB3	1.80	0.62
1:A:210:ILE:HD11	1:A:228:CYS:N	2.14	0.62
1:A:263:PHE:HZ	1:A:303:ILE:HG21	1.64	0.62
1:A:749:VAL:O	1:A:753:GLN:HG3	2.00	0.62
1:B:1:MSE:HG2	1:B:83:PHE:HD1	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:PRO:HG2	1:C:170:LEU:HD12	1.81	0.62
1:C:422:SER:HA	1:C:444:PHE:CZ	2.34	0.62
1:C:495:MSE:SE	1:C:527:LEU:HD13	2.50	0.62
1:E:210:ILE:HD11	1:E:228:CYS:CA	2.28	0.62
1:E:380:VAL:HG12	1:E:381:ILE:N	2.15	0.62
1:A:521:GLY:CA	1:A:610:SER:HA	2.30	0.62
1:C:253:MSE:HA	1:C:306:MSE:O	2.00	0.62
1:D:543:LEU:HD23	1:D:543:LEU:N	2.13	0.62
1:F:65:PRO:HG2	1:F:68:ALA:HB3	1.82	0.62
1:F:190:LEU:HG	1:F:202:PRO:CB	2.29	0.62
1:A:580:LYS:HG3	1:A:593:ASN:HD22	1.65	0.61
1:B:498:LYS:HB2	1:B:500:LEU:CD2	2.29	0.61
1:C:603:ILE:HG23	1:F:516:ASP:HA	1.81	0.61
1:C:756:LEU:HD22	1:C:770:LEU:HD21	1.82	0.61
1:D:61:TYR:OH	1:D:73:ILE:HD12	1.99	0.61
1:D:590:VAL:O	1:D:594:VAL:HG23	1.99	0.61
1:E:737:HIS:HB3	1:E:744:ARG:HD3	1.82	0.61
1:F:583:GLU:HG3	1:F:592:PHE:CD1	2.35	0.61
1:A:236:VAL:HG13	1:A:295:ASN:ND2	2.15	0.61
1:B:525:LEU:HD23	1:B:534:ARG:HA	1.81	0.61
1:C:224:ILE:HG23	1:C:338:VAL:HG13	1.82	0.61
1:D:543:LEU:HD12	1:D:549:ALA:HB3	1.82	0.61
1:E:61:TYR:CZ	1:E:73:ILE:HD12	2.34	0.61
1:E:201:ASP:N	1:E:202:PRO:CD	2.63	0.61
1:E:204:ARG:HG2	1:E:319:TRP:CE2	2.35	0.61
1:E:394:ILE:CD1	1:E:419:VAL:HB	2.28	0.61
1:E:445:ARG:HH21	1:E:452:ASN:ND2	1.97	0.61
1:C:138:PHE:HB2	1:C:389:PRO:HD3	1.82	0.61
1:C:226:LEU:HD21	1:C:351:VAL:HG12	1.81	0.61
1:D:8:VAL:O	1:D:9:GLN:HG3	2.00	0.61
1:E:111:ASP:CB	1:E:172:ARG:HH22	2.14	0.61
1:F:385:ARG:HG3	1:F:386:GLY:H	1.64	0.61
1:F:498:LYS:HE3	1:F:736:PHE:HB2	1.83	0.61
1:B:502:SER:CB	1:B:528:GLY:HA2	2.29	0.61
1:D:553:PRO:HD2	1:D:627:ARG:HA	1.82	0.61
1:E:391:PRO:HB2	1:E:418:LYS:HB2	1.82	0.61
1:F:255:LYS:HB2	1:F:323:PRO:CB	2.29	0.61
1:B:743:PRO:HG3	1:B:747:ASN:HD21	1.66	0.61
1:C:196:GLN:HG2	1:C:197:GLU:N	2.15	0.61
1:E:47:GLU:CB	1:E:80:PRO:HG2	2.30	0.61
1:A:216:VAL:HB	1:A:354:TYR:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:GLU:CG	1:C:259:THR:N	2.62	0.61
1:D:427:ASN:ND2	1:D:429:GLY:H	1.98	0.61
1:D:601:LYS:HB2	1:D:603:ILE:HG13	1.82	0.61
1:E:485:GLN:OE1	1:E:514:GLY:HA2	2.01	0.61
1:F:292:LEU:HD11	1:F:324:VAL:HG21	1.82	0.61
1:A:282:ILE:HG13	1:A:283:THR:N	2.16	0.61
1:B:125:MSE:O	1:B:127:PRO:HD3	2.01	0.61
1:B:313:HIS:HE1	1:B:327:MSE:HE2	1.64	0.61
1:B:485:GLN:CG	1:B:488:TYR:H	2.12	0.61
1:C:232:ASN:OD1	1:C:234:GLU:HB3	2.00	0.61
1:D:257:ILE:HD12	1:D:260:VAL:HG21	1.83	0.61
1:E:489:ALA:O	1:E:492:ALA:HB3	2.00	0.61
1:F:690:ALA:HB1	1:F:725:ILE:HG13	1.83	0.61
1:B:380:VAL:HG12	1:B:381:ILE:N	2.16	0.61
1:C:614:VAL:O	1:C:618:ILE:HG13	2.01	0.61
1:F:61:TYR:OH	1:F:73:ILE:HD12	2.00	0.61
1:F:106:ILE:CG2	1:F:277:TYR:HB2	2.30	0.61
1:A:727:LYS:NZ	1:C:287:LYS:HE3	2.15	0.61
1:B:491:ILE:HG22	1:B:527:LEU:HD11	1.81	0.61
1:E:670:LEU:O	1:E:673:ILE:HG12	2.01	0.61
1:F:15:VAL:HG22	1:F:103:PRO:HB3	1.82	0.61
1:F:17:PHE:O	1:F:21:VAL:HG23	2.00	0.61
1:F:154:LYS:O	1:F:154:LYS:HD3	2.01	0.61
1:F:183:VAL:HG23	1:F:184:CYS:N	2.16	0.61
1:F:633:GLU:N	1:F:634:PRO:HD2	2.16	0.61
1:C:584:SER:HB3	1:C:589:LYS:HB3	1.83	0.61
1:D:111:ASP:CB	1:D:172:ARG:HH22	2.10	0.61
1:F:614:VAL:O	1:F:618:ILE:HG13	2.01	0.61
1:A:123:ARG:NH2	1:A:173:ARG:HE	1.98	0.60
1:A:590:VAL:O	1:A:594:VAL:HG23	2.01	0.60
1:B:200:GLY:C	1:B:202:PRO:HD2	2.21	0.60
1:C:450:VAL:HG22	1:C:451:LYS:H	1.66	0.60
1:C:759:LEU:CD1	1:C:764:TYR:HB2	2.30	0.60
1:D:369:SER:N	1:D:385:ARG:HB2	2.10	0.60
1:D:542:PRO:HD3	1:D:563:LYS:HE2	1.82	0.60
1:F:370:VAL:H	1:F:382:ARG:HB3	1.65	0.60
1:A:49:ARG:O	1:A:53:ILE:HB	2.01	0.60
1:A:142:GLU:HB3	1:A:150:ASN:O	2.00	0.60
1:A:572:GLY:HA2	1:A:575:ASN:HD22	1.67	0.60
1:A:698:VAL:HG13	1:A:732:ASN:HD22	1.65	0.60
1:C:456:ILE:HG22	1:C:457:ILE:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:ILE:HG13	1:D:283:THR:N	2.16	0.60
1:D:456:ILE:HG22	1:D:457:ILE:N	2.16	0.60
1:F:35:LYS:HE2	1:F:90:LYS:NZ	2.14	0.60
1:F:506:ILE:O	1:F:711:LEU:HD12	2.00	0.60
1:D:270:GLU:HB2	1:D:373:PHE:HE2	1.66	0.60
1:E:500:LEU:HD13	1:E:736:PHE:CZ	2.36	0.60
1:F:649:LEU:HB3	1:F:684:SER:CB	2.31	0.60
1:A:524:VAL:HG22	1:A:536:ALA:CB	2.31	0.60
1:B:394:ILE:CD1	1:B:419:VAL:HB	2.25	0.60
1:B:729:VAL:CB	1:B:735:ASN:HD22	2.14	0.60
1:C:373:PHE:CE2	1:C:378:ARG:HD3	2.37	0.60
1:C:504:ILE:O	1:C:709:VAL:HA	2.01	0.60
1:E:691:ARG:NE	1:E:724:MSE:HE2	2.14	0.60
1:F:469:LEU:O	1:F:473:MSE:HB2	2.01	0.60
1:A:616:ASP:CG	1:A:634:PRO:HG3	2.22	0.60
1:C:759:LEU:HD11	1:C:764:TYR:HB2	1.83	0.60
1:D:144:LEU:HD23	1:D:146:TYR:H	1.67	0.60
1:D:148:ARG:O	1:D:151:THR:HG22	2.01	0.60
1:D:253:MSE:O	1:D:324:VAL:HA	2.02	0.60
1:E:266:VAL:HG13	1:E:270:GLU:OE2	2.01	0.60
1:E:286:LYS:HE3	1:E:290:PHE:HB2	1.84	0.60
1:E:406:GLU:HG3	1:E:407:LEU:HG	1.82	0.60
1:F:287:LYS:HG3	1:F:289:PRO:HD2	1.83	0.60
1:A:15:VAL:HG21	1:A:67:LEU:O	2.02	0.60
1:A:239:LEU:O	1:A:243:THR:HG22	2.02	0.60
1:B:373:PHE:CE2	1:B:378:ARG:HD3	2.36	0.60
1:B:408:MSE:HG3	1:B:424:TYR:CE1	2.37	0.60
1:D:504:ILE:O	1:D:709:VAL:HA	2.01	0.60
1:D:572:GLY:HA2	1:D:575:ASN:HD22	1.66	0.60
1:D:665:LEU:HD22	1:D:689:LEU:HD13	1.83	0.60
1:E:257:ILE:HD12	1:E:260:VAL:HB	1.83	0.60
1:E:759:LEU:HD11	1:E:764:TYR:HB2	1.83	0.60
1:B:35:LYS:HG3	1:B:90:LYS:HD2	1.83	0.60
1:B:263:PHE:CZ	1:B:303:ILE:HG21	2.36	0.60
1:B:759:LEU:HD11	1:B:764:TYR:HB2	1.84	0.60
1:C:552:TYR:HE1	1:C:627:ARG:NE	1.99	0.60
1:B:158:MSE:HE3	1:B:163:ARG:CZ	2.32	0.60
1:B:401:LEU:HD12	1:B:402:ALA:H	1.67	0.60
1:B:620:VAL:C	1:B:622:LEU:H	2.05	0.60
1:C:485:GLN:CB	1:C:488:TYR:HB2	2.32	0.60
1:E:6:ILE:HD12	1:E:73:ILE:HG23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:GLN:HB2	1:E:72:ARG:HD2	1.84	0.60
1:F:405:ALA:O	1:F:466:THR:HG21	2.01	0.60
1:A:282:ILE:HD12	1:A:371:ILE:O	2.02	0.60
1:A:634:PRO:HG2	1:A:635:ALA:H	1.67	0.60
1:B:653:VAL:HG13	1:B:692:ALA:CB	2.30	0.60
1:C:204:ARG:HG2	1:C:319:TRP:CZ2	2.37	0.60
1:D:371:ILE:CD1	1:D:380:VAL:HG22	2.31	0.60
1:E:30:LEU:HG	1:E:48:GLY:HA3	1.84	0.60
1:A:299:GLY:O	1:A:300:LEU:HG	2.02	0.60
1:A:587:TYR:HD1	1:A:588:GLY:N	1.93	0.60
1:B:274:LEU:HB3	1:B:307:LEU:HD11	1.84	0.60
1:B:540:TYR:HD1	1:B:540:TYR:H	1.48	0.60
1:D:34:VAL:O	1:D:89:GLU:HA	2.02	0.60
1:D:409:ASN:ND2	1:D:425:ILE:HD11	2.17	0.60
1:E:281:ILE:HG12	1:E:306:MSE:HG2	1.83	0.60
1:E:726:ARG:HH21	1:E:727:LYS:HG2	1.67	0.60
1:A:445:ARG:HH21	1:A:452:ASN:ND2	2.00	0.59
1:B:504:ILE:HG22	1:B:505:GLY:N	2.16	0.59
1:C:409:ASN:O	1:C:425:ILE:HG12	2.02	0.59
1:D:554:LEU:HD11	1:D:579:PRO:HB2	1.83	0.59
1:E:554:LEU:O	1:E:558:MSE:HG3	2.02	0.59
1:F:371:ILE:HD11	1:F:373:PHE:HE1	1.67	0.59
1:F:445:ARG:HH21	1:F:452:ASN:HD22	1.48	0.59
1:A:144:LEU:HD12	1:A:447:ILE:HG23	1.83	0.59
1:A:405:ALA:O	1:A:466:THR:HG21	2.02	0.59
1:A:723:LYS:HE2	1:C:289:PRO:HG2	1.83	0.59
1:B:219:LYS:HD3	1:B:358:HIS:H	1.66	0.59
1:B:312:THR:O	1:B:315:ILE:HG22	2.02	0.59
1:B:425:ILE:HG22	1:B:436:PHE:CE1	2.38	0.59
1:C:524:VAL:HG22	1:C:536:ALA:HB3	1.82	0.59
1:D:526:TYR:HB2	1:D:535:LEU:HD11	1.85	0.59
1:D:566:SER:N	1:D:569:GLU:HB2	2.13	0.59
1:E:261:LYS:HZ3	1:E:266:VAL:HB	1.67	0.59
1:E:329:SER:HB2	1:E:331:ASN:ND2	2.17	0.59
1:A:196:GLN:HG2	1:A:197:GLU:O	2.01	0.59
1:A:553:PRO:HG3	1:A:626:TYR:O	2.01	0.59
1:B:391:PRO:HB3	1:B:420:TYR:CE1	2.38	0.59
1:C:171:ASN:ND2	1:C:173:ARG:HB2	2.18	0.59
1:C:215:ILE:HG22	1:C:228:CYS:HB2	1.83	0.59
1:C:225:HIS:HA	1:C:330:ALA:CB	2.32	0.59
1:D:144:LEU:HD23	1:D:146:TYR:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:TYR:CE1	1:D:175:HIS:HA	2.38	0.59
1:D:614:VAL:O	1:D:618:ILE:HG13	2.02	0.59
1:E:156:PHE:CZ	1:E:186:PRO:HB3	2.38	0.59
1:E:396:PHE:CE2	1:E:759:LEU:HB2	2.36	0.59
1:F:370:VAL:HG23	1:F:381:ILE:HD11	1.83	0.59
1:A:253:MSE:HE2	1:A:317:PHE:CD1	2.37	0.59
1:A:554:LEU:O	1:A:558:MSE:HG3	2.02	0.59
1:B:107:ALA:O	1:B:134:CYS:HB2	2.02	0.59
1:C:554:LEU:O	1:C:558:MSE:HG3	2.03	0.59
1:C:724:MSE:O	1:C:728:VAL:HG23	2.03	0.59
1:D:468:LYS:HG3	1:E:587:TYR:OH	2.03	0.59
1:D:654:PRO:HG3	1:D:664:GLU:OE1	2.02	0.59
1:E:419:VAL:HG11	1:E:751:VAL:HG23	1.83	0.59
1:E:456:ILE:HG22	1:E:457:ILE:N	2.18	0.59
1:F:601:LYS:HB2	1:F:603:ILE:HG13	1.83	0.59
1:A:247:GLN:HG3	1:A:298:PRO:HG2	1.83	0.59
1:B:15:VAL:HG12	1:B:16:GLY:H	1.68	0.59
1:B:239:LEU:HD23	1:B:239:LEU:O	2.03	0.59
1:C:406:GLU:HG3	1:C:407:LEU:N	2.16	0.59
1:D:171:ASN:ND2	1:D:173:ARG:H	2.00	0.59
1:E:464:TYR:HB2	1:E:467:THR:HG23	1.84	0.59
1:F:106:ILE:HG23	1:F:277:TYR:HB2	1.84	0.59
1:A:267:SER:H	1:A:270:GLU:CD	2.06	0.59
1:B:282:ILE:HG23	1:B:283:THR:N	2.15	0.59
1:B:751:VAL:HG13	1:B:752:GLY:N	2.17	0.59
1:C:66:PRO:HG3	1:C:133:ASN:HB3	1.85	0.59
1:C:526:TYR:O	1:C:532:VAL:HG13	2.03	0.59
1:D:383:ARG:HB3	1:D:747:ASN:HD21	1.68	0.59
1:D:398:TYR:HB2	1:D:454:ASP:OD2	2.03	0.59
1:E:543:LEU:HD12	1:E:549:ALA:HB3	1.85	0.59
1:E:572:GLY:HA2	1:E:575:ASN:ND2	2.17	0.59
1:E:729:VAL:HB	1:E:735:ASN:HD22	1.66	0.59
1:F:254:ALA:HB1	1:F:259:THR:HB	1.85	0.59
1:F:265:TYR:CE2	1:F:287:LYS:HD2	2.31	0.59
1:F:370:VAL:CG2	1:F:381:ILE:HD11	2.33	0.59
1:B:281:ILE:HG12	1:B:306:MSE:CG	2.33	0.59
1:B:374:VAL:CG2	1:B:744:ARG:HH22	2.14	0.59
1:D:137:ARG:HH22	1:D:178:PRO:HG3	1.67	0.59
1:E:210:ILE:CD1	1:E:228:CYS:HA	2.32	0.59
1:E:677:SER:HB2	1:E:678:PRO:HD2	1.85	0.59
1:E:752:GLY:O	1:E:756:LEU:HB2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:253:MSE:HE1	1:F:313:HIS:ND1	2.17	0.59
1:F:519:THR:HB	1:F:608:ALA:HA	1.83	0.59
1:A:485:GLN:CG	1:A:488:TYR:H	2.16	0.59
1:B:402:ALA:HB2	1:B:457:ILE:HD12	1.84	0.59
1:C:223:GLY:HA2	1:C:362:ILE:HD12	1.85	0.59
1:D:121:ASN:HD22	1:D:123:ARG:H	1.49	0.59
1:F:181:CYS:SG	1:F:183:VAL:HG13	2.43	0.59
1:F:213:GLY:CA	1:F:235:VAL:HG11	2.33	0.59
1:A:210:ILE:HG21	1:A:325:TYR:HE1	1.67	0.59
1:A:270:GLU:N	1:A:378:ARG:HH12	2.01	0.59
1:A:408:MSE:HG3	1:A:424:TYR:HE1	1.68	0.59
1:B:111:ASP:O	1:B:114:ARG:HG2	2.02	0.59
1:B:237:ALA:HA	1:B:295:ASN:HD21	1.68	0.59
1:C:491:ILE:HG22	1:C:527:LEU:HD12	1.84	0.59
1:C:583:GLU:HG3	1:C:592:PHE:CD1	2.37	0.59
1:D:485:GLN:HE21	1:D:487:HIS:N	1.87	0.59
1:D:565:TYR:HB3	1:D:569:GLU:CB	2.33	0.59
1:E:399:ASN:O	1:E:454:ASP:HB2	2.02	0.59
1:F:253:MSE:HE3	1:F:317:PHE:CE1	2.38	0.59
1:A:447:ILE:O	1:A:448:LEU:HD23	2.02	0.59
1:A:620:VAL:C	1:A:622:LEU:H	2.06	0.59
1:C:9:GLN:O	1:C:71:ASP:HB3	2.03	0.59
1:C:247:GLN:OE1	1:C:637:LYS:HE3	2.01	0.59
1:C:591:GLU:HG2	1:F:475:ASN:ND2	2.17	0.59
1:E:274:LEU:HB3	1:E:307:LEU:HD11	1.85	0.59
1:A:371:ILE:HG13	1:A:380:VAL:HA	1.85	0.58
1:A:405:ALA:H	1:A:749:VAL:HG11	1.68	0.58
1:E:15:VAL:HG12	1:E:16:GLY:H	1.66	0.58
1:A:140:ILE:HB	1:A:152:THR:CG2	2.33	0.58
1:B:108:ILE:HD11	1:B:314:TYR:CE2	2.38	0.58
1:B:232:ASN:HB3	1:B:235:VAL:CG2	2.31	0.58
1:B:433:VAL:O	1:B:436:PHE:HB3	2.04	0.58
1:C:312:THR:HA	1:C:315:ILE:HG22	1.84	0.58
1:C:642:ALA:O	1:C:683:TYR:HB2	2.03	0.58
1:D:11:ILE:CG1	1:D:68:ALA:HA	2.29	0.58
1:D:18:ARG:HA	1:D:21:VAL:HG12	1.85	0.58
1:D:724:MSE:O	1:D:728:VAL:HG23	2.03	0.58
1:E:589:LYS:HG3	1:E:590:VAL:N	2.17	0.58
1:F:498:LYS:HB2	1:F:500:LEU:HD23	1.85	0.58
1:F:506:ILE:HG12	1:F:524:VAL:HG12	1.85	0.58
1:A:407:LEU:HD23	1:A:427:ASN:ND2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:LEU:HD12	1:A:638:LEU:HD23	1.85	0.58
1:B:34:VAL:HG12	1:B:87:TYR:HE1	1.67	0.58
1:B:154:LYS:O	1:B:154:LYS:HD3	2.02	0.58
1:B:220:GLY:H	1:B:224:ILE:HA	1.68	0.58
1:B:298:PRO:O	1:B:300:LEU:HD12	2.03	0.58
1:B:337:MSE:HG3	1:B:367:ASP:OD2	2.02	0.58
1:C:57:ILE:HG23	1:C:73:ILE:HD11	1.86	0.58
1:C:106:ILE:HG23	1:C:277:TYR:HB2	1.83	0.58
1:C:253:MSE:HG2	1:C:317:PHE:CE1	2.32	0.58
1:D:65:PRO:HG2	1:D:68:ALA:CB	2.33	0.58
1:D:247:GLN:HE22	1:D:637:LYS:HE3	1.68	0.58
1:D:370:VAL:HG22	1:D:382:ARG:HB2	1.85	0.58
1:D:331:ASN:HD22	1:D:337:MSE:CA	2.13	0.58
1:E:412:GLY:HA2	1:E:420:TYR:O	2.02	0.58
1:A:140:ILE:HB	1:A:152:THR:HG22	1.84	0.58
1:A:183:VAL:HG23	1:A:184:CYS:H	1.68	0.58
1:B:278:ARG:CG	1:B:280:PRO:HD3	2.33	0.58
1:C:500:LEU:HD13	1:C:736:PHE:CZ	2.38	0.58
1:D:216:VAL:HG23	1:D:354:TYR:O	2.03	0.58
1:E:264:ALA:HB2	1:E:286:LYS:HA	1.86	0.58
1:E:376:GLY:HA2	1:E:726:ARG:HH11	1.68	0.58
1:F:15:VAL:HG11	1:F:67:LEU:O	2.03	0.58
1:A:66:PRO:HG3	1:A:133:ASN:O	2.04	0.58
1:A:369:SER:N	1:A:385:ARG:HB2	2.19	0.58
1:A:543:LEU:H	1:A:543:LEU:HD23	1.67	0.58
1:B:329:SER:HB2	1:B:331:ASN:HD21	1.69	0.58
1:C:225:HIS:ND1	1:C:337:MSE:HE1	2.18	0.58
1:E:398:TYR:HB2	1:E:454:ASP:OD2	2.04	0.58
1:F:524:VAL:HG22	1:F:536:ALA:O	2.04	0.58
1:F:570:LEU:O	1:F:574:ILE:HG12	2.04	0.58
1:A:190:LEU:HD12	1:A:355:PHE:O	2.04	0.58
1:A:374:VAL:HG11	1:A:744:ARG:HH22	1.69	0.58
1:A:601:LYS:HB2	1:A:603:ILE:HG13	1.86	0.58
1:A:759:LEU:HD21	1:A:764:TYR:HB2	1.85	0.58
1:B:623:ASN:ND2	1:B:624:VAL:HG23	2.18	0.58
1:B:729:VAL:HG11	1:B:735:ASN:HB3	1.85	0.58
1:C:11:ILE:HG12	1:C:68:ALA:HA	1.86	0.58
1:E:490:HIS:HE1	1:E:746:ASP:HA	1.68	0.58
1:F:461:HIS:O	1:F:467:THR:HG21	2.02	0.58
1:F:580:LYS:HG3	1:F:593:ASN:ND2	2.17	0.58
1:F:583:GLU:HG3	1:F:592:PHE:CG	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:LEU:HD13	1:A:465:ASN:HB3	1.85	0.58
1:B:269:GLU:HB2	1:B:378:ARG:CZ	2.34	0.58
1:B:628:ARG:HD2	1:B:634:PRO:CD	2.34	0.58
1:C:216:VAL:HB	1:C:354:TYR:HB2	1.86	0.58
1:C:620:VAL:C	1:C:622:LEU:H	2.04	0.58
1:E:472:GLU:O	1:E:476:GLU:HG2	2.03	0.58
1:E:487:HIS:CD2	1:E:520:TRP:HB3	2.39	0.58
1:F:207:ALA:O	1:F:210:ILE:HG22	2.04	0.58
1:B:189:ARG:HB3	1:B:191:TYR:CE2	2.39	0.58
1:B:215:ILE:CD1	1:B:352:ALA:HA	2.33	0.58
1:B:554:LEU:O	1:B:558:MSE:HG3	2.03	0.58
1:D:225:HIS:HB2	1:D:328:THR:O	2.03	0.58
1:F:760:TYR:CE2	1:F:767:LYS:HG2	2.39	0.58
1:A:371:ILE:CB	1:A:380:VAL:HG13	2.33	0.58
1:A:461:HIS:HE1	1:A:463:ALA:HB3	1.67	0.58
1:C:218:ILE:O	1:C:224:ILE:HG13	2.04	0.58
1:C:264:ALA:HB1	1:C:285:ARG:O	2.03	0.58
1:D:572:GLY:HA2	1:D:575:ASN:ND2	2.19	0.58
1:E:19:PRO:O	1:E:23:ARG:HG3	2.03	0.58
1:E:401:LEU:HD12	1:E:402:ALA:H	1.69	0.58
1:F:281:ILE:HG12	1:F:306:MSE:CG	2.33	0.58
1:F:284:LEU:O	1:F:302:THR:HA	2.03	0.58
1:A:156:PHE:HZ	1:A:359:ASN:HB2	1.69	0.57
1:A:226:LEU:HD21	1:A:351:VAL:HG12	1.86	0.57
1:A:433:VAL:O	1:A:436:PHE:HB3	2.04	0.57
1:E:485:GLN:HG3	1:E:488:TYR:H	1.69	0.57
1:A:215:ILE:O	1:A:353:ASP:HB2	2.04	0.57
1:A:443:HIS:O	1:A:447:ILE:HD12	2.04	0.57
1:A:582:VAL:CG1	1:A:626:TYR:HB3	2.34	0.57
1:B:23:ARG:O	1:B:27:GLU:HB2	2.04	0.57
1:E:127:PRO:O	1:E:311:GLY:HA3	2.04	0.57
1:E:189:ARG:HD2	1:E:191:TYR:OH	2.04	0.57
1:E:265:TYR:O	1:E:284:LEU:HD13	2.04	0.57
1:F:620:VAL:C	1:F:622:LEU:H	2.06	0.57
1:B:19:PRO:O	1:B:23:ARG:HG3	2.04	0.57
1:B:283:THR:HA	1:B:303:ILE:O	2.04	0.57
1:C:373:PHE:CE1	1:C:378:ARG:HB3	2.39	0.57
1:C:455:LEU:HD21	1:C:760:TYR:HE1	1.69	0.57
1:C:590:VAL:N	1:F:475:ASN:HD21	2.02	0.57
1:E:700:ARG:HD2	1:E:704:PHE:HE2	1.68	0.57
1:F:239:LEU:O	1:F:243:THR:HG22	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:375:ASP:OD1	1:F:723:LYS:HE2	2.03	0.57
1:F:729:VAL:O	1:F:729:VAL:HG12	2.05	0.57
1:A:263:PHE:CZ	1:A:303:ILE:HG21	2.38	0.57
1:B:270:GLU:OE1	1:B:284:LEU:HD21	2.04	0.57
1:B:504:ILE:HB	1:B:709:VAL:HG12	1.84	0.57
1:B:516:ASP:HB2	1:B:518:ASN:ND2	2.19	0.57
1:B:557:LEU:O	1:B:557:LEU:HD23	2.03	0.57
1:B:579:PRO:HB3	1:B:626:TYR:CE1	2.39	0.57
1:D:560:ILE:HD12	1:D:561:LEU:N	2.18	0.57
1:E:264:ALA:CB	1:E:286:LYS:HA	2.35	0.57
1:E:394:ILE:HG22	1:E:396:PHE:H	1.69	0.57
1:E:616:ASP:HB3	1:E:634:PRO:HG3	1.86	0.57
1:F:171:ASN:ND2	1:F:173:ARG:HB2	2.20	0.57
1:F:278:ARG:HG3	1:F:280:PRO:HD3	1.86	0.57
1:F:708:ASN:N	1:F:708:ASN:ND2	2.51	0.57
1:A:183:VAL:CG2	1:A:184:CYS:H	2.17	0.57
1:A:580:LYS:NZ	1:A:590:VAL:HG22	2.20	0.57
1:B:151:THR:HG23	1:B:153:MSE:H	1.69	0.57
1:B:541:TYR:CG	1:B:560:ILE:HG22	2.39	0.57
1:B:572:GLY:HA2	1:B:575:ASN:HD22	1.69	0.57
1:C:183:VAL:HG23	1:C:184:CYS:N	2.19	0.57
1:C:273:GLU:HG3	1:C:273:GLU:O	2.04	0.57
1:D:197:GLU:O	1:D:198:ILE:HD13	2.05	0.57
1:E:653:VAL:HG13	1:E:692:ALA:HB3	1.86	0.57
1:A:193:SER:O	1:A:194:ASP:HB2	2.05	0.57
1:A:603:ILE:HG23	1:B:516:ASP:HA	1.87	0.57
1:B:37:LEU:O	1:B:37:LEU:HD13	2.04	0.57
1:B:457:ILE:HG22	1:B:458:ALA:N	2.20	0.57
1:C:88:ILE:HG22	1:C:89:GLU:N	2.19	0.57
1:C:171:ASN:ND2	1:C:173:ARG:H	2.02	0.57
1:C:203:LEU:HD21	1:C:315:ILE:HD13	1.87	0.57
1:C:690:ALA:CB	1:C:721:ILE:HG23	2.33	0.57
1:F:67:LEU:HD13	1:F:106:ILE:HD13	1.86	0.57
1:F:383:ARG:HD2	1:F:387:PHE:CD2	2.40	0.57
1:A:30:LEU:HD11	1:A:53:ILE:HA	1.86	0.57
1:A:217:ALA:O	1:A:218:ILE:HD13	2.03	0.57
1:A:401:LEU:HD12	1:A:402:ALA:H	1.70	0.57
1:B:282:ILE:HD12	1:B:371:ILE:CG2	2.35	0.57
1:D:21:VAL:HG11	1:D:34:VAL:HG21	1.87	0.57
1:E:760:TYR:CE2	1:E:767:LYS:HG2	2.40	0.57
1:A:219:LYS:HA	1:A:224:ILE:CG2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:SER:HB2	1:B:385:ARG:HB3	1.86	0.57
1:C:21:VAL:HG11	1:C:34:VAL:HG21	1.87	0.57
1:D:633:GLU:N	1:D:634:PRO:HD2	2.19	0.57
1:D:670:LEU:HA	1:D:673:ILE:HG12	1.86	0.57
1:D:700:ARG:HD2	1:D:704:PHE:HE2	1.70	0.57
1:E:52:ASP:O	1:E:56:PHE:HB2	2.04	0.57
1:F:215:ILE:HG22	1:F:228:CYS:CB	2.35	0.57
1:F:395:PRO:HG2	1:F:396:PHE:CE2	2.40	0.57
1:B:677:SER:HB2	1:B:678:PRO:HD2	1.86	0.57
1:C:21:VAL:HA	1:C:24:ILE:HG22	1.87	0.57
1:C:169:PRO:HA	1:C:174:TYR:CD2	2.40	0.57
1:C:201:ASP:N	1:C:202:PRO:CD	2.66	0.57
1:D:200:GLY:C	1:D:202:PRO:HD2	2.25	0.57
1:E:171:ASN:ND2	1:E:173:ARG:HB2	2.19	0.57
1:F:218:ILE:HD12	1:F:356:LEU:HD23	1.87	0.57
1:F:498:LYS:CB	1:F:500:LEU:HD23	2.35	0.57
1:A:202:PRO:O	1:A:203:LEU:C	2.43	0.57
1:A:384:SER:HA	1:A:388:VAL:HG23	1.86	0.57
1:B:35:LYS:HE2	1:B:90:LYS:HD2	1.87	0.57
1:B:268:PRO:C	1:B:270:GLU:H	2.09	0.57
1:B:497:GLU:OE2	1:B:741:GLU:HB3	2.05	0.57
1:B:759:LEU:CD1	1:B:764:TYR:HB2	2.35	0.57
1:C:504:ILE:HG22	1:C:505:GLY:N	2.19	0.57
1:E:288:GLU:CB	1:E:289:PRO:HD3	2.31	0.57
1:E:494:VAL:C	1:E:496:ALA:H	2.08	0.57
1:F:15:VAL:HG12	1:F:16:GLY:N	2.19	0.57
1:F:371:ILE:CD1	1:F:380:VAL:HG22	2.33	0.57
1:F:494:VAL:HG22	1:F:738:VAL:HG22	1.86	0.57
1:A:24:ILE:HG23	1:A:56:PHE:CE1	2.40	0.56
1:A:502:SER:O	1:A:503:VAL:HG13	2.05	0.56
1:B:19:PRO:HG3	1:B:174:TYR:HD1	1.69	0.56
1:B:127:PRO:HB3	1:B:312:THR:HG22	1.87	0.56
1:C:105:ASP:CG	1:C:139:THR:HG23	2.25	0.56
1:C:127:PRO:HB3	1:C:312:THR:CG2	2.28	0.56
1:D:111:ASP:HB3	1:D:172:ARG:NH1	2.14	0.56
1:D:760:TYR:HE2	1:D:767:LYS:HG2	1.70	0.56
1:E:189:ARG:HB3	1:E:191:TYR:CE2	2.40	0.56
1:E:457:ILE:HG22	1:E:458:ALA:H	1.70	0.56
1:A:102:ILE:CD1	1:A:144:LEU:HG	2.34	0.56
1:A:144:LEU:HD23	1:A:146:TYR:H	1.69	0.56
1:A:171:ASN:HD21	1:A:173:ARG:HB2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:GLU:HB2	1:A:378:ARG:CZ	2.35	0.56
1:A:335:MSE:CE	1:A:430:LYS:HG3	2.32	0.56
1:A:759:LEU:O	1:A:762:GLU:HB2	2.04	0.56
1:C:408:MSE:HG3	1:C:424:TYR:CE1	2.40	0.56
1:C:654:PRO:HG2	1:C:661:ARG:HB2	1.88	0.56
1:D:380:VAL:HG21	1:D:740:THR:HG23	1.87	0.56
1:D:495:MSE:HE2	1:D:755:PHE:HZ	1.68	0.56
1:E:122:LYS:HE3	1:E:161:PHE:CZ	2.39	0.56
1:E:331:ASN:ND2	1:E:337:MSE:HA	2.17	0.56
1:F:140:ILE:HB	1:F:152:THR:HG22	1.87	0.56
1:F:192:THR:C	1:F:194:ASP:H	2.08	0.56
1:F:301:HIS:CD2	1:F:302:THR:H	2.22	0.56
1:F:582:VAL:HG13	1:F:627:ARG:HG2	1.88	0.56
1:A:5:HIS:CE1	1:A:43:GLU:HG2	2.40	0.56
1:A:398:TYR:HB2	1:A:454:ASP:OD2	2.05	0.56
1:A:612:GLY:O	1:A:616:ASP:HB2	2.06	0.56
1:B:689:LEU:O	1:B:693:PHE:HB2	2.04	0.56
1:C:286:LYS:HE3	1:C:290:PHE:HA	1.88	0.56
1:D:567:ILE:HG12	1:D:600:ALA:HB1	1.85	0.56
1:D:665:LEU:O	1:D:669:ILE:HG13	2.05	0.56
1:E:306:MSE:HE1	1:E:309:TYR:HE2	1.70	0.56
1:E:408:MSE:HG3	1:E:424:TYR:HE1	1.69	0.56
1:E:737:HIS:O	1:E:738:VAL:C	2.44	0.56
1:F:381:ILE:HG22	1:F:717:TYR:CE1	2.40	0.56
1:F:488:TYR:O	1:F:492:ALA:HB2	2.04	0.56
1:A:136:PRO:HG3	1:A:360:ARG:NH1	2.21	0.56
1:B:296:LEU:HD12	1:B:296:LEU:H	1.70	0.56
1:B:398:TYR:HB2	1:B:454:ASP:CG	2.26	0.56
1:C:18:ARG:HH21	1:C:36:ASN:HD22	1.53	0.56
1:C:126:TYR:CD1	1:C:182:PRO:HG3	2.40	0.56
1:C:683:TYR:CZ	1:C:687:LEU:HD11	2.40	0.56
1:D:756:LEU:O	1:D:759:LEU:HB3	2.05	0.56
1:E:341:ASN:O	1:E:344:ALA:HB3	2.05	0.56
1:E:365:ARG:O	1:E:423:GLN:HG2	2.06	0.56
1:E:756:LEU:O	1:E:759:LEU:HB3	2.05	0.56
1:A:137:ARG:O	1:A:141:ILE:HG13	2.06	0.56
1:A:153:MSE:HE1	1:A:360:ARG:HD3	1.86	0.56
1:A:552:TYR:CZ	1:A:627:ARG:HD2	2.41	0.56
1:B:504:ILE:O	1:B:709:VAL:HA	2.06	0.56
1:C:137:ARG:O	1:C:141:ILE:HG13	2.05	0.56
1:D:616:ASP:O	1:D:620:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:ILE:HG12	1:E:353:ASP:OD2	2.04	0.56
1:E:224:ILE:CG1	1:E:338:VAL:HG13	2.36	0.56
1:E:379:ALA:HB3	1:E:744:ARG:NH1	2.20	0.56
1:E:633:GLU:N	1:E:634:PRO:CD	2.69	0.56
1:E:690:ALA:HB2	1:E:721:ILE:HG23	1.86	0.56
1:F:104:PRO:HD3	1:F:390:LEU:HD21	1.86	0.56
1:F:497:GLU:OE2	1:F:741:GLU:HB3	2.06	0.56
1:A:108:ILE:CG1	1:A:311:GLY:H	2.18	0.56
1:A:281:ILE:HG12	1:A:306:MSE:CG	2.32	0.56
1:A:522:GLY:HA3	1:A:611:THR:HG23	1.87	0.56
1:B:148:ARG:CZ	1:B:158:MSE:HG3	2.35	0.56
1:B:215:ILE:HG12	1:B:353:ASP:OD2	2.05	0.56
1:B:678:PRO:HG2	1:B:679:ALA:H	1.71	0.56
1:C:545:GLY:HA3	1:C:548:LEU:HD12	1.88	0.56
1:D:561:LEU:HB2	1:D:570:LEU:HD11	1.88	0.56
1:E:34:VAL:HB	1:E:87:TYR:OH	2.04	0.56
1:E:181:CYS:SG	1:E:182:PRO:N	2.79	0.56
1:F:461:HIS:CE1	1:F:463:ALA:HB3	2.40	0.56
1:F:653:VAL:HG13	1:F:692:ALA:CB	2.30	0.56
1:A:487:HIS:CE1	1:A:512:GLY:HA3	2.40	0.56
1:B:464:TYR:HB2	1:B:467:THR:HG23	1.86	0.56
1:C:310:ALA:O	1:C:313:HIS:HB2	2.06	0.56
1:C:629:HIS:HB2	1:C:633:GLU:OE1	2.06	0.56
1:D:330:ALA:O	1:D:338:VAL:HG12	2.05	0.56
1:D:339:LYS:HG3	1:D:365:ARG:NH1	2.21	0.56
1:D:401:LEU:HD12	1:D:402:ALA:H	1.71	0.56
1:F:500:LEU:HD13	1:F:503:VAL:HG11	1.87	0.56
1:A:236:VAL:CG1	1:A:295:ASN:HD22	2.18	0.56
1:A:540:TYR:HD1	1:A:540:TYR:H	1.53	0.56
1:B:261:LYS:HE2	1:B:266:VAL:HG21	1.88	0.56
1:B:498:LYS:HB2	1:B:500:LEU:HD23	1.88	0.56
1:B:655:VAL:HG22	1:B:660:ILE:HG23	1.88	0.56
1:C:457:ILE:CG2	1:C:753:GLN:HB3	2.34	0.56
1:D:228:CYS:SG	1:D:229:ASP:N	2.79	0.56
1:D:331:ASN:ND2	1:D:337:MSE:HA	2.13	0.56
1:E:558:MSE:HE1	1:E:593:ASN:OD1	2.06	0.56
1:F:344:ALA:HA	1:F:348:LEU:HD13	1.87	0.56
1:F:409:ASN:O	1:F:425:ILE:HG12	2.06	0.56
1:A:226:LEU:HD11	1:A:348:LEU:HD23	1.87	0.56
1:A:491:ILE:HG12	1:A:527:LEU:HD12	1.87	0.56
1:B:171:ASN:HD21	1:B:173:ARG:HB2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:ARG:HB2	1:B:629:HIS:CE1	2.41	0.56
1:C:286:LYS:HZ2	1:C:291:PRO:HD2	1.71	0.56
1:E:678:PRO:HG2	1:E:679:ALA:H	1.71	0.56
1:E:708:ASN:HB3	1:E:734:LEU:O	2.05	0.56
1:F:123:ARG:HH22	1:F:173:ARG:HG2	1.71	0.56
1:F:756:LEU:HD21	1:F:770:LEU:CD2	2.36	0.56
1:A:37:LEU:HB3	1:A:41:GLY:HA3	1.88	0.56
1:A:189:ARG:O	1:A:356:LEU:HD12	2.06	0.56
1:B:413:VAL:HG21	1:B:448:LEU:HD13	1.86	0.56
1:B:485:GLN:OE1	1:B:514:GLY:HA2	2.06	0.56
1:B:503:VAL:O	1:B:527:LEU:HD12	2.06	0.56
1:C:282:ILE:HG22	1:C:305:VAL:HB	1.88	0.56
1:C:379:ALA:HB3	1:C:744:ARG:NH1	2.21	0.56
1:C:524:VAL:HG23	1:C:535:LEU:HB2	1.88	0.56
1:C:650:LYS:HD2	1:C:691:ARG:NH2	2.21	0.56
1:D:504:ILE:HD12	1:D:701:ALA:HA	1.88	0.56
1:A:364:ASN:HD21	1:A:443:HIS:CD2	2.24	0.55
1:B:434:LEU:HD13	1:B:465:ASN:HB3	1.87	0.55
1:B:524:VAL:HG23	1:B:535:LEU:HB2	1.88	0.55
1:C:102:ILE:HD11	1:C:144:LEU:HG	1.88	0.55
1:C:219:LYS:NZ	1:C:362:ILE:HG12	2.20	0.55
1:C:269:GLU:O	1:C:272:GLU:HB3	2.06	0.55
1:C:516:ASP:HB2	1:C:518:ASN:ND2	2.21	0.55
1:C:582:VAL:HG11	1:C:626:TYR:O	2.05	0.55
1:D:312:THR:HA	1:D:315:ILE:HG22	1.89	0.55
1:E:700:ARG:HD2	1:E:704:PHE:CE2	2.41	0.55
1:A:247:GLN:NE2	1:A:637:LYS:HE3	2.20	0.55
1:A:371:ILE:CD1	1:A:380:VAL:HG22	2.35	0.55
1:A:456:ILE:CG2	1:A:457:ILE:H	2.16	0.55
1:C:225:HIS:NE2	1:C:327:MSE:HE3	2.21	0.55
1:C:525:LEU:HD23	1:C:534:ARG:HA	1.88	0.55
1:C:561:LEU:HB2	1:C:570:LEU:HD11	1.88	0.55
1:C:628:ARG:NH2	1:C:632:GLY:H	2.03	0.55
1:C:665:LEU:O	1:C:669:ILE:HG13	2.07	0.55
1:D:370:VAL:HG23	1:D:381:ILE:CG1	2.37	0.55
1:D:506:ILE:HB	1:D:711:LEU:HD12	1.87	0.55
1:E:380:VAL:HG12	1:E:382:ARG:H	1.71	0.55
1:E:401:LEU:O	1:E:456:ILE:HA	2.07	0.55
1:E:610:SER:O	1:E:614:VAL:HG23	2.07	0.55
1:F:53:ILE:HG23	1:F:54:GLU:HG3	1.89	0.55
1:A:190:LEU:HD13	1:A:356:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:LYS:HG2	1:B:593:ASN:HD22	1.71	0.55
1:B:587:TYR:HD1	1:B:588:GLY:N	2.00	0.55
1:C:339:LYS:HG3	1:C:365:ARG:HH12	1.70	0.55
1:C:522:GLY:CA	1:C:611:THR:HG23	2.36	0.55
1:C:554:LEU:HG	1:C:558:MSE:HE3	1.88	0.55
1:D:282:ILE:HA	1:D:371:ILE:O	2.06	0.55
1:D:624:VAL:HG12	1:D:637:LYS:HD3	1.87	0.55
1:E:338:VAL:HG21	1:E:344:ALA:HA	1.88	0.55
1:F:22:TYR:CE1	1:F:87:TYR:HB3	2.40	0.55
1:F:218:ILE:C	1:F:224:ILE:HG23	2.27	0.55
1:F:737:HIS:O	1:F:738:VAL:C	2.44	0.55
1:B:527:LEU:HD12	1:B:527:LEU:H	1.72	0.55
1:C:102:ILE:HG23	1:C:141:ILE:CD1	2.37	0.55
1:C:268:PRO:HG2	1:C:269:GLU:OE1	2.06	0.55
1:E:225:HIS:HA	1:E:330:ALA:CB	2.37	0.55
1:E:582:VAL:HG13	1:E:626:TYR:HB3	1.88	0.55
1:F:253:MSE:O	1:F:317:PHE:HZ	1.89	0.55
1:F:286:LYS:HB2	1:F:303:ILE:HD12	1.87	0.55
1:F:397:GLU:HB2	1:F:416:ASN:HA	1.88	0.55
1:C:219:LYS:HA	1:C:224:ILE:CB	2.35	0.55
1:C:601:LYS:HD3	1:F:772:LEU:HD11	1.87	0.55
1:E:196:GLN:HG2	1:E:197:GLU:O	2.07	0.55
1:F:8:VAL:HG12	1:F:12:VAL:HG11	1.88	0.55
1:F:580:LYS:HZ1	1:F:590:VAL:HG22	1.71	0.55
1:A:498:LYS:HE3	1:A:736:PHE:HB2	1.89	0.55
1:B:3:ALA:HB2	1:B:47:GLU:HA	1.89	0.55
1:B:123:ARG:HH22	1:B:173:ARG:HG2	1.72	0.55
1:B:294:GLU:HG2	1:B:294:GLU:O	2.07	0.55
1:C:196:GLN:HG2	1:C:197:GLU:O	2.07	0.55
1:D:24:ILE:HG12	1:D:56:PHE:HD1	1.72	0.55
1:D:125:MSE:O	1:D:127:PRO:HD3	2.06	0.55
1:D:457:ILE:HG21	1:D:753:GLN:HB3	1.89	0.55
1:D:522:GLY:HA2	1:D:611:THR:HG23	1.88	0.55
1:F:14:ALA:HB3	1:F:103:PRO:CD	2.36	0.55
1:F:406:GLU:HG3	1:F:407:LEU:HG	1.89	0.55
1:A:216:VAL:HG23	1:A:354:TYR:C	2.27	0.55
1:A:572:GLY:O	1:A:575:ASN:HB2	2.07	0.55
1:A:580:LYS:HZ2	1:A:590:VAL:HG13	1.71	0.55
1:B:142:GLU:O	1:B:143:ASP:HB3	2.07	0.55
1:B:491:ILE:CG2	1:B:527:LEU:HD11	2.36	0.55
1:C:123:ARG:NH2	1:C:173:ARG:HE	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:PHE:CD1	1:E:186:PRO:HG2	2.41	0.55
1:E:330:ALA:O	1:E:338:VAL:HG12	2.07	0.55
1:E:515:THR:O	1:E:516:ASP:HB2	2.05	0.55
1:F:193:SER:O	1:F:194:ASP:CB	2.54	0.55
1:F:399:ASN:HA	1:F:414:ALA:O	2.06	0.55
1:F:665:LEU:HG	1:F:669:ILE:HD11	1.88	0.55
1:A:193:SER:O	1:A:194:ASP:CB	2.54	0.55
1:A:408:MSE:HG3	1:A:424:TYR:CE1	2.41	0.55
1:A:522:GLY:CA	1:A:611:THR:HG23	2.37	0.55
1:A:727:LYS:HZ1	1:C:287:LYS:HE3	1.71	0.55
1:A:742:VAL:HG11	1:A:751:VAL:HG11	1.88	0.55
1:B:11:ILE:HG23	1:B:11:ILE:O	2.07	0.55
1:B:664:GLU:O	1:B:667:GLN:HB3	2.07	0.55
1:B:738:VAL:HB	1:B:744:ARG:HG3	1.87	0.55
1:B:749:VAL:O	1:B:753:GLN:HG3	2.06	0.55
1:C:15:VAL:HG21	1:C:67:LEU:O	2.06	0.55
1:C:249:PRO:HG3	1:C:300:LEU:CD1	2.37	0.55
1:C:670:LEU:HA	1:C:673:ILE:HG12	1.89	0.55
1:D:57:ILE:HG13	1:D:75:LYS:NZ	2.22	0.55
1:E:508:LEU:CD2	1:E:611:THR:HG21	2.37	0.55
1:E:562:SER:HB3	1:E:599:LEU:HD11	1.88	0.55
1:E:582:VAL:HG11	1:E:626:TYR:O	2.06	0.55
1:E:649:LEU:HB3	1:E:684:SER:CB	2.36	0.55
1:F:494:VAL:HG11	1:F:710:ALA:HB1	1.88	0.55
1:F:501:ASP:O	1:F:503:VAL:HG13	2.07	0.55
1:B:252:ILE:HG23	1:B:325:TYR:O	2.07	0.55
1:B:707:LYS:HG3	1:B:708:ASN:ND2	2.22	0.55
1:C:500:LEU:HD13	1:C:736:PHE:CE2	2.42	0.55
1:D:401:LEU:HD12	1:D:402:ALA:N	2.22	0.55
1:E:147:ASP:HA	1:E:177:GLU:OE2	2.07	0.55
1:A:651:PHE:HB2	1:A:688:ALA:CB	2.36	0.55
1:B:53:ILE:O	1:B:57:ILE:HG12	2.07	0.55
1:B:224:ILE:HG12	1:B:338:VAL:O	2.06	0.55
1:B:398:TYR:HB2	1:B:454:ASP:OD2	2.07	0.55
1:B:525:LEU:HA	1:B:535:LEU:HD13	1.88	0.55
