



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 11:31 am BST

PDB ID : 1EK1  
Title : CRYSTAL STRUCTURE OF MURINE SOLUBLE EPOXIDE HYDROLASE  
COMPLEXED WITH CIU INHIBITOR  
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Deposited on : 2000-03-06  
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

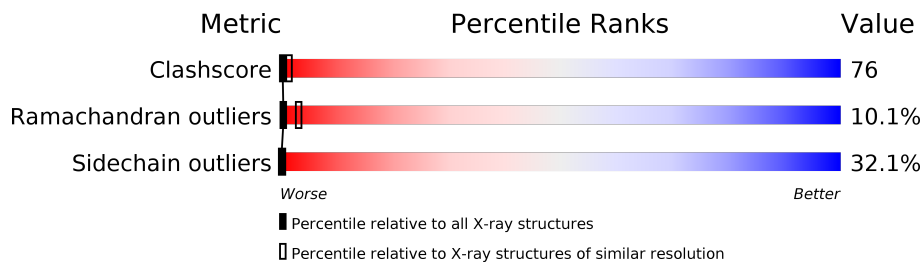
# 1 Overall quality at a glance

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	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	554	
1	B	554	

## 2 Entry composition [i](#)

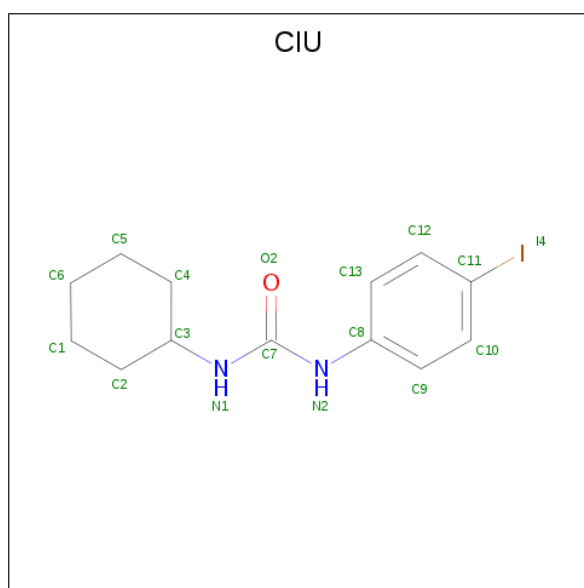
There are 3 unique types of molecules in this entry. The entry contains 8255 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 EPOXIDE HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	490	Total 3901	C 2517	N 651	O 704	S 29	61	0	0
1	B	541	Total 4299	C 2766	N 719	O 783	S 31	71	0	0

- Molecule 2 is N-CYCLOHEXYL-N'-(4-IODOPHENYL)UREA (three-letter code: CIU) (formula: C<sub>13</sub>H<sub>17</sub>IN<sub>2</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	I	N	O		
2	A	1	Total 17	C 13	I 1	N 2	O 1	0	0
2	B	1	Total 17	C 13	I 1	N 2	O 1	0	0

- Molecule 3 is water.

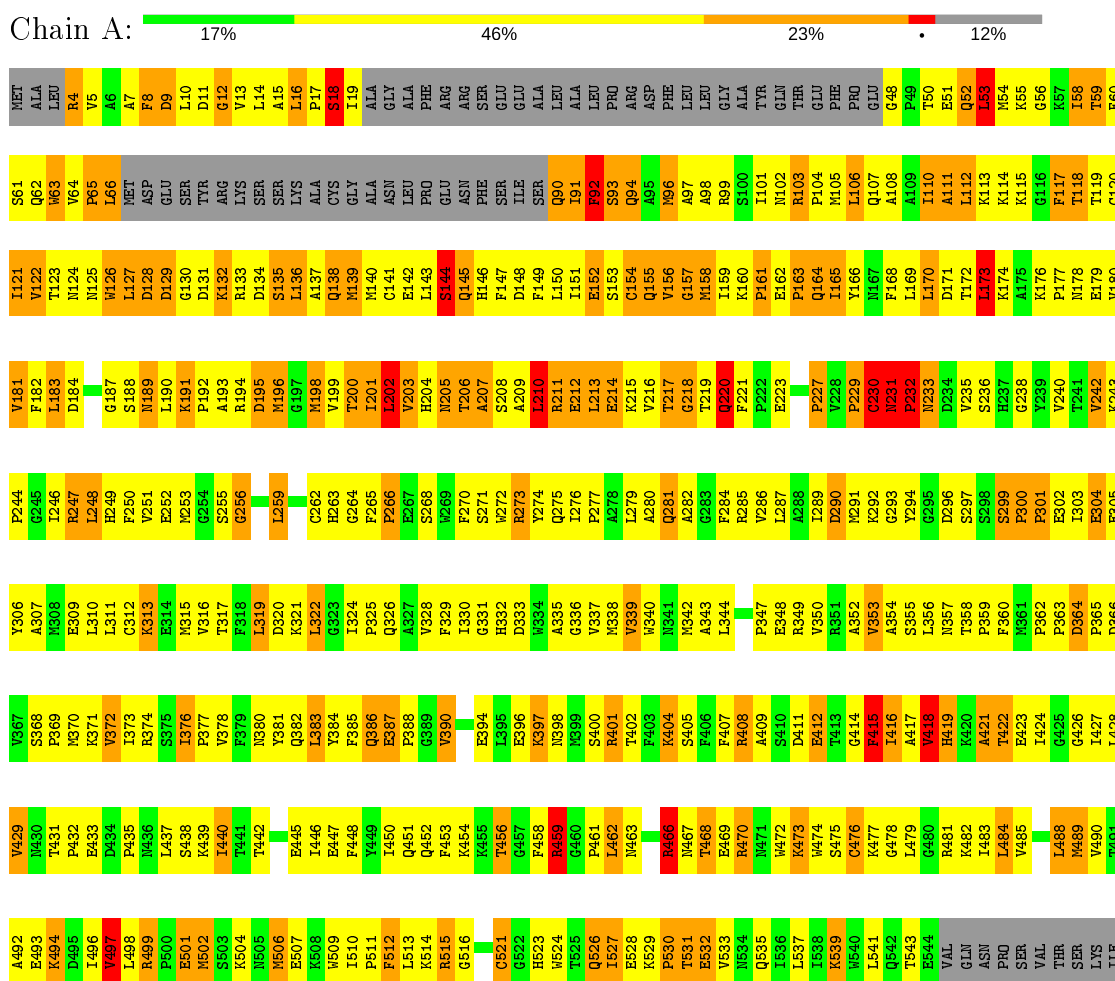
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	A	4	Total 4	O 4	0	0
3	B	17	Total 17	O 17	0	0

### 3 Residue-property plots

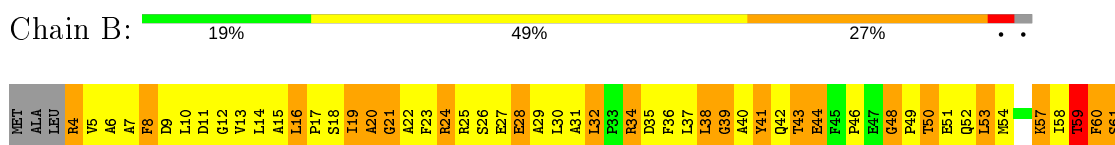
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

- Molecule 1: EPOXIDE HYDROLASE



- Molecule 1: EPOXIDE HYDROLASE



P495	P432	F369	A307	P244	D184	T123	Q62
I496	E433	M370	M308	G245	D185	M124	M63
Y497	D434	K371	E309	I246	F186	M125	V64
L498	P435	L310	L310	R247	G187	M126	P65
R499	M436	I373	L311	L248	L248	M127	M66
P500	L437	R374	C312	H249	N189	D128	L67
E501	S438	S375	K313	F250	L190	D129	D68
M502	K439	I376	E314	V251	K191	G130	E69
S503	I440	P377	M315	E252	P192	P131	S70
K504	T441	V378	V316	M253	A193	K132	Y71
M505	T442	F379	T317	G254	R194	K133	R72
M506	E445	N380	F318	S255	D195	D134	K73
E507	I446	Y381	L319	G256	M196	S135	S74
K508	L447	Q382	D320	L259	G197	L136	S75
M509	E448	L383	K321	L260	M198	A137	K76
I510	F448	L384	L322	L261	V199	Q138	A77
Y511	Y449	F385	G323	H263	T200	M139	C78
F512	I450	Q386	I324	G264	I201	M140	G79
L513	Q451	E387	P325	F265	L202	C141	A80
K514	Q452	F388	Q326	P266	V203	E142	M81
M515	F453	G389	A327	E267	H204	L143	L82
G516	K454	V390	F328	S268	N205	S144	P83
	K455		W269	W269	T206	Q145	E84
	T456	L395	F270	F270	A207	H146	N85
	G457	E396	S271	S271	S208	F147	F86
	F458	K397	W272	W272	A209	D148	S87
	R459	N398	R273	R273	L210	F149	I88
	G460	M399	Y274	Y274	R211	L150	S89
	P461	S400	Q275	Q275	E212	I151	Q90
	L462	R401	I276	I276	L213	E152	I91
	M463	T402	V337	P277	E214	S153	F92
	W464	F403	M338	E278	K215	C154	S93
	Y465	K404	V339	L279	V216	Q155	Q94
	R466	S405	W340	A280	T217	G156	A95
	T467	F406	N341	Q281	G218	F157	M96
	F468	R407	M342	A282	M158	M159	R99
	E469	R408	A343	G283	Q220	I159	S100
	R470	A409	L344	F284	F221	K160	I101
	W471	S410	P347	R285	P222	P161	M102
	W472	D411	E348	V286	E223	E162	R103
	K473	E412	R349	L287	A224	P163	P104
	W474	T413	R349	A288	P225	Q164	M105
	S475	G414	V350	I289	L226	I165	M106
	C476	E415	E351	D290	F227	Y166	Q107
	K477	I416	A352	M291	V228	M167	A108
	G478	A417	V353	K292	C229	F168	A109
	L479	V418	A354	G293	C230	L169	I110
	G480	H419	S355	Y294	N231	L170	A111
	R481	K420	L356	G295	P232	L173	L112
	K482	A421	N357	D296	N233	K113	K114
	I483	T422	T358	S297	D234	A175	K115
	L484	E423	P359	S298	V235	K176	K116
	L488	I424	F360	S299	H237	P177	G116
	M489	G425	M361	P300	G238	M178	F117
	W490	G426	P362	P301	G239	E179	T118
	T491	I427	P363	E302	Y239	V180	T119
	A492	L428	D364	I303	V240	V181	C120
	E493	W429	V367	E304	T241	F182	I121
	K494	T431	S368	Y306	K243	L483	V122

## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.90Å 143.00Å 60.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.10)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.194 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8255	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.77	1/4004 (0.0%)	0.95	11/5430 (0.2%)
1	B	0.77	0/4413	0.96	11/5984 (0.2%)
All	All	0.77	1/8417 (0.0%)	0.96	22/11414 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	CYS	CB-SG	5.35	1.91	1.82

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	ASN	C-N-CD	-12.52	93.07	120.60
1	B	231	ASN	C-N-CA	7.61	153.97	122.00
1	A	218	GLY	N-CA-C	-6.85	95.98	113.10
1	B	66	LEU	CA-CB-CG	6.57	130.41	115.30
1	A	231	ASN	N-CA-C	5.82	126.72	111.00
1	B	118	THR	N-CA-C	-5.80	95.34	111.00
1	A	353	VAL	CB-CA-C	-5.69	100.58	111.40
1	A	227	PRO	N-CA-C	-5.67	97.36	112.10
1	B	484	LEU	CA-CB-CG	-5.55	102.52	115.30
1	A	173	LEU	CA-CB-CG	5.42	127.77	115.30
1	A	484	LEU	CA-CB-CG	-5.41	102.85	115.30
1	B	353	VAL	CB-CA-C	-5.38	101.17	111.40
1	B	497	VAL	N-CA-C	-5.29	96.70	111.00
1	A	161	PRO	N-CA-C	5.28	125.83	112.10
1	B	231	ASN	N-CA-C	5.25	125.18	111.00
1	A	497	VAL	N-CA-C	-5.22	96.89	111.00
1	B	173	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	232	PRO	N-CA-C	-5.20	98.58	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	ALA	N-CA-C	-5.19	96.99	111.00
1	B	48	GLY	N-CA-C	5.18	126.06	113.10
1	A	220	GLN	N-CA-C	5.13	124.86	111.00
1	A	53	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	3901	0	3890	581	0
1	B	4299	0	4270	676	0
2	A	17	0	17	2	0
2	B	17	0	17	5	0
3	A	4	0	0	0	0
3	B	17	0	0	5	0
All	All	8255	0	8194	1220	0

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 76.

