



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:44 PM UTC

PDB ID : 1JXA / pdb_00001jxa
Title : GLUCOSAMINE 6-PHOSPHATE SYNTHASE WITH GLUCOSE 6-PHOSPHATE
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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.

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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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

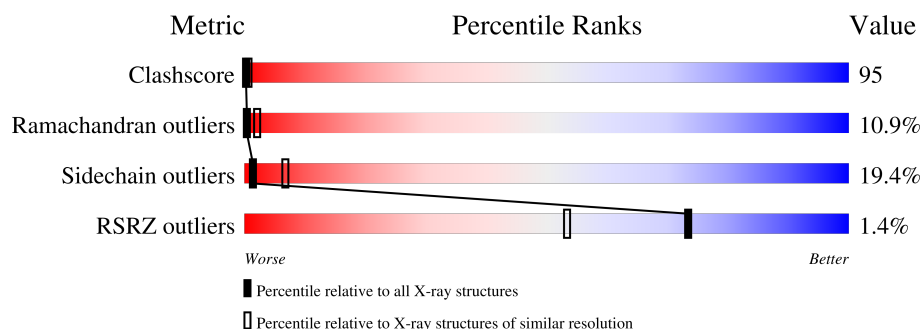
1 Overall quality at a glance

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	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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	% 16% 52% 28% .
1	B	608	% 16% 56% 26% .
1	C	608	3% 19% 61% 18% .

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.

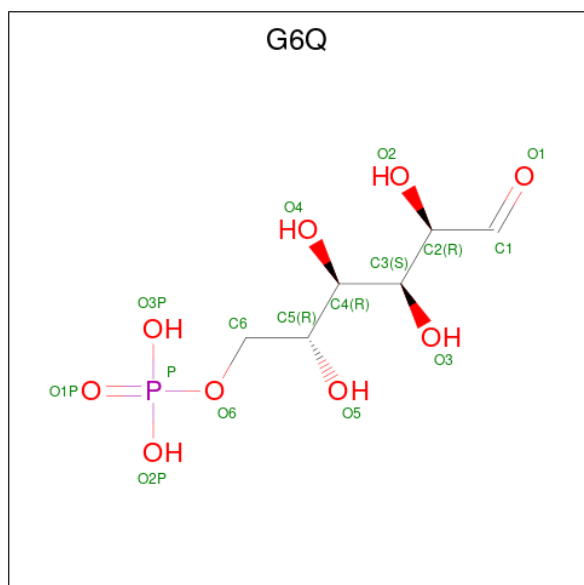
- Molecule 1 is a protein called glucosamine 6-phosphate synthase.

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 (CCD ID: 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		

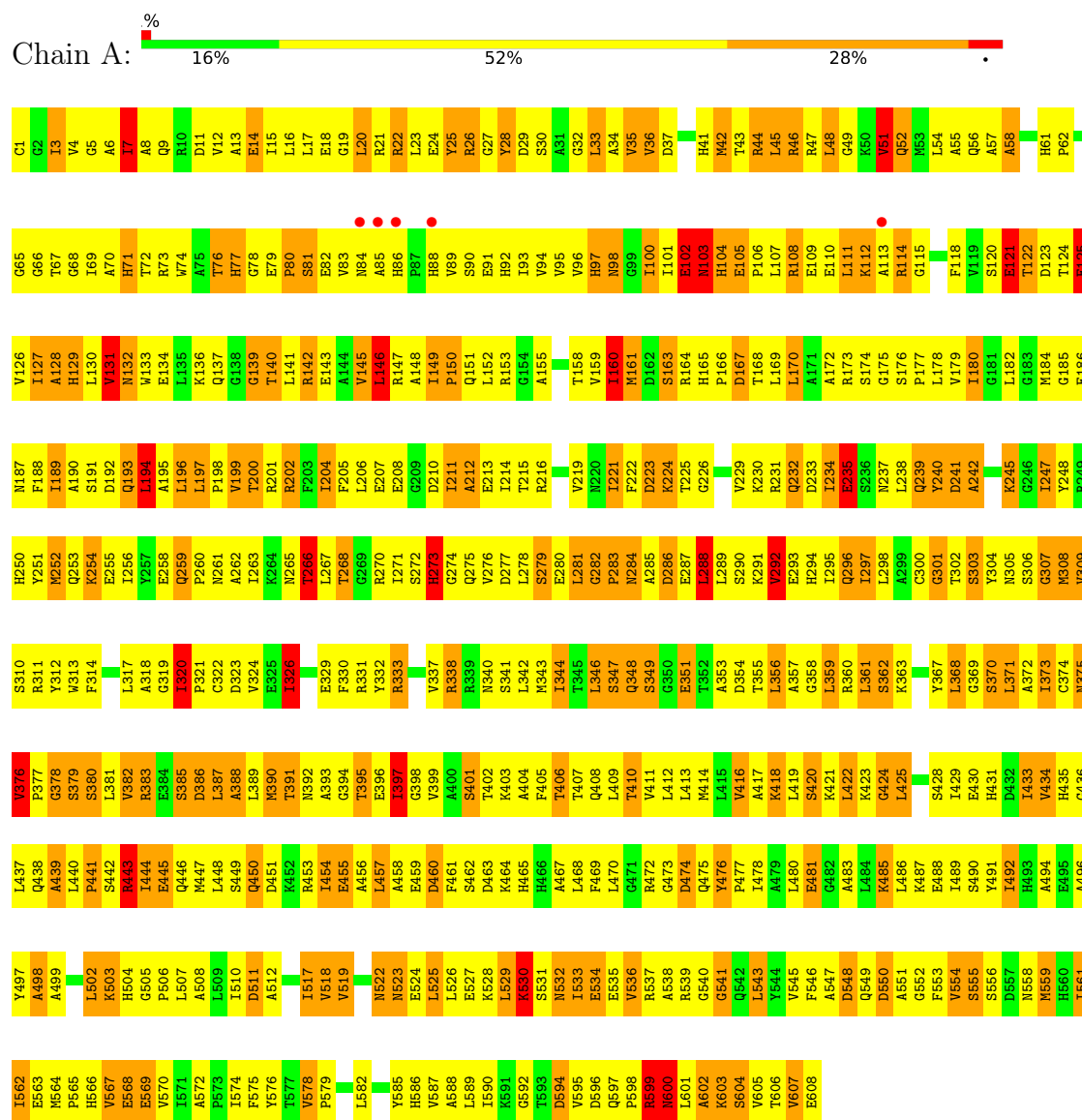
- Molecule 3 is water.

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		

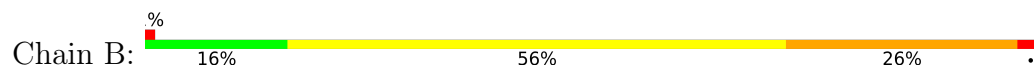
3 Residue-property plots

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





E569	P506	Q446	E384	G322	I256
V570	L507	M447	S385	D323	Y257
I571	A508	L448	D386	V324	E288
A572	L509	S449	L387	E325	Q259
P573	P573	Q450	A388	I326	P260
I574	D511	D451	L389	A327	M261
F575		K452	K390	S328	A262
F576	M514	R453	T391	E329	I263
F577		I454	N392	F330	K264
F578	I517	E455	A393	R331	N265
P579	V518	A456	G394	Y332	T266
L580		L457	T395	R333	
Q581	P521	A458	E396	K334	R270
L582	M522	E459	I397	S335	I271
L583	N523	D460	G398		S272
A584	E524	F461	V399	R338	H273
H585	L525	S462	A400		L278
H586	L526	D463	S401	S341	S279
V587	E527	K464	T402	I342	E280
A588	K528	H465	K403	M343	L281
L589	L529	H466	A404	I344	G282
I590	K530	A467	F405	T345	P283
K591	S531	L468	T406	L346	N284
G592	N532	F469	T407	S347	A285
T593	I533	L470	Q408	Q348	D286
D594	E534	G471	L409	S349	E287
V595	E535	R472	F410	G350	L288
D596	V536	G473	V411	E351	L289
Q597	R537	D474	L412	T352	S290
P598	A538	Q475	L413	A353	K291
R599	R539	Y476	M414	D354	V292
N600	G540	P477	L415	T355	E293
L601	G541	I478	V416	L356	H294
A602	Q542	A479	A417	A357	I295
K603	L543	L480	K418	G358	Q296
S604	Y544	E481		L359	I297
V605	V545	G482	K421	R360	L298
T606	F546	A483	L422	L361	A299
V607	A647	L484	K423	S362	C300
E608	D548	K485	G424	K363	G301
	Q549	L486	L425	E364	T302
	D550	K487	D426	L365	S303
	A551	E488	A427	G366	Y304
	G552	I489	S428	Y367	N305
	F553	S490	I429	L368	S306
	V554	Y491	E430	G369	G307
	S555	I492		S370	M308
	S556	H493	V434	L371	V309
	D557	A494	V435	A372	S310
	N558	E495	H435	I373	R311
	M559	A496	G436	C374	
	H560	Y497	L437	N375	F314
	I561	A498	Q438	V376	E315
	I562	A499	A439	P377	S316
	E563	G500	L440	G378	L317
	M564	E501	P441	S379	A318
	P565	I502	S442	S380	G319
	H566	R503	R443	L381	I320
	V567	H504	I444	V382	P321
	E568	G505	E445	R383	

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: G6Q

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.09	12/4776 (0.3%)	1.64	82/6467 (1.3%)
1	B	0.90	8/4776 (0.2%)	1.36	42/6467 (0.6%)
1	C	0.67	0/4776	1.13	23/6467 (0.4%)
All	All	0.90	20/14328 (0.1%)	1.39	147/19401 (0.8%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	578	VAL	CA-CB	-10.04	1.49	1.54
1	A	262	ALA	CA-CB	-6.73	1.42	1.53
1	A	93	ILE	CA-CB	-6.40	1.46	1.54
1	A	100	ILE	CG1-CD1	6.36	1.76	1.51
1	A	388	ALA	CA-CB	-6.24	1.43	1.53
1	B	55	ALA	CA-CB	-6.17	1.43	1.53
1	B	70	ALA	CA-CB	-6.14	1.45	1.53
1	B	189	ILE	CA-CB	-5.84	1.49	1.55
1	A	160	ILE	CA-CB	-5.58	1.47	1.54
1	A	292	VAL	CA-CB	-5.39	1.47	1.54
1	A	498	ALA	CA-CB	-5.37	1.44	1.53
1	B	69	ILE	CA-CB	-5.36	1.47	1.55
1	A	444	ILE	CA-CB	-5.26	1.47	1.54
1	A	483	ALA	CA-CB	-5.25	1.45	1.53
1	B	51	VAL	CA-CB	-5.24	1.46	1.54
1	A	69	ILE	CA-CB	-5.22	1.47	1.54
1	B	31	ALA	CA-CB	-5.21	1.44	1.53
1	B	7	ILE	CA-CB	-5.08	1.48	1.54
1	B	604	SER	CA-C	-5.06	1.46	1.52
1	A	100	ILE	CA-CB	-5.06	1.48	1.54

