



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:05 am GMT

PDB ID : 1JXA  
Title : GLUCOSAMINE 6-PHOSPHATE SYNTHASE WITH GLUCOSE 6-PHOSPHATE  
Authors : Teplyakov, A.; Obmolova, G.; Badet, B.; Badet-Denisot, M.A.  
Deposited on : 2001-09-06  
Resolution : 3.10 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

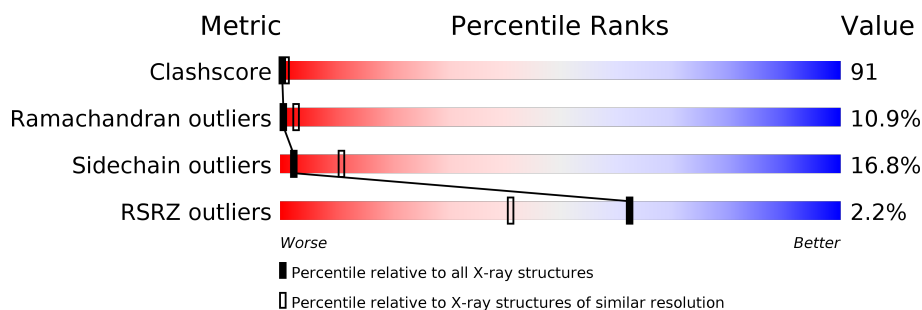
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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

Mol	Chain	Length	Quality of chain
1	A	608	<div> <div>5%</div> <div>20% 54% 23%</div> <div>•</div> </div>
1	B	608	<div> <div>17% 60% 20%</div> <div>•</div> </div>
1	C	608	<div> <div>5%</div> <div>21% 60% 17%</div> <div>•</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14156 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.

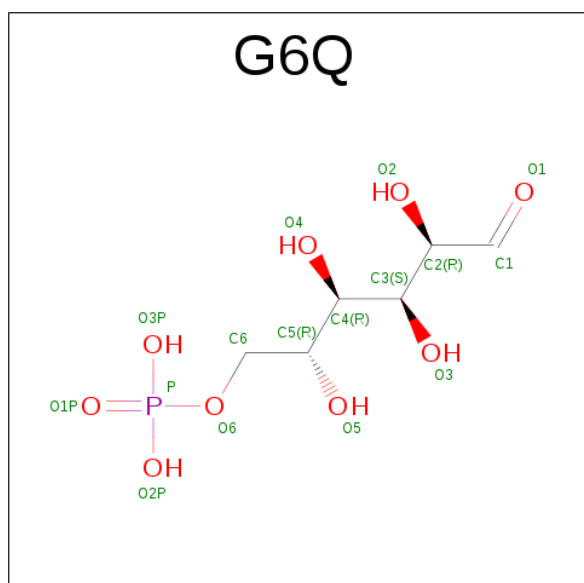
- Molecule 1 is a protein called glucosamine 6-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	608	Total	C	N	O	S	0	0	0
			4695	2953	829	896	17			
1	B	608	Total	C	N	O	S	0	0	0
			4695	2953	829	896	17			
1	C	608	Total	C	N	O	S	0	0	0
			4695	2953	829	896	17			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	421	LYS	ARG	CONFLICT	UNP P17169
B	421	LYS	ARG	CONFLICT	UNP P17169
C	421	LYS	ARG	CONFLICT	UNP P17169

- Molecule 2 is SUGAR (GLUCOSE-6-PHOSPHATE) (three-letter code: G6Q) (formula:  $C_6H_{13}O_9P$ ).

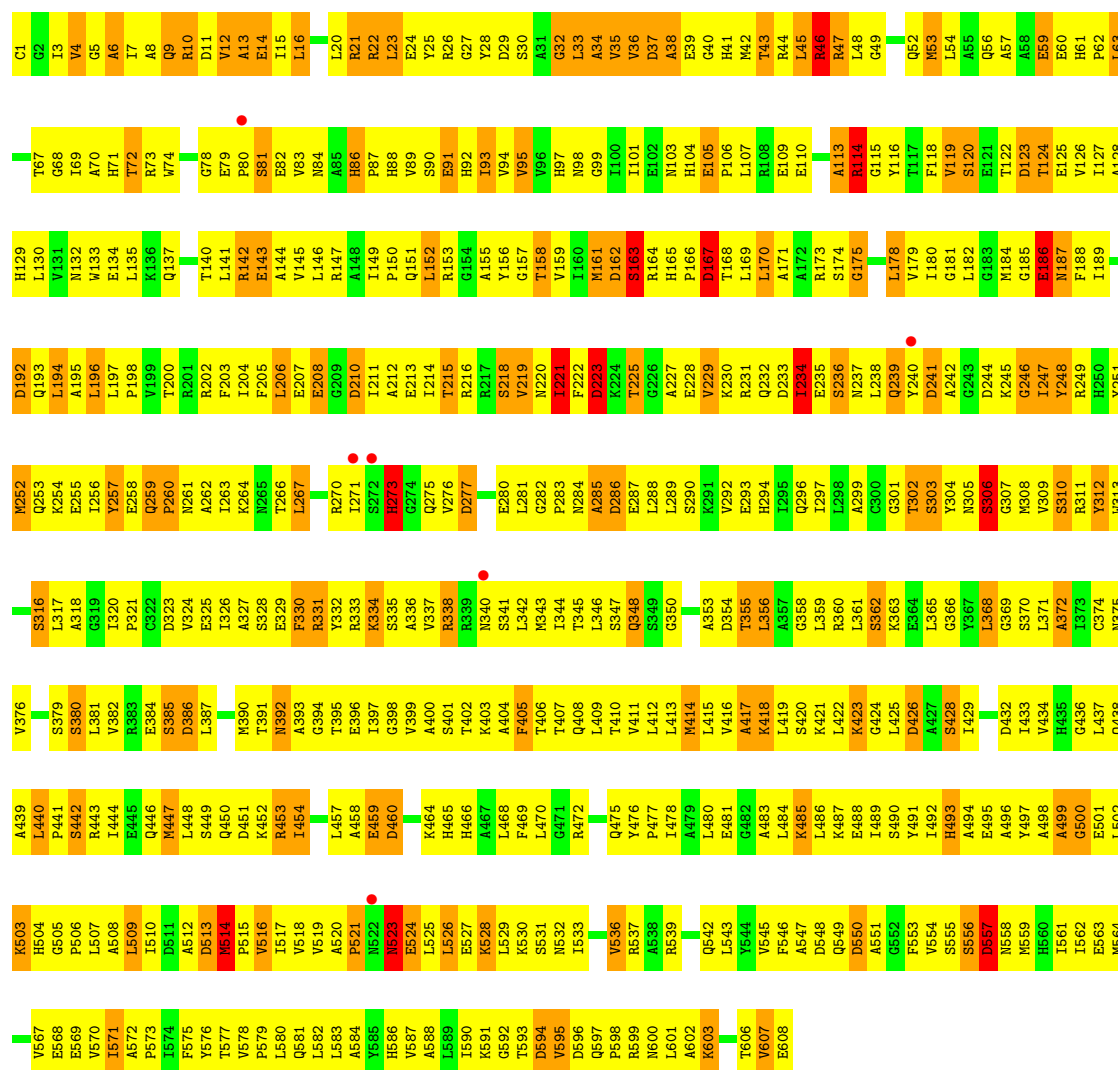


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		

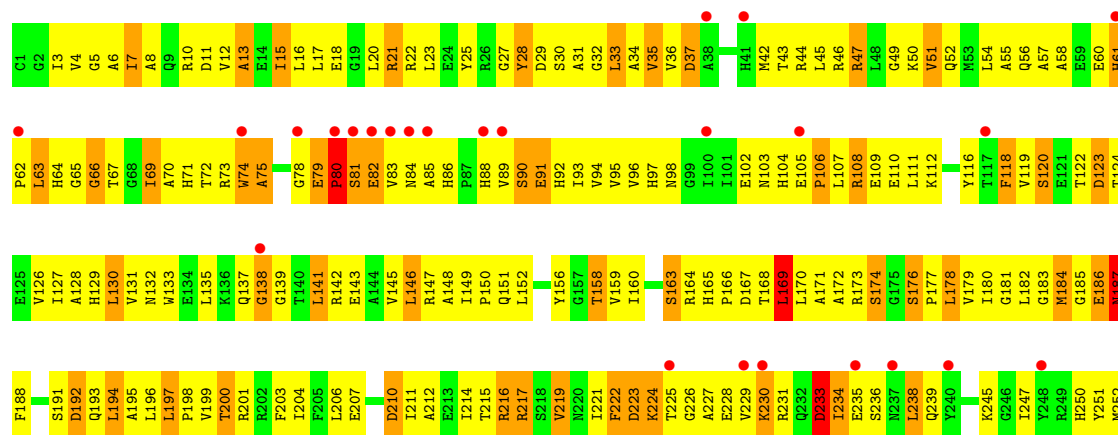
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	26	Total	O	0	0
			26	26		
3	B	10	Total	O	0	0
			10	10		
3	C	3	Total	O	0	0
			3	3		





● Molecule 1: glucosamine 6-phosphate synthase



I571	A508	M447	R383	I320	Q253
A572	L509	L448	D386	F321	K264
P573	I510	S449	D387	C322	E255
I574	D511	Q450	A388	D323	I256
F575	M514	D451	L389	V324	E257
Y576		K452	A389	E325	E258
T577		R453	R380	I326	Q259
V578	I517	I454	T391	A327	P260
P579	V518	E455	N392	S328	N261
L580		A456	A393	E329	A262
Q581	P521	L457		F330	I263
L582	N522	A458	E396	R331	K264
L583	R523	E459	I397	Y332	N265
A584	E524	D460	G398	R333	T266
Y585	L525	F461	V399	R334	
H586	L526	S462	A400	S335	
V587	E527	D463	S401		R270
A588	K528	K464	T402		I271
L589	L529	H465	K403	R338	S272
K590	K530	H466	A404		
S591	S531	A467	F405	S341	L278
G592	N532	L468	T406	I342	S279
T593	I533	F469	T407	N343	E280
D594	E534	L470	Q408	I344	L281
V595	E535	G471	L409	T345	G282
D596	V536	R472	T410	S347	P283
Q597	R537		V411	Q348	N284
P598	A538	Q475	L412	S349	A285
R599	R539	Y476	L413	E350	D286
N600	O540	P477	M414	G351	E287
L601	G541	L478	L415	T352	L288
A602	Q542	A479	V416	A353	L289
K603	L543	L480	A417	D354	S290
S604	Y544	E481	K418	T355	K291
V605	V545	G482		L356	V292
T606	F546	A483		A357	E293
V607	A547	L484	K421	G358	H294
E608	D548	K485	L422	L365	I295
	Q549	L486	K423	G366	Q296
	D550	K487	G424	Y367	I297
	A551	E488	L425	L368	L298
	G552	I489	D426	G369	L299
	F553	S490	A427	S370	A299
	Y554	Y491	S428	I371	C300
	S555	I492	I429	A372	G301
	S556	H493	E430	M308	T302
	D557	A494	D432	V309	S303
	N558	E495	I433	N310	Y304
	M559	A496	R435	S305	N305
	H560	Y497	G436	S306	S306
	I561	A498	L437	G307	G307
	I562	A499	Q438	M308	M308
	E563	G500	N375	V309	V309
	M564	E501	A439	R311	R311
	P565	L502	L440		
	H566	K503	P441		
	V567	H504	S442		
	E568	G505	R443		
	E569	P506			
	V570	L507	Q446		
					F314
					E315
					S316
					L317
					A318
					G319

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.40Å 112.40Å 185.10Å 90.00° 96.40° 90.00°	Depositor
Resolution (Å)	12.00 – 3.10 19.97 – 3.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-3.10) 92.7 (19.97-3.15)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 3.15Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.200 , 0.280 0.213 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	69.1	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 83.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	14156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: G6Q

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	0.82	1/4776 (0.0%)	1.34	47/6467 (0.7%)
1	B	0.67	0/4776	1.10	29/6467 (0.4%)
1	C	0.51	0/4776	0.90	18/6467 (0.3%)
All	All	0.68	1/14328 (0.0%)	1.13	94/19401 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	476	TYR	CD1-CE1	-5.16	1.31	1.39

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	ASP	CB-CG-OD2	9.78	127.10	118.30
1	A	22	ARG	NE-CZ-NH1	-8.83	115.88	120.30
1	B	47	ARG	NE-CZ-NH1	-8.83	115.89	120.30
1	B	142	ARG	NE-CZ-NH1	-8.83	115.89	120.30
1	B	114	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	B	167	ASP	CB-CG-OD2	8.73	126.16	118.30
1	A	216	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	A	217	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	A	216	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	A	278	LEU	CB-CG-CD1	-8.58	96.42	111.00
1	B	142	ARG	NE-CZ-NH2	8.33	124.47	120.30
1	A	37	ASP	CB-CG-OD2	7.96	125.46	118.30
1	B	46	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	B	46	ARG	NE-CZ-NH1	7.77	124.18	120.30
1	A	354	ASP	CB-CG-OD2	7.69	125.22	118.30
1	A	47	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	A	432	ASP	CB-CG-OD2	7.56	125.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	ARG	NE-CZ-NH1	-7.44	116.58	120.30
1	A	26	ARG	NE-CZ-NH1	-7.43	116.58	120.30
1	B	22	ARG	NE-CZ-NH1	-7.37	116.61	120.30
1	B	10	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	A	286	ASP	CB-CG-OD2	6.90	124.51	118.30
1	C	596	ASP	CB-CG-OD2	6.87	124.49	118.30
1	A	162	ASP	CB-CG-OD2	6.71	124.34	118.30
1	B	23	LEU	CB-CG-CD2	-6.56	99.85	111.00
1	A	426	ASP	CB-CG-OD2	6.53	124.17	118.30
1	A	3	ILE	CG1-CB-CG2	-6.49	97.13	111.40
1	B	460	ASP	CB-CG-OD2	6.45	124.10	118.30
1	A	223	ASP	CB-CG-OD2	6.27	123.95	118.30
1	C	80	PRO	N-CA-C	-6.27	95.80	112.10
1	A	47	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	B	550	ASP	CB-CG-OD2	6.13	123.82	118.30
1	B	229	VAL	CB-CA-C	-6.08	99.84	111.40
1	A	298	LEU	CB-CG-CD1	6.04	121.26	111.00
1	A	360	ARG	NE-CZ-NH2	5.99	123.29	120.30
1	C	37	ASP	CB-CG-OD2	5.97	123.67	118.30
1	C	286	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	432	ASP	CB-CG-OD2	5.92	123.63	118.30
1	B	219	VAL	CB-CA-C	-5.88	100.23	111.40
1	C	511	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	114	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	C	460	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	121	GLU	N-CA-CB	-5.79	100.18	110.60
1	A	100	ILE	CG1-CB-CG2	-5.75	98.76	111.40
1	A	130	LEU	CB-CG-CD2	5.73	120.75	111.00
1	A	451	ASP	CB-CG-OD2	5.73	123.45	118.30
1	B	386	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	557	ASP	CB-CG-OD2	5.66	123.40	118.30
1	A	111	LEU	CB-CG-CD1	-5.66	101.38	111.00
1	C	123	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	21	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	210	ASP	CB-CG-OD2	5.64	123.38	118.30
1	C	223	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	557	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	567	VAL	CB-CA-C	-5.58	100.80	111.40
1	A	233	ASP	CB-CG-OD1	5.52	123.27	118.30
1	C	432	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	354	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	286	ASP	CB-CG-OD2	5.46	123.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	596	ASP	CB-CG-OD2	5.46	123.21	118.30
1	B	277	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	426	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	594	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	192	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	463	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	196	LEU	CB-CG-CD2	-5.39	101.84	111.00
1	A	577	THR	CA-CB-CG2	-5.36	104.89	112.40
1	A	277	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	382	VAL	CA-CB-CG1	-5.34	102.89	110.90
1	A	22	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	B	192	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	217	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	594	ASP	CB-CG-OD2	5.26	123.03	118.30
1	B	162	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	270	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	A	376	VAL	CB-CA-C	-5.23	101.46	111.40
1	A	352	THR	CA-CB-CG2	-5.22	105.09	112.40
1	C	192	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	196	LEU	CA-CB-CG	-5.17	103.41	115.30
1	A	204	ILE	N-CA-C	-5.17	97.06	111.00
1	A	196	LEU	CB-CG-CD1	5.15	119.75	111.00
1	B	16	LEU	CB-CG-CD1	5.14	119.74	111.00
1	A	333	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	C	451	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	16	LEU	CA-CB-CG	-5.13	103.51	115.30
1	A	23	LEU	CB-CG-CD1	-5.12	102.30	111.00
1	B	323	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	386	ASP	CB-CG-OD2	5.08	122.88	118.30
1	A	37	ASP	CB-CG-OD1	-5.07	113.74	118.30
1	A	317	LEU	CB-CG-CD1	-5.06	102.39	111.00
1	C	233	ASP	CB-CG-OD1	5.05	122.84	118.30
1	B	223	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	599	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	C	463	ASP	CB-CG-OD2	5.03	122.82	118.30

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	4695	0	4715	862	1
1	B	4695	0	4715	918	0
1	C	4695	0	4715	826	0
2	A	16	0	10	4	0
2	B	16	0	11	2	0
3	A	26	0	0	2	0
3	B	10	0	0	2	0
3	C	3	0	0	0	0
All	All	14156	0	14166	2564	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 91.