1:C:67:LEU:HD11	1:C:106:ILE:HD11	1.89	0.55
1:C:142:GLU:HB2	1:C:150:ASN:O	2.07	0.55
1:C:315:ILE:HG23	1:C:316:LEU:N	2.22	0.55
1:C:369:SER:HB2	1:C:385:ARG:HB3	1.88	0.55
1:D:119:PRO:HA	1:D:124:TYR:CD2	2.42	0.55
1:D:737:HIS:O	1:D:738:VAL:C	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:538:ILE:HD11	1:E:611:THR:HG22	1.89	0.55
1:F:20:PHE:HE1	1:F:60:LEU:HA	1.73	0.55
1:F:503:VAL:HG11	1:F:708:ASN:OD1	2.07	0.55
1:F:545:GLY:HA3	1:F:548:LEU:HD12	1.89	0.55
1:A:245:ARG:NE	1:A:248:LYS:HB3	2.22	0.54
1:A:282:ILE:HA	1:A:371:ILE:O	2.07	0.54
1:A:724:MSE:O	1:A:728:VAL:HG23	2.07	0.54
1:B:583:GLU:OE1	1:B:583:GLU:N	2.40	0.54
1:C:114:ARG:O	1:C:118:ASP:HB2	2.07	0.54
1:E:155:GLU:O	1:E:157:PRO:HD3	2.07	0.54
1:F:237:ALA:HA	1:F:295:ASN:ND2	2.21	0.54
1:F:239:LEU:HD22	1:F:250:PHE:CZ	2.42	0.54
1:A:247:GLN:HE21	1:A:298:PRO:HG2	1.72	0.54
1:B:35:LYS:HG2	1:B:36:ASN:N	2.22	0.54
1:B:124:TYR:CE2	1:B:125:MSE:HG2	2.42	0.54
1:B:213:GLY:CA	1:B:235:VAL:HG11	2.36	0.54
1:B:528:GLY:O	1:B:529:TYR:C	2.45	0.54
1:C:102:ILE:HD12	1:C:141:ILE:HG21	1.89	0.54
1:D:140:ILE:HB	1:D:152:THR:CG2	2.38	0.54
1:E:616:ASP:HA	1:E:634:PRO:HB2	1.90	0.54
1:F:261:LYS:HZ3	1:F:266:VAL:HB	1.68	0.54
1:F:265:TYR:CD2	1:F:265:TYR:N	2.75	0.54
1:F:320:SER:O	1:F:321:LYS:C	2.46	0.54
1:A:494:VAL:HG11	1:A:710:ALA:HB1	1.89	0.54
1:C:586:LYS:CB	1:C:627:ARG:HH12	2.20	0.54
1:D:315:ILE:HG12	1:D:319:TRP:CZ3	2.40	0.54
1:D:593:ASN:O	1:D:596:LEU:HB2	2.08	0.54
1:D:601:LYS:CB	1:D:603:ILE:HG13	2.38	0.54
1:E:565:TYR:HB3	1:E:569:GLU:HB2	1.90	0.54
1:F:190:LEU:HD21	1:F:206:ALA:CB	2.32	0.54
1:F:506:ILE:HD11	1:F:697:ALA:HB2	1.88	0.54
1:A:61:TYR:CZ	1:A:73:ILE:HD12	2.42	0.54
1:A:558:MSE:HB3	1:A:570:LEU:HD21	1.89	0.54
1:A:649:LEU:HB3	1:A:684:SER:CB	2.37	0.54
1:C:227:ALA:HA	1:C:326:VAL:O	2.07	0.54
1:C:553:PRO:HB2	1:C:620:VAL:HG21	1.87	0.54
1:D:383:ARG:HH11	1:D:383:ARG:HG3	1.71	0.54
1:D:655:VAL:HG22	1:D:660:ILE:HG12	1.89	0.54
1:F:114:ARG:HG2	1:F:118:ASP:OD2	2.06	0.54
1:F:232:ASN:HB3	1:F:235:VAL:HG22	1.88	0.54
1:A:35:LYS:HG2	1:A:36:ASN:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:PHE:CE2	1:A:323:PRO:HA	2.42	0.54
1:A:385:ARG:HG3	1:A:386:GLY:N	2.22	0.54
1:B:484:VAL:HG12	1:B:770:LEU:HD13	1.89	0.54
1:C:19:PRO:O	1:C:23:ARG:HG3	2.08	0.54
1:C:370:VAL:HG23	1:C:381:ILE:HD11	1.88	0.54
1:D:140:ILE:HB	1:D:152:THR:HG22	1.89	0.54
1:D:628:ARG:CZ	1:D:632:GLY:H	2.20	0.54
1:D:711:LEU:HD23	1:D:737:HIS:NE2	2.22	0.54
1:E:273:GLU:HG2	1:E:371:ILE:HD13	1.88	0.54
1:E:434:LEU:HD13	1:E:465:ASN:HB3	1.90	0.54
1:F:215:ILE:HG21	1:F:239:LEU:HD12	1.90	0.54
1:F:341:ASN:ND2	1:F:357:LEU:HB3	2.22	0.54
1:F:391:PRO:HB3	1:F:420:TYR:CE1	2.42	0.54
1:F:729:VAL:HB	1:F:735:ASN:ND2	2.23	0.54
1:B:374:VAL:HG11	1:B:744:ARG:NH2	2.22	0.54
1:B:406:GLU:O	1:B:428:THR:HG23	2.07	0.54
1:C:738:VAL:CG2	1:C:744:ARG:HB3	2.37	0.54
1:D:484:VAL:HG12	1:D:770:LEU:HD22	1.90	0.54
1:E:50:GLU:O	1:E:53:ILE:HG22	2.08	0.54
1:E:580:LYS:HG3	1:E:593:ASN:ND2	2.20	0.54
1:F:369:SER:HB2	1:F:385:ARG:CB	2.37	0.54
1:F:651:PHE:HB2	1:F:688:ALA:HB2	1.89	0.54
1:F:739:THR:HG23	1:F:741:GLU:H	1.71	0.54
1:A:8:VAL:HA	1:A:72:ARG:O	2.08	0.54
1:A:370:VAL:HG23	1:A:381:ILE:HD11	1.88	0.54
1:B:465:ASN:O	1:B:468:LYS:HB3	2.08	0.54
1:B:682:ALA:O	1:B:686:HIS:HB2	2.07	0.54
1:D:553:PRO:HB2	1:D:620:VAL:CG2	2.38	0.54
1:E:339:LYS:HA	1:E:362:ILE:HD11	1.90	0.54
1:E:504:ILE:O	1:E:709:VAL:HA	2.06	0.54
1:F:495:MSE:HE2	1:F:755:PHE:CZ	2.42	0.54
1:A:282:ILE:HD12	1:A:371:ILE:HG23	1.89	0.54
1:B:183:VAL:HG23	1:B:184:CYS:N	2.23	0.54
1:C:215:ILE:HD11	1:C:352:ALA:HA	1.89	0.54
1:F:554:LEU:HD11	1:F:579:PRO:CB	2.36	0.54
1:B:1:MSE:HE3	1:B:2:LYS:N	2.23	0.54
1:B:403:VAL:HG11	1:B:466:THR:HB	1.90	0.54
1:C:66:PRO:CD	1:C:133:ASN:HB3	2.37	0.54
1:D:371:ILE:HB	1:D:380:VAL:HG13	1.90	0.54
1:D:522:GLY:CA	1:D:611:THR:HG23	2.38	0.54
1:D:564:VAL:HG11	1:D:667:GLN:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:312:THR:O	1:E:315:ILE:HG22	2.08	0.54
1:F:21:VAL:HG12	1:F:87:TYR:OH	2.08	0.54
1:F:103:PRO:HG2	1:F:137:ARG:HD2	1.89	0.54
1:A:219:LYS:HG2	1:A:358:HIS:CE1	2.42	0.54
1:A:395:PRO:HG2	1:A:396:PHE:CE2	2.44	0.54
1:B:553:PRO:HB2	1:B:620:VAL:HG21	1.90	0.54
1:C:215:ILE:HG12	1:C:353:ASP:OD2	2.07	0.54
1:D:103:PRO:HG2	1:D:137:ARG:HD2	1.90	0.54
1:F:225:HIS:HA	1:F:330:ALA:CB	2.33	0.54
1:F:422:SER:HA	1:F:444:PHE:CZ	2.43	0.54
1:A:197:GLU:HG2	1:A:201:ASP:OD2	2.08	0.53
1:B:520:TRP:HA	1:B:609:SER:OG	2.08	0.53
1:B:596:LEU:HD23	1:B:596:LEU:O	2.08	0.53
1:B:729:VAL:HB	1:B:735:ASN:ND2	2.23	0.53
1:C:570:LEU:HD12	1:C:573:VAL:CG1	2.38	0.53
1:D:126:TYR:OH	1:D:185:GLY:HA3	2.08	0.53
1:D:252:ILE:HD12	1:D:252:ILE:N	2.23	0.53
1:D:488:TYR:O	1:D:756:LEU:HD11	2.08	0.53
1:E:252:ILE:N	1:E:252:ILE:HD12	2.23	0.53
1:F:12:VAL:HG23	1:F:17:PHE:CD2	2.44	0.53
1:B:267:SER:O	1:B:270:GLU:HB3	2.07	0.53
1:C:18:ARG:NH2	1:C:36:ASN:HD22	2.06	0.53
1:C:152:THR:HG21	1:C:360:ARG:HG3	1.90	0.53
1:C:264:ALA:CB	1:C:286:LYS:HA	2.38	0.53
1:C:404:GLY:HA2	1:C:753:GLN:HE22	1.70	0.53
1:C:504:ILE:HG23	1:C:525:LEU:O	2.08	0.53
1:D:565:TYR:HB3	1:D:569:GLU:HB3	1.90	0.53
1:E:267:SER:HB2	1:E:270:GLU:CB	2.39	0.53
1:A:410:ALA:HB3	1:A:747:ASN:O	2.07	0.53
1:B:286:LYS:HE3	1:B:290:PHE:HB2	1.91	0.53
1:B:485:GLN:HB3	1:B:488:TYR:HB2	1.91	0.53
1:B:662:VAL:O	1:B:665:LEU:HB3	2.08	0.53
1:D:381:ILE:HG13	1:D:382:ARG:N	2.24	0.53
1:E:205:LYS:O	1:E:209:LEU:HD13	2.08	0.53
1:F:497:GLU:OE2	1:F:739:THR:HG22	2.08	0.53
1:A:374:VAL:CG2	1:A:744:ARG:HH12	2.22	0.53
1:B:115:GLU:HG2	1:B:121:ASN:ND2	2.24	0.53
1:B:330:ALA:O	1:B:338:VAL:HG12	2.08	0.53
1:B:461:HIS:CE1	1:B:463:ALA:HB3	2.43	0.53
1:B:620:VAL:HG22	1:B:625:ALA:O	2.09	0.53
1:C:380:VAL:HG12	1:C:381:ILE:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:587:TYR:CZ	1:F:468:LYS:HG3	2.43	0.53
1:D:196:GLN:HG2	1:D:197:GLU:N	2.23	0.53
1:D:261:LYS:HZ3	1:D:266:VAL:HB	1.73	0.53
1:D:288:GLU:HB3	1:D:289:PRO:CD	2.30	0.53
1:D:524:VAL:CG2	1:D:536:ALA:H	2.22	0.53
1:D:653:VAL:HG11	1:D:689:LEU:HA	1.90	0.53
1:E:581:ALA:HA	1:E:584:SER:HB3	1.90	0.53
1:E:613:ARG:HA	1:E:616:ASP:OD1	2.09	0.53
1:F:724:MSE:O	1:F:728:VAL:HG23	2.08	0.53
1:F:760:TYR:HA	1:F:765:LEU:HB3	1.89	0.53
1:B:292:LEU:HD11	1:B:324:VAL:HG21	1.89	0.53
1:B:331:ASN:ND2	1:B:337:MSE:HA	2.18	0.53
1:B:456:ILE:CG2	1:B:457:ILE:H	2.09	0.53
1:D:110:ASP:O	1:D:113:LEU:HB3	2.09	0.53
1:D:549:ALA:HA	1:D:555:ARG:HB2	1.89	0.53
1:F:19:PRO:HG3	1:F:174:TYR:O	2.09	0.53
1:F:487:HIS:O	1:F:491:ILE:HG12	2.08	0.53
1:F:560:ILE:HD12	1:F:561:LEU:N	2.24	0.53
1:F:580:LYS:NZ	1:F:590:VAL:HG22	2.23	0.53
1:F:708:ASN:HB3	1:F:734:LEU:O	2.08	0.53
1:A:267:SER:HB3	1:A:268:PRO:HD2	1.90	0.53
1:B:756:LEU:O	1:B:759:LEU:HB3	2.08	0.53
1:C:258:GLU:O	1:C:261:LYS:HG2	2.09	0.53
1:C:468:LYS:HG3	1:F:587:TYR:OH	2.08	0.53
1:D:104:PRO:HB3	1:D:387:PHE:O	2.09	0.53
1:D:190:LEU:HD13	1:D:356:LEU:HD13	1.90	0.53
1:D:247:GLN:NE2	1:D:637:LYS:HE3	2.23	0.53
1:D:320:SER:O	1:D:321:LYS:C	2.47	0.53
1:E:126:TYR:CD1	1:E:182:PRO:HG3	2.43	0.53
1:E:387:PHE:O	1:E:390:LEU:HG	2.08	0.53
1:E:613:ARG:HA	1:E:613:ARG:NE	2.22	0.53
1:F:33:TYR:OH	1:F:90:LYS:HE3	2.09	0.53
1:F:219:LYS:HG3	1:F:224:ILE:HG12	1.89	0.53
1:A:15:VAL:HG12	1:A:16:GLY:N	2.21	0.53
1:A:158:MSE:HE3	1:A:163:ARG:NH1	2.24	0.53
1:A:330:ALA:HB1	1:A:348:LEU:HD21	1.91	0.53
1:B:278:ARG:HG2	1:B:280:PRO:HD3	1.91	0.53
1:C:12:VAL:HG23	1:C:17:PHE:CG	2.42	0.53
1:C:380:VAL:HG12	1:C:381:ILE:N	2.24	0.53
1:D:274:LEU:HB3	1:D:307:LEU:HD11	1.90	0.53
1:D:329:SER:HA	1:D:337:MSE:HE2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:LYS:HA	1:D:362:ILE:HD11	1.90	0.53
1:A:415:LYS:C	1:A:417:GLY:H	2.11	0.53
1:A:468:LYS:HG3	1:B:587:TYR:OH	2.09	0.53
1:B:264:ALA:HB1	1:B:285:ARG:O	2.09	0.53
1:B:487:HIS:CD2	1:B:520:TRP:HB3	2.44	0.53
1:C:283:THR:HA	1:C:303:ILE:O	2.08	0.53
1:C:404:GLY:HA2	1:C:753:GLN:CD	2.29	0.53
1:D:380:VAL:HG12	1:D:381:ILE:N	2.24	0.53
1:D:482:LEU:HD12	1:D:483:GLN:N	2.23	0.53
1:D:580:LYS:HG3	1:D:593:ASN:ND2	2.23	0.53
1:D:601:LYS:NZ	1:E:771:MSE:HE3	2.24	0.53
1:E:170:LEU:HD12	1:E:170:LEU:H	1.74	0.53
1:E:216:VAL:HB	1:E:354:TYR:HB2	1.90	0.53
1:F:579:PRO:HB3	1:F:626:TYR:CE1	2.43	0.53
1:A:190:LEU:HB2	1:A:202:PRO:HB3	1.90	0.53
1:A:438:ARG:HG2	1:A:438:ARG:HH11	1.74	0.53
1:A:543:LEU:HD12	1:A:549:ALA:CB	2.38	0.53
1:A:633:GLU:H	1:A:634:PRO:HD2	1.73	0.53
1:B:491:ILE:HD11	1:B:507:ALA:HB2	1.91	0.53
1:C:264:ALA:HB3	1:C:284:LEU:HD13	1.91	0.53
1:C:402:ALA:HB2	1:C:457:ILE:HB	1.89	0.53
1:C:495:MSE:HE2	1:C:755:PHE:CZ	2.44	0.53
1:D:485:GLN:OE1	1:D:514:GLY:HA2	2.09	0.53
1:D:494:VAL:HG13	1:D:738:VAL:H	1.73	0.53
1:E:373:PHE:CE1	1:E:378:ARG:HB3	2.44	0.53
1:E:545:GLY:HA3	1:E:548:LEU:HB2	1.89	0.53
1:E:661:ARG:HG3	1:E:663:GLU:OE2	2.08	0.53
1:F:489:ALA:O	1:F:752:GLY:HA3	2.09	0.53
1:A:156:PHE:CZ	1:A:186:PRO:HB3	2.44	0.53
1:B:534:ARG:HG2	1:B:535:LEU:H	1.72	0.53
1:C:15:VAL:HG12	1:C:16:GLY:H	1.74	0.53
1:C:239:LEU:HD22	1:C:250:PHE:HE1	1.74	0.53
1:D:193:SER:O	1:D:194:ASP:CB	2.57	0.53
1:D:554:LEU:HD12	1:D:583:GLU:OE1	2.09	0.53
1:D:579:PRO:O	1:D:582:VAL:HG23	2.09	0.53
1:E:526:TYR:O	1:E:532:VAL:HG13	2.08	0.53
1:E:572:GLY:O	1:E:575:ASN:HB2	2.09	0.53
1:F:39:ASP:H	1:F:144:LEU:HD13	1.74	0.53
1:F:329:SER:HB2	1:F:331:ASN:ND2	2.24	0.53
1:F:759:LEU:HD11	1:F:764:TYR:HB2	1.90	0.53
1:A:49:ARG:H	1:A:49:ARG:HD2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:THR:O	1:A:316:LEU:HB2	2.09	0.52
1:A:687:LEU:HB3	1:A:724:MSE:HE3	1.90	0.52
1:B:201:ASP:N	1:B:202:PRO:CD	2.71	0.52
1:C:264:ALA:HB2	1:C:286:LYS:HA	1.90	0.52
1:C:593:ASN:O	1:C:596:LEU:HB2	2.09	0.52
1:C:651:PHE:HB2	1:C:688:ALA:CB	2.39	0.52
1:D:619:ALA:HB2	1:D:638:LEU:HB2	1.91	0.52
1:E:191:TYR:HB2	1:E:355:PHE:CB	2.31	0.52
1:E:200:GLY:C	1:E:202:PRO:HD2	2.28	0.52
1:E:522:GLY:HA3	1:E:538:ILE:HD12	1.90	0.52
1:A:270:GLU:N	1:A:378:ARG:NH1	2.57	0.52
1:B:522:GLY:H	1:B:523:GLU:CD	2.12	0.52
1:C:30:LEU:CD1	1:C:52:ASP:HB2	2.37	0.52
1:C:379:ALA:HB3	1:C:744:ARG:CZ	2.39	0.52
1:C:428:THR:HG21	1:C:466:THR:HG22	1.92	0.52
1:C:461:HIS:HE1	1:C:463:ALA:HB3	1.72	0.52
1:D:509:ASP:CG	1:D:510:GLY:H	2.12	0.52
1:D:603:ILE:HG23	1:E:516:ASP:HA	1.91	0.52
1:E:617:ALA:O	1:E:621:LEU:HB2	2.09	0.52
1:F:57:ILE:HG13	1:F:75:LYS:HZ1	1.73	0.52
1:F:205:LYS:O	1:F:209:LEU:HD13	2.08	0.52
1:F:544:PRO:HG2	1:F:555:ARG:HE	1.75	0.52
1:F:738:VAL:HB	1:F:744:ARG:HG2	1.91	0.52
1:A:266:VAL:HA	1:A:270:GLU:OE2	2.09	0.52
1:A:267:SER:O	1:A:270:GLU:HB3	2.10	0.52
1:A:695:HIS:O	1:A:698:VAL:HB	2.09	0.52
1:B:565:TYR:HB3	1:B:569:GLU:HB3	1.92	0.52
1:C:402:ALA:CB	1:C:457:ILE:HB	2.39	0.52
1:D:183:VAL:HG23	1:D:184:CYS:N	2.24	0.52
1:D:199:TYR:CG	1:D:200:GLY:N	2.77	0.52
1:F:148:ARG:CZ	1:F:158:MSE:HG3	2.39	0.52
1:F:192:THR:C	1:F:194:ASP:N	2.60	0.52
1:F:447:ILE:O	1:F:447:ILE:HG22	2.08	0.52
1:F:503:VAL:HA	1:F:706:VAL:HG11	1.91	0.52
1:A:414:ALA:HA	1:A:418:LYS:O	2.10	0.52
1:B:381:ILE:HG13	1:B:382:ARG:N	2.23	0.52
1:B:524:VAL:CG2	1:B:536:ALA:H	2.23	0.52
1:D:201:ASP:N	1:D:202:PRO:CD	2.72	0.52
1:D:504:ILE:CG2	1:D:505:GLY:N	2.72	0.52
1:E:391:PRO:HB3	1:E:420:TYR:CE1	2.45	0.52
1:F:459:ASP:OD2	1:F:486:HIS:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:641:PHE:CZ	1:F:678:PRO:HB2	2.44	0.52
1:B:453:LEU:HG	1:B:453:LEU:O	2.09	0.52
1:B:470:ALA:HB1	1:B:481:LEU:HD11	1.91	0.52
1:B:504:ILE:CG2	1:B:505:GLY:N	2.72	0.52
1:B:656:GLU:HG3	1:B:661:ARG:NH1	2.25	0.52
1:C:286:LYS:NZ	1:C:291:PRO:HD2	2.25	0.52
1:D:21:VAL:HA	1:D:24:ILE:HG22	1.91	0.52
1:D:218:ILE:O	1:D:224:ILE:HB	2.09	0.52
1:D:404:GLY:HA2	1:D:753:GLN:NE2	2.24	0.52
1:D:487:HIS:CD2	1:D:520:TRP:HB3	2.43	0.52
1:D:621:LEU:HD22	1:D:666:PHE:HD1	1.75	0.52
1:E:16:GLY:HA2	1:E:132:THR:OG1	2.08	0.52
1:E:37:LEU:O	1:E:37:LEU:HD13	2.10	0.52
1:E:102:ILE:HG12	1:E:144:LEU:HD11	1.90	0.52
1:E:202:PRO:O	1:E:203:LEU:C	2.46	0.52
1:F:401:LEU:O	1:F:456:ILE:HA	2.08	0.52
1:A:374:VAL:CG1	1:A:744:ARG:HH12	2.23	0.52
1:B:371:ILE:HG13	1:B:380:VAL:HA	1.90	0.52
1:B:385:ARG:HG3	1:B:386:GLY:H	1.75	0.52
1:D:274:LEU:HB3	1:D:307:LEU:CD1	2.40	0.52
1:D:541:TYR:CG	1:D:560:ILE:HG22	2.44	0.52
1:D:543:LEU:HD12	1:D:549:ALA:CB	2.39	0.52
1:E:412:GLY:HA3	1:E:750:ASN:ND2	2.21	0.52
1:E:560:ILE:HD12	1:E:561:LEU:N	2.24	0.52
1:F:176:ALA:O	1:F:179:THR:HG22	2.10	0.52
1:F:219:LYS:HE3	1:F:358:HIS:CE1	2.45	0.52
1:B:628:ARG:NH2	1:B:632:GLY:H	2.07	0.52
1:C:166:TYR:CE1	1:C:175:HIS:HA	2.44	0.52
1:C:579:PRO:HB3	1:C:626:TYR:CE1	2.44	0.52
1:D:78:ILE:O	1:D:80:PRO:HD3	2.09	0.52
1:D:385:ARG:HG3	1:D:386:GLY:H	1.75	0.52
1:E:110:ASP:O	1:E:113:LEU:HB3	2.09	0.52
1:E:364:ASN:HD21	1:E:443:HIS:CD2	2.27	0.52
1:F:300:LEU:HA	1:F:640:SER:OG	2.10	0.52
1:F:485:GLN:NE2	1:F:487:HIS:H	1.86	0.52
1:A:105:ASP:CG	1:A:139:THR:HG23	2.30	0.52
1:A:123:ARG:NE	1:A:173:ARG:NH2	2.58	0.52
1:A:383:ARG:H	1:A:747:ASN:ND2	2.08	0.52
1:A:690:ALA:HB2	1:A:721:ILE:HG23	1.91	0.52
1:B:412:GLY:HA3	1:B:750:ASN:ND2	2.18	0.52
1:B:594:VAL:O	1:B:594:VAL:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:ALA:HB1	1:C:320:SER:CB	2.34	0.52
1:C:269:GLU:HB2	1:C:378:ARG:NH1	2.24	0.52
1:C:409:ASN:HD22	1:C:425:ILE:CD1	2.20	0.52
1:E:279:ARG:HD3	1:E:307:LEU:HB2	1.91	0.52
1:F:369:SER:HB2	1:F:385:ARG:HB3	1.91	0.52
1:F:402:ALA:HB2	1:F:457:ILE:HD12	1.92	0.52
1:F:429:GLY:HA2	1:F:465:ASN:HD22	1.75	0.52
1:F:541:TYR:CE1	1:F:609:SER:HA	2.45	0.52
1:A:169:PRO:HA	1:A:174:TYR:CD2	2.45	0.52
1:A:447:ILE:O	1:A:447:ILE:HG22	2.10	0.52
1:B:32:GLY:H	1:B:87:TYR:HD2	1.57	0.52
1:C:215:ILE:O	1:C:353:ASP:HB2	2.10	0.52
1:C:489:ALA:HA	1:C:756:LEU:HD12	1.91	0.52
1:C:666:PHE:HA	1:C:669:ILE:HD12	1.92	0.52
1:D:451:LYS:HD3	1:D:477:LEU:HG	1.92	0.52
1:E:249:PRO:HG3	1:E:300:LEU:CD1	2.37	0.52
1:F:694:ALA:C	1:F:696:THR:H	2.13	0.52
1:A:199:TYR:CD1	1:A:200:GLY:N	2.76	0.52
1:A:254:ALA:HB1	1:A:259:THR:HB	1.92	0.52
1:A:376:GLY:C	1:A:377:LYS:HG2	2.30	0.52
1:A:738:VAL:HG12	1:A:742:VAL:O	2.10	0.52
1:B:729:VAL:O	1:B:729:VAL:HG12	2.10	0.52
1:C:32:GLY:O	1:C:87:TYR:HA	2.09	0.52
1:C:288:GLU:HB2	1:C:289:PRO:CD	2.32	0.52
1:D:226:LEU:HD21	1:D:351:VAL:HG12	1.91	0.52
1:D:403:VAL:HG11	1:D:466:THR:HB	1.92	0.52
1:D:691:ARG:HG2	1:D:695:HIS:CD2	2.45	0.52
1:E:183:VAL:CG2	1:E:184:CYS:N	2.73	0.52
1:E:247:GLN:HG3	1:E:298:PRO:CG	2.40	0.52
1:E:269:GLU:HB2	1:E:378:ARG:CZ	2.40	0.52
1:F:332:TYR:HB3	1:F:333:PRO:HD2	1.91	0.52
1:A:284:LEU:HD12	1:A:284:LEU:O	2.10	0.51
1:A:348:LEU:HD12	1:A:348:LEU:N	2.24	0.51
1:A:714:GLY:O	1:A:716:ALA:N	2.43	0.51
1:B:42:VAL:HG13	1:B:42:VAL:O	2.10	0.51
1:B:229:ASP:OD1	1:B:322:THR:HG21	2.10	0.51
1:B:403:VAL:CG1	1:B:466:THR:HB	2.40	0.51
1:B:438:ARG:HG2	1:B:438:ARG:HH11	1.75	0.51
1:B:677:SER:O	1:B:681:ILE:HG12	2.09	0.51
1:C:105:ASP:OD1	1:C:139:THR:HG23	2.10	0.51
1:C:370:VAL:CG2	1:C:381:ILE:HD11	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:PHE:CE2	1:C:759:LEU:HB2	2.44	0.51
1:C:521:GLY:CA	1:C:610:SER:HA	2.39	0.51
1:C:751:VAL:HG13	1:C:752:GLY:N	2.25	0.51
1:D:18:ARG:HB2	1:D:19:PRO:HD3	1.91	0.51
1:E:105:ASP:OD2	1:E:138:PHE:HB3	2.10	0.51
1:E:306:MSE:HE1	1:E:368:ASP:OD2	2.10	0.51
1:E:375:ASP:OD2	1:E:723:LYS:HA	2.10	0.51
1:A:383:ARG:NH2	1:A:392:ILE:HD11	2.24	0.51
1:B:15:VAL:CG1	1:B:67:LEU:HB2	2.41	0.51
1:B:252:ILE:CG2	1:B:324:VAL:HB	2.41	0.51
1:B:505:GLY:HA2	1:B:710:ALA:H	1.76	0.51
1:C:111:ASP:CB	1:C:172:ARG:HH22	2.23	0.51
1:C:408:MSE:HG3	1:C:424:TYR:HE1	1.75	0.51
1:C:584:SER:CB	1:C:589:LYS:HB3	2.39	0.51
1:D:558:MSE:HE2	1:D:574:ILE:HG13	1.93	0.51
1:E:247:GLN:OE1	1:E:637:LYS:HE3	2.10	0.51
1:F:127:PRO:HB2	1:F:188:TYR:HE2	1.75	0.51
1:F:399:ASN:O	1:F:452:ASN:HB2	2.10	0.51
1:A:258:GLU:O	1:A:261:LYS:HB2	2.11	0.51
1:B:560:ILE:HD12	1:B:561:LEU:N	2.26	0.51
1:B:620:VAL:C	1:B:622:LEU:N	2.63	0.51
1:C:625:ALA:HB2	1:C:637:LYS:HD3	1.92	0.51
1:D:169:PRO:HA	1:D:174:TYR:CD2	2.45	0.51
1:D:381:ILE:HG22	1:D:717:TYR:CZ	2.45	0.51
1:D:603:ILE:HG22	1:D:604:ASN:N	2.25	0.51
1:E:31:ARG:HG2	1:E:85:ARG:O	2.10	0.51
1:E:88:ILE:HG22	1:E:89:GLU:N	2.26	0.51
1:E:168:ASP:OD1	1:E:169:PRO:HD2	2.10	0.51
1:E:293:PRO:C	1:E:295:ASN:H	2.14	0.51
1:E:497:GLU:OE2	1:E:741:GLU:HB3	2.10	0.51
1:E:598:GLN:HG3	1:E:604:ASN:HD22	1.75	0.51
1:E:766:THR:OG1	1:E:769:ASP:HB2	2.10	0.51
1:F:8:VAL:C	1:F:9:GLN:HG3	2.30	0.51
1:F:690:ALA:CB	1:F:721:ILE:HG23	2.39	0.51
1:A:215:ILE:HD12	1:A:226:LEU:HD23	1.91	0.51
1:A:286:LYS:HE3	1:A:291:PRO:HD2	1.92	0.51
1:B:296:LEU:H	1:B:296:LEU:CD1	2.23	0.51
1:B:616:ASP:OD1	1:B:634:PRO:HG2	2.10	0.51
1:C:497:GLU:OE2	1:C:741:GLU:HB3	2.10	0.51
1:D:209:LEU:HD23	1:D:354:TYR:CE2	2.45	0.51
1:D:583:GLU:CD	1:D:583:GLU:H	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:653:VAL:HG13	1:D:692:ALA:CB	2.39	0.51
1:E:199:TYR:CD1	1:E:200:GLY:N	2.79	0.51
1:E:593:ASN:O	1:E:596:LEU:HB2	2.11	0.51
1:F:221:ILE:HG22	1:F:360:ARG:NH2	2.26	0.51
1:F:488:TYR:CE1	1:F:525:LEU:HD13	2.46	0.51
1:F:523:GLU:OE2	1:F:537:HIS:HB2	2.09	0.51
1:F:613:ARG:HH22	1:F:628:ARG:NH2	2.09	0.51
1:F:707:LYS:O	1:F:733:GLY:HA3	2.11	0.51
1:A:519:THR:HB	1:A:608:ALA:HA	1.93	0.51
1:B:534:ARG:C	1:B:535:LEU:HD12	2.31	0.51
1:C:181:CYS:SG	1:C:182:PRO:N	2.82	0.51
1:C:383:ARG:HH11	1:C:383:ARG:HG3	1.76	0.51
1:D:253:MSE:HG2	1:D:317:PHE:HE1	1.75	0.51
1:D:434:LEU:HD11	1:D:465:ASN:O	2.10	0.51
1:D:697:ALA:HB1	1:D:709:VAL:HG11	1.93	0.51
1:E:218:ILE:O	1:E:224:ILE:HB	2.11	0.51
1:E:371:ILE:CD1	1:E:380:VAL:HG22	2.40	0.51
1:E:503:VAL:HB	1:E:708:ASN:O	2.09	0.51
1:F:124:TYR:CE2	1:F:125:MSE:HG2	2.45	0.51
1:F:138:PHE:HB2	1:F:389:PRO:HD3	1.92	0.51
1:F:225:HIS:HB2	1:F:328:THR:O	2.10	0.51
1:F:253:MSE:HG2	1:F:317:PHE:CE1	2.45	0.51
1:F:374:VAL:HG21	1:F:744:ARG:NH2	2.26	0.51
1:F:495:MSE:SE	1:F:527:LEU:HD13	2.60	0.51
1:A:66:PRO:HG2	1:A:67:LEU:H	1.76	0.51
1:A:649:LEU:HB3	1:A:684:SER:HB3	1.92	0.51
1:B:404:GLY:HA2	1:B:753:GLN:NE2	2.26	0.51
1:C:487:HIS:CE1	1:C:512:GLY:HA3	2.45	0.51
1:C:739:THR:HG23	1:C:741:GLU:H	1.76	0.51
1:D:3:ALA:C	1:D:53:ILE:HD11	2.31	0.51
1:D:137:ARG:O	1:D:141:ILE:HG13	2.10	0.51
1:E:12:VAL:HA	1:E:68:ALA:CB	2.40	0.51
1:E:225:HIS:NE2	1:E:327:MSE:HE3	2.25	0.51
1:E:538:ILE:HG23	1:E:662:VAL:CG2	2.40	0.51
1:E:543:LEU:HD23	1:E:543:LEU:N	2.18	0.51
1:E:663:GLU:CD	1:E:663:GLU:H	2.13	0.51
1:E:690:ALA:CB	1:E:721:ILE:HG23	2.41	0.51
1:F:106:ILE:HB	1:F:134:CYS:HA	1.93	0.51
1:F:267:SER:HB2	1:F:270:GLU:CB	2.39	0.51
1:F:428:THR:HA	1:F:433:VAL:CG1	2.41	0.51
1:F:485:GLN:OE1	1:F:514:GLY:HA2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:491:ILE:CD1	1:F:525:LEU:HD12	2.41	0.51
1:F:551:TYR:HA	1:F:628:ARG:HD2	1.91	0.51
1:A:199:TYR:CG	1:A:200:GLY:N	2.79	0.51
1:A:408:MSE:O	1:A:747:ASN:HA	2.11	0.51
1:B:225:HIS:CA	1:B:330:ALA:HB2	2.28	0.51
1:B:409:ASN:CG	1:B:425:ILE:HD11	2.30	0.51
1:B:526:TYR:HB3	1:B:535:LEU:HD11	1.93	0.51
1:C:144:LEU:HD23	1:C:145:PRO:HA	1.91	0.51
1:C:729:VAL:HG11	1:C:735:ASN:HB3	1.91	0.51
1:C:738:VAL:HB	1:C:744:ARG:HG2	1.91	0.51
1:D:210:ILE:HD11	1:D:227:ALA:C	2.31	0.51
1:D:424:TYR:C	1:D:426:GLY:H	2.13	0.51
1:D:598:GLN:HG3	1:D:604:ASN:HB2	1.93	0.51
1:D:655:VAL:HG11	1:D:696:THR:OG1	2.11	0.51
1:E:9:GLN:NE2	1:E:40:ALA:HB1	2.25	0.51
1:E:153:MSE:SE	1:E:360:ARG:HD2	2.60	0.51
1:F:370:VAL:O	1:F:381:ILE:HG13	2.10	0.51
1:F:708:ASN:N	1:F:708:ASN:HD22	2.09	0.51
1:A:11:ILE:CG1	1:A:68:ALA:HA	2.32	0.51
1:A:554:LEU:HG	1:A:558:MSE:HE3	1.93	0.51
1:B:127:PRO:O	1:B:311:GLY:HA3	2.11	0.51
1:B:409:ASN:CB	1:B:425:ILE:HD11	2.41	0.51
1:B:476:GLU:O	1:B:477:LEU:HB3	2.11	0.51
1:B:544:PRO:HG2	1:B:555:ARG:HE	1.75	0.51
1:B:614:VAL:HG13	1:B:666:PHE:CE2	2.46	0.51
1:C:590:VAL:O	1:C:594:VAL:HG23	2.10	0.51
1:C:596:LEU:O	1:C:596:LEU:HD23	2.11	0.51
1:D:57:ILE:HG21	1:D:75:LYS:HZ1	1.76	0.51
1:D:204:ARG:HG2	1:D:319:TRP:CE2	2.46	0.51
1:D:649:LEU:HB3	1:D:684:SER:HB3	1.92	0.51
1:E:213:GLY:C	1:E:235:VAL:HG11	2.31	0.51
1:E:392:ILE:HB	1:E:419:VAL:HG12	1.93	0.51
1:E:584:SER:CB	1:E:589:LYS:HB3	2.40	0.51
1:E:633:GLU:H	1:E:634:PRO:CD	2.22	0.51
1:F:543:LEU:HD12	1:F:549:ALA:CB	2.40	0.51
1:F:554:LEU:HG	1:F:620:VAL:HG11	1.92	0.51
1:A:196:GLN:HG2	1:A:197:GLU:N	2.26	0.51
1:A:406:GLU:O	1:A:428:THR:HG23	2.10	0.51
1:A:424:TYR:C	1:A:426:GLY:H	2.14	0.51
1:A:580:LYS:HG3	1:A:593:ASN:ND2	2.26	0.51
1:C:31:ARG:HG2	1:C:85:ARG:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:LYS:HE3	1:C:290:PHE:HB3	1.93	0.51
1:C:561:LEU:HB2	1:C:570:LEU:CD1	2.40	0.51
1:C:633:GLU:N	1:C:634:PRO:HD2	2.26	0.51
1:D:33:TYR:HB2	1:D:88:ILE:O	2.11	0.51
1:D:281:ILE:HG12	1:D:306:MSE:HG2	1.91	0.51
1:E:274:LEU:C	1:E:276:SER:H	2.13	0.51
1:F:288:GLU:HB3	1:F:289:PRO:CD	2.32	0.51
1:F:491:ILE:HD11	1:F:525:LEU:HD12	1.93	0.51
1:A:225:HIS:CA	1:A:330:ALA:HB2	2.39	0.51
1:A:278:ARG:HG3	1:A:280:PRO:HD3	1.92	0.51
1:A:410:ALA:HB2	1:A:747:ASN:OD1	2.11	0.51
1:A:476:GLU:C	1:A:478:ASP:H	2.13	0.51
1:A:593:ASN:O	1:A:596:LEU:HB2	2.10	0.51
1:B:522:GLY:HA3	1:B:611:THR:HG23	1.93	0.51
1:D:492:ALA:O	1:D:495:MSE:HG2	2.11	0.51
1:D:523:GLU:HG3	1:D:537:HIS:CB	2.41	0.51
1:E:65:PRO:C	1:E:67:LEU:H	2.14	0.51
1:E:104:PRO:HD3	1:E:390:LEU:HD21	1.92	0.51
1:E:190:LEU:HB2	1:E:202:PRO:CB	2.41	0.51
1:A:455:LEU:HA	1:A:479:VAL:HG12	1.93	0.50
1:A:491:ILE:HG12	1:A:527:LEU:CD1	2.40	0.50
1:A:589:LYS:HG3	1:A:590:VAL:HG23	1.92	0.50
1:B:624:VAL:O	1:B:625:ALA:CB	2.58	0.50
1:C:138:PHE:CG	1:C:389:PRO:HD3	2.45	0.50
1:C:534:ARG:HD3	1:C:537:HIS:CD2	2.46	0.50
1:D:487:HIS:CE1	1:D:509:ASP:HB3	2.46	0.50
1:D:510:GLY:O	1:D:610:SER:HB2	2.11	0.50
1:D:612:GLY:HA2	1:D:615:LEU:HD12	1.93	0.50
1:F:308:PRO:HA	1:F:313:HIS:HB3	1.93	0.50
1:F:504:ILE:HG22	1:F:505:GLY:H	1.75	0.50
1:A:204:ARG:HG2	1:A:319:TRP:CE2	2.46	0.50
1:A:209:LEU:HA	1:A:212:LYS:HB2	1.93	0.50
1:A:543:LEU:HD23	1:A:543:LEU:N	2.26	0.50
1:B:264:ALA:HB2	1:B:286:LYS:HA	1.93	0.50
1:B:765:LEU:HD12	1:B:766:THR:H	1.76	0.50
1:C:488:TYR:CD1	1:C:525:LEU:HD13	2.46	0.50
1:C:522:GLY:HA3	1:C:611:THR:HG23	1.93	0.50
1:D:13:GLN:NE2	1:D:42:VAL:HG23	2.24	0.50
1:D:102:ILE:CG2	1:D:389:PRO:HG3	2.41	0.50
1:D:252:ILE:HG23	1:D:325:TYR:O	2.11	0.50
1:D:651:PHE:HB2	1:D:688:ALA:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:751:VAL:HG13	1:D:752:GLY:N	2.26	0.50
1:F:219:LYS:HB2	1:F:357:LEU:HA	1.93	0.50
1:F:268:PRO:HG2	1:F:378:ARG:HH22	1.76	0.50
1:F:665:LEU:O	1:F:669:ILE:HG13	2.10	0.50
1:A:218:ILE:HD12	1:A:356:LEU:HD23	1.93	0.50
1:A:252:ILE:HD12	1:A:252:ILE:N	2.25	0.50
1:A:281:ILE:HB	1:A:370:VAL:CG1	2.36	0.50
1:A:373:PHE:CD2	1:A:378:ARG:HD3	2.46	0.50
1:A:376:GLY:HA2	1:A:726:ARG:HH11	1.74	0.50
1:B:381:ILE:HA	1:B:717:TYR:OH	2.10	0.50
1:B:419:VAL:HG11	1:B:751:VAL:HG23	1.92	0.50
1:B:518:ASN:HB3	1:B:540:TYR:HE2	1.76	0.50
1:C:261:LYS:HZ2	1:C:266:VAL:HB	1.75	0.50
1:E:385:ARG:HG3	1:E:386:GLY:N	2.26	0.50
1:E:415:LYS:C	1:E:417:GLY:H	2.13	0.50
1:E:504:ILE:HG22	1:E:505:GLY:N	2.25	0.50
1:F:383:ARG:HH11	1:F:383:ARG:HG3	1.76	0.50
1:F:566:SER:H	1:F:569:GLU:HB3	1.77	0.50
1:F:686:HIS:HE1	1:F:718:ASN:ND2	2.10	0.50
1:A:106:ILE:CG2	1:A:277:TYR:HB2	2.37	0.50
1:A:370:VAL:CG2	1:A:381:ILE:HD11	2.41	0.50
1:B:35:LYS:HG3	1:B:90:LYS:HB3	1.92	0.50
1:B:65:PRO:C	1:B:67:LEU:H	2.13	0.50
1:B:537:HIS:HB3	1:B:659:LEU:HD23	1.92	0.50
1:C:142:GLU:HB2	1:C:150:ASN:C	2.32	0.50
1:C:245:ARG:NE	1:C:250:PHE:HE2	2.09	0.50
1:C:251:ALA:O	1:C:326:VAL:HA	2.11	0.50
1:C:504:ILE:HD12	1:C:701:ALA:HB2	1.93	0.50
1:D:65:PRO:HG2	1:D:68:ALA:HB3	1.92	0.50
1:D:394:ILE:HG23	1:D:755:PHE:HB2	1.93	0.50
1:D:587:TYR:OH	1:E:468:LYS:HG3	2.11	0.50
1:F:406:GLU:HG3	1:F:407:LEU:N	2.27	0.50
1:F:610:SER:O	1:F:614:VAL:HG23	2.12	0.50
1:A:319:TRP:O	1:A:320:SER:HB3	2.11	0.50
1:A:486:HIS:O	1:A:489:ALA:HB3	2.10	0.50
1:A:743:PRO:HG3	1:A:747:ASN:HD22	1.76	0.50
1:B:1:MSE:HE2	1:B:47:GLU:C	2.32	0.50
1:B:158:MSE:HE3	1:B:163:ARG:NH1	2.27	0.50
1:C:399:ASN:O	1:C:454:ASP:HB2	2.11	0.50
1:D:28:HIS:CD2	1:D:56:PHE:HB2	2.47	0.50
1:D:323:PRO:HG2	1:D:324:VAL:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:371:ILE:CG1	1:D:380:VAL:HG22	2.42	0.50
1:D:508:LEU:HB3	1:D:715:VAL:HB	1.94	0.50
1:D:748:GLY:O	1:D:751:VAL:HG12	2.11	0.50
1:E:163:ARG:O	1:E:167:GLU:HG2	2.10	0.50
1:F:189:ARG:HD2	1:F:191:TYR:OH	2.11	0.50
1:F:456:ILE:O	1:F:482:LEU:HB3	2.12	0.50
1:F:504:ILE:HD11	1:F:701:ALA:HA	1.93	0.50
1:F:756:LEU:HD21	1:F:770:LEU:HD22	1.93	0.50
1:A:65:PRO:HG2	1:A:68:ALA:CB	2.42	0.50
1:A:111:ASP:CB	1:A:172:ARG:HH22	2.25	0.50
1:B:399:ASN:O	1:B:454:ASP:HB2	2.11	0.50
1:C:138:PHE:HA	1:C:141:ILE:HD12	1.94	0.50
1:C:247:GLN:HE22	1:C:637:LYS:NZ	2.09	0.50
1:C:498:LYS:HB2	1:C:500:LEU:HD12	1.94	0.50
1:D:253:MSE:HE2	1:D:317:PHE:CE1	2.46	0.50
1:E:32:GLY:O	1:E:87:TYR:HA	2.11	0.50
1:E:192:THR:HG23	1:E:353:ASP:O	2.12	0.50
1:E:219:LYS:HG3	1:E:224:ILE:CG2	2.41	0.50
1:E:523:GLU:OE2	1:E:537:HIS:HB2	2.11	0.50
1:F:140:ILE:HG21	1:F:360:ARG:NH1	2.26	0.50
1:F:232:ASN:OD1	1:F:234:GLU:HB3	2.11	0.50
1:F:582:VAL:HG21	1:F:626:TYR:CD1	2.46	0.50
1:B:396:PHE:CE2	1:B:759:LEU:HB2	2.47	0.50
1:C:263:PHE:HE1	1:C:292:LEU:HB2	1.76	0.50
1:D:267:SER:O	1:D:270:GLU:HB3	2.11	0.50
1:D:292:LEU:HB3	1:D:296:LEU:HD22	1.92	0.50
1:D:504:ILE:H	1:D:706:VAL:HG11	1.77	0.50
1:E:284:LEU:O	1:E:302:THR:HA	2.11	0.50
1:E:535:LEU:HD23	1:E:700:ARG:HG3	1.93	0.50
1:E:714:GLY:C	1:E:716:ALA:H	2.14	0.50
1:F:4:TYR:HA	1:F:76:LYS:O	2.11	0.50
1:A:724:MSE:HE1	1:C:289:PRO:HB3	1.94	0.50
1:C:181:CYS:SG	1:C:183:VAL:HG13	2.51	0.50
1:D:219:LYS:HA	1:D:224:ILE:HG22	1.94	0.50
1:D:279:ARG:HD3	1:D:307:LEU:HB2	1.93	0.50
1:D:300:LEU:CD2	1:D:636:MSE:HE2	2.42	0.50
1:D:456:ILE:HD11	1:D:479:VAL:HB	1.94	0.50
1:D:497:GLU:OE1	1:D:738:VAL:HA	2.11	0.50
1:D:641:PHE:HZ	1:D:678:PRO:HB2	1.76	0.50
1:E:36:ASN:HA	1:E:41:GLY:O	2.12	0.50
1:E:213:GLY:CA	1:E:235:VAL:HG11	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:456:ILE:HG22	1:E:457:ILE:H	1.77	0.50
1:E:485:GLN:CG	1:E:488:TYR:H	2.23	0.50
1:E:582:VAL:CG1	1:E:626:TYR:HB3	2.40	0.50
1:F:140:ILE:HB	1:F:152:THR:CG2	2.42	0.50
1:F:233:GLU:HB2	1:F:293:PRO:HB3	1.93	0.50
1:F:476:GLU:C	1:F:478:ASP:H	2.14	0.50
1:A:177:GLU:HB2	1:A:178:PRO:HD3	1.93	0.50
1:A:582:VAL:C	1:A:584:SER:H	2.14	0.50
1:A:765:LEU:CD2	1:A:770:LEU:HD21	2.41	0.50
1:B:315:ILE:HG23	1:B:316:LEU:N	2.26	0.50
1:B:528:GLY:N	1:B:532:VAL:HG22	2.27	0.50
1:C:15:VAL:HG11	1:C:67:LEU:HB2	1.94	0.50
1:C:477:LEU:HB3	1:C:479:VAL:HG23	1.94	0.50
1:C:709:VAL:O	1:C:735:ASN:HB2	2.12	0.50
1:D:383:ARG:HD2	1:D:387:PHE:CD2	2.46	0.50
1:D:613:ARG:NE	1:D:613:ARG:HA	2.27	0.50
1:E:16:GLY:C	1:E:19:PRO:HD2	2.32	0.50
1:E:236:VAL:HG21	1:E:296:LEU:HD12	1.94	0.50
1:E:396:PHE:CZ	1:E:759:LEU:HD13	2.46	0.50
1:F:35:LYS:HE2	1:F:90:LYS:HZ2	1.76	0.50
1:F:253:MSE:HG2	1:F:317:PHE:HE1	1.76	0.50
1:F:380:VAL:HG21	1:F:740:THR:HG23	1.94	0.50
1:A:189:ARG:HA	1:A:202:PRO:HG3	1.94	0.49
1:A:381:ILE:HG22	1:A:717:TYR:CZ	2.47	0.49
1:A:427:ASN:O	1:A:433:VAL:HG21	2.11	0.49
1:A:456:ILE:CG2	1:A:457:ILE:N	2.72	0.49
1:A:557:LEU:HD23	1:A:557:LEU:O	2.12	0.49
1:B:543:LEU:HD23	1:B:543:LEU:H	1.77	0.49
1:C:123:ARG:HH22	1:C:173:ARG:HG2	1.76	0.49
1:C:224:ILE:HG22	1:C:338:VAL:O	2.12	0.49
1:C:315:ILE:CG2	1:C:316:LEU:N	2.75	0.49
1:C:427:ASN:O	1:C:433:VAL:HG11	2.12	0.49
1:D:281:ILE:HG12	1:D:306:MSE:CG	2.42	0.49
1:D:589:LYS:H	1:E:475:ASN:ND2	2.10	0.49
1:E:188:TYR:OH	1:E:312:THR:HG21	2.12	0.49
1:E:230:ALA:HB3	1:E:324:VAL:HG23	1.94	0.49