All (1220) 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:293:GLY:HA2	1:A:299:SER:HB2	1.33	1.10
1:B:141:CYS:O	1:B:144:SER:HB3	1.52	1.10
1:B:61:SER:O	1:B:64:VAL:HG23	1.51	1.09
1:B:223:GLU:H	1:B:223:GLU:CD	1.53	1.08
1:B:183:LEU:HD23	1:B:201:ILE:HD12	1.31	1.08
1:B:232:PRO:HD2	1:B:233:ASN:H	1.11	1.08
1:B:293:GLY:HA2	1:B:299:SER:HB2	1.28	1.07
1:B:49:PRO:HB2	1:B:67:MET:HG2	1.31	1.05
1:B:222:PRO:HG2	1:B:225:PRO:HG3	1.38	1.05
1:B:103:ARG:HB2	1:B:104:PRO:HD3	1.34	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ARG:HA	1:A:473:LYS:HZ3	1.19	1.04
1:B:155:GLN:OE1	1:B:155:GLN:HA	1.50	1.04
1:B:5:VAL:HG23	1:B:118:THR:O	1.57	1.04
1:B:303:ILE:HD13	1:B:463:ASN:HD21	1.17	1.03
1:B:127:LEU:HD12	1:B:127:LEU:H	1.22	1.02
1:B:424:ILE:HD13	1:B:424:ILE:H	1.19	1.02
1:A:101:ILE:HG21	1:A:106:LEU:HD12	1.42	1.02
1:A:303:ILE:HD13	1:A:463:ASN:HD21	1.23	1.01
1:B:4:ARG:HB3	1:B:4:ARG:HH11	1.26	1.01
1:A:484:LEU:HD12	1:B:129:ASP:OD2	1.61	1.00
1:B:470:ARG:HA	1:B:473:LYS:HZ3	1.21	1.00
1:B:36:PHE:HE2	1:B:82:LEU:HD13	1.27	0.99
1:A:232:PRO:HD2	1:A:233:ASN:HD22	1.24	0.99
1:B:120:CYS:HB3	1:B:149:PHE:HB2	1.43	0.99
1:A:230:CYS:O	1:A:231:ASN:HB3	1.59	0.99
1:A:377:PRO:O	1:A:419:HIS:HB3	1.63	0.99
1:B:377:PRO:O	1:B:419:HIS:HB3	1.64	0.98
1:A:214:GLU:O	1:A:217:THR:HG23	1.64	0.97
1:A:529:LYS:HB3	1:A:532:GLU:HG3	1.46	0.97
1:B:25:ARG:HA	1:B:28:GLU:HG2	1.44	0.97
1:A:380:ASN:HB3	1:A:419:HIS:HA	1.48	0.95
1:B:380:ASN:HB3	1:B:419:HIS:HA	1.49	0.95
1:B:529:LYS:HB3	1:B:532:GLU:HG3	1.47	0.95
1:A:160:LYS:HB3	1:A:189:ASN:HD21	1.28	0.94
1:B:493:GLU:HG2	1:B:494:LYS:HG2	1.50	0.94
1:B:492:ALA:HB1	1:B:521:CYS:HB3	1.51	0.93
1:A:187:GLY:HA2	1:A:190:LEU:HD12	1.48	0.92
1:B:529:LYS:O	1:B:533:VAL:HG23	1.69	0.92
1:A:183:LEU:HB3	1:A:201:ILE:HB	1.51	0.92
1:A:496:ILE:HD12	1:A:496:ILE:H	1.33	0.92
1:A:13:VAL:HG22	1:A:203:VAL:HG11	1.49	0.92
1:B:434:ASP:H	1:B:435:PRO:HD3	1.34	0.92
1:B:496:ILE:H	1:B:496:ILE:HD12	1.33	0.92
1:A:205:ASN:HD22	1:A:205:ASN:H	1.01	0.91
1:B:139:MET:O	1:B:143:LEU:HG	1.70	0.91
1:B:160:LYS:HB3	1:B:189:ASN:HD21	1.35	0.90
1:A:529:LYS:O	1:A:533:VAL:HG23	1.71	0.90
1:A:493:GLU:HG2	1:A:494:LYS:HG2	1.51	0.90
1:B:232:PRO:CD	1:B:233:ASN:H	1.83	0.90
1:B:328:VAL:HG13	1:B:330:ILE:HD11	1.54	0.90
1:A:65:PRO:HG2	1:A:66:LEU:HD22	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ILE:HG23	1:B:354:ALA:HB3	1.52	0.89
1:B:489:MET:HB2	1:B:513:LEU:HD21	1.53	0.89
1:B:293:GLY:CA	1:B:299:SER:HB2	2.02	0.89
1:B:535:GLN:HB3	1:B:539:LYS:NZ	1.88	0.89
1:B:303:ILE:HA	1:B:463:ASN:ND2	1.88	0.89
1:B:434:ASP:H	1:B:435:PRO:CD	1.85	0.88
1:B:223:GLU:N	1:B:223:GLU:CD	2.27	0.88
1:B:49:PRO:CB	1:B:67:MET:HG2	2.03	0.88
1:A:159:ILE:O	1:A:165:ILE:HD11	1.71	0.88
1:A:50:THR:OG1	1:A:66:LEU:HD11	1.73	0.88
1:A:303:ILE:HA	1:A:463:ASN:ND2	1.88	0.88
1:A:492:ALA:HB1	1:A:521:CYS:HB3	1.54	0.88
1:A:173:LEU:H	1:A:173:LEU:HD22	1.38	0.87
1:A:328:VAL:HG13	1:A:330:ILE:HD11	1.56	0.87
1:A:166:TYR:O	1:A:170:LEU:HD12	1.74	0.87
1:A:192:PRO:O	1:A:195:ASP:HB2	1.74	0.86
1:A:489:MET:HB2	1:A:513:LEU:HD21	1.56	0.86
1:B:122:VAL:HB	1:B:151:ILE:HD13	1.56	0.86
1:B:515:ARG:CG	1:B:515:ARG:HH11	1.88	0.86
1:A:535:GLN:HB3	1:A:539:LYS:NZ	1.91	0.85
1:B:328:VAL:CG1	1:B:330:ILE:HD11	2.05	0.85
1:A:330:ILE:HG23	1:A:354:ALA:HB3	1.56	0.85
1:B:16:LEU:HB2	1:B:17:PRO:HA	1.58	0.85
1:A:515:ARG:CG	1:A:515:ARG:HH11	1.89	0.85
1:A:348:GLU:HA	1:B:133:ARG:CG	2.06	0.85
1:A:8:PHE:HD2	1:A:183:LEU:HD11	1.40	0.85
1:B:232:PRO:HD2	1:B:233:ASN:N	1.90	0.85
1:A:63:TRP:C	1:A:65:PRO:HD3	1.96	0.84
1:B:329:PHE:O	1:B:330:ILE:HD13	1.77	0.84
1:B:293:GLY:HA2	1:B:299:SER:CB	2.07	0.84
1:B:49:PRO:HB2	1:B:67:MET:CG	2.07	0.84
1:B:53:LEU:HD22	1:B:126:TRP:HB2	1.60	0.84
1:B:187:GLY:HA2	1:B:190:LEU:HD12	1.60	0.83
1:A:293:GLY:CA	1:A:299:SER:HB2	2.06	0.83
1:A:155:GLN:HA	1:A:155:GLN:OE1	1.78	0.83
1:B:232:PRO:HD2	1:B:233:ASN:HD22	1.43	0.83
1:A:52:GLN:OE1	1:A:58:ILE:HD11	1.78	0.83
1:B:64:VAL:HB	1:B:65:PRO:HD3	1.60	0.83
1:B:75:SER:HB2	1:B:82:LEU:HB3	1.58	0.83
1:A:328:VAL:CG1	1:A:330:ILE:HD11	2.07	0.82
1:B:169:LEU:HD23	1:B:170:LEU:N	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASN:OD1	1:A:160:LYS:HB2	1.78	0.82
1:A:442:THR:OG1	1:A:445:GLU:HG3	1.78	0.82
1:B:13:VAL:HB	1:B:203:VAL:HG11	1.58	0.82
1:A:329:PHE:O	1:A:330:ILE:HD13	1.80	0.82
1:A:537:LEU:O	1:A:541:LEU:HD12	1.79	0.82
1:A:482:LYS:HB2	1:B:62:GLN:NE2	1.95	0.81
1:B:263:HIS:CD2	1:B:291:MET:HG2	2.15	0.81
1:B:4:ARG:CB	1:B:4:ARG:HH11	1.93	0.81
1:A:380:ASN:CB	1:A:419:HIS:HA	2.09	0.81
1:B:404:LYS:O	1:B:408:ARG:HD2	1.81	0.81
1:A:106:LEU:HD23	1:A:106:LEU:O	1.80	0.81
1:A:4:ARG:HH21	1:A:179:GLU:HB3	1.45	0.81
1:B:442:THR:OG1	1:B:445:GLU:HG3	1.80	0.81
1:A:169:LEU:HD23	1:A:173:LEU:HD21	1.63	0.81
1:A:8:PHE:CD2	1:A:183:LEU:HD11	2.16	0.81
1:B:303:ILE:HD13	1:B:463:ASN:ND2	1.96	0.80
1:B:344:LEU:HD21	1:B:478:GLY:HA3	1.64	0.80
1:B:160:LYS:HD2	1:B:189:ASN:ND2	1.95	0.80
1:A:344:LEU:HD21	1:A:478:GLY:HA3	1.63	0.80
1:A:16:LEU:HB2	1:A:17:PRO:HA	1.63	0.79
1:A:499:ARG:O	1:A:502:MET:HG3	1.82	0.79
1:B:212:GLU:C	1:B:214:GLU:H	1.83	0.79
1:A:61:SER:HB2	1:B:484:LEU:HD13	1.64	0.79
1:B:199:VAL:HG21	3:B:1002:HOH:O	1.81	0.79
1:B:499:ARG:O	1:B:502:MET:HG3	1.83	0.79
1:A:215:LYS:HG2	1:A:220:GLN:CB	2.12	0.78
1:A:301:PRO:HD2	1:A:302:GLU:H	1.48	0.78
1:B:380:ASN:CB	1:B:419:HIS:HA	2.11	0.78
1:B:36:PHE:CE2	1:B:82:LEU:HD13	2.15	0.78
1:A:137:ALA:HB1	1:B:325:PRO:O	1.83	0.78
1:A:62:GLN:O	1:A:62:GLN:HG3	1.83	0.78
1:B:73:LYS:O	1:B:77:ALA:HB3	1.83	0.78
1:A:240:VAL:HG21	1:A:322:LEU:HD12	1.65	0.78
1:A:122:VAL:HG22	1:A:122:VAL:O	1.83	0.78
1:B:347:PRO:HD2	1:B:348:GLU:OE1	1.84	0.78
1:B:515:ARG:HG3	1:B:515:ARG:HH11	1.48	0.77
1:A:483:ILE:HB	1:A:510:ILE:HG12	1.66	0.77
1:A:92:PHE:C	1:A:94:GLN:H	1.84	0.77
1:A:264:GLY:HA3	1:A:333:ASP:HB3	1.66	0.77
1:A:293:GLY:HA2	1:A:299:SER:CB	2.13	0.77
1:A:470:ARG:HA	1:A:473:LYS:NZ	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ARG:CA	1:A:473:LYS:HZ3	1.98	0.77
1:A:159:ILE:C	1:A:159:ILE:HD12	2.05	0.77
1:B:112:LEU:HD23	1:B:117:PHE:CE1	2.20	0.77
1:B:158:MET:HG2	1:B:164:GLN:HB3	1.66	0.77
1:A:404:LYS:O	1:A:408:ARG:HD2	1.85	0.76
1:B:299:SER:OG	1:B:456:THR:HG22	1.85	0.76
1:B:127:LEU:HD12	1:B:127:LEU:N	2.01	0.76
1:B:226:LEU:H	1:B:226:LEU:HD12	1.49	0.76
1:B:301:PRO:HD2	1:B:302:GLU:H	1.51	0.76
1:A:16:LEU:HB2	1:A:17:PRO:CA	2.16	0.76
1:A:193:ALA:HB1	1:A:198:MET:SD	2.24	0.76
1:B:30:LEU:HB2	1:B:32:LEU:HD13	1.65	0.76
1:B:331:GLY:N	1:B:339:VAL:HG21	2.00	0.76
1:B:7:ALA:HB2	1:B:120:CYS:SG	2.25	0.76
1:B:26:SER:C	1:B:28:GLU:H	1.86	0.76
1:B:424:ILE:HD13	1:B:424:ILE:N	2.00	0.76
1:B:470:ARG:HA	1:B:473:LYS:NZ	2.00	0.76
1:B:362:PRO:HG2	1:B:509:TRP:NE1	2.00	0.76
1:A:263:HIS:CD2	1:A:291:MET:HG2	2.21	0.76
1:B:372:VAL:HG22	1:B:373:ILE:HD13	1.67	0.76
1:B:483:ILE:HB	1:B:510:ILE:HG12	1.66	0.76
1:B:42:GLN:HB2	1:B:186:PHE:CE1	2.20	0.75
1:A:515:ARG:HG3	1:A:515:ARG:HH11	1.51	0.75
1:B:8:PHE:N	1:B:8:PHE:CD1	2.54	0.75
1:B:121:ILE:HG13	1:B:150:LEU:HD12	1.69	0.75
1:A:339:VAL:HG13	1:A:353:VAL:CG1	2.17	0.75
1:B:381:TYR:CZ	1:B:382:GLN:HG3	2.20	0.75
1:B:535:GLN:HB3	1:B:539:LYS:HZ2	1.50	0.74
1:B:264:GLY:HA3	1:B:333:ASP:HB3	1.67	0.74
1:A:62:GLN:OE1	1:B:481:ARG:HA	1.87	0.74
1:B:32:LEU:HD11	1:B:82:LEU:HD12	1.68	0.74
1:A:229:PRO:O	1:A:230:CYS:HB3	1.88	0.74
1:A:535:GLN:HB3	1:A:539:LYS:HZ2	1.50	0.74
1:B:183:LEU:CD2	1:B:201:ILE:HD12	2.16	0.74
1:B:320:ASP:OD1	1:B:349:ARG:NH2	2.20	0.74
1:B:339:VAL:HG13	1:B:353:VAL:CG1	2.17	0.74
1:A:5:VAL:HB	1:A:180:VAL:HG12	1.69	0.74
1:B:160:LYS:HD2	1:B:189:ASN:HD21	1.51	0.74
1:B:537:LEU:O	1:B:541:LEU:HD12	1.86	0.74
1:A:320:ASP:OD1	1:A:349:ARG:NH2	2.20	0.74
1:A:348:GLU:HA	1:B:133:ARG:HG2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:GLU:OE1	1:B:28:GLU:HA	1.87	0.74
1:B:48:GLY:O	1:B:52:GLN:HG2	1.88	0.73
1:A:376:ILE:H	1:A:376:ILE:HD13	1.53	0.73
1:B:183:LEU:HB3	1:B:201:ILE:HB	1.68	0.73
1:A:303:ILE:HD13	1:A:463:ASN:ND2	2.01	0.73
1:B:42:GLN:HB2	1:B:186:PHE:CZ	2.24	0.73
1:B:39:GLY:O	1:B:43:THR:HG23	1.88	0.73
1:B:122:VAL:HB	1:B:151:ILE:CD1	2.18	0.73
1:A:372:VAL:HG22	1:A:373:ILE:HD13	1.69	0.73
1:B:25:ARG:HA	1:B:28:GLU:CG	2.18	0.73
1:B:303:ILE:HA	1:B:463:ASN:HD22	1.53	0.73
1:A:467:ASN:OD1	1:A:470:ARG:HD2	1.89	0.73
1:B:230:CYS:HB3	1:B:277:PRO:HD3	1.71	0.73
1:B:240:VAL:HG21	1:B:322:LEU:HD12	1.69	0.73
1:A:205:ASN:HD22	1:A:205:ASN:N	1.80	0.73
1:B:158:MET:HG2	1:B:164:GLN:CB	2.20	0.72
1:B:68:ASP:OD1	1:B:87:SER:HA	1.90	0.72
1:A:106:LEU:CD2	1:A:110:ILE:HD11	2.18	0.72
1:A:489:MET:HG3	1:A:506:MET:SD	2.29	0.72
1:A:270:PHE:HB2	1:A:448:PHE:HE2	1.54	0.72
1:B:340:TRP:CE2	1:B:355:SER:HB2	2.24	0.72
1:B:11:ASP:OD1	1:B:99:ARG:NH1	2.21	0.72
1:A:331:GLY:N	1:A:339:VAL:HG21	2.03	0.72
1:B:103:ARG:HB2	1:B:104:PRO:CD	2.16	0.72
1:B:5:VAL:CG1	1:B:180:VAL:HG12	2.19	0.72
1:B:270:PHE:HB2	1:B:448:PHE:HE2	1.53	0.72
1:A:169:LEU:O	1:A:173:LEU:HD22	1.90	0.72
1:B:8:PHE:HB2	1:B:14:LEU:HD13	1.70	0.72
1:B:535:GLN:O	1:B:539:LYS:HD3	1.90	0.72
1:A:193:ALA:O	1:A:198:MET:HG3	1.90	0.72
1:A:329:PHE:C	1:A:330:ILE:HD13	2.10	0.72
1:A:386:GLN:O	1:A:388:PRO:HD3	1.90	0.72
1:B:96:MET:SD	1:B:136:LEU:HD22	2.29	0.72
1:A:13:VAL:HG11	1:A:183:LEU:HD12	1.70	0.72
1:A:203:VAL:O	1:A:203:VAL:HG12	1.90	0.72
1:A:205:ASN:ND2	1:A:205:ASN:H	1.83	0.72
1:A:8:PHE:HB3	1:A:183:LEU:HD11	1.72	0.72
1:B:230:CYS:H	1:B:277:PRO:CG	2.03	0.72
1:B:386:GLN:O	1:B:388:PRO:HD3	1.90	0.72
1:A:339:VAL:O	1:A:342:MET:HB2	1.89	0.71
1:A:424:ILE:HD12	1:A:426:GLY:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ASN:CG	1:A:206:THR:H	1.93	0.71
1:A:362:PRO:HG2	1:A:509:TRP:NE1	2.05	0.71
1:A:376:ILE:N	1:A:376:ILE:HD13	2.04	0.71
1:A:52:GLN:CB	1:A:55:LYS:HD2	2.20	0.71
1:B:489:MET:HG3	1:B:506:MET:SD	2.29	0.71
1:A:9:ASP:OD1	1:A:160:LYS:NZ	2.23	0.71
1:B:329:PHE:C	1:B:330:ILE:HD13	2.10	0.71
1:B:102:ASN:ND2	1:B:105:MET:HG2	2.05	0.71
1:B:204:HIS:O	1:B:205:ASN:CB	2.38	0.71
1:B:155:GLN:OE1	1:B:155:GLN:CA	2.35	0.71
1:A:10:LEU:O	1:A:12:GLY:N	2.23	0.71
1:A:347:PRO:HD2	1:A:348:GLU:OE1	1.91	0.70
1:A:232:PRO:CD	1:A:233:ASN:HD22	2.03	0.70
1:A:303:ILE:HA	1:A:463:ASN:HD22	1.54	0.70
1:B:376:ILE:HD13	1:B:376:ILE:N	2.06	0.70
1:A:340:TRP:CE2	1:A:355:SER:HB2	2.27	0.70
1:B:183:LEU:HB2	1:B:203:VAL:CG2	2.22	0.70
1:B:340:TRP:CZ2	1:B:355:SER:HB2	2.26	0.70
1:A:124:ASN:CG	1:A:160:LYS:HB2	2.12	0.70
1:A:458:PHE:O	1:A:461:PRO:HD2	1.91	0.70
1:A:535:GLN:O	1:A:539:LYS:HD3	1.91	0.70
1:B:14:LEU:HD21	1:B:147:PHE:CZ	2.27	0.70
1:B:496:ILE:H	1:B:496:ILE:CD1	2.00	0.70
1:A:122:VAL:O	1:A:122:VAL:CG2	2.39	0.70