All (2564) 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:100:ILE:CG1	1:A:100:ILE:CD1	1.76	1.63
1:A:304:TYR:CE1	1:A:326:ILE:HD13	1.47	1.48
1:A:304:TYR:CD1	1:A:326:ILE:CD1	2.18	1.26
1:B:484:LEU:O	1:B:485:LYS:HG2	1.27	1.25
1:B:223:ASP:OD2	1:B:225:THR:HG23	1.32	1.25
1:A:491:TYR:CZ	1:A:599:ARG:HD3	1.74	1.22
1:C:399:VAL:HG23	1:C:596:ASP:O	1.39	1.21
1:C:565:PRO:HG2	1:C:575:PHE:HZ	1.05	1.19
1:C:252:MET:SD	1:C:400:ALA:HB3	1.81	1.18
1:B:281:LEU:HD13	1:B:387:LEU:CD1	1.72	1.18
1:B:529:LEU:O	1:B:533:ILE:HG13	1.42	1.18
1:A:146:LEU:HG	1:A:211:ILE:HD12	1.25	1.18
1:B:406:THR:HA	1:B:409:LEU:HD12	1.21	1.18
1:B:356:LEU:HD11	1:B:360:ARG:CZ	1.73	1.18
1:B:502:LEU:HA	1:B:506:PRO:HG2	1.26	1.18
1:A:304:TYR:CD1	1:A:326:ILE:HD13	1.76	1.18
1:B:21:ARG:HG3	1:B:21:ARG:HH11	1.08	1.16
1:A:304:TYR:CE1	1:A:326:ILE:CD1	2.27	1.16
1:B:529:LEU:HG	1:B:533:ILE:HD11	1.28	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:GLU:HG3	1:A:121:GLU:O	1.47	1.14
1:C:440:LEU:HB3	1:C:441:PRO:HD3	1.21	1.14
1:B:22:ARG:HD3	1:B:194:LEU:O	1.46	1.13
1:B:281:LEU:CD1	1:B:387:LEU:HD13	1.79	1.13
1:B:523:ASN:ND2	1:B:525:LEU:H	1.44	1.12
1:B:48:LEU:HD21	1:B:81:SER:HB2	1.31	1.12
1:C:565:PRO:HG2	1:C:575:PHE:CZ	1.84	1.11
1:C:457:LEU:CD2	1:C:562:ILE:HD11	1.79	1.11
1:B:187:ASN:N	1:B:187:ASN:HD22	1.38	1.11
1:A:193:GLN:NE2	1:A:205:PHE:HZ	1.49	1.11
1:A:607:VAL:HG23	1:A:608:GLU:H	0.96	1.09
1:B:33:LEU:H	1:B:33:LEU:HD23	1.17	1.09
1:A:247:ILE:H	1:A:247:ILE:HD12	0.96	1.09
1:B:587:VAL:HA	1:B:590:ILE:HD12	1.33	1.09
1:B:532:ASN:O	1:B:536:VAL:HG22	1.53	1.09
1:A:383:ARG:HG2	1:A:383:ARG:HH11	1.14	1.09
1:A:607:VAL:HG23	1:A:608:GLU:N	1.65	1.08
1:B:32:GLY:H	1:B:54:LEU:HD22	1.16	1.08
1:A:346:LEU:CD2	1:A:408:GLN:HG2	1.83	1.08
1:A:470:LEU:HB2	1:A:518:VAL:CG2	1.83	1.08
1:B:313:TRP:CZ3	1:B:413:LEU:HD13	1.87	1.08
1:A:351:GLU:OE2	1:A:380:SER:HB2	1.53	1.07
1:B:537:ARG:HE	1:B:558:ASN:ND2	1.51	1.07
1:A:22:ARG:O	1:A:23:LEU:HD23	1.55	1.07
1:A:371:LEU:HD13	1:A:372:ALA:H	1.11	1.07
1:B:316:SER:OG	1:B:317:LEU:HG	1.52	1.06
1:A:185:GLY:O	1:A:216:ARG:HB3	1.53	1.06
1:A:95:VAL:HG11	1:A:127:ILE:HG21	1.28	1.06
1:B:36:VAL:HG12	1:B:37:ASP:H	1.21	1.06
1:B:146:LEU:HD12	1:B:211:ILE:HD13	1.34	1.05
1:C:375:ASN:HD21	1:C:393:ALA:HB3	1.11	1.05
1:B:187:ASN:H	1:B:187:ASN:ND2	1.53	1.05
1:C:375:ASN:HA	1:C:391:THR:OG1	1.55	1.05
1:B:142:ARG:HG2	1:B:142:ARG:NH1	1.72	1.04
1:C:375:ASN:ND2	1:C:393:ALA:HB3	1.70	1.04
1:B:523:ASN:HD21	1:B:525:LEU:HG	1.22	1.04
1:C:219:VAL:O	1:C:219:VAL:HG12	1.58	1.04
1:A:33:LEU:H	1:A:33:LEU:HD22	1.13	1.04
1:A:199:VAL:HG23	1:A:200:THR:H	1.17	1.04
1:B:230:LYS:O	1:B:231:ARG:HD3	1.56	1.04
1:B:32:GLY:N	1:B:54:LEU:HD22	1.70	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ASN:HD21	1:A:122:THR:HB	1.24	1.03
1:B:344:ILE:HG23	1:B:371:LEU:HD23	1.40	1.03
1:A:272:SER:O	1:A:273:HIS:HB2	1.55	1.02
1:B:313:TRP:CE3	1:B:413:LEU:HD13	1.95	1.02
1:B:356:LEU:HD11	1:B:360:ARG:NE	1.74	1.02
1:A:247:ILE:N	1:A:247:ILE:HD12	1.71	1.02
1:C:350:GLY:HA2	1:C:381:LEU:HD12	1.36	1.02
1:A:84:ASN:ND2	1:A:122:THR:HB	1.74	1.02
1:A:296:GLN:HE21	1:A:296:GLN:CA	1.70	1.01
1:A:5:GLY:HA3	1:A:189:ILE:HG22	1.42	1.01
1:C:457:LEU:HD21	1:C:562:ILE:CD1	1.89	1.01
1:C:480:LEU:HD23	1:C:496:ALA:HB1	1.37	1.01
1:A:382:VAL:HG21	1:A:390:MET:CE	1.90	1.01
1:B:507:LEU:HD12	1:B:510:ILE:HG12	1.37	1.01
1:A:296:GLN:HA	1:A:296:GLN:HE21	1.18	1.01
1:A:532:ASN:ND2	1:A:532:ASN:H	1.49	1.01
1:A:250:HIS:HB3	1:A:596:ASP:OD2	1.59	1.01
1:C:7:ILE:HG21	1:C:214:ILE:HG22	1.40	1.01
1:C:27:GLY:O	1:C:29:ASP:N	1.94	1.01
1:A:333:ARG:HG3	1:A:333:ARG:HH11	1.23	1.00
1:A:296:GLN:HA	1:A:296:GLN:NE2	1.75	1.00
1:A:17:LEU:HD21	1:A:33:LEU:CD1	1.91	1.00
1:A:7:ILE:HD11	1:A:215:THR:HA	1.43	1.00
1:A:371:LEU:CD1	1:A:372:ALA:N	2.25	1.00
1:A:103:ASN:ND2	1:A:153:ARG:H	1.58	0.99
1:B:46:ARG:O	1:B:47:ARG:HG2	1.60	0.99
1:B:537:ARG:NE	1:B:558:ASN:HD21	1.58	0.99
1:B:587:VAL:HA	1:B:590:ILE:CD1	1.93	0.99
1:C:224:LYS:CD	1:C:225:THR:HG23	1.91	0.99
1:A:71:HIS:ND1	1:A:86:HIS:HB2	1.77	0.99
1:A:193:GLN:HE21	1:A:205:PHE:HZ	1.09	0.99
1:B:142:ARG:HD3	1:B:213:GLU:OE1	1.59	0.98
1:C:373:ILE:HD13	1:C:411:VAL:HG12	1.44	0.98
1:B:559:MET:CE	1:B:561:ILE:HD11	1.92	0.98
1:C:457:LEU:HD21	1:C:562:ILE:HD11	0.99	0.98
1:C:159:VAL:HG22	1:C:171:ALA:HB1	1.44	0.98
1:A:247:ILE:CD1	1:A:247:ILE:H	1.73	0.98
1:B:122:THR:O	1:B:124:THR:N	1.94	0.98
1:A:388:ALA:O	1:A:389:LEU:HD12	1.64	0.98
1:C:565:PRO:CG	1:C:575:PHE:HZ	1.77	0.98
1:A:111:LEU:O	1:A:113:ALA:N	1.97	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:TYR:CE1	1:A:599:ARG:HD3	1.98	0.98
1:C:570:VAL:HG13	1:C:571:ILE:H	1.26	0.98
1:B:179:VAL:HG23	1:B:205:PHE:HA	1.45	0.97
1:C:18:GLU:HA	1:C:21:ARG:HH11	1.26	0.97
1:A:180:ILE:HD11	1:A:214:ILE:HD11	1.43	0.97
1:C:42:MET:HE3	1:C:44:ARG:HE	1.24	0.97
1:C:79:GLU:O	1:C:81:SER:N	1.97	0.97
1:A:356:LEU:HD21	1:A:360:ARG:NH2	1.80	0.96
1:A:371:LEU:HD13	1:A:372:ALA:N	1.78	0.96
1:C:192:ASP:OD2	1:C:194:LEU:HD22	1.66	0.95
1:B:34:ALA:HB2	1:B:87:PRO:HG2	1.47	0.95
1:B:559:MET:HE3	1:B:561:ILE:HD11	1.45	0.95
1:A:95:VAL:HG11	1:A:127:ILE:CG2	1.96	0.95
1:C:146:LEU:HD11	1:C:226:GLY:HA2	1.45	0.95
1:A:189:ILE:HD12	1:A:190:ALA:H	1.32	0.95
1:C:224:LYS:HD3	1:C:225:THR:HG23	1.46	0.94
1:A:103:ASN:HD21	1:A:153:ARG:N	1.64	0.94
1:A:421:LYS:HE2	1:A:430:GLU:OE1	1.66	0.94
1:C:170:LEU:HD22	1:C:171:ALA:H	1.32	0.94
1:A:382:VAL:HG21	1:A:390:MET:HE1	1.44	0.94
1:B:259:GLN:O	1:B:262:ALA:HB3	1.68	0.94
1:A:356:LEU:HD21	1:A:360:ARG:HH21	1.29	0.94
1:B:413:LEU:HD23	1:B:437:LEU:HD21	1.48	0.94
1:A:267:LEU:HD23	1:A:414:MET:HE1	1.50	0.94
1:A:281:LEU:HD22	1:A:387:LEU:HD12	1.50	0.94
1:A:532:ASN:HD22	1:A:532:ASN:N	1.63	0.94
1:B:289:LEU:O	1:B:292:VAL:HG23	1.68	0.93
1:C:111:LEU:HD13	1:C:116:TYR:CD2	2.03	0.93
1:C:440:LEU:HD13	1:C:571:ILE:HD12	1.48	0.93
1:A:532:ASN:H	1:A:532:ASN:HD22	1.01	0.93
1:A:607:VAL:CG2	1:A:608:GLU:H	1.81	0.93
1:A:251:TYR:O	1:A:255:GLU:HG3	1.69	0.93
1:B:146:LEU:CD1	1:B:211:ILE:HD13	1.98	0.93
1:C:451:ASP:OD2	1:C:582:LEU:HD13	1.69	0.93
1:A:105:GLU:HB3	1:A:106:PRO:HD3	1.49	0.93
1:B:24:GLU:HG2	1:B:597:GLN:NE2	1.83	0.92
1:A:603:LYS:HG3	1:A:604:SER:H	1.32	0.92
1:A:248:TYR:CD2	1:A:254:LYS:HB2	2.04	0.92
1:B:332:TYR:CE1	1:C:528:LYS:NZ	2.37	0.92
1:B:572:ALA:N	1:B:573:PRO:HD2	1.84	0.92
1:C:32:GLY:HA3	1:C:86:HIS:O	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:ILE:HD13	1:C:411:VAL:CG1	1.99	0.92
1:C:423:LYS:HD3	1:C:425:LEU:HG	1.51	0.92
1:B:371:LEU:HG	1:B:372:ALA:H	1.34	0.92
1:B:546:PHE:CE2	1:B:562:ILE:HD13	2.05	0.92
1:C:570:VAL:HG13	1:C:571:ILE:N	1.85	0.91
1:B:447:MET:HE3	1:B:564:MET:SD	2.11	0.91
1:B:63:LEU:HD12	1:B:63:LEU:H	1.32	0.91
1:A:36:VAL:CG1	1:A:42:MET:HA	1.99	0.91
1:C:476:TYR:HB3	1:C:477:PRO:HD3	1.49	0.91
1:C:485:LYS:HA	1:C:485:LYS:HE3	1.49	0.91
1:C:31:ALA:CB	1:C:51:VAL:HG22	1.99	0.91
1:A:146:LEU:HD21	1:A:226:GLY:HA2	1.49	0.91
1:B:186:GLU:O	1:B:186:GLU:CG	2.17	0.91
1:B:587:VAL:CA	1:B:590:ILE:HD12	2.00	0.91
1:A:84:ASN:HB2	1:A:121:GLU:OE1	1.70	0.90
1:A:33:LEU:O	1:A:33:LEU:HD23	1.71	0.90
1:C:4:VAL:O	1:C:4:VAL:HG12	1.70	0.90
1:C:182:LEU:HD11	1:C:204:ILE:CD1	2.00	0.90
1:C:252:MET:SD	1:C:400:ALA:CB	2.58	0.90
1:B:501:GLU:HG3	1:C:326:ILE:HD12	1.51	0.90
1:A:376:VAL:HG12	1:A:379:SER:OG	1.71	0.90
1:B:344:ILE:HD13	1:B:371:LEU:CD2	2.02	0.90
1:A:371:LEU:CD1	1:A:372:ALA:H	1.84	0.89
1:B:142:ARG:HH12	1:B:146:LEU:HD22	1.36	0.89
1:C:255:GLU:O	1:C:403:LYS:HB3	1.73	0.89
1:C:399:VAL:CG2	1:C:596:ASP:O	2.20	0.89
1:B:286:ASP:OD2	1:B:422:LEU:HD21	1.72	0.89
1:C:199:VAL:HG23	1:C:200:THR:HG22	1.52	0.89
1:C:524:GLU:CD	1:C:524:GLU:H	1.74	0.89
1:A:470:LEU:HB2	1:A:518:VAL:HG22	1.55	0.89
1:B:33:LEU:CD2	1:B:33:LEU:H	1.85	0.89
1:C:379:SER:HB2	1:C:382:VAL:HG23	1.54	0.89
1:B:447:MET:CE	1:B:564:MET:SD	2.60	0.89
1:B:162:ASP:O	1:B:164:ARG:N	2.06	0.88
1:B:214:ILE:HG22	1:B:215:THR:N	1.85	0.88
1:B:310:SER:CB	1:B:412:LEU:HD13	2.03	0.88
1:B:502:LEU:CA	1:B:506:PRO:HG2	2.03	0.88
1:A:202:ARG:HG2	1:A:202:ARG:HH11	1.38	0.88
1:A:33:LEU:N	1:A:33:LEU:HD22	1.82	0.88
1:A:5:GLY:CA	1:A:189:ILE:HG22	2.04	0.88
1:C:98:ASN:ND2	1:C:176:SER:OG	2.07	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LEU:HD11	1:C:164:ARG:HH22	1.37	0.87
1:B:142:ARG:NH1	1:B:146:LEU:HD22	1.89	0.87
1:A:304:TYR:CG	1:A:326:ILE:HD11	2.09	0.87
1:B:293:GLU:O	1:B:321:PRO:HG2	1.74	0.87
1:B:396:GLU:OE1	1:B:401:SER:OG	1.91	0.87
1:C:440:LEU:CB	1:C:441:PRO:HD3	2.04	0.87
1:C:499:ALA:O	1:C:502:LEU:HD13	1.74	0.87
1:B:187:ASN:N	1:B:187:ASN:ND2	2.09	0.87
1:B:297:ILE:HB	1:B:324:VAL:HA	1.56	0.87
1:A:423:LYS:O	1:A:425:LEU:N	2.08	0.87
1:C:130:LEU:HD23	1:C:130:LEU:O	1.75	0.87
1:A:553:PHE:HD2	1:A:559:MET:CE	1.88	0.87
1:B:48:LEU:CD2	1:B:81:SER:HB2	2.03	0.86
1:B:528:LYS:HD2	1:B:528:LYS:H	1.40	0.86
1:C:304:TYR:CE2	1:C:308:MET:HE2	2.10	0.86
1:A:567:VAL:HG22	1:A:575:PHE:CE2	2.09	0.86
1:C:578:VAL:HB	1:C:579:PRO:HD3	1.56	0.86
1:B:22:ARG:HD2	1:B:195:ALA:HA	1.58	0.86
1:C:413:LEU:O	1:C:416:VAL:HB	1.74	0.86
1:A:110:GLU:O	1:A:113:ALA:HB3	1.75	0.86
1:B:142:ARG:HH12	1:B:146:LEU:CD2	1.87	0.86
1:B:523:ASN:ND2	1:B:525:LEU:N	2.22	0.86
1:A:193:GLN:NE2	1:A:205:PHE:CZ	2.38	0.86
1:B:90:SER:O	1:B:91:GLU:HB2	1.75	0.86
1:C:480:LEU:HD23	1:C:496:ALA:CB	2.05	0.86
1:A:276:VAL:CG2	1:A:414:MET:HG2	2.05	0.85
1:C:485:LYS:CA	1:C:485:LYS:HE3	2.06	0.85
1:B:142:ARG:HH11	1:B:142:ARG:CG	1.83	0.85
1:C:499:ALA:HB1	1:C:532:ASN:OD1	1.75	0.85
1:C:294:HIS:NE2	1:C:338:ARG:HD2	1.91	0.85
1:C:373:ILE:CD1	1:C:411:VAL:HG12	2.05	0.85
1:A:105:GLU:OE2	1:A:109:GLU:HG2	1.77	0.85
1:A:207:GLU:HG3	1:A:231:ARG:NH1	1.92	0.85
1:C:343:MET:C	1:C:344:ILE:HD12	1.97	0.85
1:A:267:LEU:CD2	1:A:414:MET:CE	2.55	0.85
1:A:510:ILE:HD13	1:A:536:VAL:HB	1.59	0.85
1:B:186:GLU:HG3	1:B:186:GLU:O	1.74	0.85
1:B:221:ILE:H	1:B:221:ILE:HD12	1.41	0.85
1:B:229:VAL:HG21	1:B:231:ARG:HE	1.39	0.84
1:C:221:ILE:O	1:C:228:GLU:HG3	1.77	0.84
1:C:111:LEU:HB3	1:C:116:TYR:HD2	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:SER:HA	1:C:49:GLY:O	1.78	0.84
1:A:567:VAL:HG12	1:A:568:GLU:H	1.41	0.84
1:B:130:LEU:HD23	1:B:152:LEU:HD21	1.57	0.84
1:B:313:TRP:CE3	1:B:413:LEU:CD1	2.59	0.84
1:B:469:PHE:CE1	1:B:517:ILE:HD13	2.11	0.84
1:C:440:LEU:HB3	1:C:441:PRO:CD	2.05	0.84
1:A:128:ALA:O	1:A:130:LEU:N	2.10	0.84
1:A:279:SER:O	1:A:281:LEU:N	2.10	0.84
1:A:455:GLU:HG3	1:A:586:HIS:CE1	2.10	0.84
1:B:142:ARG:HG2	1:B:142:ARG:HH11	1.34	0.84
1:B:355:THR:O	1:B:358:GLY:N	2.10	0.84
1:C:4:VAL:O	1:C:16:LEU:HD22	1.77	0.84
1:B:600:ASN:CG	1:C:539:ARG:HG3	1.97	0.84
1:A:376:VAL:HG12	1:A:376:VAL:O	1.77	0.84
1:B:25:TYR:CE2	1:B:26:ARG:HG3	2.12	0.84
1:C:149:ILE:H	1:C:150:PRO:HD2	1.42	0.84
1:A:510:ILE:CD1	1:A:536:VAL:HB	2.08	0.84
1:C:230:LYS:O	1:C:231:ARG:HD3	1.76	0.84
1:B:520:ALA:HB2	1:B:529:LEU:CD2	2.07	0.84
1:A:346:LEU:HD22	1:A:408:GLN:HG2	1.58	0.84
1:B:458:ALA:O	1:B:460:ASP:N	2.11	0.84
1:B:484:LEU:O	1:B:485:LYS:CG	2.21	0.83
1:A:304:TYR:CG	1:A:326:ILE:CD1	2.60	0.83
1:B:147:ARG:O	1:B:150:PRO:HD2	1.78	0.83
1:B:33:LEU:HD23	1:B:33:LEU:N	1.91	0.83
1:A:140:THR:HG23	1:A:143:GLU:OE1	1.78	0.83
1:C:278:LEU:HD12	1:C:418:LYS:HG2	1.58	0.83
1:A:25:TYR:HE1	1:A:26:ARG:HG2	1.40	0.83
1:A:398:GLY:O	1:A:603:LYS:HD2	1.78	0.83
1:B:310:SER:OG	1:B:412:LEU:HD13	1.79	0.83
1:C:54:LEU:HD12	1:C:54:LEU:O	1.77	0.83
1:C:491:TYR:CZ	1:C:599:ARG:HD3	2.13	0.83
1:C:325:GLU:OE1	1:C:330:PHE:HB2	1.78	0.83
1:A:110:GLU:O	1:A:111:LEU:O	1.97	0.83
1:C:36:VAL:CG1	1:C:166:PRO:HB3	2.09	0.83
1:A:567:VAL:HG12	1:A:568:GLU:N	1.94	0.83
1:A:36:VAL:HG13	1:A:42:MET:HA	1.59	0.83
1:A:304:TYR:CD2	1:A:326:ILE:HD11	2.13	0.82
1:A:142:ARG:HD2	1:A:222:PHE:CZ	2.15	0.82
1:A:383:ARG:HH11	1:A:383:ARG:CG	1.92	0.82
1:A:25:TYR:CD1	1:A:26:ARG:N	2.48	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:MET:CE	1:A:561:ILE:HD11	2.09	0.82
1:B:294:HIS:HB3	1:B:341:SER:OG	1.80	0.82
1:A:199:VAL:HG23	1:A:200:THR:N	1.94	0.82
1:A:263:ILE:HD11	1:A:406:THR:CG2	2.10	0.81
1:A:386:ASP:O	1:A:387:LEU:HD22	1.80	0.81
1:B:310:SER:HB2	1:B:412:LEU:HD13	1.61	0.81
1:B:523:ASN:HD22	1:B:524:GLU:N	1.78	0.81
1:A:164:ARG:O	1:A:165:HIS:ND1	2.13	0.81
1:B:93:ILE:O	1:B:93:ILE:HG22	1.79	0.81
1:A:371:LEU:HD12	1:A:372:ALA:N	1.96	0.81
1:C:20:LEU:HB3	1:C:51:VAL:HG21	1.63	0.81
1:B:468:LEU:CD1	1:B:497:TYR:HD2	1.93	0.81
1:A:266:THR:HG23	1:A:391:THR:O	1.81	0.81
1:B:173:ARG:HG2	1:B:208:GLU:HA	1.63	0.81
1:A:294:HIS:CE1	1:A:338:ARG:HG2	2.16	0.81
1:B:396:GLU:OE2	1:B:401:SER:HA	1.81	0.81
1:C:149:ILE:N	1:C:150:PRO:HD2	1.93	0.81
1:C:506:PRO:C	1:C:508:ALA:H	1.83	0.81
1:A:529:LEU:HA	1:A:532:ASN:HD21	1.46	0.81
1:B:297:ILE:HD12	1:B:324:VAL:HG22	1.63	0.81
1:B:545:VAL:HB	1:B:561:ILE:HD13	1.63	0.80
1:C:305:ASN:ND2	1:C:481:GLU:OE1	2.13	0.80
1:A:17:LEU:HD21	1:A:33:LEU:HD13	1.61	0.80
1:A:21:ARG:HG2	1:A:51:VAL:HG11	1.61	0.80
1:B:122:THR:C	1:B:124:THR:H	1.82	0.80
1:B:1:CYS:N	1:B:26:ARG:O	2.15	0.80
1:A:7:ILE:HD11	1:A:215:THR:CA	2.11	0.80
1:B:214:ILE:O	1:B:215:THR:HG22	1.81	0.80
1:B:126:VAL:HG13	1:B:127:ILE:N	1.97	0.80
1:B:371:LEU:HG	1:B:372:ALA:N	1.91	0.80
1:B:600:ASN:ND2	1:C:539:ARG:HG3	1.96	0.80
1:C:353:ALA:HB1	1:C:608:GLU:OE1	1.81	0.80
1:A:331:ARG:HD3	1:A:332:TYR:CE2	2.16	0.80
1:B:118:PHE:O	1:B:120:SER:N	2.14	0.80
1:B:140:THR:HG23	1:B:143:GLU:OE1	1.81	0.80
1:C:82:GLU:HG3	1:C:83:VAL:H	1.47	0.80
1:A:84:ASN:ND2	1:A:121:GLU:O	2.13	0.80
1:A:121:GLU:O	1:A:121:GLU:CG	2.24	0.80
1:A:607:VAL:CG2	1:A:608:GLU:N	2.38	0.80
1:B:476:TYR:HB3	1:B:477:PRO:HD3	1.63	0.80
1:C:69:ILE:HD11	1:C:94:VAL:HG12	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:ARG:HE	1:B:558:ASN:HD21	0.81	0.80
1:C:36:VAL:HG12	1:C:166:PRO:CB	2.12	0.80
1:A:599:ARG:HG3	1:A:600:ASN:OD1	1.82	0.80
1:B:485:LYS:O	1:B:488:GLU:N	2.14	0.80
1:C:90:SER:HA	1:C:129:HIS:CE1	2.17	0.80
1:A:149:ILE:HB	1:A:150:PRO:HD3	1.63	0.80
1:A:308:MET:O	1:A:310:SER:N	2.16	0.79
1:A:481:GLU:OE1	1:A:481:GLU:HA	1.80	0.79
1:B:90:SER:HB2	1:B:129:HIS:ND1	1.97	0.79
1:A:182:LEU:HD11	1:A:204:ILE:HD11	1.64	0.79
1:A:356:LEU:HD12	1:A:381:LEU:HD23	1.64	0.79
1:B:270:ARG:HD3	1:B:414:MET:CE	2.12	0.79
1:A:447:MET:CE	1:A:564:MET:SD	2.70	0.79
1:B:344:ILE:HD13	1:B:371:LEU:HD23	1.62	0.79
1:A:396:GLU:HG2	1:A:603:LYS:HZ2	1.47	0.79
1:C:159:VAL:HG22	1:C:171:ALA:CB	2.11	0.79
1:A:276:VAL:HG23	1:A:414:MET:HG2	1.63	0.79
1:A:481:GLU:OE2	1:A:485:LYS:HE2	1.83	0.79
1:C:371:LEU:HA	1:C:387:LEU:HB2	1.64	0.79
1:B:433:ILE:HG13	1:B:570:VAL:HG21	1.62	0.79
1:A:223:ASP:OD1	1:A:223:ASP:C	2.21	0.79
1:A:382:VAL:O	1:A:382:VAL:HG12	1.82	0.79
1:B:276:VAL:HG13	1:B:434:VAL:HG22	1.64	0.79
1:B:97:HIS:HB2	1:B:158:THR:HB	1.64	0.79
1:C:35:VAL:HA	1:C:67:THR:O	1.81	0.79
1:B:523:ASN:HD21	1:B:525:LEU:CG	1.96	0.79
1:A:470:LEU:HB2	1:A:518:VAL:HG23	1.64	0.78
1:B:229:VAL:CG2	1:B:231:ARG:HE	1.95	0.78
1:B:413:LEU:HA	1:B:416:VAL:HG23	1.65	0.78
1:C:371:LEU:HD23	1:C:372:ALA:N	1.97	0.78
1:C:447:MET:HE1	1:C:579:PRO:HD3	1.64	0.78
1:A:410:THR:HG23	1:A:437:LEU:CD2	2.12	0.78
1:C:359:LEU:HD23	1:C:381:LEU:HD23	1.64	0.78
1:A:333:ARG:NH1	1:A:333:ARG:HG3	1.92	0.78
1:A:536:VAL:CG2	1:A:543:LEU:HD11	2.12	0.78
1:A:447:MET:HE1	1:A:564:MET:SD	2.23	0.78
1:C:532:ASN:H	1:C:532:ASN:HD22	1.28	0.78
1:A:28:TYR:CZ	1:A:597:GLN:HB3	2.18	0.78
1:B:169:LEU:O	1:B:170:LEU:HD22	1.84	0.78
1:B:483:ALA:O	1:B:487:LYS:HB3	1.83	0.78
1:C:234:ILE:CD1	1:C:236:SER:H	1.95	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:VAL:HG23	1:A:596:ASP:O	1.83	0.78
1:C:481:GLU:OE2	1:C:485:LYS:NZ	2.15	0.78
1:A:42:MET:HG3	1:A:43:THR:N	1.99	0.78
1:B:520:ALA:HB2	1:B:529:LEU:HD21	1.64	0.78
1:A:440:LEU:HB3	1:A:441:PRO:HD3	1.66	0.78
1:C:517:ILE:HD12	1:C:544:TYR:HB2	1.66	0.78
1:A:533:ILE:HG23	1:A:543:LEU:CD2	2.14	0.78
1:B:440:LEU:HB3	1:B:441:PRO:HD3	1.65	0.78
1:C:182:LEU:HD11	1:C:204:ILE:HD11	1.64	0.78
1:C:263:ILE:HG21	1:C:440:LEU:HD23	1.66	0.78
1:C:502:LEU:HB3	1:C:507:LEU:HB2	1.66	0.78
1:C:578:VAL:HB	1:C:579:PRO:CD	2.13	0.78
1:B:302:THR:OG1	1:B:481:GLU:OE2	2.00	0.78
1:B:470:LEU:HB2	1:B:518:VAL:HG22	1.63	0.77
1:B:221:ILE:HG22	1:B:222:PHE:N	1.99	0.77
1:C:486:LEU:HG	1:C:486:LEU:O	1.84	0.77
1:A:383:ARG:NH1	1:A:383:ARG:HG2	1.95	0.77
1:B:469:PHE:C	1:B:470:LEU:HD23	2.05	0.77
1:B:468:LEU:HD23	1:B:516:VAL:HG22	1.65	0.77
1:B:80:PRO:O	1:B:84:ASN:OD1	2.03	0.77
1:B:179:VAL:HG23	1:B:205:PHE:CA	2.13	0.77
1:B:267:LEU:HA	1:B:414:MET:SD	2.25	0.77
1:B:22:ARG:NH1	1:B:22:ARG:HG3	1.99	0.77
1:B:230:LYS:O	1:B:231:ARG:CD	2.32	0.77
1:A:279:SER:C	1:A:281:LEU:H	1.86	0.77
1:A:146:LEU:CD2	1:A:226:GLY:HA2	2.13	0.77
1:C:193:GLN:O	1:C:197:LEU:HG	1.84	0.77
1:C:294:HIS:CD2	1:C:338:ARG:HD2	2.18	0.77
1:C:507:LEU:O	1:C:507:LEU:HG	1.83	0.77
1:A:95:VAL:HG21	1:A:127:ILE:HG22	1.65	0.77
1:B:256:ILE:O	1:B:259:GLN:HB2	1.85	0.77
1:B:36:VAL:HG12	1:B:37:ASP:N	1.99	0.77
1:C:281:LEU:HD13	1:C:387:LEU:HD22	1.66	0.77
1:A:5:GLY:HA3	1:A:189:ILE:CG2	2.15	0.77
1:A:25:TYR:CE1	1:A:26:ARG:HG2	2.21	0.76
1:B:594:ASP:HB3	1:B:597:GLN:O	1.85	0.76
1:B:393:ALA:O	1:B:403:LYS:NZ	2.15	0.76
1:C:42:MET:CE	1:C:44:ARG:HB2	2.14	0.76
1:A:207:GLU:HG3	1:A:231:ARG:CZ	2.15	0.76
1:B:329:GLU:OE2	1:C:472:ARG:HG3	1.84	0.76
1:A:491:TYR:CE1	1:A:599:ARG:CD	2.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:THR:HG23	1:A:437:LEU:HD22	1.66	0.76
1:C:281:LEU:HD21	1:C:389:LEU:HD21	1.67	0.76
1:A:314:PHE:O	1:A:318:ALA:HB3	1.85	0.76
1:B:517:ILE:HG23	1:B:546:PHE:HE1	1.51	0.76
1:A:247:ILE:N	1:A:247:ILE:CD1	2.39	0.76
1:A:8:ALA:HB2	1:A:186:GLU:HB2	1.67	0.76
1:B:140:THR:O	1:B:143:GLU:N	2.19	0.76
1:B:501:GLU:CG	1:C:326:ILE:HD12	2.15	0.76
1:A:173:ARG:HD2	1:A:177:PRO:HA	1.68	0.76
1:A:20:LEU:HB3	1:A:51:VAL:HG21	1.68	0.76
1:B:21:ARG:HG3	1:B:21:ARG:NH1	1.88	0.76
1:A:265:ASN:O	1:A:268:THR:HB	1.86	0.76
1:A:476:TYR:HB3	1:A:477:PRO:HD3	1.68	0.76
1:A:548:ASP:OD1	1:A:550:ASP:N	2.18	0.76
1:B:15:ILE:HG21	1:B:188:PHE:CE2	2.21	0.76
1:A:33:LEU:C	1:A:33:LEU:HD23	2.03	0.75
1:C:251:TYR:CD1	1:C:397:ILE:HG21	2.21	0.75
1:C:299:ALA:HB1	1:C:303:SER:CB	2.17	0.75
1:A:199:VAL:CG2	1:A:200:THR:H	1.98	0.75
1:A:524:GLU:HG2	1:A:525:LEU:HD23	1.68	0.75
1:C:141:LEU:CD2	1:C:168:THR:OG1	2.34	0.75
1:C:380:SER:O	1:C:383:ARG:HB2	1.87	0.75
1:B:447:MET:CE	1:B:564:MET:CE	2.64	0.75
1:C:263:ILE:O	1:C:266:THR:HB	1.86	0.75
1:A:192:ASP:OD2	1:A:194:LEU:CB	2.34	0.75
1:C:216:ARG:HH21	1:C:217:ARG:NH2	1.83	0.75
1:A:522:ASN:O	1:A:522:ASN:CG	2.18	0.75
1:C:506:PRO:O	1:C:508:ALA:N	2.20	0.75
1:C:61:HIS:H	1:C:62:PRO:HD3	1.51	0.75
1:A:477:PRO:HA	1:A:480:LEU:HB2	1.68	0.75
1:A:96:VAL:HG23	1:A:96:VAL:O	1.85	0.75
1:B:200:THR:HG23	1:B:203:PHE:HE1	1.51	0.75
1:C:31:ALA:HB2	1:C:51:VAL:HG22	1.68	0.75
1:B:516:VAL:HB	1:B:543:LEU:HD23	1.68	0.75
1:B:52:GLN:HA	1:B:52:GLN:OE1	1.84	0.75
1:C:238:LEU:HD12	1:C:238:LEU:H	1.52	0.75
1:C:409:LEU:HA	1:C:412:LEU:HD12	1.66	0.75
1:B:234:ILE:HD12	1:B:235:GLU:H	1.52	0.75
1:B:521:PRO:O	1:B:526:LEU:HD22	1.86	0.75
1:B:3:ILE:HD11	1:B:98:ASN:N	2.01	0.75
1:C:404:ALA:O	1:C:408:GLN:HG3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ILE:HD12	1:B:324:VAL:CG2	2.17	0.74
1:B:281:LEU:HD13	1:B:387:LEU:HD13	0.84	0.74
1:A:267:LEU:CD2	1:A:414:MET:HE1	2.17	0.74
1:B:391:THR:O	1:B:392:ASN:C	2.26	0.74
1:B:293:GLU:O	1:B:321:PRO:CG	2.34	0.74
1:C:60:GLU:O	1:C:61:HIS:HB2	1.87	0.74
1:A:196:LEU:C	1:A:198:PRO:HD2	2.08	0.74
1:A:21:ARG:HG2	1:A:51:VAL:CG1	2.18	0.74
1:B:510:ILE:HD13	1:B:510:ILE:N	1.99	0.74
1:A:32:GLY:HA2	1:A:54:LEU:HD11	1.69	0.74
1:B:305:ASN:O	1:B:306:SER:C	2.26	0.74
1:A:308:MET:O	1:A:309:VAL:C	2.23	0.74
1:B:559:MET:O	1:B:559:MET:CG	2.35	0.74
1:A:553:PHE:HD2	1:A:559:MET:HE1	1.50	0.74
1:B:169:LEU:O	1:B:170:LEU:CD2	2.35	0.74
1:B:182:LEU:HD11	1:B:204:ILE:HD11	1.68	0.74
1:C:399:VAL:HG13	1:C:602:ALA:O	1.86	0.74
1:C:543:LEU:HD13	1:C:559:MET:CE	2.18	0.73
1:A:255:GLU:OE1	1:A:397:ILE:N	2.20	0.73
1:C:346:LEU:HD22	1:C:408:GLN:OE1	1.88	0.73
1:B:221:ILE:H	1:B:221:ILE:CD1	1.99	0.73
1:A:142:ARG:HD2	1:A:222:PHE:CE1	2.22	0.73
1:A:304:TYR:CZ	1:A:326:ILE:HD13	2.22	0.73
1:A:536:VAL:HG23	1:A:543:LEU:HD11	1.71	0.73
1:A:606:THR:O	1:A:607:VAL:O	2.05	0.73
1:C:145:VAL:HG11	1:C:170:LEU:HD11	1.71	0.73
1:A:36:VAL:HG12	1:A:41:HIS:O	1.89	0.73
1:A:391:THR:HG22	1:A:407:THR:HB	1.69	0.73
1:C:17:LEU:HD21	1:C:33:LEU:CD1	2.17	0.73
1:C:351:GLU:HG2	1:C:380:SER:HB2	1.69	0.73
1:B:21:ARG:CG	1:B:21:ARG:HH11	1.94	0.73
1:B:27:GLY:HA2	1:B:74:TRP:HB2	1.70	0.73
1:C:141:LEU:HD22	1:C:168:THR:OG1	1.88	0.73
1:A:103:ASN:HD21	1:A:153:ARG:H	0.81	0.73
1:B:88:HIS:HB2	1:B:124:THR:CG2	2.19	0.73
1:B:146:LEU:HD12	1:B:211:ILE:CD1	2.16	0.73
1:C:399:VAL:HG21	1:C:598:PRO:HD2	1.70	0.73
1:C:413:LEU:CD2	1:C:571:ILE:HG22	2.18	0.73
1:A:100:ILE:CD1	1:A:607:VAL:HA	2.19	0.73
1:A:372:ALA:HB2	1:A:385:SER:OG	1.89	0.73
1:C:599:ARG:HG3	1:C:600:ASN:ND2	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:HIS:NE2	1:C:97:HIS:O	2.21	0.73
1:B:214:ILE:CG2	1:B:215:THR:N	2.52	0.73
1:A:165:HIS:HB3	1:A:167:ASP:OD1	1.88	0.72
1:A:267:LEU:HD23	1:A:414:MET:CE	2.19	0.72
1:A:546:PHE:CE1	1:A:562:ILE:HD12	2.23	0.72
1:C:386:ASP:O	1:C:387:LEU:HG	1.89	0.72
1:A:373:ILE:HD13	1:A:411:VAL:CG1	2.20	0.72
1:A:52:GLN:HA	1:A:52:GLN:HE21	1.52	0.72
1:A:136:LYS:HB2	1:A:137:GLN:HE21	1.53	0.72
1:A:307:GLY:O	1:A:310:SER:OG	2.06	0.72
1:B:400:ALA:HA	2:B:701:G6Q:C1	2.19	0.72
1:A:165:HIS:O	1:A:167:ASP:N	2.20	0.72
1:A:304:TYR:CZ	1:A:326:ILE:CD1	2.72	0.72
1:A:399:VAL:HA	1:A:603:LYS:HB2	1.70	0.72
1:C:263:ILE:HD12	1:C:440:LEU:HD21	1.71	0.72
1:C:7:ILE:HD11	1:C:167:ASP:O	1.89	0.72
1:C:17:LEU:HD21	1:C:33:LEU:HD13	1.70	0.72
1:C:533:ILE:O	1:C:536:VAL:HG22	1.90	0.72
1:C:88:HIS:HE1	1:C:122:THR:HG21	1.55	0.72
1:B:276:VAL:HG21	1:B:417:ALA:HB3	1.72	0.72
1:B:446:GLN:O	1:B:449:SER:OG	2.07	0.72
1:B:457:LEU:CD2	1:B:562:ILE:HD11	2.20	0.72
1:A:331:ARG:HG3	1:A:332:TYR:N	2.05	0.72
1:B:301:GLY:O	1:B:304:TYR:HB3	1.89	0.72
1:C:20:LEU:HB2	1:C:51:VAL:HG11	1.70	0.72
1:C:566:HIS:O	1:C:567:VAL:HG13	1.89	0.72
1:A:376:VAL:HG12	1:A:379:SER:HG	1.54	0.71
1:B:24:GLU:HG2	1:B:597:GLN:HE21	1.53	0.71
1:A:267:LEU:HD22	1:A:414:MET:CE	2.20	0.71
1:B:529:LEU:HG	1:B:533:ILE:CD1	2.15	0.71
1:B:214:ILE:C	1:B:215:THR:HG22	2.10	0.71
1:B:415:LEU:HD11	1:B:419:LEU:HD11	1.69	0.71
1:C:309:VAL:HG22	1:C:477:PRO:HB2	1.72	0.71
1:C:31:ALA:O	1:C:54:LEU:CD2	2.39	0.71
1:B:248:TYR:CE2	1:B:254:LYS:HG3	2.26	0.71
1:B:294:HIS:CG	1:B:341:SER:HG	2.08	0.71
1:B:294:HIS:CG	1:B:341:SER:OG	2.43	0.71
1:B:45:LEU:HD11	1:B:57:ALA:HB1	1.73	0.71
1:A:202:ARG:CG	1:A:202:ARG:HH11	2.02	0.71
1:A:25:TYR:HD1	1:A:26:ARG:N	1.89	0.71
1:B:276:VAL:HG21	1:B:417:ALA:CB	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LYS:HG2	1:A:251:TYR:CE1	2.25	0.71
1:B:375:ASN:ND2	1:B:375:ASN:O	2.24	0.71
1:B:447:MET:HE1	1:B:564:MET:CE	2.20	0.71
1:B:469:PHE:O	1:B:470:LEU:HD23	1.90	0.71
1:C:180:ILE:CD1	1:C:206:LEU:HD21	2.21	0.71
1:C:98:ASN:O	1:C:156:TYR:HA	1.91	0.71
1:A:525:LEU:HD23	1:A:525:LEU:N	2.05	0.71
1:A:20:LEU:HD21	1:A:71:HIS:H	1.54	0.71
1:B:537:ARG:NE	1:B:558:ASN:ND2	2.27	0.71
1:A:294:HIS:ND1	1:A:338:ARG:HG2	2.05	0.71
1:B:559:MET:O	1:B:559:MET:HG2	1.91	0.71
1:B:63:LEU:HD12	1:B:63:LEU:N	2.06	0.71
1:C:447:MET:CE	1:C:579:PRO:HD3	2.21	0.71
1:A:522:ASN:O	1:A:522:ASN:OD1	2.09	0.70
1:A:70:ALA:O	1:A:71:HIS:HB2	1.91	0.70
1:B:263:ILE:HD12	1:B:444:ILE:CD1	2.21	0.70
1:B:583:LEU:O	1:B:587:VAL:HG23	1.91	0.70
1:A:20:LEU:HD21	1:A:71:HIS:N	2.05	0.70
1:B:254:LYS:O	1:B:258:GLU:HB2	1.90	0.70
1:B:559:MET:HE2	1:B:561:ILE:HD11	1.72	0.70
1:B:344:ILE:HD13	1:B:371:LEU:HD22	1.71	0.70
1:B:523:ASN:HD22	1:B:523:ASN:C	1.94	0.70
1:B:526:LEU:HD12	1:B:526:LEU:O	1.91	0.70
1:A:33:LEU:HA	1:A:70:ALA:HA	1.72	0.70
1:A:423:LYS:O	1:A:425:LEU:HD23	1.91	0.70
1:A:401:SER:O	1:A:485:LYS:HE3	1.90	0.70
1:C:413:LEU:HD21	1:C:571:ILE:HG22	1.72	0.70
1:A:189:ILE:HD12	1:A:190:ALA:N	2.04	0.70
1:A:333:ARG:NH1	1:A:333:ARG:CG	2.52	0.70
1:B:22:ARG:CD	1:B:194:LEU:O	2.33	0.70
1:B:468:LEU:CD1	1:B:497:TYR:CD2	2.75	0.70
1:C:536:VAL:HG23	1:C:537:ARG:N	2.07	0.70
1:A:353:ALA:CB	1:A:608:GLU:HA	2.22	0.70
1:C:457:LEU:CD2	1:C:562:ILE:CD1	2.61	0.70
1:C:570:VAL:CG1	1:C:571:ILE:H	2.04	0.70
1:A:101:ILE:HD12	1:A:152:LEU:HD22	1.74	0.70
1:B:342:LEU:HD12	1:B:369:GLY:O	1.92	0.70
1:C:151:GLN:O	1:C:152:LEU:HD23	1.90	0.70
1:A:33:LEU:N	1:A:33:LEU:CD2	2.52	0.70
1:A:8:ALA:CB	1:A:186:GLU:HB3	2.22	0.70
1:C:543:LEU:HD13	1:C:559:MET:HE2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:GLU:C	1:C:81:SER:N	2.45	0.70
1:A:7:ILE:O	1:A:7:ILE:HG12	1.90	0.70
1:A:95:VAL:CG1	1:A:127:ILE:HG21	2.16	0.69
1:B:475:GLN:HE21	1:B:519:VAL:CG2	2.04	0.69
1:C:36:VAL:HG12	1:C:166:PRO:HB3	1.71	0.69
1:C:104:HIS:O	1:C:108:ARG:HB2	1.92	0.69
1:C:156:TYR:CE1	1:C:174:SER:HB3	2.27	0.69
1:C:251:TYR:CE1	1:C:397:ILE:HG21	2.27	0.69
1:C:403:LYS:O	1:C:407:THR:HG23	1.92	0.69
1:A:146:LEU:HG	1:A:211:ILE:CD1	2.16	0.69
1:B:142:ARG:O	1:B:146:LEU:HB2	1.92	0.69
1:B:182:LEU:HD21	1:B:204:ILE:HD12	1.74	0.69
1:A:105:GLU:H	1:A:106:PRO:HD2	1.55	0.69
1:C:251:TYR:CG	1:C:397:ILE:HG21	2.27	0.69
1:C:482:GLY:HA3	1:C:580:LEU:HD13	1.73	0.69
1:A:304:TYR:CD1	1:A:326:ILE:HD11	2.17	0.69
1:B:126:VAL:HG13	1:B:127:ILE:H	1.55	0.69
1:B:25:TYR:CE2	1:B:26:ARG:CG	2.75	0.69
1:C:553:PHE:HB3	1:C:561:ILE:CD1	2.23	0.69
1:A:14:GLU:O	1:A:14:GLU:HG2	1.90	0.69
1:A:534:GLU:OE1	1:A:534:GLU:HA	1.93	0.69
1:B:289:LEU:O	1:B:292:VAL:CG2	2.40	0.69
1:B:223:ASP:OD2	1:B:225:THR:CG2	2.26	0.69
1:B:42:MET:CE	1:B:94:VAL:CG2	2.70	0.69
1:B:501:GLU:OE2	1:B:504:HIS:CD2	2.46	0.69
1:B:529:LEU:CG	1:B:533:ILE:HD11	2.17	0.69
1:C:356:LEU:CD1	1:C:380:SER:HB3	2.22	0.69
1:C:480:LEU:CD2	1:C:496:ALA:CB	2.71	0.69
1:B:164:ARG:O	1:B:165:HIS:HD2	1.76	0.69
1:A:239:GLN:O	1:A:240:TYR:C	2.31	0.69
1:C:127:ILE:HG22	1:C:152:LEU:CD1	2.22	0.69
1:C:327:ALA:O	1:C:329:GLU:N	2.23	0.69
1:C:487:LYS:O	1:C:489:ILE:N	2.26	0.69
1:A:185:GLY:O	1:A:216:ARG:CB	2.38	0.69
1:A:197:LEU:N	1:A:198:PRO:CD	2.55	0.69
1:B:517:ILE:HG23	1:B:546:PHE:CE1	2.28	0.69
1:B:24:GLU:CD	1:B:597:GLN:HE22	1.95	0.69
1:A:192:ASP:OD2	1:A:194:LEU:HB2	1.92	0.68
1:A:568:GLU:OE1	1:A:568:GLU:N	2.26	0.68
1:B:33:LEU:CD2	1:B:33:LEU:N	2.50	0.68
1:C:104:HIS:CG	1:C:123:ASP:HA	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:LEU:HD12	1:B:506:PRO:HB2	1.75	0.68
1:C:6:ALA:HB1	1:C:12:VAL:HG11	1.75	0.68
1:A:421:LYS:CE	1:A:430:GLU:OE1	2.41	0.68
1:C:234:ILE:HD12	1:C:236:SER:H	1.57	0.68
1:A:304:TYR:O	1:A:305:ASN:C	2.32	0.68
1:B:577:THR:HA	1:B:580:LEU:HD12	1.74	0.68
1:C:460:ASP:O	1:C:460:ASP:OD1	2.10	0.68
1:C:576:TYR:O	1:C:579:PRO:HD2	1.92	0.68
1:A:172:ALA:O	1:A:178:LEU:HD12	1.92	0.68
1:B:263:ILE:CD1	1:B:444:ILE:CD1	2.71	0.68
1:B:329:GLU:O	1:B:330:PHE:C	2.30	0.68
1:C:127:ILE:HG22	1:C:152:LEU:HD11	1.75	0.68
1:A:25:TYR:CE2	1:A:397:ILE:HD12	2.28	0.68
1:A:443:ARG:O	1:A:446:GLN:HB3	1.94	0.68
1:B:501:GLU:HA	1:B:504:HIS:HD2	1.57	0.68
1:B:601:LEU:HD11	1:C:505:GLY:HA2	1.76	0.68
1:A:192:ASP:OD2	1:A:194:LEU:HB3	1.94	0.68
1:A:212:ALA:HA	1:A:221:ILE:HA	1.76	0.68
1:A:304:TYR:O	1:A:307:GLY:N	2.26	0.68
1:A:4:VAL:HG12	1:A:5:GLY:N	2.09	0.68
1:C:139:GLY:HA2	1:C:143:GLU:HB3	1.76	0.68
1:C:179:VAL:O	1:C:179:VAL:HG13	1.94	0.68
1:A:313:TRP:HA	1:A:317:LEU:HD12	1.76	0.68
1:C:118:PHE:HD1	1:C:118:PHE:H	1.42	0.68
1:C:399:VAL:CG1	1:C:602:ALA:O	2.41	0.68
1:A:107:LEU:O	1:A:109:GLU:N	2.27	0.68
1:A:396:GLU:OE1	1:A:603:LYS:NZ	2.22	0.68
1:A:34:ALA:O	1:A:68:GLY:HA2	1.94	0.68
1:B:468:LEU:O	1:B:516:VAL:HA	1.94	0.68
1:B:95:VAL:O	1:B:95:VAL:HG12	1.94	0.68
1:C:570:VAL:HG13	1:C:571:ILE:HG23	1.75	0.68
1:B:516:VAL:HB	1:B:543:LEU:CD2	2.23	0.67
1:C:139:GLY:CA	1:C:143:GLU:HB3	2.25	0.67
1:C:199:VAL:CG2	1:C:200:THR:HG22	2.24	0.67
1:C:461:PHE:HZ	1:C:517:ILE:HD11	1.59	0.67
1:A:145:VAL:O	1:A:147:ARG:N	2.28	0.67
1:A:237:ASN:O	1:A:239:GLN:N	2.24	0.67
1:A:491:TYR:CZ	1:A:599:ARG:CD	2.67	0.67
1:C:17:LEU:CD2	1:C:33:LEU:HD13	2.24	0.67
1:C:343:MET:HE2	1:C:367:TYR:CE2	2.29	0.67