1:E:233:GLU:O	1:E:236:VAL:HG12	2.12	0.49
1:E:457:ILE:HG22	1:E:458:ALA:N	2.27	0.49
1:E:722:THR:O	1:E:726:ARG:HB2	2.11	0.49
1:A:61:TYR:CE2	1:A:73:ILE:HD12	2.46	0.49
1:A:230:ALA:HB2	1:A:326:VAL:CG2	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:LYS:HE3	1:A:291:PRO:CD	2.43	0.49
1:A:399:ASN:N	1:A:399:ASN:ND2	2.60	0.49
1:B:515:THR:O	1:B:516:ASP:HB2	2.12	0.49
1:C:266:VAL:HG22	1:C:284:LEU:HD22	1.93	0.49
1:C:306:MSE:HE1	1:C:368:ASP:OD2	2.12	0.49
1:C:415:LYS:C	1:C:417:GLY:H	2.15	0.49
1:C:633:GLU:H	1:C:634:PRO:HD2	1.77	0.49
1:D:329:SER:HB3	1:D:337:MSE:HE2	1.94	0.49
1:D:475:ASN:ND2	1:E:589:LYS:H	2.09	0.49
1:A:409:ASN:ND2	1:A:425:ILE:HD11	2.27	0.49
1:A:639:GLU:OE2	1:A:718:ASN:HA	2.13	0.49
1:B:22:TYR:CE1	1:B:87:TYR:HB3	2.47	0.49
1:B:379:ALA:HB2	1:B:737:HIS:HE1	1.77	0.49
1:B:409:ASN:HB3	1:B:425:ILE:HD11	1.93	0.49
1:C:20:PHE:HE1	1:C:60:LEU:HD12	1.77	0.49
1:C:130:VAL:HG23	1:C:134:CYS:SG	2.53	0.49
1:C:220:GLY:H	1:C:224:ILE:HA	1.78	0.49
1:C:406:GLU:HA	1:C:466:THR:CG2	2.42	0.49
1:C:540:TYR:HA	1:C:608:ALA:O	2.12	0.49
1:C:586:LYS:CB	1:C:627:ARG:HH22	2.25	0.49
1:C:649:LEU:CD1	1:C:650:LYS:H	2.24	0.49
1:D:394:ILE:HG22	1:D:396:PHE:H	1.76	0.49
1:D:456:ILE:HD12	1:D:480:GLU:O	2.12	0.49
1:E:278:ARG:HG3	1:E:280:PRO:HD3	1.94	0.49
1:E:398:TYR:CZ	1:E:758:GLY:HA3	2.48	0.49
1:E:759:LEU:CD1	1:E:764:TYR:HB2	2.42	0.49
1:F:714:GLY:C	1:F:716:ALA:H	2.16	0.49
1:A:111:ASP:HB3	1:A:172:ARG:NH1	2.25	0.49
1:A:148:ARG:NH1	1:A:158:MSE:HG3	2.27	0.49
1:B:398:TYR:OH	1:B:754:ALA:HA	2.13	0.49
1:B:593:ASN:C	1:B:595:VAL:H	2.16	0.49
1:B:633:GLU:N	1:B:634:PRO:HD2	2.23	0.49
1:C:287:LYS:CG	1:C:289:PRO:HD2	2.40	0.49
1:D:149:GLU:O	1:D:154:LYS:HG3	2.12	0.49
1:D:286:LYS:HD2	1:D:303:ILE:HD11	1.94	0.49
1:D:472:GLU:O	1:D:476:GLU:HG2	2.13	0.49
1:E:458:ALA:HB1	1:E:467:THR:HG22	1.94	0.49
1:F:16:GLY:C	1:F:19:PRO:HD2	2.32	0.49
1:F:201:ASP:N	1:F:202:PRO:CD	2.75	0.49
1:F:204:ARG:O	1:F:208:GLU:HG3	2.13	0.49
1:F:338:VAL:HG23	1:F:343:ARG:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:TYR:CE1	1:A:525:LEU:HD13	2.47	0.49
1:A:504:ILE:HD12	1:A:701:ALA:HA	1.94	0.49
1:C:12:VAL:HG13	1:C:13:GLN:CD	2.33	0.49
1:C:320:SER:O	1:C:322:THR:N	2.44	0.49
1:C:565:TYR:HB3	1:C:569:GLU:HB3	1.93	0.49
1:C:601:LYS:HZ2	1:F:771:MSE:HE3	1.76	0.49
1:C:760:TYR:HA	1:C:765:LEU:HB3	1.93	0.49
1:D:257:ILE:CD1	1:D:271:GLU:HG3	2.43	0.49
1:D:766:THR:OG1	1:D:769:ASP:HB2	2.11	0.49
1:E:428:THR:HA	1:E:433:VAL:CG1	2.41	0.49
1:F:280:PRO:HB2	1:F:371:ILE:HG22	1.95	0.49
1:F:504:ILE:CG2	1:F:505:GLY:N	2.76	0.49
1:A:210:ILE:HD11	1:A:228:CYS:CA	2.43	0.49
1:A:369:SER:H	1:A:385:ARG:CB	2.26	0.49
1:A:445:ARG:HH21	1:A:452:ASN:HD22	1.58	0.49
1:A:490:HIS:CG	1:A:713:GLY:HA2	2.48	0.49
1:B:191:TYR:CD1	1:B:196:GLN:HB3	2.48	0.49
1:B:205:LYS:O	1:B:209:LEU:HD13	2.12	0.49
1:B:279:ARG:CB	1:B:309:TYR:HB3	2.41	0.49
1:B:549:ALA:HA	1:B:555:ARG:CB	2.42	0.49
1:C:216:VAL:HG23	1:C:354:TYR:O	2.12	0.49
1:D:15:VAL:HG21	1:D:67:LEU:O	2.13	0.49
1:D:399:ASN:O	1:D:452:ASN:HB2	2.12	0.49
1:D:415:LYS:HD2	1:D:448:LEU:HD22	1.95	0.49
1:D:506:ILE:HB	1:D:711:LEU:CD1	2.43	0.49
1:E:370:VAL:HG22	1:E:382:ARG:HD2	1.94	0.49
1:E:541:TYR:OH	1:E:610:SER:O	2.30	0.49
1:E:583:GLU:HG3	1:E:592:PHE:CD1	2.47	0.49
1:E:613:ARG:HA	1:E:613:ARG:HE	1.78	0.49
1:F:111:ASP:HB3	1:F:172:ARG:HH12	1.76	0.49
1:F:137:ARG:O	1:F:141:ILE:HG13	2.13	0.49
1:A:19:PRO:O	1:A:23:ARG:HG3	2.13	0.49
1:A:217:ALA:HB1	1:A:224:ILE:CD1	2.41	0.49
1:A:225:HIS:HB2	1:A:328:THR:O	2.12	0.49
1:A:475:ASN:ND2	1:B:589:LYS:N	2.60	0.49
1:B:278:ARG:NH1	1:B:387:PHE:HE1	2.10	0.49
1:B:408:MSE:HG3	1:B:424:TYR:HE1	1.76	0.49
1:B:545:GLY:HA3	1:B:548:LEU:HB2	1.95	0.49
1:C:370:VAL:O	1:C:381:ILE:HG13	2.12	0.49
1:C:429:GLY:HA2	1:C:465:ASN:HD22	1.77	0.49
1:D:375:ASP:OD2	1:D:723:LYS:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:660:ILE:HG22	1:D:662:VAL:HG23	1.94	0.49
1:D:708:ASN:HB3	1:D:734:LEU:O	2.13	0.49
1:D:743:PRO:HG2	1:D:748:GLY:HA3	1.95	0.49
1:E:210:ILE:HD13	1:E:216:VAL:CG1	2.37	0.49
1:E:227:ALA:HA	1:E:326:VAL:O	2.13	0.49
1:E:282:ILE:HG23	1:E:283:THR:N	2.26	0.49
1:F:334:GLY:HA3	1:F:335:MSE:HE2	1.93	0.49
1:F:413:VAL:HG13	1:F:420:TYR:HB2	1.95	0.49
1:A:331:ASN:ND2	1:A:337:MSE:HA	2.23	0.49
1:B:495:MSE:SE	1:B:527:LEU:HD13	2.63	0.49
1:B:508:LEU:CD2	1:B:611:THR:HG21	2.41	0.49
1:B:529:TYR:HD1	1:B:764:TYR:HB3	1.78	0.49
1:C:11:ILE:HG21	1:C:69:ARG:N	2.23	0.49
1:C:170:LEU:HD12	1:C:170:LEU:N	2.27	0.49
1:C:232:ASN:OD1	1:C:235:VAL:HG22	2.13	0.49
1:C:485:GLN:OE1	1:C:514:GLY:HA2	2.13	0.49
1:D:116:LEU:HD23	1:D:129:ILE:HG21	1.95	0.49
1:E:24:ILE:HG23	1:E:56:PHE:CE1	2.47	0.49
1:E:196:GLN:N	1:E:196:GLN:NE2	2.61	0.49
1:E:255:LYS:HG2	1:E:256:ASP:OD2	2.13	0.49
1:E:384:SER:HA	1:E:388:VAL:HG23	1.93	0.49
1:E:757:GLY:C	1:E:759:LEU:H	2.16	0.49
1:F:159:CYS:SG	1:F:183:VAL:HG21	2.53	0.49
1:F:237:ALA:HA	1:F:295:ASN:HD21	1.77	0.49
1:F:385:ARG:HG3	1:F:386:GLY:N	2.28	0.49
1:F:457:ILE:HG21	1:F:753:GLN:HB3	1.95	0.49
1:A:107:ALA:O	1:A:134:CYS:HB2	2.11	0.49
1:A:404:GLY:HA2	1:A:753:GLN:CD	2.33	0.49
1:B:193:SER:O	1:B:194:ASP:CB	2.60	0.49
1:B:495:MSE:HG3	1:B:755:PHE:CZ	2.47	0.49
1:C:28:HIS:HB3	1:C:52:ASP:HB3	1.95	0.49
1:C:163:ARG:HA	1:C:166:TYR:HB3	1.95	0.49
1:D:491:ILE:HD11	1:D:505:GLY:CA	2.41	0.49
1:E:9:GLN:HE21	1:E:40:ALA:HB1	1.77	0.49
1:E:738:VAL:CG1	1:E:742:VAL:HB	2.41	0.49
1:F:242:ARG:HH22	1:F:353:ASP:CG	2.17	0.49
1:A:464:TYR:C	1:A:466:THR:N	2.67	0.49
1:A:751:VAL:HG13	1:A:752:GLY:N	2.27	0.49
1:B:31:ARG:HB3	1:B:86:PHE:O	2.13	0.49
1:B:495:MSE:SE	1:B:527:LEU:HD22	2.63	0.49
1:C:190:LEU:HB2	1:C:202:PRO:CB	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:TYR:CG	1:C:385:ARG:NH2	2.81	0.49
1:C:433:VAL:O	1:C:436:PHE:HB3	2.12	0.49
1:D:104:PRO:O	1:D:137:ARG:HB2	2.12	0.49
1:F:181:CYS:SG	1:F:182:PRO:N	2.85	0.49
1:F:725:ILE:O	1:F:729:VAL:HG23	2.13	0.49
1:A:545:GLY:HA3	1:A:548:LEU:HD12	1.95	0.48
1:A:557:LEU:HD12	1:A:620:VAL:HB	1.94	0.48
1:A:655:VAL:HG22	1:A:660:ILE:HG12	1.94	0.48
1:C:130:VAL:HG22	1:C:131:CYS:N	2.28	0.48
1:C:130:VAL:HG11	1:C:178:PRO:O	2.13	0.48
1:C:210:ILE:HG21	1:C:325:TYR:HE1	1.77	0.48
1:C:218:ILE:C	1:C:224:ILE:HG13	2.33	0.48
1:C:566:SER:N	1:C:569:GLU:HB2	2.27	0.48
1:D:376:GLY:C	1:D:377:LYS:HD2	2.33	0.48
1:D:509:ASP:CG	1:D:510:GLY:N	2.66	0.48
1:D:515:THR:O	1:D:516:ASP:HB2	2.12	0.48
1:D:519:THR:HB	1:D:608:ALA:CA	2.37	0.48
1:E:113:LEU:O	1:E:116:LEU:HG	2.13	0.48
1:E:370:VAL:HG23	1:E:381:ILE:HG13	1.95	0.48
1:F:4:TYR:CB	1:F:53:ILE:HD11	2.43	0.48
1:F:7:HIS:CD2	1:F:43:GLU:HB3	2.48	0.48
1:F:22:TYR:CD2	1:F:169:PRO:HB3	2.48	0.48
1:A:251:ALA:HB3	1:A:327:MSE:O	2.14	0.48
1:A:502:SER:CB	1:A:528:GLY:HA2	2.43	0.48
1:B:516:ASP:C	1:B:518:ASN:H	2.17	0.48
1:C:24:ILE:HG23	1:C:56:PHE:CE1	2.47	0.48
1:C:256:ASP:O	1:C:257:ILE:C	2.52	0.48
1:D:219:LYS:HA	1:D:224:ILE:HB	1.95	0.48
1:D:274:LEU:C	1:D:276:SER:H	2.17	0.48
1:D:398:TYR:HB2	1:D:454:ASP:CG	2.33	0.48
1:D:677:SER:O	1:D:681:ILE:HG12	2.13	0.48
1:E:219:LYS:HD3	1:E:358:HIS:H	1.76	0.48
1:F:146:TYR:CE1	1:F:177:GLU:HG2	2.49	0.48
1:F:601:LYS:CB	1:F:603:ILE:HG13	2.43	0.48
1:A:239:LEU:HD22	1:A:250:PHE:HZ	1.77	0.48
1:A:450:VAL:HG22	1:A:451:LYS:N	2.28	0.48
1:B:16:GLY:HA2	1:B:132:THR:OG1	2.12	0.48
1:C:225:HIS:CD2	1:C:225:HIS:N	2.81	0.48
1:C:270:GLU:N	1:C:378:ARG:NH1	2.62	0.48
1:D:392:ILE:N	1:D:392:ILE:HD12	2.29	0.48
1:E:510:GLY:O	1:E:511:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:31:ARG:HB3	1:F:86:PHE:O	2.12	0.48
1:F:124:TYR:O	1:F:125:MSE:HB2	2.13	0.48
1:F:216:VAL:O	1:F:227:ALA:HB3	2.13	0.48
1:A:116:LEU:C	1:A:118:ASP:H	2.17	0.48
1:A:144:LEU:HD23	1:A:146:TYR:N	2.27	0.48
1:B:216:VAL:O	1:B:227:ALA:HB3	2.13	0.48
1:B:406:GLU:HA	1:B:466:THR:HG21	1.96	0.48
1:B:427:ASN:O	1:B:433:VAL:HG11	2.13	0.48
1:C:375:ASP:OD2	1:C:723:LYS:HA	2.13	0.48
1:D:543:LEU:H	1:D:543:LEU:CD2	2.20	0.48
1:D:557:LEU:HD23	1:D:557:LEU:O	2.13	0.48
1:D:714:GLY:C	1:D:716:ALA:H	2.16	0.48
1:E:144:LEU:CD1	1:E:447:ILE:HG23	2.40	0.48
1:E:456:ILE:O	1:E:482:LEU:HB3	2.13	0.48
1:F:300:LEU:HD22	1:F:636:MSE:HE2	1.95	0.48
1:F:315:ILE:HG23	1:F:316:LEU:N	2.28	0.48
1:F:383:ARG:CZ	1:F:421:PRO:HG3	2.43	0.48
1:A:253:MSE:HA	1:A:306:MSE:O	2.13	0.48
1:A:309:TYR:CZ	1:A:313:HIS:NE2	2.81	0.48
1:B:170:LEU:HD12	1:B:170:LEU:H	1.79	0.48
1:C:9:GLN:NE2	1:C:40:ALA:HB1	2.28	0.48
1:C:21:VAL:HA	1:C:24:ILE:CG2	2.42	0.48
1:C:253:MSE:HG3	1:C:306:MSE:O	2.14	0.48
1:C:317:PHE:CE2	1:C:323:PRO:HA	2.45	0.48
1:D:170:LEU:HD12	1:D:170:LEU:N	2.25	0.48
1:D:399:ASN:HA	1:D:414:ALA:O	2.13	0.48
1:E:265:TYR:O	1:E:284:LEU:HD22	2.13	0.48
1:E:539:ASP:CA	1:E:659:LEU:HD11	2.40	0.48
1:F:11:ILE:HG23	1:F:11:ILE:O	2.12	0.48
1:F:15:VAL:C	1:F:17:PHE:H	2.17	0.48
1:F:182:PRO:HB3	1:F:199:TYR:OH	2.14	0.48
1:F:490:HIS:C	1:F:492:ALA:H	2.17	0.48
1:A:380:VAL:CG1	1:A:381:ILE:H	2.15	0.48
1:A:445:ARG:HH22	1:A:477:LEU:HD22	1.77	0.48
1:A:495:MSE:HG3	1:A:755:PHE:CE2	2.48	0.48
1:B:588:GLY:O	1:B:592:PHE:HD2	1.97	0.48
1:B:691:ARG:HD3	1:B:724:MSE:HE3	1.93	0.48
1:B:725:ILE:O	1:B:729:VAL:HG23	2.13	0.48
1:C:105:ASP:HA	1:C:137:ARG:HB2	1.94	0.48
1:C:265:TYR:CE2	1:C:287:LYS:HD2	2.47	0.48
1:C:415:LYS:HZ2	1:C:448:LEU:HA	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:GLY:HA2	1:C:465:ASN:ND2	2.29	0.48
1:D:105:ASP:CG	1:D:139:THR:HG23	2.33	0.48
1:D:384:SER:HA	1:D:388:VAL:CG2	2.43	0.48
1:D:690:ALA:CB	1:D:721:ILE:HG23	2.43	0.48
1:F:579:PRO:O	1:F:582:VAL:HG23	2.14	0.48
1:F:595:VAL:O	1:F:598:GLN:HB3	2.14	0.48
1:A:445:ARG:HH22	1:A:477:LEU:CD2	2.27	0.48
1:A:613:ARG:NE	1:A:613:ARG:HA	2.28	0.48
1:B:128:PHE:CD1	1:B:186:PRO:HG2	2.49	0.48
1:B:146:TYR:CE1	1:B:177:GLU:HG2	2.49	0.48
1:C:111:ASP:HB3	1:C:172:ARG:HH22	1.79	0.48
1:C:329:SER:HA	1:C:337:MSE:HE2	1.95	0.48
1:C:367:ASP:HB2	1:C:424:TYR:HB3	1.94	0.48
1:C:528:GLY:O	1:C:529:TYR:C	2.52	0.48
1:D:190:LEU:O	1:D:196:GLN:HB2	2.13	0.48
1:E:315:ILE:HG23	1:E:316:LEU:N	2.29	0.48
1:E:670:LEU:HA	1:E:673:ILE:HG12	1.94	0.48
1:F:191:TYR:HA	1:F:195:GLY:O	2.14	0.48
1:F:312:THR:O	1:F:315:ILE:HG22	2.14	0.48
1:F:534:ARG:HG2	1:F:535:LEU:N	2.28	0.48
1:A:255:LYS:HG3	1:A:317:PHE:CD2	2.49	0.48
1:A:270:GLU:HB2	1:A:373:PHE:HE2	1.79	0.48
1:A:610:SER:O	1:A:614:VAL:HG23	2.13	0.48
1:A:666:PHE:O	1:A:669:ILE:HB	2.14	0.48
1:B:140:ILE:HB	1:B:152:THR:CG2	2.44	0.48
1:B:341:ASN:O	1:B:344:ALA:HB3	2.13	0.48
1:B:595:VAL:O	1:B:595:VAL:HG12	2.13	0.48
1:C:31:ARG:HA	1:C:87:TYR:HB2	1.96	0.48
1:C:215:ILE:HD11	1:C:351:VAL:O	2.14	0.48
1:C:406:GLU:HB3	1:C:464:TYR:CG	2.48	0.48
1:C:728:VAL:C	1:C:730:GLU:H	2.17	0.48
1:D:151:THR:O	1:D:154:LYS:HB2	2.13	0.48
1:D:339:LYS:HD2	1:D:362:ILE:O	2.14	0.48
1:D:373:PHE:CE2	1:D:378:ARG:HD3	2.48	0.48
1:D:381:ILE:HA	1:D:717:TYR:OH	2.13	0.48
1:D:648:ASP:OD1	1:D:687:LEU:HD12	2.14	0.48
1:E:64:LYS:CB	1:E:65:PRO:HD2	2.43	0.48
1:E:591:GLU:O	1:E:594:VAL:HB	2.14	0.48
1:E:665:LEU:O	1:E:669:ILE:HG13	2.14	0.48
1:E:751:VAL:HG13	1:E:752:GLY:N	2.29	0.48
1:F:108:ILE:HG22	1:F:109:CYS:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:495:MSE:HB3	1:F:500:LEU:HD11	1.96	0.48
1:A:485:GLN:HB3	1:A:488:TYR:HB2	1.94	0.48
1:B:171:ASN:HD21	1:B:173:ARG:CB	2.26	0.48
1:B:335:MSE:HE2	1:B:335:MSE:N	2.29	0.48
1:B:409:ASN:O	1:B:425:ILE:HG12	2.14	0.48
1:C:9:GLN:HE21	1:C:40:ALA:C	2.16	0.48
1:C:204:ARG:HD2	1:C:204:ARG:C	2.34	0.48
1:C:525:LEU:CD2	1:C:534:ARG:HA	2.44	0.48
1:C:613:ARG:NE	1:C:613:ARG:HA	2.28	0.48
1:D:233:GLU:O	1:D:236:VAL:HG12	2.14	0.48
1:D:255:LYS:HG2	1:D:256:ASP:OD2	2.13	0.48
1:D:469:LEU:O	1:D:473:MSE:HB2	2.14	0.48
1:D:496:ALA:HB2	1:D:755:PHE:CD2	2.49	0.48
1:D:617:ALA:O	1:D:621:LEU:HB2	2.14	0.48
1:E:130:VAL:HG22	1:E:131:CYS:O	2.14	0.48
1:E:391:PRO:C	1:E:392:ILE:HD12	2.34	0.48
1:E:485:GLN:HG2	1:E:488:TYR:CD2	2.49	0.48
1:E:538:ILE:HG12	1:E:662:VAL:HG21	1.94	0.48
1:E:624:VAL:CG1	1:E:637:LYS:HB3	2.44	0.48
1:F:113:LEU:O	1:F:117:PHE:HB2	2.13	0.48
1:C:127:PRO:HG3	1:C:203:LEU:HD21	1.96	0.48
1:C:506:ILE:HG22	1:C:508:LEU:HG	1.95	0.48
1:D:218:ILE:HD12	1:D:356:LEU:HD23	1.96	0.48
1:D:263:PHE:HD1	1:D:292:LEU:HD23	1.79	0.48
1:D:403:VAL:CG1	1:D:466:THR:HB	2.44	0.48
1:D:470:ALA:HB1	1:D:481:LEU:HD11	1.96	0.48
1:D:524:VAL:HG23	1:D:535:LEU:HB2	1.96	0.48
1:E:17:PHE:HZ	1:E:60:LEU:HD21	1.77	0.48
1:E:323:PRO:HG2	1:E:324:VAL:H	1.79	0.48
1:E:455:LEU:HA	1:E:479:VAL:HG12	1.95	0.48
1:F:16:GLY:HA2	1:F:132:THR:OG1	2.13	0.48
1:F:16:GLY:O	1:F:19:PRO:HD2	2.14	0.48
1:F:690:ALA:O	1:F:725:ILE:HG12	2.13	0.48
1:A:573:VAL:HG13	1:A:574:ILE:N	2.29	0.47
1:C:149:GLU:HB2	1:C:154:LYS:HZ3	1.78	0.47
1:C:275:THR:HA	1:C:279:ARG:HE	1.79	0.47
1:C:589:LYS:HG3	1:F:475:ASN:OD1	2.14	0.47
1:D:279:ARG:HG3	1:D:309:TYR:HB3	1.96	0.47
1:D:381:ILE:HG22	1:D:717:TYR:CE1	2.48	0.47
1:E:118:ASP:HA	1:E:119:PRO:HD3	1.72	0.47
1:E:177:GLU:HB2	1:E:178:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:CYS:SG	1:E:229:ASP:N	2.87	0.47
1:E:595:VAL:O	1:E:595:VAL:HG12	2.13	0.47
1:F:50:GLU:O	1:F:53:ILE:HG22	2.15	0.47
1:F:264:ALA:HB1	1:F:286:LYS:HA	1.94	0.47
1:F:380:VAL:CG1	1:F:381:ILE:N	2.77	0.47
1:F:460:LEU:HB2	1:F:485:GLN:HA	1.96	0.47
1:A:18:ARG:HB2	1:A:19:PRO:HD3	1.96	0.47
1:A:204:ARG:HG2	1:A:319:TRP:CZ2	2.48	0.47
1:A:520:TRP:HA	1:A:609:SER:OG	2.14	0.47
1:A:534:ARG:HG2	1:A:535:LEU:H	1.76	0.47
1:B:204:ARG:HG3	1:B:319:TRP:CE2	2.49	0.47
1:B:424:TYR:CZ	1:B:426:GLY:HA2	2.50	0.47
1:B:487:HIS:CE1	1:B:512:GLY:HA3	2.49	0.47
1:C:357:LEU:N	1:C:357:LEU:HD23	2.29	0.47
1:C:380:VAL:HG23	1:C:740:THR:HA	1.96	0.47
1:C:387:PHE:O	1:C:390:LEU:HG	2.14	0.47
1:C:567:ILE:HG23	1:C:600:ALA:HB2	1.95	0.47
1:D:270:GLU:CB	1:D:373:PHE:HE2	2.26	0.47
1:D:709:VAL:O	1:D:735:ASN:HB2	2.14	0.47
1:E:651:PHE:HB2	1:E:688:ALA:HB2	1.95	0.47
1:F:301:HIS:CD2	1:F:302:THR:HG23	2.49	0.47
1:F:407:LEU:HB3	1:F:631:GLU:OE1	2.14	0.47
1:F:453:LEU:HG	1:F:453:LEU:O	2.14	0.47
1:F:485:GLN:HG3	1:F:486:HIS:N	2.29	0.47
1:F:487:HIS:CD2	1:F:520:TRP:HB3	2.49	0.47
1:F:662:VAL:O	1:F:662:VAL:HG12	2.13	0.47
1:A:247:GLN:HG3	1:A:298:PRO:CG	2.44	0.47
1:A:422:SER:HA	1:A:444:PHE:CZ	2.49	0.47
1:A:505:GLY:HA2	1:A:710:ALA:H	1.77	0.47
1:A:589:LYS:N	1:B:475:ASN:ND2	2.60	0.47
1:A:596:LEU:O	1:A:596:LEU:HD23	2.14	0.47
1:B:189:ARG:HA	1:B:202:PRO:HG3	1.97	0.47
1:B:261:LYS:NZ	1:B:266:VAL:HB	2.29	0.47
1:B:496:ALA:HB2	1:B:755:PHE:CD2	2.49	0.47
1:B:526:TYR:CB	1:B:535:LEU:HD11	2.44	0.47
1:B:553:PRO:HB2	1:B:620:VAL:CG2	2.45	0.47
1:B:756:LEU:HD21	1:B:770:LEU:HD22	1.96	0.47
1:C:370:VAL:HG23	1:C:382:ARG:HB2	1.96	0.47
1:C:487:HIS:HD2	1:C:520:TRP:HB3	1.79	0.47
1:D:394:ILE:HD12	1:D:755:PHE:HB2	1.96	0.47
1:D:485:GLN:HB3	1:D:488:TYR:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:495:MSE:SE	1:D:527:LEU:HD13	2.64	0.47
1:D:554:LEU:HD21	1:D:579:PRO:CG	2.44	0.47
1:D:629:HIS:HB2	1:D:633:GLU:OE1	2.14	0.47
1:D:702:ARG:NH2	1:D:731:ALA:O	2.48	0.47
1:E:8:VAL:HA	1:E:72:ARG:O	2.14	0.47
1:E:183:VAL:HG23	1:E:184:CYS:H	1.76	0.47
1:E:210:ILE:CD1	1:E:216:VAL:HG12	2.38	0.47
1:F:406:GLU:HG3	1:F:407:LEU:H	1.80	0.47
1:A:106:ILE:HG22	1:A:107:ALA:N	2.29	0.47
1:A:154:LYS:O	1:A:154:LYS:HD3	2.14	0.47
1:A:487:HIS:CE1	1:A:509:ASP:HB3	2.50	0.47
1:A:516:ASP:O	1:A:517:GLY:C	2.53	0.47
1:B:219:LYS:HA	1:B:224:ILE:CB	2.45	0.47
1:B:310:ALA:O	1:B:313:HIS:HB2	2.14	0.47
1:B:573:VAL:HG13	1:B:574:ILE:N	2.30	0.47
1:B:588:GLY:O	1:B:592:PHE:HB2	2.15	0.47
1:C:216:VAL:HG23	1:C:354:TYR:C	2.34	0.47
1:C:229:ASP:OD1	1:C:322:THR:HG21	2.14	0.47
1:C:309:TYR:H	1:C:313:HIS:CD2	2.32	0.47
1:C:570:LEU:HD12	1:C:573:VAL:HG11	1.96	0.47
1:C:715:VAL:HG12	1:C:715:VAL:O	2.15	0.47
1:D:219:LYS:NZ	1:D:362:ILE:HG12	2.30	0.47
1:E:124:TYR:CD2	1:E:125:MSE:HG2	2.49	0.47
1:E:181:CYS:SG	1:E:182:PRO:HD2	2.54	0.47
1:E:270:GLU:N	1:E:378:ARG:NH1	2.62	0.47
1:E:579:PRO:HB3	1:E:626:TYR:CE1	2.49	0.47
1:E:682:ALA:O	1:E:686:HIS:HB2	2.15	0.47
1:E:726:ARG:HG2	1:E:735:ASN:HD21	1.80	0.47
1:E:727:LYS:O	1:E:730:GLU:HG2	2.15	0.47
1:F:264:ALA:HB1	1:F:285:ARG:O	2.15	0.47
1:F:488:TYR:CD1	1:F:525:LEU:HD13	2.49	0.47
1:A:218:ILE:O	1:A:224:ILE:HB	2.15	0.47
1:A:406:GLU:HA	1:A:466:THR:HG21	1.95	0.47
1:A:450:VAL:HG22	1:A:451:LYS:H	1.79	0.47
1:A:460:LEU:HD12	1:A:483:GLN:HB3	1.97	0.47
1:A:566:SER:N	1:A:569:GLU:HB3	2.28	0.47
1:B:21:VAL:HG11	1:B:44:ILE:HD13	1.96	0.47
1:B:404:GLY:HA2	1:B:753:GLN:HE22	1.78	0.47
1:B:457:ILE:HG22	1:B:458:ALA:H	1.78	0.47
1:C:111:ASP:HB3	1:C:172:ARG:HH12	1.79	0.47
1:C:176:ALA:C	1:C:178:PRO:HD2	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:LEU:HB2	1:D:202:PRO:CB	2.41	0.47
1:D:498:LYS:HE3	1:D:736:PHE:HB3	1.95	0.47
1:D:642:ALA:O	1:D:683:TYR:HB2	2.14	0.47
1:E:399:ASN:O	1:E:452:ASN:HB2	2.14	0.47
1:F:183:VAL:CG2	1:F:184:CYS:N	2.77	0.47
1:A:267:SER:HB2	1:A:270:GLU:HB3	1.94	0.47
1:A:302:THR:HG21	1:A:372:ARG:HE	1.78	0.47
1:B:142:GLU:HB3	1:B:150:ASN:O	2.15	0.47
1:B:253:MSE:SE	1:B:313:HIS:ND1	2.97	0.47
1:C:8:VAL:HG13	1:C:72:ARG:O	2.15	0.47
1:C:104:PRO:HG3	1:C:390:LEU:HD11	1.95	0.47
1:C:356:LEU:C	1:C:357:LEU:HD23	2.35	0.47
1:D:183:VAL:CG2	1:D:184:CYS:N	2.78	0.47
1:D:246:PRO:CG	1:D:629:HIS:HB3	2.45	0.47
1:D:535:LEU:HD23	1:D:700:ARG:HG3	1.95	0.47
1:E:373:PHE:CE2	1:E:378:ARG:HD3	2.49	0.47
1:E:398:TYR:HB2	1:E:454:ASP:CG	2.35	0.47
1:E:413:VAL:HG21	1:E:448:LEU:HD13	1.95	0.47
1:E:553:PRO:HB2	1:E:620:VAL:CG2	2.41	0.47
1:E:665:LEU:HG	1:E:669:ILE:HD11	1.97	0.47
1:F:250:PHE:HE2	1:F:328:THR:OG1	1.96	0.47
1:A:264:ALA:HB1	1:A:285:ARG:O	2.15	0.47
1:A:582:VAL:HG13	1:A:626:TYR:HB3	1.95	0.47
1:A:660:ILE:O	1:A:662:VAL:HG23	2.14	0.47
1:A:677:SER:HB2	1:A:678:PRO:HD2	1.97	0.47
1:B:168:ASP:O	1:B:174:TYR:HB2	2.15	0.47
1:B:370:VAL:CG2	1:B:381:ILE:HD11	2.44	0.47
1:C:286:LYS:HE3	1:C:290:PHE:CA	2.43	0.47
1:C:523:GLU:CD	1:C:523:GLU:N	2.68	0.47
1:C:543:LEU:HD23	1:C:543:LEU:N	2.18	0.47
1:C:729:VAL:HB	1:C:735:ASN:HD22	1.78	0.47
1:C:760:TYR:HE2	1:C:767:LYS:HG2	1.80	0.47
1:D:1:MSE:HE3	1:D:84:ASP:N	2.30	0.47
1:D:13:GLN:HG3	1:D:42:VAL:HG23	1.97	0.47
1:D:111:ASP:CB	1:D:172:ARG:HH12	2.17	0.47
1:D:130:VAL:HG21	1:D:135:GLY:HA3	1.96	0.47
1:D:251:ALA:HB3	1:D:327:MSE:O	2.14	0.47
1:D:286:LYS:HB2	1:D:303:ILE:CD1	2.45	0.47
1:D:403:VAL:HG23	1:D:457:ILE:O	2.15	0.47
1:D:451:LYS:HD3	1:D:477:LEU:CG	2.45	0.47
1:D:504:ILE:HG22	1:D:505:GLY:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:CYS:SG	1:E:135:GLY:N	2.87	0.47
1:E:166:TYR:CE1	1:E:175:HIS:HA	2.50	0.47
1:E:252:ILE:HD13	1:E:303:ILE:CG2	2.45	0.47
1:E:266:VAL:HG22	1:E:284:LEU:HD13	1.97	0.47
1:F:283:THR:OG1	1:F:372:ARG:HB2	2.15	0.47
1:F:300:LEU:CD2	1:F:636:MSE:HE2	2.45	0.47
1:F:374:VAL:HG21	1:F:744:ARG:CZ	2.45	0.47
1:F:408:MSE:HG3	1:F:424:TYR:HE1	1.78	0.47
1:F:504:ILE:HG23	1:F:525:LEU:O	2.15	0.47
1:F:694:ALA:C	1:F:696:THR:N	2.68	0.47
1:A:1:MSE:HB2	1:A:80:PRO:HD2	1.96	0.47
1:A:128:PHE:CD1	1:A:186:PRO:HG2	2.50	0.47
1:A:129:ILE:O	1:A:130:VAL:HB	2.15	0.47
1:A:253:MSE:HE2	1:A:317:PHE:HD1	1.79	0.47
1:B:739:THR:O	1:B:742:VAL:O	2.33	0.47
1:C:451:LYS:HA	1:C:477:LEU:HD21	1.95	0.47
1:D:126:TYR:CD1	1:D:182:PRO:HG3	2.50	0.47
1:D:257:ILE:HA	1:D:260:VAL:HG23	1.96	0.47
1:E:190:LEU:O	1:E:196:GLN:HB2	2.15	0.47
1:E:193:SER:O	1:E:194:ASP:CB	2.59	0.47
1:E:245:ARG:NE	1:E:248:LYS:HB3	2.30	0.47
1:E:370:VAL:HG23	1:E:381:ILE:CG1	2.45	0.47
1:E:406:GLU:HB3	1:E:464:TYR:CG	2.50	0.47
1:F:306:MSE:O	1:F:307:LEU:HD23	2.15	0.47
1:F:509:ASP:CG	1:F:510:GLY:H	2.18	0.47
1:F:595:VAL:O	1:F:595:VAL:HG12	2.15	0.47
1:F:726:ARG:HH21	1:F:727:LYS:HG2	1.76	0.47
1:F:766:THR:OG1	1:F:769:ASP:HB2	2.14	0.47
1:A:131:CYS:SG	1:A:133:ASN:HB2	2.54	0.47
1:A:252:ILE:HG22	1:A:253:MSE:N	2.30	0.47
1:A:283:THR:OG1	1:A:372:ARG:HB2	2.15	0.47
1:A:315:ILE:HG23	1:A:316:LEU:N	2.30	0.47
1:A:515:THR:O	1:A:516:ASP:HB2	2.14	0.47
1:B:284:LEU:O	1:B:302:THR:HA	2.14	0.47
1:C:35:LYS:HG2	1:C:36:ASN:H	1.80	0.47
1:C:147:ASP:HA	1:C:177:GLU:OE2	2.15	0.47
1:C:210:ILE:HD11	1:C:228:CYS:N	2.30	0.47
1:C:456:ILE:HD11	1:C:479:VAL:HB	1.96	0.47
1:C:590:VAL:HG23	1:F:475:ASN:OD1	2.14	0.47
1:D:278:ARG:HG3	1:D:280:PRO:HD3	1.95	0.47
1:D:320:SER:HG	1:D:325:TYR:HE1	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:LEU:HA	1:E:145:PRO:C	2.36	0.47
1:E:204:ARG:HD2	1:E:204:ARG:C	2.36	0.47
1:E:566:SER:HB3	1:E:569:GLU:HG2	1.97	0.47
1:F:286:LYS:CE	1:F:290:PHE:HB2	2.45	0.47
1:F:404:GLY:HA2	1:F:753:GLN:CD	2.35	0.47
1:F:404:GLY:O	1:F:459:ASP:HB2	2.15	0.47
1:A:412:GLY:CA	1:A:750:ASN:HD22	2.22	0.47
1:A:719:GLU:O	1:A:723:LYS:HB2	2.14	0.47
1:B:6:ILE:HG22	1:B:7:HIS:H	1.80	0.47
1:B:566:SER:H	1:B:569:GLU:CB	2.28	0.47
1:B:665:LEU:O	1:B:669:ILE:HG13	2.15	0.47
1:C:66:PRO:CG	1:C:133:ASN:HB3	2.44	0.47
1:C:219:LYS:HZ2	1:C:362:ILE:HG12	1.80	0.47
1:C:251:ALA:HB3	1:C:327:MSE:O	2.14	0.47
1:C:625:ALA:HB2	1:C:637:LYS:CD	2.44	0.47
1:C:718:ASN:ND2	1:C:720:LEU:HB2	2.30	0.47
1:D:17:PHE:CZ	1:D:60:LEU:HD11	2.50	0.47
1:D:66:PRO:HG2	1:D:67:LEU:H	1.80	0.47
1:D:219:LYS:HA	1:D:224:ILE:CB	2.45	0.47
1:D:540:TYR:O	1:D:563:LYS:HE3	2.15	0.47
1:E:383:ARG:HG3	1:E:383:ARG:HH11	1.80	0.47
1:E:486:HIS:O	1:E:489:ALA:HB3	2.14	0.47
1:A:323:PRO:HG2	1:A:324:VAL:H	1.79	0.46
1:B:651:PHE:HB2	1:B:688:ALA:HB2	1.97	0.46
1:C:172:ARG:HG2	1:C:173:ARG:N	2.30	0.46
1:C:274:LEU:O	1:C:307:LEU:HD12	2.15	0.46
1:C:415:LYS:NZ	1:C:448:LEU:HA	2.30	0.46
1:C:427:ASN:ND2	1:C:429:GLY:H	2.12	0.46
1:C:558:MSE:HE1	1:C:593:ASN:OD1	2.15	0.46
1:D:288:GLU:CB	1:D:289:PRO:HD3	2.30	0.46
1:D:299:GLY:O	1:D:300:LEU:HG	2.15	0.46
1:D:371:ILE:HD11	1:D:373:PHE:HE1	1.80	0.46
1:D:409:ASN:HD22	1:D:437:MSE:HE2	1.80	0.46
1:D:589:LYS:HG3	1:D:590:VAL:N	2.25	0.46
1:D:742:VAL:CG1	1:D:751:VAL:HG11	2.45	0.46
1:E:216:VAL:O	1:E:227:ALA:HB3	2.15	0.46
1:E:287:LYS:O	1:E:288:GLU:C	2.53	0.46
1:E:485:GLN:NE2	1:E:486:HIS:H	2.13	0.46
1:F:1:MSE:CB	1:F:80:PRO:HD2	2.46	0.46
1:F:30:LEU:O	1:F:30:LEU:HD23	2.14	0.46
1:F:213:GLY:C	1:F:235:VAL:HG11	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:445:ARG:HH21	1:F:452:ASN:ND2	2.13	0.46
1:F:472:GLU:HG3	1:F:473:MSE:N	2.30	0.46
1:A:400:GLY:O	1:A:413:VAL:HG23	2.15	0.46
1:A:403:VAL:CG1	1:A:466:THR:HB	2.45	0.46
1:B:1:MSE:HE3	1:B:2:LYS:H	1.79	0.46
1:B:137:ARG:O	1:B:141:ILE:HG13	2.15	0.46
1:B:254:ALA:HB1	1:B:259:THR:CB	2.41	0.46
1:C:572:GLY:HA2	1:C:575:ASN:HD22	1.80	0.46
1:D:398:TYR:CE1	1:D:758:GLY:HA3	2.50	0.46
1:D:678:PRO:HG2	1:D:679:ALA:H	1.80	0.46
1:E:443:HIS:O	1:E:447:ILE:HD12	2.15	0.46
1:E:694:ALA:HB2	1:E:725:ILE:HG23	1.96	0.46
1:F:394:ILE:HG22	1:F:396:PHE:H	1.81	0.46
1:F:456:ILE:HD11	1:F:479:VAL:HB	1.98	0.46
1:F:507:ALA:HA	1:F:712:SER:O	2.16	0.46
1:F:584:SER:CB	1:F:589:LYS:HB3	2.46	0.46
1:A:88:ILE:HG22	1:A:89:GLU:N	2.30	0.46
1:A:123:ARG:HE	1:A:173:ARG:HH21	1.62	0.46
1:B:154:LYS:HD3	1:B:154:LYS:C	2.36	0.46
1:B:217:ALA:O	1:B:218:ILE:HD13	2.16	0.46
1:B:365:ARG:O	1:B:423:GLN:HG2	2.16	0.46
1:B:437:MSE:HG2	1:B:441:ILE:HD11	1.97	0.46
1:B:491:ILE:CD1	1:B:525:LEU:HD12	2.45	0.46
1:C:323:PRO:HG2	1:C:324:VAL:H	1.80	0.46
1:C:550:SER:O	1:C:628:ARG:HD2	2.14	0.46
1:D:158:MSE:HE1	1:D:166:TYR:CD2	2.49	0.46
1:D:455:LEU:HA	1:D:479:VAL:HG12	1.97	0.46
1:D:472:GLU:HG3	1:D:473:MSE:N	2.30	0.46
1:E:343:ARG:HG2	1:E:343:ARG:HH11	1.81	0.46
1:F:282:ILE:HA	1:F:371:ILE:O	2.15	0.46
1:A:690:ALA:CB	1:A:721:ILE:HG23	2.46	0.46
1:B:376:GLY:O	1:B:377:LYS:HG3	2.15	0.46
1:B:428:THR:HG21	1:B:437:MSE:HE1	1.96	0.46
1:B:582:VAL:CG1	1:B:626:TYR:HB3	2.46	0.46
1:B:584:SER:CB	1:B:589:LYS:HB3	2.44	0.46
1:B:707:LYS:HG3	1:B:708:ASN:CG	2.36	0.46
1:C:8:VAL:HG22	1:C:72:ARG:O	2.16	0.46
1:C:65:PRO:C	1:C:67:LEU:H	2.17	0.46
1:C:213:GLY:C	1:C:235:VAL:HG11	2.35	0.46
1:C:409:ASN:HB3	1:C:425:ILE:HD11	1.97	0.46
1:C:486:HIS:O	1:C:489:ALA:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:ARG:O	1:D:21:VAL:HG12	2.16	0.46
1:D:268:PRO:C	1:D:270:GLU:H	2.18	0.46
1:D:270:GLU:HB2	1:D:373:PHE:CE2	2.48	0.46
1:D:370:VAL:HG23	1:D:381:ILE:HG13	1.97	0.46
1:E:124:TYR:CE2	1:E:125:MSE:HG2	2.50	0.46
1:F:16:GLY:HA3	1:F:132:THR:O	2.15	0.46
1:F:279:ARG:HG3	1:F:309:TYR:HB3	1.96	0.46
1:F:335:MSE:HE2	1:F:335:MSE:N	2.30	0.46
1:F:495:MSE:HG3	1:F:755:PHE:CE2	2.50	0.46
1:A:18:ARG:HG3	1:A:18:ARG:NH1	2.30	0.46
1:B:269:GLU:HB2	1:B:378:ARG:NH2	2.31	0.46
1:B:398:TYR:CG	1:B:398:TYR:O	2.69	0.46
1:B:406:GLU:HG3	1:B:407:LEU:HG	1.97	0.46
1:B:522:GLY:CA	1:B:611:THR:HG23	2.46	0.46
1:B:555:ARG:NH2	1:B:595:VAL:HG11	2.31	0.46
1:C:330:ALA:HB1	1:C:348:LEU:HD21	1.96	0.46
1:D:123:ARG:HD3	1:D:129:ILE:HG13	1.98	0.46
1:D:225:HIS:HA	1:D:330:ALA:H	1.80	0.46
1:D:433:VAL:O	1:D:436:PHE:HB3	2.15	0.46
1:E:88:ILE:HD12	1:E:88:ILE:N	2.30	0.46
1:E:312:THR:HA	1:E:315:ILE:CG2	2.45	0.46
1:F:203:LEU:HD12	1:F:319:TRP:CZ3	2.46	0.46
1:F:374:VAL:HG21	1:F:744:ARG:NH1	2.30	0.46
1:F:380:VAL:HG23	1:F:740:THR:CA	2.39	0.46
1:F:380:VAL:HG12	1:F:381:ILE:H	1.78	0.46
1:A:210:ILE:O	1:A:229:ASP:HB2	2.15	0.46
1:A:540:TYR:HA	1:A:608:ALA:O	2.15	0.46
1:A:542:PRO:O	1:A:559:GLY:CA	2.61	0.46
1:A:582:VAL:HG11	1:A:626:TYR:HB3	1.97	0.46
1:A:616:ASP:O	1:A:619:ALA:HB3	2.15	0.46
1:B:24:ILE:HG23	1:B:56:PHE:CE1	2.50	0.46
1:B:165:GLU:HB3	1:B:171:ASN:CG	2.36	0.46
1:B:371:ILE:CD1	1:B:380:VAL:HG22	2.42	0.46
1:B:651:PHE:HB2	1:B:688:ALA:CB	2.46	0.46
1:C:273:GLU:CG	1:C:371:ILE:HD13	2.41	0.46
1:C:331:ASN:ND2	1:C:337:MSE:HA	2.20	0.46
1:C:522:GLY:HA2	1:C:611:THR:HG23	1.97	0.46
1:D:7:HIS:CD2	1:D:43:GLU:HG3	2.51	0.46
1:D:32:GLY:HA3	1:D:45:VAL:O	2.15	0.46
1:D:383:ARG:H	1:D:747:ASN:ND2	2.13	0.46
1:D:391:PRO:HB3	1:D:420:TYR:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:447:ILE:O	1:D:447:ILE:HG22	2.16	0.46
1:D:523:GLU:HG3	1:D:537:HIS:HB2	1.96	0.46
1:D:584:SER:HB3	1:D:589:LYS:HB3	1.98	0.46
1:D:618:ILE:O	1:D:622:LEU:HG	2.15	0.46
1:E:7:HIS:HB2	1:E:74:GLU:HB2	1.98	0.46
1:E:286:LYS:HD2	1:E:303:ILE:CD1	2.45	0.46
1:E:707:LYS:O	1:E:733:GLY:HA3	2.15	0.46
1:E:742:VAL:HG11	1:E:751:VAL:HG11	1.98	0.46
1:F:278:ARG:CG	1:F:280:PRO:HD3	2.46	0.46
1:A:171:ASN:ND2	1:A:173:ARG:HB2	2.30	0.46
1:A:239:LEU:O	1:A:239:LEU:HD23	2.16	0.46
1:A:239:LEU:HD13	1:A:250:PHE:CE1	2.50	0.46
1:A:276:SER:OG	1:A:278:ARG:HG2	2.15	0.46
1:A:592:PHE:O	1:A:595:VAL:HB	2.15	0.46
1:B:255:LYS:HG2	1:B:256:ASP:OD2	2.16	0.46
1:B:312:THR:HA	1:B:315:ILE:HG22	1.98	0.46
1:C:399:ASN:HD22	1:C:399:ASN:N	2.12	0.46
1:C:486:HIS:HD2	1:C:487:HIS:ND1	2.13	0.46
1:C:620:VAL:C	1:C:622:LEU:N	2.68	0.46
1:D:57:ILE:HG13	1:D:75:LYS:HZ1	1.79	0.46
1:D:749:VAL:O	1:D:753:GLN:HG3	2.16	0.46
1:E:104:PRO:HB3	1:E:387:PHE:O	2.16	0.46
1:E:570:LEU:O	1:E:574:ILE:HG12	2.16	0.46
1:E:589:LYS:HG3	1:E:590:VAL:HG23	1.97	0.46
1:F:247:GLN:HG3	1:F:298:PRO:CG	2.41	0.46
1:A:380:VAL:CG2	1:A:740:THR:HG23	2.45	0.46
1:A:664:GLU:O	1:A:667:GLN:HB3	2.16	0.46
1:B:181:CYS:SG	1:B:182:PRO:HD2	2.56	0.46
1:B:587:TYR:CD1	1:B:588:GLY:N	2.78	0.46
1:C:226:LEU:HD11	1:C:348:LEU:HD23	1.97	0.46
1:C:371:ILE:CD1	1:C:380:VAL:HG22	2.36	0.46
1:D:127:PRO:O	1:D:311:GLY:HA3	2.16	0.46
1:D:190:LEU:HD12	1:D:355:PHE:O	2.16	0.46
1:D:286:LYS:HZ3	1:D:292:LEU:HB2	1.80	0.46
1:D:380:VAL:HG23	1:D:740:THR:CA	2.42	0.46
1:D:475:ASN:HD21	1:E:590:VAL:N	2.14	0.46
1:E:16:GLY:O	1:E:19:PRO:HD2	2.16	0.46
1:E:525:LEU:HA	1:E:535:LEU:HD13	1.98	0.46
1:F:144:LEU:HA	1:F:145:PRO:C	2.36	0.46
1:F:218:ILE:O	1:F:224:ILE:HG23	2.16	0.46