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	508	ALA	N-CA-C	-9.41	101.03	114.12
1	A	397	ILE	N-CA-C	-9.27	103.69	112.96
1	A	536	VAL	N-CA-C	-9.18	101.61	110.42
1	A	394	GLY	CA-C-O	-8.80	115.57	122.52
1	A	530	LYS	N-CA-C	-8.64	101.77	111.71
1	A	474	ASP	N-CA-C	-8.47	103.44	112.93
1	A	569	GLU	N-CA-C	-8.34	105.11	114.62
1	A	73	ARG	N-CA-C	8.31	121.70	109.07
1	C	532	ASN	N-CA-C	-8.24	102.25	111.07
1	A	536	VAL	N-CA-CB	8.21	120.16	110.55
1	A	445	GLU	N-CA-C	-8.13	102.11	110.97
1	C	80	PRO	N-CA-C	-8.09	95.80	112.47
1	A	194	LEU	N-CA-C	-8.02	105.48	114.62
1	A	605	VAL	CB-CA-C	-7.64	102.02	111.88
1	A	533	ILE	N-CA-C	-7.62	102.91	110.30
1	A	395	THR	N-CA-C	-7.55	98.27	110.20
1	A	204	ILE	N-CA-C	-7.41	97.06	107.80
1	B	57	ALA	N-CA-C	-7.06	102.41	111.02
1	B	415	LEU	N-CA-C	-7.02	105.26	114.31
1	B	229	VAL	CB-CA-C	-6.98	99.84	111.29
1	A	288	LEU	N-CA-C	-6.93	102.63	112.13
1	B	603	LYS	CA-C-N	-6.86	112.05	122.81
1	B	603	LYS	C-N-CA	-6.86	112.05	122.81
1	B	501	GLU	N-CA-C	-6.79	106.19	114.75
1	A	28	TYR	N-CA-C	6.78	118.41	110.41
1	A	319	GLY	CA-C-N	-6.78	116.95	122.85
1	A	319	GLY	C-N-CA	-6.78	116.95	122.85
1	B	219	VAL	CB-CA-C	-6.74	100.23	111.29
1	A	562	ILE	N-CA-CB	-6.74	104.52	112.40
1	A	550	ASP	N-CA-C	6.66	120.39	112.93
1	C	455	GLU	N-CA-C	-6.60	104.16	111.36
1	A	9	GLN	N-CA-C	-6.59	105.24	113.55
1	B	44	ARG	N-CA-C	-6.57	100.25	110.17
1	C	580	LEU	N-CA-C	-6.56	103.75	111.03
1	C	290	SER	N-CA-C	-6.52	105.90	114.31
1	A	281	LEU	N-CA-C	-6.49	105.28	113.72
1	A	167	ASP	N-CA-C	-6.44	104.47	112.90
1	B	145	VAL	CB-CA-C	-6.44	103.73	111.97
1	A	567	VAL	CB-CA-C	-6.40	100.80	111.29
1	A	394	GLY	N-CA-C	-6.39	104.59	112.33
1	B	599	ARG	N-CA-C	6.39	120.04	110.14
1	A	522	ASN	CB-CA-C	-6.38	102.22	111.91
1	A	200	THR	N-CA-C	6.37	118.09	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	510	ILE	CB-CA-C	-6.37	105.42	112.68
1	B	3	ILE	CB-CA-C	-6.34	104.35	111.45
1	B	605	VAL	CB-CA-C	-6.33	105.46	112.68
1	B	168	THR	N-CA-C	6.30	118.12	108.42
1	B	171	ALA	N-CA-C	-6.29	99.77	109.52
1	A	416	VAL	N-CA-C	-6.26	104.64	110.53
1	B	416	VAL	N-CA-C	-6.24	104.25	110.62
1	A	498	ALA	N-CA-C	-6.21	100.65	109.96
1	B	135	LEU	N-CA-C	-6.20	104.60	111.36
1	A	160	ILE	N-CA-C	6.14	117.56	109.21
1	C	127	ILE	N-CA-C	-6.13	104.77	110.53
1	A	100	ILE	CB-CG1-CD1	6.11	126.63	113.80
1	A	98	ASN	CB-CA-C	-6.11	101.71	110.62
1	A	121	GLU	N-CA-CB	-6.10	100.18	110.49
1	A	387	LEU	N-CA-C	-6.08	100.07	109.24
1	B	347	SER	N-CA-C	6.08	118.34	108.26
1	A	529	LEU	N-CA-C	-6.05	104.25	111.69
1	B	510	ILE	N-CA-C	6.05	115.32	106.55
1	C	601	LEU	N-CA-C	6.01	116.22	108.34
1	A	450	GLN	N-CA-C	-6.00	104.41	113.89
1	A	599	ARG	N-CA-C	5.98	118.05	110.33
1	A	81	SER	N-CA-C	5.94	117.76	111.28
1	A	455	GLU	N-CA-C	-5.93	104.82	111.28
1	A	443	ARG	N-CA-C	-5.92	105.72	113.12
1	C	394	GLY	N-CA-C	-5.92	104.82	111.63
1	B	118	PHE	N-CA-C	5.87	119.26	108.58
1	B	142	ARG	NE-CZ-NH2	5.85	124.47	119.20
1	B	187	ASN	N-CA-C	5.84	118.74	110.50
1	A	235	GLU	CB-CA-C	5.81	119.44	109.51
1	A	382	VAL	CB-CA-C	-5.81	102.85	112.26
1	A	418	LYS	N-CA-C	-5.79	104.66	110.97
1	A	348	GLN	N-CA-C	-5.77	106.28	113.55
1	C	58	ALA	N-CA-C	-5.77	102.25	111.02
1	B	184	MET	N-CA-C	5.77	118.59	108.56
1	A	307	GLY	N-CA-C	-5.76	105.80	112.83
1	A	523	ASN	N-CA-CB	-5.74	102.52	110.38
1	B	53	MET	N-CA-C	-5.73	103.85	111.24
1	A	543	LEU	N-CA-C	5.72	118.02	108.02
1	C	537	ARG	N-CA-C	-5.71	104.96	111.07
1	A	266	THR	N-CA-C	5.70	118.22	111.33
1	B	313	TRP	N-CA-C	-5.69	103.94	111.96
1	B	433	ILE	N-CA-CB	-5.67	106.99	111.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	VAL	CB-CA-C	-5.66	102.00	111.29
1	A	483	ALA	N-CA-C	-5.63	103.98	111.24
1	A	545	VAL	N-CA-C	5.62	116.21	107.28
1	A	22	ARG	NE-CZ-NH1	-5.62	115.88	121.50
1	B	47	ARG	NE-CZ-NH1	-5.62	115.89	121.50
1	B	142	ARG	NE-CZ-NH1	-5.62	115.89	121.50
1	C	518	VAL	CB-CA-C	-5.61	102.27	110.62
1	A	93	ILE	N-CA-C	5.60	116.83	108.54
1	A	252	MET	N-CA-C	-5.55	104.45	111.11
1	A	254	LYS	N-CA-C	-5.55	105.31	111.36
1	C	309	VAL	CB-CA-C	-5.54	104.65	112.14
1	A	291	LYS	CA-C-N	-5.53	114.03	121.66
1	A	291	LYS	C-N-CA	-5.53	114.03	121.66
1	A	297	ILE	N-CA-C	5.52	115.81	107.75
1	B	93	ILE	CB-CA-C	-5.50	104.27	111.81
1	A	320	ILE	CB-CA-C	-5.49	104.62	110.16
1	A	58	ALA	N-CA-C	-5.47	105.72	112.72
1	C	357	ALA	N-CA-C	-5.46	104.72	111.33
1	A	429	ILE	N-CA-C	-5.46	105.52	110.82
1	B	397	ILE	N-CA-C	-5.45	107.51	112.96
1	C	346	LEU	N-CA-C	5.45	119.17	112.03
1	A	376	VAL	CB-CA-C	-5.44	101.46	111.36
1	B	525	LEU	N-CA-C	-5.43	106.43	113.16
1	A	460	ASP	CA-C-N	-5.40	114.17	122.60
1	A	460	ASP	C-N-CA	-5.40	114.17	122.60
1	A	261	ASN	N-CA-CB	5.40	119.20	110.40
1	A	242	ALA	CB-CA-C	-5.39	110.38	116.63
1	A	478	ILE	CB-CA-C	-5.39	104.98	112.04
1	B	116	TYR	N-CA-C	5.36	118.22	109.59
1	C	126	VAL	CB-CA-C	-5.35	105.03	112.04
1	B	203	PHE	N-CA-C	5.34	117.75	107.44
1	A	51	VAL	N-CA-C	-5.34	105.18	110.62
1	A	554	VAL	N-CA-C	5.29	115.73	108.12
1	C	241	ASP	N-CA-C	-5.28	104.12	110.88
1	B	537	ARG	N-CA-C	-5.28	105.42	111.07
1	C	476	TYR	N-CA-C	-5.28	105.43	112.55
1	B	122	THR	CB-CA-C	-5.27	102.02	110.14
1	B	168	THR	CB-CA-C	-5.27	101.58	110.43
1	C	545	VAL	CB-CA-C	-5.27	104.00	111.21
1	B	433	ILE	N-CA-C	-5.25	107.47	111.62
1	A	241	ASP	N-CA-C	-5.25	106.39	114.16
1	B	91	GLU	N-CA-C	-5.25	99.62	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	578	VAL	N-CA-CB	-5.24	107.01	110.52
1	C	570	VAL	CB-CA-C	-5.21	105.29	111.81
1	A	329	GLU	N-CA-C	-5.19	104.57	112.04
1	B	203	PHE	CB-CA-C	-5.19	103.86	111.23
1	B	80	PRO	N-CA-C	-5.18	101.81	112.47
1	C	452	LYS	N-CA-C	-5.17	106.82	113.02
1	A	145	VAL	N-CA-C	-5.17	106.04	110.74
1	A	121	GLU	CA-CB-CG	-5.16	103.78	114.10
1	B	518	VAL	N-CA-C	5.14	115.31	108.27
1	A	322	CYS	N-CA-C	5.10	117.66	108.48
1	C	31	ALA	N-CA-C	5.10	116.92	108.20
1	A	72	THR	CB-CA-C	-5.09	101.64	110.45
1	A	375	ASN	CB-CA-C	-5.08	101.18	109.56
1	A	131	VAL	CB-CA-C	5.08	118.38	111.88
1	A	326	ILE	N-CA-CB	-5.07	105.19	110.82
1	C	474	ASP	N-CA-C	-5.03	107.11	113.20
1	A	569	GLU	CB-CA-C	5.03	115.97	109.28
1	A	98	ASN	N-CA-C	-5.01	99.13	107.80
1	A	476	TYR	CA-C-N	5.01	124.31	118.85
1	A	476	TYR	C-N-CA	5.01	124.31	118.85

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	908	1
1	B	4695	0	4715	957	0
1	C	4695	0	4715	878	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	2700	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 95.