1:C:42:MET:HE2	1:C:44:ARG:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:C	1:A:165:HIS:ND1	2.48	0.67
1:B:37:ASP:OD2	1:B:41:HIS:HB2	1.94	0.67
1:A:197:LEU:HD11	1:A:239:GLN:HB3	1.77	0.67
1:A:376:VAL:O	1:A:379:SER:OG	2.12	0.67
1:A:342:LEU:HD12	1:A:369:GLY:O	1.94	0.67
1:A:351:GLU:OE2	1:A:380:SER:CB	2.39	0.67
1:C:204:ILE:HG12	1:C:233:ASP:HB3	1.77	0.67
1:A:567:VAL:HG22	1:A:575:PHE:CD2	2.29	0.67
1:A:8:ALA:HB1	1:A:186:GLU:HB3	1.76	0.67
1:B:194:LEU:HD23	1:B:194:LEU:O	1.94	0.67
1:C:299:ALA:HB1	1:C:303:SER:HB2	1.76	0.67
1:C:486:LEU:HD12	1:C:490:SER:OG	1.93	0.67
1:A:281:LEU:HD22	1:A:387:LEU:CD1	2.22	0.67
1:A:454:ILE:HA	1:A:457:LEU:HD23	1.76	0.67
1:B:402:THR:OG1	1:B:403:LYS:N	2.28	0.67
1:B:42:MET:SD	1:B:43:THR:N	2.67	0.67
1:B:457:LEU:HD21	1:B:562:ILE:HD11	1.77	0.67
1:A:15:ILE:O	1:A:16:LEU:C	2.32	0.67
1:A:382:VAL:HG21	1:A:390:MET:HE3	1.74	0.67
1:B:45:LEU:HG	1:B:45:LEU:O	1.93	0.67
1:C:7:ILE:O	1:C:7:ILE:HG23	1.95	0.67
1:B:520:ALA:CB	1:B:529:LEU:HD23	2.25	0.67
1:C:306:SER:HB2	1:C:346:LEU:HD13	1.76	0.67
1:C:288:LEU:HD11	1:C:368:LEU:HD21	1.77	0.67
1:C:533:ILE:O	1:C:536:VAL:CG2	2.43	0.67
1:B:306:SER:OG	1:B:346:LEU:HD13	1.95	0.66
1:B:9:GLN:O	1:B:9:GLN:OE1	2.13	0.66
1:C:156:TYR:CE2	1:C:158:THR:HG22	2.29	0.66
1:A:200:THR:OG1	1:A:201:ARG:N	2.26	0.66
1:A:248:TYR:CD2	1:A:254:LYS:CB	2.77	0.66
1:A:54:LEU:O	1:A:57:ALA:N	2.27	0.66
1:C:476:TYR:O	1:C:479:ALA:HB3	1.96	0.66
1:C:524:GLU:N	1:C:524:GLU:CD	2.49	0.66
1:C:578:VAL:O	1:C:581:GLN:HB2	1.95	0.66
1:A:485:LYS:O	1:A:488:GLU:N	2.28	0.66
1:B:270:ARG:NE	1:B:280:GLU:OE1	2.28	0.66
1:C:18:GLU:CA	1:C:21:ARG:HH11	2.07	0.66
1:A:197:LEU:N	1:A:198:PRO:HD2	2.10	0.66
1:A:346:LEU:HD21	1:A:408:GLN:HG2	1.74	0.66
1:A:529:LEU:CA	1:A:532:ASN:HD21	2.09	0.66
1:B:413:LEU:HA	1:B:416:VAL:CG2	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:SER:OG	1:B:422:LEU:HD13	1.95	0.66
1:B:513:ASP:O	1:B:514:MET:HB2	1.95	0.66
1:C:472:ARG:HD2	1:C:525:LEU:HD22	1.78	0.66
1:A:134:GLU:O	1:A:147:ARG:NH2	2.28	0.66
1:A:196:LEU:N	1:A:196:LEU:HD23	2.10	0.66
1:B:200:THR:HG23	1:B:203:PHE:CE1	2.30	0.66
1:B:22:ARG:CD	1:B:195:ALA:HA	2.25	0.66
1:C:170:LEU:HD13	1:C:171:ALA:N	2.10	0.66
1:B:486:LEU:O	1:B:490:SER:HB3	1.95	0.66
1:B:502:LEU:O	1:B:506:PRO:HD2	1.95	0.66
1:A:88:HIS:HD2	1:A:124:THR:CG2	2.09	0.66
1:A:434:VAL:HG12	1:A:435:HIS:N	2.11	0.66
1:B:399:VAL:HA	1:B:603:LYS:HD2	1.78	0.66
1:B:520:ALA:HB2	1:B:529:LEU:HD23	1.78	0.66
1:C:107:LEU:HA	1:C:110:GLU:HB3	1.75	0.66
1:C:90:SER:HG	1:C:129:HIS:CE1	2.13	0.66
1:B:187:ASN:HD22	1:B:187:ASN:H	0.74	0.66
1:B:56:GLN:O	1:B:57:ALA:C	2.31	0.66
1:B:576:TYR:O	1:B:579:PRO:HG2	1.96	0.66
1:B:88:HIS:HB2	1:B:124:THR:HG22	1.77	0.66
1:C:95:VAL:HG21	1:C:128:ALA:HA	1.78	0.66
1:B:234:ILE:CG1	1:B:235:GLU:N	2.59	0.66
1:A:107:LEU:O	1:A:108:ARG:C	2.33	0.65
1:A:399:VAL:HG21	1:A:597:GLN:HA	1.77	0.65
1:C:204:ILE:HG23	1:C:231:ARG:HB2	1.78	0.65
1:C:283:PRO:HG2	1:C:284:ASN:H	1.60	0.65
1:C:304:TYR:CZ	1:C:308:MET:HE2	2.31	0.65
1:C:251:TYR:CD2	1:C:397:ILE:HG21	2.31	0.65
1:A:121:GLU:O	1:A:122:THR:HB	1.96	0.65
1:A:204:ILE:HG13	1:A:233:ASP:HB3	1.77	0.65
1:B:502:LEU:HG	1:B:507:LEU:HB2	1.78	0.65
1:C:201:ARG:O	1:C:203:PHE:CD2	2.50	0.65
1:C:368:LEU:HD23	1:C:369:GLY:N	2.11	0.65
1:A:136:LYS:HB2	1:A:137:GLN:NE2	2.10	0.65
1:A:388:ALA:C	1:A:389:LEU:HD12	2.16	0.65
1:A:437:LEU:O	1:A:439:ALA:N	2.27	0.65
1:A:559:MET:HE2	1:A:561:ILE:HD11	1.78	0.65
1:B:162:ASP:C	1:B:164:ARG:H	1.99	0.65
1:B:263:ILE:HD12	1:B:444:ILE:HD12	1.79	0.65
1:C:197:LEU:H	1:C:198:PRO:CD	2.09	0.65
1:C:28:TYR:O	1:C:50:LYS:HB3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ASP:C	1:A:511:ASP:OD1	2.33	0.65
1:A:396:GLU:HG2	1:A:603:LYS:NZ	2.10	0.65
1:A:48:LEU:HD13	1:A:82:GLU:HG3	1.77	0.65
1:B:413:LEU:C	1:B:415:LEU:H	1.98	0.65
1:A:305:ASN:ND2	1:A:481:GLU:HA	2.12	0.65
1:A:559:MET:HE3	1:A:561:ILE:HD11	1.78	0.65
1:B:252:MET:CE	1:B:489:ILE:HD13	2.27	0.65
1:A:273:HIS:O	1:A:275:GLN:N	2.29	0.65
1:A:346:LEU:HD11	1:A:412:LEU:HD11	1.78	0.65
1:A:480:LEU:HD23	1:A:496:ALA:HB3	1.79	0.65
1:A:182:LEU:HD11	1:A:204:ILE:CD1	2.27	0.65
1:A:221:ILE:HG22	1:A:229:VAL:HB	1.78	0.65
1:B:311:ARG:O	1:B:313:TRP:N	2.30	0.65
1:B:572:ALA:HB3	1:B:573:PRO:CD	2.27	0.65
1:C:295:ILE:O	1:C:295:ILE:HG22	1.96	0.65
1:C:412:LEU:O	1:C:416:VAL:HG23	1.97	0.65
1:A:447:MET:HE3	1:A:564:MET:SD	2.36	0.65
1:A:602:ALA:O	1:A:603:LYS:O	2.15	0.65
1:B:294:HIS:CB	1:B:341:SER:OG	2.45	0.65
1:C:373:ILE:CD1	1:C:411:VAL:CG1	2.70	0.65
1:C:447:MET:O	1:C:449:SER:N	2.30	0.65
1:C:476:TYR:CB	1:C:477:PRO:HD3	2.24	0.65
1:B:185:GLY:O	1:B:186:GLU:HB3	1.97	0.65
1:B:231:ARG:HA	3:B:706:HOH:O	1.95	0.65
1:B:235:GLU:O	1:B:236:SER:O	2.15	0.65
1:C:104:HIS:NE2	1:C:108:ARG:HG3	2.11	0.65
1:A:103:ASN:O	1:A:106:PRO:HD2	1.97	0.64
1:A:141:LEU:C	1:A:143:GLU:H	2.00	0.64
1:A:229:VAL:HG11	1:A:231:ARG:CZ	2.26	0.64
1:B:229:VAL:HG11	1:B:231:ARG:HH21	1.61	0.64
1:C:31:ALA:O	1:C:54:LEU:HD22	1.96	0.64
1:A:8:ALA:HB2	1:A:186:GLU:CB	2.26	0.64
1:A:324:VAL:O	1:A:324:VAL:HG12	1.95	0.64
1:A:603:LYS:CG	1:A:604:SER:H	2.09	0.64
1:A:105:GLU:HB3	1:A:106:PRO:CD	2.27	0.64
1:A:234:ILE:HD12	1:A:235:GLU:O	1.97	0.64
1:A:248:TYR:CG	1:A:254:LYS:HB2	2.31	0.64
1:A:382:VAL:CG2	1:A:390:MET:HE3	2.28	0.64
1:B:492:ILE:O	1:B:494:ALA:N	2.29	0.64
1:C:506:PRO:C	1:C:508:ALA:N	2.49	0.64
1:B:179:VAL:HG13	1:B:179:VAL:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:HIS:CE1	1:C:122:THR:HG21	2.32	0.64
1:C:219:VAL:O	1:C:219:VAL:CG1	2.32	0.64
1:B:24:GLU:CG	1:B:597:GLN:NE2	2.58	0.64
1:C:158:THR:HG23	1:C:172:ALA:O	1.97	0.64
1:B:524:GLU:CD	1:B:524:GLU:H	2.01	0.64
1:B:78:GLY:H	1:C:538:ALA:HB2	1.63	0.64
1:A:32:GLY:HA2	1:A:54:LEU:HD21	1.77	0.64
1:B:90:SER:CB	1:B:129:HIS:ND1	2.60	0.64
1:A:292:VAL:HG21	1:A:342:LEU:HB2	1.78	0.64
1:B:289:LEU:C	1:B:292:VAL:HG23	2.16	0.64
1:B:42:MET:HG3	1:B:163:SER:HB3	1.80	0.64
1:C:179:VAL:CG2	1:C:203:PHE:HB3	2.27	0.64
1:A:304:TYR:CD1	1:A:326:ILE:HD12	2.29	0.64
1:A:374:CYS:HB3	1:A:390:MET:HE3	1.80	0.64
1:A:578:VAL:N	1:A:579:PRO:HD2	2.12	0.64
1:C:356:LEU:HD11	1:C:380:SER:HB3	1.79	0.64
1:B:220:ASN:O	1:B:222:PHE:CD2	2.51	0.64
1:B:359:LEU:HA	1:B:362:SER:HB3	1.79	0.64
1:B:475:GLN:HE21	1:B:519:VAL:HG21	1.63	0.64
1:B:587:VAL:O	1:B:590:ILE:HD12	1.98	0.64
1:B:71:HIS:ND1	1:B:72:THR:N	2.46	0.64
1:C:448:LEU:O	1:C:451:ASP:OD1	2.15	0.64
1:C:7:ILE:HG21	1:C:214:ILE:CG2	2.21	0.64
1:A:36:VAL:HG12	1:A:41:HIS:C	2.19	0.63
1:B:14:GLU:O	1:B:15:ILE:C	2.34	0.63
1:B:310:SER:HB2	1:B:412:LEU:CD1	2.28	0.63
1:A:382:VAL:CG2	1:A:390:MET:CE	2.72	0.63
1:B:413:LEU:O	1:B:415:LEU:N	2.31	0.63
1:C:565:PRO:O	1:C:566:HIS:O	2.17	0.63
1:A:185:GLY:O	1:A:216:ARG:O	2.16	0.63
1:A:33:LEU:C	1:A:33:LEU:CD2	2.67	0.63
1:A:383:ARG:NH1	1:A:383:ARG:CG	2.57	0.63
1:B:379:SER:O	1:B:382:VAL:N	2.18	0.63
1:C:50:LYS:O	1:C:52:GLN:N	2.30	0.63
1:A:304:TYR:CE2	1:A:326:ILE:HD11	2.33	0.63
1:B:105:GLU:HB3	1:B:106:PRO:HD3	1.79	0.63
1:B:316:SER:HG	1:B:317:LEU:HG	1.62	0.63
1:B:413:LEU:O	1:B:416:VAL:N	2.27	0.63
1:B:42:MET:CE	1:B:94:VAL:HG21	2.26	0.63
1:B:89:VAL:HG12	1:B:94:VAL:HG13	1.81	0.63
1:C:486:LEU:O	1:C:490:SER:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:O	1:A:112:LYS:C	2.36	0.63
1:A:15:ILE:O	1:A:18:GLU:N	2.31	0.63
1:A:481:GLU:OE1	1:A:481:GLU:CA	2.46	0.63
1:A:536:VAL:HG21	1:A:543:LEU:HD11	1.80	0.63
1:C:107:LEU:O	1:C:109:GLU:N	2.31	0.63
1:B:594:ASP:CB	1:B:597:GLN:O	2.46	0.63
1:B:251:TYR:CD2	1:B:397:ILE:HG21	2.34	0.63
1:C:234:ILE:HD12	1:C:235:GLU:N	2.14	0.63
1:B:398:GLY:O	1:B:603:LYS:NZ	2.28	0.63
1:B:485:LYS:O	1:B:486:LEU:C	2.37	0.63
1:C:370:SER:HG	1:C:386:ASP:H	1.45	0.63
1:C:564:MET:HB3	1:C:565:PRO:HD2	1.79	0.63
1:A:110:GLU:O	1:A:113:ALA:CB	2.44	0.63
1:B:503:LYS:HE3	1:B:503:LYS:HA	1.81	0.63
1:C:36:VAL:HG11	1:C:166:PRO:HB3	1.79	0.63
1:C:327:ALA:C	1:C:329:GLU:H	2.01	0.63
1:A:74:TRP:CE3	1:A:602:ALA:HB3	2.33	0.62
1:B:391:THR:HG22	1:B:411:VAL:HG21	1.80	0.62
1:B:470:LEU:CB	1:B:518:VAL:HG22	2.29	0.62
1:C:182:LEU:HD11	1:C:204:ILE:HD12	1.77	0.62
1:A:102:GLU:N	1:A:153:ARG:O	2.30	0.62
1:A:251:TYR:HB3	1:A:255:GLU:OE2	1.99	0.62
1:C:299:ALA:HB1	1:C:303:SER:HB3	1.81	0.62
1:C:3:ILE:HD11	1:C:98:ASN:HB2	1.79	0.62
1:A:338:ARG:HD3	1:A:338:ARG:N	2.14	0.62
1:B:475:GLN:NE2	1:B:519:VAL:HG21	2.15	0.62
1:B:518:VAL:HG11	1:B:529:LEU:HD11	1.80	0.62
1:C:105:GLU:HB2	1:C:106:PRO:HD3	1.80	0.62
1:C:216:ARG:HH21	1:C:217:ARG:HH22	1.47	0.62
1:C:251:TYR:CG	1:C:397:ILE:CG2	2.82	0.62
1:A:207:GLU:HG2	1:A:231:ARG:HD2	1.80	0.62
1:A:32:GLY:HA2	1:A:54:LEU:CD1	2.29	0.62
1:A:76:THR:C	1:A:78:GLY:H	2.03	0.62
1:B:15:ILE:HG21	1:B:188:PHE:HE2	1.63	0.62
1:B:37:ASP:C	1:B:37:ASP:OD1	2.37	0.62
1:C:23:LEU:O	1:C:23:LEU:HD12	1.99	0.62
1:A:120:SER:OG	1:A:121:GLU:HG2	1.99	0.62
1:A:8:ALA:CB	1:A:186:GLU:CB	2.77	0.62
1:B:539:ARG:HB3	1:C:600:ASN:OD1	1.98	0.62
1:C:521:PRO:HA	1:C:548:ASP:HB2	1.82	0.62
1:C:80:PRO:O	1:C:84:ASN:OD1	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:O	1:A:114:ARG:N	2.33	0.62
1:A:237:ASN:C	1:A:239:GLN:H	2.03	0.62
1:B:507:LEU:CD1	1:B:510:ILE:HG12	2.22	0.62
1:A:141:LEU:HD23	1:A:170:LEU:HD23	1.80	0.62
1:A:17:LEU:CD2	1:A:33:LEU:CD1	2.72	0.62
1:A:569:GLU:HA	1:A:572:ALA:HB2	1.82	0.62
1:B:129:HIS:O	1:B:132:ASN:HB3	2.00	0.62
1:C:245:LYS:O	1:C:254:LYS:HD3	1.99	0.62
1:A:103:ASN:O	1:A:105:GLU:N	2.32	0.62
1:C:185:GLY:HA2	1:C:217:ARG:HG3	1.81	0.62
1:A:510:ILE:CD1	1:A:536:VAL:CG1	2.77	0.62
1:A:89:VAL:HG23	1:A:89:VAL:O	1.98	0.62
1:B:178:LEU:CD1	1:B:189:ILE:HD11	2.30	0.62
1:B:182:LEU:HD21	1:B:204:ILE:CD1	2.29	0.62
1:B:477:PRO:HA	1:B:480:LEU:HD12	1.81	0.62
1:B:516:VAL:HG12	1:B:516:VAL:O	1.98	0.62
1:C:158:THR:OG1	1:C:160:ILE:HD12	1.99	0.62
1:C:170:LEU:HD22	1:C:171:ALA:N	2.11	0.62
1:C:341:SER:OG	1:C:367:TYR:CD2	2.53	0.62
1:B:607:VAL:O	1:B:608:GLU:C	2.38	0.62
1:C:544:TYR:CE2	1:C:560:HIS:HD2	2.18	0.62
1:A:553:PHE:CD2	1:A:559:MET:CE	2.77	0.61
1:B:359:LEU:HD11	1:B:381:LEU:HD12	1.82	0.61
1:C:224:LYS:HD3	1:C:225:THR:N	2.15	0.61
1:C:234:ILE:HD13	1:C:236:SER:H	1.65	0.61
1:C:359:LEU:O	1:C:362:SER:OG	2.18	0.61
1:A:205:PHE:HE2	1:A:234:ILE:HD11	1.66	0.61
1:A:489:ILE:HG13	1:A:588:ALA:HB2	1.81	0.61
1:C:42:MET:HE3	1:C:44:ARG:NE	2.07	0.61
1:A:239:GLN:O	1:A:241:ASP:N	2.33	0.61
1:A:347:SER:HB2	1:A:381:LEU:CD1	2.30	0.61
1:A:356:LEU:HA	1:A:381:LEU:HD21	1.82	0.61
1:A:510:ILE:CD1	1:A:536:VAL:CB	2.79	0.61
1:B:305:ASN:O	1:B:306:SER:O	2.17	0.61
1:B:439:ALA:O	1:B:443:ARG:HG2	2.00	0.61
1:B:587:VAL:C	1:B:590:ILE:HD12	2.20	0.61
1:A:310:SER:O	1:A:313:TRP:N	2.34	0.61
1:B:124:THR:O	1:B:127:ILE:N	2.33	0.61
1:A:375:ASN:HA	1:A:391:THR:OG1	2.00	0.61
1:B:42:MET:HE1	1:B:94:VAL:CG2	2.31	0.61
1:C:180:ILE:HD11	1:C:206:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:TYR:CZ	1:C:397:ILE:HG21	2.36	0.61
1:C:565:PRO:O	1:C:566:HIS:C	2.39	0.61
1:A:342:LEU:O	1:A:342:LEU:HG	2.00	0.61
1:A:529:LEU:O	1:A:532:ASN:ND2	2.33	0.61
1:B:220:ASN:O	1:B:222:PHE:CE2	2.53	0.61
1:C:173:ARG:HG3	1:C:178:LEU:HB2	1.81	0.61
1:A:17:LEU:CD2	1:A:33:LEU:HD13	2.31	0.61
1:B:3:ILE:O	1:B:4:VAL:CG2	2.49	0.61
1:B:572:ALA:N	1:B:573:PRO:CD	2.60	0.61
1:C:467:ALA:O	1:C:494:ALA:HA	2.00	0.61
1:C:90:SER:O	1:C:91:GLU:HB2	2.01	0.61
1:A:453:ARG:O	1:A:456:ALA:HB3	2.00	0.61
1:A:469:PHE:CZ	1:A:517:ILE:HD13	2.36	0.61
1:A:485:LYS:O	1:A:486:LEU:C	2.37	0.61
1:B:186:GLU:HG2	1:B:186:GLU:O	2.00	0.61
1:B:192:ASP:OD1	1:B:194:LEU:HB2	2.00	0.61
1:B:528:LYS:O	1:B:531:SER:HB3	2.01	0.61
1:C:263:ILE:CG2	1:C:440:LEU:HD23	2.31	0.61
1:C:545:VAL:HB	1:C:561:ILE:HD13	1.81	0.61
1:A:204:ILE:CG1	1:A:233:ASP:HB3	2.31	0.61
1:A:276:VAL:HG12	1:A:430:GLU:OE2	2.01	0.61
1:A:448:LEU:C	1:A:450:GLN:H	2.04	0.61
1:B:63:LEU:H	1:B:63:LEU:CD1	2.09	0.61
1:B:42:MET:HE2	1:B:94:VAL:CG2	2.31	0.61
1:C:28:TYR:HB2	1:C:50:LYS:HD3	1.82	0.61
1:C:250:HIS:HB3	1:C:596:ASP:OD1	2.00	0.61
1:A:272:SER:O	1:A:273:HIS:CB	2.40	0.61
1:B:167:ASP:OD1	1:B:167:ASP:C	2.39	0.61
1:B:549:GLN:HA	1:B:563:GLU:OE2	2.01	0.61
1:C:111:LEU:HB3	1:C:116:TYR:CD2	2.31	0.61
1:C:318:ALA:C	1:C:320:ILE:H	2.02	0.61
1:C:485:LYS:O	1:C:584:ALA:HB1	2.00	0.61
1:C:529:LEU:HA	1:C:532:ASN:ND2	2.16	0.61
1:B:130:LEU:CD2	1:B:152:LEU:HD21	2.28	0.60
1:B:294:HIS:ND1	1:B:341:SER:OG	2.35	0.60
1:C:359:LEU:HD23	1:C:381:LEU:CD2	2.31	0.60
1:C:4:VAL:O	1:C:4:VAL:CG1	2.43	0.60
1:A:276:VAL:HG21	1:A:414:MET:HG2	1.81	0.60
1:B:122:THR:C	1:B:124:THR:N	2.49	0.60
1:B:214:ILE:C	1:B:215:THR:CG2	2.69	0.60
1:B:22:ARG:CG	1:B:22:ARG:HH11	2.13	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ARG:HD3	1:B:414:MET:HE1	1.80	0.60
1:C:93:ILE:HG21	1:C:131:VAL:HB	1.83	0.60
1:A:128:ALA:C	1:A:130:LEU:H	2.05	0.60
1:B:338:ARG:NE	1:C:321:PRO:HB3	2.15	0.60
1:C:12:VAL:O	1:C:13:ALA:C	2.39	0.60
1:C:42:MET:HE3	1:C:44:ARG:HB2	1.83	0.60
1:A:3:ILE:HG22	1:A:191:SER:HB3	1.82	0.60
1:A:510:ILE:HD11	1:A:536:VAL:CG1	2.31	0.60
1:A:503:LYS:HD3	1:A:535:GLU:CD	2.22	0.60
1:A:603:LYS:HG3	1:A:604:SER:N	2.10	0.60
1:C:279:SER:O	1:C:280:GLU:C	2.40	0.60
1:A:207:GLU:N	1:A:210:ASP:OD2	2.34	0.60
1:B:105:GLU:H	1:B:106:PRO:HD2	1.66	0.60
1:A:472:ARG:HG2	1:A:525:LEU:HD12	1.83	0.60
1:C:399:VAL:HG13	1:C:603:LYS:HA	1.83	0.60
1:A:180:ILE:CD1	1:A:214:ILE:HD11	2.23	0.60
1:A:279:SER:C	1:A:281:LEU:N	2.51	0.60
1:B:113:ALA:O	1:B:115:GLY:N	2.34	0.60
1:B:67:THR:OG1	1:B:166:PRO:O	2.17	0.60
1:B:294:HIS:O	1:B:341:SER:HA	2.01	0.60
1:C:69:ILE:HG21	1:C:159:VAL:HG12	1.83	0.60
1:C:255:GLU:OE2	1:C:397:ILE:N	2.33	0.60
1:B:493:HIS:CD2	1:C:466:HIS:ND1	2.70	0.60
1:C:555:SER:OG	1:C:561:ILE:HB	2.01	0.60
1:A:103:ASN:C	1:A:105:GLU:H	2.05	0.60
1:A:133:TRP:CZ3	1:A:134:GLU:OE2	2.55	0.60
1:B:1:CYS:HA	1:B:72:THR:O	2.02	0.60
1:B:329:GLU:O	1:B:330:PHE:O	2.20	0.60
1:C:29:ASP:OD2	1:C:75:ALA:N	2.33	0.60
1:B:454:ILE:O	1:B:457:LEU:HB3	2.01	0.60
1:C:178:LEU:HB3	1:C:206:LEU:HD12	1.82	0.60
1:A:175:GLY:N	1:A:208:GLU:OE2	2.34	0.60
1:B:152:LEU:N	1:B:152:LEU:HD23	2.17	0.60
1:B:214:ILE:HG22	1:B:215:THR:H	1.66	0.60
1:B:520:ALA:CB	1:B:529:LEU:CD2	2.80	0.60
1:B:572:ALA:H	1:B:573:PRO:HD2	1.67	0.60
1:C:286:ASP:OD1	1:C:422:LEU:HD11	2.02	0.60
1:C:251:TYR:CE2	1:C:397:ILE:HG21	2.37	0.60
1:C:44:ARG:HD3	1:C:46:ARG:HD3	1.84	0.60
1:C:95:VAL:O	1:C:96:VAL:HG13	2.01	0.60
1:A:353:ALA:HB1	1:A:608:GLU:OE2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:GLU:HG2	1:B:229:VAL:H	1.66	0.59
1:B:594:ASP:O	1:B:595:VAL:C	2.39	0.59
1:C:74:TRP:CZ3	1:C:602:ALA:HB2	2.37	0.59
1:B:32:GLY:HA3	1:B:46:ARG:HA	1.84	0.59
1:C:18:GLU:OE2	1:C:21:ARG:NH1	2.35	0.59
1:A:371:LEU:CD1	1:A:371:LEU:C	2.66	0.59
1:B:118:PHE:C	1:B:120:SER:H	2.04	0.59
1:B:32:GLY:CA	1:B:54:LEU:HD22	2.31	0.59
1:B:394:GLY:HA3	1:B:403:LYS:NZ	2.17	0.59
1:B:454:ILE:HD12	1:B:582:LEU:HD12	1.84	0.59
1:B:487:LYS:HD3	1:C:509:LEU:HD11	1.84	0.59
1:C:135:LEU:HD11	1:C:164:ARG:NH2	2.12	0.59
1:C:33:LEU:HA	1:C:70:ALA:HA	1.85	0.59
1:C:565:PRO:O	1:C:567:VAL:HG13	2.02	0.59
1:A:20:LEU:O	1:A:21:ARG:C	2.39	0.59
1:A:434:VAL:O	1:A:435:HIS:C	2.41	0.59
1:B:221:ILE:HG22	1:B:222:PHE:H	1.65	0.59
1:A:18:GLU:OE1	1:A:18:GLU:HA	2.02	0.59
1:A:312:TYR:CZ	1:A:473:GLY:O	2.56	0.59
1:A:474:ASP:C	1:A:474:ASP:OD1	2.40	0.59
1:A:510:ILE:CG2	1:A:511:ASP:N	2.65	0.59
1:B:241:ASP:HB3	1:B:244:ASP:O	2.03	0.59
1:B:334:LYS:HD2	1:B:334:LYS:C	2.23	0.59
1:B:421:LYS:O	1:B:424:GLY:N	2.36	0.59
1:C:594:ASP:HB3	1:C:597:GLN:O	2.02	0.59
1:A:297:ILE:HB	1:A:324:VAL:HA	1.84	0.59
1:B:254:LYS:O	1:B:258:GLU:CB	2.51	0.59
1:B:359:LEU:HD13	1:B:384:GLU:O	2.02	0.59
1:B:447:MET:HE3	1:B:564:MET:CE	2.29	0.59
1:B:42:MET:CE	1:B:94:VAL:HG22	2.33	0.59
1:B:501:GLU:CG	1:C:326:ILE:HG21	2.32	0.59
1:A:531:SER:O	1:A:534:GLU:N	2.36	0.59
1:B:344:ILE:CG2	1:B:371:LEU:HD23	2.25	0.59
1:C:173:ARG:HB2	1:C:178:LEU:HD13	1.85	0.59
1:C:234:ILE:CD1	1:C:238:LEU:HD11	2.33	0.59
1:A:102:GLU:O	1:A:104:HIS:N	2.36	0.59
1:B:436:GLY:O	1:B:571:ILE:HD13	2.02	0.59
1:C:130:LEU:HD22	1:C:148:ALA:HB1	1.83	0.59
1:C:20:LEU:CB	1:C:51:VAL:HG11	2.32	0.59
1:A:149:ILE:O	1:A:151:GLN:N	2.36	0.59
1:A:187:ASN:ND2	1:A:219:VAL:HG22	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LEU:CB	1:A:51:VAL:HG21	2.33	0.59
1:B:261:ASN:O	1:B:264:LYS:HB3	2.03	0.59
1:A:526:LEU:O	1:A:529:LEU:HB3	2.03	0.58
1:B:14:GLU:HG2	1:B:15:ILE:N	2.18	0.58
1:B:468:LEU:HD13	1:B:497:TYR:CD2	2.38	0.58
1:C:265:ASN:O	1:C:392:ASN:HB2	2.03	0.58
1:C:343:MET:CE	1:C:367:TYR:CE2	2.85	0.58
1:A:13:ALA:O	1:A:15:ILE:N	2.36	0.58
1:A:318:ALA:HB1	1:A:320:ILE:HG13	1.84	0.58
1:A:519:VAL:HG12	1:A:576:TYR:HD2	1.67	0.58
1:B:276:VAL:HG23	1:B:276:VAL:O	2.03	0.58
1:B:29:ASP:O	1:B:49:GLY:N	2.25	0.58
1:B:304:TYR:CE2	1:B:308:MET:HE2	2.37	0.58
1:B:419:LEU:O	1:B:423:LYS:HG2	2.02	0.58
1:C:224:LYS:HD2	1:C:225:THR:HG23	1.84	0.58
1:C:308:MET:HB2	1:C:477:PRO:HB3	1.85	0.58
1:A:105:GLU:H	1:A:106:PRO:CD	2.16	0.58
1:A:221:ILE:HG21	1:A:231:ARG:HG2	1.84	0.58
1:A:268:THR:HG22	1:A:268:THR:O	2.02	0.58
1:A:32:GLY:HA2	1:A:54:LEU:CD2	2.33	0.58
1:A:373:ILE:HD13	1:A:411:VAL:HG11	1.85	0.58
1:B:404:ALA:HA	1:B:407:THR:HG1	1.68	0.58
1:B:578:VAL:N	1:B:579:PRO:HD2	2.18	0.58
1:C:90:SER:OG	1:C:129:HIS:ND1	2.35	0.58
1:C:18:GLU:HA	1:C:21:ARG:NH1	2.09	0.58
1:C:371:LEU:HD11	1:C:389:LEU:HD11	1.84	0.58
1:C:263:ILE:HD12	1:C:440:LEU:CD2	2.33	0.58
1:A:503:LYS:HD3	1:A:535:GLU:OE2	2.03	0.58
1:A:47:ARG:NE	1:A:57:ALA:HB2	2.18	0.58
1:B:240:TYR:CE1	1:B:241:ASP:HB2	2.37	0.58
1:B:263:ILE:CD1	1:B:444:ILE:HD11	2.33	0.58
1:C:418:LYS:O	1:C:422:LEU:HB2	2.03	0.58
1:A:270:ARG:O	1:A:277:ASP:N	2.32	0.58
1:A:375:ASN:OD1	1:A:393:ALA:HB3	2.04	0.58
1:A:551:ALA:CB	1:A:553:PHE:HD1	2.17	0.58
1:B:273:HIS:O	1:B:275:GLN:HG3	2.03	0.58
1:B:523:ASN:OD1	1:B:525:LEU:HB2	2.03	0.58
1:C:311:ARG:HA	1:C:322:CYS:SG	2.44	0.58
1:C:318:ALA:O	1:C:320:ILE:N	2.37	0.58
1:A:128:ALA:C	1:A:130:LEU:N	2.55	0.58
1:B:356:LEU:CD1	1:B:360:ARG:NE	2.57	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:MET:HB3	1:B:370:SER:CB	2.32	0.58
1:C:197:LEU:N	1:C:198:PRO:CD	2.66	0.58
1:A:161:MET:HB2	1:A:169:LEU:HD23	1.86	0.58
1:A:36:VAL:HG12	1:A:42:MET:HA	1.85	0.58
1:A:510:ILE:CD1	1:A:536:VAL:HG12	2.34	0.58
1:A:491:TYR:CG	1:A:599:ARG:NH1	2.71	0.58
1:B:546:PHE:CE2	1:B:562:ILE:CD1	2.83	0.58
1:A:355:THR:O	1:A:355:THR:HG22	2.04	0.58
1:B:168:THR:HG22	1:B:169:LEU:N	2.19	0.58
1:B:221:ILE:CG2	1:B:222:PHE:N	2.66	0.58
1:C:11:ASP:OD1	1:C:65:GLY:O	2.22	0.58
1:C:184:MET:HA	1:C:184:MET:HE2	1.85	0.58
1:C:5:GLY:HA2	1:C:69:ILE:HA	1.84	0.58
1:A:305:ASN:O	1:A:308:MET:HB2	2.03	0.58
1:A:436:GLY:O	1:A:437:LEU:C	2.43	0.58
1:C:476:TYR:HB3	1:C:477:PRO:CD	2.29	0.58
1:C:565:PRO:CG	1:C:575:PHE:CZ	2.65	0.58
1:C:80:PRO:O	1:C:84:ASN:CG	2.42	0.58
1:A:88:HIS:HD2	1:A:124:THR:HG21	1.68	0.58
1:A:356:LEU:HD21	1:A:360:ARG:CZ	2.33	0.58
1:A:523:ASN:HD22	1:A:524:GLU:N	2.02	0.58
1:A:84:ASN:HB2	1:A:121:GLU:CD	2.24	0.58
1:B:331:ARG:HA	1:B:361:LEU:HD22	1.86	0.58
1:A:161:MET:HB2	1:A:169:LEU:CD2	2.34	0.57
1:A:530:LYS:O	1:A:530:LYS:HD2	2.03	0.57
1:A:97:HIS:C	1:A:97:HIS:ND1	2.57	0.57
1:B:453:ARG:NH1	1:B:453:ARG:HG3	2.19	0.57
1:B:523:ASN:HD22	1:B:525:LEU:H	1.44	0.57
1:B:526:LEU:HD11	1:B:553:PHE:HE1	1.68	0.57
1:C:300:CYS:H	1:C:303:SER:HB2	1.68	0.57
1:A:382:VAL:CG1	1:A:382:VAL:O	2.52	0.57
1:A:79:GLU:O	1:A:81:SER:N	2.37	0.57
1:B:98:ASN:O	1:B:157:GLY:N	2.36	0.57
1:B:343:MET:HB3	1:B:370:SER:HA	1.85	0.57
1:B:346:LEU:HD22	1:B:408:GLN:HG2	1.85	0.57
1:C:118:PHE:N	1:C:118:PHE:CD1	2.72	0.57
1:C:278:LEU:HD21	1:C:414:MET:HE3	1.86	0.57
1:A:192:ASP:O	1:A:194:LEU:N	2.37	0.57
1:A:409:LEU:CD1	1:A:574:ILE:HG12	2.34	0.57
1:B:36:VAL:HG21	1:B:163:SER:HA	1.87	0.57
1:B:523:ASN:C	1:B:523:ASN:ND2	2.56	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:VAL:HA	1:C:171:ALA:HA	1.85	0.57
1:A:164:ARG:O	1:A:165:HIS:CG	2.57	0.57
1:A:532:ASN:ND2	1:A:532:ASN:N	2.23	0.57
1:B:3:ILE:O	1:B:4:VAL:HG23	2.04	0.57
1:C:74:TRP:CH2	1:C:602:ALA:HB2	2.40	0.57
1:C:80:PRO:HG2	1:C:84:ASN:ND2	2.19	0.57
1:A:255:GLU:OE2	1:A:398:GLY:N	2.37	0.57
1:B:24:GLU:CG	1:B:597:GLN:HE22	2.16	0.57
1:C:159:VAL:HG13	1:C:171:ALA:HB2	1.87	0.57
1:C:346:LEU:HD22	1:C:408:GLN:HB3	1.86	0.57
1:C:587:VAL:O	1:C:590:ILE:HG22	2.04	0.57
1:C:71:HIS:HD2	1:C:96:VAL:HB	1.69	0.57
1:A:155:ALA:HB1	1:A:175:GLY:HA3	1.86	0.57
1:A:46:ARG:HD2	1:A:82:GLU:O	2.04	0.57
1:B:238:LEU:HD11	1:B:240:TYR:HE2	1.69	0.57
1:B:337:VAL:O	1:B:337:VAL:HG23	2.04	0.57
1:B:3:ILE:HG22	1:B:4:VAL:N	2.19	0.57
1:C:532:ASN:H	1:C:532:ASN:ND2	2.01	0.57
1:A:304:TYR:CE1	1:A:326:ILE:HD11	2.36	0.57
1:A:7:ILE:HD13	1:A:214:ILE:HG22	1.87	0.57
1:A:90:SER:HB3	1:A:128:ALA:HB1	1.84	0.57
1:B:134:GLU:OE1	1:B:134:GLU:HA	2.04	0.57
1:B:406:THR:O	1:B:409:LEU:HB2	2.04	0.57
1:B:318:ALA:O	1:B:423:LYS:HE3	2.05	0.57
1:B:559:MET:HE3	1:B:561:ILE:CD1	2.26	0.57
1:C:564:MET:HG3	1:C:576:TYR:CE1	2.40	0.57
1:A:344:ILE:O	1:A:344:ILE:HG22	2.03	0.57
1:A:540:GLY:O	1:A:541:GLY:C	2.41	0.57
1:B:193:GLN:O	1:B:195:ALA:N	2.38	0.57
1:C:549:GLN:HB2	1:C:564:MET:O	2.05	0.57
1:A:202:ARG:NH1	1:A:202:ARG:CG	2.64	0.57
1:A:330:PHE:C	1:A:330:PHE:CD1	2.78	0.57
1:B:140:THR:O	1:B:141:LEU:C	2.43	0.57
1:B:417:ALA:O	1:B:419:LEU:N	2.38	0.57
1:B:515:PRO:O	1:B:516:VAL:HG23	2.05	0.57
1:C:350:GLY:CA	1:C:381:LEU:HD12	2.24	0.57
1:A:447:MET:CE	1:A:575:PHE:CE1	2.88	0.57
1:A:305:ASN:ND2	1:A:481:GLU:OE1	2.38	0.57
1:A:507:LEU:O	1:A:507:LEU:HD12	2.05	0.57
1:A:28:TYR:CE1	1:A:597:GLN:HB3	2.40	0.57
1:C:130:LEU:HD13	1:C:152:LEU:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLU:O	1:A:111:LEU:C	2.42	0.56
1:A:585:TYR:O	1:A:588:ALA:HB3	2.05	0.56
1:B:331:ARG:HG3	1:B:332:TYR:N	2.20	0.56
1:B:379:SER:O	1:B:381:LEU:N	2.38	0.56
1:B:86:HIS:N	1:B:86:HIS:CD2	2.73	0.56
1:C:197:LEU:HD23	1:C:203:PHE:HZ	1.70	0.56
1:C:289:LEU:O	1:C:422:LEU:HD22	2.05	0.56
1:C:36:VAL:O	1:C:36:VAL:HG12	2.04	0.56
1:A:440:LEU:CD2	1:A:574:ILE:HD12	2.35	0.56
1:A:598:PRO:CG	1:A:601:LEU:HD12	2.35	0.56
1:A:7:ILE:CD1	1:A:215:THR:CA	2.82	0.56
1:B:44:ARG:CZ	1:B:46:ARG:HH21	2.17	0.56
1:B:3:ILE:C	1:B:4:VAL:HG23	2.26	0.56
1:C:283:PRO:CG	1:C:284:ASN:H	2.18	0.56
1:C:309:VAL:CG2	1:C:477:PRO:HB2	2.35	0.56
1:C:533:ILE:HG22	1:C:559:MET:CE	2.36	0.56
1:A:346:LEU:O	1:A:408:GLN:NE2	2.37	0.56
1:A:447:MET:HE2	1:A:575:PHE:CE1	2.39	0.56
1:B:92:HIS:CD2	1:B:164:ARG:HE	2.24	0.56
1:B:249:ARG:O	1:B:249:ARG:HG2	2.04	0.56
1:B:60:GLU:O	1:B:62:PRO:HD3	2.05	0.56
1:C:130:LEU:CD1	1:C:152:LEU:HD21	2.36	0.56
1:C:28:TYR:HB2	1:C:50:LYS:CD	2.35	0.56
1:A:184:MET:C	1:A:186:GLU:H	2.09	0.56
1:A:296:GLN:NE2	1:A:296:GLN:CA	2.40	0.56
1:B:127:ILE:HG12	1:B:152:LEU:CD1	2.36	0.56
1:B:309:VAL:HG21	1:B:478:ILE:HD11	1.88	0.56
1:B:498:ALA:O	1:B:500:GLY:N	2.38	0.56
1:C:107:LEU:HA	1:C:110:GLU:CB	2.34	0.56
1:C:187:ASN:O	1:C:188:PHE:CG	2.59	0.56
1:C:348:GLN:HG2	1:C:375:ASN:HB3	1.86	0.56
1:C:379:SER:CB	1:C:382:VAL:HG23	2.31	0.56
1:B:234:ILE:HG13	1:B:235:GLU:N	2.20	0.56
1:B:586:HIS:O	1:B:590:ILE:CD1	2.53	0.56
1:C:149:ILE:N	1:C:150:PRO:CD	2.65	0.56
1:A:76:THR:O	1:A:78:GLY:N	2.38	0.56
1:A:71:HIS:CE1	1:A:86:HIS:CG	2.94	0.56
1:B:338:ARG:NH2	1:C:315:GLU:OE2	2.39	0.56
1:B:425:LEU:HG	1:B:426:ASP:H	1.71	0.56
1:B:433:ILE:CG1	1:B:570:VAL:HG21	2.35	0.56
1:A:263:ILE:HD11	1:A:406:THR:HG21	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ALA:O	1:A:71:HIS:CB	2.53	0.56
1:B:133:TRP:O	1:B:137:GLN:HG2	2.05	0.56
1:B:468:LEU:HD23	1:B:516:VAL:CG2	2.36	0.56
1:B:468:LEU:HD11	1:B:470:LEU:HD21	1.87	0.56
1:C:216:ARG:NH2	1:C:217:ARG:NH2	2.52	0.56
1:C:447:MET:C	1:C:449:SER:N	2.58	0.56
1:A:102:GLU:C	1:A:104:HIS:H	2.08	0.56
1:A:277:ASP:OD1	1:A:277:ASP:C	2.44	0.56
1:A:476:TYR:N	1:A:477:PRO:CD	2.68	0.56
1:A:553:PHE:CD2	1:A:559:MET:HE3	2.41	0.56
1:B:253:GLN:O	1:B:256:ILE:N	2.38	0.56
1:C:141:LEU:HD21	1:C:168:THR:OG1	2.05	0.56
1:C:47:ARG:HE	1:C:47:ARG:HA	1.70	0.56
1:C:82:GLU:HG3	1:C:83:VAL:N	2.18	0.56
1:A:145:VAL:C	1:A:147:ARG:H	2.09	0.56
1:A:165:HIS:C	1:A:167:ASP:H	2.07	0.56
1:A:28:TYR:HE1	1:A:602:ALA:HA	1.70	0.56
1:B:276:VAL:CG1	1:B:434:VAL:HG22	2.32	0.56
1:B:283:PRO:C	1:B:285:ALA:H	2.09	0.56
1:B:447:MET:HG2	1:B:575:PHE:CZ	2.40	0.56
1:C:15:ILE:HD11	1:C:199:VAL:HG11	1.88	0.56
1:C:185:GLY:CA	1:C:217:ARG:HG3	2.36	0.56
1:C:480:LEU:HA	1:C:496:ALA:HB2	1.88	0.56
1:A:25:TYR:HE2	1:A:397:ILE:HD12	1.71	0.56
1:A:313:TRP:CA	1:A:317:LEU:HD12	2.36	0.56
1:A:485:LYS:NZ	2:A:700:G6Q:O1	2.39	0.56
1:B:134:GLU:O	1:B:147:ARG:NH2	2.34	0.56
1:B:466:HIS:CE1	1:C:466:HIS:CE1	2.94	0.56
1:B:79:GLU:O	1:B:80:PRO:C	2.44	0.56
1:C:42:MET:CG	1:C:43:THR:N	2.68	0.56
1:C:480:LEU:HA	1:C:496:ALA:CB	2.36	0.56
1:C:566:HIS:O	1:C:567:VAL:CG1	2.54	0.56
1:A:371:LEU:HD12	1:A:371:LEU:C	2.25	0.56
1:A:373:ILE:HD13	1:A:411:VAL:HG12	1.87	0.56
1:B:8:ALA:O	1:B:216:ARG:HD3	2.06	0.56
1:B:484:LEU:C	1:B:485:LYS:HG2	2.18	0.56
1:C:156:TYR:HE2	1:C:158:THR:HG22	1.71	0.56
1:B:501:GLU:CD	1:C:326:ILE:HD12	2.25	0.56
1:C:36:VAL:CG1	1:C:166:PRO:CB	2.76	0.56
1:C:47:ARG:NE	1:C:47:ARG:HA	2.21	0.56
1:A:259:GLN:O	1:A:263:ILE:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:SER:OG	2:A:700:G6Q:O2P	2.14	0.55
1:B:162:ASP:C	1:B:162:ASP:OD1	2.43	0.55
1:B:159:VAL:HG22	1:B:171:ALA:HB2	1.88	0.55
1:B:286:ASP:CB	1:B:422:LEU:HD11	2.36	0.55
1:B:252:MET:HE2	1:B:489:ILE:HD13	1.88	0.55
1:C:502:LEU:HD12	1:C:502:LEU:N	2.21	0.55
1:C:544:TYR:CE2	1:C:560:HIS:CD2	2.93	0.55
1:C:3:ILE:CD1	1:C:98:ASN:HB2	2.35	0.55
1:A:122:THR:OG1	1:A:123:ASP:N	2.39	0.55
1:A:375:ASN:HD21	1:A:393:ALA:HB3	1.71	0.55
1:B:5:GLY:CA	1:B:189:ILE:HG23	2.36	0.55
1:C:179:VAL:HG21	1:C:203:PHE:HB3	1.89	0.55
1:C:487:LYS:C	1:C:489:ILE:H	2.08	0.55
1:C:543:LEU:CD1	1:C:559:MET:HE3	2.35	0.55
1:C:8:ALA:HA	1:C:186:GLU:HA	1.86	0.55
1:A:318:ALA:CB	1:A:320:ILE:HG13	2.35	0.55
1:A:338:ARG:HD3	1:A:338:ARG:H	1.71	0.55
1:A:413:LEU:HG	1:A:433:ILE:CG2	2.36	0.55
1:B:468:LEU:HD12	1:B:497:TYR:HD2	1.68	0.55
1:B:99:GLY:HA3	1:B:156:TYR:HA	1.88	0.55
1:B:221:ILE:N	1:B:221:ILE:HD12	2.15	0.55
1:B:24:GLU:OE2	1:B:597:GLN:NE2	2.26	0.55
1:C:297:ILE:HD12	1:C:324:VAL:HG22	1.88	0.55
1:C:517:ILE:CD1	1:C:544:TYR:HB2	2.35	0.55
1:A:282:GLY:O	1:A:284:ASN:N	2.40	0.55
1:B:101:ILE:N	1:B:123:ASP:OD2	2.39	0.55
1:B:20:LEU:O	1:B:21:ARG:C	2.45	0.55
1:B:259:GLN:N	1:B:260:PRO:HD2	2.21	0.55
1:C:330:PHE:C	1:C:332:TYR:H	2.09	0.55
1:C:56:GLN:O	1:C:60:GLU:HB2	2.07	0.55
1:A:437:LEU:C	1:A:439:ALA:H	2.08	0.55
1:B:164:ARG:O	1:B:165:HIS:CD2	2.59	0.55
1:B:476:TYR:CD1	1:B:498:ALA:HB2	2.40	0.55
1:C:61:HIS:N	1:C:62:PRO:HD3	2.20	0.55
1:A:7:ILE:CD1	1:A:215:THR:HA	2.29	0.55
1:A:254:LYS:O	1:A:258:GLU:HG3	2.06	0.55
1:B:234:ILE:CD1	1:B:235:GLU:H	2.19	0.55
1:B:486:LEU:O	1:B:490:SER:CB	2.55	0.55
1:B:480:LEU:HA	1:B:496:ALA:CB	2.36	0.55
1:C:476:TYR:O	1:C:479:ALA:N	2.40	0.55
1:A:210:ASP:OD1	1:A:231:ARG:NH2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:VAL:CG1	1:B:127:ILE:N	2.69	0.55
1:B:237:ASN:C	1:B:239:GLN:HE22	2.10	0.55
1:B:447:MET:HE1	1:B:564:MET:HE2	1.89	0.55
1:C:126:VAL:HG23	1:C:127:ILE:N	2.20	0.55
1:C:216:ARG:HE	1:C:217:ARG:CZ	2.19	0.55
1:C:345:THR:HG21	1:C:381:LEU:HD22	1.89	0.55
1:C:80:PRO:HB2	1:C:84:ASN:OD1	2.07	0.55
1:A:131:VAL:O	1:A:134:GLU:HB2	2.06	0.55
1:A:206:LEU:HD22	1:A:210:ASP:CB	2.36	0.55
1:A:486:LEU:HD21	1:A:492:ILE:HG21	1.89	0.55
1:B:413:LEU:CD2	1:B:571:ILE:HG22	2.37	0.55
1:C:197:LEU:H	1:C:198:PRO:HD2	1.72	0.55
1:C:204:ILE:CG1	1:C:233:ASP:HB3	2.36	0.55
1:A:118:PHE:N	1:A:118:PHE:CD1	2.74	0.55
1:B:334:LYS:CD	1:B:335:SER:N	2.70	0.55
1:C:370:SER:HG	1:C:386:ASP:N	2.05	0.55
1:C:79:GLU:HB3	1:C:81:SER:OG	2.08	0.55
1:A:567:VAL:CG2	1:A:575:PHE:CD2	2.89	0.54
1:A:37:ASP:HA	1:A:65:GLY:HA2	1.89	0.54
1:B:444:ILE:O	1:B:448:LEU:HG	2.07	0.54
1:B:526:LEU:HD11	1:B:553:PHE:CE1	2.41	0.54
1:A:486:LEU:HD11	1:A:587:VAL:HG11	1.88	0.54
1:A:602:ALA:O	1:A:603:LYS:C	2.44	0.54
1:B:110:GLU:OE2	1:B:114:ARG:NH2	2.41	0.54
1:B:304:TYR:O	1:B:305:ASN:C	2.44	0.54
1:C:376:VAL:HG13	1:C:377:PRO:HD2	1.89	0.54
1:A:510:ILE:HG22	1:A:511:ASP:N	2.22	0.54