1:B:343:ALA:HB2	1:B:353:VAL:HG21	1.73	0.70
1:A:230:CYS:O	1:A:230:CYS:SG	2.50	0.69
1:A:299:SER:OG	1:A:456:THR:HG22	1.91	0.69
1:A:160:LYS:HB3	1:A:189:ASN:ND2	2.07	0.69
1:B:376:ILE:HD13	1:B:376:ILE:H	1.57	0.69
1:B:470:ARG:CA	1:B:473:LYS:HZ3	2.01	0.69
1:A:50:THR:HA	1:A:63:TRP:HE1	1.56	0.69
1:B:208:SER:HA	1:B:211:ARG:HB2	1.74	0.69
1:A:381:TYR:CZ	1:A:382:GLN:HG3	2.27	0.69
1:B:8:PHE:O	1:B:121:ILE:HG22	1.90	0.69
1:B:211:ARG:HA	1:B:214:GLU:HG2	1.73	0.69
1:B:414:GLY:O	1:B:431:THR:HG23	1.92	0.69
1:B:416:ILE:HG23	1:B:427:ILE:HG22	1.74	0.69
1:A:343:ALA:HB2	1:A:353:VAL:HG21	1.74	0.69
1:A:92:PHE:C	1:A:94:GLN:N	2.45	0.69
1:B:467:ASN:OD1	1:B:470:ARG:HD2	1.93	0.69
1:B:6:ALA:HB2	1:B:181:VAL:HG13	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:LYS:HB3	1:B:189:ASN:ND2	2.07	0.68
1:A:496:ILE:H	1:A:496:ILE:CD1	2.00	0.68
1:B:67:MET:HA	1:B:70:SER:HB3	1.75	0.68
1:A:176:LYS:HB3	1:A:178:ASN:ND2	2.08	0.68
1:A:426:GLY:O	1:A:429:VAL:HG23	1.93	0.68
1:B:158:MET:HB3	1:B:164:GLN:HB2	1.74	0.68
1:B:203:VAL:HG12	1:B:203:VAL:O	1.94	0.68
1:B:339:VAL:O	1:B:342:MET:HB2	1.92	0.68
1:A:529:LYS:HB3	1:A:532:GLU:CG	2.24	0.68
1:B:71:TYR:HE2	1:B:88:ILE:HD13	1.56	0.68
1:B:499:ARG:HB3	1:B:501:GLU:CD	2.14	0.68
1:A:127:LEU:HG	1:A:154:CYS:SG	2.32	0.67
1:B:232:PRO:CD	1:B:233:ASN:N	2.48	0.67
1:A:232:PRO:HD2	1:A:233:ASN:N	2.09	0.67
1:A:263:HIS:NE2	1:A:291:MET:HB2	2.07	0.67
1:B:160:LYS:CB	1:B:189:ASN:HD21	2.08	0.67
1:A:200:THR:C	1:A:201:ILE:HG12	2.14	0.67
1:B:231:ASN:OD1	1:B:270:PHE:HE1	1.78	0.67
1:B:483:ILE:HD12	1:B:510:ILE:HD11	1.76	0.67
1:A:8:PHE:HB3	1:A:183:LEU:CD1	2.24	0.67
1:A:304:GLU:H	1:A:304:GLU:CD	1.97	0.67
1:B:43:THR:O	1:B:44:GLU:HB2	1.94	0.67
1:B:173:LEU:O	1:B:174:LYS:HD2	1.93	0.67
1:B:304:GLU:H	1:B:304:GLU:CD	1.98	0.67
1:B:458:PHE:O	1:B:461:PRO:HD2	1.94	0.67
1:B:60:PHE:O	1:B:63:TRP:HB3	1.95	0.67
1:A:180:VAL:O	1:A:180:VAL:HG23	1.94	0.66
1:A:499:ARG:HB3	1:A:501:GLU:CD	2.16	0.66
1:B:211:ARG:O	1:B:215:LYS:HD2	1.96	0.66
1:B:75:SER:OG	1:B:76:LYS:N	2.25	0.66
1:B:64:VAL:HB	1:B:65:PRO:CD	2.22	0.66
1:A:115:LYS:HE3	1:A:219:THR:OG1	1.96	0.66
1:B:424:ILE:H	1:B:424:ILE:CD1	1.98	0.66
1:A:13:VAL:HG22	1:A:203:VAL:CG1	2.24	0.66
1:B:428:LEU:HA	1:B:431:THR:OG1	1.95	0.66
1:A:240:VAL:CG2	1:A:322:LEU:HD12	2.24	0.66
1:B:232:PRO:CD	1:B:233:ASN:HD22	2.08	0.66
1:A:101:ILE:HD13	1:A:106:LEU:HD12	1.77	0.66
1:A:101:ILE:HD11	1:A:142:GLU:HG2	1.78	0.66
1:A:190:LEU:CD2	1:A:200:THR:HG22	2.25	0.66
1:A:5:VAL:HG13	1:A:118:THR:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:HD21	1:A:206:THR:HG22	1.79	0.65
1:A:230:CYS:O	1:A:231:ASN:CB	2.36	0.65
1:A:490:VAL:HG22	1:A:516:GLY:HA3	1.77	0.65
1:B:458:PHE:O	1:B:462:LEU:HD12	1.95	0.65
1:A:227:PRO:HG2	1:A:274:TYR:HD1	1.60	0.65
1:A:326:GLN:NE2	1:B:134:ASP:HA	2.11	0.65
1:B:229:PRO:HA	1:B:273:ARG:O	1.96	0.65
1:A:133:ARG:HG2	1:B:348:GLU:HA	1.78	0.65
1:B:497:VAL:O	1:B:498:LEU:HB2	1.97	0.65
1:B:490:VAL:HG22	1:B:516:GLY:HA3	1.77	0.65
1:A:232:PRO:CD	1:A:233:ASN:N	2.56	0.65
1:A:497:VAL:O	1:A:498:LEU:HB2	1.97	0.65
1:A:340:TRP:CZ2	1:A:355:SER:HB2	2.31	0.65
1:A:159:ILE:O	1:A:159:ILE:HD12	1.97	0.65
1:B:230:CYS:H	1:B:277:PRO:HG2	1.61	0.65
1:A:13:VAL:O	1:A:105:MET:HG2	1.96	0.65
1:A:348:GLU:HA	1:B:133:ARG:CD	2.25	0.65
1:B:119:THR:N	1:B:148:ASP:OD2	2.30	0.65
1:B:5:VAL:HG13	1:B:180:VAL:HG12	1.78	0.65
1:A:350:VAL:O	1:B:133:ARG:NH1	2.31	0.64
1:B:204:HIS:O	1:B:205:ASN:HB2	1.97	0.64
1:A:126:TRP:NE1	1:A:128:ASP:OD1	2.20	0.64
1:B:106:LEU:HD21	1:B:146:HIS:CD2	2.33	0.64
1:B:86:PHE:CD1	1:B:87:SER:N	2.65	0.64
1:B:240:VAL:CG2	1:B:322:LEU:HD12	2.28	0.64
1:B:434:ASP:N	1:B:435:PRO:CD	2.52	0.64
1:A:216:VAL:O	1:A:217:THR:C	2.36	0.64
1:A:478:GLY:HA2	1:A:481:ARG:HG3	1.78	0.64
1:A:50:THR:CA	1:A:63:TRP:HE1	2.09	0.64
1:B:300:PRO:HG2	1:B:305:GLU:HG2	1.80	0.64
1:A:125:ASN:O	1:A:126:TRP:HB3	1.96	0.64
1:A:270:PHE:HB2	1:A:448:PHE:CE2	2.33	0.64
1:A:4:ARG:NH2	1:A:179:GLU:HB3	2.10	0.64
1:B:270:PHE:HB2	1:B:448:PHE:CE2	2.33	0.64
1:A:232:PRO:HD2	1:A:233:ASN:ND2	2.07	0.63
1:A:458:PHE:O	1:A:462:LEU:HD12	1.98	0.63
1:B:101:ILE:HD11	1:B:143:LEU:HD21	1.81	0.63
1:B:386:GLN:NE2	1:B:468:THR:OG1	2.32	0.63
1:B:303:ILE:CD1	1:B:463:ASN:HD21	2.01	0.63
1:B:23:PHE:O	1:B:27:GLU:HG3	1.99	0.63
1:B:293:GLY:O	1:B:456:THR:HG21	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ASN:O	1:A:383:LEU:N	2.27	0.63
1:A:242:VAL:HG12	1:A:317:THR:HB	1.80	0.62
1:A:386:GLN:NE2	1:A:468:THR:OG1	2.32	0.62
1:B:331:GLY:H	1:B:339:VAL:HG21	1.62	0.62
1:B:176:LYS:HB3	1:B:178:ASN:ND2	2.15	0.62
1:A:193:ALA:CB	1:A:198:MET:SD	2.88	0.62
1:A:381:TYR:CE2	1:A:418:VAL:HG12	2.33	0.62
1:B:156:VAL:HG23	1:B:157:GLY:H	1.64	0.62
1:B:529:LYS:HB3	1:B:532:GLU:CG	2.24	0.62
1:B:159:ILE:O	1:B:165:ILE:HD11	1.98	0.62
1:B:524:TRP:O	1:B:528:GLU:HB3	1.99	0.62
1:A:159:ILE:CD1	1:A:159:ILE:C	2.67	0.62
1:A:300:PRO:HG2	1:A:305:GLU:HG2	1.81	0.62
1:B:16:LEU:CB	1:B:17:PRO:HA	2.26	0.62
1:A:191:LYS:CB	1:A:192:PRO:HD3	2.29	0.62
1:A:483:ILE:HD12	1:A:510:ILE:HD11	1.80	0.62
1:A:62:GLN:NE2	1:B:482:LYS:HB2	2.15	0.62
1:A:64:VAL:N	1:A:65:PRO:HD3	2.13	0.62
1:A:90:GLN:HG3	1:A:91:ILE:N	2.14	0.62
1:A:415:PHE:HD1	1:A:416:ILE:H	1.48	0.61
1:B:263:HIS:NE2	1:B:291:MET:HB2	2.13	0.61
1:B:387:GLU:HB3	1:B:390:VAL:HG21	1.82	0.61
1:A:215:LYS:HG2	1:A:220:GLN:HB2	1.82	0.61
1:B:177:PRO:O	1:B:198:MET:HA	2.00	0.61
1:B:535:GLN:HB3	1:B:539:LYS:HZ3	1.61	0.61
1:A:156:VAL:O	1:A:158:MET:HG3	2.00	0.61
1:A:510:ILE:O	1:A:513:LEU:HB2	2.01	0.61
1:B:478:GLY:HA2	1:B:481:ARG:HG3	1.81	0.61
1:A:331:GLY:H	1:A:339:VAL:HG21	1.65	0.61
1:A:482:LYS:CB	1:B:62:GLN:NE2	2.63	0.61
1:B:380:ASN:O	1:B:383:LEU:N	2.31	0.61
1:B:32:LEU:HD21	1:B:82:LEU:CD1	2.31	0.61
1:A:121:ILE:HD11	1:A:147:PHE:CD1	2.36	0.61
1:A:190:LEU:HD23	1:A:200:THR:HG22	1.82	0.61
1:B:121:ILE:HG13	1:B:150:LEU:CD1	2.30	0.61
1:B:169:LEU:O	1:B:173:LEU:HD22	2.00	0.61
1:A:102:ASN:O	1:A:105:MET:HB3	2.01	0.61
1:A:231:ASN:HB2	1:A:232:PRO:HB3	1.82	0.61
1:B:26:SER:C	1:B:28:GLU:N	2.54	0.61
1:A:207:ALA:C	1:A:210:LEU:HB2	2.21	0.61
1:B:301:PRO:CD	1:B:302:GLU:H	2.13	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LEU:HD23	1:B:37:LEU:HG	1.81	0.60
1:A:535:GLN:HB3	1:A:539:LYS:HZ3	1.66	0.60
1:B:426:GLY:HA3	1:B:429:VAL:CG2	2.31	0.60
1:B:72:ARG:HH11	1:B:72:ARG:CB	2.14	0.60
1:B:50:THR:HG23	1:B:63:TRP:HZ2	1.66	0.60
1:A:128:ASP:O	1:A:133:ARG:HG3	2.01	0.60
1:A:291:MET:O	1:A:292:LYS:C	2.40	0.60
1:A:428:LEU:O	1:A:431:THR:HB	2.01	0.60
1:B:415:PHE:HD1	1:B:416:ILE:H	1.49	0.60
1:A:289:ILE:CG2	1:A:290:ASP:N	2.64	0.60
1:A:293:GLY:O	1:A:456:THR:HG21	2.01	0.60
1:B:458:PHE:C	1:B:461:PRO:HD2	2.22	0.60
1:A:301:PRO:CD	1:A:302:GLU:H	2.13	0.60
1:B:211:ARG:HA	1:B:214:GLU:CG	2.31	0.60
1:A:405:SER:OG	1:A:431:THR:HG21	2.01	0.59
1:A:524:TRP:O	1:A:528:GLU:HB3	2.01	0.59
1:B:230:CYS:HB3	1:B:277:PRO:HG3	1.82	0.59
1:B:134:ASP:OD1	1:B:135:SER:N	2.31	0.59
1:A:101:ILE:CD1	1:A:142:GLU:HG2	2.32	0.59
1:A:173:LEU:O	1:A:174:LYS:HB2	2.02	0.59
1:A:99:ARG:O	1:A:99:ARG:HG3	2.02	0.59
1:B:210:LEU:O	1:B:214:GLU:HB3	2.01	0.59
1:B:380:ASN:OD1	1:B:421:ALA:HB3	2.02	0.59
1:B:442:THR:H	1:B:445:GLU:HB2	1.68	0.59
1:A:481:ARG:HG2	1:B:57:LYS:O	2.01	0.59
1:A:442:THR:H	1:A:445:GLU:HB2	1.68	0.59
1:B:13:VAL:O	1:B:105:MET:HG3	2.02	0.59
1:A:289:ILE:HG22	1:A:290:ASP:N	2.15	0.59
1:A:453:PHE:HE2	1:A:461:PRO:HG2	1.68	0.59
1:B:242:VAL:HG12	1:B:317:THR:HB	1.84	0.59
1:B:7:ALA:HA	1:B:120:CYS:O	2.02	0.59
1:B:137:ALA:O	1:B:141:CYS:N	2.34	0.59
1:B:381:TYR:O	1:B:384:TYR:HB3	2.02	0.59
1:A:7:ALA:HB2	1:A:120:CYS:SG	2.42	0.59
1:A:210:LEU:O	1:A:214:GLU:CB	2.50	0.59
1:A:50:THR:HG23	1:A:63:TRP:HZ2	1.68	0.59
1:A:381:TYR:O	1:A:384:TYR:HB3	2.02	0.59
1:A:303:ILE:CD1	1:A:463:ASN:HD21	2.07	0.59
1:A:381:TYR:CD2	1:A:418:VAL:HG12	2.38	0.59
1:A:458:PHE:C	1:A:461:PRO:HD2	2.23	0.59
1:A:488:LEU:HD13	1:A:490:VAL:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ARG:HB3	1:A:179:GLU:HB2	1.84	0.59
1:A:138:GLN:HA	1:B:325:PRO:HB3	1.85	0.58
1:B:510:ILE:O	1:B:513:LEU:HB2	2.02	0.58
1:A:123:THR:HA	1:A:160:LYS:HE2	1.84	0.58
1:A:131:ASP:C	1:A:133:ARG:H	2.05	0.58
1:A:387:GLU:HB3	1:A:390:VAL:HG21	1.84	0.58
1:B:189:ASN:O	1:B:192:PRO:HD2	2.02	0.58
1:A:141:CYS:O	1:A:144:SER:HB3	2.03	0.58
1:B:291:MET:O	1:B:292:LYS:C	2.41	0.58
1:A:386:GLN:NE2	1:A:466:ARG:HA	2.19	0.58
1:A:4:ARG:NH2	1:A:179:GLU:CB	2.67	0.58
1:B:205:ASN:CG	1:B:206:THR:H	2.07	0.58
1:A:115:LYS:HZ1	1:A:218:GLY:HA3	1.68	0.58
1:B:161:PRO:HB2	1:B:192:PRO:HG2	1.85	0.58
1:B:230:CYS:SG	1:B:276:ILE:HG21	2.44	0.58
1:A:134:ASP:O	1:A:138:GLN:HG3	2.04	0.58
1:A:242:VAL:CG1	1:A:317:THR:HB	2.34	0.58
1:B:269:TRP:HA	3:B:1016:HOH:O	2.03	0.57
1:A:144:SER:OG	1:A:145:GLN:N	2.36	0.57
1:B:255:SER:O	1:B:256:GLY:O	2.21	0.57
1:B:62:GLN:O	1:B:65:PRO:HD2	2.05	0.57
1:B:124:ASN:HA	1:B:153:SER:HB3	1.85	0.57
1:B:205:ASN:HB3	1:B:207:ALA:H	1.69	0.57
1:B:453:PHE:HE2	1:B:461:PRO:HG2	1.68	0.57
1:A:469:GLU:HG3	1:A:473:LYS:NZ	2.18	0.57
1:B:212:GLU:C	1:B:214:GLU:N	2.55	0.57
1:B:214:GLU:HG3	1:B:215:LYS:N	2.19	0.57
1:A:139:MET:O	1:A:143:LEU:HD12	2.05	0.57
1:A:381:TYR:N	1:A:418:VAL:O	2.30	0.57
1:B:6:ALA:CB	1:B:181:VAL:HG13	2.35	0.57
1:B:72:ARG:HG2	1:B:72:ARG:O	2.05	0.57
1:A:270:PHE:O	1:A:273:ARG:HB3	2.05	0.57
1:B:243:LYS:HB3	1:B:246:ILE:HD13	1.87	0.57
1:B:24:ARG:HH21	1:B:35:ASP:N	2.03	0.57
1:B:420:LYS:C	1:B:424:ILE:HD11	2.25	0.57
1:B:94:GLN:HA	1:B:94:GLN:NE2	2.20	0.57
1:A:200:THR:O	1:A:201:ILE:HG12	2.05	0.56
1:B:165:ILE:O	1:B:166:TYR:C	2.42	0.56
1:B:222:PRO:CG	1:B:225:PRO:HG3	2.22	0.56
1:B:13:VAL:CB	1:B:203:VAL:HG11	2.31	0.56
1:A:202:LEU:O	1:A:203:VAL:HB	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ALA:O	1:B:112:LEU:HD12	2.05	0.56
1:B:386:GLN:NE2	1:B:466:ARG:HA	2.20	0.56
1:A:227:PRO:HG2	1:A:274:TYR:CD1	2.40	0.56
1:A:64:VAL:HG22	1:A:64:VAL:O	2.06	0.56
1:A:92:PHE:CD1	1:A:92:PHE:O	2.59	0.56
1:A:212:GLU:O	1:A:215:LYS:HB2	2.05	0.56
1:A:347:PRO:O	1:B:133:ARG:HD2	2.05	0.56
1:B:79:GLY:O	1:B:80:ALA:HB3	2.05	0.56
1:A:16:LEU:HA	1:A:17:PRO:O	2.06	0.56
1:A:187:GLY:CA	1:A:190:LEU:HD12	2.29	0.56
1:A:332:HIS:HB2	1:A:356:LEU:HB2	1.88	0.56
1:B:8:PHE:CE1	1:B:147:PHE:HE2	2.23	0.56
1:B:165:ILE:O	1:B:168:PHE:N	2.35	0.56
1:B:12:GLY:HA3	1:B:185:ASP:HB3	1.87	0.56
1:A:513:LEU:HD23	1:A:514:LYS:O	2.05	0.56
1:A:122:VAL:HA	1:A:151:ILE:O	2.06	0.56
1:A:50:THR:OG1	1:A:66:LEU:CD1	2.52	0.56
1:A:96:MET:O	1:A:99:ARG:HG2	2.06	0.56
1:B:115:LYS:HE3	1:B:219:THR:CG2	2.36	0.56
1:B:153:SER:HB2	1:B:159:ILE:HG22	1.87	0.56
1:A:96:MET:SD	1:A:136:LEU:HD22	2.46	0.55
1:B:187:GLY:HA2	1:B:190:LEU:CD1	2.35	0.55
