



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 06:04 PM EST

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

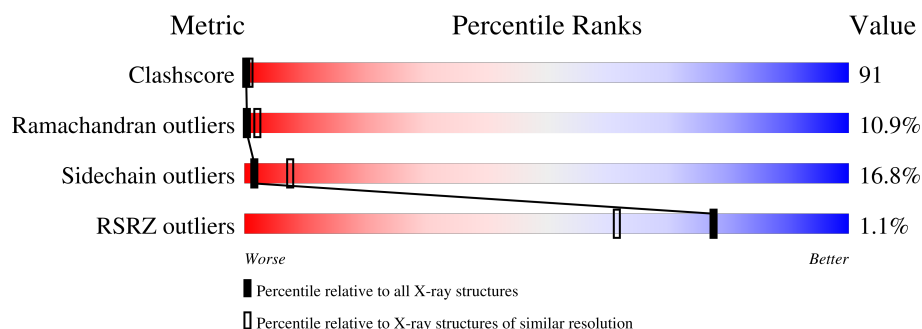
1 Overall quality at a glance

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	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

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

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	G6Q	A	700	-	X	-	-

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.

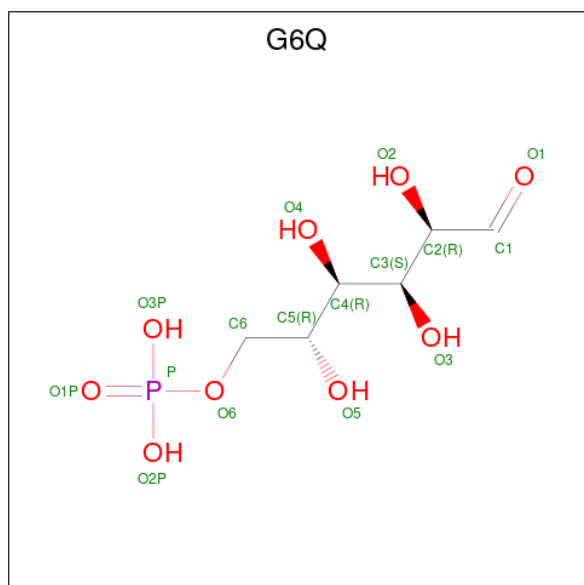
- Molecule 1 is a protein called glucosamine 6-phosphate synthase.

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 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		

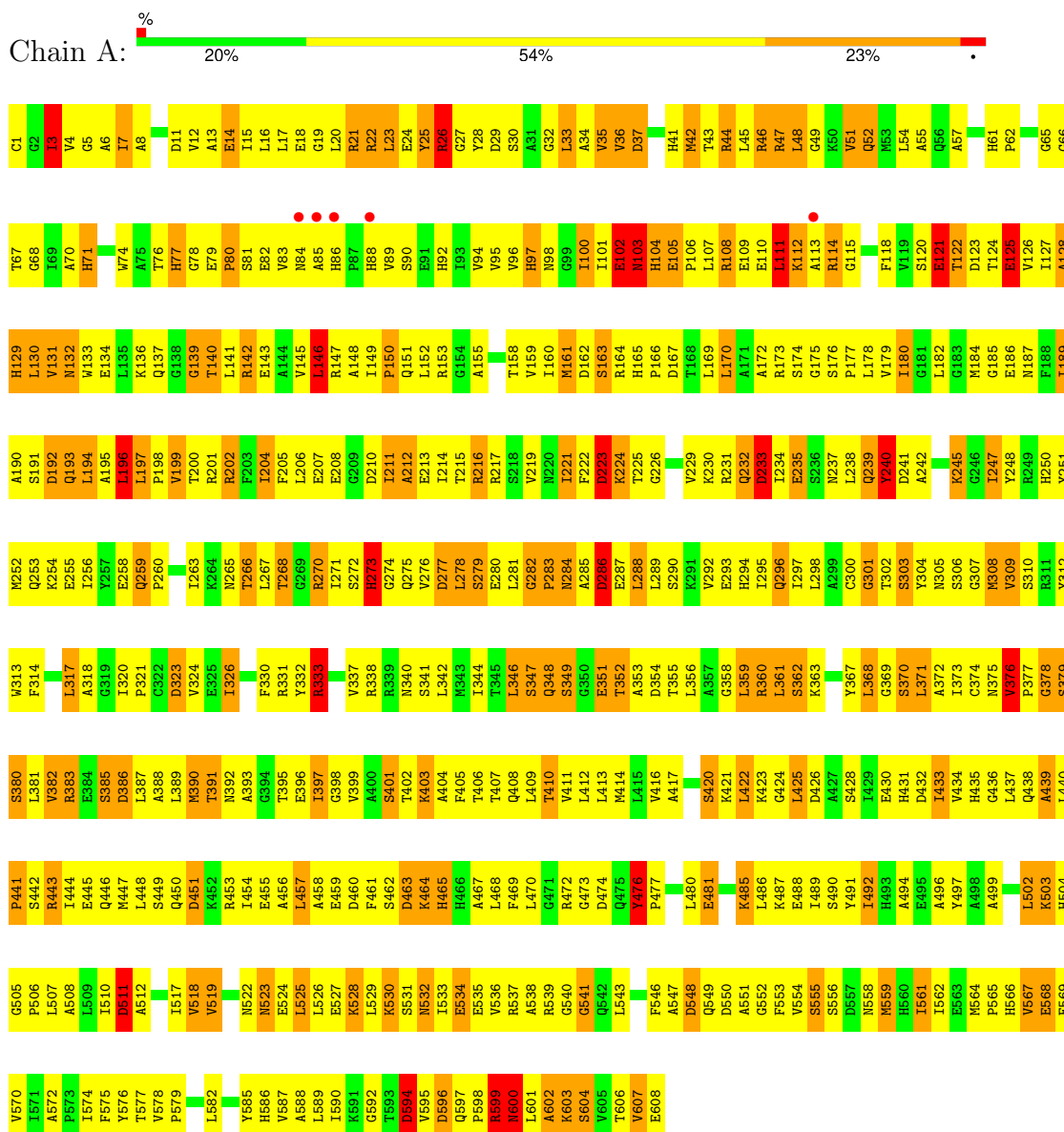
- Molecule 3 is water.

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		

3 Residue-property plots

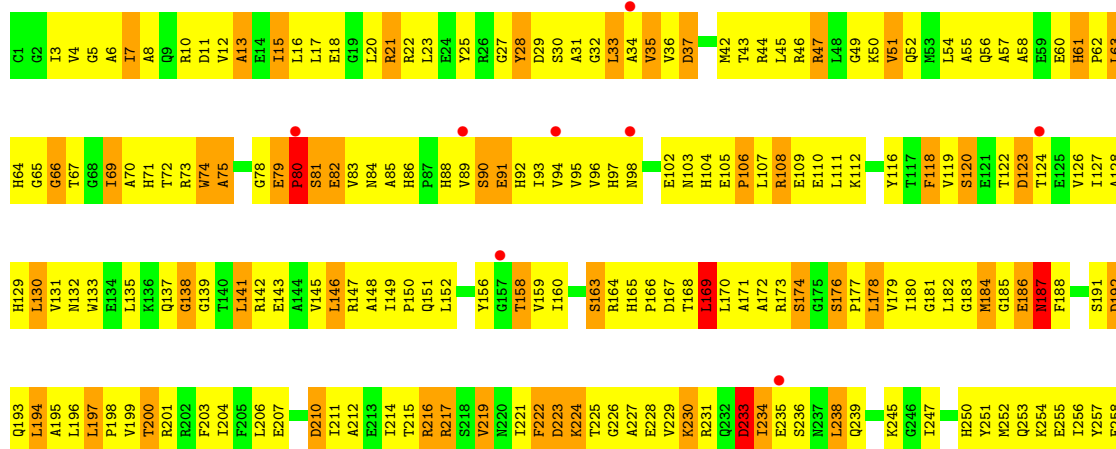
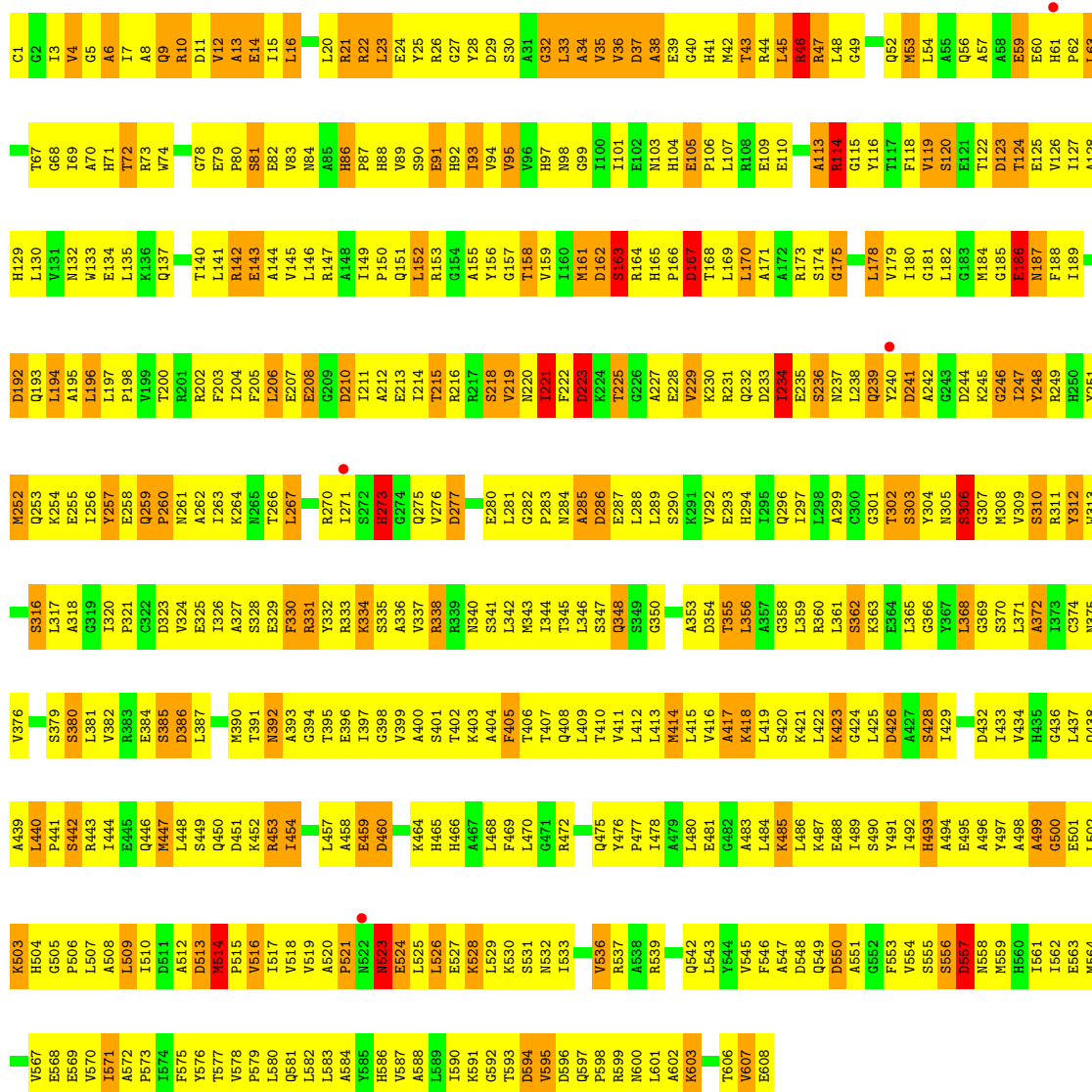
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: glucosamine 6-phosphate synthase