1:A:121:ASN:HD22	1:A:123:ARG:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:TYR:C	1:A:466:THR:H	2.19	0.46
1:A:580:LYS:C	1:A:582:VAL:H	2.18	0.46
1:A:670:LEU:HA	1:A:673:ILE:HG12	1.98	0.46
1:A:759:LEU:CD2	1:A:764:TYR:HB2	2.46	0.46
1:B:189:ARG:O	1:B:356:LEU:HA	2.15	0.46
1:B:410:ALA:HB3	1:B:747:ASN:O	2.16	0.46
1:D:114:ARG:O	1:D:118:ASP:HB2	2.16	0.46
1:D:268:PRO:HG2	1:D:378:ARG:HH22	1.81	0.46
1:E:335:MSE:CE	1:E:430:LYS:HG3	2.46	0.46
1:E:541:TYR:CG	1:E:560:ILE:HG22	2.51	0.46
1:E:545:GLY:HA3	1:E:548:LEU:HD12	1.98	0.46
1:F:205:LYS:HA	1:F:208:GLU:HG3	1.98	0.46
1:F:380:VAL:CG2	1:F:740:THR:HG23	2.46	0.46
1:F:413:VAL:CG1	1:F:420:TYR:HB2	2.46	0.46
1:F:460:LEU:CD2	1:F:515:THR:HG22	2.45	0.46
1:F:542:PRO:HD2	1:F:563:LYS:HG3	1.98	0.46
1:A:126:TYR:OH	1:A:185:GLY:HA3	2.15	0.46
1:A:225:HIS:CD2	1:A:327:MSE:HB3	2.51	0.46
1:A:365:ARG:O	1:A:423:GLN:HG2	2.16	0.46
1:A:445:ARG:NH2	1:A:452:ASN:ND2	2.63	0.46
1:A:543:LEU:HD23	1:A:606:ALA:O	2.16	0.46
1:A:660:ILE:HG22	1:A:662:VAL:HG22	1.97	0.46
1:B:205:LYS:O	1:B:208:GLU:HB3	2.16	0.46
1:B:228:CYS:SG	1:B:235:VAL:HG23	2.56	0.46
1:B:538:ILE:HG23	1:B:662:VAL:CG2	2.46	0.46
1:C:485:GLN:CG	1:C:488:TYR:H	2.20	0.46
1:C:582:VAL:HG21	1:C:626:TYR:HB3	1.97	0.46
1:C:726:ARG:HH21	1:C:727:LYS:HA	1.81	0.46
1:C:738:VAL:HG21	1:C:744:ARG:HB3	1.98	0.46
1:D:410:ALA:HB3	1:D:747:ASN:O	2.16	0.46
1:D:432:GLU:H	1:D:432:GLU:CD	2.19	0.46
1:E:20:PHE:CZ	1:E:63:LYS:HB3	2.51	0.46
1:E:219:LYS:HA	1:E:224:ILE:HB	1.98	0.46
1:E:301:HIS:CD2	1:E:301:HIS:N	2.83	0.46
1:E:369:SER:HB2	1:E:385:ARG:HB3	1.97	0.46
1:F:163:ARG:HA	1:F:166:TYR:HB3	1.97	0.46
1:F:191:TYR:CD1	1:F:196:GLN:HB3	2.50	0.46
1:A:288:GLU:CB	1:A:289:PRO:HD3	2.34	0.45
1:A:310:ALA:O	1:A:311:GLY:C	2.54	0.45
1:A:651:PHE:HB2	1:A:688:ALA:HB2	1.97	0.45
1:B:15:VAL:HG12	1:B:16:GLY:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:PHE:O	1:B:24:ILE:HG22	2.16	0.45
1:B:25:ALA:HA	1:B:56:PHE:HE1	1.80	0.45
1:B:751:VAL:HG13	1:B:752:GLY:H	1.80	0.45
1:C:151:THR:O	1:C:154:LYS:HB2	2.17	0.45
1:C:557:LEU:O	1:C:561:LEU:HG	2.15	0.45
1:C:595:VAL:O	1:C:595:VAL:HG12	2.16	0.45
1:C:649:LEU:HD12	1:C:650:LYS:N	2.31	0.45
1:D:88:ILE:N	1:D:88:ILE:HD12	2.30	0.45
1:D:233:GLU:HA	1:D:236:VAL:HG12	1.98	0.45
1:D:406:GLU:HG3	1:D:407:LEU:N	2.31	0.45
1:E:270:GLU:HB2	1:E:373:PHE:CE2	2.34	0.45
1:E:738:VAL:CG2	1:E:744:ARG:HG2	2.35	0.45
1:F:749:VAL:O	1:F:753:GLN:HG3	2.16	0.45
1:A:9:GLN:NE2	1:A:40:ALA:HB1	2.31	0.45
1:A:383:ARG:HD2	1:A:387:PHE:CD2	2.52	0.45
1:A:451:LYS:HD3	1:A:477:LEU:HD11	1.97	0.45
1:B:139:THR:HG21	1:B:222:GLY:HA3	1.97	0.45
1:C:163:ARG:NH1	1:C:163:ARG:HB2	2.31	0.45
1:C:274:LEU:HD23	1:C:274:LEU:HA	1.71	0.45
1:C:485:GLN:CG	1:C:488:TYR:HB2	2.46	0.45
1:C:495:MSE:HE2	1:C:755:PHE:HZ	1.81	0.45
1:D:116:LEU:HG	1:D:117:PHE:N	2.32	0.45
1:D:138:PHE:HB2	1:D:389:PRO:HD3	1.97	0.45
1:D:144:LEU:HA	1:D:145:PRO:C	2.37	0.45
1:D:181:CYS:HG	1:D:183:VAL:HG22	1.82	0.45
1:D:261:LYS:HA	1:D:264:ALA:O	2.16	0.45
1:D:475:ASN:ND2	1:E:591:GLU:H	2.13	0.45
1:E:62:LYS:O	1:E:63:LYS:HG3	2.16	0.45
1:E:269:GLU:HB2	1:E:378:ARG:NH2	2.32	0.45
1:F:13:GLN:HB2	1:F:42:VAL:HG22	1.98	0.45
1:F:263:PHE:HD1	1:F:292:LEU:HD23	1.81	0.45
1:A:216:VAL:O	1:A:227:ALA:HB3	2.16	0.45
1:A:558:MSE:HE1	1:A:593:ASN:OD1	2.16	0.45
1:A:737:HIS:O	1:A:738:VAL:C	2.55	0.45
1:B:743:PRO:HG3	1:B:747:ASN:ND2	2.32	0.45
1:D:203:LEU:HD21	1:D:315:ILE:HG21	1.99	0.45
1:D:253:MSE:HE1	1:D:313:HIS:CG	2.51	0.45
1:D:370:VAL:CG2	1:D:381:ILE:HD11	2.47	0.45
1:D:557:LEU:HD23	1:D:557:LEU:C	2.37	0.45
1:D:752:GLY:O	1:D:756:LEU:HB2	2.16	0.45
1:F:217:ALA:HA	1:F:226:LEU:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:506:ILE:CD1	1:F:694:ALA:HA	2.46	0.45
1:F:619:ALA:HA	1:F:638:LEU:HD13	1.97	0.45
1:F:642:ALA:HB1	1:F:683:TYR:HA	1.98	0.45
1:A:134:CYS:SG	1:A:135:GLY:N	2.90	0.45
1:A:158:MSE:HE3	1:A:163:ARG:HH12	1.81	0.45
1:A:168:ASP:O	1:A:174:TYR:HD2	2.00	0.45
1:A:293:PRO:C	1:A:295:ASN:H	2.19	0.45
1:A:739:THR:O	1:A:740:THR:C	2.55	0.45
1:B:738:VAL:HG12	1:B:742:VAL:O	2.17	0.45
1:C:67:LEU:HD21	1:C:106:ILE:HD11	1.98	0.45
1:C:140:ILE:HB	1:C:152:THR:CG2	2.46	0.45
1:C:154:LYS:C	1:C:156:PHE:H	2.18	0.45
1:C:239:LEU:HD22	1:C:250:PHE:CE1	2.51	0.45
1:C:398:TYR:CE1	1:C:758:GLY:HA3	2.51	0.45
1:D:165:GLU:HB3	1:D:171:ASN:ND2	2.31	0.45
1:E:15:VAL:HG12	1:E:16:GLY:N	2.31	0.45
1:E:485:GLN:NE2	1:E:486:HIS:N	2.64	0.45
1:F:589:LYS:HG3	1:F:590:VAL:HG23	1.98	0.45
1:A:38:GLY:C	1:A:40:ALA:H	2.20	0.45
1:A:240:ARG:HB3	1:A:245:ARG:O	2.17	0.45
1:A:288:GLU:HB3	1:A:289:PRO:CD	2.33	0.45
1:A:320:SER:O	1:A:322:THR:N	2.50	0.45
1:B:265:TYR:HE2	1:B:287:LYS:HD2	1.81	0.45
1:B:331:ASN:HD22	1:B:337:MSE:CA	2.23	0.45
1:C:411:PHE:CZ	1:C:441:ILE:HA	2.51	0.45
1:C:742:VAL:CG1	1:C:751:VAL:HG11	2.47	0.45
1:D:142:GLU:O	1:D:143:ASP:HB2	2.16	0.45
1:D:365:ARG:O	1:D:423:GLN:HG2	2.16	0.45
1:D:391:PRO:HB2	1:D:418:LYS:HB2	1.98	0.45
1:F:321:LYS:HB2	1:F:322:THR:H	1.61	0.45
1:A:219:LYS:HG3	1:A:224:ILE:HG22	1.98	0.45
1:A:235:VAL:HG23	1:A:236:VAL:N	2.32	0.45
1:A:553:PRO:HB2	1:A:620:VAL:CG2	2.33	0.45
1:A:591:GLU:O	1:A:594:VAL:HB	2.16	0.45
1:B:134:CYS:SG	1:B:135:GLY:N	2.89	0.45
1:B:268:PRO:C	1:B:270:GLU:N	2.69	0.45
1:B:288:GLU:HB3	1:B:289:PRO:CD	2.33	0.45
1:B:374:VAL:CG1	1:B:744:ARG:HH22	2.28	0.45
1:C:148:ARG:NH2	1:C:156:PHE:O	2.49	0.45
1:C:331:ASN:HD22	1:C:337:MSE:CA	2.20	0.45
1:D:249:PRO:HG3	1:D:300:LEU:CD1	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:LYS:HE3	1:D:291:PRO:CD	2.46	0.45
1:D:455:LEU:HD13	1:D:456:ILE:O	2.16	0.45
1:E:447:ILE:HG22	1:E:447:ILE:O	2.17	0.45
1:E:524:VAL:HG23	1:E:536:ALA:H	1.81	0.45
1:E:551:TYR:O	1:E:628:ARG:HB3	2.16	0.45
1:E:579:PRO:O	1:E:582:VAL:HG23	2.17	0.45
1:F:179:THR:HG23	1:F:179:THR:O	2.17	0.45
1:F:557:LEU:HD11	1:F:621:LEU:HA	1.99	0.45
1:F:585:LEU:HB2	1:F:627:ARG:NH1	2.31	0.45
1:A:475:ASN:HD21	1:B:590:VAL:N	2.14	0.45
1:A:633:GLU:N	1:A:634:PRO:CD	2.79	0.45
1:B:130:VAL:HG11	1:B:178:PRO:O	2.17	0.45
1:B:445:ARG:C	1:B:447:ILE:H	2.20	0.45
1:B:524:VAL:HG22	1:B:536:ALA:H	1.81	0.45
1:B:765:LEU:HD21	1:B:770:LEU:CD2	2.40	0.45
1:C:306:MSE:CE	1:C:309:TYR:HE2	2.30	0.45
1:C:592:PHE:O	1:C:595:VAL:HB	2.17	0.45
1:C:717:TYR:CE1	1:C:744:ARG:HG3	2.51	0.45
1:D:31:ARG:HG2	1:D:85:ARG:HA	1.98	0.45
1:D:202:PRO:O	1:D:203:LEU:C	2.54	0.45
1:D:239:LEU:HD23	1:D:239:LEU:C	2.37	0.45
1:D:589:LYS:HG3	1:D:590:VAL:HG23	1.98	0.45
1:E:335:MSE:HE1	1:E:430:LYS:HG3	1.99	0.45
1:E:370:VAL:CG2	1:E:381:ILE:HD11	2.46	0.45
1:E:397:GLU:HB2	1:E:416:ASN:HA	1.99	0.45
1:E:414:ALA:HB2	1:E:419:VAL:HA	1.99	0.45
1:E:415:LYS:HD3	1:E:448:LEU:CD2	2.44	0.45
1:E:450:VAL:HG22	1:E:451:LYS:N	2.31	0.45
1:F:252:ILE:HG23	1:F:325:TYR:O	2.17	0.45
1:F:270:GLU:N	1:F:378:ARG:NH1	2.64	0.45
1:F:398:TYR:O	1:F:398:TYR:CG	2.70	0.45
1:F:428:THR:HA	1:F:433:VAL:HG11	1.99	0.45
1:F:613:ARG:HA	1:F:613:ARG:NE	2.29	0.45
1:F:620:VAL:C	1:F:622:LEU:N	2.69	0.45
1:A:124:TYR:CD2	1:A:125:MSE:HG2	2.51	0.45
1:A:532:VAL:HG12	1:A:533:GLU:N	2.32	0.45
1:A:589:LYS:HG2	1:B:475:ASN:OD1	2.17	0.45
1:B:530:GLU:O	1:B:531:ASP:HB2	2.16	0.45
1:B:616:ASP:HA	1:B:634:PRO:HB2	1.99	0.45
1:B:766:THR:OG1	1:B:769:ASP:HB2	2.17	0.45
1:C:61:TYR:CD2	1:C:61:TYR:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ARG:CB	1:C:309:TYR:HB3	2.47	0.45
1:C:394:ILE:CD1	1:C:419:VAL:HB	2.47	0.45
1:C:534:ARG:HG2	1:C:535:LEU:N	2.31	0.45
1:D:345:PHE:C	1:D:347:GLU:H	2.20	0.45
1:D:387:PHE:O	1:D:390:LEU:HG	2.17	0.45
1:D:565:TYR:HB3	1:D:569:GLU:HB2	1.98	0.45
1:D:581:ALA:HA	1:D:584:SER:HB3	1.98	0.45
1:D:582:VAL:C	1:D:584:SER:H	2.19	0.45
1:E:151:THR:O	1:E:154:LYS:HB2	2.16	0.45
1:E:393:GLU:HA	1:E:417:GLY:O	2.17	0.45
1:E:460:LEU:HD12	1:E:483:GLN:HB3	1.98	0.45
1:E:629:HIS:HB2	1:E:633:GLU:OE1	2.17	0.45
1:F:274:LEU:HB3	1:F:307:LEU:HD11	1.99	0.45
1:F:282:ILE:HG23	1:F:283:THR:N	2.32	0.45
1:F:369:SER:OG	1:F:384:SER:N	2.49	0.45
1:F:429:GLY:HA2	1:F:465:ASN:ND2	2.32	0.45
1:A:3:ALA:HB2	1:A:47:GLU:CA	2.44	0.45
1:A:108:ILE:CG1	1:A:310:ALA:HA	2.34	0.45
1:A:292:LEU:HB3	1:A:296:LEU:HD22	1.99	0.45
1:A:653:VAL:CG1	1:A:692:ALA:HB3	2.46	0.45
1:B:219:LYS:HE2	1:B:358:HIS:O	2.17	0.45
1:B:250:PHE:CD2	1:B:328:THR:HG21	2.52	0.45
1:B:270:GLU:CD	1:B:284:LEU:HD21	2.37	0.45
1:B:415:LYS:C	1:B:417:GLY:H	2.19	0.45
1:B:443:HIS:O	1:B:447:ILE:HD12	2.16	0.45
1:C:196:GLN:CG	1:C:197:GLU:N	2.77	0.45
1:C:553:PRO:HB2	1:C:620:VAL:CG2	2.46	0.45
1:D:306:MSE:HE1	1:D:309:TYR:HE2	1.82	0.45
1:D:376:GLY:HA2	1:D:726:ARG:HH11	1.81	0.45
1:E:230:ALA:HB3	1:E:324:VAL:CG2	2.47	0.45
1:E:286:LYS:HE3	1:E:290:PHE:CB	2.46	0.45
1:E:474:ALA:HB2	1:E:481:LEU:HD13	1.98	0.45
1:E:521:GLY:CA	1:E:610:SER:HA	2.46	0.45
1:F:89:GLU:HG3	1:F:175:HIS:CE1	2.52	0.45
1:F:373:PHE:CD2	1:F:378:ARG:HD3	2.52	0.45
1:A:207:ALA:HB1	1:A:320:SER:CB	2.42	0.45
1:A:225:HIS:HA	1:A:330:ALA:H	1.82	0.45
1:A:263:PHE:HE1	1:A:292:LEU:HG	1.81	0.45
1:A:428:THR:HG21	1:A:466:THR:HG22	1.99	0.45
1:A:466:THR:OG1	1:A:467:THR:N	2.50	0.45
1:A:738:VAL:HB	1:A:744:ARG:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LYS:HB2	1:B:357:LEU:HA	1.99	0.45
1:B:371:ILE:CB	1:B:380:VAL:HG13	2.43	0.45
1:B:461:HIS:HB2	1:B:513:TYR:CB	2.47	0.45
1:B:614:VAL:HG13	1:B:666:PHE:CZ	2.52	0.45
1:C:270:GLU:O	1:C:274:LEU:HB2	2.16	0.45
1:C:641:PHE:CE2	1:C:679:ALA:HA	2.52	0.45
1:D:142:GLU:HB3	1:D:150:ASN:C	2.36	0.45
1:D:292:LEU:HD12	1:D:296:LEU:HD21	1.99	0.45
1:D:552:TYR:CD1	1:D:627:ARG:HG3	2.52	0.45
1:D:739:THR:OG1	1:D:740:THR:N	2.49	0.45
1:E:232:ASN:HB3	1:E:235:VAL:CG2	2.46	0.45
1:E:504:ILE:CG2	1:E:505:GLY:N	2.80	0.45
1:F:11:ILE:HG12	1:F:15:VAL:HG21	1.98	0.45
1:F:294:GLU:O	1:F:294:GLU:HG2	2.17	0.45
1:F:384:SER:HB2	1:F:385:ARG:H	1.57	0.45
1:F:573:VAL:HG13	1:F:574:ILE:N	2.31	0.45
1:A:157:PRO:O	1:A:184:CYS:HB2	2.16	0.44
1:A:409:ASN:CG	1:A:425:ILE:HD11	2.37	0.44
1:A:709:VAL:O	1:A:735:ASN:HB2	2.17	0.44
1:B:159:CYS:SG	1:B:183:VAL:HG21	2.58	0.44
1:B:270:GLU:OE2	1:B:284:LEU:HD21	2.17	0.44
1:B:506:ILE:HG22	1:B:508:LEU:HG	1.98	0.44
1:B:568:ASP:O	1:B:571:GLU:HB3	2.17	0.44
1:C:144:LEU:HA	1:C:145:PRO:C	2.37	0.44
1:C:292:LEU:HD13	1:C:293:PRO:CD	2.43	0.44
1:C:487:HIS:CD2	1:C:520:TRP:HB3	2.51	0.44
1:D:118:ASP:HA	1:D:119:PRO:HD3	1.74	0.44
1:D:191:TYR:HA	1:D:195:GLY:O	2.17	0.44
1:D:246:PRO:HG2	1:D:629:HIS:HB3	1.97	0.44
1:D:274:LEU:HD21	1:D:282:ILE:HG22	1.99	0.44
1:D:300:LEU:HD21	1:D:636:MSE:HE2	1.99	0.44
1:D:447:ILE:N	1:D:447:ILE:HD12	2.32	0.44
1:E:24:ILE:HG12	1:E:56:PHE:CD1	2.51	0.44
1:E:257:ILE:HA	1:E:260:VAL:CG2	2.46	0.44
1:E:372:ARG:NH2	1:E:717:TYR:HB3	2.31	0.44
1:E:522:GLY:HA2	1:E:611:THR:HG23	1.98	0.44
1:E:523:GLU:HB2	1:E:525:LEU:HD21	1.99	0.44
1:F:44:ILE:HG22	1:F:45:VAL:H	1.82	0.44
1:F:413:VAL:HG11	1:F:448:LEU:HD11	1.99	0.44
1:A:116:LEU:HG	1:A:117:PHE:N	2.32	0.44
1:A:251:ALA:O	1:A:326:VAL:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ASN:HA	1:A:414:ALA:O	2.17	0.44
1:A:732:ASN:OD1	1:A:733:GLY:N	2.51	0.44
1:B:7:HIS:CD2	1:B:43:GLU:HB3	2.52	0.44
1:B:487:HIS:CE1	1:B:509:ASP:HB3	2.52	0.44
1:C:34:VAL:HG23	1:C:43:GLU:O	2.18	0.44
1:C:66:PRO:HD3	1:C:133:ASN:HB3	1.99	0.44
1:C:233:GLU:HB2	1:C:293:PRO:HB3	1.99	0.44
1:C:554:LEU:CG	1:C:558:MSE:HE3	2.47	0.44
1:C:614:VAL:HG13	1:C:666:PHE:CE2	2.53	0.44
1:D:253:MSE:HA	1:D:306:MSE:O	2.16	0.44
1:D:312:THR:O	1:D:315:ILE:HG22	2.18	0.44
1:D:552:TYR:HD1	1:D:627:ARG:HG3	1.82	0.44
1:D:584:SER:CB	1:D:589:LYS:HB3	2.47	0.44
1:E:425:ILE:HG22	1:E:436:PHE:CD1	2.52	0.44
1:E:543:LEU:HD12	1:E:549:ALA:CB	2.46	0.44
1:F:35:LYS:CG	1:F:90:LYS:HD2	2.41	0.44
1:F:62:LYS:C	1:F:64:LYS:H	2.20	0.44
1:F:67:LEU:CD1	1:F:106:ILE:HD13	2.47	0.44
1:F:497:GLU:CD	1:F:739:THR:HG22	2.37	0.44
1:F:522:GLY:CA	1:F:611:THR:HG23	2.47	0.44
1:F:524:VAL:CG2	1:F:536:ALA:H	2.30	0.44
1:F:619:ALA:HB2	1:F:638:LEU:HD22	1.98	0.44
1:F:639:GLU:OE2	1:F:718:ASN:HA	2.16	0.44
1:A:263:PHE:O	1:A:264:ALA:HB2	2.18	0.44
1:A:529:TYR:CE1	1:A:759:LEU:HD11	2.52	0.44
1:A:772:LEU:HD11	1:B:601:LYS:HD3	1.99	0.44
1:B:15:VAL:HG21	1:B:67:LEU:O	2.18	0.44
1:B:383:ARG:NH1	1:B:387:PHE:HB3	2.32	0.44
1:B:401:LEU:HD12	1:B:402:ALA:N	2.32	0.44
1:C:128:PHE:CD1	1:C:186:PRO:HG2	2.53	0.44
1:C:412:GLY:HA3	1:C:750:ASN:ND2	2.32	0.44
1:C:501:ASP:O	1:C:503:VAL:HG22	2.17	0.44
1:C:567:ILE:HG12	1:C:600:ALA:HB1	1.99	0.44
1:D:257:ILE:HD12	1:D:260:VAL:CG2	2.47	0.44
1:D:281:ILE:CB	1:D:370:VAL:HG12	2.36	0.44
1:D:286:LYS:HE3	1:D:291:PRO:HD2	2.00	0.44
1:D:399:ASN:N	1:D:399:ASN:ND2	2.66	0.44
1:D:504:ILE:HG13	1:D:706:VAL:HG21	1.99	0.44
1:D:601:LYS:HZ2	1:E:771:MSE:HE3	1.82	0.44
1:F:329:SER:HA	1:F:337:MSE:HE2	1.99	0.44
1:F:567:ILE:HG12	1:F:600:ALA:HB1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:748:GLY:O	1:F:751:VAL:HG12	2.16	0.44
1:A:252:ILE:CG2	1:A:324:VAL:HB	2.48	0.44
1:A:312:THR:HA	1:A:315:ILE:HG22	2.00	0.44
1:B:6:ILE:HG13	1:B:57:ILE:HD12	1.98	0.44
1:B:25:ALA:HA	1:B:56:PHE:CE1	2.52	0.44
1:B:319:TRP:O	1:B:320:SER:O	2.36	0.44
1:B:337:MSE:CE	1:B:367:ASP:HA	2.41	0.44
1:C:317:PHE:HE2	1:C:323:PRO:CA	2.27	0.44
1:D:219:LYS:HG3	1:D:224:ILE:CG2	2.43	0.44
1:D:261:LYS:HD3	1:D:266:VAL:CG2	2.47	0.44
1:D:281:ILE:HG23	1:D:306:MSE:HG3	2.00	0.44
1:E:286:LYS:CE	1:E:290:PHE:HB2	2.46	0.44
1:E:498:LYS:HB2	1:E:500:LEU:CD1	2.48	0.44
1:A:35:LYS:HG2	1:A:36:ASN:N	2.33	0.44
1:A:401:LEU:HD12	1:A:402:ALA:N	2.32	0.44
1:A:582:VAL:HB	1:A:583:GLU:OE1	2.18	0.44
1:A:748:GLY:O	1:A:751:VAL:HG12	2.18	0.44
1:B:313:HIS:CE1	1:B:327:MSE:HE2	2.49	0.44
1:B:422:SER:HA	1:B:444:PHE:CZ	2.53	0.44
1:B:495:MSE:HA	1:B:500:LEU:HD21	2.00	0.44
1:B:541:TYR:CB	1:B:560:ILE:HG22	2.48	0.44
1:B:572:GLY:O	1:B:575:ASN:HB2	2.17	0.44
1:B:714:GLY:C	1:B:716:ALA:H	2.20	0.44
1:B:738:VAL:HG23	1:B:744:ARG:HG2	1.99	0.44
1:C:30:LEU:O	1:C:30:LEU:HD23	2.18	0.44
1:C:87:TYR:C	1:C:88:ILE:HG13	2.37	0.44
1:C:124:TYR:CE2	1:C:125:MSE:HG2	2.52	0.44
1:C:219:LYS:HE3	1:C:358:HIS:ND1	2.33	0.44
1:C:278:ARG:CZ	1:C:387:PHE:HE1	2.29	0.44
1:C:450:VAL:HG22	1:C:451:LYS:N	2.30	0.44
1:C:504:ILE:CG2	1:C:505:GLY:N	2.81	0.44
1:D:219:LYS:HA	1:D:224:ILE:CG2	2.46	0.44
1:D:286:LYS:NZ	1:D:292:LEU:HB2	2.32	0.44
1:D:396:PHE:O	1:D:417:GLY:HA2	2.18	0.44
1:D:413:VAL:HG21	1:D:448:LEU:HD13	1.99	0.44
1:D:482:LEU:HD11	1:D:770:LEU:HD13	2.00	0.44
1:E:410:ALA:CA	1:E:425:ILE:HD11	2.47	0.44
1:F:215:ILE:CG2	1:F:239:LEU:HD12	2.47	0.44
1:F:219:LYS:HG2	1:F:358:HIS:NE2	2.32	0.44
1:F:230:ALA:HB2	1:F:325:TYR:O	2.17	0.44
1:F:443:HIS:O	1:F:447:ILE:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:476:GLU:C	1:F:478:ASP:N	2.70	0.44
1:F:736:PHE:CD2	1:F:736:PHE:N	2.84	0.44
1:A:104:PRO:HG3	1:A:390:LEU:HD11	2.00	0.44
1:A:144:LEU:HA	1:A:145:PRO:C	2.37	0.44
1:A:188:TYR:CE1	1:A:358:HIS:HD2	2.36	0.44
1:A:381:ILE:HG13	1:A:382:ARG:N	2.33	0.44
1:A:415:LYS:O	1:A:417:GLY:N	2.48	0.44
1:A:587:TYR:OH	1:B:468:LYS:HG3	2.18	0.44
1:B:144:LEU:HA	1:B:145:PRO:C	2.37	0.44
1:B:370:VAL:HG23	1:B:381:ILE:HD11	1.99	0.44
1:B:653:VAL:CG1	1:B:692:ALA:HB3	2.43	0.44
1:C:132:THR:HG23	1:C:133:ASN:OD1	2.18	0.44
1:C:134:CYS:SG	1:C:135:GLY:N	2.90	0.44
1:C:192:THR:C	1:C:194:ASP:N	2.69	0.44
1:C:233:GLU:O	1:C:236:VAL:HG12	2.18	0.44
1:C:239:LEU:HD23	1:C:239:LEU:C	2.38	0.44
1:C:451:LYS:O	1:C:452:ASN:C	2.55	0.44
1:D:130:VAL:HG22	1:D:131:CYS:O	2.17	0.44
1:D:216:VAL:HB	1:D:354:TYR:HB2	1.99	0.44
1:D:225:HIS:CA	1:D:330:ALA:HB2	2.40	0.44
1:D:312:THR:O	1:D:316:LEU:HB2	2.18	0.44
1:D:315:ILE:HG23	1:D:316:LEU:N	2.32	0.44
1:D:462:PRO:HG2	1:E:604:ASN:ND2	2.32	0.44
1:D:491:ILE:CG2	1:D:527:LEU:HD21	2.44	0.44
1:D:541:TYR:CZ	1:D:609:SER:HA	2.53	0.44
1:D:599:LEU:O	1:D:599:LEU:HD22	2.17	0.44
1:D:759:LEU:CD1	1:D:764:TYR:HB2	2.46	0.44
1:E:278:ARG:CZ	1:E:387:PHE:HE1	2.30	0.44
1:F:142:GLU:HB3	1:F:150:ASN:C	2.38	0.44
1:F:286:LYS:HE3	1:F:290:PHE:HB2	1.99	0.44
1:F:521:GLY:CA	1:F:610:SER:HA	2.41	0.44
1:F:599:LEU:O	1:F:599:LEU:HD13	2.17	0.44
1:F:742:VAL:HG13	1:F:743:PRO:HD2	2.00	0.44
1:A:612:GLY:HA2	1:A:615:LEU:HD23	1.99	0.44
1:A:615:LEU:HD21	1:A:635:ALA:CB	2.47	0.44
1:B:210:ILE:HD11	1:B:228:CYS:CA	2.48	0.44
1:B:253:MSE:HE2	1:B:317:PHE:CD1	2.52	0.44
1:B:405:ALA:H	1:B:749:VAL:HG11	1.83	0.44
1:C:283:THR:OG1	1:C:372:ARG:HB2	2.17	0.44
1:C:401:LEU:HD12	1:C:412:GLY:O	2.18	0.44
1:C:485:GLN:CD	1:C:514:GLY:HA2	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:LEU:HG	1:D:117:PHE:H	1.83	0.44
1:D:269:GLU:HB2	1:D:378:ARG:NH2	2.33	0.44
1:D:383:ARG:CZ	1:D:421:PRO:HG3	2.48	0.44
1:D:428:THR:HG21	1:D:466:THR:HG22	2.00	0.44
1:D:570:LEU:HD12	1:D:573:VAL:CG1	2.48	0.44
1:D:727:LYS:O	1:D:730:GLU:HG2	2.17	0.44
1:E:677:SER:O	1:E:681:ILE:HG12	2.17	0.44
1:F:1:MSE:HG2	1:F:83:PHE:HD1	1.83	0.44
1:F:9:GLN:HB2	1:F:72:ARG:HH21	1.83	0.44
1:F:14:ALA:HA	1:F:146:TYR:CD1	2.52	0.44
1:F:401:LEU:HD12	1:F:412:GLY:O	2.18	0.44
1:F:457:ILE:HA	1:F:482:LEU:O	2.17	0.44
1:F:565:TYR:HB3	1:F:569:GLU:HG2	2.00	0.44
1:A:213:GLY:O	1:A:235:VAL:HG11	2.17	0.44
1:A:343:ARG:HG2	1:A:343:ARG:HH11	1.83	0.44
1:A:567:ILE:HG23	1:A:600:ALA:HB2	1.99	0.44
1:A:584:SER:HA	1:A:587:TYR:O	2.17	0.44
1:A:653:VAL:HG23	1:A:662:VAL:HA	1.99	0.44
1:B:54:GLU:C	1:B:56:PHE:H	2.20	0.44
1:B:181:CYS:SG	1:B:182:PRO:N	2.91	0.44
1:B:288:GLU:CB	1:B:289:PRO:CD	2.94	0.44
1:B:506:ILE:HD11	1:B:694:ALA:HA	1.99	0.44
1:C:18:ARG:O	1:C:21:VAL:HG12	2.18	0.44
1:C:45:VAL:O	1:C:45:VAL:HG12	2.16	0.44
1:C:485:GLN:HE21	1:C:486:HIS:N	2.16	0.44
1:C:560:ILE:HD12	1:C:561:LEU:N	2.33	0.44
1:D:252:ILE:HD13	1:D:303:ILE:HG22	1.99	0.44
1:D:579:PRO:HB3	1:D:626:TYR:CE1	2.52	0.44
1:E:341:ASN:HB3	1:E:357:LEU:HD13	2.00	0.44
1:E:756:LEU:HD21	1:E:770:LEU:HD22	2.00	0.44
1:F:125:MSE:O	1:F:315:ILE:HD12	2.18	0.44
1:F:251:ALA:O	1:F:326:VAL:HA	2.18	0.44
1:F:270:GLU:HA	1:F:373:PHE:HE2	1.83	0.44
1:F:315:ILE:HG12	1:F:319:TRP:CZ3	2.53	0.44
1:F:364:ASN:HD21	1:F:443:HIS:CD2	2.34	0.44
1:F:543:LEU:HG	1:F:543:LEU:O	2.17	0.44
1:F:707:LYS:HB3	1:F:708:ASN:HD22	1.83	0.44
1:A:455:LEU:HB3	1:A:480:GLU:HB3	2.00	0.44
1:B:1:MSE:HG2	1:B:83:PHE:CD1	2.50	0.44
1:B:249:PRO:CG	1:B:300:LEU:HD13	2.37	0.44
1:B:293:PRO:O	1:B:296:LEU:HD13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:GLY:HA2	1:B:420:TYR:O	2.17	0.44
1:B:413:VAL:CG1	1:B:420:TYR:HB2	2.47	0.44
1:B:687:LEU:HD22	1:B:724:MSE:SE	2.68	0.44
1:C:261:LYS:HA	1:C:261:LYS:HD2	1.82	0.44
1:C:447:ILE:C	1:C:448:LEU:HD23	2.38	0.44
1:C:491:ILE:HD12	1:C:525:LEU:HD12	2.00	0.44
1:C:518:ASN:HB3	1:C:540:TYR:HE2	1.82	0.44
1:C:581:ALA:HA	1:C:584:SER:HB3	1.98	0.44
1:C:603:ILE:HD11	1:F:772:LEU:HD21	1.99	0.44
1:E:163:ARG:O	1:E:166:TYR:HB3	2.18	0.44
1:F:12:VAL:HG22	1:F:42:VAL:HG11	2.00	0.44
1:A:50:GLU:HA	1:A:53:ILE:HG22	2.01	0.43
1:A:163:ARG:HB2	1:A:163:ARG:NH1	2.21	0.43
1:A:312:THR:HA	1:A:315:ILE:CG2	2.48	0.43
1:A:373:PHE:CE2	1:A:378:ARG:HD3	2.53	0.43
1:A:568:ASP:O	1:A:571:GLU:HB3	2.16	0.43
1:B:8:VAL:O	1:B:9:GLN:HG3	2.18	0.43
1:B:338:VAL:O	1:B:338:VAL:HG13	2.18	0.43
1:B:525:LEU:C	1:B:535:LEU:HD13	2.39	0.43
1:B:584:SER:HA	1:B:587:TYR:O	2.18	0.43
1:B:651:PHE:CE2	1:B:669:ILE:HA	2.49	0.43
1:C:24:ILE:HD11	1:C:59:ASP:HB2	2.00	0.43
1:C:130:VAL:CG2	1:C:131:CYS:N	2.81	0.43
1:C:140:ILE:HB	1:C:152:THR:HG22	1.99	0.43
1:C:299:GLY:C	1:C:300:LEU:HG	2.38	0.43
1:C:339:LYS:HB2	1:C:339:LYS:HE3	1.79	0.43
1:C:370:VAL:CG2	1:C:382:ARG:HB2	2.48	0.43
1:C:409:ASN:CG	1:C:410:ALA:H	2.22	0.43
1:D:189:ARG:HD2	1:D:191:TYR:OH	2.18	0.43
1:D:383:ARG:NH2	1:D:390:LEU:O	2.51	0.43
1:D:504:ILE:CG2	1:D:505:GLY:H	2.31	0.43
1:D:643:PHE:C	1:D:645:GLY:H	2.21	0.43
1:E:401:LEU:O	1:E:456:ILE:HG23	2.18	0.43
1:E:718:ASN:HB3	1:E:721:ILE:HB	2.00	0.43
1:F:613:ARG:HH22	1:F:628:ARG:HH22	1.66	0.43
1:F:629:HIS:HB2	1:F:633:GLU:OE1	2.17	0.43
1:A:148:ARG:HH22	1:A:158:MSE:HG3	1.83	0.43
1:A:253:MSE:HE2	1:A:317:PHE:CE1	2.53	0.43
1:A:373:PHE:CE1	1:A:378:ARG:HB3	2.52	0.43
1:B:65:PRO:HG2	1:B:68:ALA:HB3	1.99	0.43
1:B:492:ALA:CB	1:B:756:LEU:HD12	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:691:ARG:HH11	1:B:695:HIS:HD2	1.65	0.43
1:C:190:LEU:O	1:C:196:GLN:HA	2.19	0.43
1:C:226:LEU:HD12	1:C:330:ALA:HA	2.00	0.43
1:C:270:GLU:N	1:C:378:ARG:HH12	2.16	0.43
1:D:12:VAL:HG22	1:D:17:PHE:CE1	2.53	0.43
1:D:198:ILE:HG22	1:D:199:TYR:N	2.33	0.43
1:D:589:LYS:HG3	1:E:475:ASN:HD21	1.83	0.43
1:E:181:CYS:SG	1:E:182:PRO:CD	3.06	0.43
1:E:334:GLY:HA3	1:E:335:MSE:HE2	2.00	0.43
1:E:578:CYS:O	1:E:578:CYS:SG	2.76	0.43
1:E:616:ASP:HB3	1:E:634:PRO:CG	2.47	0.43
1:E:729:VAL:HG12	1:E:733:GLY:O	2.18	0.43
1:F:282:ILE:HG22	1:F:305:VAL:HB	1.99	0.43
1:F:368:ASP:HA	1:F:385:ARG:HD3	2.00	0.43
1:F:383:ARG:NH1	1:F:387:PHE:HB3	2.32	0.43
1:F:487:HIS:NE2	1:F:520:TRP:HB3	2.33	0.43
1:A:36:ASN:OD1	1:A:42:VAL:HG22	2.18	0.43
1:A:269:GLU:O	1:A:272:GLU:HB3	2.18	0.43
1:A:329:SER:HB2	1:A:331:ASN:ND2	2.31	0.43
1:A:341:ASN:O	1:A:344:ALA:HB3	2.18	0.43
1:B:409:ASN:ND2	1:B:425:ILE:HD11	2.33	0.43
1:C:18:ARG:NH2	1:C:36:ASN:ND2	2.66	0.43
1:C:543:LEU:HD12	1:C:549:ALA:HB3	2.00	0.43
1:D:102:ILE:HD12	1:D:141:ILE:HG21	2.00	0.43
1:D:204:ARG:HD2	1:D:204:ARG:C	2.38	0.43
1:D:338:VAL:HG11	1:D:348:LEU:HD11	1.99	0.43
1:D:491:ILE:HD11	1:D:505:GLY:C	2.38	0.43
1:E:18:ARG:HD2	1:E:175:HIS:ND1	2.33	0.43
1:E:236:VAL:HG13	1:E:295:ASN:ND2	2.32	0.43
1:E:620:VAL:HG13	1:E:626:TYR:HD1	1.82	0.43
1:F:52:ASP:O	1:F:56:PHE:HB3	2.19	0.43
1:F:526:TYR:CB	1:F:535:LEU:HD11	2.47	0.43
1:F:757:GLY:C	1:F:759:LEU:H	2.21	0.43
1:F:759:LEU:CD1	1:F:764:TYR:HB2	2.48	0.43
1:A:406:GLU:HA	1:A:466:THR:CG2	2.48	0.43
1:A:560:ILE:HD12	1:A:561:LEU:N	2.33	0.43
1:A:603:ILE:HD11	1:B:772:LEU:HD21	2.00	0.43
1:A:654:PRO:HG2	1:A:661:ARG:HB2	2.01	0.43
1:B:39:ASP:CG	1:B:40:ALA:H	2.22	0.43
1:B:106:ILE:CG2	1:B:277:TYR:HB2	2.37	0.43
1:B:396:PHE:CZ	1:B:759:LEU:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:LEU:O	1:C:212:LYS:HB3	2.17	0.43
1:C:348:LEU:HD12	1:C:348:LEU:N	2.33	0.43
1:D:18:ARG:CB	1:D:19:PRO:HD3	2.48	0.43
1:D:163:ARG:HB2	1:D:163:ARG:NH1	2.28	0.43
1:E:395:PRO:HG2	1:E:396:PHE:CE2	2.52	0.43
1:F:213:GLY:HA3	1:F:235:VAL:HG11	2.00	0.43
1:F:360:ARG:HG2	1:F:360:ARG:HH11	1.83	0.43
1:F:564:VAL:HG11	1:F:667:GLN:HB2	1.99	0.43
1:F:694:ALA:O	1:F:696:THR:N	2.51	0.43
1:F:729:VAL:CB	1:F:735:ASN:HD22	2.29	0.43
1:A:12:VAL:HG13	1:A:17:PHE:CD2	2.53	0.43
1:A:12:VAL:HG13	1:A:17:PHE:CG	2.53	0.43
1:A:151:THR:O	1:A:154:LYS:HB2	2.18	0.43
1:A:595:VAL:HG12	1:A:595:VAL:O	2.18	0.43
1:B:282:ILE:HA	1:B:371:ILE:O	2.18	0.43
1:B:296:LEU:HD12	1:B:296:LEU:N	2.32	0.43
1:C:28:HIS:CE1	1:C:55:ALA:HB1	2.54	0.43
1:C:197:GLU:OE2	1:D:124:TYR:CD1	2.71	0.43
1:C:364:ASN:HD21	1:C:443:HIS:CD2	2.35	0.43
1:C:472:GLU:HG3	1:C:473:MSE:N	2.32	0.43
1:D:20:PHE:CZ	1:D:64:LYS:HA	2.54	0.43
1:D:36:ASN:HA	1:D:42:VAL:HG22	2.01	0.43
1:D:163:ARG:HA	1:D:166:TYR:HB3	1.99	0.43
1:D:539:ASP:CA	1:D:659:LEU:HD11	2.45	0.43
1:D:589:LYS:CG	1:E:475:ASN:HD21	2.31	0.43
1:D:595:VAL:O	1:D:595:VAL:HG12	2.19	0.43
1:E:207:ALA:HB1	1:E:320:SER:HB2	2.00	0.43
1:E:494:VAL:O	1:E:496:ALA:N	2.51	0.43
1:F:221:ILE:HG22	1:F:360:ARG:HH21	1.82	0.43
1:F:227:ALA:HA	1:F:326:VAL:O	2.19	0.43
1:F:302:THR:O	1:F:303:ILE:HG13	2.17	0.43
1:F:323:PRO:HG2	1:F:324:VAL:H	1.83	0.43
1:A:339:LYS:HG3	1:A:365:ARG:NH1	2.33	0.43
1:A:406:GLU:HG3	1:A:407:LEU:N	2.33	0.43
1:A:501:ASP:O	1:A:502:SER:C	2.56	0.43
1:B:14:ALA:HA	1:B:146:TYR:CD1	2.54	0.43
1:B:17:PHE:CZ	1:B:60:LEU:HG	2.54	0.43
1:B:219:LYS:CD	1:B:358:HIS:H	2.30	0.43
1:B:230:ALA:HB2	1:B:325:TYR:O	2.18	0.43
1:B:323:PRO:HG2	1:B:324:VAL:H	1.83	0.43
1:C:742:VAL:HG11	1:C:751:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ILE:CD1	1:D:144:LEU:HG	2.40	0.43
1:D:614:VAL:HG13	1:D:666:PHE:CZ	2.53	0.43
1:E:279:ARG:CB	1:E:309:TYR:HB3	2.48	0.43
1:E:294:GLU:HG2	1:E:294:GLU:O	2.19	0.43
1:E:370:VAL:HG22	1:E:382:ARG:HB2	2.00	0.43
1:E:425:ILE:HG22	1:E:436:PHE:CE1	2.53	0.43
1:E:502:SER:CB	1:E:528:GLY:HA2	2.48	0.43
1:E:584:SER:HB3	1:E:589:LYS:HB3	1.99	0.43
1:F:383:ARG:CZ	1:F:421:PRO:CG	2.97	0.43
1:F:490:HIS:C	1:F:492:ALA:N	2.70	0.43
1:F:498:LYS:HB2	1:F:500:LEU:CD2	2.47	0.43
1:A:625:ALA:HB2	1:A:637:LYS:CD	2.42	0.43
1:A:742:VAL:CG1	1:A:751:VAL:HG11	2.48	0.43
1:B:118:ASP:HA	1:B:119:PRO:HD3	1.74	0.43
1:B:209:LEU:O	1:B:212:LYS:HB2	2.18	0.43
1:B:253:MSE:HE1	1:B:313:HIS:ND1	2.34	0.43
1:B:485:GLN:HG3	1:B:487:HIS:N	2.34	0.43
1:B:547:ASP:O	1:B:550:SER:HB2	2.19	0.43
1:B:593:ASN:C	1:B:595:VAL:N	2.71	0.43
1:B:686:HIS:CD2	1:B:720:LEU:HD12	2.54	0.43
1:C:5:HIS:HB3	1:C:76:LYS:HD2	2.00	0.43
1:C:224:ILE:CG2	1:C:338:VAL:HG13	2.48	0.43
1:C:261:LYS:CE	1:C:266:VAL:HB	2.49	0.43
1:C:543:LEU:H	1:C:543:LEU:CD2	2.23	0.43
1:C:570:LEU:HA	1:C:573:VAL:HG12	2.01	0.43
1:D:404:GLY:HA2	1:D:753:GLN:HE22	1.82	0.43
1:D:564:VAL:HG13	1:D:667:GLN:NE2	2.30	0.43
1:E:19:PRO:HG2	1:E:132:THR:HG21	2.01	0.43
1:E:392:ILE:HB	1:E:419:VAL:CG1	2.49	0.43
1:F:118:ASP:HA	1:F:119:PRO:HD3	1.75	0.43
1:F:263:PHE:O	1:F:264:ALA:HB2	2.17	0.43
1:F:485:GLN:HG2	1:F:488:TYR:CD2	2.54	0.43
1:F:577:CYS:SG	1:F:579:PRO:HD3	2.59	0.43
1:F:739:THR:O	1:F:742:VAL:O	2.37	0.43
1:A:110:ASP:O	1:A:113:LEU:HB3	2.19	0.43
1:A:226:LEU:HD12	1:A:330:ALA:CB	2.49	0.43
1:A:348:LEU:HB3	1:A:351:VAL:HB	2.01	0.43
1:A:434:LEU:HD11	1:A:465:ASN:O	2.18	0.43
1:A:457:ILE:CG2	1:A:753:GLN:HB3	2.41	0.43
1:A:665:LEU:O	1:A:669:ILE:HG13	2.18	0.43
1:A:766:THR:OG1	1:A:769:ASP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:VAL:HG12	1:B:87:TYR:CE1	2.49	0.43
1:B:159:CYS:O	1:B:160:ASP:C	2.57	0.43
1:B:286:LYS:CE	1:B:290:PHE:HB2	2.49	0.43
1:B:406:GLU:HA	1:B:466:THR:CG2	2.49	0.43
1:B:494:VAL:HG22	1:B:738:VAL:CG2	2.40	0.43
1:B:506:ILE:HD12	1:B:725:ILE:HG23	2.00	0.43
1:C:396:PHE:CZ	1:C:759:LEU:HD13	2.54	0.43
1:C:560:ILE:H	1:C:560:ILE:HG13	1.61	0.43
1:C:564:VAL:HG11	1:C:667:GLN:HG3	2.01	0.43
1:C:621:LEU:O	1:C:622:LEU:HD23	2.18	0.43
1:D:319:TRP:O	1:D:320:SER:C	2.55	0.43
1:D:380:VAL:CG2	1:D:740:THR:HG23	2.47	0.43
1:D:415:LYS:C	1:D:417:GLY:H	2.22	0.43
1:D:738:VAL:HG11	1:D:742:VAL:HG12	2.01	0.43
1:E:171:ASN:HD21	1:E:173:ARG:HB2	1.82	0.43
1:E:286:LYS:HE3	1:E:290:PHE:CA	2.48	0.43
1:E:286:LYS:HE3	1:E:290:PHE:HA	2.01	0.43
1:E:370:VAL:H	1:E:382:ARG:CB	2.32	0.43
1:F:12:VAL:HG23	1:F:17:PHE:CG	2.53	0.43
1:F:25:ALA:HB1	1:F:30:LEU:O	2.19	0.43
1:F:123:ARG:NH2	1:F:173:ARG:HG2	2.33	0.43
1:A:468:LYS:HA	1:B:587:TYR:OH	2.18	0.43
1:A:584:SER:CB	1:A:589:LYS:HB3	2.43	0.43
1:A:654:PRO:O	1:A:660:ILE:HG23	2.19	0.43
1:B:110:ASP:O	1:B:113:LEU:HB3	2.19	0.43
1:B:743:PRO:HG2	1:B:748:GLY:HA3	2.00	0.43
1:C:372:ARG:HD2	1:C:373:PHE:N	2.34	0.43
1:D:252:ILE:CG2	1:D:324:VAL:HB	2.49	0.43
1:D:455:LEU:C	1:D:455:LEU:HD12	2.39	0.43
1:D:583:GLU:HG3	1:D:592:PHE:CD1	2.53	0.43
1:E:154:LYS:O	1:E:154:LYS:HD3	2.19	0.43
1:E:170:LEU:HD12	1:E:170:LEU:N	2.34	0.43
1:E:315:ILE:CG2	1:E:316:LEU:N	2.82	0.43
1:F:371:ILE:HD12	1:F:380:VAL:CG2	2.44	0.43
1:F:456:ILE:CG2	1:F:457:ILE:N	2.81	0.43
1:A:29:ASN:O	1:A:31:ARG:HD2	2.19	0.43
1:A:34:VAL:O	1:A:34:VAL:HG13	2.19	0.43
1:A:177:GLU:HB2	1:A:178:PRO:CD	2.49	0.43
1:A:339:LYS:HE2	1:A:365:ARG:HH12	1.84	0.43
1:A:476:GLU:C	1:A:478:ASP:N	2.72	0.43
1:B:545:GLY:HA3	1:B:548:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:VAL:HG12	1:B:618:ILE:HD11	2.01	0.43
1:C:399:ASN:N	1:C:399:ASN:ND2	2.67	0.43