1:A:399:VAL:CG2	1:A:596:ASP:O	2.56	0.54
1:B:45:LEU:HD21	1:B:57:ALA:HB3	1.90	0.54
1:C:434:VAL:C	1:C:436:GLY:H	2.08	0.54
1:C:443:ARG:O	1:C:446:GLN:N	2.40	0.54
1:C:486:LEU:O	1:C:490:SER:CB	2.55	0.54
1:C:523:ASN:ND2	1:C:569:GLU:OE2	2.41	0.54
1:A:348:GLN:C	1:A:348:GLN:NE2	2.61	0.54
1:A:371:LEU:HD22	1:A:387:LEU:HB3	1.89	0.54
1:A:414:MET:HE3	1:A:437:LEU:HD13	1.89	0.54
1:A:461:PHE:O	1:A:462:SER:C	2.43	0.54
1:B:271:ILE:HG21	1:B:438:GLN:NE2	2.22	0.54
1:B:350:GLY:O	1:B:381:LEU:CB	2.56	0.54
1:B:313:TRP:HZ2	1:B:573:PRO:HG3	1.71	0.54
1:C:286:ASP:OD1	1:C:422:LEU:CD1	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:MET:O	1:A:43:THR:OG1	2.21	0.54
1:A:523:ASN:HD22	1:A:524:GLU:H	1.53	0.54
1:A:600:ASN:OD1	1:A:600:ASN:N	2.40	0.54
1:C:234:ILE:HD12	1:C:236:SER:N	2.23	0.54
1:C:304:TYR:OH	1:C:308:MET:CE	2.56	0.54
1:C:456:ALA:HA	1:C:459:GLU:OE2	2.08	0.54
1:C:95:VAL:CG1	1:C:96:VAL:N	2.71	0.54
1:A:44:ARG:O	1:A:45:LEU:HD12	2.06	0.54
1:A:455:GLU:HG3	1:A:586:HIS:ND1	2.21	0.54
1:B:162:ASP:OD1	1:B:164:ARG:HB2	2.08	0.54
1:C:572:ALA:N	1:C:573:PRO:CD	2.70	0.54
1:A:430:GLU:O	1:A:431:HIS:C	2.43	0.54
1:B:12:VAL:O	1:B:16:LEU:HB2	2.07	0.54
1:C:356:LEU:HD21	1:C:360:ARG:NH2	2.22	0.54
1:A:6:ALA:O	1:A:169:LEU:HD11	2.08	0.54
1:A:25:TYR:CD1	1:A:25:TYR:C	2.81	0.54
1:A:441:PRO:O	1:A:445:GLU:HG3	2.07	0.54
1:A:448:LEU:O	1:A:450:GLN:N	2.37	0.54
1:A:606:THR:C	1:A:607:VAL:O	2.43	0.54
1:B:413:LEU:CA	1:B:416:VAL:HG23	2.35	0.54
1:B:28:TYR:CE1	1:B:602:ALA:HA	2.42	0.54
1:C:270:ARG:O	1:C:271:ILE:HD13	2.08	0.54
1:C:278:LEU:HD12	1:C:418:LYS:CG	2.35	0.54
1:C:281:LEU:HD13	1:C:387:LEU:CD2	2.36	0.54
1:C:443:ARG:HB3	1:C:575:PHE:CE1	2.43	0.54
1:C:28:TYR:C	1:C:50:LYS:HB3	2.28	0.54
1:C:547:ALA:HB2	1:C:553:PHE:CD2	2.42	0.54
1:C:567:VAL:HG11	1:C:575:PHE:CD2	2.42	0.54
1:C:523:ASN:CG	1:C:569:GLU:OE2	2.46	0.54
1:B:118:PHE:CD2	1:B:125:GLU:HG2	2.43	0.54
1:B:346:LEU:HD22	1:B:408:GLN:CG	2.38	0.54
1:B:549:GLN:HG3	1:B:550:ASP:N	2.23	0.54
1:A:124:THR:C	1:A:126:VAL:H	2.10	0.54
1:A:133:TRP:O	1:A:137:GLN:HG2	2.08	0.54
1:A:180:ILE:HG13	1:A:189:ILE:HD13	1.90	0.54
1:A:393:ALA:O	1:A:403:LYS:NZ	2.37	0.54
1:A:346:LEU:HD22	1:A:408:GLN:HE21	1.73	0.54
1:A:553:PHE:HB3	1:A:561:ILE:HG13	1.89	0.54
1:B:546:PHE:CD2	1:B:562:ILE:HD13	2.43	0.54
1:B:490:SER:OG	1:B:587:VAL:HG12	2.08	0.54
1:C:127:ILE:HG13	1:C:128:ALA:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:MET:HE1	1:C:185:GLY:N	2.23	0.54
1:C:251:TYR:CD2	1:C:397:ILE:CG2	2.91	0.54
1:C:330:PHE:O	1:C:332:TYR:N	2.41	0.54
1:C:505:GLY:O	1:C:508:ALA:HB2	2.08	0.54
1:A:253:GLN:HB2	1:A:585:TYR:CZ	2.43	0.53
1:A:302:THR:HG23	1:A:405:PHE:CD1	2.44	0.53
1:A:314:PHE:CE1	1:A:416:VAL:HG22	2.43	0.53
1:B:236:SER:OG	1:B:237:ASN:N	2.41	0.53
1:B:33:LEU:HG	1:B:34:ALA:N	2.22	0.53
1:C:95:VAL:CG2	1:C:128:ALA:HA	2.38	0.53
1:A:302:THR:CG2	1:A:405:PHE:CD1	2.91	0.53
1:A:54:LEU:O	1:A:55:ALA:C	2.46	0.53
1:A:250:HIS:CB	1:A:596:ASP:OD2	2.44	0.53
1:A:28:TYR:CZ	1:A:597:GLN:CB	2.89	0.53
1:B:246:GLY:O	1:B:247:ILE:C	2.46	0.53
1:B:334:LYS:HD2	1:B:335:SER:N	2.24	0.53
1:B:340:ASN:HB3	1:B:368:LEU:HD11	1.90	0.53
1:C:224:LYS:NZ	1:C:225:THR:HG23	2.24	0.53
1:A:97:HIS:HA	1:A:158:THR:HA	1.91	0.53
1:A:178:LEU:HD23	1:A:190:ALA:O	2.08	0.53
1:A:348:GLN:NE2	1:A:349:SER:N	2.55	0.53
1:B:90:SER:HB2	1:B:129:HIS:CE1	2.42	0.53
1:C:507:LEU:O	1:C:507:LEU:CG	2.53	0.53
1:A:267:LEU:HD21	1:A:437:LEU:HD22	1.90	0.53
1:A:491:TYR:CE1	1:A:599:ARG:HG2	2.43	0.53
1:B:10:ARG:NH2	1:B:186:GLU:OE2	2.31	0.53
1:B:22:ARG:HD2	1:B:195:ALA:CA	2.35	0.53
1:B:404:ALA:HA	1:B:407:THR:OG1	2.08	0.53
1:B:497:TYR:CE1	1:B:506:PRO:HB3	2.44	0.53
1:C:310:SER:HB3	1:C:412:LEU:HD13	1.90	0.53
1:C:456:ALA:HB1	1:C:459:GLU:OE2	2.09	0.53
1:A:229:VAL:HG12	1:A:230:LYS:N	2.24	0.53
1:A:511:ASP:OD1	1:A:512:ALA:N	2.41	0.53
1:B:105:GLU:C	1:B:107:LEU:H	2.12	0.53
1:B:311:ARG:C	1:B:313:TRP:H	2.12	0.53
1:B:44:ARG:HD2	1:B:87:PRO:O	2.08	0.53
1:B:505:GLY:N	1:B:506:PRO:CD	2.72	0.53
1:C:107:LEU:O	1:C:108:ARG:C	2.47	0.53
1:C:375:ASN:CA	1:C:391:THR:OG1	2.43	0.53
1:C:69:ILE:HG13	1:C:96:VAL:HG22	1.90	0.53
1:A:134:GLU:OE1	1:A:147:ARG:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:GLU:HG2	1:B:15:ILE:H	1.73	0.53
1:B:214:ILE:CG2	1:B:215:THR:H	2.17	0.53
1:B:238:LEU:CD1	1:B:240:TYR:HE2	2.22	0.53
1:C:95:VAL:HG11	1:C:127:ILE:HG13	1.90	0.53
1:A:100:ILE:HD12	1:A:607:VAL:HA	1.90	0.53
1:A:414:MET:HG3	1:A:437:LEU:CD1	2.39	0.53
1:A:16:LEU:HD11	1:A:68:GLY:HA3	1.90	0.53
1:B:44:ARG:NH1	1:B:89:VAL:HG13	2.24	0.53
1:C:137:GLN:O	1:C:138:GLY:O	2.27	0.53
1:C:45:LEU:HD21	1:C:57:ALA:O	2.09	0.53
1:A:346:LEU:HD22	1:A:408:GLN:CG	2.35	0.53
1:A:491:TYR:OH	1:A:599:ARG:HD3	2.07	0.53
1:B:207:GLU:O	1:B:210:ASP:HB2	2.08	0.53
1:B:33:LEU:HA	1:B:70:ALA:HA	1.91	0.53
1:B:350:GLY:O	1:B:381:LEU:HB2	2.08	0.53
1:C:417:ALA:HB2	1:C:433:ILE:HG21	1.91	0.53
1:C:455:GLU:HG3	1:C:586:HIS:CE1	2.44	0.53
1:B:601:LEU:HD22	1:C:503:LYS:O	2.09	0.53
1:A:13:ALA:C	1:A:15:ILE:H	2.12	0.53
1:A:304:TYR:CE1	1:A:324:VAL:O	2.62	0.53
1:A:294:HIS:HD2	1:A:321:PRO:O	1.92	0.53
1:A:4:VAL:CG1	1:A:5:GLY:N	2.72	0.53
1:B:405:PHE:CE2	1:B:481:GLU:HG2	2.43	0.53
1:B:42:MET:HE1	1:B:94:VAL:HG21	1.87	0.53
1:B:499:ALA:C	1:B:501:GLU:H	2.13	0.53
1:B:79:GLU:HB3	1:B:80:PRO:HD2	1.91	0.53
1:C:236:SER:O	1:C:238:LEU:HD12	2.09	0.53
1:B:500:GLY:HA3	1:C:328:SER:OG	2.09	0.53
1:C:288:LEU:HD11	1:C:368:LEU:CD2	2.39	0.53
1:C:379:SER:O	1:C:382:VAL:N	2.42	0.53
1:A:18:GLU:HG3	1:A:22:ARG:HD2	1.90	0.53
1:A:293:GLU:HB2	1:A:340:ASN:HB2	1.91	0.53
1:A:450:GLN:O	1:A:451:ASP:C	2.47	0.53
1:A:551:ALA:HB1	1:A:553:PHE:CD1	2.43	0.53
1:B:168:THR:HG22	1:B:169:LEU:O	2.09	0.53
1:B:207:GLU:O	1:B:208:GLU:C	2.45	0.53
1:B:228:GLU:CG	1:B:229:VAL:H	2.22	0.53
1:B:287:GLU:HB3	1:B:288:LEU:HD12	1.90	0.53
1:B:498:ALA:O	1:B:499:ALA:C	2.46	0.53
1:C:344:ILE:CG2	1:C:345:THR:N	2.71	0.53
1:C:533:ILE:HG22	1:C:559:MET:HE1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:C	1:A:143:GLU:N	2.63	0.52
1:A:206:LEU:HD22	1:A:210:ASP:HB2	1.91	0.52
1:A:304:TYR:CZ	1:A:326:ILE:HD11	2.43	0.52
1:A:529:LEU:HA	1:A:532:ASN:ND2	2.19	0.52
1:B:25:TYR:CD2	1:B:26:ARG:HG3	2.44	0.52
1:B:92:HIS:CD2	1:B:164:ARG:NE	2.77	0.52
1:C:256:ILE:HG22	1:C:257:TYR:N	2.22	0.52
1:C:42:MET:HG2	1:C:43:THR:N	2.25	0.52
1:C:548:ASP:O	1:C:550:ASP:N	2.42	0.52
1:C:572:ALA:N	1:C:573:PRO:HD2	2.24	0.52
1:A:346:LEU:HD22	1:A:408:GLN:NE2	2.24	0.52
1:A:95:VAL:HG12	1:A:96:VAL:N	2.23	0.52
1:B:168:THR:CG2	1:B:169:LEU:N	2.73	0.52
1:B:155:ALA:HB1	1:B:175:GLY:HA3	1.91	0.52
1:B:25:TYR:CZ	1:B:26:ARG:HG3	2.44	0.52
1:B:334:LYS:C	1:B:334:LYS:CD	2.78	0.52
1:C:300:CYS:SG	1:C:327:ALA:HB3	2.48	0.52
1:C:405:PHE:HA	1:C:408:GLN:NE2	2.24	0.52
1:C:440:LEU:HD13	1:C:571:ILE:CD1	2.30	0.52
1:C:599:ARG:O	1:C:601:LEU:N	2.42	0.52
1:A:103:ASN:ND2	1:A:103:ASN:N	2.56	0.52
1:A:141:LEU:CD2	1:A:170:LEU:HD23	2.40	0.52
1:B:101:ILE:O	1:B:104:HIS:HB3	2.10	0.52
1:B:348:GLN:O	1:B:376:VAL:HG23	2.09	0.52
1:B:346:LEU:CD2	1:B:408:GLN:HG2	2.39	0.52
1:B:528:LYS:H	1:B:528:LYS:CD	2.18	0.52
1:C:456:ALA:CB	1:C:459:GLU:OE2	2.57	0.52
1:A:275:GLN:OE1	1:A:421:LYS:NZ	2.36	0.52
1:A:375:ASN:ND2	1:A:393:ALA:HB3	2.23	0.52
1:B:22:ARG:HG2	1:B:194:LEU:HD22	1.91	0.52
1:C:314:PHE:CE1	1:C:416:VAL:HG22	2.45	0.52
1:A:277:ASP:OD1	1:A:278:LEU:N	2.43	0.52
1:A:331:ARG:HD3	1:A:332:TYR:CZ	2.44	0.52
1:B:22:ARG:NH1	1:B:22:ARG:CG	2.58	0.52
1:B:483:ALA:O	1:B:487:LYS:HE3	2.09	0.52
1:C:564:MET:HG3	1:C:576:TYR:HE1	1.74	0.52
1:B:539:ARG:HD2	1:C:600:ASN:OD1	2.09	0.52
1:A:26:ARG:HE	1:A:604:SER:HB3	1.75	0.52
1:A:391:THR:HG22	1:A:407:THR:CB	2.39	0.52
1:A:410:THR:CG2	1:A:437:LEU:HD22	2.38	0.52
1:B:164:ARG:C	1:B:165:HIS:CD2	2.83	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:PHE:CE2	1:C:199:VAL:HG23	2.45	0.52
1:C:206:LEU:HB3	1:C:210:ASP:CG	2.30	0.52
1:C:537:ARG:HG3	1:C:543:LEU:HD12	1.91	0.52
1:A:296:GLN:C	1:A:296:GLN:HE21	2.13	0.52
1:A:267:LEU:HD21	1:A:410:THR:CG2	2.40	0.52
1:A:47:ARG:CZ	1:A:57:ALA:CB	2.87	0.52
1:B:221:ILE:CG2	1:B:222:PHE:H	2.21	0.52
1:B:228:GLU:HG2	1:B:229:VAL:N	2.24	0.52
1:B:3:ILE:CD1	1:B:98:ASN:HB3	2.39	0.52
1:B:501:GLU:HA	1:B:504:HIS:CD2	2.43	0.52
1:B:553:PHE:CD2	1:B:561:ILE:HD12	2.45	0.52
1:B:34:ALA:CB	1:B:87:PRO:HG2	2.31	0.52
1:B:3:ILE:CD1	1:B:98:ASN:CB	2.87	0.52
1:C:111:LEU:HB2	1:C:118:PHE:CE1	2.45	0.52
1:C:188:PHE:HD2	1:C:200:THR:HG21	1.75	0.52
1:C:344:ILE:HG22	1:C:345:THR:N	2.24	0.52
1:A:173:ARG:HG3	1:A:178:LEU:HB2	1.92	0.52
1:A:414:MET:HG3	1:A:437:LEU:HD13	1.92	0.52
1:A:96:VAL:CG2	1:A:96:VAL:O	2.55	0.52
1:B:276:VAL:HG13	1:B:434:VAL:CG2	2.38	0.52
1:B:42:MET:HE2	1:B:94:VAL:HG21	1.89	0.52
1:C:234:ILE:HD13	1:C:238:LEU:HD11	1.91	0.52
1:C:409:LEU:HD23	1:C:412:LEU:HD12	1.92	0.52
1:A:599:ARG:O	1:A:601:LEU:HG	2.10	0.52
1:B:193:GLN:C	1:B:195:ALA:N	2.59	0.52
1:B:282:GLY:O	1:B:285:ALA:HB2	2.10	0.52
1:B:38:ALA:HB3	1:B:39:GLU:CD	2.30	0.52
1:B:470:LEU:HB2	1:B:518:VAL:CG2	2.38	0.52
1:A:125:GLU:OE1	1:A:125:GLU:O	2.28	0.52
1:A:124:THR:O	1:A:127:ILE:HB	2.10	0.52
1:A:356:LEU:CD2	1:A:360:ARG:NH2	2.64	0.52
1:A:11:ASP:HA	1:A:65:GLY:O	2.10	0.52
1:B:11:ASP:C	1:B:13:ALA:H	2.12	0.52
1:B:3:ILE:HD11	1:B:157:GLY:O	2.10	0.52
1:B:493:HIS:HD2	1:C:466:HIS:ND1	2.07	0.52
1:C:142:ARG:HG2	1:C:146:LEU:HB2	1.92	0.52
1:C:28:TYR:HB2	1:C:50:LYS:HB3	1.92	0.52
1:C:468:LEU:HD12	1:C:495:GLU:HB3	1.91	0.52
1:A:286:ASP:OD1	1:A:286:ASP:N	2.42	0.51
1:A:547:ALA:O	1:A:548:ASP:C	2.47	0.51
1:B:68:GLY:C	1:B:69:ILE:HG23	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:MET:C	1:C:449:SER:H	2.14	0.51
1:B:487:LYS:HG3	1:C:509:LEU:HD21	1.92	0.51
1:A:142:ARG:HG2	1:A:142:ARG:O	2.09	0.51
1:A:18:GLU:OE1	1:A:18:GLU:CA	2.57	0.51
1:A:589:LEU:O	1:A:592:GLY:N	2.44	0.51
1:B:88:HIS:HB2	1:B:124:THR:HG21	1.91	0.51
1:B:259:GLN:O	1:B:262:ALA:CB	2.51	0.51
1:C:33:LEU:HD23	1:C:33:LEU:N	2.25	0.51
1:C:564:MET:HB3	1:C:565:PRO:CD	2.40	0.51
1:A:223:ASP:OD1	1:A:224:LYS:N	2.44	0.51
1:B:134:GLU:OE1	1:B:134:GLU:CA	2.56	0.51
1:B:229:VAL:HG21	1:B:231:ARG:NE	2.17	0.51
1:B:313:TRP:CZ3	1:B:413:LEU:CD1	2.76	0.51
1:B:313:TRP:CE3	1:B:413:LEU:HD12	2.45	0.51
1:C:224:LYS:NZ	1:C:225:THR:CG2	2.74	0.51
1:C:318:ALA:C	1:C:320:ILE:N	2.64	0.51
1:C:547:ALA:CB	1:C:553:PHE:HD2	2.23	0.51
1:A:255:GLU:CD	1:A:398:GLY:H	2.14	0.51
1:A:594:ASP:O	1:A:595:VAL:C	2.48	0.51
1:B:251:TYR:N	1:B:596:ASP:OD1	2.43	0.51
1:B:53:MET:O	1:B:54:LEU:C	2.47	0.51
1:B:56:GLN:HA	1:B:59:GLU:HB2	1.93	0.51
1:C:204:ILE:CG2	1:C:231:ARG:HB2	2.41	0.51
1:C:28:TYR:HB2	1:C:50:LYS:CB	2.40	0.51
1:C:405:PHE:CD2	1:C:577:THR:HG21	2.46	0.51
1:A:288:LEU:O	1:A:289:LEU:C	2.49	0.51
1:A:361:LEU:O	1:A:362:SER:C	2.49	0.51
1:A:469:PHE:O	1:A:496:ALA:HA	2.11	0.51
1:B:294:HIS:HA	1:B:321:PRO:HG2	1.93	0.51
1:B:68:GLY:C	1:B:69:ILE:CG2	2.79	0.51
1:C:173:ARG:HB2	1:C:178:LEU:CD1	2.40	0.51
1:C:423:LYS:HD3	1:C:425:LEU:CG	2.34	0.51
1:A:142:ARG:HG3	1:A:213:GLU:HB2	1.91	0.51
1:B:405:PHE:CD2	1:B:577:THR:HG21	2.46	0.51
1:B:440:LEU:N	1:B:441:PRO:CD	2.73	0.51
1:B:559:MET:O	1:B:561:ILE:HG12	2.10	0.51
1:C:281:LEU:CD1	1:C:285:ALA:HB1	2.41	0.51
1:C:281:LEU:HD21	1:C:389:LEU:CD2	2.39	0.51
1:C:434:VAL:C	1:C:436:GLY:N	2.64	0.51
1:A:132:ASN:OD1	1:A:132:ASN:C	2.49	0.51
1:A:143:GLU:O	1:A:147:ARG:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ASP:OD1	1:A:225:THR:N	2.44	0.51
1:B:105:GLU:C	1:B:107:LEU:N	2.64	0.51
1:B:417:ALA:O	1:B:420:SER:N	2.44	0.51
1:B:45:LEU:HD21	1:B:57:ALA:CB	2.40	0.51
1:B:504:HIS:CD2	1:C:300:CYS:HB3	2.45	0.51
1:B:90:SER:O	1:B:91:GLU:CB	2.51	0.51
1:B:93:ILE:CD1	1:B:93:ILE:N	2.73	0.51
1:C:308:MET:N	1:C:324:VAL:HG11	2.26	0.51
1:C:487:LYS:C	1:C:489:ILE:N	2.64	0.51
1:C:74:TRP:CH2	1:C:602:ALA:CB	2.94	0.51
1:A:296:GLN:HE21	1:A:297:ILE:N	2.07	0.51
1:A:29:ASP:O	1:A:49:GLY:N	2.30	0.51
1:A:36:VAL:O	1:A:65:GLY:CA	2.59	0.51
1:B:343:MET:HE2	1:B:362:SER:HB2	1.92	0.51
1:B:36:VAL:HG23	1:B:161:MET:SD	2.50	0.51
1:B:472:ARG:NH1	1:B:532:ASN:HD21	2.08	0.51
1:B:600:ASN:CB	1:C:539:ARG:HG3	2.41	0.51
1:C:158:THR:OG1	1:C:160:ILE:CD1	2.58	0.51
1:C:201:ARG:O	1:C:203:PHE:CE2	2.63	0.51
1:A:440:LEU:HD22	1:A:574:ILE:HD12	1.93	0.51
1:A:92:HIS:O	1:A:163:SER:OG	2.26	0.51
1:B:193:GLN:O	1:B:194:LEU:C	2.48	0.51
1:B:472:ARG:HH21	1:C:332:TYR:HE2	1.59	0.51
1:B:606:THR:HG22	3:B:707:HOH:O	2.10	0.51
1:C:547:ALA:HB2	1:C:553:PHE:HD2	1.76	0.51
1:A:411:VAL:O	1:A:414:MET:N	2.44	0.51
1:A:486:LEU:CD2	1:A:492:ILE:HG21	2.41	0.51
1:B:182:LEU:HD11	1:B:204:ILE:CD1	2.41	0.51
1:C:476:TYR:CB	1:C:477:PRO:CD	2.88	0.51
1:C:517:ILE:N	1:C:517:ILE:HD13	2.25	0.51
1:C:530:LYS:HG2	1:C:553:PHE:CE1	2.46	0.51
1:C:553:PHE:HB3	1:C:561:ILE:HD12	1.93	0.51
1:A:603:LYS:CG	1:A:604:SER:N	2.71	0.50
1:A:396:GLU:CG	1:A:603:LYS:NZ	2.73	0.50
1:B:179:VAL:HG23	1:B:204:ILE:O	2.11	0.50
1:B:220:ASN:O	1:B:221:ILE:O	2.28	0.50
1:B:276:VAL:HG21	1:B:417:ALA:HB1	1.94	0.50
1:B:331:ARG:HH11	1:B:354:ASP:HA	1.76	0.50
1:A:159:VAL:HG12	1:A:159:VAL:O	2.10	0.50
1:A:179:VAL:HG23	1:A:205:PHE:HA	1.93	0.50
1:A:260:PRO:HG3	1:A:444:ILE:HG22	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:LEU:HA	1:B:387:LEU:O	2.10	0.50
1:B:523:ASN:ND2	1:B:524:GLU:OE2	2.44	0.50
1:B:523:ASN:HD21	1:B:525:LEU:CB	2.25	0.50
1:B:447:MET:CE	1:B:564:MET:HE1	2.41	0.50
1:C:187:ASN:OD1	1:C:219:VAL:CG2	2.60	0.50
1:C:351:GLU:O	1:C:352:THR:C	2.46	0.50
1:C:489:ILE:HG13	1:C:588:ALA:HB2	1.93	0.50
1:A:296:GLN:NE2	1:A:323:ASP:HB2	2.26	0.50
1:B:101:ILE:HB	1:B:123:ASP:HB2	1.92	0.50
1:B:103:ASN:OD1	1:B:153:ARG:HB2	2.11	0.50
1:B:213:GLU:HG2	1:B:213:GLU:O	2.11	0.50
1:B:270:ARG:HD3	1:B:414:MET:HE3	1.91	0.50
1:B:302:THR:HG22	1:B:303:SER:N	2.24	0.50
1:B:307:GLY:O	1:B:324:VAL:HG21	2.11	0.50
1:B:333:ARG:O	1:B:333:ARG:HG3	2.11	0.50
1:B:453:ARG:HH21	1:B:562:ILE:HA	1.76	0.50
1:B:20:LEU:HD22	1:B:72:THR:OG1	2.12	0.50
1:C:370:SER:OG	1:C:386:ASP:N	2.35	0.50
1:C:443:ARG:O	1:C:447:MET:N	2.43	0.50
1:C:4:VAL:HB	1:C:70:ALA:HB3	1.94	0.50
1:B:311:ARG:C	1:B:313:TRP:N	2.65	0.50
1:B:528:LYS:HD2	1:B:528:LYS:N	2.20	0.50
1:B:67:THR:HG22	1:B:68:GLY:N	2.27	0.50
1:C:127:ILE:O	1:C:128:ALA:C	2.50	0.50
1:C:265:ASN:O	1:C:392:ASN:CB	2.59	0.50
1:A:134:GLU:HG3	1:A:148:ALA:HB2	1.93	0.50
1:B:159:VAL:HA	1:B:171:ALA:HA	1.92	0.50
1:C:7:ILE:O	1:C:216:ARG:HA	2.12	0.50
1:C:256:ILE:O	1:C:259:GLN:N	2.45	0.50
1:C:353:ALA:HB2	1:C:606:THR:O	2.12	0.50
1:A:140:THR:O	1:A:143:GLU:HB2	2.12	0.50
1:A:266:THR:HG22	1:A:270:ARG:NH1	2.27	0.50
1:A:477:PRO:O	1:A:480:LEU:HB2	2.11	0.50
1:A:536:VAL:O	1:A:537:ARG:C	2.50	0.50
1:A:47:ARG:CZ	1:A:57:ALA:HB2	2.42	0.50
1:B:146:LEU:CD1	1:B:211:ILE:CD1	2.81	0.50
1:B:127:ILE:HG12	1:B:152:LEU:HD11	1.93	0.50
1:B:276:VAL:CG2	1:B:417:ALA:HB1	2.42	0.50
1:B:485:LYS:O	1:B:487:LYS:N	2.44	0.50
1:B:557:ASP:OD1	1:B:557:ASP:N	2.43	0.50
1:C:291:LYS:O	1:C:293:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:GLN:HG3	1:A:404:ALA:CB	2.42	0.50
1:A:533:ILE:HG23	1:A:543:LEU:HD23	1.90	0.50
1:B:158:THR:HG23	1:B:158:THR:O	2.12	0.50
1:B:32:GLY:HA2	1:B:45:LEU:O	2.12	0.50
1:B:486:LEU:HD13	1:B:584:ALA:HA	1.93	0.50
1:B:501:GLU:O	1:B:506:PRO:CD	2.60	0.50
1:B:454:ILE:HD12	1:B:582:LEU:CD1	2.42	0.50
1:B:30:SER:OG	1:B:73:ARG:HB3	2.12	0.50
1:C:83:VAL:HG11	1:C:119:VAL:O	2.12	0.50
1:C:447:MET:HE1	1:C:575:PHE:O	2.12	0.50
1:A:190:ALA:HB2	1:A:196:LEU:HD11	1.94	0.50
1:B:359:LEU:CD1	1:B:381:LEU:HD12	2.39	0.50
1:B:524:GLU:CD	1:B:524:GLU:N	2.65	0.50
1:B:523:ASN:O	1:B:526:LEU:HB2	2.12	0.50
1:C:158:THR:CG2	1:C:172:ALA:O	2.59	0.50
1:C:181:GLY:O	1:C:182:LEU:HG	2.11	0.50
1:C:263:ILE:HD11	1:C:406:THR:HG22	1.94	0.50
1:C:82:GLU:CG	1:C:83:VAL:H	2.22	0.50
1:A:252:MET:O	1:A:256:ILE:N	2.37	0.50
1:A:300:CYS:O	1:A:303:SER:N	2.44	0.50
1:C:330:PHE:HE1	1:C:335:SER:HB3	1.77	0.50
1:C:74:TRP:CE3	1:C:74:TRP:HA	2.45	0.50
1:B:90:SER:O	1:B:132:ASN:ND2	2.42	0.49
1:B:92:HIS:O	1:B:162:ASP:HA	2.13	0.49
1:B:94:VAL:O	1:B:95:VAL:HG23	2.12	0.49
1:C:565:PRO:HD2	1:C:575:PHE:CE2	2.47	0.49
1:C:79:GLU:HB3	1:C:81:SER:HG	1.76	0.49
1:A:567:VAL:HG21	1:A:575:PHE:CG	2.48	0.49
1:B:359:LEU:HD11	1:B:381:LEU:CD1	2.40	0.49
1:B:33:LEU:CB	1:B:70:ALA:HB2	2.42	0.49
1:C:525:LEU:O	1:C:528:LYS:HB2	2.12	0.49
1:C:447:MET:HE1	1:C:578:VAL:HB	1.94	0.49
1:A:103:ASN:C	1:A:106:PRO:HD2	2.32	0.49
1:A:164:ARG:HB2	1:A:165:HIS:ND1	2.27	0.49
1:A:271:ILE:HG22	1:A:271:ILE:O	2.12	0.49
1:A:308:MET:C	1:A:310:SER:N	2.65	0.49
1:B:345:THR:HG21	1:B:359:LEU:HD21	1.94	0.49
1:B:396:GLU:CD	1:B:401:SER:HA	2.33	0.49
1:B:525:LEU:HA	1:B:528:LYS:HD3	1.93	0.49
1:C:263:ILE:HG21	1:C:440:LEU:CD2	2.39	0.49
1:C:316:SER:OG	1:C:317:LEU:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ILE:HG22	1:A:326:ILE:O	2.12	0.49
1:A:330:PHE:HD1	1:A:331:ARG:N	2.11	0.49
1:A:552:GLY:O	1:A:553:PHE:C	2.50	0.49
1:B:520:ALA:O	1:B:547:ALA:HA	2.12	0.49
1:B:572:ALA:HB3	1:B:573:PRO:HD3	1.94	0.49
1:B:90:SER:HB3	1:B:128:ALA:HB1	1.94	0.49
1:C:145:VAL:HG11	1:C:170:LEU:CD1	2.41	0.49
1:C:433:ILE:O	1:C:436:GLY:N	2.38	0.49
1:A:251:TYR:CG	1:A:397:ILE:HG21	2.47	0.49
1:B:234:ILE:HD12	1:B:235:GLU:N	2.22	0.49
1:B:252:MET:O	1:B:256:ILE:HG13	2.13	0.49
1:A:251:TYR:O	1:A:252:MET:C	2.49	0.49
1:B:346:LEU:HD11	1:B:412:LEU:HD11	1.93	0.49
1:B:92:HIS:HD2	1:B:164:ARG:HE	1.59	0.49
1:C:259:GLN:N	1:C:260:PRO:HD2	2.28	0.49
1:C:283:PRO:CG	1:C:284:ASN:N	2.76	0.49
1:C:304:TYR:CZ	1:C:308:MET:CE	2.95	0.49
1:C:480:LEU:CD2	1:C:496:ALA:HB3	2.40	0.49
1:C:20:LEU:HD11	1:C:70:ALA:HB1	1.94	0.49
1:A:281:LEU:HD21	1:A:389:LEU:HD11	1.94	0.49
1:A:33:LEU:O	1:A:33:LEU:CD2	2.51	0.49
1:A:374:CYS:SG	1:A:375:ASN:N	2.86	0.49
1:A:417:ALA:HB1	1:A:430:GLU:HG3	1.94	0.49
1:A:518:VAL:HG11	1:A:533:ILE:HD11	1.94	0.49
1:C:188:PHE:CD2	1:C:200:THR:HG21	2.48	0.49
1:C:498:ALA:O	1:C:499:ALA:C	2.51	0.49
1:A:273:HIS:C	1:A:275:GLN:H	2.15	0.49
1:B:180:ILE:HG22	1:B:181:GLY:N	2.26	0.49
1:B:406:THR:CA	1:B:409:LEU:HD12	2.16	0.49
1:B:515:PRO:O	1:B:516:VAL:CG2	2.60	0.49
1:B:530:LYS:HA	1:B:533:ILE:HD12	1.94	0.49
1:C:31:ALA:HB2	1:C:51:VAL:CG2	2.40	0.49
1:A:6:ALA:CB	1:A:12:VAL:HB	2.42	0.49
1:A:13:ALA:C	1:A:15:ILE:N	2.66	0.49
1:A:76:THR:C	1:A:78:GLY:N	2.65	0.49
1:B:91:GLU:CD	1:B:132:ASN:HD21	2.16	0.49
1:C:393:ALA:HB2	1:C:407:THR:HG21	1.95	0.49
1:A:42:MET:CE	1:A:43:THR:H	2.26	0.49
1:A:551:ALA:CB	1:A:553:PHE:CD1	2.96	0.49
1:A:401:SER:OG	2:A:700:G6Q:H2	2.13	0.49
1:B:185:GLY:O	1:B:186:GLU:CB	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:VAL:O	1:B:311:ARG:N	2.46	0.49
1:B:442:SER:OG	1:B:443:ARG:NH1	2.46	0.49
1:B:499:ALA:O	1:B:501:GLU:N	2.43	0.49
1:C:346:LEU:CD2	1:C:408:GLN:HB3	2.42	0.49
1:C:408:GLN:O	1:C:412:LEU:HG	2.13	0.49
1:C:531:SER:O	1:C:535:GLU:HG3	2.12	0.49
1:B:594:ASP:HB3	1:B:597:GLN:C	2.34	0.48
1:C:165:HIS:N	1:C:166:PRO:HD3	2.28	0.48
1:C:16:LEU:O	1:C:20:LEU:HG	2.13	0.48
1:C:344:ILE:N	1:C:344:ILE:HD12	2.28	0.48
1:C:359:LEU:CD2	1:C:381:LEU:CD2	2.91	0.48
1:B:332:TYR:HE1	1:C:528:LYS:HZ1	1.58	0.48
1:C:567:VAL:HG11	1:C:575:PHE:CG	2.48	0.48
1:B:144:ALA:O	1:B:147:ARG:HB2	2.12	0.48
1:B:14:GLU:OE2	1:B:15:ILE:HG13	2.13	0.48
1:B:371:LEU:CG	1:B:372:ALA:H	2.16	0.48
1:B:415:LEU:CD1	1:B:419:LEU:HD11	2.40	0.48
1:B:433:ILE:HG13	1:B:570:VAL:CG2	2.37	0.48
1:B:502:LEU:O	1:B:506:PRO:CD	2.62	0.48
1:C:308:MET:HB3	1:C:477:PRO:HG3	1.96	0.48
1:C:460:ASP:O	1:C:461:PHE:HD1	1.96	0.48
1:C:469:PHE:HA	1:C:517:ILE:O	2.13	0.48
1:A:118:PHE:HD2	1:A:125:GLU:OE1	1.96	0.48
1:A:16:LEU:HD11	1:A:68:GLY:CA	2.43	0.48
1:B:343:MET:CE	1:B:362:SER:HB2	2.43	0.48
1:C:17:LEU:HD21	1:C:33:LEU:HD11	1.93	0.48
1:A:292:VAL:HG21	1:A:342:LEU:CB	2.43	0.48
1:A:491:TYR:HE1	1:A:599:ARG:HG2	1.78	0.48
1:B:36:VAL:HA	1:B:42:MET:HA	1.95	0.48
1:B:501:GLU:O	1:B:506:PRO:HD2	2.12	0.48
1:B:457:LEU:HD23	1:B:562:ILE:HD11	1.95	0.48
1:C:187:ASN:O	1:C:188:PHE:CD1	2.66	0.48
1:C:469:PHE:CE2	1:C:482:GLY:C	2.86	0.48
1:C:540:GLY:O	1:C:541:GLY:O	2.30	0.48
1:C:82:GLU:O	1:C:85:ALA:HB3	2.13	0.48
1:A:131:VAL:HG11	1:A:160:ILE:HG21	1.94	0.48
1:B:23:LEU:HD21	1:B:195:ALA:HB2	1.95	0.48
1:B:413:LEU:HD12	1:B:416:VAL:HG21	1.95	0.48
1:B:453:ARG:HH11	1:B:453:ARG:CG	2.27	0.48
1:B:45:LEU:HD11	1:B:57:ALA:CB	2.42	0.48
1:C:107:LEU:O	1:C:110:GLU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:VAL:HG11	1:C:163:SER:HA	1.94	0.48
1:C:251:TYR:CD1	1:C:397:ILE:CG2	2.93	0.48
1:C:327:ALA:C	1:C:329:GLU:N	2.67	0.48
1:A:281:LEU:HD21	1:A:389:LEU:CD1	2.44	0.48
1:A:314:PHE:CD1	1:A:416:VAL:HG22	2.49	0.48
1:A:388:ALA:O	1:A:389:LEU:CD1	2.50	0.48
1:B:162:ASP:C	1:B:164:ARG:N	2.61	0.48
1:B:219:VAL:HG12	1:B:220:ASN:N	2.26	0.48
1:B:440:LEU:N	1:B:441:PRO:HD2	2.29	0.48
1:B:509:LEU:C	1:B:510:ILE:HD13	2.34	0.48
1:B:556:SER:C	1:B:558:ASN:H	2.15	0.48
1:C:139:GLY:HA3	1:C:143:GLU:HB3	1.96	0.48
1:C:31:ALA:HB1	1:C:51:VAL:HG22	1.89	0.48
1:A:24:GLU:O	1:A:27:GLY:O	2.32	0.48
1:A:504:HIS:NE2	3:A:707:HOH:O	2.35	0.48
1:A:567:VAL:HG22	1:A:575:PHE:CZ	2.49	0.48
1:B:276:VAL:HG11	1:B:417:ALA:CB	2.43	0.48
1:B:313:TRP:CH2	1:B:413:LEU:HD13	2.43	0.48
1:B:275:GLN:CA	1:B:434:VAL:HG11	2.44	0.48
1:B:4:VAL:O	1:B:4:VAL:HG12	2.13	0.48
1:C:92:HIS:HB2	1:C:163:SER:HB2	1.95	0.48
1:C:470:LEU:HA	1:C:497:TYR:O	2.14	0.48
1:A:21:ARG:CG	1:A:51:VAL:HG11	2.39	0.48
1:B:169:LEU:O	1:B:170:LEU:HD23	2.11	0.48
1:B:304:TYR:O	1:B:307:GLY:N	2.47	0.48
1:C:96:VAL:HG23	1:C:159:VAL:HB	1.95	0.48
1:C:489:ILE:HD11	1:C:584:ALA:O	2.13	0.48
1:A:457:LEU:HG	1:A:562:ILE:HD11	1.96	0.48
1:A:523:ASN:ND2	1:A:524:GLU:N	2.62	0.48
1:A:553:PHE:CD2	1:A:559:MET:HE1	2.39	0.48
1:A:578:VAL:N	1:A:579:PRO:CD	2.77	0.48
1:B:196:LEU:HD23	1:B:196:LEU:HA	1.29	0.48
1:B:197:LEU:N	1:B:198:PRO:CD	2.77	0.48
1:B:34:ALA:C	1:B:35:VAL:CG1	2.81	0.48
1:B:453:ARG:HH11	1:B:453:ARG:HG3	1.78	0.48
1:C:12:VAL:HG13	1:C:66:GLY:O	2.14	0.48
1:C:307:GLY:C	1:C:324:VAL:HG21	2.33	0.48
1:C:480:LEU:HD22	1:C:496:ALA:HB3	1.95	0.48
1:A:103:ASN:ND2	1:A:103:ASN:H	2.12	0.48
1:A:155:ALA:HA	1:A:174:SER:O	2.14	0.48
1:A:348:GLN:O	1:A:375:ASN:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:LEU:O	1:A:460:ASP:N	2.42	0.48
1:C:348:GLN:CG	1:C:375:ASN:HB3	2.44	0.48
1:B:509:LEU:HD11	1:C:493:HIS:HA	1.95	0.48
1:C:25:TYR:CE1	1:C:603:LYS:HG2	2.49	0.48
1:A:16:LEU:HD11	1:A:68:GLY:C	2.34	0.47
1:A:4:VAL:HG21	1:A:19:GLY:HA3	1.95	0.47
1:A:296:GLN:HG2	1:A:367:TYR:OH	2.13	0.47
1:C:112:LYS:HA	1:C:116:TYR:O	2.14	0.47
1:C:453:ARG:O	1:C:457:LEU:HD13	2.13	0.47
1:C:529:LEU:HG	1:C:533:ILE:HD11	1.96	0.47
1:A:301:GLY:O	1:A:302:THR:C	2.52	0.47
1:A:266:THR:CG2	1:A:391:THR:O	2.58	0.47
1:A:411:VAL:O	1:A:414:MET:HB2	2.14	0.47
1:A:436:GLY:O	1:A:439:ALA:N	2.47	0.47
1:B:396:GLU:OE2	1:B:401:SER:CA	2.58	0.47
1:B:400:ALA:O	1:B:402:THR:HG23	2.14	0.47
1:C:27:GLY:O	1:C:29:ASP:OD1	2.32	0.47
1:C:583:LEU:O	1:C:583:LEU:HD12	2.14	0.47
1:A:52:GLN:CA	1:A:52:GLN:HE21	2.25	0.47
1:A:559:MET:O	1:A:559:MET:CG	2.61	0.47
1:B:101:ILE:HB	1:B:104:HIS:HB3	1.97	0.47
1:B:145:VAL:O	1:B:149:ILE:HG12	2.15	0.47
1:B:288:LEU:HD12	1:B:288:LEU:N	2.29	0.47
1:B:307:GLY:C	1:B:324:VAL:HG21	2.34	0.47
1:B:356:LEU:CD1	1:B:360:ARG:HD2	2.44	0.47
1:B:3:ILE:HD12	1:B:98:ASN:HB3	1.97	0.47
1:B:476:TYR:CE1	1:B:498:ALA:HB2	2.49	0.47
1:B:3:ILE:CG2	1:B:4:VAL:N	2.77	0.47
1:B:588:ALA:O	1:B:592:GLY:N	2.47	0.47
1:C:104:HIS:ND1	1:C:123:ASP:HA	2.28	0.47
1:C:214:ILE:O	1:C:214:ILE:HG22	2.13	0.47
1:B:501:GLU:HG2	1:C:326:ILE:HG21	1.96	0.47
1:C:536:VAL:CG2	1:C:537:ARG:N	2.76	0.47
1:A:103:ASN:C	1:A:105:GLU:N	2.68	0.47
1:A:223:ASP:CG	1:A:224:LYS:N	2.65	0.47
1:A:551:ALA:HB3	1:A:553:PHE:HD1	1.80	0.47
1:B:286:ASP:O	1:B:287:GLU:C	2.50	0.47
1:C:216:ARG:HE	1:C:217:ARG:NH1	2.12	0.47
1:C:245:LYS:HD2	1:C:251:TYR:CZ	2.49	0.47
1:C:251:TYR:HB3	1:C:397:ILE:HB	1.95	0.47
1:C:413:LEU:O	1:C:416:VAL:CB	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:VAL:CG2	1:C:43:THR:HB	2.45	0.47
1:C:35:VAL:HG23	1:C:43:THR:HB	1.96	0.47
1:C:460:ASP:O	1:C:461:PHE:CD1	2.68	0.47
1:C:572:ALA:O	1:C:576:TYR:HD2	1.97	0.47
1:C:11:ASP:HA	1:C:65:GLY:O	2.14	0.47
1:A:145:VAL:C	1:A:147:ARG:N	2.68	0.47
1:A:231:ARG:O	1:A:232:GLN:O	2.31	0.47
1:A:241:ASP:OD2	1:A:254:LYS:HE3	2.14	0.47
1:A:443:ARG:HG2	1:A:443:ARG:HH11	1.79	0.47
1:A:528:LYS:O	1:A:531:SER:HB3	2.14	0.47
1:A:250:HIS:CE1	1:A:595:VAL:HB	2.50	0.47
1:C:159:VAL:HA	1:C:171:ALA:CB	2.45	0.47
1:C:22:ARG:HG2	1:C:22:ARG:HH11	1.80	0.47
1:C:376:VAL:CG1	1:C:377:PRO:HD2	2.43	0.47
1:C:393:ALA:HB1	1:C:403:LYS:HG3	1.97	0.47
1:A:98:ASN:HB3	1:A:176:SER:OG	2.15	0.47
1:B:48:LEU:HD21	1:B:81:SER:CB	2.22	0.47
1:B:94:VAL:C	1:B:95:VAL:HG23	2.34	0.47
1:C:159:VAL:HG12	1:C:159:VAL:O	2.14	0.47
1:C:259:GLN:N	1:C:260:PRO:CD	2.78	0.47
1:B:240:TYR:CD1	1:B:241:ASP:HB2	2.50	0.47
1:B:79:GLU:O	1:B:81:SER:N	2.48	0.47
1:C:142:ARG:CG	1:C:146:LEU:HB2	2.44	0.47
1:C:306:SER:HB2	1:C:346:LEU:CD1	2.42	0.47
1:C:373:ILE:HD12	1:C:412:LEU:HD23	1.96	0.47
1:C:439:ALA:O	1:C:440:LEU:C	2.53	0.47
1:C:544:TYR:CZ	1:C:560:HIS:HD2	2.31	0.47
1:C:578:VAL:CB	1:C:579:PRO:CD	2.82	0.47
1:A:173:ARG:HH21	1:A:208:GLU:HB2	1.80	0.47
1:A:22:ARG:C	1:A:23:LEU:HD23	2.30	0.47
1:A:250:HIS:ND1	1:A:595:VAL:HB	2.30	0.47
1:B:484:LEU:HA	1:B:484:LEU:HD12	1.63	0.47
1:B:488:GLU:OE1	2:B:701:G6Q:C1	2.61	0.47
1:B:78:GLY:H	1:C:538:ALA:CB	2.28	0.47
1:C:374:CYS:O	1:C:390:MET:HA	2.15	0.47
1:C:485:LYS:CE	1:C:485:LYS:HA	2.33	0.47
1:C:486:LEU:O	1:C:490:SER:OG	2.32	0.47
1:A:443:ARG:CG	1:A:443:ARG:HH11	2.28	0.47
1:A:48:LEU:HD12	1:A:48:LEU:HA	1.51	0.47
1:B:223:ASP:OD1	1:B:227:ALA:HB3	2.15	0.47
1:B:256:ILE:HG22	1:B:257:TYR:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:LEU:HD11	1:B:360:ARG:CD	2.44	0.47
1:C:239:GLN:HG2	1:C:239:GLN:O	2.14	0.47
1:C:45:LEU:HD21	1:C:57:ALA:CB	2.44	0.47
1:C:526:LEU:O	1:C:527:GLU:C	2.49	0.47
1:C:557:ASP:O	1:C:560:HIS:HE1	1.98	0.47
1:C:576:TYR:O	1:C:577:THR:C	2.53	0.47
1:A:245:LYS:HG2	1:A:251:TYR:CZ	2.50	0.47
1:A:358:GLY:O	1:A:359:LEU:C	2.51	0.47
1:A:534:GLU:CA	1:A:534:GLU:OE1	2.63	0.47
1:B:276:VAL:HG21	1:B:418:LYS:H	1.79	0.47
1:B:337:VAL:O	1:B:338:ARG:O	2.32	0.47
1:B:564:MET:HG3	1:B:576:TYR:CE2	2.50	0.47
1:C:130:LEU:HD23	1:C:130:LEU:C	2.35	0.47
1:C:263:ILE:HD11	1:C:406:THR:CG2	2.45	0.47
1:C:283:PRO:HG2	1:C:284:ASN:N	2.28	0.47
1:B:140:THR:O	1:B:144:ALA:N	2.42	0.47
1:B:179:VAL:CG2	1:B:205:PHE:HA	2.29	0.47
1:B:28:TYR:CE1	1:B:602:ALA:CB	2.98	0.47
1:B:331:ARG:HD3	1:B:332:TYR:CE2	2.50	0.47
1:B:532:ASN:O	1:B:536:VAL:CG2	2.43	0.47
1:C:69:ILE:CG2	1:C:169:LEU:HD11	2.45	0.47
1:A:103:ASN:N	1:A:103:ASN:HD22	2.11	0.46
1:A:195:ALA:O	1:A:198:PRO:HD2	2.15	0.46
1:A:305:ASN:HD22	1:A:481:GLU:HG2	1.80	0.46
1:A:502:LEU:HB3	1:A:507:LEU:HB2	1.96	0.46
1:B:347:SER:HB3	1:B:381:LEU:HD23	1.97	0.46
1:B:84:ASN:O	1:B:88:HIS:NE2	2.42	0.46
1:C:126:VAL:O	1:C:130:LEU:HB2	2.15	0.46
1:C:34:ALA:O	1:C:35:VAL:HG13	2.14	0.46
1:C:32:GLY:CA	1:C:86:HIS:O	2.55	0.46
1:A:409:LEU:HD13	1:A:574:ILE:HG12	1.98	0.46
1:A:490:SER:O	1:A:491:TYR:HB2	2.14	0.46
1:A:76:THR:HG22	1:A:77:HIS:N	2.30	0.46
1:B:451:ASP:O	1:B:452:LYS:C	2.53	0.46
1:B:475:GLN:HE22	1:B:576:TYR:HB2	1.81	0.46
1:C:223:ASP:OD1	1:C:223:ASP:N	2.47	0.46
1:C:304:TYR:OH	1:C:308:MET:HE1	2.14	0.46
1:C:381:LEU:C	1:C:383:ARG:N	2.67	0.46
1:C:502:LEU:H	1:C:502:LEU:CD1	2.29	0.46
1:C:523:ASN:ND2	1:C:569:GLU:CD	2.69	0.46
1:C:571:ILE:HG13	1:C:571:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:HIS:C	1:A:167:ASP:N	2.67	0.46
1:A:248:TYR:CB	1:A:254:LYS:HB2	2.46	0.46
1:A:25:TYR:HD1	1:A:25:TYR:C	2.17	0.46
1:A:440:LEU:HD21	1:A:574:ILE:CD1	2.45	0.46
1:B:149:ILE:HB	1:B:150:PRO:HD3	1.97	0.46
1:B:355:THR:O	1:B:356:LEU:C	2.53	0.46
1:B:509:LEU:HD23	1:B:509:LEU:O	2.16	0.46
1:B:564:MET:HG3	1:B:576:TYR:HE2	1.80	0.46
1:C:129:HIS:O	1:C:131:VAL:N	2.49	0.46
1:C:255:GLU:OE1	1:C:396:GLU:HG2	2.16	0.46
1:B:495:GLU:OE1	1:C:493:HIS:NE2	2.46	0.46
1:A:326:ILE:HA	1:A:326:ILE:HD12	1.64	0.46
1:C:327:ALA:O	1:C:330:PHE:N	2.38	0.46
1:C:36:VAL:HG21	1:C:163:SER:OG	2.16	0.46
1:C:573:PRO:O	1:C:574:ILE:C	2.51	0.46