• Molecule 1: glucosamine 6-phosphate synthase





T577	V578	P579	L580	Q581	L582	L583	A584	Y585	H586	V587	A588	L589	T590	K591	G592	T593	D594	V595	D596	Q597	P598	R599	N600	L601	A602	K603	S604	V605	T606	V607	E608																															
■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■																															
Q259	P260	N261	A262	I263	K264	N265	T266				R270	I271	S272			L278	S279	E280	L281	G282	P283	N284	A285	D286	E287	L288	L289	S290	K291	V292	E293	H294	I295	Q296	I297	L298	A299	C300	G301	T302	S303	Y304	N305	S306	G307	M308	V309	S310	R311		F314	E315	L316	A317	I318	G319	I320	P321	C322	D323	V324	E325
I326	A327	S328	E329	F330	R331	Y332	R333	K334	S335		R338			S341	L342	M343	I344	T345	L346	S347	Q348	S349	G350	E351	T352	A353	D354	T355	L356	A357	G358	L359	R360	L361	S362		L365	G366	Y367	L368	G369	S370	L371	A372	I373	C374	N375	V376	P377	G378	S379	S380	L381	V382	R383		D386	L387	A388	V389	L389	
R390	T391	N392	A393		E396	I397	G398	V399	A400	S401	T402	K403	A404	F405	T406	T407	Q408	L409	T410	V411	L412	L413	M414	L415	V416	A417	K418		K421	L422	K423	G424	L425	D426	A427	S428	I429	E430	H431	D432	I433	V434	H435	G436	L437	Q438	A439	L440	P441	S442	R443		Q446	M447	L448	S449	Q450	D451	K452			
R453	I454	E455	A456	L457	A458	E459	D460	F461	S462	D463	K464	H465	H466	A467	L468	F469	L470	G471	R472		Q475	Y476	P477	L478	A479	L480	E481	G482	A483	L484	K485	L486	K487	E488	I489	S490	Y491	L492	H493	A494	E495	A496	Y497	A498	A499	G500	E501	L502	K503	H504	G505	P506	L507	A508	L509	I510	D511		M514			
	L517	V518		P521	N522	H523	E524	L525	L526	E527	K528	L529	K530	S531	N532	L533	E534	F535	V536	R537	A538	R539	G540	G541	G542	L543	Y544	V545	F546	A547	D548	Q549	D550	A551	G552	F553	V554	S555	S556	D557	N558	M559	H560	L561	L562	E563	M564	P565	H566	V567	E568	E569	V570	L571	A572	P573	L574	F575	Y576			