All (2700) 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:A:447:MET:HE1	1:A:564:MET:SD	1.84	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:270:ARG:HD3	1:B:414:MET:HE1	1.26	1.17
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:C:42:MET:HE3	1:C:44:ARG:HB2	1.18	1.16
1:B:529:LEU:HG	1:B:533:ILE:HD11	1.28	1.14
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:A:559:MET:HE3	1:A:561:ILE:HD11	1.28	1.13
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:A:382:VAL:HG21	1:A:390:MET:HE1	1.21	1.12
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:42:MET:HE2	1:B:94:VAL:HG21	1.33	1.07
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: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
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:B:447:MET:HE1	1:B:564:MET:HE1	1.39	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:607:VAL:HG23	1:A:608:GLU:N	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:42:MET:HE2	1:B:94:VAL:CG2	1.95	0.97
1:B:447:MET:HE1	1:B:564:MET:CE	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:553:PHE:HD2	1:A:559:MET:HE1	1.31	0.94
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:B:259:GLN:O	1:B:262:ALA:HB3	1.68	0.94
1:B:559:MET:HE2	1:B:561:ILE:HD11	1.46	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: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:187:ASN:H	1:B:187:ASN:ND2	1.53	0.94
1:C:524:GLU:CD	1:C:524:GLU:H	1.74	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:A:382:VAL:CG2	1:A:390:MET:HE1	1.99	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:447:MET:HE3	1:B:564:MET:SD	2.11	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:C:304:TYR:CE2	1:C:308:MET:HE2	2.06	0.90
1:C:343:MET:C	1:C:344:ILE:HD12	1.97	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:B:600:ASN:CG	1:C:539:ARG:HG3	1.97	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: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:B:214:ILE:HG22	1:B:215:THR:N	1.85	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:184:MET:HE2	1:C:185:GLY:N	1.88	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: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:506:PRO:C	1:C:508:ALA:H	1.83	0.85
1:C:294:HIS:NE2	1:C:338:ARG:HD2	1.91	0.85
1:B:122:THR:C	1:B:124:THR:H	1.82	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ALA:O	1:A:130:LEU:N	2.10	0.84
1:A:279:SER:O	1:A:281:LEU:N	2.10	0.84
1:A:455:GLU:HG3	1:A:586:HIS:CE1	2.10	0.84
1:B:142:ARG:HG2	1:B:142:ARG:HH11	1.34	0.84
1:B:355:THR:O	1:B:358:GLY:N	2.10	0.84
1:C:4:VAL:O	1:C:16:LEU:HD22	1.77	0.84
1: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:A:223:ASP:OD1	1:A:223:ASP:C	2.21	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
1:A:553:PHE:CD2	1:A:559:MET:HE1	2.15	0.82
1:B:294:HIS:HB3	1:B:341:SER:OG	1.80	0.82
1:A:33:LEU:HD23	1:A:33:LEU:C	2.03	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:279:SER:C	1:A:281:LEU:H	1.86	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:469:PHE:C	1:B:470:LEU:HD23	2.05	0.81
1:C:42:MET:HE3	1:C:44:ARG:CB	2.08	0.81
1:C:149:ILE:N	1:C:150:PRO:HD2	1.93	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: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: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
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:522:ASN:CG	1:A:522:ASN:O	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:396:GLU:HG2	1:A:603:LYS:HZ2	1.47	0.79
1:B:344:ILE:HD13	1:B:371:LEU:HD23	1.62	0.79
1:B:391:THR:O	1:B:392:ASN:C	2.26	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:196:LEU:C	1:A:198:PRO:HD2	2.08	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:A:559:MET:CE	1:A:561:ILE:HD11	2.09	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: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:B:305:ASN:O	1:B:306:SER:C	2.26	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:A:410:THR:HG23	1:A:437:LEU:CD2	2.12	0.78
1:B:126:VAL:HG13	1:B:127:ILE:N	1.97	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: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:A:267:LEU:HD23	1:A:414:MET:HE1	1.65	0.78
1:B:169:LEU:O	1:B:170:LEU:HD22	1.84	0.78
1:B:483:ALA:O	1:B:487:LYS:HB3	1.83	0.78
1:C:234:ILE:CD1	1:C:236:SER:H	1.95	0.78
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:308:MET:O	1:A:309:VAL:C	2.23	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:B:270:ARG:HD3	1:B:414:MET:CE	2.12	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: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:447:MET:CE	1:A:564:MET:SD	2.70	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: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:C:304:TYR:CZ	1:C:308:MET:HE2	2.20	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:A:207:GLU:HG3	1:A:231:ARG:CZ	2.15	0.76
1:B:329:GLU:OE2	1:C:472:ARG:HG3	1.84	0.76
1:A:491:TYR:CE1	1:A:599:ARG:CD	2.68	0.76
1:A:410:THR:HG23	1:A:437:LEU:HD22	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:214:ILE:C	1:B:215:THR:HG22	2.10	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: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:B:523:ASN:HD22	1:B:523:ASN:C	1.94	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ILE:HD12	1:B:324:VAL:CG2	2.17	0.74
1:C:79:GLU:C	1:C:81:SER:N	2.45	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: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:559:MET:CG	1:B:559:MET:O	2.35	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:239:GLN:O	1:A:240:TYR:C	2.31	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:B:24:GLU:CD	1:B:597:GLN:HE22	1.95	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:C:184:MET:HE2	1:C:184:MET:C	2.14	0.73
1:A:103:ASN:HD21	1:A:153:ARG:H	0.81	0.73
1:A:377:PRO:HA	1:A:390:MET:HE2	1.70	0.73
1:B:88:HIS:HB2	1:B:124:THR:CG2	2.19	0.73
1:B:146:LEU:HD12	1:B:211:ILE:CD1	2.16	0.73
1:C:399:VAL:HG21	1:C:598:PRO:HD2	1.70	0.73
1:C:413:LEU:CD2	1:C:571:ILE:HG22	2.18	0.73
1:A:100:ILE:CD1	1:A:607:VAL:HA	2.19	0.73
1:A:304:TYR:O	1:A:305:ASN:C	2.32	0.73
1:A:372:ALA:HB2	1:A:385:SER:OG	1.89	0.73
1:C:599:ARG:HG3	1:C:600:ASN:ND2	2.04	0.73
1:B:329:GLU:O	1:B:330:PHE:C	2.30	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:HIS:NE2	1:C:97:HIS:O	2.21	0.73
1:B:214:ILE:CG2	1:B:215:THR:N	2.52	0.73
1:A:165:HIS:HB3	1:A:167:ASP:OD1	1.88	0.72
1:A:267:LEU:HD23	1:A:414:MET:CE	2.19	0.72
1:A:546:PHE:CE1	1:A:562:ILE:HD12	2.23	0.72
1:C:386:ASP:O	1:C:387:LEU:HG	1.89	0.72
1:A: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:164:ARG:C	1:A:165:HIS:ND1	2.48	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: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:A:15:ILE:O	1:A:16:LEU:C	2.32	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:36:VAL:HG12	1:B:37:ASP:N	1.99	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:B:304:TYR:CE2	1:B:308:MET:HE2	2.25	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:390:MET:HA	1:B:390:MET:HE2	1.72	0.71
1:C:447:MET:CE	1:C:579:PRO:HD3	2.21	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: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: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:O	1:B:559:MET:HG2	1.91	0.70
1:B:56:GLN:O	1:B:57:ALA:C	2.31	0.70
1:B:344:ILE:HD13	1:B:371:LEU:HD22	1.71	0.70
1:B:526:LEU:O	1:B:526:LEU:HD12	1.91	0.70
1:C:343:MET:HE2	1:C:367:TYR:CE2	2.26	0.70
1:A:33:LEU:HA	1:A:70:ALA:HA	1.72	0.70
1:A:107:LEU:O	1:A:108:ARG:C	2.33	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:A:511:ASP:C	1:A:511:ASP:OD1	2.33	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:B:559:MET:HE3	1:B:561:ILE:HD11	1.71	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:A:388:ALA:C	1:A:389:LEU:HD12	2.16	0.70
1:B:162:ASP:C	1:B:164:ARG:H	1.99	0.70
1:C:457:LEU:CD2	1:C:562:ILE:CD1	2.61	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:33:LEU:N	1:A:33:LEU:CD2	2.52	0.70
1:B:413:LEU:C	1:B:415:LEU:H	1.98	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:141:LEU:C	1:A:143:GLU:H	2.00	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:C:506:PRO:C	1:C:508:ALA:N	2.49	0.69
1:B:524:GLU:H	1:B:524:GLU:CD	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:LEU:CD1	1:C:559:MET:HE3	2.22	0.69
1:A:185:GLY:O	1:A:216:ARG:CB	2.38	0.69
1:A:197:LEU:N	1:A:198:PRO:CD	2.55	0.69
1:B:517:ILE:HG23	1:B:546:PHE:CE1	2.28	0.69
1: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
1:B:33:LEU:CD2	1:B:33:LEU:N	2.50	0.68
1:B:289:LEU:C	1:B:292:VAL:HG23	2.16	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:374:CYS:HB3	1:A:390:MET:HE3	1.76	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:B:14:GLU:O	1:B:15:ILE:C	2.34	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: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:111:LEU:O	1:A:112:LYS:C	2.36	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:B:252:MET:HE2	1:B:489:ILE:HD13	1.76	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:36:VAL:HG12	1:A:41:HIS:C	2.19	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:C:543:LEU:HD13	1:C:559:MET:HE3	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:485:LYS:O	1:B:486:LEU:C	2.37	0.67
1:A:33:LEU:C	1:A:33:LEU:CD2	2.67	0.67
1:B:447:MET:CE	1:B:564:MET:HE1	2.20	0.67
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:327:ALA:C	1:C:329:GLU:H	2.01	0.67
1:C:461:PHE:HZ	1:C:517:ILE:HD11	1.59	0.67
1:A:145:VAL:O	1:A:147:ARG:N	2.28	0.67
1:A:237:ASN:O	1:A:239:GLN:N	2.24	0.67
1:A:491:TYR:CZ	1:A:599:ARG:CD	2.67	0.67
1:C:17:LEU:CD2	1:C:33:LEU:HD13	2.24	0.67
1: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:B:37:ASP:C	1:B:37:ASP:OD1	2.37	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:237:ASN:C	1:A:239:GLN:H	2.03	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:457:LEU:HD21	1:B:562:ILE:HD11	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:607:VAL:O	1:B:608:GLU:C	2.38	0.66
1:C:476:TYR:O	1:C:479:ALA:HB3	1.96	0.66
1:C:578:VAL:O	1:C:581:GLN:HB2	1.95	0.66
1:A:485:LYS:O	1:A:488:GLU:N	2.28	0.66
1:B:270:ARG:NE	1:B:280:GLU:OE1	2.28	0.66
1:C:18:GLU:CA	1:C:21:ARG:HH11	2.07	0.66
1:A:197:LEU:N	1:A:198:PRO:HD2	2.10	0.66
1:A:346:LEU:HD21	1:A:408:GLN:HG2	1.74	0.66
1:A:529:LEU:CA	1:A:532:ASN:HD21	2.09	0.66
1:B: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:B:587:VAL:C	1:B:590:ILE:HD12	2.20	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:C:524:GLU:CD	1:C:524:GLU:N	2.49	0.66
1:C:565:PRO:O	1:C:566:HIS:C	2.39	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: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:A:485:LYS:O	1:A:486:LEU:C	2.37	0.66
1:B:234:ILE:CG1	1:B:235:GLU:N	2.59	0.66
1:A:76:THR:C	1:A:78:GLY:H	2.03	0.65
1:A:399:VAL:HG21	1:A:597:GLN:HA	1.77	0.65
1:B:214:ILE:C	1:B:215:THR:CG2	2.69	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:318:ALA:C	1:C:320:ILE:H	2.02	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:437:LEU:O	1:A:439:ALA:N	2.27	0.65
1:B:263:ILE:HD12	1:B:444:ILE:HD12	1.79	0.65
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:B:167:ASP:C	1:B:167:ASP:OD1	2.39	0.65
1:C:12:VAL:O	1:C:13:ALA:C	2.39	0.65
1:A:128:ALA:C	1:A:130:LEU:H	2.05	0.65
1:A:305:ASN:ND2	1:A:481:GLU:HA	2.12	0.65
1:A:503:LYS:HD3	1:A:535:GLU:CD	2.22	0.65
1:B:252:MET:CE	1:B:489:ILE:HD13	2.27	0.65
1:C:279:SER:O	1:C:280:GLU:C	2.40	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:448:LEU:C	1:A:450:GLN:H	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:370:SER:HG	1:C:386:ASP:H	1.46	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:B:316:SER:HG	1:B:317:LEU:HG	1.62	0.64
1:B:594:ASP:O	1:B:595:VAL:C	2.39	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:B:492:ILE:O	1:B:494:ALA:N	2.29	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:B:118:PHE:C	1:B:120:SER:H	2.04	0.64
1:C:158:THR:HG23	1:C:172:ALA:O	1.97	0.64
1:A:20:LEU:O	1:A:21:ARG:C	2.39	0.64
1:A:103:ASN:C	1:A:105:GLU:H	2.05	0.64
1:A:434:VAL:O	1:A:435:HIS:C	2.41	0.64
1:B:78:GLY:H	1:C:538:ALA:HB2	1.63	0.64
1:A:32:GLY:HA2	1:A:54:LEU:HD21	1.77	0.64
1:A:371:LEU:CD1	1:A:371:LEU:C	2.66	0.64
1:B:90:SER:CB	1:B:129:HIS:ND1	2.60	0.64
1:B:334:LYS:HD2	1:B:334:LYS:C	2.23	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:LEU:O	1:C:451:ASP:OD1	2.15	0.64
1:B:310:SER:HB2	1:B:412:LEU:CD1	2.28	0.63
1:B:413:LEU:O	1:B:415:LEU:N	2.31	0.63
1:C:565:PRO:O	1:C:566:HIS:O	2.17	0.63
1:A:185:GLY:O	1:A:216:ARG:O	2.16	0.63
1:A: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: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: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: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:A:128:ALA:C	1:A:130:LEU:N	2.55	0.63
1:B:398:GLY:O	1:B:603:LYS:NZ	2.28	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:447:MET:HE1	1:C:579:PRO:HD3	1.81	0.63
1:A:74:TRP:CE3	1:A:602:ALA:HB3	2.33	0.62
1:A:436:GLY:O	1:A:437:LEU:C	2.43	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:80:PRO:O	1:C:84:ASN:CG	2.42	0.62
1:C:299:ALA:HB1	1:C:303:SER:HB3	1.81	0.62
1:A:84:ASN:HB2	1:A:121:GLU:CD	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:97:HIS:C	1:A:97:HIS:ND1	2.57	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: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
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: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:474:ASP:C	1:A:474:ASP:OD1	2.40	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:B:523:ASN:ND2	1:B:523:ASN:C	2.56	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:B:67:THR:OG1	1:B:166:PRO:O	2.17	0.62
1:B:122:THR:C	1:B:124:THR:N	2.49	0.62
1:B:402:THR:OG1	1:B:403:LYS:N	2.28	0.62
1:B:481:GLU:OE2	1:B:485:LYS:NZ	2.25	0.62