1:A:328:VAL:HG22	1:A:352:ALA:HB3	1.87	0.55
1:B:20:ALA:O	1:B:23:PHE:N	2.37	0.55
1:B:363:PRO:HB2	1:B:472:TRP:CD1	2.42	0.55
1:A:210:LEU:O	1:A:214:GLU:HB2	2.07	0.55
1:A:243:LYS:HB3	1:A:246:ILE:HD13	1.88	0.55
1:B:229:PRO:O	1:B:230:CYS:C	2.43	0.55
1:B:463:ASN:HA	1:B:466:ARG:HG3	1.88	0.55
1:A:363:PRO:HB2	1:A:472:TRP:CD1	2.41	0.55
1:B:106:LEU:O	1:B:109:ALA:HB3	2.07	0.55
1:B:160:LYS:CD	1:B:189:ASN:HD21	2.19	0.55
1:B:230:CYS:HB3	1:B:277:PRO:CD	2.34	0.55
1:B:25:ARG:C	1:B:28:GLU:HB2	2.27	0.55
1:A:242:VAL:HG12	1:A:317:THR:CG2	2.37	0.55
1:A:90:GLN:CG	1:A:91:ILE:N	2.70	0.55
1:B:126:TRP:HD1	1:B:127:LEU:O	1.89	0.55
1:B:242:VAL:CG1	1:B:317:THR:HB	2.37	0.55
1:A:279:LEU:O	1:A:282:ALA:HB3	2.07	0.55
1:B:131:ASP:C	1:B:133:ARG:H	2.10	0.55
1:B:328:VAL:HG22	1:B:352:ALA:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:PHE:HA	1:B:524:TRP:NE1	2.21	0.55
1:A:16:LEU:HA	1:A:17:PRO:C	2.28	0.55
1:B:182:PHE:O	1:B:201:ILE:HG13	2.07	0.55
1:B:50:THR:HG23	1:B:63:TRP:CZ2	2.41	0.55
1:A:303:ILE:HA	1:A:463:ASN:HD21	1.71	0.55
1:A:385:PHE:O	1:A:387:GLU:N	2.40	0.55
1:B:38:LEU:O	1:B:40:ALA:N	2.40	0.55
1:A:125:ASN:HD22	1:A:152:GLU:HB3	1.72	0.55
1:A:12:GLY:HA3	1:A:18:SER:OG	2.07	0.55
1:A:463:ASN:HA	1:A:466:ARG:HG3	1.87	0.55
1:B:281:GLN:O	1:B:282:ALA:C	2.43	0.55
1:B:468:THR:HA	3:B:1005:HOH:O	2.07	0.55
1:B:279:LEU:O	1:B:282:ALA:HB3	2.07	0.54
1:B:333:ASP:OD2	1:B:523:HIS:NE2	2.36	0.54
1:A:482:LYS:HB2	1:B:62:GLN:HE22	1.72	0.54
1:B:206:THR:O	1:B:207:ALA:CB	2.55	0.54
1:B:72:ARG:CD	1:B:73:LYS:HZ1	2.21	0.54
1:B:242:VAL:HG12	1:B:317:THR:CG2	2.37	0.54
1:B:477:LYS:C	1:B:479:LEU:H	2.09	0.54
1:A:428:LEU:O	1:A:431:THR:CB	2.55	0.54
1:B:134:ASP:O	1:B:135:SER:C	2.45	0.54
1:B:214:GLU:O	1:B:214:GLU:OE1	2.26	0.54
1:A:177:PRO:O	1:A:198:MET:HB3	2.07	0.54
1:A:202:LEU:O	1:A:203:VAL:CB	2.56	0.54
1:A:381:TYR:CE1	1:A:382:GLN:HG3	2.42	0.54
1:B:194:ARG:HB2	1:B:200:THR:HG21	1.88	0.54
1:B:177:PRO:O	1:B:197:GLY:O	2.25	0.54
1:B:215:LYS:O	1:B:219:THR:O	2.25	0.54
1:B:107:GLN:HG2	1:B:225:PRO:HG2	1.90	0.54
1:B:332:HIS:HB2	1:B:356:LEU:HB2	1.90	0.54
1:B:58:ILE:O	1:B:58:ILE:HG13	2.07	0.54
1:B:92:PHE:C	1:B:94:GLN:H	2.11	0.54
1:A:499:ARG:HB3	1:A:501:GLU:OE2	2.08	0.54
1:B:362:PRO:HG2	1:B:509:TRP:CE2	2.42	0.54
1:B:270:PHE:CD2	1:B:448:PHE:CD2	2.95	0.54
1:A:209:ALA:O	1:A:213:LEU:N	2.41	0.54
1:A:537:LEU:O	1:A:541:LEU:CD1	2.54	0.54
1:A:92:PHE:HD1	1:A:92:PHE:O	1.90	0.54
1:B:193:ALA:HB1	1:B:198:MET:HG3	1.90	0.54
1:B:205:ASN:OD1	1:B:207:ALA:O	2.26	0.54
1:B:272:TRP:O	1:B:274:TYR:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ILE:HG22	1:A:102:ASN:N	2.23	0.54
1:A:293:GLY:C	1:A:299:SER:HB2	2.28	0.54
1:A:535:GLN:C	1:A:539:LYS:HD3	2.28	0.54
1:A:53:LEU:HB3	1:A:58:ILE:HD12	1.90	0.54
1:B:183:LEU:HD23	1:B:201:ILE:CD1	2.21	0.54
1:B:293:GLY:C	1:B:299:SER:HB2	2.28	0.54
1:B:376:ILE:H	1:B:376:ILE:CD1	2.16	0.54
1:A:477:LYS:C	1:A:479:LEU:H	2.10	0.54
1:A:60:PHE:O	1:A:63:TRP:HB3	2.08	0.54
1:B:32:LEU:CD2	1:B:37:LEU:HG	2.38	0.54
1:A:101:ILE:CG2	1:A:102:ASN:N	2.71	0.53
1:A:111:ALA:O	1:A:114:LYS:N	2.40	0.53
1:B:61:SER:OG	1:B:129:ASP:OD1	2.26	0.53
1:B:180:VAL:O	1:B:199:VAL:HG23	2.09	0.53
1:A:348:GLU:HA	1:B:133:ARG:HD2	1.90	0.53
1:B:183:LEU:HB2	1:B:203:VAL:HG23	1.90	0.53
1:B:325:PRO:HA	1:B:349:ARG:NH1	2.23	0.53
1:B:381:TYR:N	1:B:418:VAL:O	2.29	0.53
1:B:50:THR:HA	1:B:63:TRP:HE1	1.74	0.53
1:A:117:PHE:CD1	1:A:117:PHE:N	2.75	0.53
1:A:122:VAL:HA	1:A:151:ILE:HB	1.91	0.53
1:A:433:GLU:HA	1:A:433:GLU:OE1	2.08	0.53
1:B:61:SER:O	1:B:65:PRO:HD2	2.09	0.53
1:A:13:VAL:HG22	1:A:203:VAL:HG21	1.90	0.53
1:B:535:GLN:C	1:B:539:LYS:HD3	2.28	0.53
1:A:263:HIS:O	1:A:335:ALA:HB2	2.09	0.53
1:B:173:LEU:HD22	1:B:173:LEU:H	1.73	0.53
1:B:173:LEU:O	1:B:174:LYS:HB2	2.08	0.53
1:B:381:TYR:CD2	1:B:418:VAL:HG12	2.44	0.53
1:A:168:PHE:C	1:A:168:PHE:CD2	2.82	0.53
1:A:255:SER:O	1:A:256:GLY:O	2.27	0.53
1:A:300:PRO:CG	1:A:305:GLU:HG2	2.39	0.53
1:A:482:LYS:N	1:B:62:GLN:HE22	2.06	0.53
1:A:92:PHE:O	1:A:94:GLN:N	2.42	0.53
1:B:16:LEU:HD23	1:B:102:ASN:HB2	1.90	0.53
1:A:108:ALA:O	1:A:112:LEU:HD12	2.08	0.53
1:A:125:ASN:N	1:A:153:SER:OG	2.42	0.53
1:A:272:TRP:O	1:A:274:TYR:N	2.41	0.53
1:B:124:ASN:HA	1:B:153:SER:CB	2.38	0.53
1:A:16:LEU:CA	1:A:17:PRO:C	2.77	0.53
1:B:232:PRO:HG2	1:B:233:ASN:ND2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LEU:HD21	1:B:82:LEU:HD11	1.90	0.53
1:B:488:LEU:HD13	1:B:490:VAL:HG23	1.90	0.53
1:B:499:ARG:HB3	1:B:501:GLU:OE2	2.07	0.53
1:B:72:ARG:CD	1:B:73:LYS:NZ	2.72	0.53
1:A:515:ARG:HG2	1:A:515:ARG:HH11	1.70	0.53
1:B:523:HIS:CD2	2:B:1200:CIU:HC41	2.44	0.53
1:B:381:TYR:CE2	1:B:418:VAL:HG12	2.44	0.53
1:B:513:LEU:HD23	1:B:514:LYS:O	2.09	0.53
1:B:515:ARG:HH11	1:B:515:ARG:HG2	1.71	0.53
1:A:183:LEU:HA	1:A:201:ILE:O	2.09	0.53
1:B:385:PHE:O	1:B:387:GLU:N	2.42	0.53
1:B:40:ALA:HB2	1:B:71:TYR:OH	2.09	0.53
1:B:9:ASP:OD1	1:B:160:LYS:NZ	2.35	0.53
1:A:270:PHE:CD2	1:A:448:PHE:CD2	2.97	0.52
1:B:300:PRO:CG	1:B:305:GLU:HG2	2.39	0.52
1:A:249:HIS:ND1	1:A:296:ASP:HB2	2.23	0.52
1:A:52:GLN:CA	1:A:55:LYS:HD2	2.39	0.52
1:B:118:THR:CA	1:B:148:ASP:OD2	2.57	0.52
1:B:469:GLU:HG3	1:B:473:LYS:NZ	2.23	0.52
1:A:256:GLY:N	1:A:285:ARG:HB2	2.24	0.52
1:A:482:LYS:CB	1:B:62:GLN:HE22	2.21	0.52
1:A:162:GLU:O	1:A:164:GLN:N	2.42	0.52
1:B:112:LEU:HB3	1:B:117:PHE:CD1	2.44	0.52
1:A:206:THR:O	1:A:207:ALA:HB2	2.09	0.52
1:A:489:MET:HE3	1:A:490:VAL:N	2.25	0.52
1:B:156:VAL:HG23	1:B:157:GLY:N	2.24	0.52
1:B:191:LYS:HB3	1:B:192:PRO:HD3	1.92	0.52
1:B:20:ALA:O	1:B:22:ALA:N	2.43	0.52
1:A:213:LEU:O	1:A:216:VAL:HB	2.10	0.52
1:A:407:PHE:HA	1:A:524:TRP:NE1	2.24	0.52
1:B:64:VAL:CB	1:B:65:PRO:CD	2.87	0.52
1:B:270:PHE:CE1	1:B:273:ARG:HD3	2.45	0.52
1:B:230:CYS:HB3	1:B:277:PRO:CG	2.39	0.52
1:B:458:PHE:HB3	1:B:462:LEU:CD1	2.40	0.52
1:A:136:LEU:HD12	1:A:140:MET:HG2	1.91	0.52
1:A:94:GLN:O	1:A:97:ALA:N	2.43	0.52
1:A:119:THR:OG1	1:A:147:PHE:HA	2.10	0.52
1:B:459:ARG:HG2	1:B:459:ARG:HH11	1.75	0.52
1:A:304:GLU:CD	1:A:304:GLU:N	2.62	0.52
1:A:53:LEU:CD1	1:A:53:LEU:C	2.79	0.52
1:A:205:ASN:ND2	1:A:207:ALA:H	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLN:OE1	1:A:53:LEU:N	2.43	0.51
1:A:8:PHE:HE1	1:A:147:PHE:HE2	1.58	0.51
1:B:134:ASP:O	1:B:137:ALA:N	2.43	0.51
1:B:13:VAL:CG2	1:B:14:LEU:N	2.72	0.51
1:B:4:ARG:HD2	1:B:179:GLU:HB2	1.91	0.51
1:B:523:HIS:CD2	1:B:524:TRP:CZ3	2.98	0.51
1:B:54:MET:CB	1:B:159:ILE:HG21	2.39	0.51
1:B:263:HIS:O	1:B:335:ALA:HB2	2.10	0.51
1:A:53:LEU:HD13	1:A:53:LEU:C	2.30	0.51
1:B:247:ARG:HG2	1:B:248:LEU:N	2.26	0.51
1:A:17:PRO:HD2	1:A:99:ARG:HA	1.92	0.51
1:A:115:LYS:NZ	1:A:218:GLY:HA3	2.25	0.51
1:B:42:GLN:HB2	1:B:186:PHE:HE1	1.72	0.51
1:B:303:ILE:HA	1:B:463:ASN:HD21	1.74	0.51
1:B:515:ARG:CG	1:B:515:ARG:NH1	2.59	0.51
1:B:72:ARG:HD3	1:B:73:LYS:NZ	2.25	0.51
1:B:13:VAL:HG22	1:B:14:LEU:N	2.25	0.51
1:B:86:PHE:CE1	1:B:87:SER:O	2.63	0.51
1:A:106:LEU:O	1:A:106:LEU:CD2	2.56	0.51
1:A:265:PHE:CD1	1:A:265:PHE:C	2.84	0.51
1:A:276:ILE:HG22	1:A:277:PRO:HD3	1.93	0.51
1:B:289:ILE:CG2	1:B:290:ASP:N	2.73	0.51
1:B:30:LEU:O	1:B:31:ALA:C	2.48	0.51
1:B:72:ARG:NH1	1:B:72:ARG:HB2	2.25	0.51
1:A:380:ASN:HB2	1:A:419:HIS:HA	1.93	0.51
1:A:438:SER:C	1:A:440:ILE:H	2.14	0.51
1:A:459:ARG:HG2	1:A:459:ARG:HH11	1.75	0.51
1:B:162:GLU:HB3	1:B:164:GLN:HG2	1.92	0.51
1:B:303:ILE:CD1	1:B:463:ASN:ND2	2.68	0.51
1:A:124:ASN:ND2	1:A:160:LYS:HB2	2.26	0.51
1:A:113:LYS:NZ	1:A:146:HIS:HA	2.26	0.51
1:A:259:LEU:CD1	1:A:279:LEU:HD13	2.41	0.51
1:A:205:ASN:CG	1:A:206:THR:N	2.63	0.51
1:A:300:PRO:HB2	1:A:301:PRO:CD	2.41	0.51
1:A:50:THR:HG23	1:A:63:TRP:CZ2	2.45	0.51
1:B:191:LYS:CB	1:B:192:PRO:HD3	2.40	0.51
1:B:299:SER:CB	1:B:456:THR:HG22	2.40	0.51
1:B:417:ALA:H	1:B:427:ILE:HG22	1.75	0.51
1:B:473:LYS:HB2	1:B:473:LYS:NZ	2.25	0.51
1:A:52:GLN:HA	1:A:55:LYS:HD2	1.92	0.51
1:B:208:SER:O	1:B:209:ALA:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ARG:HB2	1:B:72:ARG:HH11	1.75	0.51
1:A:325:PRO:O	1:B:137:ALA:HB1	2.11	0.50
1:A:337:VAL:CG2	2:A:1100:CIU:H12	2.41	0.50
1:A:299:SER:CB	1:A:456:THR:HG22	2.40	0.50
1:A:90:GLN:HG3	1:A:91:ILE:H	1.75	0.50
1:B:420:LYS:O	1:B:424:ILE:CD1	2.59	0.50
1:A:207:ALA:O	1:A:210:LEU:HB2	2.11	0.50
1:B:276:ILE:HG22	1:B:277:PRO:HD3	1.93	0.50
1:A:124:ASN:OD1	1:A:160:LYS:N	2.45	0.50
1:A:9:ASP:HB2	1:A:160:LYS:HZ3	1.76	0.50
1:A:362:PRO:HG2	1:A:509:TRP:CE2	2.46	0.50
1:B:54:MET:HB2	1:B:159:ILE:HG21	1.92	0.50
1:A:117:PHE:HD1	1:A:117:PHE:N	2.10	0.50
1:A:446:ILE:O	1:A:450:ILE:HG13	2.12	0.50
1:A:458:PHE:HB3	1:A:462:LEU:CD1	2.41	0.50
1:B:127:LEU:CD1	1:B:127:LEU:N	2.66	0.50
1:B:89:SER:OG	1:B:90:GLN:N	2.44	0.50
1:A:5:VAL:O	1:A:180:VAL:HA	2.11	0.50
1:A:106:LEU:HD23	1:A:110:ILE:HD11	1.92	0.50
1:A:319:LEU:N	1:A:319:LEU:HD23	2.27	0.50
1:A:145:GLN:HE22	1:B:321:LYS:HD2	1.76	0.50
1:B:44:GLU:O	1:B:46:PRO:HD3	2.11	0.50
1:A:211:ARG:O	1:A:215:LYS:N	2.45	0.50
1:A:511:PRO:C	1:A:512:PHE:CG	2.85	0.50
1:A:12:GLY:HA2	1:A:15:ALA:O	2.12	0.50
1:A:473:LYS:HB2	1:A:473:LYS:NZ	2.27	0.50
1:B:270:PHE:CD2	1:B:448:PHE:HD2	2.28	0.50
1:A:281:GLN:O	1:A:282:ALA:C	2.49	0.50
1:A:385:PHE:O	1:A:386:GLN:C	2.49	0.50
1:A:401:ARG:O	1:A:402:THR:C	2.49	0.50
1:A:512:PHE:O	1:A:513:LEU:C	2.49	0.50
1:B:304:GLU:N	1:B:304:GLU:CD	2.64	0.50
1:A:108:ALA:O	1:A:111:ALA:HB3	2.11	0.49
1:A:376:ILE:H	1:A:376:ILE:CD1	2.13	0.49
1:B:202:LEU:HD12	1:B:204:HIS:HB2	1.92	0.49
1:B:210:LEU:O	1:B:212:GLU:N	2.45	0.49
1:B:265:PHE:C	1:B:265:PHE:CD1	2.85	0.49
1:B:289:ILE:HG22	1:B:290:ASP:N	2.26	0.49
1:A:145:GLN:NE2	1:B:321:LYS:HD2	2.27	0.49
1:A:307:ALA:O	1:A:311:LEU:HG	2.12	0.49
1:A:417:ALA:O	1:A:421:ALA:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:GLU:O	1:B:214:GLU:N	2.44	0.49
1:B:8:PHE:O	1:B:121:ILE:HA	2.11	0.49
1:B:91:ILE:O	1:B:91:ILE:CG1	2.61	0.49
1:A:155:GLN:C	1:A:157:GLY:H	2.15	0.49
1:A:190:LEU:HB3	1:A:200:THR:CG2	2.43	0.49
1:B:128:ASP:O	1:B:133:ARG:HG3	2.12	0.49
1:B:319:LEU:HD23	1:B:319:LEU:N	2.27	0.49
1:B:374:ARG:HG2	1:B:383:LEU:HD11	1.95	0.49
1:B:309:GLU:HA	1:B:474:TRP:CZ2	2.47	0.49
1:B:526:GLN:NE2	1:B:527:ILE:CD1	2.75	0.49
1:B:406:PHE:CD2	2:B:1200:CIU:HC12	2.47	0.49
1:B:190:LEU:HD12	1:B:202:LEU:HD23	1.94	0.49
1:B:249:HIS:ND1	1:B:296:ASP:HB2	2.28	0.49
1:B:512:PHE:O	1:B:513:LEU:C	2.49	0.49
1:A:180:VAL:O	1:A:180:VAL:CG2	2.61	0.49
1:B:136:LEU:O	1:B:136:LEU:HD12	2.13	0.49
1:B:160:LYS:HA	1:B:165:ILE:HD11	1.94	0.49
1:B:515:ARG:HG3	1:B:515:ARG:NH1	2.22	0.49
1:B:86:PHE:CG	1:B:87:SER:N	2.81	0.49
1:A:165:ILE:O	1:A:169:LEU:N	2.43	0.49
1:A:238:GLY:HA2	1:B:238:GLY:HA2	1.93	0.49
1:B:126:TRP:HA	1:B:154:CYS:CB	2.43	0.49
1:B:8:PHE:HA	1:B:183:LEU:HD12	1.93	0.49