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.40Å 112.40Å 185.10Å 90.00° 96.40° 90.00°	Depositor
Resolution (Å)	12.00 – 3.10 12.00 – 3.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-3.10) 91.0 (12.00-3.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (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.	wwPDB-VP
Wilson B-factor (Å ²)	67.7	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14156	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	920	0
1	C	4695	0	4715	826	0
2	A	16	0	10	4	0
2	B	16	0	11	4	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	2566	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 (2566) 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:A:304:TYR:CD1	1:A:326:ILE:HD13	1.76	1.18
1:B:502:LEU:HA	1:B:506:PRO:HG2	1.26	1.18
1:B:21:ARG:HH11	1:B:21:ARG:HG3	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:A:193:GLN:NE2	1:A:205:PHE:HZ	1.49	1.11
1:B:187:ASN:HD22	1:B:187:ASN:N	1.38	1.11
1:A:607:VAL:HG23	1:A:608:GLU:H	0.96	1.09
1:A:247:ILE:H	1:A:247:ILE:HD12	0.96	1.09
1:B:33:LEU:HD23	1:B:33:LEU:H	1.17	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:A:33:LEU:HD22	1:A:33:LEU:H	1.13	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: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:A:84:ASN:HD21	1:A:122:THR:HB	1.24	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLY:N	1:B:54:LEU:HD22	1.70	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:HD12	1:A:247:ILE:N	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:5:GLY:HA3	1:A:189:ILE:HG22	1.42	1.01
1:A:296:GLN:CA	1:A:296:GLN:HE21	1.70	1.01
1:C:457:LEU:HD21	1:C:562:ILE:CD1	1.89	1.01
1:A:382:VAL:HG21	1:A:390:MET:CE	1.90	1.01
1:C:480:LEU:HD23	1:C:496:ALA:HB1	1.37	1.01
1:A:296:GLN:HE21	1:A:296:GLN:HA	1.18	1.01
1:A:532:ASN:H	1:A:532:ASN:ND2	1.49	1.01
1:B:507:LEU:HD12	1:B:510:ILE:HG12	1.37	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:296:GLN:HA	1:A:296:GLN:NE2	1.75	1.00
1:A:333:ARG:HG3	1:A:333:ARG:HH11	1.23	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:H	1:A:247:ILE:CD1	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:63:LEU:H	1:B:63:LEU:HD12	1.32	0.91
1:B:447:MET:HE3	1:B:564:MET:SD	2.11	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:CG	1:B:186:GLU:O	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:H	1:B:33:LEU:CD2	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:33:LEU:HD22	1:A:33:LEU:N	1.82	0.88
1:A:202:ARG:HG2	1:A:202:ARG:HH11	1.38	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:H	1:B:528:LYS:HD2	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:HE3	1:C:485:LYS:CA	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:O	1:B:186:GLU:HG3	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:B:600:ASN:CG	1:C:539:ARG:HG3	1.97	0.84
1:C:4:VAL:O	1:C:16:LEU:HD22	1.77	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:33:LEU:HD23	1:B:33:LEU:N	1.91	0.83
1:B:147:ARG:O	1:B:150:PRO:HD2	1.78	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:A:164:ARG:O	1:A:165:HIS:ND1	2.13	0.81
1:B:523:ASN:HD22	1:B:524:GLU:N	1.78	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:1:CYS:N	1:B:26:ARG:O	2.15	0.80
1:B:122:THR:C	1:B:124:THR:H	1.82	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:HA	1:A:481:GLU:OE1	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:B:347:SER:OG	2:B:701:G6Q:O2P	2.01	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:97:HIS:HB2	1:B:158:THR:HB	1.64	0.79
1:B:276:VAL:HG13	1:B:434:VAL:HG22	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:HG3	1:A:333:ARG:NH1	1.92	0.78
1:A:447:MET:HE1	1:A:564:MET:SD	2.23	0.78
1:A:536:VAL:CG2	1:A:543:LEU:HD11	2.12	0.78
1:C:532:ASN:HD22	1:C:532:ASN:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ILE:CD1	1:C:236:SER:H	1.95	0.78
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:HG2	1:A:383:ARG:NH1	1.95	0.77
1:B:469:PHE:C	1:B:470:LEU:HD23	2.05	0.77
1:B:80:PRO:O	1:B:84:ASN:OD1	2.03	0.77
1:B:468:LEU:HD23	1:B:516:VAL:HG22	1.65	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:HG3	1:B:22:ARG:NH1	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:B:488:GLU:OE1	2:B:701:G6Q:O1	2.03	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:HG	1:C:507:LEU:O	1.83	0.77
1:A:95:VAL:HG21	1:A:127:ILE:HG22	1.65	0.77
1:B:36:VAL:HG12	1:B:37:ASP:N	1.99	0.77
1:B:256:ILE:O	1:B:259:GLN:HB2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:8:ALA:HB2	1:A:186:GLU:HB2	1.67	0.76
1:A:247:ILE:N	1:A:247:ILE:CD1	2.39	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:20:LEU:HB3	1:A:51:VAL:HG21	1.68	0.76
1:A:173:ARG:HD2	1:A:177:PRO:HA	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:HD23	1:A:33:LEU:C	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:CG	1:A:522:ASN:O	2.18	0.75
1:C:61:HIS:H	1:C:62:PRO:HD3	1.51	0.75
1:C:506:PRO:O	1:C:508:ALA:N	2.20	0.75
1:A:96:VAL:HG23	1:A:96:VAL:O	1.85	0.75
1:A:477:PRO:HA	1:A:480:LEU:HB2	1.68	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:52:GLN:OE1	1:B:52:GLN:HA	1.84	0.75
1:B:516:VAL:HB	1:B:543:LEU:HD23	1.68	0.75
1:C:238:LEU:H	1:C:238:LEU:HD12	1.52	0.75
1:C:409:LEU:HA	1:C:412:LEU:HD12	1.66	0.75
1:B:3:ILE:HD11	1:B:98:ASN:N	2.01	0.75
1:B:234:ILE:HD12	1:B:235:GLU:H	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:PRO:O	1:B:526:LEU:HD22	1.86	0.75
1:C:404:ALA:O	1:C:408:GLN:HG3	1.86	0.75
1:B:281:LEU:HD13	1:B:387:LEU:HD13	0.84	0.74
1:B:297:ILE:HD12	1:B:324:VAL:CG2	2.17	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:CG	1:B:559:MET:O	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:HH11	1:B:21:ARG:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:52:GLN:HE21	1:A:52:GLN:HA	1.52	0.72
1:A:373:ILE:HD13	1:A:411:VAL:CG1	2.20	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:88:HIS:HE1	1:C:122:THR:HG21	1.55	0.72
1:C:533:ILE:O	1:C:536:VAL:HG22	1.90	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:31:ALA:O	1:C:54:LEU:CD2	2.39	0.71
1:C:309:VAL:HG22	1:C:477:PRO:HB2	1.72	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:45:LEU:HD11	1:B:57:ALA:HB1	1.73	0.71
1:B:294:HIS:CG	1:B:341:SER:OG	2.43	0.71
1:A:25:TYR:HD1	1:A:26:ARG:N	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:HH11	1:A:202:ARG:CG	2.02	0.71
1:B:276:VAL:HG21	1:B:417:ALA:CB	2.21	0.71
1:A:245:LYS:HG2	1:A:251:TYR:CE1	2.25	0.71
1:B:375:ASN:O	1:B:375:ASN:ND2	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:98:ASN:O	1:C:156:TYR:HA	1.91	0.71
1:C:180:ILE:CD1	1:C:206:LEU:HD21	2.21	0.71
1:A:20:LEU:HD21	1:A:71:HIS:H	1.54	0.71
1:A:525:LEU:HD23	1:A:525:LEU:N	2.05	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:63:LEU:HD12	1:B:63:LEU:N	2.06	0.71
1:B:559:MET:O	1:B:559:MET:HG2	1.91	0.71
1:C:447:MET:CE	1:C:579:PRO:HD3	2.21	0.71
1:A:70:ALA:O	1:A:71:HIS:HB2	1.91	0.70
1:A:522:ASN:O	1:A:522:ASN:OD1	2.09	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:O	1:B:526:LEU:HD12	1.91	0.70
1:A:33:LEU:HA	1:A:70:ALA:HA	1.72	0.70
1:A:401:SER:O	1:A:485:LYS:HE3	1.90	0.70
1:A:423:LYS:O	1:A:425:LEU:HD23	1.91	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:8:ALA:CB	1:A:186:GLU:HB3	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:N	1:A:33:LEU:CD2	2.52	0.70
1:C:79:GLU:C	1:C:81:SER:N	2.45	0.70
1:C:543:LEU:HD13	1:C:559:MET:HE2	1.74	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:25:TYR:CE2	1:B:26:ARG:CG	2.75	0.69
1:B:126:VAL:HG13	1:B:127:ILE:H	1.55	0.69
1:C:553:PHE:HB3	1:C:561:ILE:CD1	2.23	0.69
1:A:14:GLU:HG2	1:A:14:GLU:O	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:42:MET:CE	1:B:94:VAL:CG2	2.70	0.69
1:B:223:ASP:OD2	1:B:225:THR:CG2	2.26	0.69
1:B:164:ARG:O	1:B:165:HIS:HD2	1.76	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: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:24:GLU:CD	1:B:597:GLN:HE22	1.95	0.69
1:B:517:ILE:HG23	1:B:546:PHE:CE1	2.28	0.69
1:A:192:ASP:OD2	1:A:194:LEU:HB2	1.92	0.68
1:A:568:GLU:N	1:A:568:GLU:OE1	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:4:VAL:HG12	1:A:5:GLY:N	2.09	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:C:139:GLY:HA2	1:C:143:GLU:HB3	1.76	0.68
1:C:179:VAL:HG13	1:C:179:VAL:O	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:34:ALA:O	1:A:68:GLY:HA2	1.94	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:B:95:VAL:O	1:B:95:VAL:HG12	1.94	0.68
1:B:468:LEU:O	1:B:516:VAL:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:MET:HE2	1:C:44:ARG:HB2	1.75	0.67
1:C:343:MET:HE2	1:C:367:TYR:CE2	2.29	0.67
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:8:ALA:HB1	1:A:186:GLU:HB3	1.76	0.67
1:A:567:VAL:HG22	1:A:575:PHE:CD2	2.29	0.67
1:B:194:LEU:O	1:B:194:LEU:HD23	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:42:MET:SD	1:B:43:THR:N	2.67	0.67
1:B:402:THR:OG1	1:B:403:LYS:N	2.28	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:O	1:B:45:LEU:HG	1.93	0.67
1:C:7:ILE:HG23	1:C:7:ILE:O	1.95	0.67
1:B:520:ALA:CB	1:B:529:LEU:HD23	2.25	0.67
1:C:288:LEU:HD11	1:C:368:LEU:HD21	1.77	0.67
1:C:306:SER:HB2	1:C:346:LEU:HD13	1.76	0.67
1:C:533:ILE:O	1:C:536:VAL:CG2	2.43	0.67
1:B:9:GLN:OE1	1:B:9:GLN:O	2.13	0.66
1:B:306:SER:OG	1:B:346:LEU:HD13	1.95	0.66
1:C:156:TYR:CE2	1:C:158:THR:HG22	2.29	0.66
1:A:54:LEU:O	1:A:57:ALA:N	2.27	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:C:476:TYR:O	1:C:479:ALA:HB3	1.96	0.66
1:C:524:GLU:CD	1:C:524:GLU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:LEU:CA	1:A:532:ASN:HD21	2.09	0.66
1:B:290:SER:OG	1:B:422:LEU:HD13	1.95	0.66
1:B:413:LEU:HA	1:B:416:VAL:CG2	2.24	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:22:ARG:CD	1:B:195:ALA:HA	2.25	0.66
1:B:200:THR:HG23	1:B:203:PHE:CE1	2.30	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:90:SER:HG	1:C:129:HIS:CE1	2.13	0.66
1:C:107:LEU:HA	1:C:110:GLU:HB3	1.75	0.66
1:B:56:GLN:O	1:B:57:ALA:C	2.31	0.66
1:B:88:HIS:HB2	1:B:124:THR:HG22	1.77	0.66
1:B:187:ASN:HD22	1:B:187:ASN:H	0.74	0.66
1:B:576:TYR:O	1:B:579:PRO:HG2	1.96	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:251:TYR:CD2	1:C:397:ILE:HG21	2.31	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:TYR:O	1:C:50:LYS:HB3	1.95	0.65
1:C:197:LEU:H	1:C:198:PRO:CD	2.09	0.65
1:A:48:LEU:HD13	1:A:82:GLU:HG3	1.77	0.65
1:A:396:GLU:HG2	1:A:603:LYS:NZ	2.10	0.65
1:A:511:ASP:C	1:A:511:ASP:OD1	2.33	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:HG22	1:C:295:ILE:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:PRO:C	1:C:508:ALA:N	2.49	0.64
1:B:179:VAL:O	1:B:179:VAL:HG13	1.97	0.64
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:78:GLY:H	1:C:538:ALA:HB2	1.63	0.64
1:B:524:GLU:H	1:B:524:GLU:CD	2.01	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:42:MET:HG3	1:B:163:SER:HB3	1.80	0.64
1:B:289:LEU:C	1:B:292:VAL:HG23	2.16	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:71:HIS:ND1	1:B:72:THR:N	2.46	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:C:7:ILE:HG21	1:C:214:ILE:CG2	2.21	0.64
1:C:448:LEU:O	1:C:451:ASP:OD1	2.15	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:33:LEU:C	1:A:33:LEU:CD2	2.67	0.63
1:A:185:GLY:O	1:A:216:ARG:O	2.16	0.63
1:A:383:ARG:CG	1:A:383:ARG:NH1	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:LEU:O	1:B:416:VAL:N	2.27	0.63
1:C:486:LEU:O	1:C:490:SER:HB2	1.98	0.63
1:A:15:ILE:O	1:A:18:GLU:N	2.31	0.63
1:A:111:LEU:O	1:A:112:LYS:C	2.36	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:HA	1:B:503:LYS:HE3	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:3:ILE:HD11	1:C:98:ASN:HB2	1.79	0.62
1:C:299:ALA:HB1	1:C:303:SER:HB3	1.81	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: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:A:207:GLU:HG2	1:A:231:ARG:HD2	1.80	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:8:ALA:CB	1:A:186:GLU:CB	2.77	0.62
1:A:120:SER:OG	1:A:121:GLU:HG2	1.99	0.62
1:B:539:ARG:HB3	1:C:600:ASN:OD1	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:PRO:O	1:C:84:ASN:OD1	2.17	0.62
1:C:521:PRO:HA	1:C:548:ASP:HB2	1.82	0.62
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:17:LEU:CD2	1:A:33:LEU:CD1	2.72	0.62
1:A:141:LEU:HD23	1:A:170:LEU:HD23	1.80	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:89:VAL:HG23	1:A:89:VAL:O	1.98	0.62
1:A:510:ILE:CD1	1:A:536:VAL:CG1	2.77	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:O	1:B:516:VAL:HG12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HG	1:A:342:LEU:O	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:90:SER:O	1:C:91:GLU:HB2	2.01	0.61