1:C:768:GLU:C	1:C:770:LEU:H	2.23	0.43
1:D:108:ILE:HG13	1:D:310:ALA:HA	2.01	0.43
1:D:487:HIS:HE1	1:D:509:ASP:HB3	1.81	0.43
1:D:488:TYR:HE1	1:D:525:LEU:HB3	1.84	0.43
1:E:283:THR:OG1	1:E:372:ARG:HB2	2.19	0.43
1:E:757:GLY:C	1:E:759:LEU:N	2.73	0.43
1:F:24:ILE:HD13	1:F:60:LEU:HD13	2.00	0.43
1:F:578:CYS:O	1:F:578:CYS:SG	2.77	0.43
1:B:116:LEU:HD23	1:B:129:ILE:HG21	2.01	0.42
1:B:131:CYS:SG	1:B:133:ASN:HB2	2.59	0.42
1:C:74:GLU:O	1:C:74:GLU:HG2	2.18	0.42
1:C:138:PHE:CB	1:C:389:PRO:HD3	2.47	0.42
1:C:183:VAL:CG2	1:C:184:CYS:N	2.81	0.42
1:C:204:ARG:HD2	1:C:204:ARG:O	2.18	0.42
1:C:263:PHE:O	1:C:264:ALA:HB2	2.18	0.42
1:C:591:GLU:O	1:C:595:VAL:HG23	2.19	0.42
1:D:520:TRP:HZ2	1:D:534:ARG:HH21	1.67	0.42
1:D:711:LEU:O	1:D:712:SER:HB2	2.19	0.42
1:E:225:HIS:HB2	1:E:328:THR:O	2.19	0.42
1:E:450:VAL:HG22	1:E:451:LYS:H	1.84	0.42
1:E:455:LEU:HA	1:E:479:VAL:CG1	2.49	0.42
1:E:755:PHE:O	1:E:755:PHE:CG	2.72	0.42
1:F:265:TYR:N	1:F:265:TYR:HD2	2.14	0.42
1:F:381:ILE:HG22	1:F:717:TYR:CZ	2.54	0.42
1:F:524:VAL:O	1:F:525:LEU:HD23	2.19	0.42
1:A:265:TYR:O	1:A:284:LEU:HB2	2.18	0.42
1:A:399:ASN:O	1:A:454:ASP:HB2	2.19	0.42
1:A:726:ARG:HH21	1:A:727:LYS:CG	2.32	0.42
1:B:57:ILE:HG21	1:B:75:LYS:HE2	2.01	0.42
1:B:171:ASN:ND2	1:B:173:ARG:H	2.17	0.42
1:B:427:ASN:HD21	1:B:429:GLY:H	1.65	0.42
1:B:540:TYR:CD1	1:B:540:TYR:N	2.87	0.42
1:B:654:PRO:HG2	1:B:661:ARG:HB2	2.01	0.42
1:B:670:LEU:O	1:B:673:ILE:HG12	2.19	0.42
1:C:129:ILE:HG13	1:C:130:VAL:H	1.84	0.42
1:C:503:VAL:HA	1:C:706:VAL:CG1	2.50	0.42
1:D:21:VAL:HA	1:D:24:ILE:CG2	2.49	0.42
1:D:335:MSE:HE2	1:D:335:MSE:N	2.33	0.42
1:D:475:ASN:HD22	1:E:591:GLU:HG2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:719:GLU:O	1:D:719:GLU:HG3	2.19	0.42
1:E:210:ILE:HD11	1:E:228:CYS:N	2.34	0.42
1:E:225:HIS:HE2	1:E:327:MSE:HE3	1.84	0.42
1:E:371:ILE:CB	1:E:380:VAL:HG13	2.41	0.42
1:E:381:ILE:HG22	1:E:717:TYR:CE1	2.54	0.42
1:F:371:ILE:CG1	1:F:380:VAL:HG22	2.49	0.42
1:F:541:TYR:OH	1:F:610:SER:N	2.52	0.42
1:A:181:CYS:SG	1:A:182:PRO:N	2.91	0.42
1:A:370:VAL:CG2	1:A:382:ARG:HB2	2.50	0.42
1:A:485:GLN:HB3	1:A:488:TYR:HD2	1.83	0.42
1:A:567:ILE:HG12	1:A:600:ALA:HB1	2.00	0.42
1:B:9:GLN:HG2	1:B:40:ALA:HA	2.00	0.42
1:B:381:ILE:HG22	1:B:717:TYR:CE1	2.54	0.42
1:B:552:TYR:HA	1:B:553:PRO:HD2	1.92	0.42
1:C:188:TYR:CE1	1:C:312:THR:HG21	2.54	0.42
1:C:364:ASN:ND2	1:C:443:HIS:NE2	2.68	0.42
1:C:372:ARG:O	1:C:379:ALA:O	2.37	0.42
1:C:628:ARG:CZ	1:C:632:GLY:H	2.32	0.42
1:D:475:ASN:ND2	1:E:591:GLU:HG2	2.34	0.42
1:D:543:LEU:N	1:D:543:LEU:CD2	2.82	0.42
1:E:523:GLU:CD	1:E:537:HIS:HB2	2.40	0.42
1:F:38:GLY:CA	1:F:144:LEU:HB3	2.49	0.42
1:F:210:ILE:HD11	1:F:228:CYS:N	2.33	0.42
1:F:219:LYS:HA	1:F:224:ILE:HG23	2.00	0.42
1:F:537:HIS:HE2	1:F:659:LEU:HD22	1.82	0.42
1:A:172:ARG:C	1:A:174:TYR:H	2.23	0.42
1:A:504:ILE:HG22	1:A:709:VAL:HG12	2.00	0.42
1:A:702:ARG:C	1:A:704:PHE:H	2.22	0.42
1:B:18:ARG:HB3	1:B:175:HIS:ND1	2.34	0.42
1:B:256:ASP:O	1:B:258:GLU:N	2.52	0.42
1:B:391:PRO:HB2	1:B:418:LYS:HB2	2.01	0.42
1:B:455:LEU:HD13	1:B:456:ILE:O	2.20	0.42
1:C:35:LYS:O	1:C:36:ASN:HB2	2.20	0.42
1:C:204:ARG:HA	1:C:319:TRP:CZ3	2.54	0.42
1:C:639:GLU:OE2	1:C:718:ASN:HA	2.19	0.42
1:D:30:LEU:HD22	1:D:52:ASP:O	2.19	0.42
1:D:171:ASN:HD22	1:D:173:ARG:H	1.67	0.42
1:D:486:HIS:CD2	1:D:490:HIS:HE2	2.36	0.42
1:D:738:VAL:HG12	1:D:742:VAL:O	2.19	0.42
1:E:30:LEU:HD23	1:E:30:LEU:O	2.19	0.42
1:E:107:ALA:HB2	1:E:309:TYR:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:PHE:HB2	1:E:389:PRO:HD3	2.01	0.42
1:E:261:LYS:NZ	1:E:266:VAL:HB	2.34	0.42
1:E:405:ALA:O	1:E:466:THR:HG21	2.19	0.42
1:E:528:GLY:O	1:E:529:TYR:C	2.56	0.42
1:E:570:LEU:HA	1:E:573:VAL:HG12	2.01	0.42
1:E:771:MSE:O	1:E:772:LEU:HD23	2.19	0.42
1:F:369:SER:HB2	1:F:385:ARG:HB2	2.00	0.42
1:F:504:ILE:CG2	1:F:505:GLY:H	2.33	0.42
1:A:210:ILE:HD11	1:A:228:CYS:HA	2.02	0.42
1:A:215:ILE:HD11	1:A:352:ALA:HA	2.02	0.42
1:A:253:MSE:SE	1:A:313:HIS:ND1	3.03	0.42
1:A:587:TYR:OH	1:B:468:LYS:HA	2.19	0.42
1:A:687:LEU:HD22	1:A:724:MSE:CE	2.44	0.42
1:A:708:ASN:OD1	1:A:708:ASN:N	2.52	0.42
1:B:251:ALA:HB3	1:B:327:MSE:O	2.20	0.42
1:B:385:ARG:HG3	1:B:386:GLY:N	2.35	0.42
1:B:528:GLY:H	1:B:532:VAL:HG22	1.85	0.42
1:C:18:ARG:HH21	1:C:36:ASN:ND2	2.15	0.42
1:C:204:ARG:HG2	1:C:319:TRP:CH2	2.55	0.42
1:C:232:ASN:CG	1:C:235:VAL:HG22	2.40	0.42
1:C:260:VAL:HG12	1:C:266:VAL:CG2	2.49	0.42
1:C:487:HIS:HE1	1:C:509:ASP:HB3	1.85	0.42
1:C:526:TYR:CB	1:C:535:LEU:HD11	2.49	0.42
1:D:401:LEU:O	1:D:456:ILE:HA	2.20	0.42
1:D:610:SER:HB3	1:D:613:ARG:CG	2.50	0.42
1:E:137:ARG:C	1:E:141:ILE:HG13	2.39	0.42
1:E:199:TYR:CG	1:E:200:GLY:N	2.87	0.42
1:E:451:LYS:O	1:E:452:ASN:C	2.57	0.42
1:E:599:LEU:O	1:E:599:LEU:HD22	2.19	0.42
1:F:20:PHE:CE1	1:F:60:LEU:HD12	2.54	0.42
1:F:23:ARG:HD3	1:F:169:PRO:O	2.19	0.42
1:F:399:ASN:O	1:F:454:ASP:HB2	2.20	0.42
1:A:427:ASN:C	1:A:429:GLY:H	2.22	0.42
1:A:438:ARG:HG2	1:A:438:ARG:NH1	2.34	0.42
1:A:504:ILE:CG2	1:A:505:GLY:N	2.82	0.42
1:B:19:PRO:HA	1:B:174:TYR:CD1	2.54	0.42
1:B:406:GLU:HG3	1:B:407:LEU:N	2.35	0.42
1:B:413:VAL:O	1:B:420:TYR:N	2.53	0.42
1:B:570:LEU:HD12	1:B:573:VAL:CG1	2.50	0.42
1:B:639:GLU:HB2	1:B:718:ASN:HD21	1.83	0.42
1:C:9:GLN:HE21	1:C:41:GLY:N	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:ILE:CG2	1:C:89:GLU:H	2.23	0.42
1:C:270:GLU:HA	1:C:373:PHE:HE2	1.84	0.42
1:C:383:ARG:CZ	1:C:387:PHE:HB3	2.50	0.42
1:C:508:LEU:CD2	1:C:611:THR:HG21	2.48	0.42
1:D:664:GLU:HA	1:D:667:GLN:HG3	2.01	0.42
1:E:58:GLU:HA	1:E:61:TYR:HD2	1.85	0.42
1:E:438:ARG:NH2	1:E:469:LEU:HD21	2.34	0.42
1:E:503:VAL:HA	1:E:706:VAL:HG11	2.00	0.42
1:E:729:VAL:CB	1:E:735:ASN:HD22	2.30	0.42
1:F:19:PRO:HA	1:F:174:TYR:HD1	1.81	0.42
1:F:177:GLU:N	1:F:178:PRO:HD2	2.35	0.42
1:F:301:HIS:CD2	1:F:302:THR:N	2.87	0.42
1:F:343:ARG:HD3	1:F:343:ARG:HA	1.81	0.42
1:F:500:LEU:HD22	1:F:736:PHE:CZ	2.54	0.42
1:F:520:TRP:HZ2	1:F:534:ARG:HH21	1.67	0.42
1:A:88:ILE:HD12	1:A:88:ILE:N	2.34	0.42
1:A:229:ASP:OD1	1:A:322:THR:HG21	2.20	0.42
1:A:365:ARG:HH21	1:A:436:PHE:HD2	1.67	0.42
1:A:495:MSE:HE2	1:A:755:PHE:HZ	1.84	0.42
1:A:765:LEU:HD12	1:A:766:THR:H	1.84	0.42
1:B:102:ILE:CD1	1:B:103:PRO:HD2	2.50	0.42
1:C:20:PHE:CE1	1:C:60:LEU:HD12	2.55	0.42
1:C:122:LYS:HD3	1:D:198:ILE:HD11	2.01	0.42
1:C:148:ARG:HH21	1:C:158:MSE:N	2.18	0.42
1:C:381:ILE:HG22	1:C:717:TYR:CZ	2.55	0.42
1:C:482:LEU:HD21	1:C:757:GLY:HA2	2.01	0.42
1:C:649:LEU:CG	1:C:650:LYS:H	2.33	0.42
1:C:718:ASN:HD22	1:C:720:LEU:HB2	1.83	0.42
1:D:7:HIS:NE2	1:D:43:GLU:HG3	2.35	0.42
1:D:252:ILE:HG12	1:D:296:LEU:HD23	2.01	0.42
1:D:253:MSE:O	1:D:317:PHE:HZ	2.01	0.42
1:D:320:SER:HB3	1:D:325:TYR:OH	2.19	0.42
1:D:383:ARG:HD2	1:D:387:PHE:HD2	1.84	0.42
1:D:520:TRP:HE1	1:D:534:ARG:NH2	2.17	0.42
1:D:597:ASN:HB3	1:D:601:LYS:HE3	2.01	0.42
1:D:726:ARG:HH21	1:D:727:LYS:HG2	1.85	0.42
1:E:293:PRO:C	1:E:295:ASN:N	2.72	0.42
1:E:503:VAL:HG11	1:E:708:ASN:OD1	2.19	0.42
1:F:171:ASN:HD21	1:F:173:ARG:HB2	1.82	0.42
1:F:216:VAL:HG23	1:F:354:TYR:C	2.40	0.42
1:F:766:THR:HG21	1:F:769:ASP:OD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:HIS:NE2	1:A:521:GLY:HA2	2.35	0.42
1:A:561:LEU:CB	1:A:570:LEU:HD13	2.50	0.42
1:A:577:CYS:SG	1:A:579:PRO:HD3	2.59	0.42
1:B:226:LEU:CD1	1:B:330:ALA:HA	2.50	0.42
1:B:264:ALA:CB	1:B:286:LYS:HA	2.50	0.42
1:B:420:TYR:HB3	1:B:444:PHE:HE1	1.85	0.42
1:B:544:PRO:O	1:B:549:ALA:HB2	2.20	0.42
1:B:580:LYS:C	1:B:582:VAL:H	2.22	0.42
1:B:751:VAL:CG1	1:B:752:GLY:N	2.82	0.42
1:C:102:ILE:HG21	1:C:389:PRO:HG3	2.01	0.42
1:C:253:MSE:HB3	1:C:325:TYR:HB2	2.02	0.42
1:C:487:HIS:CE1	1:C:509:ASP:HB3	2.55	0.42
1:D:65:PRO:HB2	1:D:66:PRO:HD2	2.00	0.42
1:E:8:VAL:HG13	1:E:70:ILE:HG23	2.01	0.42
1:E:34:VAL:HG23	1:E:44:ILE:HG12	2.02	0.42
1:E:79:PRO:HA	1:E:80:PRO:HD3	1.89	0.42
1:E:247:GLN:HG3	1:E:298:PRO:HG2	2.02	0.42
1:E:530:GLU:HG3	1:E:531:ASP:OD2	2.20	0.42
1:E:543:LEU:HB2	1:E:549:ALA:CB	2.50	0.42
1:F:35:LYS:HE2	1:F:90:LYS:HZ3	1.82	0.42
1:F:293:PRO:C	1:F:295:ASN:H	2.23	0.42
1:F:412:GLY:HA2	1:F:420:TYR:O	2.18	0.42
1:F:621:LEU:HD22	1:F:666:PHE:HD1	1.84	0.42
1:F:702:ARG:NH2	1:F:731:ALA:O	2.53	0.42
1:A:123:ARG:NH2	1:A:173:ARG:NE	2.68	0.42
1:A:235:VAL:O	1:A:238:GLU:HB2	2.19	0.42
1:B:257:ILE:O	1:B:260:VAL:HB	2.20	0.42
1:B:610:SER:HB3	1:B:613:ARG:CG	2.50	0.42
1:B:672:ALA:O	1:B:676:ALA:HB3	2.20	0.42
1:B:738:VAL:HG11	1:B:742:VAL:HG12	2.01	0.42
1:C:202:PRO:O	1:C:203:LEU:C	2.57	0.42
1:C:385:ARG:CG	1:C:386:GLY:N	2.74	0.42
1:C:424:TYR:C	1:C:426:GLY:H	2.23	0.42
1:D:284:LEU:O	1:D:302:THR:HA	2.19	0.42
1:D:287:LYS:HG3	1:D:288:GLU:N	2.35	0.42
1:E:11:ILE:HG23	1:E:12:VAL:N	2.34	0.42
1:E:19:PRO:HA	1:E:174:TYR:CD1	2.54	0.42
1:E:702:ARG:C	1:E:704:PHE:H	2.23	0.42
1:F:38:GLY:HA2	1:F:145:PRO:HA	2.01	0.42
1:F:215:ILE:O	1:F:215:ILE:HG13	2.20	0.42
1:F:279:ARG:HG3	1:F:309:TYR:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:385:ARG:HD2	1:F:385:ARG:HA	1.91	0.42
1:A:197:GLU:C	1:A:198:ILE:HG12	2.41	0.42
1:A:230:ALA:O	1:A:292:LEU:HD12	2.20	0.42
1:A:247:GLN:NE2	1:A:298:PRO:HG2	2.34	0.42
1:A:670:LEU:O	1:A:673:ILE:HG12	2.20	0.42
1:B:16:GLY:HA3	1:B:132:THR:HG23	2.02	0.42
1:B:225:HIS:CD2	1:B:225:HIS:N	2.86	0.42
1:B:281:ILE:HA	1:B:305:VAL:O	2.19	0.42
1:B:524:VAL:O	1:B:535:LEU:HB2	2.20	0.42
1:C:65:PRO:HG2	1:C:68:ALA:HB3	2.00	0.42
1:C:301:HIS:ND1	1:C:640:SER:HB3	2.35	0.42
1:C:466:THR:OG1	1:C:467:THR:N	2.53	0.42
1:C:515:THR:O	1:C:516:ASP:HB2	2.18	0.42
1:C:766:THR:OG1	1:C:769:ASP:HB2	2.20	0.42
1:D:239:LEU:HD22	1:D:250:PHE:CZ	2.55	0.42
1:D:329:SER:HB2	1:D:331:ASN:ND2	2.29	0.42
1:D:329:SER:CA	1:D:337:MSE:HE2	2.49	0.42
1:D:580:LYS:HD2	1:D:590:VAL:HA	2.01	0.42
1:D:690:ALA:HB2	1:D:721:ILE:HG23	2.02	0.42
1:E:12:VAL:O	1:E:12:VAL:HG22	2.20	0.42
1:E:183:VAL:CG2	1:E:184:CYS:H	2.31	0.42
1:E:748:GLY:O	1:E:751:VAL:HG12	2.19	0.42
1:F:210:ILE:HD11	1:F:227:ALA:O	2.20	0.42
1:F:339:LYS:HG3	1:F:365:ARG:NH1	2.34	0.42
1:F:376:GLY:HA2	1:F:726:ARG:HH11	1.84	0.42
1:F:391:PRO:C	1:F:392:ILE:HD12	2.41	0.42
1:F:481:LEU:HD12	1:F:482:LEU:H	1.84	0.42
1:F:536:ALA:HA	1:F:658:GLU:O	2.20	0.42
1:A:123:ARG:HE	1:A:173:ARG:NH2	2.16	0.41
1:A:209:LEU:N	1:A:209:LEU:HD12	2.35	0.41
1:A:359:ASN:O	1:A:360:ARG:C	2.58	0.41
1:A:589:LYS:CG	1:A:590:VAL:H	2.22	0.41
1:B:15:VAL:HG13	1:B:67:LEU:HB2	2.01	0.41
1:B:166:TYR:CZ	1:B:175:HIS:HA	2.55	0.41
1:C:209:LEU:N	1:C:209:LEU:HD12	2.35	0.41
1:D:278:ARG:CG	1:D:280:PRO:HD3	2.49	0.41
1:D:561:LEU:HB2	1:D:570:LEU:CD1	2.50	0.41
1:D:639:GLU:HB2	1:D:718:ASN:HD21	1.85	0.41
1:E:543:LEU:HD23	1:E:606:ALA:O	2.20	0.41
1:F:383:ARG:CZ	1:F:387:PHE:HB3	2.50	0.41
1:F:615:LEU:HD23	1:F:635:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:SER:HB3	1:A:527:LEU:O	2.20	0.41
1:B:67:LEU:HD22	1:B:106:ILE:HD13	2.01	0.41
1:B:166:TYR:CE1	1:B:175:HIS:HA	2.54	0.41
1:B:281:ILE:CB	1:B:370:VAL:HG12	2.42	0.41
1:B:283:THR:OG1	1:B:372:ARG:HB2	2.20	0.41
1:B:481:LEU:HD12	1:B:482:LEU:N	2.33	0.41
1:B:724:MSE:O	1:B:728:VAL:HG23	2.20	0.41
1:C:121:ASN:ND2	1:C:123:ARG:H	2.17	0.41
1:C:168:ASP:O	1:C:174:TYR:HD2	2.03	0.41
1:C:177:GLU:N	1:C:178:PRO:HD2	2.35	0.41
1:C:189:ARG:HA	1:C:202:PRO:HG3	2.02	0.41
1:C:190:LEU:O	1:C:196:GLN:HB2	2.19	0.41
1:C:553:PRO:CG	1:C:620:VAL:HG21	2.50	0.41
1:C:580:LYS:C	1:C:582:VAL:H	2.23	0.41
1:D:128:PHE:CG	1:D:186:PRO:HG2	2.56	0.41
1:D:168:ASP:O	1:D:174:TYR:HD2	2.03	0.41
1:D:257:ILE:HD11	1:D:271:GLU:HG3	2.01	0.41
1:D:474:ALA:C	1:D:476:GLU:H	2.23	0.41
1:D:700:ARG:HD2	1:D:704:PHE:CE2	2.52	0.41
1:E:18:ARG:HB2	1:E:19:PRO:CD	2.38	0.41
1:E:18:ARG:HH12	1:E:36:ASN:ND2	2.19	0.41
1:E:522:GLY:HA3	1:E:538:ILE:CD1	2.50	0.41
1:E:526:TYR:CB	1:E:535:LEU:HD11	2.50	0.41
1:E:739:THR:O	1:E:742:VAL:O	2.37	0.41
1:F:312:THR:HA	1:F:315:ILE:HG22	2.02	0.41
1:F:387:PHE:O	1:F:390:LEU:HG	2.20	0.41
1:F:409:ASN:HD22	1:F:425:ILE:CD1	2.28	0.41
1:A:86:PHE:O	1:A:88:ILE:HD12	2.19	0.41
1:B:19:PRO:HG3	1:B:174:TYR:O	2.19	0.41
1:B:21:VAL:HG11	1:B:44:ILE:HG21	2.02	0.41
1:B:140:ILE:HB	1:B:152:THR:HG22	2.01	0.41
1:B:190:LEU:O	1:B:196:GLN:HB2	2.20	0.41
1:B:540:TYR:HD2	1:B:607:TYR:HB3	1.85	0.41
1:C:148:ARG:NH2	1:C:158:MSE:N	2.68	0.41
1:C:217:ALA:HB1	1:C:224:ILE:HD11	2.02	0.41
1:C:472:GLU:O	1:C:476:GLU:HG2	2.20	0.41
1:D:312:THR:HA	1:D:315:ILE:CG2	2.50	0.41
1:E:7:HIS:CB	1:E:74:GLU:HB2	2.51	0.41
1:E:106:ILE:HG22	1:E:107:ALA:N	2.35	0.41
1:E:312:THR:CA	1:E:315:ILE:HG22	2.47	0.41
1:E:410:ALA:HA	1:E:425:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:VAL:HG22	1:F:131:CYS:O	2.20	0.41
1:F:247:GLN:OE1	1:F:637:LYS:HE3	2.21	0.41
1:F:299:GLY:O	1:F:300:LEU:HG	2.20	0.41
1:F:584:SER:HB3	1:F:589:LYS:HB3	2.02	0.41
1:A:1:MSE:N	1:A:80:PRO:HD2	2.36	0.41
1:A:1:MSE:HE3	1:A:2:LYS:H	1.85	0.41
1:A:370:VAL:HG23	1:A:382:ARG:HB2	2.02	0.41
1:A:487:HIS:CD2	1:A:520:TRP:HB3	2.56	0.41
1:A:488:TYR:CD1	1:A:525:LEU:HD13	2.55	0.41
1:A:504:ILE:HD12	1:A:701:ALA:CA	2.51	0.41
1:A:520:TRP:HZ2	1:A:534:ARG:HH21	1.68	0.41
1:B:65:PRO:O	1:B:67:LEU:N	2.54	0.41
1:B:125:MSE:HE3	1:B:319:TRP:CH2	2.56	0.41
1:B:161:PHE:O	1:B:164:SER:HB3	2.20	0.41
1:B:258:GLU:O	1:B:261:LYS:N	2.52	0.41
1:B:321:LYS:HA	1:B:321:LYS:HD3	1.93	0.41
1:B:558:MSE:HE1	1:B:593:ASN:ND2	2.36	0.41
1:B:582:VAL:HB	1:B:583:GLU:OE1	2.21	0.41
1:C:493:SER:HB2	1:C:751:VAL:HG13	2.01	0.41
1:D:219:LYS:HB2	1:D:357:LEU:HA	2.02	0.41
1:D:248:LYS:HA	1:D:249:PRO:HD3	1.97	0.41
1:E:55:ALA:O	1:E:59:ASP:HB2	2.19	0.41
1:E:493:SER:HB2	1:E:742:VAL:HG11	2.02	0.41
1:F:38:GLY:HA2	1:F:144:LEU:HB3	2.02	0.41
1:F:39:ASP:HB3	1:F:144:LEU:HD13	2.02	0.41
1:F:209:LEU:HA	1:F:212:LYS:CG	2.50	0.41
1:F:415:LYS:O	1:F:416:ASN:HB2	2.20	0.41
1:A:180:ALA:HB1	1:A:185:GLY:HA3	2.02	0.41
1:A:456:ILE:N	1:A:456:ILE:HD12	2.36	0.41
1:A:506:ILE:HD11	1:A:694:ALA:HA	2.02	0.41
1:A:738:VAL:HG11	1:A:742:VAL:HG12	2.02	0.41
1:B:1:MSE:HB2	1:B:80:PRO:HD2	2.02	0.41
1:B:18:ARG:N	1:B:19:PRO:CD	2.83	0.41
1:B:368:ASP:HA	1:B:385:ARG:HD3	2.03	0.41
1:B:383:ARG:CZ	1:B:387:PHE:HB3	2.50	0.41
1:C:123:ARG:NH2	1:C:173:ARG:NE	2.67	0.41
1:C:292:LEU:HD12	1:C:296:LEU:CD2	2.47	0.41
1:C:503:VAL:HA	1:C:706:VAL:HG11	2.03	0.41
1:D:188:TYR:CD2	1:D:203:LEU:HD13	2.55	0.41
1:D:236:VAL:HG21	1:D:296:LEU:HD12	2.03	0.41
1:D:278:ARG:NH1	1:D:387:PHE:HE1	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:MSE:HE1	1:D:309:TYR:CE2	2.54	0.41
1:D:595:VAL:O	1:D:598:GLN:HB3	2.20	0.41
1:D:752:GLY:O	1:D:756:LEU:HD12	2.19	0.41
1:E:130:VAL:HG21	1:E:135:GLY:HA3	2.03	0.41
1:E:488:TYR:CD1	1:E:525:LEU:HD13	2.55	0.41
1:E:700:ARG:HH11	1:E:704:PHE:HE2	1.67	0.41
1:F:11:ILE:O	1:F:11:ILE:HG12	2.20	0.41
1:F:186:PRO:HB3	1:F:359:ASN:HB2	2.03	0.41
1:F:398:TYR:CE1	1:F:758:GLY:HA3	2.56	0.41
1:F:557:LEU:HD23	1:F:561:LEU:HD12	2.02	0.41
1:F:620:VAL:HG22	1:F:625:ALA:O	2.20	0.41
1:F:633:GLU:N	1:F:634:PRO:CD	2.81	0.41
1:A:132:THR:HG23	1:A:133:ASN:OD1	2.21	0.41
1:A:286:LYS:HB2	1:A:303:ILE:CD1	2.51	0.41
1:A:329:SER:CA	1:A:337:MSE:HE2	2.45	0.41
1:A:399:ASN:N	1:A:399:ASN:HD22	2.19	0.41
1:B:14:ALA:HA	1:B:146:TYR:CE1	2.56	0.41
1:B:108:ILE:HG13	1:B:108:ILE:O	2.21	0.41
1:B:116:LEU:HB3	1:B:129:ILE:HD13	2.03	0.41
1:B:180:ALA:HB1	1:B:185:GLY:HA3	2.02	0.41
1:B:265:TYR:HE2	1:B:287:LYS:CD	2.33	0.41
1:B:508:LEU:HD11	1:B:725:ILE:CD1	2.51	0.41
1:C:37:LEU:HB2	1:C:41:GLY:HA3	2.03	0.41
1:C:181:CYS:SG	1:C:182:PRO:HD2	2.60	0.41
1:C:371:ILE:CB	1:C:380:VAL:HG13	2.49	0.41
1:C:591:GLU:HG3	1:F:471:MSE:O	2.20	0.41
1:D:261:LYS:HD3	1:D:266:VAL:HG21	2.03	0.41
1:D:265:TYR:O	1:D:284:LEU:HD13	2.20	0.41
1:D:290:PHE:HA	1:D:291:PRO:HD3	1.90	0.41
1:D:493:SER:HB2	1:D:751:VAL:CG1	2.50	0.41
1:E:12:VAL:CA	1:E:68:ALA:HB1	2.48	0.41
1:E:498:LYS:CB	1:E:500:LEU:HD11	2.51	0.41
1:E:501:ASP:O	1:E:503:VAL:HG13	2.20	0.41
1:E:582:VAL:C	1:E:584:SER:H	2.23	0.41
1:E:628:ARG:NH2	1:E:632:GLY:H	2.19	0.41
1:F:35:LYS:HG2	1:F:36:ASN:H	1.86	0.41
1:F:111:ASP:HB2	1:F:172:ARG:NH2	2.27	0.41
1:F:510:GLY:HA2	1:F:610:SER:OG	2.19	0.41
1:F:522:GLY:HA3	1:F:611:THR:HG23	2.03	0.41
1:A:738:VAL:HB	1:A:744:ARG:CG	2.51	0.41
1:B:5:HIS:CD2	1:B:78:ILE:HD12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LEU:HD23	1:B:30:LEU:O	2.20	0.41
1:B:370:VAL:HG23	1:B:381:ILE:CG1	2.51	0.41
1:C:104:PRO:HB3	1:C:387:PHE:O	2.21	0.41
1:C:171:ASN:HD21	1:C:173:ARG:HB2	1.82	0.41
1:D:502:SER:CB	1:D:528:GLY:HA2	2.48	0.41
1:D:582:VAL:HG22	1:D:626:TYR:HB3	2.03	0.41
1:E:1:MSE:HB2	1:E:80:PRO:HD2	2.03	0.41
1:E:612:GLY:O	1:E:615:LEU:HB2	2.20	0.41
1:E:687:LEU:HD22	1:E:724:MSE:SE	2.70	0.41
1:F:88:ILE:HD12	1:F:88:ILE:N	2.35	0.41
1:F:140:ILE:HG21	1:F:360:ARG:HH11	1.85	0.41
1:F:455:LEU:HD12	1:F:455:LEU:C	2.41	0.41
1:F:474:ALA:C	1:F:476:GLU:H	2.22	0.41
1:A:264:ALA:O	1:A:265:TYR:HD2	2.03	0.41
1:A:469:LEU:O	1:A:470:ALA:C	2.59	0.41
1:A:472:GLU:HG3	1:A:473:MSE:N	2.36	0.41
1:A:578:CYS:O	1:A:578:CYS:SG	2.79	0.41
1:A:620:VAL:C	1:A:622:LEU:N	2.72	0.41
1:A:691:ARG:HG3	1:A:724:MSE:HG3	2.03	0.41
1:A:756:LEU:O	1:A:759:LEU:HB3	2.21	0.41
1:B:202:PRO:O	1:B:203:LEU:C	2.58	0.41
1:C:108:ILE:HG22	1:C:309:TYR:O	2.20	0.41
1:C:413:VAL:CG2	1:C:448:LEU:HD12	2.51	0.41
1:C:564:VAL:HG12	1:C:565:TYR:CD1	2.56	0.41
1:D:65:PRO:HG2	1:D:68:ALA:HB2	2.02	0.41
1:D:66:PRO:HD3	1:D:133:ASN:HD22	1.86	0.41
1:D:279:ARG:HG3	1:D:279:ARG:HH11	1.85	0.41
1:D:317:PHE:O	1:D:318:HIS:C	2.59	0.41
1:D:383:ARG:HB3	1:D:747:ASN:ND2	2.34	0.41
1:D:598:GLN:CG	1:D:604:ASN:HB2	2.50	0.41
1:D:757:GLY:C	1:D:759:LEU:H	2.22	0.41
1:E:142:GLU:HB3	1:E:150:ASN:C	2.41	0.41
1:E:219:LYS:HA	1:E:224:ILE:CB	2.51	0.41
1:E:461:HIS:CE1	1:E:463:ALA:HB3	2.56	0.41
1:F:621:LEU:O	1:F:622:LEU:HD23	2.21	0.41
1:A:111:ASP:HB2	1:A:172:ARG:HH22	1.86	0.41
1:A:339:LYS:HG3	1:A:365:ARG:HH12	1.84	0.41
1:A:376:GLY:HA2	1:A:726:ARG:NH1	2.35	0.41
1:A:409:ASN:CG	1:A:410:ALA:H	2.24	0.41
1:A:413:VAL:HG13	1:A:420:TYR:HB2	2.02	0.41
1:A:456:ILE:HD12	1:A:480:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:ILE:HG22	1:A:505:GLY:N	2.35	0.41
1:A:528:GLY:O	1:A:529:TYR:C	2.59	0.41
1:A:535:LEU:HD23	1:A:700:ARG:HG3	2.03	0.41
1:A:587:TYR:CD1	1:A:588:GLY:N	2.74	0.41
1:A:613:ARG:O	1:A:616:ASP:HB3	2.21	0.41
1:A:737:HIS:HD2	1:A:744:ARG:NE	2.19	0.41
1:B:21:VAL:CG1	1:B:44:ILE:HD13	2.51	0.41
1:B:102:ILE:HD13	1:B:102:ILE:HA	1.91	0.41
1:B:171:ASN:ND2	1:B:173:ARG:CB	2.84	0.41
1:B:190:LEU:HB2	1:B:202:PRO:HB3	2.02	0.41
1:B:221:ILE:HD11	1:B:309:TYR:CE1	2.56	0.41
1:B:250:PHE:O	1:B:252:ILE:HD12	2.21	0.41
1:B:252:ILE:CD1	1:B:296:LEU:HD23	2.51	0.41
1:B:256:ASP:O	1:B:257:ILE:C	2.59	0.41
1:B:286:LYS:HB2	1:B:303:ILE:CD1	2.51	0.41
1:B:482:LEU:HD12	1:B:483:GLN:N	2.35	0.41
1:B:619:ALA:HB1	1:B:625:ALA:CB	2.50	0.41
1:B:639:GLU:OE2	1:B:718:ASN:HA	2.21	0.41
1:B:656:GLU:HG3	1:B:661:ARG:CZ	2.51	0.41
1:C:12:VAL:HG13	1:C:13:GLN:N	2.32	0.41
1:C:102:ILE:CD1	1:C:144:LEU:HG	2.51	0.41
1:C:154:LYS:HD3	1:C:154:LYS:O	2.21	0.41
1:C:204:ARG:HG2	1:C:319:TRP:CE2	2.56	0.41
1:C:253:MSE:HE1	1:C:313:HIS:CG	2.56	0.41
1:C:309:TYR:CZ	1:C:385:ARG:NH1	2.83	0.41
1:C:341:ASN:O	1:C:344:ALA:HB3	2.21	0.41
1:C:534:ARG:C	1:C:535:LEU:HD12	2.41	0.41
1:C:601:LYS:HB3	1:C:603:ILE:HG13	2.03	0.41
1:C:601:LYS:CB	1:C:603:ILE:HG13	2.51	0.41
1:D:134:CYS:SG	1:D:135:GLY:N	2.93	0.41
1:D:203:LEU:HD21	1:D:315:ILE:CG2	2.51	0.41
1:D:233:GLU:HA	1:D:236:VAL:CG1	2.50	0.41
1:D:247:GLN:HG3	1:D:298:PRO:CG	2.38	0.41
1:D:348:LEU:HD12	1:D:348:LEU:N	2.36	0.41
1:D:422:SER:HA	1:D:444:PHE:CZ	2.56	0.41
1:D:427:ASN:O	1:D:433:VAL:HG11	2.21	0.41
1:D:447:ILE:O	1:D:448:LEU:HD23	2.21	0.41
1:D:451:LYS:HG3	1:D:451:LYS:O	2.21	0.41
1:D:695:HIS:CE1	1:D:728:VAL:HG13	2.55	0.41
1:D:760:TYR:CE2	1:D:767:LYS:HG2	2.53	0.41
1:E:22:TYR:CE1	1:E:87:TYR:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:GLU:HB3	1:E:289:PRO:CD	2.38	0.41
1:E:653:VAL:HG13	1:E:653:VAL:O	2.21	0.41
1:E:688:ALA:O	1:E:691:ARG:HB3	2.21	0.41
1:E:690:ALA:HB2	1:E:721:ILE:HG12	2.03	0.41
1:F:64:LYS:CB	1:F:65:PRO:HD2	2.51	0.41
1:F:137:ARG:NH2	1:F:178:PRO:HG3	2.31	0.41
1:F:220:GLY:H	1:F:224:ILE:HA	1.85	0.41
1:F:270:GLU:CA	1:F:373:PHE:HE2	2.34	0.41
1:F:552:TYR:O	1:F:555:ARG:HG3	2.20	0.41
1:F:596:LEU:O	1:F:600:ALA:N	2.54	0.41
1:F:601:LYS:HD2	1:F:603:ILE:HD11	2.03	0.41
1:A:286:LYS:HD2	1:A:303:ILE:HD11	2.02	0.41
1:A:399:ASN:N	1:A:454:ASP:OD1	2.54	0.41
1:A:618:ILE:HG22	1:A:638:LEU:HD21	2.03	0.41
1:B:15:VAL:HG21	1:B:68:ALA:HB2	2.03	0.41
1:B:20:PHE:HE1	1:B:60:LEU:HA	1.86	0.41
1:B:42:VAL:O	1:B:42:VAL:HG22	2.21	0.41
1:B:309:TYR:CD1	1:B:309:TYR:C	2.94	0.41
1:B:373:PHE:CZ	1:B:378:ARG:HD3	2.55	0.41
1:B:497:GLU:OE1	1:B:738:VAL:HA	2.21	0.41
1:B:598:GLN:HG3	1:B:604:ASN:HB2	2.03	0.41
1:B:626:TYR:C	1:B:627:ARG:HG2	2.40	0.41
1:B:761:LEU:O	1:B:761:LEU:HD12	2.20	0.41
1:C:320:SER:O	1:C:321:LYS:C	2.58	0.41
1:C:404:GLY:HA2	1:C:753:GLN:OE1	2.21	0.41
1:C:494:VAL:HG11	1:C:710:ALA:HB1	2.02	0.41
1:C:526:TYR:HB2	1:C:535:LEU:HD11	2.03	0.41
1:C:554:LEU:HD23	1:C:583:GLU:OE2	2.21	0.41
1:D:147:ASP:HA	1:D:177:GLU:OE2	2.21	0.41
1:D:148:ARG:CZ	1:D:158:MSE:HG3	2.51	0.41
1:D:177:GLU:N	1:D:178:PRO:HD2	2.36	0.41
1:D:339:LYS:O	1:D:340:ASP:C	2.59	0.41
1:D:557:LEU:O	1:D:561:LEU:HG	2.21	0.41
1:D:694:ALA:O	1:D:698:VAL:HG23	2.20	0.41
1:E:8:VAL:O	1:E:42:VAL:HB	2.21	0.41
1:E:13:GLN:NE2	1:E:18:ARG:NH2	2.69	0.41
1:E:198:ILE:O	1:E:199:TYR:HB3	2.21	0.41
1:E:433:VAL:O	1:E:436:PHE:N	2.52	0.41
1:F:153:MSE:HA	1:F:156:PHE:HD2	1.86	0.41
1:F:500:LEU:HD12	1:F:501:ASP:O	2.21	0.41
1:A:50:GLU:O	1:A:53:ILE:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ILE:HD13	1:A:303:ILE:CG2	2.51	0.40
1:A:496:ALA:HB2	1:A:755:PHE:CD2	2.56	0.40
1:A:630:TYR:HD1	1:A:631:GLU:N	2.19	0.40
1:B:460:LEU:CD2	1:B:515:THR:HG22	2.51	0.40
1:B:524:VAL:CG2	1:B:536:ALA:HB3	2.47	0.40
1:C:31:ARG:HG2	1:C:85:ARG:C	2.42	0.40
1:C:406:GLU:HA	1:C:466:THR:HG21	2.03	0.40
1:C:543:LEU:HD12	1:C:549:ALA:CB	2.51	0.40
1:D:170:LEU:H	1:D:170:LEU:CD1	2.29	0.40
1:D:171:ASN:HD21	1:D:173:ARG:HB2	1.86	0.40
1:D:205:LYS:HB2	1:D:205:LYS:HE3	1.84	0.40
1:D:522:GLY:H	1:D:523:GLU:CD	2.23	0.40
1:E:66:PRO:HD2	1:E:133:ASN:HD21	1.85	0.40
1:E:209:LEU:O	1:E:212:LYS:HB2	2.20	0.40
1:E:218:ILE:HD12	1:E:356:LEU:CD2	2.51	0.40
1:E:739:THR:O	1:E:740:THR:C	2.60	0.40
1:F:249:PRO:CG	1:F:300:LEU:HD13	2.45	0.40
1:F:552:TYR:HA	1:F:553:PRO:HD2	1.89	0.40
1:F:615:LEU:HD23	1:F:635:ALA:CB	2.52	0.40
1:A:38:GLY:C	1:A:40:ALA:N	2.74	0.40
1:A:148:ARG:C	1:A:150:ASN:H	2.25	0.40
1:A:307:LEU:HB3	1:A:308:PRO:HD2	2.01	0.40
1:A:398:TYR:O	1:A:398:TYR:CG	2.74	0.40
1:A:683:TYR:O	1:A:687:LEU:HG	2.22	0.40
1:A:694:ALA:O	1:A:697:ALA:N	2.54	0.40
1:B:15:VAL:HG11	1:B:67:LEU:HB2	2.02	0.40
1:B:224:ILE:HG12	1:B:338:VAL:HG13	2.03	0.40
1:B:242:ARG:HD3	1:B:351:VAL:O	2.21	0.40
1:B:332:TYR:HB3	1:B:333:PRO:HD2	2.03	0.40
1:B:365:ARG:O	1:B:366:ALA:HB2	2.21	0.40
1:B:413:VAL:HG11	1:B:448:LEU:HD11	2.03	0.40
1:B:525:LEU:CA	1:B:535:LEU:HD13	2.51	0.40
1:B:616:ASP:O	1:B:619:ALA:HB3	2.21	0.40
1:C:6:ILE:HG13	1:C:57:ILE:HD11	2.04	0.40
1:C:142:GLU:O	1:C:143:ASP:HB2	2.20	0.40
1:C:282:ILE:HA	1:C:371:ILE:O	2.22	0.40
1:C:370:VAL:HG23	1:C:381:ILE:CD1	2.51	0.40
1:D:163:ARG:HH11	1:D:163:ARG:CB	2.32	0.40
1:D:279:ARG:HH11	1:D:279:ARG:CG	2.34	0.40
1:D:453:LEU:HG	1:D:453:LEU:O	2.21	0.40
1:D:649:LEU:HD23	1:D:651:PHE:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:VAL:O	1:E:89:GLU:HA	2.21	0.40
1:E:279:ARG:N	1:E:280:PRO:CD	2.84	0.40
1:E:383:ARG:O	1:E:384:SER:HB3	2.21	0.40
1:F:451:LYS:O	1:F:451:LYS:HG3	2.22	0.40
1:F:553:PRO:HG3	1:F:626:TYR:O	2.21	0.40
1:F:743:PRO:HG2	1:F:748:GLY:CA	2.49	0.40
1:A:108:ILE:HG13	1:A:311:GLY:N	2.32	0.40
1:A:561:LEU:HB3	1:A:570:LEU:HD13	2.02	0.40
1:A:642:ALA:HB1	1:A:683:TYR:HA	2.03	0.40
1:B:253:MSE:HE2	1:B:317:PHE:HD1	1.86	0.40
1:B:278:ARG:O	1:B:279:ARG:C	2.60	0.40
1:B:303:ILE:HG22	1:B:304:GLY:N	2.36	0.40
1:C:172:ARG:HG2	1:C:173:ARG:HD3	2.03	0.40
1:D:35:LYS:O	1:D:42:VAL:HG13	2.22	0.40
1:D:104:PRO:HD3	1:D:390:LEU:HD21	2.04	0.40
1:D:210:ILE:HD13	1:D:216:VAL:CG1	2.47	0.40
1:D:292:LEU:HD11	1:D:324:VAL:HG21	2.02	0.40
1:D:383:ARG:HG3	1:D:383:ARG:NH1	2.37	0.40
1:D:437:MSE:HE1	1:D:466:THR:HG22	2.03	0.40
1:D:497:GLU:OE2	1:D:738:VAL:HG12	2.22	0.40
1:D:727:LYS:HA	1:D:730:GLU:HG2	2.03	0.40
1:E:73:ILE:HG22	1:E:73:ILE:O	2.21	0.40
1:E:140:ILE:HB	1:E:152:THR:CG2	2.51	0.40
1:E:252:ILE:CG2	1:E:324:VAL:HB	2.51	0.40
1:E:415:LYS:O	1:E:417:GLY:N	2.54	0.40
1:F:270:GLU:CB	1:F:373:PHE:HE2	2.34	0.40
1:F:394:ILE:HG23	1:F:755:PHE:HB2	2.04	0.40
1:F:532:VAL:HG12	1:F:533:GLU:N	2.37	0.40
1:F:582:VAL:O	1:F:627:ARG:HD2	2.21	0.40
1:F:722:THR:O	1:F:722:THR:HG22	2.22	0.40
1:A:21:VAL:HA	1:A:24:ILE:CG2	2.52	0.40
1:A:116:LEU:C	1:A:116:LEU:HD12	2.42	0.40
1:A:154:LYS:HD3	1:A:154:LYS:C	2.42	0.40
1:A:207:ALA:C	1:A:209:LEU:N	2.75	0.40
1:A:219:LYS:HB2	1:A:357:LEU:HA	2.03	0.40
1:A:228:CYS:O	1:A:326:VAL:HB	2.22	0.40
1:A:457:ILE:HA	1:A:482:LEU:O	2.21	0.40
1:A:561:LEU:HD22	1:A:565:TYR:CE2	2.57	0.40
1:A:588:GLY:O	1:A:592:PHE:CD2	2.75	0.40
1:B:207:ALA:HB1	1:B:320:SER:CB	2.52	0.40
1:B:217:ALA:HA	1:B:226:LEU:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:MSE:HA	1:B:306:MSE:HB2	2.04	0.40
1:B:259:THR:O	1:B:263:PHE:HB2	2.22	0.40
1:B:278:ARG:HG3	1:B:280:PRO:HD3	2.03	0.40
1:B:582:VAL:HG11	1:B:626:TYR:HB3	2.04	0.40
1:C:106:ILE:HG12	1:C:277:TYR:CD1	2.56	0.40
1:C:312:THR:HA	1:C:315:ILE:CG2	2.49	0.40
1:C:424:TYR:HD1	1:C:747:ASN:HD22	1.68	0.40
1:C:737:HIS:O	1:C:738:VAL:C	2.58	0.40
1:D:125:MSE:HE3	1:D:319:TRP:CH2	2.56	0.40
1:D:152:THR:HG23	1:D:153:MSE:N	2.36	0.40
1:D:219:LYS:HG2	1:D:358:HIS:CE1	2.55	0.40
1:D:729:VAL:O	1:D:729:VAL:HG12	2.21	0.40
1:E:11:ILE:O	1:E:13:GLN:N	2.55	0.40
1:E:239:LEU:HD22	1:E:250:PHE:CZ	2.56	0.40
1:E:261:LYS:HD3	1:E:266:VAL:CG2	2.51	0.40
1:E:406:GLU:HB3	1:E:464:TYR:CD2	2.56	0.40
1:E:459:ASP:C	1:E:461:HIS:H	2.25	0.40
1:F:413:VAL:CG2	1:F:448:LEU:HD13	2.48	0.40
1:F:614:VAL:HG11	1:F:662:VAL:HG11	2.03	0.40
1:F:771:MSE:O	1:F:772:LEU:HD23	2.21	0.40
1:A:12:VAL:HG12	1:A:13:GLN:N	2.37	0.40
1:A:90:LYS:HE2	1:A:90:LYS:HB3	1.93	0.40
1:A:105:ASP:OD1	1:A:139:THR:HG23	2.22	0.40
1:A:196:GLN:HE21	1:A:196:GLN:N	2.19	0.40
1:B:153:MSE:HE1	1:B:360:ARG:NE	2.36	0.40
1:B:228:CYS:O	1:B:326:VAL:HG23	2.21	0.40
1:B:248:LYS:HA	1:B:249:PRO:HD3	1.97	0.40
1:C:128:PHE:CE1	1:C:186:PRO:HG2	2.57	0.40
1:C:394:ILE:HD11	1:C:419:VAL:CG1	2.51	0.40
1:C:516:ASP:HB2	1:C:518:ASN:HD22	1.84	0.40
1:C:555:ARG:NH1	1:C:592:PHE:CE1	2.90	0.40
1:C:618:ILE:HG13	1:C:618:ILE:H	1.71	0.40
1:D:6:ILE:O	1:D:43:GLU:HA	2.22	0.40
1:D:394:ILE:HG23	1:D:395:PRO:HD2	2.02	0.40
1:D:395:PRO:HG2	1:D:396:PHE:CE2	2.55	0.40
1:D:506:ILE:HG23	1:D:693:PHE:CE1	2.57	0.40
1:D:543:LEU:HB2	1:D:549:ALA:CB	2.52	0.40
1:D:612:GLY:O	1:D:615:LEU:HB2	2.22	0.40
1:E:278:ARG:H	1:E:278:ARG:HG2	1.72	0.40
1:E:399:ASN:HA	1:E:414:ALA:O	2.22	0.40
1:F:8:VAL:O	1:F:9:GLN:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:413:VAL:HG11	1:F:448:LEU:CD1	2.52	0.40
1:F:524:VAL:HG23	1:F:536:ALA:H	1.86	0.40
1:F:557:LEU:HD11	1:F:621:LEU:CA	2.50	0.40
1:F:601:LYS:CD	1:F:603:ILE:HD11	2.51	0.40
1:F:620:VAL:HG13	1:F:626:TYR:CE1	2.57	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ARG:NH1	1:A:204:ARG:NH1[12_554]	1.95	0.25