1:B:182:PHE:C	1:B:183:LEU:HG	2.33	0.49
1:A:173:LEU:N	1:A:173:LEU:HD22	2.18	0.49
1:A:215:LYS:HG2	1:A:220:GLN:CA	2.42	0.49
1:B:32:LEU:HD12	1:B:32:LEU:H	1.78	0.49
1:B:438:SER:C	1:B:440:ILE:H	2.16	0.49
1:B:286:VAL:C	1:B:287:LEU:HD12	2.32	0.49
1:A:8:PHE:CB	1:A:183:LEU:HD11	2.43	0.49
1:A:247:ARG:HG2	1:A:248:LEU:N	2.28	0.49
1:A:286:VAL:C	1:A:287:LEU:HD12	2.33	0.49
1:A:302:GLU:HB3	1:A:304:GLU:OE1	2.11	0.49
1:B:381:TYR:CG	1:B:382:GLN:N	2.81	0.49
1:A:187:GLY:HA2	1:A:190:LEU:CD1	2.33	0.48
1:A:207:ALA:O	1:A:208:SER:HB3	2.12	0.48
1:A:242:VAL:HG12	1:A:317:THR:CB	2.43	0.48
1:A:440:ILE:HA	1:A:440:ILE:HD12	1.66	0.48
1:A:484:LEU:HD13	1:B:61:SER:HB2	1.93	0.48
1:B:293:GLY:O	1:B:299:SER:HB2	2.13	0.48
1:B:408:ARG:O	1:B:524:TRP:HD1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:GLN:NE2	1:B:134:ASP:CA	2.76	0.48
1:B:176:LYS:HB3	1:B:178:ASN:HD22	1.76	0.48
1:B:328:VAL:HG12	1:B:330:ILE:HD11	1.93	0.48
1:A:381:TYR:CG	1:A:382:GLN:N	2.81	0.48
1:B:103:ARG:CB	1:B:104:PRO:HD3	2.23	0.48
1:B:106:LEU:HD21	1:B:146:HIS:HD2	1.78	0.48
1:B:306:TYR:CD1	1:B:306:TYR:N	2.82	0.48
1:B:350:VAL:HG11	1:B:353:VAL:HG22	1.94	0.48
1:B:469:GLU:O	1:B:472:TRP:HB3	2.12	0.48
1:B:5:VAL:HB	1:B:118:THR:OG1	2.13	0.48
1:B:92:PHE:C	1:B:94:GLN:N	2.67	0.48
1:B:93:SER:O	1:B:132:LYS:HG3	2.13	0.48
1:B:101:ILE:CD1	1:B:143:LEU:HD21	2.44	0.48
1:B:194:ARG:HB2	1:B:200:THR:CG2	2.43	0.48
1:B:385:PHE:HE1	1:B:427:ILE:HD11	1.78	0.48
1:B:63:TRP:O	1:B:63:TRP:CG	2.67	0.48
1:A:270:PHE:CD2	1:A:448:PHE:HD2	2.32	0.48
1:A:63:TRP:CE3	1:A:63:TRP:O	2.66	0.48
1:B:256:GLY:N	1:B:285:ARG:HB2	2.28	0.48
1:A:182:PHE:CD1	1:A:183:LEU:N	2.81	0.48
1:A:211:ARG:HB2	1:A:215:LYS:NZ	2.27	0.48
1:A:270:PHE:CE1	1:A:273:ARG:HD3	2.49	0.48
1:A:333:ASP:OD2	1:A:523:HIS:NE2	2.36	0.48
1:A:380:ASN:HB3	1:A:418:VAL:O	2.14	0.48
1:B:340:TRP:CZ2	1:B:489:MET:HG2	2.49	0.48
1:B:446:ILE:O	1:B:450:ILE:HG13	2.14	0.48
1:A:102:ASN:ND2	1:A:105:MET:HB2	2.28	0.48
1:A:293:GLY:O	1:A:299:SER:HB2	2.14	0.48
1:A:459:ARG:CG	1:A:459:ARG:HH11	2.27	0.48
1:B:30:LEU:CB	1:B:32:LEU:HD13	2.38	0.48
1:B:511:PRO:C	1:B:512:PHE:CG	2.87	0.48
1:A:136:LEU:HD12	1:A:140:MET:CG	2.44	0.48
1:A:181:VAL:HG23	1:A:182:PHE:N	2.29	0.48
1:A:13:VAL:HG22	1:A:203:VAL:CB	2.44	0.48
1:A:332:HIS:ND1	1:A:333:ASP:HB2	2.28	0.48
1:A:350:VAL:HG11	1:A:353:VAL:HG22	1.95	0.48
1:A:48:GLY:O	1:A:52:GLN:HG3	2.14	0.48
1:B:10:LEU:O	1:B:15:ALA:HB3	2.13	0.48
1:A:248:LEU:HA	1:A:297:SER:HB3	1.95	0.48
1:B:25:ARG:HA	1:B:28:GLU:HB2	1.94	0.48
1:B:259:LEU:CD1	1:B:279:LEU:HD13	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:GLU:OE1	1:A:217:THR:HG21	2.14	0.47
1:B:475:SER:C	1:B:477:LYS:H	2.18	0.47
1:A:123:THR:HA	1:A:160:LYS:CE	2.44	0.47
1:B:149:PHE:CE2	1:B:173:LEU:HD13	2.50	0.47
1:B:302:GLU:HB3	1:B:304:GLU:OE1	2.14	0.47
1:B:38:LEU:HD22	1:B:42:GLN:HB3	1.95	0.47
1:B:64:VAL:O	1:B:65:PRO:C	2.50	0.47
1:B:340:TRP:NE1	1:B:355:SER:HB2	2.29	0.47
1:B:381:TYR:CE1	1:B:382:GLN:HG3	2.49	0.47
1:B:305:GLU:HB3	1:B:306:TYR:CD1	2.49	0.47
1:B:416:ILE:HG23	1:B:417:ALA:N	2.29	0.47
1:A:291:MET:HA	1:A:291:MET:CE	2.45	0.47
1:A:340:TRP:NE1	1:A:355:SER:HB2	2.28	0.47
1:B:115:LYS:HE3	1:B:219:THR:HG23	1.96	0.47
1:B:231:ASN:OD1	1:B:270:PHE:CE1	2.62	0.47
1:B:74:SER:O	1:B:75:SER:O	2.32	0.47
1:A:301:PRO:CD	1:A:302:GLU:N	2.78	0.47
1:B:158:MET:CB	1:B:164:GLN:HB2	2.43	0.47
1:B:219:THR:HB	1:B:220:GLN:H	1.32	0.47
1:B:223:GLU:OE2	1:B:223:GLU:N	2.46	0.47
1:B:499:ARG:CB	1:B:501:GLU:OE2	2.63	0.47
1:B:76:LYS:HA	1:B:80:ALA:O	2.14	0.47
1:A:132:LYS:O	1:A:135:SER:HB2	2.14	0.47
1:A:252:GLU:HG2	3:B:1013:HOH:O	2.13	0.47
1:B:202:LEU:CD1	1:B:204:HIS:CD2	2.97	0.47
1:B:380:ASN:O	1:B:381:TYR:C	2.53	0.47
1:A:122:VAL:HG11	1:A:169:LEU:HD11	1.96	0.47
1:B:131:ASP:C	1:B:133:ARG:N	2.68	0.47
1:B:16:LEU:O	1:B:100:SER:N	2.45	0.47
1:B:300:PRO:HB2	1:B:301:PRO:CD	2.45	0.47
1:B:428:LEU:N	1:B:428:LEU:CD1	2.78	0.47
1:A:177:PRO:O	1:A:198:MET:CB	2.63	0.47
1:A:469:GLU:O	1:A:472:TRP:HB3	2.15	0.47
1:A:501:GLU:O	1:A:504:LYS:HG2	2.15	0.47
1:B:229:PRO:HB3	1:B:274:TYR:CD1	2.49	0.47
1:B:270:PHE:O	1:B:273:ARG:HB3	2.14	0.47
1:B:401:ARG:O	1:B:402:THR:C	2.54	0.47
1:A:103:ARG:HG2	1:A:103:ARG:H	1.19	0.47
1:A:136:LEU:O	1:A:137:ALA:C	2.53	0.47
1:A:347:PRO:O	1:B:133:ARG:CD	2.63	0.47
1:B:490:VAL:HA	1:B:516:GLY:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ILE:HG23	1:A:417:ALA:N	2.30	0.46
1:A:475:SER:C	1:A:477:LYS:H	2.18	0.46
1:A:163:PRO:HA	1:A:166:TYR:CD1	2.50	0.46
1:A:380:ASN:O	1:A:381:TYR:C	2.53	0.46
1:A:511:PRO:O	1:A:512:PHE:CG	2.69	0.46
1:A:52:GLN:HB3	1:A:55:LYS:HD2	1.96	0.46
1:A:50:THR:HA	1:A:63:TRP:NE1	2.26	0.46
1:B:73:LYS:C	1:B:75:SER:H	2.19	0.46
1:B:8:PHE:HD1	1:B:120:CYS:O	1.99	0.46
1:A:103:ARG:N	1:A:104:PRO:HD2	2.31	0.46
1:A:340:TRP:CZ2	1:A:489:MET:HG2	2.50	0.46
1:A:408:ARG:O	1:A:524:TRP:HD1	1.99	0.46
1:A:523:HIS:CD2	1:A:524:TRP:CZ3	3.02	0.46
1:A:53:LEU:HA	1:A:58:ILE:HG13	1.98	0.46
1:B:16:LEU:CB	1:B:17:PRO:CA	2.92	0.46
1:B:193:ALA:HA	1:B:196:MET:HG3	1.96	0.46
1:A:101:ILE:HD13	1:A:106:LEU:CD1	2.44	0.46
1:A:137:ALA:O	1:A:140:MET:HB2	2.16	0.46
1:A:123:THR:CA	1:A:160:LYS:HE2	2.45	0.46
1:B:124:ASN:HA	1:B:153:SER:OG	2.15	0.46
1:B:232:PRO:CG	1:B:233:ASN:HD22	2.29	0.46
1:B:28:GLU:O	1:B:30:LEU:N	2.48	0.46
1:B:380:ASN:HB3	1:B:418:VAL:O	2.15	0.46
1:A:259:LEU:HD11	1:A:279:LEU:HD13	1.97	0.46
1:A:515:ARG:CG	1:A:515:ARG:NH1	2.60	0.46
1:B:385:PHE:O	1:B:386:GLN:C	2.53	0.46
1:B:434:ASP:N	1:B:435:PRO:HD2	2.30	0.46
1:B:442:THR:HG23	1:B:445:GLU:OE1	2.15	0.46
1:B:459:ARG:CG	1:B:459:ARG:HH11	2.28	0.46
1:A:180:VAL:HG23	1:A:198:MET:CE	2.46	0.46
1:A:400:SER:O	1:A:404:LYS:HG2	2.16	0.46
1:A:489:MET:CE	1:A:490:VAL:N	2.78	0.46
1:A:53:LEU:CD1	1:A:54:MET:N	2.78	0.46
1:A:294:TYR:CZ	1:A:461:PRO:HB3	2.51	0.46
1:A:499:ARG:CB	1:A:501:GLU:OE2	2.63	0.46
1:B:10:LEU:HD12	1:B:15:ALA:HB2	1.98	0.46
1:B:242:VAL:HG12	1:B:317:THR:CB	2.46	0.46
1:B:193:ALA:C	1:B:195:ASP:H	2.19	0.46
1:B:25:ARG:HA	1:B:28:GLU:CB	2.46	0.46
1:B:248:LEU:HA	1:B:297:SER:HB3	1.98	0.46
1:B:48:GLY:HA3	1:B:49:PRO:HD3	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ILE:C	1:A:305:GLU:N	2.67	0.46
1:A:374:ARG:HG2	1:A:383:LEU:HD11	1.97	0.46
1:A:450:ILE:O	1:A:454:LYS:HG2	2.16	0.46
1:A:529:LYS:HA	1:A:529:LYS:HD3	1.74	0.46
1:B:161:PRO:CB	1:B:192:PRO:HG2	2.46	0.46
1:A:305:GLU:HB3	1:A:306:TYR:CD1	2.51	0.46
1:A:416:ILE:CG2	1:A:417:ALA:N	2.79	0.46
1:B:10:LEU:CD1	1:B:15:ALA:HB2	2.46	0.46
1:B:332:HIS:ND1	1:B:333:ASP:HB2	2.31	0.46
1:B:416:ILE:HG23	1:B:427:ILE:CG2	2.45	0.46
1:B:408:ARG:HH21	1:B:412:GLU:HG2	1.81	0.45
1:B:294:TYR:CZ	1:B:461:PRO:HB3	2.51	0.45
1:B:77:ALA:O	1:B:78:CYS:HB2	2.16	0.45
1:A:368:SER:HB3	1:A:371:LYS:CG	2.46	0.45
1:B:378:VAL:HG22	1:B:418:VAL:HG11	1.98	0.45
1:A:303:ILE:CD1	1:A:463:ASN:ND2	2.74	0.45
1:B:14:LEU:HD22	1:B:121:ILE:HG21	1.98	0.45
1:A:484:LEU:CD1	1:B:129:ASP:OD2	2.50	0.45
1:B:364:ASP:N	1:B:364:ASP:OD1	2.50	0.45
1:B:400:SER:O	1:B:404:LYS:HG2	2.17	0.45
1:A:129:ASP:OD2	1:B:484:LEU:HD12	2.16	0.45
1:A:442:THR:HG23	1:A:445:GLU:OE1	2.16	0.45
1:A:490:VAL:HA	1:A:516:GLY:O	2.17	0.45
1:A:60:PHE:CE1	1:A:92:PHE:CZ	3.04	0.45
1:B:416:ILE:CG2	1:B:417:ALA:N	2.79	0.45
1:A:7:ALA:O	1:A:182:PHE:HA	2.16	0.45
1:A:309:GLU:HA	1:A:474:TRP:CZ2	2.51	0.45
1:A:512:PHE:N	1:A:512:PHE:CD1	2.85	0.45
1:B:301:PRO:CD	1:B:302:GLU:N	2.78	0.45
1:B:419:HIS:N	1:B:419:HIS:ND1	2.64	0.45
1:B:537:LEU:O	1:B:541:LEU:CD1	2.60	0.45
1:A:407:PHE:C	1:A:408:ARG:HG2	2.37	0.45
1:A:106:LEU:HD23	1:A:106:LEU:C	2.37	0.45
1:A:369:PRO:O	1:A:372:VAL:HG13	2.17	0.45
1:A:526:GLN:NE2	1:A:527:ILE:CD1	2.80	0.45
1:B:119:THR:HB	1:B:147:PHE:CD2	2.52	0.45
1:B:307:ALA:O	1:B:311:LEU:HG	2.16	0.45
1:B:380:ASN:HB2	1:B:419:HIS:HA	1.96	0.45
1:B:476:CYS:HA	1:B:479:LEU:CD1	2.46	0.45
1:B:511:PRO:O	1:B:512:PHE:CG	2.70	0.45
1:A:207:ALA:HA	1:A:210:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:GLN:CB	1:B:186:PHE:CE1	2.97	0.45
1:B:270:PHE:CZ	1:B:273:ARG:HD3	2.52	0.45
1:B:526:GLN:HE22	1:B:527:ILE:HD11	1.81	0.45
1:B:61:SER:C	1:B:64:VAL:HG23	2.28	0.45
1:A:106:LEU:CD2	1:A:106:LEU:C	2.86	0.45
1:A:168:PHE:CE2	1:A:172:THR:OG1	2.69	0.45
1:A:279:LEU:HA	1:A:279:LEU:HD23	1.79	0.45
1:A:306:TYR:CD1	1:A:306:TYR:N	2.85	0.45
1:B:132:LYS:H	1:B:132:LYS:HD3	1.81	0.45
1:B:50:THR:HA	1:B:63:TRP:NE1	2.30	0.45
1:A:209:ALA:HA	1:A:212:GLU:HB2	1.99	0.45
1:A:336:GLY:HA2	1:A:339:VAL:HB	1.98	0.45
1:A:470:ARG:CA	1:A:473:LYS:NZ	2.71	0.45
1:A:4:ARG:HH21	1:A:179:GLU:CB	2.19	0.45
1:B:232:PRO:HG2	1:B:233:ASN:HD22	1.81	0.45
1:B:229:PRO:CA	1:B:273:ARG:O	2.63	0.45
1:B:27:GLU:HG2	1:B:37:LEU:HB2	1.99	0.45
1:B:9:ASP:O	1:B:13:VAL:HG22	2.17	0.45
1:A:202:LEU:O	1:A:203:VAL:HG23	2.17	0.44
1:A:271:SER:HA	1:A:273:ARG:NH1	2.32	0.44
1:A:470:ARG:N	1:A:473:LYS:NZ	2.65	0.44
1:B:173:LEU:O	1:B:174:LYS:CB	2.64	0.44
1:B:206:THR:O	1:B:207:ALA:HB3	2.17	0.44
1:B:73:LYS:HA	1:B:73:LYS:HD3	1.65	0.44
1:A:231:ASN:HB2	1:A:232:PRO:CB	2.46	0.44
1:A:312:CYS:SG	1:A:338:MET:HG3	2.57	0.44
1:A:515:ARG:HG3	1:A:515:ARG:NH1	2.25	0.44
1:A:58:ILE:HA	1:A:62:GLN:OE1	2.17	0.44
1:B:303:ILE:C	1:B:305:GLU:N	2.70	0.44
1:B:49:PRO:HD2	1:B:67:MET:CE	2.47	0.44
1:A:177:PRO:O	1:A:198:MET:HA	2.17	0.44
1:A:386:GLN:NE2	1:A:468:THR:HG1	2.15	0.44
1:B:150:LEU:HA	1:B:150:LEU:HD12	1.84	0.44
1:B:24:ARG:O	1:B:27:GLU:HB2	2.18	0.44
1:A:124:ASN:HA	1:A:153:SER:OG	2.18	0.44
1:A:173:LEU:CD2	1:A:173:LEU:H	2.20	0.44
1:A:215:LYS:HG2	1:A:220:GLN:HB3	1.99	0.44
1:A:339:VAL:HG13	1:A:353:VAL:HG13	1.97	0.44
1:B:183:LEU:CB	1:B:203:VAL:HG23	2.47	0.44
1:B:404:LYS:HG3	1:B:435:PRO:HB2	1.99	0.44
1:B:82:LEU:HA	1:B:83:PRO:HD2	1.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:LEU:HD11	1:B:204:HIS:CD2	2.52	0.44
1:B:20:ALA:O	1:B:21:GLY:C	2.55	0.44
1:B:293:GLY:HA2	1:B:299:SER:HA	2.00	0.44
1:B:428:LEU:N	1:B:428:LEU:HD13	2.32	0.44
1:B:523:HIS:HD2	1:B:524:TRP:CH2	2.36	0.44
1:A:476:CYS:HA	1:A:479:LEU:CD1	2.48	0.44
1:B:122:VAL:CB	1:B:151:ILE:CD1	2.94	0.44
1:B:210:LEU:C	1:B:212:GLU:H	2.20	0.44
1:B:265:PHE:HA	1:B:266:PRO:HA	1.80	0.44
1:B:336:GLY:HA2	1:B:339:VAL:HB	1.99	0.44
1:A:171:ASP:O	1:A:174:LYS:HG3	2.17	0.44
1:A:404:LYS:HG3	1:A:435:PRO:HB2	1.99	0.44
1:A:488:LEU:HD22	1:A:489:MET:N	2.32	0.44
1:B:73:LYS:O	1:B:75:SER:N	2.51	0.44
1:A:10:LEU:C	1:A:12:GLY:N	2.70	0.44
1:A:305:GLU:O	1:A:310:LEU:HD23	2.18	0.44
1:A:372:VAL:O	1:A:376:ILE:HD11	2.18	0.44
1:A:380:ASN:OD1	1:A:422:THR:N	2.50	0.44
1:B:160:LYS:CG	1:B:189:ASN:HD21	2.31	0.44
1:B:216:VAL:HG12	1:B:217:THR:N	2.32	0.44
1:B:91:ILE:HG12	1:B:91:ILE:O	2.17	0.44