1:C:467:ALA:O	1:C:494:ALA:HA	2.00	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:O	1:B:186:GLU:HG2	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:42:MET:HE2	1:B:94:VAL:CG2	2.31	0.61
1:B:63:LEU:H	1:B:63:LEU:CD1	2.09	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:C	1:B:167:ASP:OD1	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:4:VAL:O	1:C:4:VAL:CG1	2.43	0.60
1:C:359:LEU:HD23	1:C:381:LEU:CD2	2.31	0.60
1:A:276:VAL:HG21	1:A:414:MET:HG2	1.81	0.60
1:B:22:ARG:HH11	1:B:22:ARG:CG	2.13	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:503:LYS:HD3	1:A:535:GLU:CD	2.22	0.60
1:A:510:ILE:HD11	1:A:536:VAL:CG1	2.31	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:67:THR:OG1	1:B:166:PRO:O	2.17	0.60
1:B:113:ALA:O	1:B:115:GLY:N	2.34	0.60
1:B:294:HIS:O	1:B:341:SER:HA	2.01	0.60
1:B:493:HIS:CD2	1:C:466:HIS:ND1	2.70	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: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: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:C:251:TYR:CE2	1:C:397:ILE:HG21	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:ASP:OD1	1:C:422:LEU:HD11	2.02	0.60
1:A:353:ALA:HB1	1:A:608:GLU:OE2	2.02	0.59
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:32:GLY:CA	1:B:54:LEU:HD22	2.31	0.59
1:B:118:PHE:C	1:B:120:SER:H	2.04	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:33:LEU:HA	1:C:70:ALA:HA	1.85	0.59
1:C:135:LEU:HD11	1:C:164:ARG:NH2	2.12	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:HA	1:A:18:GLU:OE1	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:42:MET:CE	1:B:94:VAL:HG22	2.33	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: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:20:LEU:CB	1:C:51:VAL:HG11	2.32	0.59
1:C:130:LEU:HD22	1:C:148:ALA:HB1	1.83	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: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
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:29:ASP:O	1:B:49:GLY:N	2.25	0.58
1:B:276:VAL:HG23	1:B:276:VAL:O	2.03	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:32:GLY:HA2	1:A:54:LEU:CD2	2.33	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:O	1:A:268:THR:HG22	2.02	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:18:GLU:HA	1:C:21:ARG:NH1	2.09	0.58
1:C:90:SER:OG	1:C:129:HIS:ND1	2.35	0.58
1:C:263:ILE:HD12	1:C:440:LEU:CD2	2.33	0.58
1:C:371:LEU:HD11	1:C:389:LEU:HD11	1.84	0.58
1:A:47:ARG:NE	1:A:57:ALA:HB2	2.18	0.58
1:A:503:LYS:HD3	1:A:535:GLU:OE2	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ALA:C	1:A:130:LEU:N	2.55	0.58
1:B:343:MET:HB3	1:B:370:SER:CB	2.32	0.58
1:B:356:LEU:CD1	1:B:360:ARG:NE	2.57	0.58
1:C:197:LEU:N	1:C:198:PRO:CD	2.66	0.58
1:A:36:VAL:HG12	1:A:42:MET:HA	1.85	0.58
1:A:161:MET:HB2	1:A:169:LEU:HD23	1.86	0.58
1:A:491:TYR:CG	1:A:599:ARG:NH1	2.71	0.58
1:A:510:ILE:CD1	1:A:536:VAL:HG12	2.34	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:5:GLY:HA2	1:C:69:ILE:HA	1.84	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: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:80:PRO:O	1:C:84:ASN:CG	2.42	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:A:84:ASN:HB2	1:A:121:GLU:CD	2.24	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:B:331:ARG:HA	1:B:361:LEU:HD22	1.86	0.58
1:A:97:HIS:C	1:A:97:HIS:ND1	2.57	0.57
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:B:453:ARG:HG3	1:B:453:ARG:NH1	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:79:GLU:O	1:A:81:SER:N	2.37	0.57
1:A:382:VAL:O	1:A:382:VAL:CG1	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:VAL:HG21	1:B:163:SER:HA	1.87	0.57
1:B:523:ASN:ND2	1:B:523:ASN:C	2.56	0.57
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:71:HIS:HD2	1:C:96:VAL:HB	1.69	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:A:46:ARG:HD2	1:A:82:GLU:O	2.04	0.57
1:A:155:ALA:HB1	1:A:175:GLY:HA3	1.86	0.57
1:B:3:ILE:HG22	1:B:4:VAL:N	2.19	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:C:532:ASN:H	1:C:532:ASN:ND2	2.01	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:A:304:TYR:CE1	1:A:326:ILE:HD11	2.36	0.57
1:B:134:GLU:OE1	1:B:134:GLU:HA	2.04	0.57
1:B:318:ALA:O	1:B:423:LYS:HE3	2.05	0.57
1:B:406:THR:O	1:B:409:LEU:HB2	2.04	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:HG22	1:A:344:ILE:O	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:CG	1:A:202:ARG:NH1	2.64	0.57
1:A:330:PHE:CD1	1:A:330:PHE:C	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:28:TYR:CE1	1:A:597:GLN:HB3	2.40	0.57
1:A:305:ASN:ND2	1:A:481:GLU:OE1	2.38	0.57
1:A:447:MET:CE	1:A:575:PHE:CE1	2.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:LEU:HD12	1:A:507:LEU:O	2.05	0.57
1:C:130:LEU:HD13	1:C:152:LEU:HD11	1.87	0.57
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:86:HIS:CD2	1:B:86:HIS:N	2.73	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:C:36:VAL:HG12	1:C:36:VAL:O	2.04	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:A:7:ILE:CD1	1:A:215:THR:CA	2.82	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:B:3:ILE:C	1:B:4:VAL:HG23	2.26	0.56
1:B:44:ARG:CZ	1:B:46:ARG:HH21	2.17	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:184:MET:C	1:A:186:GLU:H	2.09	0.56
1:A:296:GLN:CA	1:A:296:GLN:NE2	2.40	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:60:GLU:O	1:B:62:PRO:HD3	2.05	0.56
1:B:92:HIS:CD2	1:B:164:ARG:HE	2.24	0.56
1:B:127:ILE:HG12	1:B:152:LEU:CD1	2.36	0.56
1:B:249:ARG:HG2	1:B:249:ARG:O	2.04	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:28:TYR:HB2	1:C:50:LYS:CD	2.35	0.56
1:C:107:LEU:HA	1:C:110:GLU:CB	2.34	0.56
1:C:130:LEU:CD1	1:C:152:LEU:HD21	2.36	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:71:HIS:CE1	1:A:86:HIS:CG	2.94	0.56
1:A:76:THR:O	1:A:78:GLY:N	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:ILE:CG1	1:B:570:VAL:HG21	2.35	0.56
1:A:70:ALA:O	1:A:71:HIS:CB	2.53	0.56
1:A:263:ILE:HD11	1:A:406:THR:HG21	1.85	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:C	1:A:277:ASP:OD1	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:47:ARG:HA	1:C:47:ARG:HE	1.70	0.56
1:C:82:GLU:HG3	1:C:83:VAL:N	2.18	0.56
1:C:141:LEU:HD21	1:C:168:THR:OG1	2.05	0.56
1:A:28:TYR:HE1	1:A:602:ALA:HA	1.70	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: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:79:GLU:O	1:B:80:PRO:C	2.44	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: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: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:HA	1:C:47:ARG:NE	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:TYR:HE2	1:C:158:THR:HG22	1.71	0.56
1:A:259:GLN:O	1:A:263:ILE:HG13	2.07	0.55
1:A:347:SER:OG	2:A:700:G6Q:O2P	2.14	0.55
1:B:159:VAL:HG22	1:B:171:ALA:HB2	1.88	0.55
1:B:162:ASP:C	1:B:162:ASP:OD1	2.43	0.55
1:B:252:MET:HE2	1:B:489:ILE:HD13	1.88	0.55
1:B:286:ASP:CB	1:B:422:LEU:HD11	2.36	0.55
1:C:3:ILE:CD1	1:C:98:ASN:HB2	2.35	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: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:8:ALA:HA	1:C:186:GLU:HA	1.86	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: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:99:GLY:HA3	1:B:156:TYR:HA	1.88	0.55
1:B:468:LEU:HD12	1:B:497:TYR:HD2	1.68	0.55
1:B:24:GLU:OE2	1:B:597:GLN:NE2	2.26	0.55
1:B:221:ILE:HD12	1:B:221:ILE:N	2.15	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:20:LEU:O	1:B:21:ARG:C	2.45	0.55
1:B:101:ILE:N	1:B:123:ASP:OD2	2.39	0.55
1:B:259:GLN:N	1:B:260:PRO:HD2	2.21	0.55
1:C:56:GLN:O	1:C:60:GLU:HB2	2.07	0.55
1:C:330:PHE:C	1:C:332:TYR:H	2.09	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:480:LEU:HA	1:B:496:ALA:CB	2.36	0.55
1:B:486:LEU:O	1:B:490:SER:CB	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:80:PRO:HB2	1:C:84:ASN:OD1	2.07	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: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:79:GLU:HB3	1:C:81:SER:OG	2.08	0.55
1:C:370:SER:HG	1:C:386:ASP:N	2.05	0.55
1:A:37:ASP:HA	1:A:65:GLY:HA2	1.89	0.54
1:A:567:VAL:CG2	1:A:575:PHE:CD2	2.89	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:399:VAL:CG2	1:A:596:ASP:O	2.56	0.54
1:A:510:ILE:HG22	1:A:511:ASP:N	2.22	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:NE2	1:A:348:GLN:C	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:313:TRP:HZ2	1:B:573:PRO:HG3	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:GLY:O	1:B:381:LEU:CB	2.56	0.54
1:C:286:ASP:OD1	1:C:422:LEU:CD1	2.55	0.54
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:95:VAL:CG1	1:C:96:VAL:N	2.71	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: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:28:TYR:CE1	1:B:602:ALA:HA	2.42	0.54
1:B:413:LEU:CA	1:B:416:VAL:HG23	2.35	0.54
1:C:28:TYR:C	1:C:50:LYS:HB3	2.28	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:523:ASN:CG	1:C:569:GLU:OE2	2.46	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: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:346:LEU:HD22	1:A:408:GLN:HE21	1.73	0.54
1:A:393:ALA:O	1:A:403:LYS:NZ	2.37	0.54
1:A:553:PHE:HB3	1:A:561:ILE:HG13	1.89	0.54
1:B:490:SER:OG	1:B:587:VAL:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:PHE:CD2	1:B:562:ILE:HD13	2.43	0.54
1:C:127:ILE:HG13	1:C:128:ALA:N	2.23	0.54
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:33:LEU:HG	1:B:34:ALA:N	2.22	0.53
1:B:236:SER:OG	1:B:237:ASN:N	2.41	0.53
1:C:95:VAL:CG2	1:C:128:ALA:HA	2.38	0.53
1:A:28:TYR:CZ	1:A:597:GLN:CB	2.89	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:302:THR:CG2	1:A:405:PHE:CD1	2.91	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:44:ARG:HD2	1:B:87:PRO:O	2.08	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:505:GLY:N	1:B:506:PRO:CD	2.72	0.53
1:C:69:ILE:HG13	1:C:96:VAL:HG22	1.90	0.53
1:C:107:LEU:O	1:C:108:ARG:C	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:ASN:CA	1:C:391:THR:OG1	2.43	0.53
1:A:134:GLU:OE1	1:A:147:ARG:HB2	2.08	0.53
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:16:LEU:HD11	1:A:68:GLY:HA3	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:B:44:ARG:NH1	1:B:89:VAL:HG13	2.24	0.53
1:C:45:LEU:HD21	1:C:57:ALA:O	2.09	0.53
1:C:137:GLN:O	1:C:138:GLY:O	2.27	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:33:LEU:HA	1:B:70:ALA:HA	1.91	0.53
1:B:207:GLU:O	1:B:210:ASP:HB2	2.08	0.53
1:B:350:GLY:O	1:B:381:LEU:HB2	2.08	0.53
1:B:601:LEU:HD22	1:C:503:LYS:O	2.09	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:A:4:VAL:CG1	1:A:5:GLY:N	2.72	0.53
1:A:13:ALA:C	1:A:15:ILE:H	2.12	0.53
1:A:294:HIS:HD2	1:A:321:PRO:O	1.92	0.53
1:A:304:TYR:CE1	1:A:324:VAL:O	2.62	0.53
1:B:42:MET:HE1	1:B:94:VAL:HG21	1.87	0.53
1:B:79:GLU:HB3	1:B:80:PRO:HD2	1.91	0.53
1:B:405:PHE:CE2	1:B:481:GLU:HG2	2.43	0.53
1:B:499:ALA:C	1:B:501:GLU:H	2.13	0.53
1:B:500:GLY:HA3	1:C:328:SER:OG	2.09	0.53
1:C:236:SER:O	1:C:238:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:42:MET:HG2	1:C:43:THR:N	2.25	0.52
1:C:256:ILE:HG22	1:C:257:TYR:N	2.22	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:95:VAL:HG12	1:A:96:VAL:N	2.23	0.52
1:A:346:LEU:HD22	1:A:408:GLN:NE2	2.24	0.52
1:B:25:TYR:CZ	1:B:26:ARG:HG3	2.44	0.52
1:B:155:ALA:HB1	1:B:175:GLY:HA3	1.91	0.52
1:B:168:THR:CG2	1:B:169:LEU:N	2.73	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:346:LEU:CD2	1:B:408:GLN:HG2	2.39	0.52
1:B:348:GLN:O	1:B:376:VAL:HG23	2.09	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:B:539:ARG:HD2	1:C:600:ASN:OD1	2.09	0.52
1:C:564:MET:HG3	1:C:576:TYR:HE1	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:47:ARG:CZ	1:A:57:ALA:CB	2.87	0.52
1:A:267:LEU:HD21	1:A:410:THR:CG2	2.40	0.52
1:A:296:GLN:HE21	1:A:296:GLN:C	2.13	0.52
1:B:3:ILE:CD1	1:B:98:ASN:HB3	2.39	0.52
1:B:3:ILE:CD1	1:B:98:ASN:CB	2.87	0.52
1:B:34:ALA:CB	1:B:87:PRO:HG2	2.31	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: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: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:96:VAL:O	1:A:96:VAL:CG2	2.55	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:B:42:MET:HE2	1:B:94:VAL:HG21	1.89	0.52
1:B:276:VAL:HG13	1:B:434:VAL:CG2	2.38	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:38:ALA:HB3	1:B:39:GLU:CD	2.30	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:470:LEU:HB2	1:B:518:VAL:CG2	2.38	0.52