1:A:267:LEU:CD2	1:A:414:MET:HE3	2.42	0.46
1:A:599:ARG:CG	1:A:600:ASN:OD1	2.60	0.46
1:B:178:LEU:HD11	1:B:189:ILE:HD11	1.98	0.46
1:B:179:VAL:HG23	1:B:204:ILE:C	2.36	0.46
1:B:5:GLY:HA3	1:B:189:ILE:CG2	2.45	0.46
1:B:21:ARG:CG	1:B:21:ARG:NH1	2.61	0.46
1:B:343:MET:O	1:B:371:LEU:N	2.49	0.46
1:B:556:SER:O	1:B:558:ASN:N	2.49	0.46
1:B:577:THR:O	1:B:581:GLN:HG3	2.16	0.46
1:C:255:GLU:OE2	1:C:398:GLY:N	2.43	0.46
1:C:361:LEU:O	1:C:365:LEU:HG	2.16	0.46
1:C:314:PHE:CD1	1:C:416:VAL:HG22	2.51	0.46
1:C:570:VAL:CG1	1:C:571:ILE:N	2.59	0.46
1:A:36:VAL:HG12	1:A:42:MET:CA	2.46	0.46
1:A:44:ARG:O	1:A:45:LEU:CD1	2.64	0.46
1:A:597:GLN:HA	1:A:598:PRO:HD2	1.82	0.46
1:B:316:SER:OG	1:B:317:LEU:N	2.48	0.46
1:C:567:VAL:HG11	1:C:575:PHE:CE2	2.51	0.46
1:C:56:GLN:C	1:C:58:ALA:H	2.18	0.46
1:A:124:THR:C	1:A:126:VAL:N	2.69	0.46
1:A:285:ALA:C	1:A:287:GLU:H	2.18	0.46
1:A:447:MET:HE2	1:A:447:MET:HB2	1.73	0.46
1:A:464:LYS:C	1:A:465:HIS:ND1	2.69	0.46
1:A:533:ILE:HG23	1:A:543:LEU:HD22	1.97	0.46
1:B:270:ARG:HA	1:B:277:ASP:HB3	1.98	0.46
1:C:130:LEU:HD11	1:C:152:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:487:LYS:HD3	1:C:494:ALA:O	2.15	0.46
1:C:443:ARG:NH1	1:C:568:GLU:OE2	2.44	0.46
1:C:599:ARG:HG3	1:C:600:ASN:HD22	1.77	0.46
1:C:93:ILE:O	1:C:93:ILE:HG22	2.16	0.46
1:A:195:ALA:O	1:A:198:PRO:CD	2.64	0.46
1:A:251:TYR:H	1:A:596:ASP:CG	2.17	0.46
1:A:457:LEU:HD21	1:A:562:ILE:HD13	1.97	0.46
1:A:486:LEU:HD21	1:A:492:ILE:HD12	1.98	0.46
1:A:86:HIS:CE1	1:A:124:THR:HG1	2.33	0.46
1:B:97:HIS:CB	1:B:158:THR:HB	2.42	0.46
1:C:331:ARG:O	1:C:332:TYR:CD1	2.69	0.46
1:C:373:ILE:HD13	1:C:411:VAL:HG11	1.94	0.46
1:B:487:LYS:HG3	1:C:509:LEU:HD11	1.97	0.46
1:B:332:TYR:CZ	1:C:528:LYS:NZ	2.69	0.46
1:C:69:ILE:HG13	1:C:96:VAL:CG2	2.46	0.46
1:A:12:VAL:O	1:A:16:LEU:HG	2.16	0.46
1:A:146:LEU:CD2	1:A:226:GLY:CA	2.89	0.46
1:A:305:ASN:HD22	1:A:481:GLU:CG	2.29	0.46
1:A:528:LYS:O	1:A:532:ASN:ND2	2.49	0.46
1:B:237:ASN:C	1:B:239:GLN:NE2	2.69	0.46
1:B:334:LYS:HD3	1:B:335:SER:N	2.31	0.46
1:B:306:SER:HA	1:B:405:PHE:HE1	1.81	0.46
1:B:468:LEU:CG	1:B:470:LEU:HD21	2.46	0.46
1:C:178:LEU:O	1:C:206:LEU:HG	2.16	0.46
1:C:359:LEU:HD22	1:C:381:LEU:HD22	1.98	0.46
1:C:498:ALA:O	1:C:500:GLY:N	2.49	0.46
1:A:134:GLU:OE1	1:A:147:ARG:CB	2.64	0.46
1:A:510:ILE:O	1:A:511:ASP:HB3	2.15	0.46
1:B:293:GLU:OE2	1:B:340:ASN:ND2	2.49	0.46
1:B:32:GLY:CA	1:B:54:LEU:CD2	2.94	0.46
1:C:105:GLU:N	1:C:106:PRO:HD2	2.30	0.46
1:C:201:ARG:NH1	1:C:239:GLN:HG3	2.31	0.46
1:C:525:LEU:O	1:C:526:LEU:C	2.54	0.46
1:C:60:GLU:O	1:C:61:HIS:CB	2.58	0.46
1:B:179:VAL:HG22	1:B:180:ILE:O	2.16	0.45
1:B:5:GLY:HA3	1:B:189:ILE:HG23	1.97	0.45
1:B:337:VAL:CG1	1:B:365:LEU:HD22	2.47	0.45
1:B:523:ASN:ND2	1:B:525:LEU:CB	2.79	0.45
1:C:188:PHE:CE2	1:C:199:VAL:CG2	2.99	0.45
1:C:345:THR:HB	1:C:381:LEU:HD13	1.98	0.45
1:A:118:PHE:HA	1:A:125:GLU:OE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:HD21	1:A:33:LEU:HD12	1.92	0.45
1:A:476:TYR:CB	1:A:477:PRO:HD3	2.36	0.45
1:A:510:ILE:HD12	1:A:536:VAL:HG12	1.97	0.45
1:B:228:GLU:CG	1:B:229:VAL:N	2.78	0.45
1:B:241:ASP:OD2	1:B:254:LYS:HE2	2.15	0.45
1:B:286:ASP:O	1:B:290:SER:OG	2.26	0.45
1:B:426:ASP:OD1	1:B:428:SER:HB3	2.15	0.45
1:C:255:GLU:HA	1:C:403:LYS:HD3	1.98	0.45
1:C:356:LEU:O	1:C:357:ALA:C	2.55	0.45
1:C:553:PHE:HB3	1:C:561:ILE:HD11	1.97	0.45
1:A:121:GLU:O	1:A:122:THR:CB	2.57	0.45
1:A:25:TYR:C	1:A:27:GLY:H	2.19	0.45
1:A:440:LEU:HD21	1:A:574:ILE:HG21	1.98	0.45
1:A:491:TYR:CE1	1:A:599:ARG:CG	2.99	0.45
1:B:46:ARG:O	1:B:47:ARG:CG	2.48	0.45
1:B:586:HIS:O	1:B:590:ILE:HD11	2.16	0.45
1:A:18:GLU:O	1:A:19:GLY:C	2.54	0.45
1:A:347:SER:HB2	1:A:381:LEU:HD11	1.98	0.45
1:A:448:LEU:C	1:A:450:GLN:N	2.69	0.45
1:A:28:TYR:CE2	1:A:597:GLN:CB	2.99	0.45
1:B:259:GLN:N	1:B:260:PRO:CD	2.80	0.45
1:B:305:ASN:N	1:B:305:ASN:OD1	2.49	0.45
1:B:350:GLY:HA3	1:B:374:CYS:SG	2.57	0.45
1:B:440:LEU:HD12	1:B:440:LEU:O	2.17	0.45
1:B:505:GLY:N	1:B:506:PRO:HD2	2.31	0.45
1:B:570:VAL:HG13	1:B:571:ILE:HG23	1.97	0.45
1:B:3:ILE:HD11	1:B:98:ASN:CB	2.47	0.45
1:C:104:HIS:CD2	1:C:108:ARG:HB2	2.51	0.45
1:C:417:ALA:HB2	1:C:433:ILE:HD12	1.98	0.45
1:C:495:GLU:OE1	1:C:497:TYR:CE2	2.69	0.45
1:C:454:ILE:HG23	1:C:583:LEU:HB2	1.97	0.45
1:C:583:LEU:HD12	1:C:587:VAL:HG23	1.98	0.45
1:A:124:THR:O	1:A:126:VAL:N	2.50	0.45
1:B:118:PHE:HD2	1:B:125:GLU:HG2	1.80	0.45
1:B:130:LEU:HD11	1:B:151:GLN:NE2	2.32	0.45
1:B:264:LYS:HD3	1:B:264:LYS:C	2.36	0.45
1:B:502:LEU:C	1:B:506:PRO:HD2	2.37	0.45
1:B:515:PRO:HA	1:B:542:GLN:O	2.17	0.45
1:C:18:GLU:CD	1:C:21:ARG:NH1	2.69	0.45
1:C:27:GLY:C	1:C:29:ASP:N	2.67	0.45
1:A:111:LEU:C	1:A:113:ALA:N	2.66	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLY:H	1:A:208:GLU:CD	2.20	0.45
1:A:178:LEU:O	1:A:206:LEU:HB2	2.17	0.45
1:A:20:LEU:O	1:A:22:ARG:N	2.50	0.45
1:A:28:TYR:CE2	1:A:597:GLN:HB2	2.52	0.45
1:A:294:HIS:ND1	1:A:338:ARG:HB2	2.31	0.45
1:A:347:SER:CB	1:A:381:LEU:HD12	2.47	0.45
1:B:330:PHE:O	1:B:333:ARG:HG3	2.15	0.45
1:B:37:ASP:O	1:B:38:ALA:C	2.54	0.45
1:B:3:ILE:HG13	1:B:98:ASN:HB2	1.97	0.45
1:B:515:PRO:C	1:B:516:VAL:HG23	2.36	0.45
1:B:44:ARG:NH1	1:B:88:HIS:HA	2.31	0.45
1:C:127:ILE:CG2	1:C:152:LEU:HD13	2.46	0.45
1:C:259:GLN:O	1:C:260:PRO:C	2.53	0.45
1:C:298:LEU:O	1:C:299:ALA:HB2	2.17	0.45
1:C:390:MET:N	1:C:390:MET:SD	2.89	0.45
1:C:511:ASP:OD1	1:C:514:MET:HB2	2.17	0.45
1:C:546:PHE:CE1	1:C:562:ILE:HD12	2.51	0.45
1:C:74:TRP:HA	1:C:74:TRP:HE3	1.81	0.45
1:A:348:GLN:CD	1:A:348:GLN:C	2.76	0.45
1:A:48:LEU:HD13	1:A:48:LEU:N	2.32	0.45
1:A:42:MET:SD	1:A:94:VAL:HG21	2.57	0.45
1:B:149:ILE:N	1:B:150:PRO:CD	2.79	0.45
1:B:270:ARG:O	1:B:277:ASP:N	2.44	0.45
1:C:95:VAL:HG11	1:C:127:ILE:CD1	2.46	0.45
1:C:270:ARG:HD3	1:C:414:MET:CE	2.47	0.45
1:C:518:VAL:HB	1:C:545:VAL:HG13	1.97	0.45
1:A:295:ILE:HG22	1:A:295:ILE:O	2.15	0.45
1:A:356:LEU:CD1	1:A:380:SER:HB3	2.47	0.45
1:A:399:VAL:HG13	1:A:603:LYS:N	2.31	0.45
1:A:3:ILE:HG23	1:A:3:ILE:HD13	1.37	0.45
1:A:421:LYS:O	1:A:422:LEU:C	2.54	0.45
1:A:491:TYR:CD1	1:A:599:ARG:NH1	2.84	0.45
1:A:61:HIS:N	1:A:62:PRO:HD3	2.31	0.45
1:B:240:TYR:HE1	1:B:254:LYS:HZ1	1.64	0.45
1:B:404:ALA:O	1:B:408:GLN:NE2	2.50	0.45
1:C:211:ILE:HG22	1:C:212:ALA:N	2.32	0.45
1:C:371:LEU:HA	1:C:387:LEU:CB	2.40	0.45
1:C:456:ALA:O	1:C:459:GLU:CD	2.55	0.45
1:C:29:ASP:OD2	1:C:74:TRP:HE3	2.00	0.45
1:A:123:ASP:O	1:A:126:VAL:HB	2.17	0.45
1:A:523:ASN:ND2	1:A:524:GLU:H	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:MET:O	1:A:559:MET:HG3	2.16	0.45
1:B:181:GLY:HA2	1:B:203:PHE:HD1	1.81	0.45
1:B:468:LEU:HD11	1:B:470:LEU:CD2	2.46	0.45
1:B:399:VAL:HG21	1:B:598:PRO:HD2	1.99	0.45
1:C:288:LEU:O	1:C:288:LEU:HD12	2.17	0.45
1:B:509:LEU:CD1	1:C:493:HIS:HA	2.47	0.45
1:A:301:GLY:O	1:A:303:SER:N	2.50	0.45
1:B:126:VAL:CG1	1:B:127:ILE:H	2.24	0.45
1:B:299:ALA:HB1	1:B:303:SER:HB3	1.99	0.45
1:B:569:GLU:OE1	1:B:569:GLU:HA	2.18	0.45
1:B:61:HIS:CD2	1:B:61:HIS:C	2.89	0.45
1:C:131:VAL:C	1:C:133:TRP:N	2.70	0.45
1:C:173:ARG:CG	1:C:178:LEU:HB2	2.47	0.45
1:C:255:GLU:HB3	1:C:403:LYS:HD3	1.99	0.45
1:C:447:MET:O	1:C:448:LEU:C	2.53	0.45
1:A:502:LEU:HD12	1:A:502:LEU:HA	1.70	0.44
1:B:123:ASP:C	1:B:126:VAL:HG12	2.38	0.44
1:B:281:LEU:HD22	1:B:387:LEU:HB3	1.99	0.44
1:B:338:ARG:CZ	1:C:321:PRO:HB3	2.47	0.44
1:B:379:SER:O	1:B:380:SER:C	2.55	0.44
1:B:588:ALA:HB1	1:B:593:THR:OG1	2.17	0.44
1:C:356:LEU:HD21	1:C:360:ARG:CZ	2.47	0.44
1:C:389:LEU:O	1:C:390:MET:O	2.35	0.44
1:C:400:ALA:O	1:C:401:SER:C	2.56	0.44
1:C:413:LEU:O	1:C:416:VAL:N	2.50	0.44
1:C:456:ALA:CA	1:C:459:GLU:OE2	2.65	0.44
1:C:510:ILE:HD13	1:C:514:MET:HG2	1.99	0.44
1:C:71:HIS:ND1	1:C:72:THR:N	2.64	0.44
1:C:42:MET:SD	1:C:94:VAL:HG21	2.57	0.44
1:A:294:HIS:HE2	1:A:323:ASP:CG	2.20	0.44
1:B:110:GLU:OE2	1:B:114:ARG:CZ	2.66	0.44
1:B:32:GLY:CA	1:B:46:ARG:HA	2.46	0.44
1:B:251:TYR:CD2	1:B:397:ILE:CG2	3.00	0.44
1:C:405:PHE:HD2	1:C:577:THR:HG21	1.81	0.44
1:C:67:THR:HG22	1:C:169:LEU:HD23	1.98	0.44
1:A:251:TYR:CG	1:A:397:ILE:CG2	3.01	0.44
1:A:71:HIS:ND1	1:A:86:HIS:CB	2.66	0.44
1:B:14:GLU:O	1:B:16:LEU:N	2.50	0.44
1:B:327:ALA:O	1:B:328:SER:C	2.54	0.44
1:B:335:SER:O	1:B:337:VAL:N	2.51	0.44
1:C:178:LEU:HD22	1:C:206:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ILE:HD11	1:C:238:LEU:HD11	1.98	0.44
1:C:254:LYS:O	1:C:256:ILE:N	2.50	0.44
1:C:36:VAL:HG12	1:C:166:PRO:CG	2.48	0.44
1:A:296:GLN:HE22	1:A:323:ASP:HB2	1.83	0.44
1:B:179:VAL:O	1:B:179:VAL:CG1	2.64	0.44
1:B:299:ALA:HB3	1:B:304:TYR:HA	2.00	0.44
1:B:372:ALA:HB2	1:B:385:SER:OG	2.18	0.44
1:C:107:LEU:C	1:C:109:GLU:N	2.70	0.44
1:C:343:MET:HG3	1:C:344:ILE:N	2.32	0.44
1:B:260:PRO:HG3	1:B:444:ILE:HG22	2.00	0.44
1:B:421:LYS:O	1:B:422:LEU:C	2.56	0.44
1:B:458:ALA:O	1:B:459:GLU:C	2.53	0.44
1:B:44:ARG:NH1	1:B:46:ARG:HH21	2.15	0.44
1:C:215:THR:O	1:C:216:ARG:C	2.56	0.44
1:C:502:LEU:H	1:C:502:LEU:HD12	1.82	0.44
1:A:164:ARG:O	1:A:165:HIS:CE1	2.70	0.44
1:A:409:LEU:O	1:A:410:THR:C	2.56	0.44
1:A:567:VAL:CG1	1:A:568:GLU:H	2.22	0.44
1:A:585:TYR:CZ	1:A:589:LEU:HD11	2.53	0.44
1:B:252:MET:HE1	1:B:489:ILE:HD13	2.00	0.44
1:B:579:PRO:HA	1:B:582:LEU:HD12	1.99	0.44
1:C:179:VAL:O	1:C:179:VAL:CG1	2.64	0.44
1:C:18:GLU:HA	1:C:21:ARG:HD2	2.00	0.44
1:A:88:HIS:CD2	1:A:124:THR:HG21	2.52	0.44
1:A:212:ALA:HB2	1:A:221:ILE:HG13	2.00	0.44
1:A:292:VAL:HG23	1:A:368:LEU:HD12	2.00	0.44
1:A:440:LEU:HB3	1:A:441:PRO:CD	2.42	0.44
1:B:281:LEU:CD1	1:B:387:LEU:CD1	2.63	0.44
1:B:391:THR:O	1:B:393:ALA:N	2.49	0.44
1:B:447:MET:HE3	1:B:564:MET:HE1	1.95	0.44
1:A:352:THR:HG22	1:A:353:ALA:N	2.33	0.44
1:A:530:LYS:C	1:A:530:LYS:HD2	2.38	0.44
1:A:12:VAL:HG13	1:A:66:GLY:HA2	2.00	0.44
1:B:42:MET:O	1:B:43:THR:OG1	2.30	0.44
1:B:490:SER:O	1:B:491:TYR:HB2	2.17	0.44
1:C:36:VAL:CG1	1:C:166:PRO:HG3	2.46	0.44
1:C:557:ASP:OD1	1:C:557:ASP:N	2.37	0.44
1:A:241:ASP:O	1:A:242:ALA:HB3	2.18	0.44
1:A:85:ALA:O	1:A:88:HIS:CE1	2.71	0.44
1:A:89:VAL:CG2	1:A:89:VAL:O	2.65	0.44
1:B:412:LEU:HA	1:B:412:LEU:HD23	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:TYR:CD1	1:B:491:TYR:N	2.81	0.44
1:C:12:VAL:O	1:C:15:ILE:N	2.51	0.44
1:C:127:ILE:CG2	1:C:152:LEU:CD1	2.92	0.44
1:C:251:TYR:O	1:C:255:GLU:HG3	2.17	0.44
1:C:278:LEU:CD2	1:C:414:MET:HE3	2.48	0.44
1:C:351:GLU:HG2	1:C:380:SER:CB	2.44	0.44
1:A:136:LYS:CB	1:A:137:GLN:NE2	2.79	0.43
1:A:199:VAL:CG2	1:A:200:THR:N	2.64	0.43
1:A:250:HIS:HB3	1:A:596:ASP:CG	2.36	0.43
1:A:34:ALA:HB1	1:A:42:MET:HE1	2.00	0.43
1:A:476:TYR:CD1	1:A:476:TYR:C	2.87	0.43
1:B:179:VAL:HG23	1:B:205:PHE:N	2.33	0.43
1:B:202:ARG:O	1:B:203:PHE:CD1	2.71	0.43
1:B:294:HIS:CD2	1:B:338:ARG:HG2	2.53	0.43
1:B:34:ALA:HB2	1:B:87:PRO:CG	2.34	0.43
1:B:354:ASP:O	1:B:355:THR:C	2.51	0.43
1:B:433:ILE:O	1:B:437:LEU:HG	2.18	0.43
1:B:485:LYS:C	1:B:487:LYS:N	2.69	0.43
1:B:480:LEU:HD23	1:B:496:ALA:HB3	1.99	0.43
1:C:107:LEU:HD12	1:C:107:LEU:N	2.32	0.43
1:A:178:LEU:HD22	1:A:189:ILE:HD11	1.99	0.43
1:A:35:VAL:HG21	3:A:702:HOH:O	2.19	0.43
1:A:589:LEU:O	1:A:590:ILE:C	2.57	0.43
1:B:124:THR:HG22	1:B:125:GLU:N	2.32	0.43
1:B:348:GLN:C	1:B:348:GLN:OE1	2.57	0.43
1:B:308:MET:HB2	1:B:477:PRO:HB3	2.00	0.43
1:B:580:LEU:O	1:B:581:GLN:C	2.55	0.43
1:C:259:GLN:CG	1:C:403:LYS:HA	2.48	0.43
1:C:3:ILE:HG22	1:C:4:VAL:N	2.33	0.43
1:B:600:ASN:HA	1:C:539:ARG:CZ	2.48	0.43
1:C:565:PRO:C	1:C:566:HIS:O	2.55	0.43
1:C:98:ASN:HD21	1:C:176:SER:HG	1.64	0.43
1:A:239:GLN:C	1:A:241:ASP:N	2.72	0.43
1:A:36:VAL:O	1:A:65:GLY:HA2	2.18	0.43
1:A:48:LEU:HD11	1:A:81:SER:C	2.39	0.43
1:A:253:GLN:HB2	1:A:585:TYR:CE2	2.53	0.43
1:B:20:LEU:HA	1:B:20:LEU:HD23	1.65	0.43
1:B:453:ARG:NH2	1:B:563:GLU:H	2.15	0.43
1:B:507:LEU:HD12	1:B:507:LEU:O	2.17	0.43
1:B:567:VAL:HG11	1:B:575:PHE:CE1	2.53	0.43
1:B:8:ALA:O	1:B:216:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:HIS:C	1:C:131:VAL:N	2.72	0.43
1:C:373:ILE:HD11	1:C:411:VAL:HG12	1.95	0.43
1:C:505:GLY:O	1:C:508:ALA:CB	2.65	0.43
1:A:344:ILE:HG12	1:A:371:LEU:HB3	2.00	0.43
1:A:36:VAL:O	1:A:65:GLY:HA3	2.18	0.43
1:B:397:ILE:HA	1:B:397:ILE:HD13	1.67	0.43
1:B:3:ILE:C	1:B:4:VAL:CG2	2.87	0.43
1:B:405:PHE:HD2	1:B:577:THR:HG21	1.83	0.43
1:C:255:GLU:CB	1:C:403:LYS:HD3	2.48	0.43
1:C:463:ASP:OD1	1:C:464:LYS:N	2.51	0.43
1:A:132:ASN:OD1	1:A:133:TRP:N	2.52	0.43
1:A:173:ARG:NH2	1:A:208:GLU:HB2	2.33	0.43
1:A:239:GLN:OE1	1:A:240:TYR:N	2.52	0.43
1:A:330:PHE:CD1	1:A:331:ARG:N	2.86	0.43
1:B:220:ASN:O	1:B:221:ILE:C	2.57	0.43
1:B:470:LEU:N	1:B:470:LEU:HD23	2.33	0.43
1:B:606:THR:O	1:B:606:THR:HG22	2.19	0.43
1:C:135:LEU:CD1	1:C:164:ARG:HH22	2.20	0.43
1:C:467:ALA:N	1:C:493:HIS:O	2.51	0.43
1:C:86:HIS:NE2	1:C:97:HIS:CE1	2.87	0.43
1:A:111:LEU:O	1:A:113:ALA:CA	2.65	0.43
1:A:211:ILE:O	1:A:212:ALA:C	2.57	0.43
1:A:437:LEU:C	1:A:439:ALA:N	2.71	0.43
1:A:491:TYR:CD2	1:A:599:ARG:NH1	2.86	0.43
1:B:267:LEU:HB3	1:B:414:MET:SD	2.59	0.43
1:B:283:PRO:C	1:B:285:ALA:N	2.71	0.43
1:B:483:ALA:O	1:B:487:LYS:CB	2.62	0.43
1:B:487:LYS:HE2	1:B:494:ALA:O	2.19	0.43
1:B:549:GLN:C	1:B:551:ALA:H	2.22	0.43
1:B:553:PHE:HD2	1:B:559:MET:CE	2.31	0.43
1:B:578:VAL:O	1:B:582:LEU:HG	2.19	0.43
1:C:187:ASN:OD1	1:C:219:VAL:HG21	2.18	0.43
1:C:203:PHE:O	1:C:233:ASP:HB2	2.17	0.43
1:C:258:GLU:O	1:C:262:ALA:HB2	2.19	0.43
1:C:306:SER:N	1:C:405:PHE:HE1	2.17	0.43
1:C:576:TYR:C	1:C:579:PRO:HD2	2.39	0.43
1:A:149:ILE:C	1:A:151:GLN:H	2.22	0.43
1:A:251:TYR:CD2	1:A:397:ILE:HG21	2.53	0.43
1:A:300:CYS:O	1:A:301:GLY:C	2.57	0.43
1:A:413:LEU:HA	1:A:413:LEU:HD12	1.84	0.43
1:B:237:ASN:HA	1:B:239:GLN:HE22	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:LEU:O	1:B:416:VAL:HG23	2.19	0.43
1:B:468:LEU:CD1	1:B:470:LEU:HD21	2.49	0.43
1:B:504:HIS:CE1	1:C:300:CYS:CB	3.01	0.43
1:C:259:GLN:HG2	1:C:403:LYS:HA	2.01	0.43
1:C:405:PHE:CZ	1:C:409:LEU:HD11	2.54	0.43
1:C:571:ILE:HB	1:C:574:ILE:HD12	2.00	0.43
1:C:588:ALA:HB1	1:C:593:THR:HG23	2.00	0.43
1:A:401:SER:H	2:A:700:G6Q:H2	1.84	0.43
1:B:180:ILE:CD1	1:B:206:LEU:HD21	2.49	0.43
1:B:249:ARG:O	1:B:249:ARG:CG	2.65	0.43
1:B:476:TYR:HB3	1:B:477:PRO:CD	2.44	0.43
1:B:578:VAL:HG23	1:B:578:VAL:H	1.53	0.43
1:C:289:LEU:O	1:C:422:LEU:CD2	2.65	0.43
1:C:353:ALA:HB2	1:C:606:THR:C	2.39	0.43
1:A:196:LEU:C	1:A:198:PRO:CD	2.83	0.43
1:B:219:VAL:C	1:B:220:ASN:OD1	2.58	0.43
1:B:258:GLU:O	1:B:262:ALA:HB2	2.19	0.43
1:B:267:LEU:O	1:B:270:ARG:HB2	2.19	0.43
1:B:283:PRO:O	1:B:285:ALA:N	2.52	0.43
1:B:555:SER:C	1:B:556:SER:HG	2.22	0.43
1:B:553:PHE:CD2	1:B:559:MET:CE	3.02	0.43
1:C:197:LEU:HD23	1:C:203:PHE:CZ	2.51	0.43
1:C:270:ARG:HD3	1:C:414:MET:HE1	2.01	0.43
1:C:447:MET:HE3	1:C:578:VAL:CG1	2.49	0.43
1:A:122:THR:HG23	1:A:125:GLU:CB	2.49	0.43
1:A:457:LEU:O	1:A:459:GLU:N	2.52	0.43
1:B:312:TYR:O	1:B:316:SER:HB3	2.19	0.43
1:B:356:LEU:CD1	1:B:360:ARG:CD	2.96	0.43
1:B:519:VAL:HG11	1:B:576:TYR:HB3	2.01	0.43
1:C:485:LYS:N	1:C:485:LYS:HE3	2.34	0.43
1:C:83:VAL:HG12	1:C:120:SER:OG	2.19	0.43
1:A:178:LEU:HA	1:A:190:ALA:O	2.19	0.42
1:A:377:PRO:O	1:A:378:GLY:C	2.58	0.42
1:A:529:LEU:C	1:A:531:SER:N	2.71	0.42
1:A:251:TYR:N	1:A:596:ASP:OD2	2.42	0.42
1:B:169:LEU:HA	1:B:169:LEU:HD23	1.70	0.42
1:B:170:LEU:HA	1:B:212:ALA:O	2.19	0.42
1:B:234:ILE:CD1	1:B:235:GLU:N	2.80	0.42
1:B:294:HIS:HE1	1:B:296:GLN:HB2	1.84	0.42
1:B:458:ALA:C	1:B:460:ASP:N	2.70	0.42
1:C:298:LEU:HG	1:C:343:MET:SD	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:LEU:HD13	1:C:380:SER:HB3	2.00	0.42
1:C:63:LEU:N	1:C:63:LEU:HD22	2.34	0.42
1:A:141:LEU:O	1:A:143:GLU:N	2.51	0.42
1:A:510:ILE:HD11	1:A:536:VAL:HG12	1.97	0.42
1:A:585:TYR:CE1	1:A:595:VAL:HG11	2.54	0.42
1:B:294:HIS:O	1:B:342:LEU:N	2.46	0.42
1:B:443:ARG:O	1:B:446:GLN:HB3	2.19	0.42
1:B:478:ILE:HG13	1:B:573:PRO:HA	2.00	0.42
1:C:89:VAL:O	1:C:129:HIS:NE2	2.53	0.42
1:C:131:VAL:O	1:C:133:TRP:N	2.53	0.42
1:C:178:LEU:HD22	1:C:206:LEU:HD12	2.01	0.42
1:C:281:LEU:HD12	1:C:285:ALA:HB1	2.00	0.42
1:C:320:ILE:HA	1:C:321:PRO:HD3	1.89	0.42
1:C:88:HIS:NE2	1:C:124:THR:HB	2.34	0.42
1:A:139:GLY:HA2	1:A:143:GLU:OE1	2.20	0.42
1:A:14:GLU:O	1:A:14:GLU:CG	2.63	0.42
1:A:388:ALA:C	1:A:389:LEU:CD1	2.86	0.42
1:A:412:LEU:O	1:A:413:LEU:C	2.56	0.42
1:A:42:MET:HE3	1:A:43:THR:H	1.84	0.42
1:A:463:ASP:OD1	1:A:463:ASP:N	2.51	0.42
1:A:538:ALA:C	1:A:539:ARG:HG2	2.39	0.42
1:A:598:PRO:HG3	1:A:601:LEU:HD12	2.00	0.42
1:B:293:GLU:HG3	1:B:340:ASN:HB2	2.02	0.42
1:B:513:ASP:O	1:B:514:MET:CB	2.61	0.42
1:B:583:LEU:HD12	1:B:587:VAL:HG23	1.99	0.42
1:B:5:GLY:O	1:B:6:ALA:HB2	2.20	0.42
1:B:90:SER:OG	1:B:90:SER:O	2.36	0.42
1:C:251:TYR:CD1	1:C:397:ILE:CB	3.02	0.42
1:C:302:THR:HG22	1:C:302:THR:O	2.18	0.42
1:C:348:GLN:HB3	1:C:348:GLN:HE21	1.49	0.42
1:C:429:ILE:O	1:C:430:GLU:C	2.57	0.42
1:C:453:ARG:NH1	1:C:563:GLU:O	2.52	0.42
1:C:546:PHE:CE2	1:C:579:PRO:HB2	2.53	0.42
1:C:585:TYR:CZ	1:C:589:LEU:HD11	2.54	0.42
1:C:73:ARG:HG2	1:C:74:TRP:H	1.83	0.42
1:A:360:ARG:O	1:A:363:LYS:HB2	2.19	0.42
1:A:305:ASN:HD22	1:A:481:GLU:HA	1.84	0.42
1:A:506:PRO:C	1:A:508:ALA:N	2.73	0.42
1:B:193:GLN:C	1:B:195:ALA:H	2.23	0.42
1:B:46:ARG:HG2	1:B:46:ARG:H	1.59	0.42
1:C:234:ILE:HD12	1:C:235:GLU:CA	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ALA:O	1:A:149:ILE:C	2.57	0.42
1:A:338:ARG:N	1:A:338:ARG:CD	2.81	0.42
1:B:218:SER:OG	1:B:219:VAL:N	2.51	0.42
1:B:343:MET:HB3	1:B:370:SER:CA	2.49	0.42
1:B:266:THR:CG2	1:B:411:VAL:HG23	2.50	0.42
1:C:127:ILE:HA	1:C:130:LEU:CB	2.50	0.42
1:C:234:ILE:HD12	1:C:234:ILE:C	2.40	0.42
1:C:348:GLN:O	1:C:348:GLN:NE2	2.52	0.42
1:C:381:LEU:O	1:C:383:ARG:N	2.53	0.42
1:C:426:ASP:OD1	1:C:428:SER:OG	2.33	0.42
1:C:90:SER:OG	1:C:129:HIS:CG	2.73	0.42
1:A:266:THR:HG22	1:A:270:ARG:HH12	1.84	0.42
1:A:529:LEU:CA	1:A:532:ASN:ND2	2.79	0.42
1:A:554:VAL:HG12	1:A:555:SER:O	2.20	0.42
1:B:238:LEU:HD23	1:B:242:ALA:HA	2.01	0.42
1:B:246:GLY:O	1:B:248:TYR:N	2.53	0.42
1:B:374:CYS:SG	1:B:375:ASN:N	2.92	0.42
1:B:464:LYS:C	1:B:465:HIS:ND1	2.73	0.42
1:B:523:ASN:C	1:B:525:LEU:H	2.22	0.42
1:C:89:VAL:O	1:C:129:HIS:CE1	2.72	0.42
1:C:224:LYS:CE	1:C:225:THR:HG23	2.48	0.42
1:C:583:LEU:CD1	1:C:587:VAL:HG23	2.50	0.42
1:A:105:GLU:C	1:A:107:LEU:N	2.73	0.42
1:A:237:ASN:O	1:A:239:GLN:OE1	2.38	0.42
1:A:248:TYR:CD2	1:A:254:LYS:CG	3.03	0.42
1:A:356:LEU:HD13	1:A:380:SER:HB3	2.01	0.42
1:A:3:ILE:HD12	1:A:3:ILE:HG21	1.53	0.42
1:A:421:LYS:C	1:A:423:LYS:N	2.73	0.42
1:B:107:LEU:HD23	1:B:107:LEU:HA	1.84	0.42
1:B:453:ARG:NH1	1:B:453:ARG:CG	2.81	0.42
1:B:83:VAL:O	1:B:88:HIS:HE1	2.02	0.42
1:C:135:LEU:C	1:C:137:GLN:H	2.23	0.42
1:C:409:LEU:O	1:C:412:LEU:N	2.53	0.42
1:C:476:TYR:O	1:C:479:ALA:CB	2.66	0.42
1:C:486:LEU:HD11	1:C:587:VAL:HG11	2.02	0.42
1:A:266:THR:HA	1:A:392:ASN:ND2	2.34	0.42
1:A:505:GLY:C	1:A:507:LEU:N	2.72	0.42
1:A:565:PRO:O	1:A:566:HIS:C	2.58	0.42
1:B:286:ASP:HB3	1:B:422:LEU:CD1	2.50	0.42
1:B:376:VAL:O	1:B:379:SER:OG	2.19	0.42
1:B:507:LEU:HD12	1:B:510:ILE:CG1	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:ILE:CG2	1:C:559:MET:CE	2.98	0.42
1:C:61:HIS:H	1:C:62:PRO:CD	2.27	0.42
1:C:79:GLU:N	1:C:80:PRO:CD	2.83	0.42
1:A:86:HIS:CE1	1:A:124:THR:OG1	2.73	0.42
1:B:205:PHE:CD1	1:B:205:PHE:N	2.88	0.42
1:B:425:LEU:HG	1:B:426:ASP:N	2.35	0.42
1:B:555:SER:C	1:B:556:SER:OG	2.58	0.42
1:B:61:HIS:O	1:B:61:HIS:CG	2.70	0.42
1:B:33:LEU:HB3	1:B:70:ALA:HB2	2.01	0.42
1:C:18:GLU:OE2	1:C:21:ARG:CZ	2.68	0.42
1:C:532:ASN:HD22	1:C:532:ASN:N	2.06	0.42
1:C:523:ASN:OD1	1:C:569:GLU:OE2	2.36	0.42
1:A:36:VAL:CG1	1:A:42:MET:CA	2.84	0.42
1:A:599:ARG:C	1:A:601:LEU:H	2.23	0.42
1:A:80:PRO:HB2	1:A:83:VAL:HB	2.02	0.42
1:B:308:MET:CB	1:B:477:PRO:HB3	2.50	0.42
1:B:356:LEU:HD12	1:B:360:ARG:HD2	2.01	0.42
1:B:450:GLN:O	1:B:454:ILE:HG13	2.20	0.42
1:B:433:ILE:CG1	1:B:570:VAL:CG2	2.97	0.42
1:C:330:PHE:C	1:C:332:TYR:N	2.73	0.42
1:C:379:SER:O	1:C:380:SER:C	2.58	0.42
1:C:408:GLN:O	1:C:409:LEU:C	2.58	0.42
1:A:133:TRP:CE3	1:A:134:GLU:OE2	2.73	0.41
1:A:306:SER:O	1:A:307:GLY:C	2.57	0.41
1:A:375:ASN:CG	1:A:393:ALA:HB3	2.39	0.41
1:A:32:GLY:CA	1:A:54:LEU:HD21	2.48	0.41
1:B:20:LEU:HD11	1:B:70:ALA:HB1	2.02	0.41
1:B:297:ILE:CD1	1:B:324:VAL:HG22	2.44	0.41
1:C:386:ASP:C	1:C:387:LEU:HG	2.40	0.41
1:C:530:LYS:HA	1:C:533:ILE:HD12	2.02	0.41
1:C:250:HIS:NE2	1:C:589:LEU:HD21	2.35	0.41
1:C:93:ILE:HG21	1:C:131:VAL:CB	2.49	0.41
1:A:32:GLY:HA3	1:A:45:LEU:O	2.20	0.41
1:A:529:LEU:C	1:A:532:ASN:ND2	2.74	0.41
1:A:74:TRP:CZ2	1:A:601:LEU:HA	2.55	0.41
1:B:22:ARG:HG2	1:B:194:LEU:CD2	2.50	0.41
1:B:255:GLU:O	1:B:403:LYS:HB3	2.21	0.41
1:B:326:ILE:HG23	1:C:501:GLU:OE2	2.20	0.41
1:B:408:GLN:O	1:B:412:LEU:HB2	2.20	0.41
1:B:468:LEU:HD21	1:B:470:LEU:HD21	2.02	0.41
1:B:483:ALA:HB1	1:B:494:ALA:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:LEU:HB2	1:C:118:PHE:HE1	1.85	0.41
1:C:184:MET:CE	1:C:185:GLY:N	2.82	0.41
1:C:224:LYS:HZ2	1:C:225:THR:CG2	2.31	0.41
1:C:300:CYS:O	1:C:303:SER:HB2	2.19	0.41
1:C:502:LEU:CD1	1:C:502:LEU:N	2.82	0.41
1:B:23:LEU:HD23	1:B:23:LEU:HA	1.84	0.41
1:B:306:SER:OG	1:B:307:GLY:N	2.53	0.41
1:B:276:VAL:CG2	1:B:417:ALA:CB	2.93	0.41
1:B:34:ALA:HA	1:B:43:THR:O	2.20	0.41
1:C:111:LEU:CD1	1:C:116:TYR:CD2	2.91	0.41
1:C:95:VAL:HG13	1:C:96:VAL:H	1.85	0.41
1:A:100:ILE:CD1	1:A:607:VAL:CA	2.95	0.41
1:A:224:LYS:HE2	1:A:224:LYS:HB3	1.80	0.41
1:A:276:VAL:CG1	1:A:276:VAL:O	2.68	0.41
1:A:324:VAL:CG1	1:A:324:VAL:O	2.64	0.41
1:A:45:LEU:CD2	1:A:57:ALA:O	2.68	0.41
1:A:67:THR:HG22	1:A:161:MET:SD	2.60	0.41
1:B:237:ASN:CA	1:B:239:GLN:HE22	2.33	0.41
1:B:503:LYS:HE2	1:C:601:LEU:HD23	2.03	0.41
1:C:489:ILE:HD11	1:C:584:ALA:C	2.40	0.41
1:C:525:LEU:O	1:C:528:LYS:N	2.53	0.41
1:C:565:PRO:HD2	1:C:575:PHE:HE2	1.84	0.41
1:A:131:VAL:CG2	1:A:145:VAL:HG22	2.50	0.41
1:A:231:ARG:C	1:A:232:GLN:O	2.58	0.41
1:A:312:TYR:CE2	1:A:473:GLY:O	2.72	0.41
1:A:48:LEU:CD1	1:A:48:LEU:N	2.78	0.41
1:A:527:GLU:O	1:A:528:LYS:C	2.58	0.41
1:A:548:ASP:OD1	1:A:549:GLN:N	2.53	0.41
1:A:567:VAL:CG1	1:A:568:GLU:N	2.66	0.41
1:A:574:ILE:HG21	1:A:574:ILE:HD13	1.74	0.41
1:A:353:ALA:HB2	1:A:607:VAL:O	2.20	0.41
1:B:118:PHE:CD1	1:B:118:PHE:N	2.88	0.41
1:B:119:VAL:HG23	1:B:119:VAL:O	2.18	0.41
1:B:180:ILE:HG13	1:B:206:LEU:HD21	2.02	0.41
1:B:309:VAL:CG2	1:B:477:PRO:HB2	2.50	0.41
1:B:576:TYR:C	1:B:579:PRO:HD2	2.41	0.41
1:C:105:GLU:O	1:C:108:ARG:HB3	2.20	0.41
1:C:359:LEU:CD2	1:C:381:LEU:HD22	2.50	0.41
1:C:27:GLY:H	1:C:602:ALA:HB1	1.86	0.41
1:C:71:HIS:HD2	1:C:96:VAL:CB	2.34	0.41
1:A:128:ALA:O	1:A:129:HIS:C	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:TYR:CD1	1:A:397:ILE:HG21	2.55	0.41
1:A:497:TYR:CZ	1:A:506:PRO:HB3	2.56	0.41
1:B:105:GLU:HB3	1:B:106:PRO:CD	2.48	0.41
1:B:527:GLU:O	1:B:528:LYS:C	2.59	0.41
1:B:553:PHE:HD2	1:B:561:ILE:CD1	2.33	0.41
1:C:145:VAL:O	1:C:147:ARG:N	2.53	0.41
1:C:173:ARG:HE	1:C:177:PRO:HA	1.85	0.41
1:A:178:LEU:HD23	1:A:178:LEU:HA	1.44	0.41
1:A:247:ILE:HD13	1:A:248:TYR:CD2	2.56	0.41
1:A:276:VAL:HG13	1:A:276:VAL:O	2.19	0.41
1:A:282:GLY:HA2	1:A:283:PRO:HD2	1.85	0.41
1:A:307:GLY:C	1:A:324:VAL:HG11	2.41	0.41
1:A:409:LEU:HA	1:A:409:LEU:HD23	1.78	0.41
1:A:457:LEU:O	1:A:458:ALA:C	2.57	0.41
1:A:480:LEU:HD23	1:A:480:LEU:HA	1.58	0.41
1:A:467:ALA:O	1:A:494:ALA:HA	2.20	0.41
1:A:525:LEU:O	1:A:526:LEU:C	2.59	0.41
1:A:535:GLU:O	1:A:536:VAL:C	2.56	0.41
1:A:28:TYR:CE1	1:A:602:ALA:HA	2.53	0.41
1:B:313:TRP:HZ2	1:B:573:PRO:CG	2.34	0.41
1:B:549:GLN:C	1:B:551:ALA:N	2.74	0.41
1:C:169:LEU:HD13	1:C:169:LEU:HA	1.87	0.41
1:C:192:ASP:OD2	1:C:194:LEU:HB2	2.21	0.41
1:B:600:ASN:HA	1:C:539:ARG:NE	2.35	0.41
1:C:399:VAL:HG11	1:C:602:ALA:O	2.18	0.41
1:C:61:HIS:O	1:C:63:LEU:HD22	2.20	0.41
1:A:104:HIS:O	1:A:104:HIS:CG	2.74	0.41
1:A:107:LEU:C	1:A:109:GLU:N	2.74	0.41
1:A:16:LEU:HB3	1:A:70:ALA:HB2	2.02	0.41
1:A:356:LEU:HA	1:A:381:LEU:CD2	2.48	0.41
1:A:45:LEU:HD12	1:A:45:LEU:HA	1.89	0.41
1:B:103:ASN:C	1:B:105:GLU:H	2.22	0.41
1:B:146:LEU:HD12	1:B:146:LEU:HA	1.83	0.41
1:B:234:ILE:CG1	1:B:235:GLU:H	2.29	0.41
1:B:325:GLU:OE2	1:B:333:ARG:NH2	2.51	0.41
1:B:520:ALA:HA	1:B:521:PRO:HD3	1.79	0.41
1:C:165:HIS:N	1:C:166:PRO:CD	2.83	0.41
1:C:466:HIS:HA	1:C:493:HIS:O	2.21	0.41
1:C:472:ARG:O	1:C:475:GLN:HB2	2.20	0.41
1:C:576:TYR:C	1:C:578:VAL:N	2.69	0.41
1:A:499:ALA:HB1	1:A:532:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ILE:H	1:B:234:ILE:HG23	1.63	0.41
1:B:281:LEU:CD2	1:B:387:LEU:HB3	2.51	0.41
1:B:452:LYS:HD3	1:B:452:LYS:HA	1.81	0.41
1:B:491:TYR:CD2	1:B:599:ARG:CZ	3.04	0.41
1:B:537:ARG:CZ	1:B:558:ASN:HD21	2.28	0.41
1:B:599:ARG:O	1:B:600:ASN:HB2	2.21	0.41
1:C:421:LYS:HB3	1:C:421:LYS:HE3	1.64	0.41
1:C:514:MET:HB2	1:C:514:MET:HE3	1.85	0.41
1:C:447:MET:CE	1:C:578:VAL:HB	2.51	0.41
1:A:74:TRP:CZ3	1:A:602:ALA:O	2.74	0.41
1:B:271:ILE:O	1:B:271:ILE:HG22	2.20	0.41
1:B:371:LEU:O	1:B:372:ALA:HB2	2.21	0.41
1:B:390:MET:CE	1:B:390:MET:HA	2.51	0.41
1:B:454:ILE:CD1	1:B:582:LEU:HD12	2.48	0.41
1:B:7:ILE:HD13	1:B:215:THR:HA	2.02	0.41
1:C:127:ILE:HA	1:C:130:LEU:HB3	2.03	0.41
1:C:166:PRO:O	1:C:167:ASP:C	2.59	0.41
1:C:263:ILE:O	1:C:266:THR:CB	2.63	0.41
1:C:437:LEU:O	1:C:440:LEU:CB	2.69	0.41
1:A:454:ILE:HD12	1:A:582:LEU:HD12	2.03	0.41
1:A:457:LEU:CD2	1:A:562:ILE:HD13	2.52	0.41
1:A:440:LEU:HD21	1:A:574:ILE:HD12	2.03	0.41
1:B:130:LEU:HD11	1:B:151:GLN:HE22	1.85	0.41
1:B:267:LEU:CB	1:B:414:MET:SD	3.09	0.41
1:B:7:ILE:H	1:B:7:ILE:HG22	1.50	0.41
1:C:7:ILE:HD13	1:C:168:THR:O	2.20	0.41
1:C:528:LYS:O	1:C:531:SER:N	2.52	0.41
1:C:45:LEU:CD2	1:C:57:ALA:O	2.69	0.41
1:A:102:GLU:C	1:A:104:HIS:N	2.72	0.40
1:A:359:LEU:HD11	1:A:370:SER:HB3	2.03	0.40
1:A:440:LEU:CD2	1:A:574:ILE:CD1	2.99	0.40
1:A:457:LEU:HD21	1:A:562:ILE:CD1	2.51	0.40
1:B:359:LEU:O	1:B:363:LYS:HG2	2.22	0.40
1:B:480:LEU:O	1:B:483:ALA:N	2.54	0.40
1:B:554:VAL:HG23	1:B:554:VAL:O	2.20	0.40
1:B:8:ALA:O	1:B:9:GLN:HB2	2.20	0.40
1:C:173:ARG:HD3	1:C:207:GLU:O	2.21	0.40
1:B:504:HIS:NE2	1:C:300:CYS:SG	2.95	0.40
1:B:600:ASN:O	1:C:507:LEU:HD23	2.21	0.40
1:B:487:LYS:CD	1:C:509:LEU:HD11	2.50	0.40
1:A:26:ARG:HH11	1:A:26:ARG:HG3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLU:O	1:B:110:GLU:C	2.59	0.40
1:B:159:VAL:HG22	1:B:171:ALA:CB	2.49	0.40
1:B:601:LEU:O	1:B:602:ALA:HB2	2.22	0.40
1:C:230:LYS:C	1:C:231:ARG:HD3	2.37	0.40
1:C:33:LEU:CD2	1:C:54:LEU:HD21	2.52	0.40
1:C:28:TYR:CD2	1:C:50:LYS:HD3	2.56	0.40
1:C:55:ALA:O	1:C:58:ALA:HB3	2.20	0.40
1:B:116:TYR:HE2	1:B:133:TRP:HB2	1.86	0.40
1:B:390:MET:HE2	1:B:390:MET:HA	2.02	0.40
1:C:102:GLU:O	1:C:104:HIS:N	2.48	0.40
1:C:96:VAL:CG2	1:C:159:VAL:HB	2.52	0.40
1:C:184:MET:HE2	1:C:184:MET:CA	2.50	0.40
1:C:222:PHE:HA	1:C:228:GLU:HA	2.03	0.40
1:B:504:HIS:CE1	1:C:300:CYS:HB3	2.56	0.40
1:C:314:PHE:CE1	1:C:416:VAL:CG2	3.03	0.40
1:C:480:LEU:O	1:C:483:ALA:N	2.53	0.40
1:A:149:ILE:HB	1:A:150:PRO:CD	2.44	0.40
1:A:267:LEU:HD22	1:A:414:MET:HE2	2.02	0.40
1:A:305:ASN:O	1:A:308:MET:N	2.54	0.40
1:A:34:ALA:HB1	1:A:42:MET:CE	2.51	0.40
1:A:402:THR:OG1	1:A:403:LYS:N	2.54	0.40
1:B:105:GLU:N	1:B:106:PRO:HD2	2.34	0.40
1:B:4:VAL:O	1:B:16:LEU:HD21	2.21	0.40
1:B:24:GLU:CD	1:B:597:GLN:NE2	2.70	0.40
1:B:320:ILE:HA	1:B:321:PRO:HD2	1.93	0.40
1:B:458:ALA:C	1:B:460:ASP:H	2.25	0.40
1:B:507:LEU:O	1:B:509:LEU:N	2.54	0.40
1:C:331:ARG:HD2	1:C:354:ASP:HA	2.02	0.40
1:C:480:LEU:O	1:C:483:ALA:HB3	2.22	0.40
1:C:547:ALA:O	1:C:549:GLN:N	2.53	0.40
1:C:553:PHE:CB	1:C:561:ILE:HD12	2.50	0.40
1:C:86:HIS:CD2	1:C:88:HIS:NE2	2.89	0.40
1:A:133:TRP:HZ3	1:A:134:GLU:OE2	2.02	0.40
1:A:197:LEU:HA	1:A:197:LEU:HD22	1.51	0.40
1:A:22:ARG:O	1:A:194:LEU:HD23	2.22	0.40
1:A:417:ALA:HA	1:A:420:SER:HB3	2.04	0.40
1:A:601:LEU:O	1:A:602:ALA:HB2	2.22	0.40
1:B:572:ALA:CB	1:B:573:PRO:CD	2.91	0.40
1:B:48:LEU:CD1	1:B:82:GLU:HB2	2.51	0.40
1:C:6:ALA:CB	1:C:12:VAL:HG11	2.47	0.40
1:C:159:VAL:HA	1:C:171:ALA:CA	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:MET:O	1:C:253:GLN:C	2.59	0.40
1:C:407:THR:HG23	1:C:407:THR:H	1.63	0.40
1:C:580:LEU:O	1:C:583:LEU:N	2.54	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:487:LYS:NZ	1:A:497:TYR:OH[2_555]	2.05	0.15