1:A:272:TRP:C	1:A:274:TYR:H	2.21	0.44
1:A:364:ASP:HA	1:A:365:PRO:HD2	1.84	0.44
1:B:101:ILE:CG2	1:B:102:ASN:N	2.80	0.44
1:B:202:LEU:O	1:B:204:HIS:N	2.45	0.44
1:B:5:VAL:O	1:B:180:VAL:HA	2.17	0.44
1:A:93:SER:O	1:A:132:LYS:HB2	2.17	0.43
1:B:272:TRP:C	1:B:274:TYR:H	2.21	0.43
1:B:306:TYR:HD2	1:B:464:TRP:CD1	2.36	0.43
1:B:32:LEU:CD2	1:B:36:PHE:HD2	2.31	0.43
1:A:236:SER:HB2	1:B:322:LEU:HG	1.99	0.43
1:B:132:LYS:H	1:B:132:LYS:CD	2.31	0.43
1:B:158:MET:HG2	1:B:164:GLN:HB2	1.96	0.43
1:A:156:VAL:O	1:A:158:MET:N	2.51	0.43
1:A:205:ASN:OD1	1:A:208:SER:HB2	2.19	0.43
1:A:398:ASN:OD1	1:A:400:SER:HB3	2.18	0.43
1:A:404:LYS:HG2	1:A:404:LYS:H	1.37	0.43
1:B:291:MET:HA	1:B:291:MET:CE	2.49	0.43
1:B:440:ILE:HD12	1:B:440:ILE:HA	1.70	0.43
1:B:488:LEU:HD22	1:B:489:MET:N	2.33	0.43
1:A:102:ASN:ND2	1:A:105:MET:CB	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:SER:O	1:A:139:MET:HB3	2.18	0.43
1:A:207:ALA:CA	1:A:210:LEU:HB2	2.49	0.43
1:B:142:GLU:HG3	1:B:281:GLN:OE1	2.18	0.43
1:A:124:ASN:OD1	1:A:160:LYS:CB	2.58	0.43
1:A:140:MET:HE3	1:A:140:MET:HA	2.00	0.43
1:A:265:PHE:HA	1:A:266:PRO:HA	1.81	0.43
1:A:368:SER:HB3	1:A:371:LYS:HG3	2.01	0.43
1:B:134:ASP:O	1:B:136:LEU:N	2.51	0.43
1:A:160:LYS:HA	1:A:161:PRO:HA	1.83	0.43
1:A:122:VAL:O	1:A:160:LYS:HE2	2.19	0.43
1:A:270:PHE:CZ	1:A:273:ARG:HD3	2.53	0.43
1:A:364:ASP:OD1	1:A:364:ASP:N	2.50	0.43
1:A:396:GLU:O	1:A:397:LYS:C	2.57	0.43
1:A:53:LEU:HD12	1:A:54:MET:N	2.32	0.43
1:A:59:THR:OG1	1:A:60:PHE:N	2.51	0.43
1:B:115:LYS:NZ	1:B:218:GLY:O	2.47	0.43
1:B:271:SER:HA	1:B:273:ARG:NH1	2.34	0.43
1:B:414:GLY:O	1:B:415:PHE:O	2.35	0.43
1:B:458:PHE:O	1:B:459:ARG:C	2.57	0.43
1:B:501:GLU:H	1:B:501:GLU:HG3	1.42	0.43
1:B:537:LEU:HA	1:B:537:LEU:HD23	1.74	0.43
1:B:61:SER:HA	1:B:64:VAL:CG2	2.48	0.43
1:A:181:VAL:HB	1:A:199:VAL:HB	2.01	0.43
1:B:246:ILE:HD12	1:B:246:ILE:N	2.34	0.43
1:A:337:VAL:HG21	2:A:1100:CIU:H12	2.01	0.43
1:A:149:PHE:CD2	1:A:173:LEU:HD12	2.54	0.43
1:A:159:ILE:O	1:A:165:ILE:CD1	2.55	0.43
1:A:190:LEU:HD22	1:A:200:THR:HG22	1.98	0.43
1:A:313:LYS:O	1:A:316:VAL:HB	2.18	0.43
1:A:481:ARG:HA	1:B:62:GLN:OE1	2.18	0.43
1:A:501:GLU:H	1:A:501:GLU:HG3	1.42	0.43
1:B:32:LEU:HD23	1:B:36:PHE:HD2	1.84	0.43
1:B:501:GLU:O	1:B:504:LYS:HG2	2.19	0.43
1:B:50:THR:CA	1:B:63:TRP:HE1	2.31	0.43
1:A:170:LEU:HD21	1:A:177:PRO:HA	2.00	0.43
1:A:263:HIS:NE2	1:A:291:MET:CB	2.79	0.43
1:A:280:ALA:HA	1:A:284:PHE:O	2.18	0.43
1:A:489:MET:HE3	1:A:490:VAL:H	1.83	0.43
1:A:533:VAL:O	1:A:537:LEU:HB2	2.19	0.43
1:B:162:GLU:HA	1:B:163:PRO:HD2	1.81	0.43
1:B:183:LEU:CB	1:B:203:VAL:CG2	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ILE:HB	1:B:429:VAL:HG11	2.01	0.43
1:A:178:ASN:OD1	1:A:179:GLU:N	2.52	0.43
1:A:263:HIS:CD2	1:A:291:MET:H	2.37	0.43
1:A:459:ARG:CG	1:A:459:ARG:NH1	2.82	0.43
1:B:187:GLY:O	1:B:190:LEU:HB2	2.19	0.43
1:B:28:GLU:C	1:B:30:LEU:N	2.72	0.43
1:B:313:LYS:O	1:B:316:VAL:HB	2.19	0.43
1:B:368:SER:HB3	1:B:371:LYS:CG	2.49	0.43
1:A:13:VAL:CG2	1:A:203:VAL:HG21	2.49	0.42
1:A:271:SER:C	1:A:273:ARG:H	2.23	0.42
1:A:300:PRO:CB	1:A:301:PRO:CD	2.97	0.42
1:A:422:THR:HG1	1:A:422:THR:H	1.42	0.42
1:B:6:ALA:HB2	1:B:181:VAL:CG1	2.45	0.42
1:A:195:ASP:O	1:A:196:MET:C	2.58	0.42
1:A:250:PHE:CD2	1:A:251:VAL:N	2.87	0.42
1:A:414:GLY:O	1:A:415:PHE:O	2.36	0.42
1:A:58:ILE:HG22	1:A:62:GLN:CD	2.40	0.42
1:B:126:TRP:CD1	1:B:126:TRP:C	2.92	0.42
1:B:178:ASN:CG	1:B:179:GLU:N	2.73	0.42
1:B:293:GLY:HA2	1:B:299:SER:CA	2.48	0.42
1:B:322:LEU:HD23	3:B:1013:HOH:O	2.19	0.42
1:B:407:PHE:C	1:B:408:ARG:HG2	2.39	0.42
1:A:408:ARG:HH21	1:A:412:GLU:HG2	1.83	0.42
1:A:440:ILE:HG23	1:A:440:ILE:O	2.19	0.42
1:A:511:PRO:HB2	1:A:512:PHE:CE1	2.54	0.42
1:A:97:ALA:O	1:A:99:ARG:N	2.52	0.42
1:B:276:ILE:HB	1:B:277:PRO:HD3	2.00	0.42
1:B:280:ALA:HA	1:B:284:PHE:O	2.19	0.42
1:A:97:ALA:HB2	1:A:132:LYS:HG2	2.01	0.42
1:A:160:LYS:CB	1:A:189:ASN:HD21	2.13	0.42
1:B:272:TRP:C	1:B:274:TYR:N	2.73	0.42
1:B:325:PRO:O	1:B:326:GLN:HG3	2.20	0.42
1:B:63:TRP:NE1	1:B:67:MET:HG3	2.34	0.42
1:A:272:TRP:C	1:A:274:TYR:N	2.73	0.42
1:A:277:PRO:O	1:A:280:ALA:HB3	2.19	0.42
1:A:294:TYR:CE2	1:A:461:PRO:HB3	2.55	0.42
1:B:440:ILE:O	1:B:440:ILE:HG23	2.20	0.42
1:B:470:ARG:CA	1:B:473:LYS:NZ	2.72	0.42
1:B:53:LEU:HA	1:B:53:LEU:HD23	1.82	0.42
1:B:96:MET:HB3	1:B:96:MET:HE2	1.76	0.42
1:A:276:ILE:HG22	1:A:277:PRO:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:PRO:O	1:A:326:GLN:HG3	2.20	0.42
1:B:169:LEU:HG	1:B:173:LEU:HD21	2.02	0.42
1:B:19:ILE:HD13	1:B:19:ILE:HA	1.77	0.42
1:B:339:VAL:HG13	1:B:353:VAL:HG13	1.98	0.42
1:A:513:LEU:CD2	1:A:514:LYS:O	2.67	0.42
1:B:122:VAL:CA	1:B:151:ILE:HD12	2.50	0.42
1:B:248:LEU:HD13	1:B:248:LEU:HA	1.93	0.42
1:B:276:ILE:HG22	1:B:277:PRO:CD	2.49	0.42
1:B:309:GLU:HA	1:B:474:TRP:CE2	2.55	0.42
1:A:138:GLN:CA	1:B:325:PRO:HB3	2.49	0.42
1:B:529:LYS:HA	1:B:529:LYS:HD3	1.70	0.42
1:B:54:MET:HB3	1:B:159:ILE:CG2	2.49	0.42
1:A:128:ASP:O	1:A:133:ARG:CG	2.67	0.42
1:A:303:ILE:O	1:A:304:GLU:C	2.58	0.42
1:A:55:LYS:HG3	1:A:159:ILE:HG23	2.02	0.42
1:B:163:PRO:HA	1:B:166:TYR:HD1	1.84	0.42
1:B:42:GLN:HB2	1:B:186:PHE:HZ	1.80	0.42
1:B:49:PRO:HD2	1:B:67:MET:HE2	2.01	0.42
1:A:378:VAL:HG22	1:A:418:VAL:HG11	2.01	0.42
1:B:406:PHE:HD2	2:B:1200:CIU:HC12	1.85	0.42
1:B:177:PRO:C	1:B:197:GLY:O	2.58	0.42
1:B:337:VAL:O	1:B:341:ASN:ND2	2.52	0.42
1:B:378:VAL:HA	1:B:419:HIS:CD2	2.55	0.42
1:B:469:GLU:HG3	1:B:473:LYS:HZ1	1.85	0.42
1:B:72:ARG:HD3	1:B:73:LYS:HZ1	1.83	0.42
1:A:92:PHE:CD1	1:A:92:PHE:C	2.93	0.42
1:B:118:THR:HA	1:B:148:ASP:OD2	2.18	0.42
1:B:168:PHE:CD2	1:B:168:PHE:C	2.92	0.42
1:B:183:LEU:HB2	1:B:203:VAL:HG21	2.00	0.42
1:B:271:SER:C	1:B:273:ARG:H	2.23	0.42
1:B:329:PHE:HB3	1:B:339:VAL:HG22	2.02	0.42
1:B:386:GLN:HE22	1:B:468:THR:HG1	1.67	0.42
1:B:43:THR:O	1:B:44:GLU:CB	2.66	0.42
1:B:8:PHE:CE1	1:B:147:PHE:CE2	3.06	0.42
1:A:229:PRO:HB2	1:A:230:CYS:H	1.69	0.41
1:A:246:ILE:N	1:A:246:ILE:HD12	2.35	0.41
1:B:103:ARG:H	1:B:103:ARG:HG2	1.54	0.41
1:B:358:THR:HA	1:B:359:PRO:HD3	1.83	0.41
1:B:72:ARG:O	1:B:75:SER:HB3	2.20	0.41
1:A:121:ILE:HB	1:A:150:LEU:CD1	2.51	0.41
1:B:190:LEU:CD1	1:B:202:LEU:HD23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:MET:SD	1:B:454:LYS:HE3	2.60	0.41
1:A:191:LYS:HB3	1:A:192:PRO:HD3	2.02	0.41
1:A:360:PHE:O	1:A:362:PRO:HD3	2.19	0.41
1:B:132:LYS:N	1:B:132:LYS:CD	2.84	0.41
1:B:284:PHE:N	1:B:284:PHE:CD1	2.89	0.41
1:B:148:ASP:N	1:B:148:ASP:OD1	2.54	0.41
1:B:243:LYS:CB	1:B:246:ILE:HD13	2.50	0.41
1:B:250:PHE:CD2	1:B:251:VAL:N	2.88	0.41
1:B:326:GLN:HG2	1:B:348:GLU:O	2.21	0.41
1:A:190:LEU:HB3	1:A:200:THR:HG21	2.02	0.41
1:B:160:LYS:HA	1:B:165:ILE:CD1	2.49	0.41
1:B:187:GLY:HA2	1:B:190:LEU:HB2	2.02	0.41
1:B:233:ASN:N	1:B:233:ASN:HD22	2.19	0.41
1:B:360:PHE:O	1:B:362:PRO:HD3	2.20	0.41
1:B:396:GLU:O	1:B:397:LYS:C	2.58	0.41
1:B:427:ILE:HB	1:B:428:LEU:HD13	2.02	0.41
1:B:431:THR:O	1:B:432:PRO:C	2.59	0.41
1:B:459:ARG:NH1	1:B:459:ARG:CG	2.83	0.41
1:B:489:MET:CE	1:B:490:VAL:N	2.82	0.41
1:A:205:ASN:CG	1:A:207:ALA:H	2.23	0.41
1:A:220:GLN:NE2	1:A:220:GLN:O	2.54	0.41
1:A:262:CYS:C	1:A:272:TRP:HZ2	2.24	0.41
1:A:396:GLU:O	1:A:398:ASN:N	2.53	0.41
1:A:54:MET:O	1:A:154:CYS:CA	2.69	0.41
1:B:259:LEU:HD11	1:B:279:LEU:HD13	2.03	0.41
1:B:406:PHE:HE2	2:B:1200:CIU:HC11	1.85	0.41
1:A:54:MET:O	1:A:154:CYS:HA	2.21	0.41
1:A:321:LYS:HE3	1:B:234:ASP:HB2	2.03	0.41
1:A:394:GLU:OE1	1:A:427:ILE:HG22	2.21	0.41
1:A:532:GLU:HG2	1:A:532:GLU:H	1.56	0.41
1:A:58:ILE:HG22	1:A:62:GLN:OE1	2.20	0.41
1:B:42:GLN:CB	1:B:186:PHE:HE1	2.32	0.41
1:A:149:PHE:HD2	1:A:173:LEU:HD12	1.86	0.41
1:A:210:LEU:O	1:A:214:GLU:HB3	2.19	0.41
1:B:259:LEU:HB3	1:B:328:VAL:HB	2.01	0.41
1:B:340:TRP:HZ2	1:B:489:MET:HG2	1.85	0.41
1:B:420:LYS:O	1:B:424:ILE:HD11	2.20	0.41
1:B:470:ARG:N	1:B:473:LYS:NZ	2.68	0.41
1:B:4:ARG:CG	1:B:4:ARG:HH11	2.30	0.41
1:A:208:SER:OG	1:A:209:ALA:N	2.52	0.41
1:A:293:GLY:HA2	1:A:299:SER:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:TRP:HZ2	1:A:489:MET:HG2	1.85	0.41
1:A:58:ILE:HG22	1:A:62:GLN:HG3	2.03	0.41
1:A:62:GLN:HE22	1:B:482:LYS:N	2.19	0.41
1:B:112:LEU:CD2	1:B:117:PHE:CE1	3.00	0.41
1:B:214:GLU:O	1:B:215:LYS:C	2.58	0.41
1:A:322:LEU:HG	1:B:236:SER:HB2	2.02	0.41
1:B:272:TRP:HA	1:B:275:GLN:OE1	2.21	0.41
1:A:231:ASN:HB2	1:A:232:PRO:CA	2.51	0.41
1:A:276:ILE:CB	1:A:277:PRO:HD3	2.51	0.41
1:A:329:PHE:HB3	1:A:339:VAL:HG22	2.03	0.41
1:A:513:LEU:C	1:A:513:LEU:HD23	2.41	0.41
1:B:159:ILE:O	1:B:162:GLU:HB2	2.21	0.41
1:A:112:LEU:HA	1:A:115:LYS:HB3	2.03	0.41
1:A:126:TRP:C	1:A:126:TRP:CD1	2.94	0.41
1:A:134:ASP:O	1:A:135:SER:C	2.59	0.41
1:A:191:LYS:CB	1:A:192:PRO:CD	2.97	0.41
1:A:458:PHE:O	1:A:459:ARG:C	2.60	0.41
1:A:64:VAL:N	1:A:65:PRO:CD	2.83	0.41
1:B:276:ILE:CB	1:B:277:PRO:HD3	2.50	0.41
1:B:404:LYS:HG2	1:B:404:LYS:H	1.35	0.41
1:B:395:LEU:HD23	1:B:428:LEU:HD21	2.03	0.41
1:B:294:TYR:CE2	1:B:461:PRO:HB3	2.55	0.41
1:A:7:ALA:N	1:A:181:VAL:O	2.51	0.40
1:A:94:GLN:O	1:A:97:ALA:HB3	2.21	0.40
1:B:122:VAL:O	1:B:122:VAL:HG22	2.20	0.40
1:B:149:PHE:CD2	1:B:173:LEU:HD13	2.56	0.40
1:B:173:LEU:HB2	1:B:174:LYS:H	1.64	0.40
1:B:203:VAL:O	1:B:203:VAL:CG1	2.65	0.40
1:B:28:GLU:C	1:B:30:LEU:H	2.24	0.40
1:B:372:VAL:O	1:B:376:ILE:HD11	2.21	0.40
1:B:405:SER:O	1:B:408:ARG:CG	2.68	0.40
1:B:479:LEU:HA	1:B:479:LEU:HD23	1.82	0.40
1:B:178:ASN:C	1:B:180:VAL:H	2.25	0.40
1:A:137:ALA:CB	1:B:325:PRO:O	2.61	0.40
1:B:431:THR:O	1:B:432:PRO:O	2.40	0.40
1:B:4:ARG:NH1	1:B:4:ARG:CG	2.85	0.40
1:A:358:THR:HA	1:A:359:PRO:HD3	1.82	0.40
1:A:4:ARG:NH2	1:A:179:GLU:HB2	2.36	0.40
1:A:530:PRO:O	1:A:531:THR:C	2.59	0.40
1:B:119:THR:H	1:B:148:ASP:CG	2.24	0.40
1:B:524:TRP:CZ2	2:B:1200:CIU:HC62	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ASP:N	1:B:129:ASP:OD1	2.52	0.40
1:B:134:ASP:C	1:B:136:LEU:N	2.75	0.40
1:B:398:ASN:OD1	1:B:400:SER:HB3	2.21	0.40
1:B:41:TYR:OH	1:B:126:TRP:HZ3	2.04	0.40
1:A:138:GLN:HG2	1:B:325:PRO:CG	2.52	0.40
1:A:17:PRO:O	1:A:18:SER:O	2.39	0.40
1:A:405:SER:O	1:A:408:ARG:CG	2.69	0.40
1:A:56:GLY:HA2	1:A:127:LEU:HD11	2.03	0.40
1:A:91:ILE:O	1:A:91:ILE:HG22	2.20	0.40
1:B:8:PHE:CB	1:B:14:LEU:HD13	2.47	0.40
1:B:228:VAL:O	1:B:277:PRO:HG2	2.22	0.40
1:B:276:ILE:CG2	1:B:277:PRO:HD3	2.52	0.40
1:B:325:PRO:HA	1:B:349:ARG:HH12	1.86	0.40
1:B:364:ASP:HB2	1:B:367:VAL:CG2	2.52	0.40
1:B:59:THR:OG1	1:B:60:PHE:N	2.52	0.40
1:A:276:ILE:HB	1:A:277:PRO:HD3	2.03	0.40
1:A:284:PHE:N	1:A:284:PHE:CD1	2.89	0.40
1:A:326:GLN:HG2	1:A:348:GLU:O	2.21	0.40
1:A:339:VAL:CG1	1:A:353:VAL:CG1	2.95	0.40
1:B:249:HIS:CG	1:B:250:PHE:N	2.89	0.40
1:B:305:GLU:O	1:B:310:LEU:HD23	2.22	0.40