1:A:11:ASP:HA	1:A:65:GLY:O	2.10	0.52
1:A:124:THR:O	1:A:127:ILE:HB	2.10	0.52
1:A:125:GLU:O	1:A:125:GLU:OE1	2.28	0.52
1:A:356:LEU:CD2	1:A:360:ARG:NH2	2.64	0.52
1:B:3:ILE:HD11	1:B:157:GLY:O	2.10	0.52
1:B:11:ASP:C	1:B:13:ALA:H	2.12	0.52
1:B:493:HIS:HD2	1:C:466:HIS:ND1	2.07	0.52
1:C:28:TYR:HB2	1:C:50:LYS:HB3	1.92	0.52
1:C:142:ARG:HG2	1:C:146:LEU:HB2	1.92	0.52
1:C:468:LEU:HD12	1:C:495:GLU:HB3	1.91	0.52
1:A:286:ASP:N	1:A:286:ASP:OD1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:487:LYS:HG3	1:C:509:LEU:HD21	1.92	0.51
1:C:447:MET:C	1:C:449:SER:H	2.14	0.51
1:A:18:GLU:OE1	1:A:18:GLU:CA	2.57	0.51
1:A:142:ARG:HG2	1:A:142:ARG:O	2.09	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:N	1:C:33:LEU:HD23	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: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:B:251:TYR:N	1:B:596:ASP:OD1	2.43	0.51
1:C:28:TYR:HB2	1:C:50:LYS:CB	2.40	0.51
1:C:204:ILE:CG2	1:C:231:ARG:HB2	2.41	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:68:GLY:C	1:B:69:ILE:CG2	2.79	0.51
1:B:294:HIS:HA	1:B:321:PRO:HG2	1.93	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:HD21	1:C:389:LEU:CD2	2.39	0.51
1:C:281:LEU:CD1	1:C:285:ALA:HB1	2.41	0.51
1:C:434:VAL:C	1:C:436:GLY:N	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASN:C	1:A:132:ASN:OD1	2.49	0.51
1:A:143:GLU:O	1:A:147:ARG:HG3	2.11	0.51
1:A:223:ASP:OD1	1:A:225:THR:N	2.44	0.51
1:B:45:LEU:HD21	1:B:57:ALA:CB	2.40	0.51
1:B:90:SER:O	1:B:91:GLU:CB	2.51	0.51
1:B:93:ILE:N	1:B:93:ILE:CD1	2.73	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:504:HIS:CD2	1:C:300:CYS:HB3	2.45	0.51
1:C:74:TRP:CH2	1:C:602:ALA:CB	2.94	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: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:A:296:GLN:HE21	1:A:297:ILE:N	2.07	0.51
1:B:36:VAL:HG23	1:B:161:MET:SD	2.50	0.51
1:B:343:MET:HE2	1:B:362:SER:HB2	1.92	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:92:HIS:O	1:A:163:SER:OG	2.26	0.51
1:A:440:LEU:HD22	1:A:574:ILE:HD12	1.93	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:HD13	1:C:517:ILE:N	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:396:GLU:CG	1:A:603:LYS:NZ	2.73	0.50
1:A:603:LYS:CG	1:A:604:SER:N	2.71	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:O	1:A:159:VAL:HG12	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:371:LEU:HA	1:B:387:LEU:O	2.10	0.50
1:B:447:MET:CE	1:B:564:MET:HE1	2.41	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: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:20:LEU:HD22	1:B:72:THR:OG1	2.12	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:HG3	1:B:333:ARG:O	2.11	0.50
1:B:453:ARG:HH21	1:B:562:ILE:HA	1.76	0.50
1:C:4:VAL:HB	1:C:70:ALA:HB3	1.94	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:B:67:THR:HG22	1:B:68:GLY:N	2.27	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: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:47:ARG:CZ	1:A:57:ALA:HB2	2.42	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:B:127:ILE:HG12	1:B:152:LEU:HD11	1.93	0.50
1:B:146:LEU:CD1	1:B:211:ILE:CD1	2.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:ASP:N	1:B:557:ASP:OD1	2.43	0.50
1:C:291:LYS:O	1:C:293:GLU:HG3	2.12	0.50
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:30:SER:OG	1:B:73:ARG:HB3	2.12	0.50
1:B:32:GLY:HA2	1:B:45:LEU:O	2.12	0.50
1:B:158:THR:O	1:B:158:THR:HG23	2.12	0.50
1:B:454:ILE:HD12	1:B:582:LEU:CD1	2.42	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: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:523:ASN:O	1:B:526:LEU:HB2	2.12	0.50
1:B:524:GLU:N	1:B:524:GLU:CD	2.65	0.50
1:C:82:GLU:CG	1:C:83:VAL:H	2.22	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: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:74:TRP:HA	1:C:74:TRP:CE3	2.45	0.50
1:C:330:PHE:HE1	1:C:335:SER:HB3	1.77	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:79:GLU:HB3	1:C:81:SER:HG	1.76	0.49
1:C:565:PRO:HD2	1:C:575:PHE:CE2	2.47	0.49
1:A:567:VAL:HG21	1:A:575:PHE:CG	2.48	0.49
1:B:33:LEU:CB	1:B:70:ALA:HB2	2.42	0.49
1:B:359:LEU:HD11	1:B:381:LEU:CD1	2.40	0.49
1:C:447:MET:HE1	1:C:578:VAL:HB	1.94	0.49
1:C:525:LEU:O	1:C:528:LYS:HB2	2.12	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:O	1:A:271:ILE:HG22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:326:ILE:O	1:A:326:ILE:HG22	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:90:SER:HB3	1:B:128:ALA:HB1	1.94	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: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:92:HIS:HD2	1:B:164:ARG:HE	1.59	0.49
1:B:346:LEU:HD11	1:B:412:LEU:HD11	1.93	0.49
1:C:20:LEU:HD11	1:C:70:ALA:HB1	1.94	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:A:33:LEU:O	1:A:33:LEU:CD2	2.51	0.49
1:A:281:LEU:HD21	1:A:389:LEU:HD11	1.94	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:401:SER:OG	2:A:700:G6Q:H2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ALA:CB	1:A:553:PHE:CD1	2.96	0.49
1:B:185:GLY:O	1:B:186:GLU:CB	2.61	0.49
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:332:TYR:HE1	1:C:528:LYS:HZ1	1.58	0.48
1:B:594:ASP:HB3	1:B:597:GLN:C	2.34	0.48
1:C:16:LEU:O	1:C:20:LEU:HG	2.13	0.48
1:C:165:HIS:N	1:C:166:PRO:HD3	2.28	0.48
1:C:344:ILE:HD12	1:C:344:ILE:N	2.28	0.48
1:C:359:LEU:CD2	1:C:381:LEU:CD2	2.91	0.48
1:C:567:VAL:HG11	1:C:575:PHE:CG	2.48	0.48
1:B:14:GLU:OE2	1:B:15:ILE:HG13	2.13	0.48
1:B:144:ALA:O	1:B:147:ARG:HB2	2.12	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:16:LEU:HD11	1:A:68:GLY:CA	2.43	0.48
1:A:118:PHE:HD2	1:A:125:GLU:OE1	1.96	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:457:LEU:HD23	1:B:562:ILE:HD11	1.95	0.48
1:B:501:GLU:O	1:B:506:PRO:HD2	2.12	0.48
1:C:82:GLU:O	1:C:85:ALA:HB3	2.13	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: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:45:LEU:HD11	1:B:57:ALA:CB	2.42	0.48
1:B:413:LEU:HD12	1:B:416:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:ARG:HH11	1:B:453:ARG:CG	2.27	0.48
1:C:36:VAL:HG11	1:C:163:SER:HA	1.94	0.48
1:C:107:LEU:O	1:C:110:GLU:N	2.47	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:31:ALA:HB1	1:C:51:VAL:HG22	1.89	0.48
1:C:139:GLY:HA3	1:C:143:GLU:HB3	1.96	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:4:VAL:O	1:B:4:VAL:HG12	2.13	0.48
1:B:275:GLN:CA	1:B:434:VAL:HG11	2.44	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: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:34:ALA:C	1:B:35:VAL:CG1	2.81	0.48
1:B:196:LEU:HA	1:B:196:LEU:HD23	1.29	0.48
1:B:197:LEU:N	1:B:198:PRO:CD	2.77	0.48
1:B:453:ARG:HG3	1:B:453:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:457:LEU:O	1:A:460:ASP:N	2.42	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:C:348:GLN:CG	1:C:375:ASN:HB3	2.44	0.48
1:A:4:VAL:HG21	1:A:19:GLY:HA3	1.95	0.47
1:A:16:LEU:HD11	1:A:68:GLY:C	2.34	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:266:THR:CG2	1:A:391:THR:O	2.58	0.47
1:A:301:GLY:O	1:A:302:THR:C	2.52	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:HD12	1:C:583:LEU:O	2.14	0.47
1:A:52:GLN:HE21	1:A:52:GLN:CA	2.25	0.47
1:A:559:MET:O	1:A:559:MET:CG	2.61	0.47
1:B:3:ILE:HD12	1:B:98:ASN:HB3	1.97	0.47
1:B:3:ILE:CG2	1:B:4:VAL:N	2.77	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:476:TYR:CE1	1:B:498:ALA:HB2	2.49	0.47
1:B:501:GLU:HG2	1:C:326:ILE:HG21	1.96	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:HG22	1:C:214:ILE:O	2.13	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:11:ASP:HA	1:C:65:GLY:O	2.14	0.47
1:C:35:VAL:CG2	1:C:43:THR:HB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:VAL:HG23	1:C:43:THR:HB	1.96	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
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: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:250:HIS:CE1	1:A:595:VAL:HB	2.50	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:C:22:ARG:HG2	1:C:22:ARG:HH11	1.80	0.47
1:C:159:VAL:HA	1:C:171:ALA:CB	2.45	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:A:22:ARG:C	1:A:23:LEU:HD23	2.30	0.47
1:A:173:ARG:HH21	1:A:208:GLU:HB2	1.80	0.47
1:A:250:HIS:ND1	1:A:595:VAL:HB	2.30	0.47
1:B:78:GLY:H	1:C:538:ALA:CB	2.28	0.47
1:B:79:GLU:O	1:B:81:SER:N	2.48	0.47
1:B:240:TYR:CD1	1:B:241:ASP:HB2	2.50	0.47
1:B:484:LEU:HD12	1:B:484:LEU:HA	1.63	0.47
1:B:488:GLU:OE1	2:B:701:G6Q:C1	2.61	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:374:CYS:O	1:C:390:MET:HA	2.15	0.47
1:C:439:ALA:O	1:C:440:LEU:C	2.53	0.47
1:C:485:LYS:HA	1:C:485:LYS:CE	2.33	0.47
1:C:486:LEU:O	1:C:490:SER:OG	2.32	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:48:LEU:HA	1:A:48:LEU:HD12	1.51	0.47
1:A:443:ARG:HH11	1:A:443:ARG:CG	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:356:LEU:HD11	1:B:360:ARG:CD	2.44	0.47
1:C:45:LEU:HD21	1:C:57:ALA:CB	2.44	0.47
1:C:239:GLN:O	1:C:239:GLN:HG2	2.14	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:OE1	1:A:534:GLU:CA	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:28:TYR:CE1	1:B:602:ALA:CB	2.98	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: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:84:ASN:O	1:B:88:HIS:NE2	2.42	0.46
1:B:347:SER:HB3	1:B:381:LEU:HD23	1.97	0.46
1:C:32:GLY:CA	1:C:86:HIS:O	2.55	0.46
1:C:34:ALA:O	1:C:35:VAL:HG13	2.14	0.46
1:C:126:VAL:O	1:C:130:LEU:HB2	2.15	0.46
1:A:76:THR:HG22	1:A:77:HIS:N	2.30	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: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:CD1	1:C:502:LEU:H	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:25:TYR:HD1	1:A:25:TYR:C	2.17	0.46
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: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:495:GLU:OE1	1:C:493:HIS:NE2	2.46	0.46
1:B:509:LEU:O	1:B:509:LEU:HD23	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:A:326:ILE:HD12	1:A:326:ILE:HA	1.64	0.46
1:C:36:VAL:HG21	1:C:163:SER:OG	2.16	0.46
1:C:327:ALA:O	1:C:330:PHE:N	2.38	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:5:GLY:HA3	1:B:189:ILE:CG2	2.45	0.46
1:B:21:ARG:NH1	1:B:21:ARG:CG	2.61	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: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:314:PHE:CD1	1:C:416:VAL:HG22	2.51	0.46
1:C:361:LEU:O	1:C:365:LEU:HG	2.16	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:56:GLN:C	1:C:58:ALA:H	2.18	0.46
1:C:567:VAL:HG11	1:C:575:PHE:CE2	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ARG:HA	1:B:277:ASP:HB3	1.98	0.46
1:C:93:ILE:O	1:C:93:ILE:HG22	2.16	0.46
1:C:130:LEU:HD11	1:C:152:LEU:HD21	1.98	0.46
1:C:443:ARG:NH1	1:C:568:GLU:OE2	2.44	0.46
1:C:487:LYS:HD3	1:C:494:ALA:O	2.15	0.46
1:C:599:ARG:HG3	1:C:600:ASN:HD22	1.77	0.46
1:A:86:HIS:CE1	1:A:124:THR:HG1	2.33	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:B:97:HIS:CB	1:B:158:THR:HB	2.42	0.46
1:B:332:TYR:CZ	1:C:528:LYS:NZ	2.69	0.46
1:B:487:LYS:HG3	1:C:509:LEU:HD11	1.97	0.46
1:C:69:ILE:HG13	1:C:96:VAL:CG2	2.46	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: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:306:SER:HA	1:B:405:PHE:HE1	1.81	0.46
1:B:334:LYS:HD3	1:B:335:SER:N	2.31	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:32:GLY:CA	1:B:54:LEU:CD2	2.94	0.46
1:B:293:GLU:OE2	1:B:340:ASN:ND2	2.49	0.46
1:C:60:GLU:O	1:C:61:HIS:CB	2.58	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:B:5:GLY:HA3	1:B:189:ILE:HG23	1.97	0.45
1:B:179:VAL:HG22	1:B:180:ILE:O	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:THR:HB	1:C:381:LEU:HD13	1.98	0.45
1:A:17:LEU:HD21	1:A:33:LEU:HD12	1.92	0.45
1:A:118:PHE:HA	1:A:125:GLU:OE2	2.16	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:25:TYR:C	1:A:27:GLY:H	2.19	0.45
1:A:121:GLU:O	1:A:122:THR:CB	2.57	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:28:TYR:CE2	1:A:597:GLN:CB	2.99	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:B:3:ILE:HD11	1:B:98:ASN:CB	2.47	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: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:454:ILE:HG23	1:C:583:LEU:HB2	1.97	0.45
1:C:495:GLU:OE1	1:C:497:TYR:CE2	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:GLY:C	1:C:29:ASP:N	2.67	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:111:LEU:C	1:A:113:ALA:N	2.66	0.45