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	606/608 (100%)	417 (69%)	128 (21%)	61 (10%)	1	4
1	B	606/608 (100%)	423 (70%)	113 (19%)	70 (12%)	0	2
1	C	606/608 (100%)	374 (62%)	164 (27%)	68 (11%)	0	2
All	All	1818/1824 (100%)	1214 (67%)	405 (22%)	199 (11%)	0	3

All (199) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	71	HIS
1	A	77	HIS
1	A	103	ASN
1	A	111	LEU
1	A	112	LYS
1	A	125	GLU
1	A	128	ALA
1	A	129	HIS

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Mol	Chain	Res	Type
1	A	199	VAL
1	A	212	ALA
1	A	238	LEU
1	A	240	TYR
1	A	273	HIS
1	A	280	GLU
1	A	283	PRO
1	A	424	GLY
1	A	485	LYS
1	A	541	GLY
1	A	600	ASN
1	A	603	LYS
1	A	604	SER
1	A	607	VAL
1	B	4	VAL
1	B	9	GLN
1	B	13	ALA
1	B	81	SER
1	B	91	GLU
1	B	119	VAL
1	B	123	ASP
1	B	163	SER
1	B	186	GLU
1	B	221	ILE
1	B	234	ILE
1	B	236	SER
1	B	285	ALA
1	B	312	TYR
1	B	330	PHE
1	B	338	ARG
1	B	414	MET
1	B	417	ALA
1	B	459	GLU
1	B	485	LYS
1	B	493	HIS
1	B	499	ALA
1	B	603	LYS
1	C	7	ILE
1	C	28	TYR
1	C	61	HIS
1	C	64	HIS
1	C	81	SER