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	762/772 (99%)	530 (70%)	179 (24%)	53 (7%)	1	12
1	B	758/772 (98%)	565 (74%)	145 (19%)	48 (6%)	1	14
1	C	750/772 (97%)	540 (72%)	170 (23%)	40 (5%)	1	16
1	D	761/772 (99%)	580 (76%)	148 (19%)	33 (4%)	2	18
1	E	758/772 (98%)	566 (75%)	149 (20%)	43 (6%)	1	15
1	F	758/772 (98%)	562 (74%)	171 (23%)	25 (3%)	3	21
All	All	4547/4632 (98%)	3343 (74%)	962 (21%)	242 (5%)	1	16

All (242) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	ASP
1	A	203	LEU
1	A	264	ALA

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Mol	Chain	Res	Type
1	A	311	GLY
1	B	42	VAL
1	B	625	ALA
1	C	255	LYS
1	C	291	PRO
1	C	323	PRO
1	C	363	LEU
1	C	624	VAL
1	D	11	ILE
1	D	321	LYS
1	D	384	SER
1	D	603	ILE
1	D	738	VAL
1	E	255	LYS
1	E	384	SER
1	E	624	VAL
1	F	194	ASP
1	F	202	PRO
1	F	203	LEU
1	F	321	LYS
1	F	603	ILE
1	F	738	VAL
1	A	13	GLN
1	A	202	PRO
1	A	268	PRO
1	A	291	PRO
1	A	321	LYS
1	A	323	PRO
1	A	351	VAL
1	A	384	SER
1	A	428	THR
1	A	429	GLY
1	A	499	ASN
1	A	603	ILE
1	A	609	SER
1	A	624	VAL
1	A	725	ILE
1	B	291	PRO
1	B	320	SER
1	B	323	PRO
1	B	366	ALA
1	B	455	LEU