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: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:3:ILE:HG13	1:B:98:ASN:HB2	1.97	0.45
1:B:37:ASP:O	1:B:38:ALA:C	2.54	0.45
1:B:44:ARG:NH1	1:B:88:HIS:HA	2.31	0.45
1:B:330:PHE:O	1:B:333:ARG:HG3	2.15	0.45
1:B:515:PRO:C	1:B:516:VAL:HG23	2.36	0.45
1:C:74:TRP:HA	1:C:74:TRP:HE3	1.81	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:A:42:MET:SD	1:A:94:VAL:HG21	2.57	0.45
1:A:48:LEU:HD13	1:A:48:LEU:N	2.32	0.45
1:A:348:GLN:C	1:A:348:GLN:CD	2.76	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:3:ILE:HG23	1:A:3:ILE:HD13	1.37	0.45
1:A:61:HIS:N	1:A:62:PRO:HD3	2.31	0.45
1:A:295:ILE:O	1:A:295:ILE:HG22	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: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: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:29:ASP:OD2	1:C:74:TRP:HE3	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:399:VAL:HG21	1:B:598:PRO:HD2	1.99	0.45
1:B:468:LEU:HD11	1:B:470:LEU:CD2	2.46	0.45
1:B:509:LEU:CD1	1:C:493:HIS:HA	2.47	0.45
1:C:288:LEU:HD12	1:C:288:LEU:O	2.17	0.45
1:A:301:GLY:O	1:A:303:SER:N	2.50	0.45
1:B:61:HIS:C	1:B:61:HIS:CD2	2.89	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: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:42:MET:SD	1:C:94:VAL:HG21	2.57	0.44
1:C:71:HIS:ND1	1:C:72:THR:N	2.64	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:A:294:HIS:HE2	1:A:323:ASP:CG	2.20	0.44
1:B:32:GLY:CA	1:B:46:ARG:HA	2.46	0.44
1:B:110:GLU:OE2	1:B:114:ARG:CZ	2.66	0.44
1:B:251:TYR:CD2	1:B:397:ILE:CG2	3.00	0.44
1:C:67:THR:HG22	1:C:169:LEU:HD23	1.98	0.44
1:C:405:PHE:HD2	1:C:577:THR:HG21	1.81	0.44
1:A:71:HIS:ND1	1:A:86:HIS:CB	2.66	0.44
1:A:251:TYR:CG	1:A:397:ILE:CG2	3.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:SER:O	1:B:337:VAL:N	2.51	0.44
1:C:36:VAL:HG12	1:C:166:PRO:CG	2.48	0.44
1:C:178:LEU:HD22	1:C:206:LEU:CD1	2.47	0.44
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: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:44:ARG:NH1	1:B:46:ARG:HH21	2.15	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:C:215:THR:O	1:C:216:ARG:C	2.56	0.44
1:C:502:LEU:HD12	1:C:502:LEU:H	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:18:GLU:HA	1:C:21:ARG:HD2	2.00	0.44
1:C:179:VAL:O	1:C:179:VAL:CG1	2.64	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:12:VAL:HG13	1:A:66:GLY:HA2	2.00	0.44
1:A:352:THR:HG22	1:A:353:ALA:N	2.33	0.44
1:A:530:LYS:HD2	1:A:530:LYS:C	2.38	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:85:ALA:O	1:A:88:HIS:CE1	2.71	0.44
1:A:89:VAL:O	1:A:89:VAL:CG2	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ASP:O	1:A:242:ALA:HB3	2.18	0.44
1:B:412:LEU:HD23	1:B:412:LEU:HA	1.80	0.44
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:34:ALA:HB1	1:A:42:MET:HE1	2.00	0.43
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:476:TYR:C	1:A:476:TYR:CD1	2.87	0.43
1:B:34:ALA:HB2	1:B:87:PRO:CG	2.34	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: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:480:LEU:HD23	1:B:496:ALA:HB3	1.99	0.43
1:B:485:LYS:C	1:B:487:LYS:N	2.69	0.43
1:C:107:LEU:N	1:C:107:LEU:HD12	2.32	0.43
1:A:35:VAL:HG21	3:A:702:HOH:O	2.19	0.43
1:A:178:LEU:HD22	1:A:189:ILE:HD11	1.99	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:308:MET:HB2	1:B:477:PRO:HB3	2.00	0.43
1:B:348:GLN:C	1:B:348:GLN:OE1	2.57	0.43
1:B:580:LEU:O	1:B:581:GLN:C	2.55	0.43
1:B:600:ASN:HA	1:C:539:ARG:CZ	2.48	0.43
1:C:3:ILE:HG22	1:C:4:VAL:N	2.33	0.43
1:C:98:ASN:HD21	1:C:176:SER:HG	1.64	0.43
1:C:259:GLN:CG	1:C:403:LYS:HA	2.48	0.43
1:C:565:PRO:C	1:C:566:HIS:O	2.55	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:239:GLN:C	1:A:241:ASP:N	2.72	0.43
1:A:253:GLN:HB2	1:A:585:TYR:CE2	2.53	0.43
1:B:8:ALA:O	1:B:216:ARG:HB2	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:36:VAL:O	1:A:65:GLY:HA3	2.18	0.43
1:A:344:ILE:HG12	1:A:371:LEU:HB3	2.00	0.43
1:B:3:ILE:C	1:B:4:VAL:CG2	2.87	0.43
1:B:397:ILE:HD13	1:B:397:ILE:HA	1.67	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:HD23	1:B:470:LEU:N	2.33	0.43
1:B:606:THR:HG22	1:B:606:THR:O	2.19	0.43
1:C:86:HIS:NE2	1:C:97:HIS:CE1	2.87	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:LEU:HD12	1:A:413:LEU:HA	1.84	0.43
1:B:237:ASN:HA	1:B:239:GLN:HE22	1.82	0.43
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:H	1:B:578:VAL:HG23	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:553:PHE:CD2	1:B:559:MET:CE	3.02	0.43
1:B:555:SER:C	1:B:556:SER:HG	2.22	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:83:VAL:HG12	1:C:120:SER:OG	2.19	0.43
1:C:485:LYS:HE3	1:C:485:LYS:N	2.34	0.43
1:A:178:LEU:HA	1:A:190:ALA:O	2.19	0.42
1:A:251:TYR:N	1:A:596:ASP:OD2	2.42	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:B:169:LEU:HD23	1:B:169:LEU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:ALA:C	1:B:460:ASP:N	2.70	0.42
1:C:63:LEU:HD22	1:C:63:LEU:N	2.34	0.42
1:C:298:LEU:HG	1:C:343:MET:SD	2.59	0.42
1:C:356:LEU:HD13	1:C:380:SER:HB3	2.00	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:88:HIS:NE2	1:C:124:THR:HB	2.34	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:A:14:GLU:O	1:A:14:GLU:CG	2.63	0.42
1:A:42:MET:HE3	1:A:43:THR:H	1.84	0.42
1:A:139:GLY:HA2	1:A:143:GLU:OE1	2.20	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: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:5:GLY:O	1:B:6:ALA:HB2	2.20	0.42
1:B:90:SER:O	1:B:90:SER:OG	2.36	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:C:73:ARG:HG2	1:C:74:TRP:H	1.83	0.42
1:C:251:TYR:CD1	1:C:397:ILE:CB	3.02	0.42
1:C:302:THR:O	1:C:302:THR:HG22	2.18	0.42
1:C:348:GLN:HE21	1:C:348:GLN:HB3	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:A:305:ASN:HD22	1:A:481:GLU:HA	1.84	0.42
1:A:360:ARG:O	1:A:363:LYS:HB2	2.19	0.42
1:A:506:PRO:C	1:A:508:ALA:N	2.73	0.42
1:B:46:ARG:H	1:B:46:ARG:HG2	1.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:GLN:C	1:B:195:ALA:H	2.23	0.42
1:C:234:ILE:HD12	1:C:235:GLU:CA	2.48	0.42
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:266:THR:CG2	1:B:411:VAL:HG23	2.50	0.42
1:B:343:MET:HB3	1:B:370:SER:CA	2.49	0.42
1:C:90:SER:OG	1:C:129:HIS:CG	2.73	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:NE2	1:C:348:GLN:O	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: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:3:ILE:HD12	1:A:3:ILE:HG21	1.53	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:421:LYS:C	1:A:423:LYS:N	2.73	0.42
1:B:83:VAL:O	1:B:88:HIS:HE1	2.02	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:533:ILE:CG2	1:C:559:MET:CE	2.98	0.42
1:A:86:HIS:CE1	1:A:124:THR:OG1	2.73	0.42
1:B:33:LEU:HB3	1:B:70:ALA:HB2	2.01	0.42
1:B:61:HIS:O	1:B:61:HIS:CG	2.70	0.42
1:B:205:PHE:N	1:B:205:PHE:CD1	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:C:18:GLU:OE2	1:C:21:ARG:CZ	2.68	0.42
1:C:523:ASN:OD1	1:C:569:GLU:OE2	2.36	0.42
1:C:532:ASN:HD22	1:C:532:ASN:N	2.06	0.42
1:A:36:VAL:CG1	1:A:42:MET:CA	2.84	0.42
1:A:80:PRO:HB2	1:A:83:VAL:HB	2.02	0.42
1:A:599:ARG:C	1:A:601:LEU:H	2.23	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:433:ILE:CG1	1:B:570:VAL:CG2	2.97	0.42
1:B:450:GLN:O	1:B:454:ILE:HG13	2.20	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:32:GLY:CA	1:A:54:LEU:HD21	2.48	0.41
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: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:93:ILE:HG21	1:C:131:VAL:CB	2.49	0.41
1:C:250:HIS:NE2	1:C:589:LEU:HD21	2.35	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:A:32:GLY:HA3	1:A:45:LEU:O	2.20	0.41
1:A:74:TRP:CZ2	1:A:601:LEU:HA	2.55	0.41
1:A:529:LEU:C	1:A:532:ASN:ND2	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:N	1:C:502:LEU:CD1	2.82	0.41
1:B:23:LEU:HA	1:B:23:LEU:HD23	1.84	0.41
1:B:34:ALA:HA	1:B:43:THR:O	2.20	0.41
1:B:276:VAL:CG2	1:B:417:ALA:CB	2.93	0.41
1:B:306:SER:OG	1:B:307:GLY:N	2.53	0.41
1:C:95:VAL:HG13	1:C:96:VAL:H	1.85	0.41
1:C:111:LEU:CD1	1:C:116:TYR:CD2	2.91	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:A:100:ILE:CD1	1:A:607:VAL:CA	2.95	0.41
1:A:224:LYS:HB3	1:A:224:LYS:HE2	1.80	0.41
1:A:276:VAL:O	1:A:276:VAL:CG1	2.68	0.41
1:A:324:VAL:O	1:A:324:VAL:CG1	2.64	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:48:LEU:N	1:A:48:LEU:CD1	2.78	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:353:ALA:HB2	1:A:607:VAL:O	2.20	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:B:118:PHE:CD1	1:B:118:PHE:N	2.88	0.41
1:B:119:VAL:O	1:B:119:VAL:HG23	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: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:C:105:GLU:O	1:C:108:ARG:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:LEU:CD2	1:C:381:LEU:HD22	2.50	0.41
1:A:128:ALA:O	1:A:129:HIS:C	2.54	0.41
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:28:TYR:CE1	1:A:602:ALA:HA	2.53	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:O	1:A:276:VAL:HG13	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:HD23	1:A:409:LEU:HA	1.78	0.41
1:A:457:LEU:O	1:A:458:ALA:C	2.57	0.41
1:A:467:ALA:O	1:A:494:ALA:HA	2.20	0.41
1:A:480:LEU:HD23	1:A:480:LEU:HA	1.58	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: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:B:600:ASN:HA	1:C:539:ARG:NE	2.35	0.41
1:C:61:HIS:O	1:C:63:LEU:HD22	2.20	0.41
1:C:169:LEU:HA	1:C:169:LEU:HD13	1.87	0.41
1:C:192:ASP:OD2	1:C:194:LEU:HB2	2.21	0.41
1:C:399:VAL:HG11	1:C:602:ALA:O	2.18	0.41
1:A:16:LEU:HB3	1:A:70:ALA:HB2	2.02	0.41
1:A:45:LEU:HD12	1:A:45:LEU:HA	1.89	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:356:LEU:HA	1:A:381:LEU:CD2	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:576:TYR:C	1:C:578:VAL:N	2.69	0.41
1:A:74:TRP:CZ3	1:A:602:ALA:O	2.74	0.41
1:A:499:ALA:HB1	1:A:532:ASN:OD1	2.20	0.41
1:B:7:ILE:HD13	1:B:215:THR:HA	2.02	0.41
1:B:234:ILE:H	1:B:234:ILE:HG23	1.63	0.41
1:B:271:ILE:O	1:B:271:ILE:HG22	2.20	0.41
1:B:281:LEU:CD2	1:B:387:LEU:HB3	2.51	0.41
1:B:371:LEU:O	1:B:372:ALA:HB2	2.21	0.41
1:B:390:MET:HA	1:B:390:MET:CE	2.51	0.41
1:B:452:LYS:HA	1:B:452:LYS:HD3	1.81	0.41
1:B:454:ILE:CD1	1:B:582:LEU:HD12	2.48	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: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:421:LYS:HE3	1:C:421:LYS:HB3	1.64	0.41
1:C:437:LEU:O	1:C:440:LEU:CB	2.69	0.41
1:C:447:MET:CE	1:C:578:VAL:HB	2.51	0.41
1:C:514:MET:HB2	1:C:514:MET:HE3	1.85	0.41
1:A:440:LEU:HD21	1:A:574:ILE:HD12	2.03	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:B:7:ILE:H	1:B:7:ILE:HG22	1.50	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:C:7:ILE:HD13	1:C:168:THR:O	2.20	0.41
1:C:45:LEU:CD2	1:C:57:ALA:O	2.69	0.41
1:C:528:LYS:O	1:C:531:SER:N	2.52	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:8:ALA:O	1:B:9:GLN:HB2	2.20	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:487:LYS:CD	1:C:509:LEU:HD11	2.50	0.40
1:B:504:HIS:NE2	1:C:300:CYS:SG	2.95	0.40
1:B:554:VAL:HG23	1:B:554:VAL:O	2.20	0.40
1:B:600:ASN:O	1:C:507:LEU:HD23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ARG:HD3	1:C:207:GLU:O	2.21	0.40
1:A:26:ARG:HG3	1:A:26:ARG:HH11	1.86	0.40
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:28:TYR:CD2	1:C:50:LYS:HD3	2.56	0.40
1:C:33:LEU:CD2	1:C:54:LEU:HD21	2.52	0.40
1:C:55:ALA:O	1:C:58:ALA:HB3	2.20	0.40
1:C:230:LYS:C	1:C:231:ARG:HD3	2.37	0.40
1:B:116:TYR:HE2	1:B:133:TRP:HB2	1.86	0.40
1:B:390:MET:HA	1:B:390:MET:HE2	2.02	0.40
1:B:504:HIS:CE1	1:C:300:CYS:HB3	2.56	0.40
1:C:96:VAL:CG2	1:C:159:VAL:HB	2.52	0.40
1:C:102:GLU:O	1:C:104:HIS:N	2.48	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: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:34:ALA:HB1	1:A:42:MET:CE	2.51	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:402:THR:OG1	1:A:403:LYS:N	2.54	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:105:GLU:N	1:B:106:PRO:HD2	2.34	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:86:HIS:CD2	1:C:88:HIS:NE2	2.89	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:A:22:ARG:O	1:A:194:LEU:HD23	2.22	0.40
1:A:133:TRP:HZ3	1:A:134:GLU:OE2	2.02	0.40
1:A:197:LEU:HD22	1:A:197:LEU:HA	1.51	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:48:LEU:CD1	1:B:82:GLU:HB2	2.51	0.40
1:B:572:ALA:CB	1:B:573:PRO:CD	2.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	0	3
1	B	606/608 (100%)	423 (70%)	113 (19%)	70 (12%)	0	1
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	2