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Mol	Chain	Res	Type
1	C	227	ALA
1	C	328	SER
1	C	331	ARG
1	C	349	SER
1	C	488	GLU
1	C	499	ALA
1	C	541	GLY
1	C	550	ASP
1	C	595	VAL
1	A	104	HIS
1	A	108	ARG
1	A	142	ARG
1	A	146	LEU
1	A	193	GLN
1	A	232	GLN
1	A	274	GLY
1	A	282	GLY
1	A	309	VAL
1	A	385	SER
1	A	438	GLN
1	A	449	SER
1	B	38	ALA
1	B	45	LEU
1	B	113	ALA
1	B	241	ASP
1	B	284	ASN
1	B	310	SER
1	B	336	ALA
1	B	353	ALA
1	B	366	GLY
1	B	368	LEU
1	B	386	ASP
1	B	418	LYS
1	B	512	ALA
1	B	516	VAL
1	B	595	VAL
1	C	13	ALA
1	C	51	VAL
1	C	78	GLY
1	C	82	GLU
1	C	108	ARG
1	C	130	LEU

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Mol	Chain	Res	Type
1	C	138	GLY
1	C	141	LEU
1	C	146	LEU
1	C	169	LEU
1	C	187	ASN
1	C	233	ASP
1	C	283	PRO
1	C	367	TYR
1	C	368	LEU
1	C	370	SER
1	C	390	MET
1	C	448	LEU
1	C	461	PHE
1	C	507	LEU
1	C	523	ASN
1	C	549	GLN
1	C	566	HIS
1	C	600	ASN
1	A	14	GLU
1	A	105	GLU
1	A	121	GLU
1	A	196	LEU
1	A	284	ASN
1	A	286	ASP
1	A	425	LEU
1	A	439	ALA
1	A	568	GLU
1	A	594	ASP
1	A	602	ALA
1	B	95	VAL
1	B	114	ARG
1	B	175	GLY
1	B	247	ILE
1	B	372	ALA
1	B	380	SER
1	B	508	ALA
1	B	557	ASP
1	C	37	ASP
1	C	66	GLY
1	C	103	ASN
1	C	299	ALA
1	C	319	GLY