1:C:544:TYR:CE2	1:C:560:HIS:HD2	2.18	0.62
1:A:437:LEU:C	1:A:439:ALA:H	2.08	0.61
1:A:540:GLY:O	1:A:541:GLY:C	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:330:PHE:CD1	1:A:330:PHE:C	2.78	0.61
1:A:489:ILE:HG13	1:A:588:ALA:HB2	1.81	0.61
1:B:140:THR:O	1:B:141:LEU:C	2.43	0.61
1:A:239:GLN:O	1:A:241:ASP:N	2.33	0.61
1:A:267:LEU:CD2	1:A:414:MET:HE3	2.28	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:A:110:GLU:O	1:A:111:LEU:C	2.42	0.61
1:A:310:SER:O	1:A:313:TRP:N	2.34	0.61
1:B:124:THR:O	1:B:127:ILE:N	2.33	0.61
1:A:375:ASN:HA	1:A:391:THR:OG1	2.00	0.61
1:B:3:ILE:C	1:B:4:VAL:HG23	2.26	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: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:467:ALA:O	1:C:494:ALA:HA	2.00	0.61
1:A:184:MET:C	1:A:186:GLU:H	2.09	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: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: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:42:MET:CE	1:C:44:ARG:HE	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:HIS:HB3	1:C:596:ASP:OD1	2.00	0.61
1:A:271:ILE:HD11	1:A:414:MET:HE2	1.83	0.61
1:A:272:SER:O	1:A:273:HIS:CB	2.40	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: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:A:102:GLU:C	1:A:104:HIS:H	2.08	0.60
1:A:277:ASP:C	1:A:277:ASP:OD1	2.44	0.60
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:145:VAL:C	1:A:147:ARG:H	2.09	0.60
1:A:165:HIS:C	1:A:167:ASP:H	2.07	0.60
1:A:276:VAL:HG21	1:A:414:MET:HG2	1.81	0.60
1:A:559:MET:HE3	1:A:561:ILE:CD1	2.17	0.60
1:B:22:ARG:HH11	1:B:22:ARG:CG	2.13	0.60
1:B:283:PRO:C	1:B:285:ALA:H	2.09	0.60
1:C:93:ILE:HG21	1:C:131:VAL:HB	1.83	0.60
1:B:79:GLU:O	1:B:80:PRO:C	2.44	0.60
1:B:338:ARG:NE	1:C:321:PRO:HB3	2.15	0.60
1:C:42:MET:HE1	1:C:44:ARG:HH21	1.66	0.60
1:C:487:LYS:C	1:C:489:ILE:H	2.08	0.60
1:A:3:ILE:HG22	1:A:191:SER:HB3	1.82	0.60
1:A:371:LEU:HD12	1:A:371:LEU:C	2.25	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:B:162:ASP:C	1:B:162:ASP:OD1	2.43	0.60
1:B:484:LEU:C	1:B:485:LYS:HG2	2.18	0.60
1:B:501:GLU:CD	1:C:326:ILE:HD12	2.25	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:C:90:SER:O	1:C:91:GLU:HB2	2.01	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:C:447:MET:C	1:C:449:SER:N	2.58	0.60
1:A:180:ILE:CD1	1:A:214:ILE:HD11	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:20:LEU:O	1:B:21:ARG:C	2.45	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:C:330:PHE:C	1:C:332:TYR:H	2.09	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
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:C:74:TRP:CZ3	1:C:602:ALA:HB2	2.37	0.59
1:C:278:LEU:HD21	1:C:414:MET:HE3	1.84	0.59
1:A:553:PHE:CD2	1:A:559:MET:CE	2.77	0.59
1:B:32:GLY:HA3	1:B:46:ARG:HA	1.84	0.59
1:B:237:ASN:C	1:B:239:GLN:HE22	2.10	0.59
1:C:18:GLU:OE2	1:C:21:ARG:NH1	2.35	0.59
1:B:32:GLY:CA	1:B:54:LEU:HD22	2.31	0.59
1:B:394:GLY:HA3	1:B:403:LYS:NZ	2.17	0.59
1:B:454:ILE:HD12	1:B:582:LEU:HD12	1.84	0.59
1:B:487:LYS:HD3	1:C:509:LEU:HD11	1.84	0.59
1:C: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: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: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:421:LYS:O	1:B:424:GLY:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:304:TYR:O	1:B:305:ASN:C	2.44	0.59
1:B:359:LEU:HD13	1:B:384:GLU:O	2.02	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:347:SER:OG	2:A:700:G6Q:O2P	2.14	0.59
1:A:461:PHE:O	1:A:462:SER:C	2.43	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
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:A:602:ALA:O	1:A:603:LYS:C	2.44	0.59
1:B:261:ASN:O	1:B:264:LYS:HB3	2.03	0.59
1:A:348:GLN:NE2	1:A:348:GLN:C	2.61	0.58
1:A:430:GLU:O	1:A:431:HIS:C	2.43	0.58
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:C:434:VAL:C	1:C:436:GLY:H	2.08	0.58
1:A:13:ALA:O	1:A:15:ILE:N	2.36	0.58
1:A:25:TYR:CD1	1:A:25:TYR:C	2.81	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:A:606:THR:C	1:A:607:VAL:O	2.43	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:419:LEU:O	1:B:423:LYS:HG2	2.02	0.58
1:C:28:TYR:C	1:C:50:LYS:HB3	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:523:ASN:CG	1:C:569:GLU:OE2	2.46	0.58
1:A:47:ARG:NE	1:A:57:ALA:HB2	2.18	0.58
1:A:124:THR:C	1:A:126:VAL:H	2.10	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:42:MET:HE1	1:C:44:ARG:HE	1.69	0.58
1:C:418:LYS:O	1:C:422:LEU:HB2	2.03	0.58
1:A:270:ARG:O	1:A:277:ASP:N	2.32	0.58
1:A:375:ASN:OD1	1:A:393:ALA:HB3	2.04	0.58
1:A:551:ALA:CB	1:A:553:PHE:HD1	2.17	0.58
1:B:273:HIS:O	1:B:275:GLN:HG3	2.03	0.58
1:B:523:ASN:OD1	1:B:525:LEU:HB2	2.03	0.58
1:C:311:ARG:HA	1:C:322:CYS:SG	2.44	0.58
1:C:318:ALA:O	1:C:320:ILE:N	2.37	0.58
1:A:54:LEU:O	1:A:55:ALA:C	2.46	0.58
1:B:246:GLY:O	1:B:247:ILE:C	2.46	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:A:305:ASN:O	1:A:308:MET:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:ARG:C	1:B:313:TRP:H	2.12	0.58
1:C:107:LEU:O	1:C:108:ARG:C	2.47	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: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: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:105:GLU:C	1:B:107:LEU:H	2.12	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: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:A:13:ALA:C	1:A:15:ILE:H	2.12	0.57
1:A:192:ASP:O	1:A:194:LEU:N	2.37	0.57
1:A:409:LEU:CD1	1:A:574:ILE:HG12	2.34	0.57
1:B:36:VAL:HG21	1:B:163:SER:HA	1.87	0.57
1:B:498:ALA:O	1:B:499:ALA:C	2.46	0.57
1:B:499:ALA:C	1:B:501:GLU:H	2.13	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:450:GLN:O	1:A:451:ASP:C	2.47	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:B:207:GLU:O	1:B:208:GLU:C	2.45	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:C:341:SER:OG	1:C:367:TYR:CD2	2.53	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:B:334:LYS:C	1:B:334:LYS:CD	2.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:564:MET:HG3	1:C:576:TYR:CE1	2.40	0.57
1:A:141:LEU:C	1:A:143:GLU:N	2.63	0.57
1:A:344:ILE:HG22	1:A:344:ILE:O	2.03	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: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:252:MET:HE3	1:A:402:THR:HG21	1.86	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
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:296:GLN:HE21	1:A:296:GLN:C	2.13	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:C:562:ILE:HG22	1:C:564:MET:HE3	1.87	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:44:ARG:CZ	1:B:46:ARG:HH21	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:GLN:C	1:B:195:ALA:N	2.59	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: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:B:38:ALA:HB3	1:B:39:GLU:CD	2.30	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:206:LEU:HB3	1:C:210:ASP:CG	2.30	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:A:547:ALA:O	1:A:548:ASP:C	2.47	0.56
1:B:164:ARG:C	1:B:165:HIS:CD2	2.83	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:68:GLY:C	1:B:69:ILE:HG23	2.30	0.56
1:B:338:ARG:NH2	1:C:315:GLU:OE2	2.39	0.56
1:B:425:LEU:HG	1:B:426:ASP:H	1.71	0.56
1:B:433:ILE:CG1	1:B:570:VAL:HG21	2.35	0.56
1:A: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:53:MET:O	1:B:54:LEU:C	2.47	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:A:255:GLU:CD	1:A:398:GLY:H	2.14	0.56
1:A:361:LEU:O	1:A:362:SER:C	2.49	0.56
1:A:476:TYR:N	1:A:477:PRO:CD	2.68	0.56
1:B:253:GLN:O	1:B:256:ILE:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:22:ARG:C	1:A:23:LEU:HD23	2.30	0.56
1:A:28:TYR:HE1	1:A:602:ALA:HA	1.70	0.56
1:A:288:LEU:O	1:A:289:LEU:C	2.49	0.56
1:B:276:VAL:CG1	1:B:434:VAL:HG22	2.32	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:132:ASN:C	1:A:132:ASN:OD1	2.49	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:68:GLY:C	1:B:69:ILE:CG2	2.79	0.56
1:B:134:GLU:O	1:B:147:ARG:NH2	2.34	0.56
1:B:413:LEU:C	1:B:415:LEU:N	2.62	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:377:PRO:HA	1:C:390:MET:HE2	1.88	0.56
1:C:434:VAL:C	1:C:436:GLY:N	2.64	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: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: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
1:C:156:TYR:HE2	1:C:158:THR:HG22	1.71	0.56
1:C:487:LYS:C	1:C:489:ILE:N	2.64	0.56
1:A:259:GLN:O	1:A:263:ILE:HG13	2.07	0.55
1:B:159:VAL:HG22	1:B:171:ALA:HB2	1.88	0.55
1:B:286:ASP:CB	1:B:422:LEU:HD11	2.36	0.55
1:B:304:TYR:CZ	1:B:308:MET:HE2	2.40	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:B:193:GLN:O	1:B:194:LEU:C	2.48	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:11:ASP:C	1:B:13:ALA:H	2.12	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:351:GLU:O	1:C:352:THR:C	2.46	0.55
1:C:382:VAL:HG11	1:C:390:MET:HE1	1.88	0.55
1:C:517:ILE:CD1	1:C:544:TYR:HB2	2.35	0.55
1:A:282:GLY:O	1:A:284:ASN:N	2.40	0.55
1:B:101:ILE:N	1:B:123:ASP:OD2	2.39	0.55
1:B: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: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:311:ARG:C	1:B:313:TRP:N	2.65	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
1:C:127:ILE:O	1:C:128:ALA:C	2.50	0.55
1:C:476:TYR:O	1:C:479:ALA:N	2.40	0.55
1:A:210:ASP:OD1	1:A:231:ARG:NH2	2.38	0.55
1:A:536:VAL:O	1:A:537:ARG:C	2.50	0.55
1:B:126:VAL:CG1	1:B:127:ILE:N	2.69	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:C:447:MET:HE1	1:C:575:PHE:O	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:298:LEU:HD11	1:A:343:MET:HE1	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:C:447:MET:C	1:C:449:SER:H	2.14	0.54
1:A:486:LEU:HD11	1:A:587:VAL:HG11	1.88	0.54
1:B:110:GLU:OE2	1:B:114:ARG:NH2	2.41	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: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:279:SER:C	1:A:281:LEU:N	2.51	0.54
1:A:308:MET:C	1:A:310:SER:N	2.65	0.54
1:A:348:GLN:C	1:A:348:GLN:CD	2.76	0.54
1:A:371:LEU:HD22	1:A:387:LEU:HB3	1.89	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
1:B:350:GLY:O	1:B:381:LEU:CB	2.56	0.54
1:B:396:GLU:CD	1:B:401:SER:HA	2.33	0.54
1:C:286:ASP:OD1	1:C:422:LEU:CD1	2.55	0.54
1:C:543:LEU:HD13	1:C:559:MET:HE2	1.89	0.54
1:A:42:MET:O	1:A:43:THR:OG1	2.21	0.54
1:A:103:ASN:C	1:A:106:PRO:HD2	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:251:TYR:O	1:A:252:MET:C	2.49	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: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: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:498:ALA:O	1:C:499:ALA:C	2.51	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:A:74:TRP:CD1	1:A:76:THR:HG1	2.26	0.54
1:A:552:GLY:O	1:A:553:PHE:C	2.50	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:C:318:ALA:C	1:C:320:ILE:N	2.64	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:273:HIS:C	1:A:275:GLN:H	2.15	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
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: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:252:MET:HE2	1:A:256:ILE:HD11	1.90	0.53
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:91:GLU:CD	1:B:132:ASN:HD21	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:594:ASP:HB3	1:B:597:GLN:C	2.34	0.53
1:C:469:PHE:CE2	1:C:482:GLY:C	2.86	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:298:LEU:HD11	1:B:343:MET:HE1	1.90	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: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:C:327:ALA:C	1:C:329:GLU:N	2.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:509:LEU:C	1:B:510:ILE:HD13	2.34	0.53
1:B:556:SER:C	1:B:558:ASN:H	2.15	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: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: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: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: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:228:GLU:CG	1:B:229:VAL:H	2.22	0.53
1:B:234:ILE:HG13	1:B:235:GLU:N	2.20	0.53
1:B:287:GLU:HB3	1:B:288:LEU:HD12	1.90	0.53
1:C:344:ILE:CG2	1:C:345:THR:N	2.71	0.53
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:34:ALA:C	1:B:35:VAL:CG1	2.81	0.52
1:B:94:VAL:C	1:B:95:VAL:HG23	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:GLU:C	1:B:107:LEU:N	2.64	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:C:300:CYS:SG	1:C:327:ALA:HB3	2.48	0.52
1:C:307:GLY:C	1:C:324:VAL:HG21	2.33	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:A:382:VAL:O	1:A:382:VAL:CG1	2.52	0.52
1:A:594:ASP:O	1:A:595:VAL:C	2.48	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:13:ALA:C	1:A:15:ILE:N	2.66	0.52
1:A:145:VAL:C	1:A:147:ARG:N	2.68	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:251:TYR:H	1:A:596:ASP:CG	2.17	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:236:SER:OG	1:B:237:ASN:N	2.41	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:16:LEU:HD11	1:A:68:GLY:C	2.34	0.52
1:A:26:ARG:HE	1:A:604:SER:HB3	1.75	0.52
1:A:103:ASN:C	1:A:105:GLU:N	2.68	0.52
1:A:223:ASP:CG	1:A:224:LYS:N	2.65	0.52
1:A:391:THR:HG22	1:A:407:THR:CB	2.39	0.52
1:A:410:THR:CG2	1:A:437:LEU:HD22	2.38	0.52
1:B:286:ASP:O	1:B:287:GLU:C	2.50	0.52
1:B:307:GLY:C	1:B:324:VAL:HG21	2.34	0.52
1:C:188:PHE:CE2	1:C:199:VAL:HG23	2.45	0.52
1:C:537:ARG:HG3	1:C:543:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:C:439:ALA:O	1:C:440:LEU:C	2.53	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: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:C:526:LEU:O	1:C:527:GLU:C	2.49	0.52
1:C:576:TYR:O	1:C:577:THR:C	2.53	0.52
1:A:286:ASP:N	1:A:286:ASP:OD1	2.42	0.51
1:A:358:GLY:O	1:A:359:LEU:C	2.51	0.51
1:B:487:LYS:HG3	1:C:509:LEU:HD21	1.92	0.51
1:C:382:VAL:CG1	1:C:390:MET:HE1	2.40	0.51
1:A:18:GLU:OE1	1:A:18:GLU:CA	2.57	0.51
1:A:589:LEU:O	1:A:592:GLY:N	2.44	0.51