There are no symmetry-related clashes.

## 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	484/554 (87%)	345 (71%)	90 (19%)	49 (10%)	0   3
1	B	539/554 (97%)	384 (71%)	101 (19%)	54 (10%)	0   3
All	All	1023/1108 (92%)	729 (71%)	191 (19%)	103 (10%)	0   3

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	18	SER
1	A	63	TRP
1	A	65	PRO
1	A	91	ILE
1	A	144	SER
1	A	203	VAL
1	A	207	ALA
1	A	212	GLU
1	A	217	THR
1	A	229	PRO
1	A	230	CYS
1	A	256	GLY
1	A	415	PHE
1	A	466	ARG
1	B	18	SER
1	B	32	LEU
1	B	44	GLU
1	B	59	THR
1	B	75	SER
1	B	78	CYS
1	B	89	SER
1	B	174	LYS
1	B	205	ASN
1	B	207	ALA
1	B	211	ARG
1	B	225	PRO
1	B	232	PRO
1	B	256	GLY
1	B	415	PHE
1	B	421	ALA
1	B	434	ASP
1	B	435	PRO
1	B	466	ARG
1	A	98	ALA
1	A	126	TRP
1	A	130	GLY
1	A	156	VAL
1	A	163	PRO
1	A	210	LEU
1	A	273	ARG
1	A	301	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	386	GLN
1	A	397	LYS
1	A	421	ALA
1	A	543	THR
1	B	21	GLY
1	B	39	GLY
1	B	63	TRP
1	B	74	SER
1	B	203	VAL
1	B	213	LEU
1	B	216	VAL
1	B	219	THR
1	B	273	ARG
1	B	386	GLN
1	B	397	LYS
1	B	543	THR
1	A	111	ALA
1	A	157	GLY
1	A	164	GLN
1	A	202	LEU
1	A	244	PRO
1	A	409	ALA
1	B	29	ALA
1	B	73	LYS
1	B	179	GLU
1	B	244	PRO
1	B	301	PRO
1	B	409	ALA
1	B	459	ARG
1	A	12	GLY
1	A	92	PHE
1	A	231	ASN
1	A	232	PRO
1	A	459	ARG
1	B	34	ARG
1	A	195	ASP
1	A	423	GLU
1	A	476	CYS
1	B	20	ALA
1	B	90	GLN
1	B	229	PRO
1	B	423	GLU