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Mol	Chain	Res	Type
1	C	378	GLY
1	C	429	ILE
1	C	548	ASP
1	C	598	PRO
1	A	80	PRO
1	A	308	MET
1	A	548	ASP
1	B	6	ALA
1	B	43	THR
1	B	167	ASP
1	B	194	LEU
1	B	246	GLY
1	B	273	HIS
1	B	356	LEU
1	B	405	PHE
1	B	500	GLY
1	C	75	ALA
1	C	91	GLU
1	C	132	ASN
1	C	174	SER
1	C	195	ALA
1	C	280	GLU
1	C	383	ARG
1	C	459	GLU
1	C	551	ALA
1	A	102	GLU
1	A	122	THR
1	A	150	PRO
1	A	166	PRO
1	A	245	LYS
1	A	301	GLY
1	A	386	ASP
1	A	511	ASP
1	B	34	ALA
1	B	306	SER
1	B	331	ARG
1	B	355	THR
1	B	392	ASN
1	B	514	MET
1	B	521	PRO
1	B	523	ASN
1	C	106	PRO

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Mol	Chain	Res	Type
1	C	216	ARG
1	C	260	PRO
1	C	442	SER
1	A	410	THR
1	B	105	GLU
1	B	410	THR
1	C	80	PRO
1	C	197	LEU
1	C	433	ILE
1	A	139	GLY
1	B	12	VAL
1	C	219	VAL
1	B	32	GLY
1	B	36	VAL
1	C	573	PRO
1	B	40	GLY
1	B	260	PRO
1	C	183	GLY
1	C	229	VAL
1	C	398	GLY
1	A	115	GLY
1	A	378	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	500/500 (100%)	393 (79%)	107 (21%)	1	5
1	B	500/500 (100%)	422 (84%)	78 (16%)	3	13
1	C	500/500 (100%)	433 (87%)	67 (13%)	4	19
All	All	1500/1500 (100%)	1248 (83%)	252 (17%)	2	11

All (252) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	CYS
1	A	3	ILE
1	A	25	TYR
1	A	26	ARG
1	A	30	SER
1	A	33	LEU
1	A	35	VAL
1	A	36	VAL
1	A	42	MET
1	A	44	ARG
1	A	46	ARG
1	A	48	LEU
1	A	51	VAL
1	A	52	GLN
1	A	97	HIS
1	A	102	GLU
1	A	103	ASN
1	A	114	ARG
1	A	125	GLU
1	A	131	VAL
1	A	132	ASN
1	A	140	THR
1	A	146	LEU
1	A	161	MET
1	A	163	SER
1	A	170	LEU
1	A	180	ILE
1	A	189	ILE
1	A	194	LEU
1	A	197	LEU
1	A	202	ARG
1	A	211	ILE
1	A	221	ILE
1	A	223	ASP
1	A	224	LYS
1	A	233	ASP
1	A	235	GLU
1	A	239	GLN
1	A	240	TYR
1	A	247	ILE
1	A	259	GLN
1	A	266	THR
1	A	268	THR

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Mol	Chain	Res	Type
1	A	273	HIS
1	A	279	SER
1	A	288	LEU
1	A	290	SER
1	A	296	GLN
1	A	303	SER
1	A	326	ILE
1	A	333	ARG
1	A	337	VAL
1	A	341	SER
1	A	346	LEU
1	A	347	SER
1	A	348	GLN
1	A	349	SER
1	A	351	GLU
1	A	359	LEU
1	A	361	LEU
1	A	362	SER
1	A	368	LEU
1	A	370	SER
1	A	371	LEU
1	A	376	VAL
1	A	379	SER
1	A	380	SER
1	A	383	ARG
1	A	390	MET
1	A	391	THR
1	A	395	THR
1	A	397	ILE
1	A	401	SER
1	A	403	LYS
1	A	420	SER
1	A	422	LEU
1	A	428	SER
1	A	433	ILE
1	A	441	PRO
1	A	442	SER
1	A	443	ARG
1	A	457	LEU
1	A	464	LYS
1	A	465	HIS
1	A	468	LEU

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Mol	Chain	Res	Type
1	A	476	TYR
1	A	481	GLU
1	A	492	ILE
1	A	502	LEU
1	A	503	LYS
1	A	511	ASP
1	A	518	VAL
1	A	519	VAL
1	A	523	ASN
1	A	525	LEU
1	A	528	LYS
1	A	530	LYS
1	A	532	ASN
1	A	534	GLU
1	A	555	SER
1	A	556	SER
1	A	558	ASN
1	A	559	MET
1	A	561	ILE
1	A	570	VAL
1	A	599	ARG
1	A	600	ASN
1	B	14	GLU
1	B	21	ARG
1	B	33	LEU
1	B	35	VAL
1	B	37	ASP
1	B	46	ARG
1	B	53	MET
1	B	59	GLU
1	B	63	LEU
1	B	72	THR
1	B	86	HIS
1	B	93	ILE
1	B	120	SER
1	B	124	THR
1	B	135	LEU
1	B	143	GLU
1	B	152	LEU
1	B	158	THR
1	B	161	MET
1	B	163	SER

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Mol	Chain	Res	Type
1	B	170	LEU
1	B	174	SER
1	B	178	LEU
1	B	184	MET
1	B	186	GLU
1	B	187	ASN
1	B	206	LEU
1	B	208	GLU
1	B	210	ASP
1	B	215	THR
1	B	218	SER
1	B	221	ILE
1	B	223	ASP
1	B	225	THR
1	B	232	GLN
1	B	233	ASP
1	B	234	ILE
1	B	239	GLN
1	B	245	LYS
1	B	248	TYR
1	B	252	MET
1	B	257	TYR
1	B	259	GLN
1	B	267	LEU
1	B	273	HIS
1	B	302	THR
1	B	303	SER
1	B	306	SER
1	B	316	SER
1	B	334	LYS
1	B	348	GLN
1	B	362	SER
1	B	385	SER
1	B	395	THR
1	B	423	LYS
1	B	428	SER
1	B	429	ILE
1	B	440	LEU
1	B	442	SER
1	B	447	MET
1	B	453	ARG
1	B	454	ILE

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Mol	Chain	Res	Type
1	B	503	LYS
1	B	509	LEU
1	B	513	ASP
1	B	514	MET
1	B	523	ASN
1	B	524	GLU
1	B	526	LEU
1	B	528	LYS
1	B	536	VAL
1	B	548	ASP
1	B	556	SER
1	B	568	GLU
1	B	571	ILE
1	B	591	LYS
1	B	594	ASP
1	B	607	VAL
1	C	10	ARG
1	C	15	ILE
1	C	21	ARG
1	C	33	LEU
1	C	35	VAL
1	C	47	ARG
1	C	63	LEU
1	C	69	ILE
1	C	74	TRP
1	C	79	GLU
1	C	90	SER
1	C	118	PHE
1	C	120	SER
1	C	158	THR
1	C	163	SER
1	C	169	LEU
1	C	176	SER
1	C	178	LEU
1	C	184	MET
1	C	186	GLU
1	C	187	ASN
1	C	191	SER
1	C	194	LEU
1	C	196	LEU
1	C	200	THR
1	C	217	ARG

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Mol	Chain	Res	Type
1	C	222	PHE
1	C	224	LYS
1	C	230	LYS
1	C	234	ILE
1	C	238	LEU
1	C	247	ILE
1	C	272	SER
1	C	306	SER
1	C	322	CYS
1	C	328	SER
1	C	333	ARG
1	C	334	LYS
1	C	338	ARG
1	C	348	GLN
1	C	349	SER
1	C	368	LEU
1	C	390	MET
1	C	402	THR
1	C	421	LYS
1	C	452	LYS
1	C	457	LEU
1	C	461	PHE
1	C	462	SER
1	C	485	LYS
1	C	490	SER
1	C	497	TYR
1	C	518	VAL
1	C	523	ASN
1	C	524	GLU
1	C	527	GLU
1	C	528	LYS
1	C	531	SER
1	C	532	ASN
1	C	534	GLU
1	C	539	ARG
1	C	545	VAL
1	C	557	ASP
1	C	590	ILE
1	C	591	LYS
1	C	593	THR
1	C	604	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such



sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	56	GLN
1	A	84	ASN
1	A	88	HIS
1	A	103	ASN
1	A	137	GLN
1	A	151	GLN
1	A	265	ASN
1	A	296	GLN
1	A	305	ASN
1	A	392	ASN
1	A	435	HIS
1	A	438	GLN
1	A	523	ASN
1	A	532	ASN
1	A	549	GLN
1	B	61	HIS
1	B	64	HIS
1	B	86	HIS
1	B	137	GLN
1	B	151	GLN
1	B	165	HIS
1	B	187	ASN
1	B	239	GLN
1	B	250	HIS
1	B	296	GLN
1	B	375	ASN
1	B	438	GLN
1	B	466	HIS
1	B	475	GLN
1	B	493	HIS
1	B	523	ASN
1	B	532	ASN
1	B	558	ASN
1	B	600	ASN
1	C	98	ASN
1	C	137	GLN
1	C	193	GLN
1	C	239	GLN
1	C	250	HIS
1	C	265	ASN
1	C	340	ASN

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Mol	Chain	Res	Type
1	C	348	GLN
1	C	375	ASN
1	C	438	GLN
1	C	465	HIS
1	C	523	ASN
1	C	560	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	G6Q	A	700	-	15,15,15	2.12	5 (33%)	20,21,21	2.70	12 (60%)
2	G6Q	B	701	1	15,15,15	1.39	3 (20%)	20,21,21	1.95	5 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G6Q	A	700	-	-	0/18/20/20	0/0/0/0
2	G6Q	B	701	1	-	0/18/20/20	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	G6Q	O5-C5	-3.26	1.36	1.43
2	B	701	G6Q	C3-C2	-2.82	1.48	1.53
2	A	700	G6Q	P-O2P	-2.61	1.44	1.54
2	B	701	G6Q	O4-C4	-2.53	1.37	1.43
2	A	700	G6Q	C3-C2	-2.52	1.49	1.53
2	A	700	G6Q	C6-C5	-2.28	1.48	1.51
2	B	701	G6Q	C2-C1	2.15	1.54	1.50
2	A	700	G6Q	C2-C1	4.51	1.58	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	G6Q	O1-C1-C2	-4.71	112.30	125.13
2	A	700	G6Q	O1-C1-C2	-4.59	112.63	125.13
2	A	700	G6Q	O2-C2-C1	-4.32	100.05	110.30
2	B	701	G6Q	O2-C2-C1	-4.03	100.73	110.30
2	A	700	G6Q	O3P-P-O1P	-3.37	97.30	110.50
2	A	700	G6Q	O3-C3-C4	-3.09	102.08	109.46
2	B	701	G6Q	O3-C3-C4	-2.48	103.53	109.46
2	A	700	G6Q	C3-C2-C1	-2.06	104.62	111.10
2	A	700	G6Q	O6-P-O1P	2.14	112.47	106.47
2	B	701	G6Q	O6-P-O1P	2.18	112.60	106.47
2	A	700	G6Q	O4-C4-C3	2.22	114.77	109.46
2	A	700	G6Q	O3P-P-O6	2.39	113.08	106.73
2	A	700	G6Q	C4-C3-C2	2.98	118.82	113.54
2	B	701	G6Q	O4-C4-C3	3.18	117.06	109.46
2	A	700	G6Q	O3P-P-O2P	3.30	120.94	107.61
2	A	700	G6Q	O5-C5-C4	3.98	118.95	109.09
2	A	700	G6Q	O6-C6-C5	4.67	121.82	109.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	G6Q	4	0
2	B	701	G6Q	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	608/608 (100%)	-0.73	5 (0%) 86 71	9, 38, 101, 133	0
1	B	608/608 (100%)	-0.52	6 (0%) 82 67	19, 78, 125, 138	0
1	C	608/608 (100%)	0.05	30 (4%) 30 14	44, 113, 137, 151	0
All	All	1824/1824 (100%)	-0.40	41 (2%) 62 41	9, 79, 131, 151	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	ASN	8.6
1	C	89	VAL	5.6
1	C	81	SER	5.5
1	B	240	TYR	4.7
1	B	522	ASN	4.6
1	A	85	ALA	4.6
1	C	84	ASN	4.6
1	C	83	VAL	3.3
1	C	237	ASN	3.2
1	C	82	GLU	3.2
1	C	105	GLU	3.1
1	C	41	HIS	3.0
1	C	117	THR	2.9
1	A	81	SER	2.8
1	C	138	GLY	2.8
1	C	88	HIS	2.8
1	C	80	PRO	2.8
1	C	229	VAL	2.8
1	C	78	GLY	2.6
1	C	62	PRO	2.5
1	C	225	THR	2.5
1	C	248	TYR	2.5
1	A	88	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	351	GLU	2.5
1	C	74	TRP	2.4
1	C	240	TYR	2.4
1	C	38	ALA	2.4
1	B	80	PRO	2.3
1	B	340	ASN	2.3
1	C	230	LYS	2.3
1	C	522	ASN	2.3
1	C	85	ALA	2.3
1	A	83	VAL	2.3
1	C	61	HIS	2.3
1	C	435	HIS	2.3
1	C	347	SER	2.2
1	B	272	SER	2.2
1	C	100	ILE	2.2
1	C	235	GLU	2.1
1	B	271	ILE	2.0
1	C	287	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	G6Q	B	701	16/16	0.94	0.17	0.78	62,73,81,84	0
2	G6Q	A	700	16/16	0.96	0.13	0.38	25,31,35,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.