1:B:88:HIS:HB2	1:B:124:THR:HG21	1.91	0.51
1:B:259:GLN:O	1:B:262:ALA:CB	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:LEU:N	1:C:33:LEU:HD23	2.25	0.51
1:C:130:LEU:HD23	1:C:130:LEU:C	2.35	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:547:ALA:CB	1:C:553:PHE:HD2	2.23	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:142:ARG:HG2	1:A:142:ARG:O	2.09	0.51
1:A:469:PHE:O	1:A:496:ALA:HA	2.11	0.51
1:B:294:HIS:HA	1:B:321:PRO:HG2	1.93	0.51
1:B:451:ASP:O	1:B:452:LYS:C	2.53	0.51
1:C:173:ARG:HB2	1:C:178:LEU:CD1	2.40	0.51
1:C:381:LEU:C	1:C:383:ARG:N	2.67	0.51
1:C:423:LYS:HD3	1:C:425:LEU:CG	2.34	0.51
1:C:523:ASN:ND2	1:C:569:GLU:CD	2.69	0.51
1:A:25:TYR:HD1	1:A:25:TYR:C	2.17	0.51
1:A:142:ARG:HG3	1:A:213:GLU:HB2	1.91	0.51
1:B:355:THR:O	1:B:356:LEU:C	2.53	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:524:GLU:N	1:B:524:GLU:CD	2.65	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:A:143:GLU:O	1:A:147:ARG:HG3	2.11	0.51
1:A:165:HIS:C	1:A:167:ASP:N	2.67	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:179:VAL:HG23	1:B:204:ILE:C	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:573:PRO:O	1:C:574:ILE:C	2.51	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: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: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:124:THR:C	1:A:126:VAL:N	2.69	0.51
1:A:285:ALA:C	1:A:287:GLU:H	2.18	0.51
1:A:411:VAL:O	1:A:414:MET:N	2.44	0.51
1:A:464:LYS:C	1:A:465:HIS:ND1	2.69	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:B:458:ALA:O	1:B:459:GLU:C	2.53	0.50
1:C:56:GLN:C	1:C:58:ALA:H	2.18	0.50
1:A:159:VAL:O	1:A:159:VAL:HG12	2.10	0.50
1:A:179:VAL:HG23	1:A:205:PHE:HA	1.93	0.50
1:A:260:PRO:HG3	1:A:444:ILE:HG22	1.91	0.50
1:B:371:LEU:HA	1:B:387:LEU:O	2.10	0.50
1:B:523:ASN:ND2	1:B:524:GLU:OE2	2.44	0.50
1:B:523:ASN:HD21	1:B:525:LEU:CB	2.25	0.50
1:C:187:ASN:OD1	1:C:219:VAL:CG2	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:525:LEU:O	1:C:526:LEU:C	2.54	0.50
1:A:376:VAL:HG12	1:A:379:SER:HG	1.73	0.50
1:B:67:THR:HG22	1:B:68:GLY:N	2.27	0.50
1:B:528:LYS:HD2	1:B:528:LYS:N	2.20	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:C:356:LEU:O	1:C:357:ALA:C	2.55	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:294:HIS:HE2	1:A:323:ASP:CG	2.20	0.50
1:A:477:PRO:O	1:A:480:LEU:HB2	2.11	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:237:ASN:C	1:B:239:GLN:NE2	2.69	0.50
1:B:276:VAL:CG2	1:B:417:ALA:HB1	2.42	0.50
1:B:485:LYS:O	1:B:487:LYS:N	2.44	0.50
1:B:557:ASP: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:18:GLU:O	1:A:19:GLY:C	2.54	0.50
1:A:25:TYR:C	1:A:27:GLY:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLY:HA2	1:B:45:LEU:O	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:27:GLY:C	1:C:29:ASP:N	2.67	0.50
1:C:83:VAL:HG11	1:C:119:VAL:O	2.12	0.50
1:A:190:ALA:HB2	1:A:196:LEU:HD11	1.94	0.50
1:B:264:LYS:HD3	1:B:264:LYS:C	2.36	0.50
1:B:359:LEU:CD1	1:B:381:LEU:HD12	2.39	0.50
1:B:502:LEU:C	1:B:506:PRO:HD2	2.37	0.50
1:B:523:ASN:O	1:B:526:LEU:HB2	2.12	0.50
1:C:18:GLU:CD	1:C:21:ARG:NH1	2.69	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:111:LEU:C	1:A:113:ALA:N	2.66	0.50
1:A:175:GLY:H	1:A:208:GLU:CD	2.20	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:B:37:ASP:O	1:B:38:ALA:C	2.54	0.50
1:C:74:TRP:HA	1:C:74:TRP:CE3	2.45	0.50
1:C:259:GLN:O	1:C:260:PRO:C	2.53	0.50
1:C:330:PHE:HE1	1:C:335:SER:HB3	1.77	0.50
1:A:34:ALA:HB1	1:A:42:MET:HE1	1.94	0.49
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:B:515:PRO:C	1:B:516:VAL:HG23	2.36	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:421:LYS:O	1:A:422:LEU:C	2.54	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:456:ALA:O	1:C:459:GLU:CD	2.55	0.49
1:C:525:LEU:O	1:C:528:LYS:HB2	2.12	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:B:345:THR:HG21	1:B:359:LEU:HD21	1.94	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: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:B:61:HIS:C	1:B:61:HIS:CD2	2.89	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:C:447:MET:O	1:C:448:LEU:C	2.53	0.49
1:A:251:TYR:CG	1:A:397:ILE:HG21	2.47	0.49
1:A:563:GLU:O	1:A:564:MET:HE2	2.13	0.49
1:B:123:ASP:C	1:B:126:VAL:HG12	2.38	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:B:379:SER:O	1:B:380:SER:C	2.55	0.49
1:C:131:VAL:C	1:C:133:TRP:N	2.70	0.49
1:C:400:ALA:O	1:C:401:SER:C	2.56	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: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:B:327:ALA:O	1:B:328:SER:C	2.54	0.49
1:C:107:LEU:C	1:C:109:GLU:N	2.70	0.49
1:C:188:PHE:CD2	1:C:200:THR:HG21	2.48	0.49
1:C:304:TYR:OH	1:C:308:MET:HE2	2.11	0.49
1:C:316:SER:OG	1:C:317:LEU:N	2.44	0.49
1:A:301:GLY:O	1:A:302:THR:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:THR:O	1:B:158:THR:HG23	2.12	0.49
1:C:215:THR:O	1:C:216:ARG:C	2.56	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
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: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: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:A:250:HIS:HB3	1:A:596:ASP:CG	2.36	0.48
1:A:388:ALA:C	1:A:389:LEU:CD1	2.86	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:196:LEU:C	1:A:198:PRO:CD	2.83	0.48
1:A:292:VAL:HG21	1:A:342:LEU:CB	2.43	0.48
1:A:382:VAL:CG2	1:A:390:MET:CE	2.72	0.48
1:A:476:TYR:C	1:A:476:TYR:CD1	2.87	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:421:LYS:O	1:B:422:LEU:C	2.56	0.48
1:B:457:LEU:HD23	1:B:562:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:GLU:O	1:B:506:PRO:HD2	2.12	0.48
1:B:580:LEU:O	1:B:581:GLN:C	2.55	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: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:A:423:LYS:O	1:A:424:GLY:C	2.52	0.48
1:A:589:LEU:O	1:A:590:ILE:C	2.57	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:348:GLN:C	1:B:348:GLN:OE1	2.57	0.48
1:B:413:LEU:HD12	1:B:416:VAL:HG21	1.95	0.48
1:B:453:ARG:HH11	1:B:453:ARG:CG	2.27	0.48
1: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:565:PRO:C	1:C:566:HIS:O	2.55	0.48
1:A:48:LEU:HD11	1:A:81:SER:C	2.39	0.48
1:A:239:GLN:C	1:A:241:ASP:N	2.72	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:440:LEU:N	1:B:441:PRO:HD2	2.29	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:409:LEU:O	1:A:410:THR:C	2.56	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:3:ILE:C	1:B:4:VAL:CG2	2.87	0.48
1:B:4:VAL:O	1:B:4:VAL:HG12	2.13	0.48
1:B:219:VAL:HG12	1:B:220:ASN:N	2.26	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:A:237:ASN:C	1:A:239:GLN:N	2.72	0.48
1:A:530:LYS:HD2	1:A:530:LYS:C	2.38	0.48
1:B:169:LEU:O	1:B:170:LEU:HD23	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ASN:O	1:B:221:ILE:C	2.57	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:578:VAL:N	1:A:579:PRO:CD	2.77	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:283:PRO:C	1:B:285:ALA:N	2.71	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:184:MET:HE2	1:C:184:MET:CA	2.43	0.48
1:C:480:LEU:HD22	1:C:496:ALA:HB3	1.95	0.48
1:C:576:TYR:C	1:C:579:PRO:HD2	2.39	0.48
1:A:103:ASN:ND2	1:A:103:ASN:H	2.12	0.48
1:A:149:ILE:C	1:A:151:GLN:H	2.22	0.48
1:A:155:ALA:HA	1:A:174:SER:O	2.14	0.48
1:A:300:CYS:O	1:A:301:GLY:C	2.57	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:C:353:ALA:HB2	1:C:606:THR:C	2.39	0.48
1:A:4:VAL:HG21	1:A:19:GLY:HA3	1.95	0.47
1:A:296:GLN:HG2	1:A:367:TYR:OH	2.13	0.47
1:B:354:ASP:O	1:B:355:THR:C	2.51	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: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:219:VAL:C	1:B:220:ASN:OD1	2.58	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:B:555:SER:C	1:B:556:SER:HG	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:377:PRO:O	1:A:378:GLY:C	2.58	0.47
1:A:551:ALA:HB3	1:A:553:PHE:HD1	1.80	0.47
1:B:458:ALA:C	1:B:460:ASP:N	2.70	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
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:C:576:TYR:C	1:C:578:VAL:N	2.69	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:412:LEU:O	1:A:413:LEU:C	2.56	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:234:ILE:HD12	1:C:234:ILE:C	2.40	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:A:529:LEU:C	1:A:531:SER:N	2.71	0.47
1:B:48:LEU:HD21	1:B:81:SER:CB	2.22	0.47
1:C:159:VAL:HG12	1:C:159:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:GLN:N	1:C:260:PRO:CD	2.78	0.47
1:C:429:ILE:O	1:C:430:GLU:C	2.57	0.47
1:A:102:GLU:C	1:A:104:HIS:N	2.72	0.47
1:A:148:ALA:O	1:A:149:ILE:C	2.57	0.47
1:A:173:ARG:HH21	1:A:208:GLU:HB2	1.80	0.47
1:A:211:ILE:O	1:A:212:ALA:C	2.57	0.47
1:A:250:HIS:ND1	1:A:595:VAL:HB	2.30	0.47
1:A:267:LEU:CD2	1:A:414:MET:HE1	2.28	0.47
1:A:538:ALA:C	1:A:539:ARG:HG2	2.39	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:270:ARG:HD3	1:C:414:MET:HE1	1.97	0.47
1:C:306:SER:HB2	1:C:346:LEU:CD1	2.42	0.47
1:C:344:ILE:HD12	1:C:344:ILE:N	2.28	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: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:76:THR:C	1:A:78:GLY:N	2.65	0.47
1:A:443:ARG:HH11	1:A:443:ARG:CG	2.28	0.47
1:B:223:ASP:OD1	1:B:227:ALA:HB3	2.15	0.47
1:B:256:ILE:HG22	1:B:257:TYR:N	2.28	0.47
1:B:356:LEU:HD11	1:B:360:ARG:CD	2.44	0.47
1:B:464:LYS:C	1:B:465:HIS:ND1	2.73	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:557:ASP:O	1:C:560:HIS:HE1	1.98	0.47
1:A:245:LYS:HG2	1:A:251:TYR:CZ	2.50	0.47
1:A:421:LYS:C	1:A:423:LYS:N	2.73	0.47
1:A:534:GLU:OE1	1:A:534:GLU:CA	2.63	0.47
1:A:565:PRO:O	1:A:566:HIS:C	2.58	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:523:ASN:C	1:B:525:LEU:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:GLN:C	1:B:551:ALA:H	2.22	0.47
1:B:564:MET:HG3	1:B:576:TYR:CE2	2.50	0.47
1:C:135:LEU:C	1:C:137:GLN:H	2.23	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:A:599:ARG:C	1:A:601:LEU:H	2.23	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: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:475:GLN:HE22	1:B:576:TYR:HB2	1.81	0.46
1:B:555:SER:C	1:B:556:SER:OG	2.58	0.46
1:C:223:ASP:OD1	1:C:223:ASP:N	2.47	0.46
1:C:379:SER:O	1:C:380:SER:C	2.58	0.46
1:C:408:GLN:O	1:C:409:LEU:C	2.58	0.46
1:C:502:LEU:CD1	1:C:502:LEU:H	2.29	0.46
1:C:571:ILE:O	1:C:571:ILE:HG13	2.15	0.46
1:A:248:TYR:CB	1:A:254:LYS:HB2	2.46	0.46
1:A:306:SER:O	1:A:307:GLY:C	2.57	0.46
1:A:375:ASN:CG	1:A:393:ALA:HB3	2.39	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:485:LYS:C	1:B:487:LYS:N	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:ASP:C	1:C:387:LEU:HG	2.40	0.46
1:A:326:ILE:HD12	1:A:326:ILE:HA	1.64	0.46
1:A:529:LEU:C	1:A:532:ASN:ND2	2.74	0.46
1:B:103:ASN:C	1:B:105:GLU:H	2.22	0.46
1:B:374:CYS:HB3	1:B:390:MET:HE1	1.97	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: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: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: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:489:ILE:HD11	1:C:584:ALA:C	2.40	0.46
1:C:567:VAL:HG11	1:C:575:PHE:CE2	2.51	0.46
1:A:231:ARG:C	1:A:232:GLN:O	2.58	0.46
1:A:527:GLU:O	1:A:528:LYS:C	2.58	0.46
1:A:533:ILE:HG23	1:A:543:LEU:HD22	1.97	0.46
1:B:270:ARG:HA	1:B:277:ASP:HB3	1.98	0.46
1:B:576:TYR:C	1:B:579:PRO:HD2	2.41	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:128:ALA:O	1:A:129:HIS:C	2.54	0.46
1:A:195:ALA:O	1:A:198:PRO:CD	2.64	0.46
1:A:457:LEU:O	1:A:458:ALA:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:GLU:O	1:B:528:LYS:C	2.59	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:C:533:ILE:HG22	1:C:559:MET:HE1	1.96	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:525:LEU:O	1:A:526:LEU:C	2.59	0.46
1:A:528:LYS:O	1:A:532:ASN:ND2	2.49	0.46
1:A:535:GLU:O	1:A:536:VAL:C	2.56	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:330:PHE:C	1:C:332:TYR:N	2.73	0.46
1:C:359:LEU:HD22	1:C:381:LEU:HD22	1.98	0.46
1:C:426:ASP:OD1	1:C:428:SER:OG	2.33	0.46
1:C:498:ALA:O	1:C:500:GLY:N	2.49	0.46
1:A:76:THR:HG22	1:A:77:HIS:N	2.30	0.46
1:A:107:LEU:C	1:A:109:GLU:N	2.74	0.46
1:A:134:GLU:OE1	1:A:147:ARG:CB	2.64	0.46
1:A:307:GLY:C	1:A:324:VAL:HG11	2.41	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:193:GLN:C	1:B:195:ALA:H	2.23	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:447:MET:HE3	1:C:578:VAL:CG1	2.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:376:VAL:O	1:B:379:SER:OG	2.19	0.45
1:B:426:ASP:OD1	1:B:428:SER:HB3	2.15	0.45
1:C:166:PRO:O	1:C:167:ASP:C	2.59	0.45
1:C:255:GLU:HA	1:C:403:LYS:HD3	1.98	0.45
1:C:553:PHE:HB3	1:C:561:ILE:HD11	1.97	0.45
1:A:121:GLU:O	1:A:122:THR:CB	2.57	0.45
1:A: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:28:TYR:CE2	1:A:597:GLN:CB	2.99	0.45
1:A:86:HIS:CE1	1:A:124:THR:HG1	2.34	0.45
1:A:105:GLU:C	1:A:107:LEU:N	2.73	0.45
1:A:347:SER:HB2	1:A:381:LEU:HD11	1.98	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:109:GLU:O	1:B:110:GLU:C	2.59	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:459:GLU:O	1:B:462:SER:OG	2.15	0.45
1:B:515:PRO:HA	1:B:542:GLN:O	2.17	0.45
1:C:230:LYS:C	1:C:231:ARG:HD3	2.37	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:GLY:C	1:A:507:LEU:N	2.72	0.45
1:B:3:ILE:HG13	1:B:98:ASN:HB2	1.97	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: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: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: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:B:458:ALA:C	1:B:460:ASP:H	2.25	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:457:LEU:C	1:C:459:GLU:N	2.75	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:491:TYR:CD1	1:A:599:ARG:NH1	2.84	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:129:HIS:C	1:C:131:VAL:N	2.72	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:532:ASN:O	1:C:533:ILE:C	2.60	0.45