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Mol	Chain	Res	Type
1	B	529	TYR
1	B	741	GLU
1	C	41	GLY
1	C	321	LYS
1	C	362	ILE
1	C	384	SER
1	C	531	ASP
1	C	586	LYS
1	C	718	ASN
1	D	13	GLN
1	D	194	ASP
1	D	319	TRP
1	D	632	GLY
1	D	644	LYS
1	D	715	VAL
1	E	194	ASP
1	E	203	LEU
1	E	319	TRP
1	E	320	SER
1	E	429	GLY
1	E	495	MSE
1	E	603	ILE
1	E	632	GLY
1	E	715	VAL
1	E	738	VAL
1	F	291	PRO
1	F	363	LEU
1	F	384	SER
1	F	545	GLY
1	A	130	VAL
1	A	255	LYS
1	A	329	SER
1	A	363	LEU
1	A	424	TYR
1	A	657	GLY
1	A	714	GLY
1	A	715	VAL
1	A	732	ASN
1	B	81	GLN
1	B	83	PHE
1	B	194	ASP
1	B	268	PRO

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Mol	Chain	Res	Type
1	B	321	LYS
1	B	360	ARG
1	B	384	SER
1	B	715	VAL
1	B	738	VAL
1	C	29	ASN
1	C	234	GLU
1	C	360	ARG
1	C	423	GLN
1	C	539	ASP
1	C	609	SER
1	C	738	VAL
1	D	49	ARG
1	D	143	ASP
1	D	291	PRO
1	D	320	SER
1	D	323	PRO
1	E	12	VAL
1	E	83	PHE
1	E	199	TYR
1	E	202	PRO
1	E	268	PRO
1	E	291	PRO
1	E	586	LYS
1	E	648	ASP
1	E	718	ASN
1	F	715	VAL
1	A	113	LEU
1	A	502	SER
1	A	516	ASP
1	A	539	ASP
1	A	551	TYR
1	B	12	VAL
1	B	143	ASP
1	B	247	GLN
1	B	255	LYS
1	B	330	ALA
1	B	521	GLY
1	B	609	SER
1	C	143	ASP
1	C	361	LYS
1	C	521	GLY