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

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Mol	Chain	Res	Type
1	A	128	ALA
1	A	129	HIS
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

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Mol	Chain	Res	Type
1	C	64	HIS
1	C	81	SER
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

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Mol	Chain	Res	Type
1	C	108	ARG
1	C	130	LEU
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

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Mol	Chain	Res	Type
1	C	299	ALA
1	C	319	GLY
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

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Mol	Chain	Res	Type
1	B	523	ASN
1	C	106	PRO
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	4
1	B	500/500 (100%)	422 (84%)	78 (16%)	2	9
1	C	500/500 (100%)	433 (87%)	67 (13%)	3	13
All	All	1500/1500 (100%)	1248 (83%)	252 (17%)	1	7

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

Sometimes 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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	701	-	14,15,15	1.36	2 (14%)	19,21,21	1.87	5 (26%)
2	G6Q	A	700	-	14,15,15	1.92	5 (35%)	19,21,21	2.84	12 (63%)

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	B	701	-	-	8/19/20/20	-
2	G6Q	A	700	-	-	9/19/20/20	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	G6Q	O5-C5	-3.41	1.36	1.43
2	B	701	G6Q	C3-C2	-2.96	1.48	1.53
2	A	700	G6Q	P-O2P	-2.88	1.44	1.54
2	A	700	G6Q	C3-C2	-2.64	1.49	1.53
2	A	700	G6Q	C6-C5	-2.53	1.48	1.51
2	B	701	G6Q	O4-C4	-2.35	1.37	1.43
2	A	700	G6Q	P-O3P	-2.07	1.47	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	G6Q	O6-C6-C5	4.67	121.82	109.36
2	A	700	G6Q	C6-C5-C4	-4.61	103.52	112.22
2	A	700	G6Q	O2-C2-C1	-4.59	100.05	110.48
2	B	701	G6Q	O2-C2-C1	-4.29	100.73	110.48
2	A	700	G6Q	O5-C5-C4	4.15	118.95	109.25
2	A	700	G6Q	O3P-P-O2P	3.50	120.94	107.80
2	A	700	G6Q	O3P-P-O1P	-3.47	97.30	110.83
2	B	701	G6Q	O4-C4-C3	3.25	117.06	109.46
2	A	700	G6Q	O3-C3-C4	-3.16	102.08	109.46
2	A	700	G6Q	C4-C3-C2	3.04	118.82	113.49
2	B	701	G6Q	C6-C5-C4	-2.86	106.82	112.22
2	B	701	G6Q	O3-C3-C4	-2.54	103.53	109.46
2	A	700	G6Q	O3P-P-O6	2.46	113.08	106.67
2	B	701	G6Q	O6-P-O1P	2.28	112.60	106.44
2	A	700	G6Q	O4-C4-C3	2.27	114.77	109.46
2	A	700	G6Q	O6-P-O1P	2.23	112.47	106.44
2	A	700	G6Q	C3-C2-C1	-2.11	104.62	111.03

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700	G6Q	C4-C5-C6-O6
2	A	700	G6Q	O5-C5-C6-O6
2	A	700	G6Q	C6-O6-P-O1P

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Mol	Chain	Res	Type	Atoms
2	A	700	G6Q	C6-O6-P-O2P
2	A	700	G6Q	C6-O6-P-O3P
2	B	701	G6Q	O2-C2-C3-O3
2	B	701	G6Q	O5-C5-C6-O6
2	B	701	G6Q	O3-C3-C4-O4
2	B	701	G6Q	C2-C3-C4-O4
2	B	701	G6Q	O3-C3-C4-C5
2	A	700	G6Q	O3-C3-C4-O4
2	A	700	G6Q	O3-C3-C4-C5
2	B	701	G6Q	O2-C2-C3-C4
2	A	700	G6Q	C2-C3-C4-O4
2	A	700	G6Q	O2-C2-C3-O3
2	B	701	G6Q	O4-C4-C5-O5
2	B	701	G6Q	C1-C2-C3-O3