1:A:123:ASP:O	1:A:126:VAL:HB	2.17	0.45
1:A:523:ASN:ND2	1:A:524:GLU:H	2.15	0.45
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:253:GLN:O	1:B:254:LYS:C	2.60	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:C:447:MET:HE3	1:C:579:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:GLY:O	1:A:303:SER:N	2.50	0.45
1:A:506:PRO:C	1:A:508:ALA:H	2.24	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: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:371:LEU:HD23	1:C:371:LEU:C	2.42	0.45
1:C:608:GLU:H	1:C:608:GLU:CD	2.15	0.45
1:A:423:LYS:C	1:A:425:LEU:N	2.74	0.44
1:A:502:LEU:HD12	1:A:502:LEU:HA	1.70	0.44
1:B:24:GLU:CD	1:B:597:GLN:NE2	2.70	0.44
1:B:60:GLU:C	1:B:62:PRO:HD3	2.42	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:523:ASN:CG	1:B:525:LEU:HB2	2.41	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:348:GLN:O	1:C:348:GLN:CD	2.61	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: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:330:PHE:O	1:A:331:ARG:C	2.60	0.44
1:A:405:PHE:O	1:A:406:THR:C	2.61	0.44
1:B:32:GLY:CA	1:B:46:ARG:HA	2.46	0.44
1:B:51:VAL:O	1:B:52:GLN:C	2.58	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:102:GLU:C	1:C:104:HIS:H	2.24	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:175:GLY:O	1:A:176:SER:C	2.61	0.44
1:A:251:TYR:CG	1:A:397:ILE:CG2	3.01	0.44
1:A:447:MET:HE2	1:A:575:PHE:CE1	2.52	0.44
1:B:14:GLU:O	1:B:16:LEU:N	2.50	0.44
1:B:286:ASP:CG	1:B:422:LEU:HD11	2.42	0.44
1:B:335:SER:O	1:B:337:VAL:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:LEU:C	1:B:421:LYS:H	2.25	0.44
1:C:21:ARG:C	1:C:23:LEU:H	2.25	0.44
1:C:36:VAL:HG12	1:C:166:PRO:CG	2.48	0.44
1:C:94:VAL:HB	1:C:161:MET:HE2	1.99	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:252:MET:O	1:C:253:GLN:C	2.59	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:127:ILE:O	1:B:128:ALA:C	2.60	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:B:417:ALA:C	1:B:419:LEU:N	2.76	0.44
1:B:573:PRO:O	1:B:574:ILE:C	2.61	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:523:ASN:C	1:B:525:LEU:N	2.76	0.44
1:C:124:THR:C	1:C:126:VAL:N	2.75	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: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: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:101:ILE:O	1:C:102:GLU:C	2.60	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:C:443:ARG:O	1:C:444:ILE:C	2.60	0.44
1:A:12:VAL:HG13	1:A:66:GLY:HA2	2.00	0.44
1:A:56:GLN:C	1:A:58:ALA:H	2.25	0.44
1:A:441:PRO:C	1:A:443:ARG:H	2.26	0.44
1:A:448:LEU:C	1:A:450:GLN:N	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:VAL:CG1	1:C:166:PRO:HG3	2.46	0.44
1:C:411:VAL:O	1:C:412:LEU:C	2.61	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
1:A:187:ASN:C	1:A:188:PHE:CD2	2.96	0.44
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:304:TYR:CZ	1:C:308:MET:CE	2.95	0.44
1:C:343:MET:HE2	1:C:343:MET:HB2	1.86	0.44
1:C:351:GLU:HG2	1:C:380:SER:CB	2.44	0.44
1:C:580:LEU:O	1:C:581:GLN:C	2.61	0.44
1:A:112:LYS:O	1:A:113:ALA:C	2.61	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:252:MET:HE3	1:A:402:THR:CG2	2.47	0.43
1:A:267:LEU:HD22	1:A:414:MET:HE2	1.98	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: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: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: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: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:42:MET:HE1	1:C:44:ARG:NH2	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:A:36:VAL:O	1:A:65:GLY:HA2	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:ARG:NH2	1:B:563:GLU:H	2.15	0.43
1:B:507:LEU:HD12	1:B:507:LEU:O	2.17	0.43
1:B:567:VAL:HG11	1:B:575:PHE:CE1	2.53	0.43
1: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:A:411:VAL:O	1:A:412:LEU:C	2.61	0.43
1:B:298:LEU:CD1	1:B:343:MET:HE1	2.48	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:79:GLU:O	1:A:80:PRO:C	2.60	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:258:GLU:O	1:A:259:GLN:C	2.61	0.43
1:A:305:ASN:O	1:A:306:SER:C	2.61	0.43
1:A:330:PHE:CD1	1:A:331:ARG:N	2.86	0.43
1:A:360:ARG:O	1:A:361:LEU:C	2.61	0.43
1:B:470:LEU:HD23	1:B:470:LEU:N	2.33	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:331:ARG:HH12	1:C:608:GLU:CD	2.25	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:273:HIS:C	1:A:275:GLN:N	2.74	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: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: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:466:HIS:HB2	1:C:514:MET:HE1	2.00	0.43
1:C:573:PRO:C	1:C:575:PHE:N	2.76	0.43
1:A:251:TYR:CD2	1:A:397:ILE:HG21	2.53	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:310:SER:O	1:A:311:ARG:C	2.61	0.43
1:A:330:PHE:C	1:A:330:PHE:HD1	2.25	0.43
1:A:401:SER:H	2:A:700:G6Q:H2	1.84	0.43
1:A:506:PRO:C	1:A:508:ALA:N	2.73	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:131:VAL:C	1:C:133:TRP:H	2.26	0.43
1:C:289:LEU:O	1:C:422:LEU:CD2	2.65	0.43
1:C:543:LEU:HD12	1:C:559:MET:HE3	1.99	0.43
1:B:33:LEU:HD23	1:B:33:LEU:C	2.44	0.43
1:B:107:LEU:O	1:B:108:ARG:C	2.60	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:501:GLU:CD	1:C:326:ILE:CD1	2.92	0.43
1:B:553:PHE:CD2	1:B:559:MET:CE	3.02	0.43
1:C:42:MET:HE3	1:C:44:ARG:HE	1.84	0.43
1:C:80:PRO:HB2	1:C:84:ASN:CG	2.44	0.43
1:C:197:LEU:HD23	1:C:203:PHE:CZ	2.51	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:B:549:GLN:C	1:B:551:ALA:N	2.74	0.43
1:C:83:VAL:HG12	1:C:120:SER:OG	2.19	0.43
1:C:405:PHE:O	1:C:406:THR:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:450:GLN:O	1:B:451:ASP:C	2.61	0.42
1:B:507:LEU:C	1:B:509:LEU:H	2.26	0.42
1:C:63:LEU:HD22	1:C:63:LEU:N	2.34	0.42
1:C:103:ASN:C	1:C:106:PRO:HD2	2.44	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:285:ALA:C	1:A:287:GLU:N	2.75	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:335:SER:O	1:B:336:ALA:C	2.62	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:256:ILE:C	1:C:258:GLU:N	2.76	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:139:GLY:HA2	1:A:143:GLU:OE1	2.20	0.42
1:A:187:ASN:C	1:A:188:PHE:CG	2.97	0.42
1:A:463:ASP:OD1	1:A:463:ASP:N	2.51	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:458:ALA:O	1:A:459:GLU:C	2.62	0.42
1:B:46:ARG:H	1:B:46:ARG:HG2	1.59	0.42
1:B:402:THR:C	1:B:404:ALA:H	2.26	0.42
1:B:526:LEU:HD12	1:B:526:LEU:C	2.43	0.42
1:C:234:ILE:HD12	1:C:235:GLU:CA	2.48	0.42
1:C:599:ARG:O	1:C:600:ASN:C	2.61	0.42
1:A:338:ARG:N	1:A:338:ARG:CD	2.81	0.42
1:A:356:LEU:O	1:A:357:ALA:C	2.62	0.42
1:A:473:GLY:C	1:A:475:GLN:H	2.26	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:135:LEU:C	1:C:137:GLN:N	2.75	0.42
1:C:300:CYS:O	1:C:301:GLY:C	2.61	0.42
1:C:348:GLN:O	1:C:348:GLN:NE2	2.52	0.42
1:C:381:LEU:O	1:C:383:ARG:N	2.53	0.42
1:A:42:MET:C	1:A:43:THR:OG1	2.62	0.42
1:A:266:THR:HG22	1:A:270:ARG:HH12	1.84	0.42
1:A:419:LEU:O	1:A:420:SER:C	2.62	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:A:562:ILE:O	1:A:563:GLU:C	2.61	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:503:LYS:C	1:B:505:GLY:H	2.28	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: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:574:ILE:O	1:A:575:PHE:C	2.61	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:235:GLU:O	1:B:236:SER:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:ARG:NH1	1:B:453:ARG:CG	2.81	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:196:LEU:O	1:A:197:LEU:C	2.61	0.42
1:A:266:THR:HA	1:A:392:ASN:ND2	2.34	0.42
1:B:286:ASP:HB3	1:B:422:LEU:CD1	2.50	0.42
1:B:475:GLN:O	1:B:476:TYR:C	2.63	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:502:LEU:C	1:C:504:HIS:N	2.78	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:A:524:GLU:H	1:A:524:GLU:CD	2.27	0.42
1:B:33:LEU:HB3	1:B:70:ALA:HB2	2.01	0.42
1:B:205:PHE:N	1:B:205:PHE:CD1	2.88	0.42
1:B:302:THR:OG1	1:B:481:GLU:CD	2.62	0.42
1:B:352:THR:O	1:B:353:ALA:C	2.62	0.42
1:B:425:LEU:HG	1:B:426:ASP:N	2.35	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:90:SER:O	1:A:91:GLU:C	2.62	0.42
1:A:164:ARG:C	1:A:165:HIS:CG	2.97	0.42
1:B:63:LEU:C	1:B:64:HIS:HD2	2.28	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:449:SER:C	1:B:451:ASP:H	2.27	0.42
1:B:450:GLN:O	1:B:454:ILE:HG13	2.20	0.42
1:C:272:SER:O	1:C:273:HIS:C	2.62	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:473:GLY:C	1:A:475:GLN:N	2.77	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:B:363:LYS:C	1:B:365:LEU:H	2.27	0.41
1:B:405:PHE:O	1:B:406:THR:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:423:LYS:C	1:A:425:LEU:H	2.27	0.41
1:A:437:LEU:C	1:A:439:ALA:N	2.71	0.41
1:B:22:ARG:HG2	1:B:194:LEU:CD2	2.50	0.41
1:B:255:GLU:O	1:B:403:LYS:HB3	2.21	0.41
1:B:326:ILE:HG23	1:C:501:GLU:OE2	2.20	0.41
1:B:408:GLN:O	1:B:412:LEU:HB2	2.20	0.41
1:B:468:LEU:HD21	1:B:470:LEU:HD21	2.02	0.41
1:B:483:ALA:HB1	1:B:494:ALA:O	2.20	0.41
1:C:111:LEU:HB2	1:C:118:PHE:HE1	1.85	0.41
1:C:224:LYS:HZ2	1:C:225:THR:CG2	2.31	0.41
1:C:283:PRO:C	1:C:285:ALA:H	2.28	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:B:522:ASN:O	1:B:523:ASN:C	2.63	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:90:SER:O	1:B:90:SER:OG	2.36	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:525:LEU:O	1:C:528:LYS:N	2.53	0.41
1:C:540:GLY:O	1:C:541:GLY:C	2.63	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:ALA:O	1:A:499:ALA:C	2.62	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: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
1:C:359:LEU:CD2	1:C:381:LEU:HD22	2.50	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: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:C:568:GLU:CD	1:C:568:GLU:H	2.28	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:282:GLY:HA2	1:A:283:PRO:HD2	1.85	0.41
1:A:409:LEU:HD23	1:A:409:LEU:HA	1.78	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:B:306:SER:O	1:B:307:GLY:C	2.63	0.41
1:B:313:TRP:HZ2	1:B:573:PRO:CG	2.34	0.41
1:B:359:LEU:O	1:B:360:ARG:C	2.62	0.41
1:B:554:VAL:O	1:B:555:SER:C	2.64	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:356:LEU:HA	1:A:381:LEU:CD2	2.48	0.41
1:A:357:ALA:O	1:A:358:GLY:C	2.62	0.41
1:B:146:LEU:HD12	1:B:146:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:451:ASP:C	1:B:453:ARG:N	2.76	0.41
1:B:520:ALA:HA	1:B:521:PRO:HD3	1.79	0.41
1:C:25:TYR:CD1	1:C:25:TYR:C	2.98	0.41
1:C:142:ARG:C	1:C:144:ALA:H	2.28	0.41
1:C:165:HIS:N	1:C:166:PRO:CD	2.83	0.41
1:C:385:SER:C	1:C:387:LEU:H	2.29	0.41
1:C:466:HIS:HA	1:C:493:HIS:O	2.21	0.41
1:C:472:ARG:O	1:C:475:GLN:HB2	2.20	0.41
1:C:514:MET:HB2	1:C:514:MET:HE2	1.69	0.41
1:A:74:TRP:CZ3	1:A:602:ALA:O	2.74	0.41
1:A:266:THR:HG23	1:A:391:THR:C	2.44	0.41
1:A:441:PRO:C	1:A:443:ARG:N	2.78	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:101:ILE:O	1:B:102:GLU:C	2.62	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: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:556:SER:C	1:B:558:ASN:N	2.79	0.41
1:B:599:ARG:O	1:B:600:ASN:HB2	2.21	0.41
1:B:606:THR:HG22	1:B:606:THR:O	2.19	0.41
1:C:127:ILE:HA	1:C:130:LEU:HB3	2.03	0.41
1:C:263:ILE:O	1:C:266:THR:CB	2.63	0.41
1:C:389:LEU:C	1:C:390:MET:O	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:533:ILE:CG2	1:C:559:MET:HE2	2.51	0.41
1:C:552:GLY:O	1:C:553:PHE:C	2.64	0.41
1:C:599:ARG:C	1:C:601:LEU:N	2.78	0.41
1:A:354:ASP:O	1:A:355:THR:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:309:VAL:O	1:B:310:SER:C	2.61	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:352:THR:O	1:C:353:ALA:C	2.64	0.41
1:C:528:LYS:O	1:C:531:SER:N	2.52	0.41
1:A:37:ASP:C	1:A:37:ASP:OD1	2.62	0.40
1:A:301:GLY:C	1:A:303:SER:N	2.78	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:53:MET:C	1:B:55:ALA:N	2.78	0.40
1:B:103:ASN:C	1:B:105:GLU:N	2.78	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:529:LEU:C	1:B:533:ILE:HG13	2.33	0.40
1:B:600:ASN:O	1:C:507:LEU:HD23	2.21	0.40
1:C:173:ARG:HD3	1:C:207:GLU:O	2.21	0.40
1:C:368:LEU:HD23	1:C:368:LEU:C	2.47	0.40
1:C:501:GLU:O	1:C:502:LEU:C	2.65	0.40
1:A:26:ARG:HG3	1:A:26:ARG:HH11	1.86	0.40
1:A:505:GLY:C	1:A:507:LEU:H	2.30	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:291:LYS:O	1:C:292:VAL:C	2.62	0.40
1:C:389:LEU:O	1:C:390:MET:C	2.62	0.40
1:A:184:MET:C	1:A:186:GLU:N	2.74	0.40
1:A:267:LEU:HA	1:A:414:MET:HE1	2.03	0.40
1:A:393:ALA:C	1:A:403:LYS:HZ2	2.24	0.40
1:B:16:LEU:HD11	1:B:68:GLY:C	2.46	0.40
1:B:116:TYR:HE2	1:B:133:TRP:HB2	1.86	0.40
1:B:229:VAL:C	1:B:230:LYS:HD3	2.47	0.40
1:B:504:HIS:CE1	1:C:300:CYS:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:526:LEU:C	1:A:526:LEU:HD12	2.47	0.40
1:B:4:VAL:O	1:B:16:LEU:HD21	2.21	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: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:166:PRO:C	1:C:168:THR:N	2.78	0.40
1:C:254:LYS:C	1:C:256:ILE:N	2.80	0.40
1:C:331:ARG:HD2	1:C:354:ASP:HA	2.02	0.40
1:C:480:LEU:O	1:C:483:ALA:HB3	2.22	0.40
1:C:547:ALA:O	1:C:549:GLN:N	2.53	0.40
1:C:553:PHE:CB	1:C:561:ILE:HD12	2.50	0.40
1:C:566:HIS:C	1:C:567:VAL:HG13	2.45	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:276:VAL:O	1:A:276:VAL:HG13	2.19	0.40
1:A:417:ALA:HA	1:A:420:SER:HB3	2.04	0.40
1:B:20:LEU:C	1:B:22:ARG:N	2.74	0.40
1:B:48:LEU:CD1	1:B:82:GLU:HB2	2.51	0.40
1:B:61:HIS:O	1:B:61:HIS:CG	2.70	0.40
1:B:124:THR:C	1:B:126:VAL:N	2.75	0.40
1:B:507:LEU:C	1:B:509:LEU:N	2.80	0.40
1:B:554:VAL:O	1:B:554:VAL:HG23	2.20	0.40
1:B:572:ALA:CB	1:B:573:PRO:CD	2.91	0.40
1:C:6:ALA:CB	1:C:12:VAL:HG11	2.47	0.40
1:C:159:VAL:HA	1:C:171:ALA:CA	2.49	0.40
1:C:363:LYS:C	1:C:365:LEU:N	2.78	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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
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