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Mol	Chain	Res	Type
1	C	729	VAL
1	D	268	PRO
1	D	339	LYS
1	D	346	GLU
1	D	586	LYS
1	E	63	LYS
1	E	323	PRO
1	E	410	ALA
1	E	460	LEU
1	E	741	GLU
1	F	63	LYS
1	F	83	PHE
1	F	540	TYR
1	F	648	ASP
1	F	695	HIS
1	A	117	PHE
1	A	214	TYR
1	A	416	ASN
1	A	425	ILE
1	A	453	LEU
1	A	514	GLY
1	A	581	ALA
1	A	667	GLN
1	A	718	ASN
1	B	66	PRO
1	B	296	LEU
1	B	311	GLY
1	B	333	PRO
1	B	460	LEU
1	B	499	ASN
1	B	514	GLY
1	B	623	ASN
1	B	630	TYR
1	B	678	PRO
1	C	36	ASN
1	C	88	ILE
1	C	324	VAL
1	C	499	ASN
1	C	603	ILE
1	C	652	GLU
1	D	130	VAL
1	D	180	ALA

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Mol	Chain	Res	Type
1	D	424	TYR
1	E	15	VAL
1	E	36	ASN
1	E	66	PRO
1	E	127	PRO
1	E	416	ASN
1	E	678	PRO
1	F	6	ILE
1	F	234	GLU
1	F	514	GLY
1	F	521	GLY
1	A	12	VAL
1	A	143	ASP
1	A	405	ALA
1	A	521	GLY
1	B	137	ARG
1	B	633	GLU
1	C	268	PRO
1	C	567	ILE
1	D	329	SER
1	D	425	ILE
1	D	741	GLU
1	F	632	GLY
1	A	249	PRO
1	B	82	GLY
1	B	130	VAL
1	B	511	VAL
1	C	715	VAL
1	E	73	ILE
1	E	426	GLY
1	F	15	VAL
1	F	323	PRO
1	A	326	VAL
1	A	738	VAL
1	B	362	ILE
1	B	517	GLY
1	B	522	GLY
1	C	11	ILE
1	C	45	VAL
1	D	66	PRO
1	D	333	PRO
1	A	511	VAL

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Mol	Chain	Res	Type
1	A	634	PRO
1	B	202	PRO
1	B	603	ILE
1	B	705	GLY
1	D	429	GLY
1	E	521	GLY
1	F	324	VAL
1	A	41	GLY
1	C	127	PRO
1	C	202	PRO
1	C	257	ILE
1	D	41	GLY
1	D	73	ILE
1	D	403	VAL
1	E	333	PRO
1	E	351	VAL
1	E	425	ILE
1	F	511	VAL
1	A	698	VAL
1	B	257	ILE
1	B	729	VAL
1	C	130	VAL
1	C	511	VAL
1	E	186	PRO
1	E	249	PRO
1	E	311	GLY
1	E	389	PRO
1	D	389	PRO
1	C	389	PRO

### 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	632/627 (101%)	575 (91%)	57 (9%)	8	25
1	B	630/627 (100%)	574 (91%)	56 (9%)	8	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	626/627 (100%)	569 (91%)	57 (9%)	7	25
1	D	632/627 (101%)	584 (92%)	48 (8%)	11	30
1	E	630/627 (100%)	579 (92%)	51 (8%)	9	29
1	F	630/627 (100%)	573 (91%)	57 (9%)	8	25
All	All	3780/3762 (100%)	3454 (91%)	326 (9%)	8	27

All (326) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	30	LEU
1	A	49	ARG
1	A	60	LEU
1	A	69	ARG
1	A	89	GLU
1	A	91	SER
1	A	111	ASP
1	A	116	LEU
1	A	117	PHE
1	A	163	ARG
1	A	173	ARG
1	A	181	CYS
1	A	187	SER
1	A	188	TYR
1	A	193	SER
1	A	196	GLN
1	A	221	ILE
1	A	224	ILE
1	A	228	CYS
1	A	250	PHE
1	A	284	LEU
1	A	300	LEU
1	A	306	MSE
1	A	317	PHE
1	A	320	SER
1	A	328	THR
1	A	347	GLU
1	A	357	LEU
1	A	375	ASP
1	A	399	ASN
1	A	438	ARG

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Mol	Chain	Res	Type
1	A	455	LEU
1	A	482	LEU
1	A	500	LEU
1	A	502	SER
1	A	516	ASP
1	A	523	GLU
1	A	529	TYR
1	A	537	HIS
1	A	547	ASP
1	A	587	TYR
1	A	615	LEU
1	A	627	ARG
1	A	640	SER
1	A	648	ASP
1	A	663	GLU
1	A	668	SER
1	A	708	ASN
1	A	718	ASN
1	A	719	GLU
1	A	735	ASN
1	A	736	PHE
1	A	738	VAL
1	A	755	PHE
1	A	756	LEU
1	A	771	MSE
1	B	7	HIS
1	B	11	ILE
1	B	33	TYR
1	B	86	PHE
1	B	102	ILE
1	B	112	CYS
1	B	117	PHE
1	B	134	CYS
1	B	162	CYS
1	B	177	GLU
1	B	181	CYS
1	B	193	SER
1	B	221	ILE
1	B	224	ILE
1	B	225	HIS
1	B	228	CYS
1	B	241	ARG

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Mol	Chain	Res	Type
1	B	250	PHE
1	B	256	ASP
1	B	278	ARG
1	B	282	ILE
1	B	309	TYR
1	B	317	PHE
1	B	320	SER
1	B	328	THR
1	B	337	MSE
1	B	369	SER
1	B	375	ASP
1	B	411	PHE
1	B	428	THR
1	B	438	ARG
1	B	439	GLU
1	B	444	PHE
1	B	445	ARG
1	B	471	MSE
1	B	482	LEU
1	B	488	TYR
1	B	490	HIS
1	B	500	LEU
1	B	516	ASP
1	B	527	LEU
1	B	540	TYR
1	B	547	ASP
1	B	587	TYR
1	B	592	PHE
1	B	653	VAL
1	B	663	GLU
1	B	699	GLU
1	B	704	PHE
1	B	718	ASN
1	B	736	PHE
1	B	738	VAL
1	B	747	ASN
1	B	755	PHE
1	B	760	TYR
1	B	771	MSE
1	C	33	TYR
1	C	61	TYR
1	C	89	GLU

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Mol	Chain	Res	Type
1	C	117	PHE
1	C	120	THR
1	C	129	ILE
1	C	142	GLU
1	C	148	ARG
1	C	164	SER
1	C	172	ARG
1	C	173	ARG
1	C	181	CYS
1	C	193	SER
1	C	196	GLN
1	C	225	HIS
1	C	233	GLU
1	C	257	ILE
1	C	258	GLU
1	C	261	LYS
1	C	267	SER
1	C	274	LEU
1	C	278	ARG
1	C	284	LEU
1	C	292	LEU
1	C	306	MSE
1	C	313	HIS
1	C	317	PHE
1	C	337	MSE
1	C	357	LEU
1	C	370	VAL
1	C	375	ASP
1	C	382	ARG
1	C	403	VAL
1	C	427	ASN
1	C	488	TYR
1	C	502	SER
1	C	516	ASP
1	C	523	GLU
1	C	541	TYR
1	C	543	LEU
1	C	548	LEU
1	C	587	TYR
1	C	605	THR
1	C	616	ASP
1	C	624	VAL

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Mol	Chain	Res	Type
1	C	648	ASP
1	C	663	GLU
1	C	693	PHE
1	C	718	ASN
1	C	724	MSE
1	C	726	ARG
1	C	736	PHE
1	C	738	VAL
1	C	744	ARG
1	C	756	LEU
1	C	760	TYR
1	C	766	THR
1	D	7	HIS
1	D	60	LEU
1	D	112	CYS
1	D	113	LEU
1	D	117	PHE
1	D	164	SER
1	D	181	CYS
1	D	188	TYR
1	D	201	ASP
1	D	221	ILE
1	D	242	ARG
1	D	250	PHE
1	D	262	SER
1	D	267	SER
1	D	270	GLU
1	D	295	ASN
1	D	306	MSE
1	D	313	HIS
1	D	317	PHE
1	D	367	ASP
1	D	375	ASP
1	D	382	ARG
1	D	399	ASN
1	D	403	VAL
1	D	423	GLN
1	D	427	ASN
1	D	437	MSE
1	D	473	MSE
1	D	475	ASN
1	D	494	VAL

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Mol	Chain	Res	Type
1	D	541	TYR
1	D	543	LEU
1	D	551	TYR
1	D	587	TYR
1	D	605	THR
1	D	653	VAL
1	D	693	PHE
1	D	708	ASN
1	D	718	ASN
1	D	719	GLU
1	D	724	MSE
1	D	736	PHE
1	D	737	HIS
1	D	738	VAL
1	D	755	PHE
1	D	760	TYR
1	D	766	THR
1	D	771	MSE
1	E	33	TYR
1	E	62	LYS
1	E	67	LEU
1	E	75	LYS
1	E	84	ASP
1	E	110	ASP
1	E	112	CYS
1	E	117	PHE
1	E	128	PHE
1	E	147	ASP
1	E	172	ARG
1	E	181	CYS
1	E	196	GLN
1	E	224	ILE
1	E	225	HIS
1	E	241	ARG
1	E	259	THR
1	E	267	SER
1	E	278	ARG
1	E	283	THR
1	E	301	HIS
1	E	309	TYR
1	E	313	HIS
1	E	317	PHE

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Mol	Chain	Res	Type
1	E	328	THR
1	E	342	GLU
1	E	375	ASP
1	E	403	VAL
1	E	423	GLN
1	E	427	ASN
1	E	444	PHE
1	E	500	LEU
1	E	525	LEU
1	E	541	TYR
1	E	587	TYR
1	E	596	LEU
1	E	605	THR
1	E	616	ASP
1	E	630	TYR
1	E	643	PHE
1	E	663	GLU
1	E	668	SER
1	E	686	HIS
1	E	693	PHE
1	E	708	ASN
1	E	718	ASN
1	E	736	PHE
1	E	738	VAL
1	E	747	ASN
1	E	755	PHE
1	E	760	TYR
1	F	22	TYR
1	F	84	ASP
1	F	113	LEU
1	F	116	LEU
1	F	117	PHE
1	F	147	ASP
1	F	175	HIS
1	F	181	CYS
1	F	203	LEU
1	F	225	HIS
1	F	228	CYS
1	F	233	GLU
1	F	238	GLU
1	F	250	PHE
1	F	262	SER

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Mol	Chain	Res	Type
1	F	284	LEU
1	F	301	HIS
1	F	312	THR
1	F	317	PHE
1	F	328	THR
1	F	342	GLU
1	F	369	SER
1	F	384	SER
1	F	403	VAL
1	F	423	GLN
1	F	427	ASN
1	F	459	ASP
1	F	473	MSE
1	F	487	HIS
1	F	490	HIS
1	F	533	GLU
1	F	537	HIS
1	F	541	TYR
1	F	554	LEU
1	F	587	TYR
1	F	593	ASN
1	F	596	LEU
1	F	599	LEU
1	F	605	THR
1	F	627	ARG
1	F	628	ARG
1	F	640	SER
1	F	643	PHE
1	F	653	VAL
1	F	663	GLU
1	F	686	HIS
1	F	695	HIS
1	F	704	PHE
1	F	708	ASN
1	F	719	GLU
1	F	736	PHE
1	F	738	VAL
1	F	750	ASN
1	F	755	PHE
1	F	760	TYR
1	F	766	THR
1	F	771	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	121	ASN
1	A	171	ASN
1	A	196	GLN
1	A	247	GLN
1	A	295	ASN
1	A	331	ASN
1	A	427	ASN
1	A	452	ASN
1	A	475	ASN
1	A	485	GLN
1	A	575	ASN
1	A	593	ASN
1	A	718	ASN
1	A	737	HIS
1	A	747	ASN
1	A	750	ASN
1	B	5	HIS
1	B	13	GLN
1	B	36	ASN
1	B	121	ASN
1	B	171	ASN
1	B	247	GLN
1	B	295	ASN
1	B	318	HIS
1	B	331	ASN
1	B	399	ASN
1	B	427	ASN
1	B	475	ASN
1	B	483	GLN
1	B	485	GLN
1	B	490	HIS
1	B	575	ASN
1	B	593	ASN
1	B	623	ASN
1	B	667	GLN
1	B	695	HIS
1	B	735	ASN
1	B	747	ASN
1	B	750	ASN
1	C	9	GLN

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Mol	Chain	Res	Type
1	C	121	ASN
1	C	133	ASN
1	C	171	ASN
1	C	247	GLN
1	C	295	ASN
1	C	331	ASN
1	C	399	ASN
1	C	409	ASN
1	C	427	ASN
1	C	465	ASN
1	C	475	ASN
1	C	486	HIS
1	C	518	ASN
1	C	575	ASN
1	C	718	ASN
1	C	750	ASN
1	D	5	HIS
1	D	9	GLN
1	D	26	HIS
1	D	28	HIS
1	D	121	ASN
1	D	133	ASN
1	D	171	ASN
1	D	295	ASN
1	D	331	ASN
1	D	409	ASN
1	D	427	ASN
1	D	452	ASN
1	D	475	ASN
1	D	483	GLN
1	D	485	GLN
1	D	575	ASN
1	D	593	ASN
1	D	597	ASN
1	D	604	ASN
1	D	708	ASN
1	D	718	ASN
1	D	735	ASN
1	D	747	ASN
1	D	750	ASN
1	E	5	HIS
1	E	7	HIS

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Mol	Chain	Res	Type
1	E	13	GLN
1	E	36	ASN
1	E	121	ASN
1	E	133	ASN
1	E	171	ASN
1	E	196	GLN
1	E	295	ASN
1	E	301	HIS
1	E	331	ASN
1	E	364	ASN
1	E	427	ASN
1	E	452	ASN
1	E	475	ASN
1	E	485	GLN
1	E	575	ASN
1	E	593	ASN
1	E	604	ASN
1	E	686	HIS
1	E	718	ASN
1	E	747	ASN
1	E	750	ASN
1	E	753	GLN
1	F	7	HIS
1	F	171	ASN
1	F	295	ASN
1	F	301	HIS
1	F	331	ASN
1	F	341	ASN
1	F	427	ASN
1	F	452	ASN
1	F	465	ASN
1	F	475	ASN
1	F	593	ASN
1	F	604	ASN
1	F	686	HIS
1	F	708	ASN
1	F	750	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	748/772 (96%)	0.30	26 (3%)	47	36	97, 155, 228, 284	0
1	B	744/772 (96%)	0.49	39 (5%)	34	27	115, 179, 293, 361	0
1	C	739/772 (95%)	0.28	22 (2%)	52	39	118, 171, 229, 257	0
1	D	747/772 (96%)	0.34	27 (3%)	46	35	125, 189, 267, 339	0
1	E	744/772 (96%)	0.36	28 (3%)	44	34	110, 183, 285, 327	0
1	F	744/772 (96%)	0.47	35 (4%)	37	30	138, 191, 298, 348	0
All	All	4466/4632 (96%)	0.38	177 (3%)	43	33	97, 179, 272, 361	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	198	ILE	6.1
1	D	198	ILE	6.0
1	E	198	ILE	6.0
1	A	37	LEU	5.6
1	F	604	ASN	5.4
1	F	320	SER	5.2
1	F	198	ILE	4.8
1	D	200	GLY	4.8
1	C	320	SER	4.8
1	B	37	LEU	4.5
1	B	453	LEU	4.5
1	A	320	SER	4.4
1	B	199	TYR	4.4
1	B	51	GLU	4.3
1	C	198	ILE	4.2
1	C	604	ASN	4.1
1	A	198	ILE	4.1
1	E	542	PRO	4.1
1	D	320	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	320	SER	4.0
1	B	542	PRO	3.9
1	F	2	LYS	3.9
1	E	37	LEU	3.9
1	E	70	ILE	3.9
1	F	453	LEU	3.9
1	C	99	ASP	3.9
1	E	585	LEU	3.8
1	F	193	SER	3.7
1	E	2	LYS	3.7
1	E	604	ASN	3.6
1	F	37	LEU	3.6
1	B	31	ARG	3.6
1	B	513	TYR	3.6
1	C	376	GLY	3.6
1	B	17	PHE	3.5
1	E	62	LYS	3.4
1	C	740	THR	3.4
1	D	2	LYS	3.4
1	F	199	TYR	3.4
1	C	197	GLU	3.4
1	C	453	LEU	3.3
1	E	173	ARG	3.3
1	F	202	PRO	3.3
1	D	588	GLY	3.3
1	E	36	ASN	3.3
1	D	37	LEU	3.2
1	B	2	LYS	3.2
1	C	37	LEU	3.2
1	D	81	GLN	3.2
1	A	732	ASN	3.2
1	D	737	HIS	3.1
1	D	728	VAL	3.0
1	B	52	ASP	3.0
1	F	584	SER	3.0
1	D	99	ASP	3.0
1	A	453	LEU	3.0
1	D	30	LEU	3.0
1	D	587	TYR	3.0
1	E	18	ARG	2.9
1	B	40	ALA	2.9
1	C	585	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	586	LYS	2.9
1	A	740	THR	2.9
1	E	376	GLY	2.9
1	B	585	LEU	2.9
1	B	628	ARG	2.9
1	A	78	ILE	2.9
1	B	683	TYR	2.9
1	D	542	PRO	2.8
1	F	40	ALA	2.8
1	A	376	GLY	2.8
1	E	172	ARG	2.8
1	B	70	ILE	2.8
1	E	199	TYR	2.8
1	F	62	LYS	2.8
1	B	16	GLY	2.8
1	D	453	LEU	2.7
1	B	45	VAL	2.7
1	F	86	PHE	2.7
1	F	691	ARG	2.7
1	A	38	GLY	2.7
1	B	35	LYS	2.7
1	E	588	GLY	2.7
1	F	585	LEU	2.6
1	C	731	ALA	2.6
1	A	604	ASN	2.6
1	E	453	LEU	2.6
1	C	270	GLU	2.6
1	D	29	ASN	2.6
1	D	584	SER	2.6
1	B	604	ASN	2.6
1	A	99	ASP	2.5
1	E	648	ASP	2.5
1	F	36	ASN	2.5
1	A	378	ARG	2.5
1	B	531	ASP	2.5
1	C	193	SER	2.5
1	F	10	GLY	2.5
1	A	626	TYR	2.5
1	B	378	ARG	2.5
1	B	626	TYR	2.4
1	F	586	LYS	2.4
1	B	280	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	603	ILE	2.4
1	F	603	ILE	2.4
1	A	36	ASN	2.4
1	C	47	GLU	2.4
1	C	635	ALA	2.4
1	B	648	ASP	2.4
1	F	513	TYR	2.4
1	D	585	LEU	2.4
1	E	60	LEU	2.4
1	B	29	ASN	2.4
1	B	62	LYS	2.4
1	C	157	PRO	2.4
1	F	91	SER	2.4
1	D	40	ALA	2.3
1	E	683	TYR	2.3
1	A	193	SER	2.3
1	E	320	SER	2.3
1	D	199	TYR	2.3
1	B	200	GLY	2.3
1	F	587	TYR	2.3
1	F	48	GLY	2.3
1	D	290	PHE	2.3
1	A	587	TYR	2.3
1	B	587	TYR	2.3
1	A	584	SER	2.3
1	B	193	SER	2.3
1	A	178	PRO	2.3
1	A	585	LEU	2.2
1	E	653	VAL	2.2
1	F	588	GLY	2.2
1	D	78	ILE	2.2
1	B	142	GLU	2.2
1	D	197	GLU	2.2
1	E	46	VAL	2.2
1	F	51	GLU	2.2
1	A	589	LYS	2.2
1	A	197	GLU	2.2
1	E	603	ILE	2.2
1	F	115	GLU	2.2
1	E	193	SER	2.2
1	A	10	GLY	2.2
1	E	715	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	740	THR	2.2
1	C	589	LYS	2.2
1	D	263	PHE	2.2
1	B	26	HIS	2.2
1	F	72	ARG	2.2
1	B	588	GLY	2.2
1	F	30	LEU	2.2
1	D	405	ALA	2.1
1	B	79	PRO	2.1
1	E	17	PHE	2.1
1	F	516	ASP	2.1
1	B	178	PRO	2.1
1	B	173	ARG	2.1
1	F	427	ASN	2.1
1	E	14	ALA	2.1
1	A	92	SER	2.1
1	B	50	GLU	2.1
1	A	117	PHE	2.1
1	C	626	TYR	2.1
1	F	175	HIS	2.1
1	C	201	ASP	2.1
1	A	588	GLY	2.1
1	B	14	ALA	2.0
1	C	737	HIS	2.0
1	D	586	LYS	2.0
1	E	270	GLU	2.0
1	F	589	LYS	2.0
1	F	625	ALA	2.0
1	D	605	THR	2.0
1	C	373	PHE	2.0
1	F	17	PHE	2.0
1	D	262	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	B	1003	1/1	0.92	0.07	180,180,180,180	0
2	ZN	F	1002	1/1	0.95	0.08	213,213,213,213	0
2	ZN	D	1003	1/1	0.96	0.06	202,202,202,202	0
2	ZN	D	1001	1/1	0.97	0.10	157,157,157,157	0
2	ZN	A	1003	1/1	0.97	0.07	178,178,178,178	0
2	ZN	C	1003	1/1	0.97	0.05	156,156,156,156	0
2	ZN	B	1002	1/1	0.98	0.03	187,187,187,187	0
2	ZN	A	1001	1/1	0.98	0.14	144,144,144,144	0
2	ZN	C	1001	1/1	0.98	0.09	143,143,143,143	0
2	ZN	E	1002	1/1	0.98	0.04	175,175,175,175	0
2	ZN	F	1001	1/1	0.98	0.07	187,187,187,187	0
2	ZN	C	1002	1/1	0.98	0.10	147,147,147,147	0
2	ZN	F	1003	1/1	0.98	0.04	179,179,179,179	0
2	ZN	B	1001	1/1	0.99	0.07	170,170,170,170	0
2	ZN	E	1003	1/1	0.99	0.04	183,183,183,183	0
2	ZN	D	1002	1/1	0.99	0.06	149,149,149,149	0
2	ZN	A	1002	1/1	0.99	0.05	113,113,113,113	0
2	ZN	E	1001	1/1	0.99	0.08	152,152,152,152	0

## 6.5 Other polymers

There are no such residues in this entry.