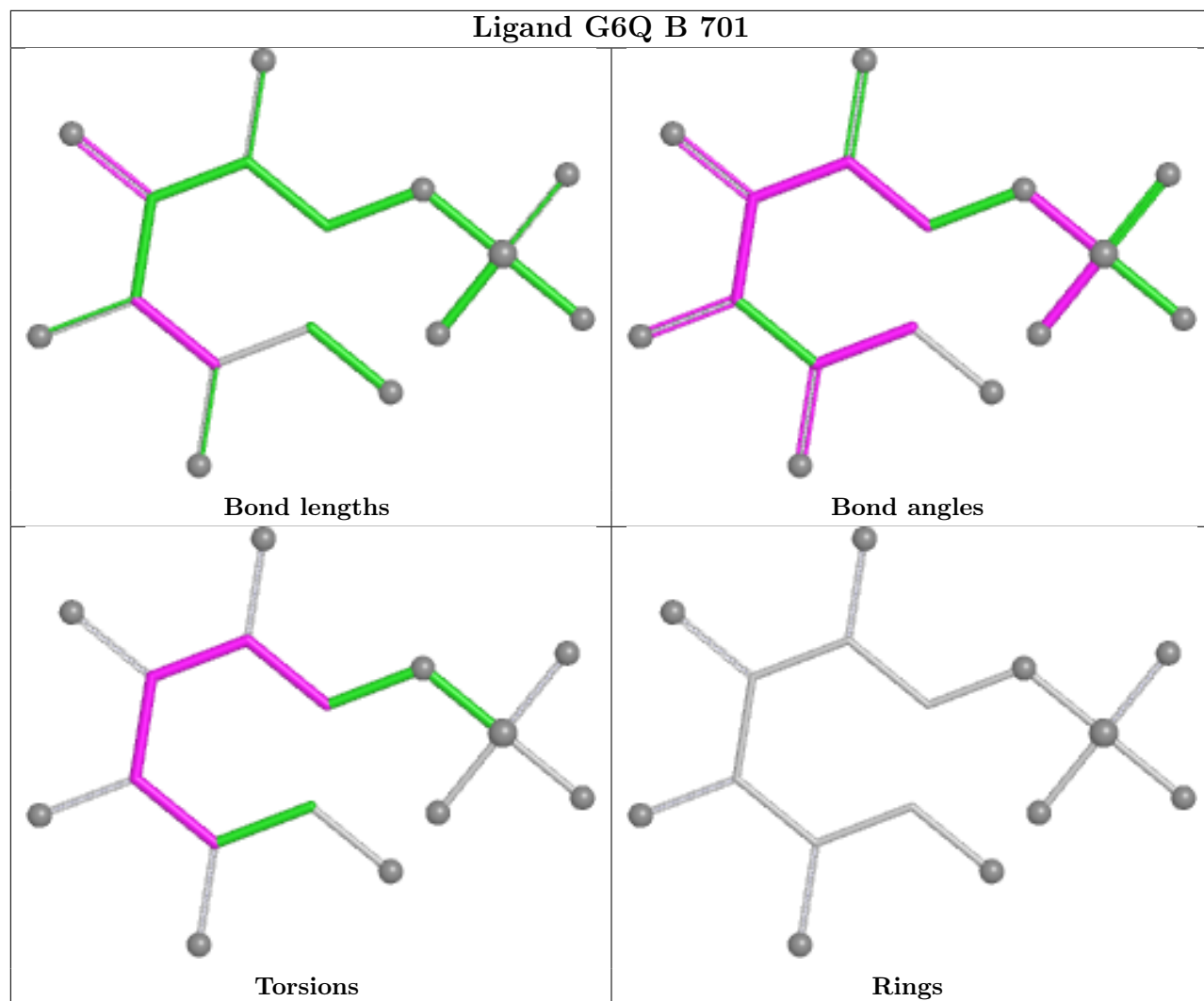
There are no ring outliers.

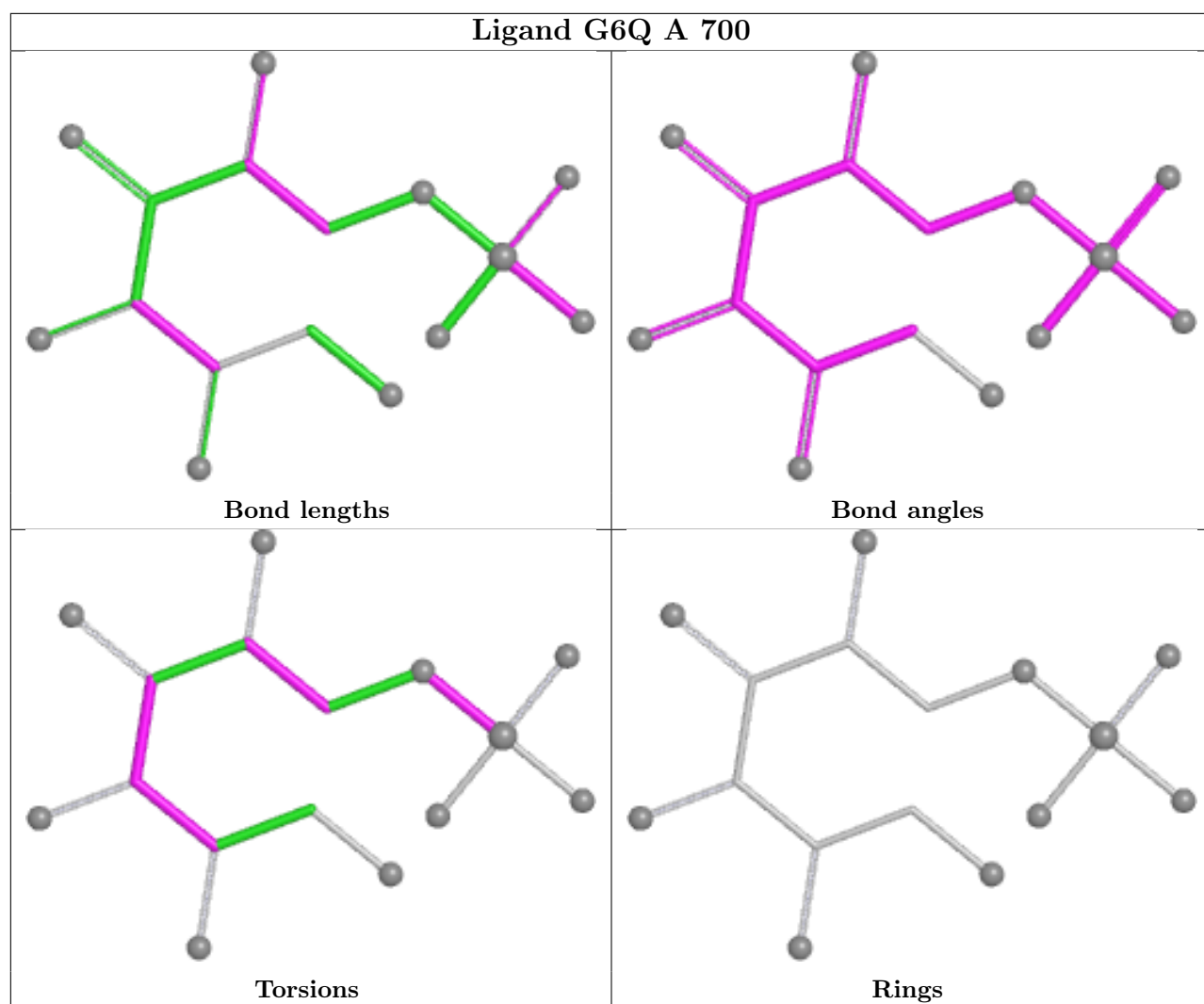
2 monomers are involved in 8 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand G6Q B 701





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	608/608 (100%)	-0.80	5 (0%) 82 68	9, 38, 101, 133	0
1	B	608/608 (100%)	-0.50	4 (0%) 84 70	19, 78, 125, 138	0
1	C	608/608 (100%)	0.01	11 (1%) 67 49	44, 113, 137, 151	0
All	All	1824/1824 (100%)	-0.43	20 (1%) 77 61	9, 79, 131, 151	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	ASN	4.0
1	C	124	THR	3.0
1	C	435	HIS	2.9
1	C	522	ASN	2.7
1	A	88	HIS	2.6
1	C	34	ALA	2.5
1	C	94	VAL	2.4
1	B	240	TYR	2.3
1	A	85	ALA	2.3
1	A	86	HIS	2.3
1	C	89	VAL	2.3
1	C	80	PRO	2.2
1	C	393	ALA	2.2
1	B	271	ILE	2.2
1	A	113	ALA	2.1
1	C	157	GLY	2.1
1	C	235	GLU	2.1
1	C	98	ASN	2.1
1	B	522	ASN	2.0
1	B	61	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

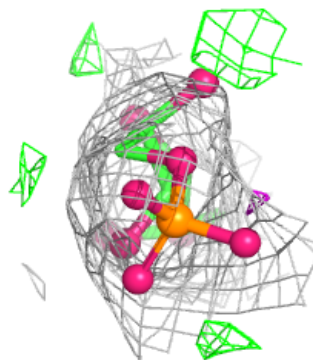
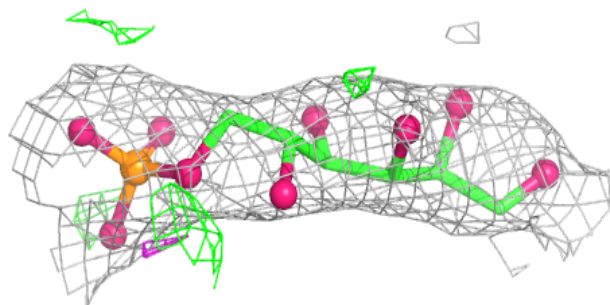
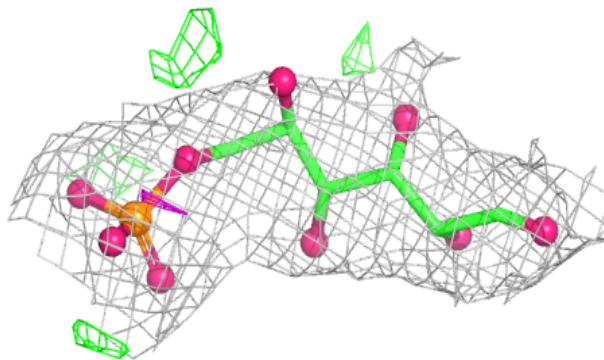
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	G6Q	B	701	16/16	0.90	0.10	62,73,81,84	0
2	G6Q	A	700	16/16	0.94	0.11	25,31,35,36	0

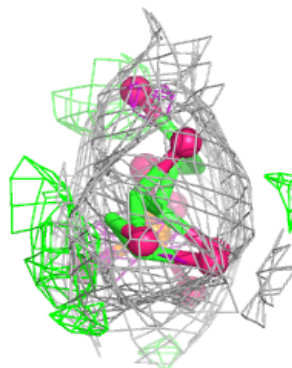
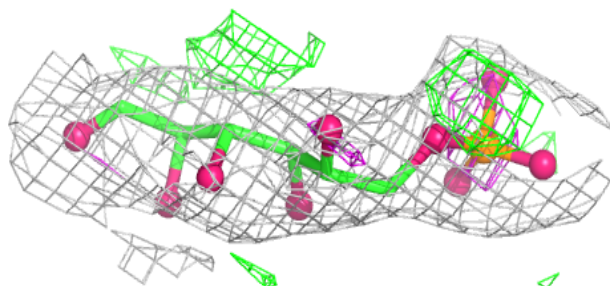
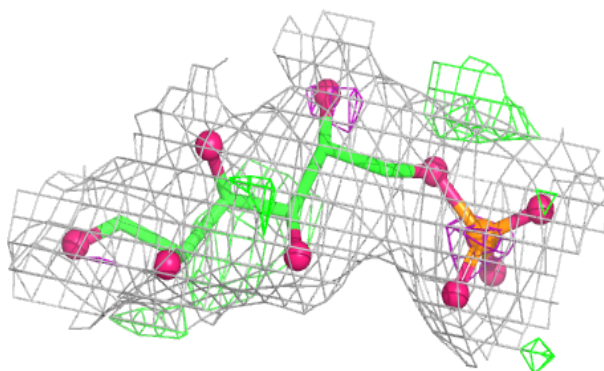
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around G6Q B 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around G6Q A 700:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.