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

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

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

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

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Mol	Chain	Res	Type
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%)	383 (77%)	117 (23%)	1	4
1	B	500/500 (100%)	401 (80%)	99 (20%)	1	6
1	C	500/500 (100%)	425 (85%)	75 (15%)	3	13
All	All	1500/1500 (100%)	1209 (81%)	291 (19%)	1	7

All (291) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	CYS
1	A	3	ILE
1	A	7	ILE
1	A	20	LEU
1	A	25	TYR
1	A	26	ARG
1	A	30	SER
1	A	33	LEU
1	A	35	VAL
1	A	36	VAL

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Mol	Chain	Res	Type
1	A	42	MET
1	A	44	ARG
1	A	45	LEU
1	A	46	ARG
1	A	48	LEU
1	A	51	VAL
1	A	52	GLN
1	A	76	THR
1	A	97	HIS
1	A	102	GLU
1	A	103	ASN
1	A	114	ARG
1	A	125	GLU
1	A	127	ILE
1	A	131	VAL
1	A	132	ASN
1	A	140	THR
1	A	146	LEU
1	A	149	ILE
1	A	160	ILE
1	A	161	MET
1	A	163	SER
1	A	168	THR
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	234	ILE
1	A	235	GLU
1	A	239	GLN
1	A	247	ILE
1	A	259	GLN
1	A	266	THR
1	A	268	THR
1	A	273	HIS
1	A	279	SER

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Mol	Chain	Res	Type
1	A	288	LEU
1	A	290	SER
1	A	292	VAL
1	A	296	GLN
1	A	303	SER
1	A	320	ILE
1	A	326	ILE
1	A	333	ARG
1	A	337	VAL
1	A	338	ARG
1	A	341	SER
1	A	344	ILE
1	A	346	LEU
1	A	347	SER
1	A	349	SER
1	A	351	GLU
1	A	356	LEU
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	373	ILE
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	406	THR
1	A	418	LYS
1	A	420	SER
1	A	422	LEU
1	A	428	SER
1	A	433	ILE
1	A	434	VAL
1	A	441	PRO
1	A	442	SER

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Mol	Chain	Res	Type
1	A	443	ARG
1	A	454	ILE
1	A	457	LEU
1	A	468	LEU
1	A	481	GLU
1	A	492	ILE
1	A	502	LEU
1	A	503	LYS
1	A	517	ILE
1	A	518	VAL
1	A	519	VAL
1	A	525	LEU
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	42	MET
1	B	45	LEU
1	B	46	ARG
1	B	48	LEU
1	B	52	GLN
1	B	59	GLU
1	B	63	LEU
1	B	72	THR
1	B	86	HIS
1	B	93	ILE
1	B	97	HIS
1	B	107	LEU
1	B	120	SER
1	B	124	THR

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Mol	Chain	Res	Type
1	B	135	LEU
1	B	140	THR
1	B	143	GLU
1	B	146	LEU
1	B	152	LEU
1	B	158	THR
1	B	161	MET
1	B	162	ASP
1	B	163	SER
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	252	MET
1	B	255	GLU
1	B	259	GLN
1	B	267	LEU
1	B	273	HIS
1	B	297	ILE
1	B	302	THR
1	B	303	SER
1	B	306	SER
1	B	316	SER
1	B	320	ILE
1	B	326	ILE
1	B	334	LYS
1	B	344	ILE

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Mol	Chain	Res	Type
1	B	348	GLN
1	B	362	SER
1	B	385	SER
1	B	390	MET
1	B	395	THR
1	B	397	ILE
1	B	415	LEU
1	B	423	LYS
1	B	428	SER
1	B	429	ILE
1	B	433	ILE
1	B	440	LEU
1	B	442	SER
1	B	447	MET
1	B	449	SER
1	B	453	ARG
1	B	454	ILE
1	B	468	LEU
1	B	472	ARG
1	B	503	LYS
1	B	509	LEU
1	B	510	ILE
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	567	VAL
1	B	568	GLU
1	B	571	ILE
1	B	578	VAL
1	B	590	ILE
1	B	591	LYS
1	B	607	VAL
1	C	15	ILE
1	C	23	LEU
1	C	33	LEU
1	C	35	VAL

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Mol	Chain	Res	Type
1	C	50	LYS
1	C	63	LEU
1	C	69	ILE
1	C	74	TRP
1	C	79	GLU
1	C	90	SER
1	C	101	ILE
1	C	118	PHE
1	C	120	SER
1	C	141	LEU
1	C	158	THR
1	C	163	SER
1	C	169	LEU
1	C	170	LEU
1	C	176	SER
1	C	178	LEU
1	C	184	MET
1	C	191	SER
1	C	194	LEU
1	C	196	LEU
1	C	200	THR
1	C	222	PHE
1	C	224	LYS
1	C	234	ILE
1	C	238	LEU
1	C	247	ILE
1	C	263	ILE
1	C	272	SER
1	C	306	SER
1	C	320	ILE
1	C	322	CYS
1	C	326	ILE
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	362	SER
1	C	368	LEU
1	C	382	VAL
1	C	390	MET

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Mol	Chain	Res	Type
1	C	402	THR
1	C	433	ILE
1	C	452	LYS
1	C	454	ILE
1	C	457	LEU
1	C	461	PHE
1	C	462	SER
1	C	485	LYS
1	C	490	SER
1	C	492	ILE
1	C	497	TYR
1	C	503	LYS
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	537	ARG
1	C	539	ARG
1	C	545	VAL
1	C	557	ASP
1	C	570	VAL
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 (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	56	GLN
1	A	77	HIS
1	A	84	ASN
1	A	88	HIS
1	A	103	ASN
1	A	137	GLN
1	A	151	GLN
1	A	187	ASN

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Mol	Chain	Res	Type
1	A	265	ASN
1	A	296	GLN
1	A	305	ASN
1	A	435	HIS
1	A	438	GLN
1	A	523	ASN
1	A	532	ASN
1	A	549	GLN
1	A	566	HIS
1	B	61	HIS
1	B	64	HIS
1	B	86	HIS
1	B	104	HIS
1	B	151	GLN
1	B	165	HIS
1	B	187	ASN
1	B	239	GLN
1	B	250	HIS
1	B	261	ASN
1	B	265	ASN
1	B	375	ASN
1	B	438	GLN
1	B	450	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	56	GLN
1	C	61	HIS
1	C	98	ASN
1	C	132	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
1	C	348	GLN
1	C	375	ASN

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Mol	Chain	Res	Type
1	C	438	GLN
1	C	465	HIS
1	C	523	ASN
1	C	558	ASN
1	C	560	HIS
1	C	586	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	G6Q	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

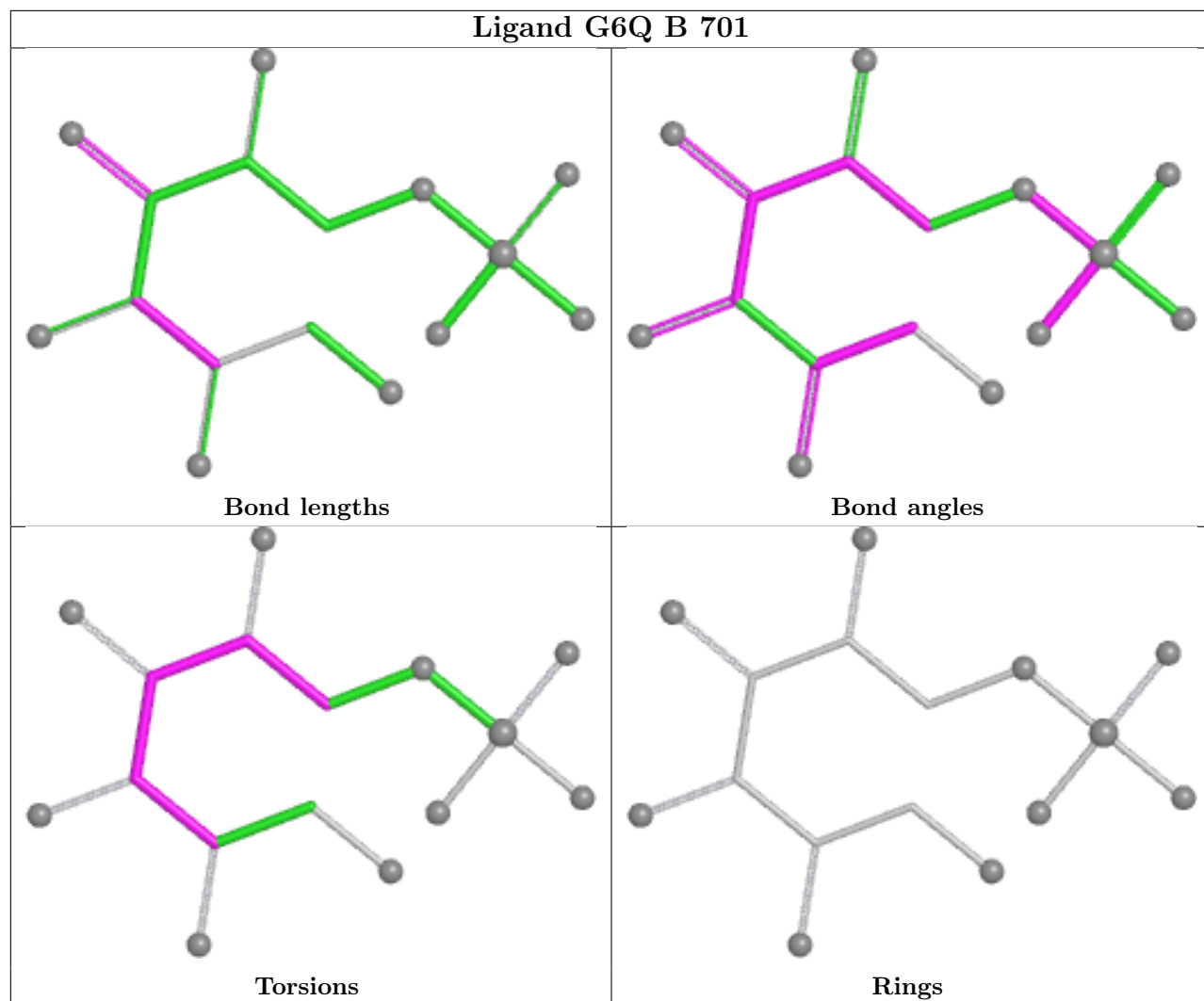
There are no ring outliers.

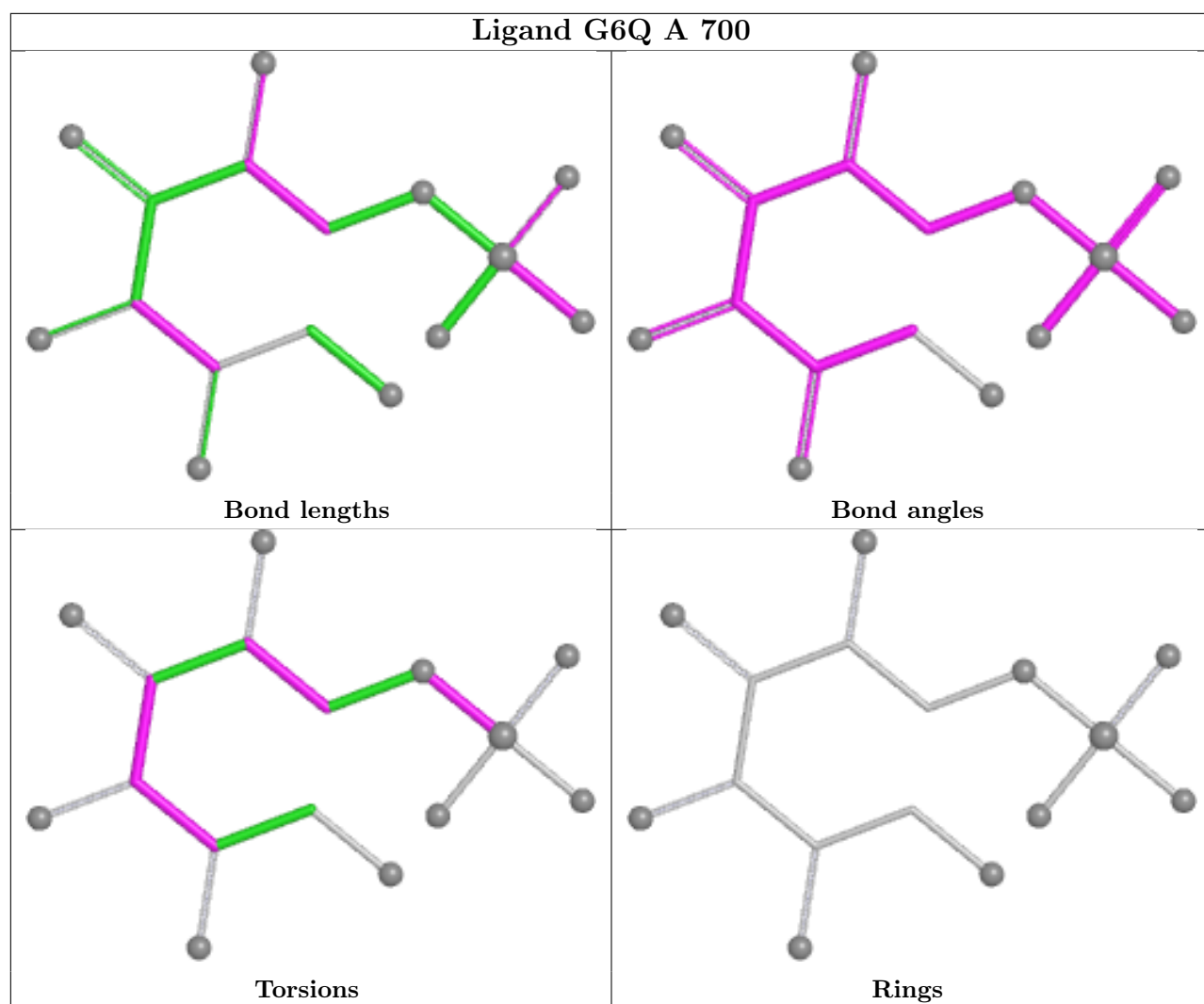
2 monomers are involved in 8 short contacts:

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%)	-0.65	5 (0%) 82 65	9, 38, 101, 133	0
1	B	608/608 (100%)	-0.35	4 (0%) 84 68	19, 78, 125, 138	0
1	C	608/608 (100%)	0.16	17 (2%) 55 34	44, 113, 137, 151	0
All	All	1824/1824 (100%)	-0.28	26 (1%) 73 53	9, 79, 131, 151	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	ASN	4.1
1	C	124	THR	3.2
1	C	435	HIS	3.0
1	C	522	ASN	2.8
1	A	88	HIS	2.8
1	C	34	ALA	2.6
1	C	94	VAL	2.5
1	B	240	TYR	2.5
1	A	86	HIS	2.4
1	C	80	PRO	2.4
1	A	85	ALA	2.4
1	C	89	VAL	2.4
1	C	393	ALA	2.3
1	B	271	ILE	2.3
1	C	157	GLY	2.3
1	A	113	ALA	2.3
1	C	235	GLU	2.2
1	C	98	ASN	2.2
1	B	61	HIS	2.2
1	B	522	ASN	2.2
1	C	181	GLY	2.1
1	C	96	VAL	2.1
1	C	236	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	61	HIS	2.0
1	C	25	TYR	2.0
1	C	65	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

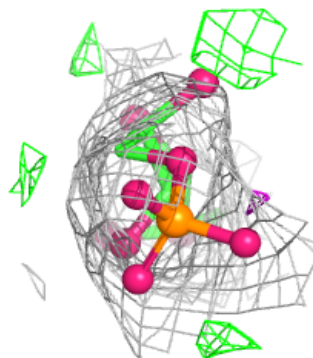
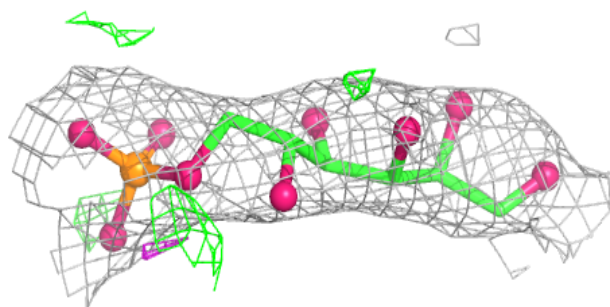
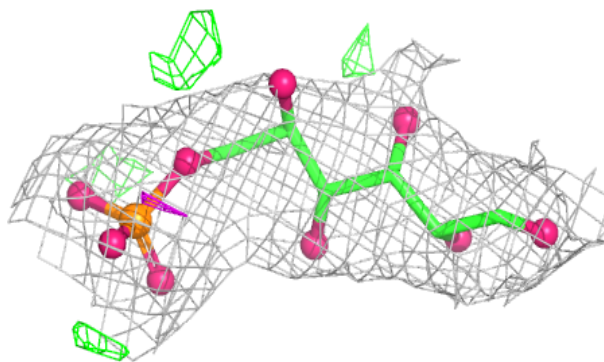
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å 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

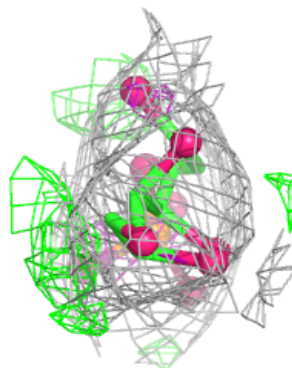
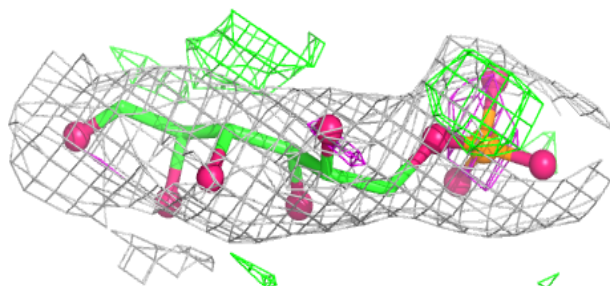
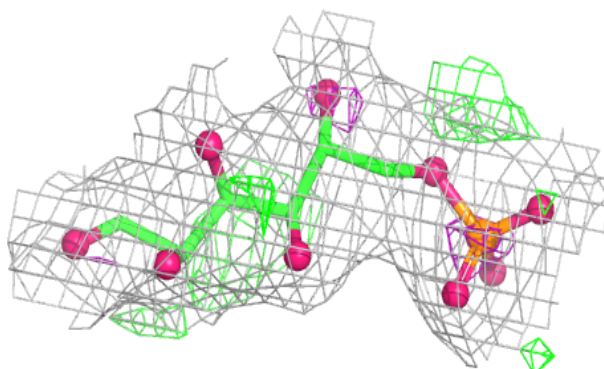
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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