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Mol	Chain	Res	Type
1	B	432	PRO
1	B	534	ASN
1	A	145	GLN
1	A	506	MET
1	A	530	PRO
1	B	111	ALA
1	B	418	VAL
1	B	530	PRO
1	A	300	PRO
1	A	390	VAL
1	A	432	PRO
1	B	165	ILE
1	B	300	PRO
1	B	390	VAL
1	A	418	VAL
1	B	103	ARG
1	B	197	GLY
1	A	266	PRO
1	B	266	PRO

### 5.3.2 Protein sidechains [i](#)

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	427/480 (89%)	291 (68%)	136 (32%)	0 0
1	B	468/480 (98%)	317 (68%)	151 (32%)	0 0
All	All	895/960 (93%)	608 (68%)	287 (32%)	0 0

All (287) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	8	PHE
1	A	9	ASP
1	A	14	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	16	LEU
1	A	18	SER
1	A	19	ILE
1	A	51	GLU
1	A	52	GLN
1	A	53	LEU
1	A	58	ILE
1	A	59	THR
1	A	66	LEU
1	A	90	GLN
1	A	92	PHE
1	A	93	SER
1	A	94	GLN
1	A	96	MET
1	A	103	ARG
1	A	106	LEU
1	A	107	GLN
1	A	110	ILE
1	A	112	LEU
1	A	117	PHE
1	A	118	THR
1	A	121	ILE
1	A	122	VAL
1	A	127	LEU
1	A	128	ASP
1	A	129	ASP
1	A	132	LYS
1	A	135	SER
1	A	136	LEU
1	A	138	GLN
1	A	139	MET
1	A	144	SER
1	A	148	ASP
1	A	152	GLU
1	A	154	CYS
1	A	155	GLN
1	A	158	MET
1	A	165	ILE
1	A	170	LEU
1	A	173	LEU
1	A	181	VAL
1	A	183	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	184	ASP
1	A	188	SER
1	A	189	ASN
1	A	191	LYS
1	A	194	ARG
1	A	196	MET
1	A	198	MET
1	A	200	THR
1	A	201	ILE
1	A	202	LEU
1	A	204	HIS
1	A	205	ASN
1	A	206	THR
1	A	210	LEU
1	A	211	ARG
1	A	213	LEU
1	A	214	GLU
1	A	220	GLN
1	A	221	PHE
1	A	223	GLU
1	A	230	CYS
1	A	231	ASN
1	A	233	ASN
1	A	235	VAL
1	A	242	VAL
1	A	247	ARG
1	A	248	LEU
1	A	253	MET
1	A	259	LEU
1	A	268	SER
1	A	275	GLN
1	A	281	GLN
1	A	290	ASP
1	A	299	SER
1	A	304	GLU
1	A	313	LYS
1	A	315	MET
1	A	319	LEU
1	A	322	LEU
1	A	324	ILE
1	A	339	VAL
1	A	357	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	364	ASP
1	A	366	ASP
1	A	370	MET
1	A	372	VAL
1	A	376	ILE
1	A	383	LEU
1	A	387	GLU
1	A	401	ARG
1	A	404	LYS
1	A	408	ARG
1	A	411	ASP
1	A	412	GLU
1	A	415	PHE
1	A	416	ILE
1	A	418	VAL
1	A	419	HIS
1	A	422	THR
1	A	429	VAL
1	A	437	LEU
1	A	439	LYS
1	A	440	ILE
1	A	447	GLU
1	A	451	GLN
1	A	452	GLN
1	A	456	THR
1	A	459	ARG
1	A	462	LEU
1	A	466	ARG
1	A	468	THR
1	A	470	ARG
1	A	473	LYS
1	A	485	VAL
1	A	488	LEU
1	A	489	MET
1	A	494	LYS
1	A	497	VAL
1	A	499	ARG
1	A	501	GLU
1	A	502	MET
1	A	507	GLU
1	A	512	PHE
1	A	515	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	521	CYS
1	A	526	GLN
1	A	527	ILE
1	A	531	THR
1	A	532	GLU
1	A	539	LYS
1	B	4	ARG
1	B	8	PHE
1	B	16	LEU
1	B	19	ILE
1	B	24	ARG
1	B	28	GLU
1	B	34	ARG
1	B	38	LEU
1	B	41	TYR
1	B	43	THR
1	B	50	THR
1	B	51	GLU
1	B	53	LEU
1	B	57	LYS
1	B	59	THR
1	B	60	PHE
1	B	61	SER
1	B	62	GLN
1	B	64	VAL
1	B	66	LEU
1	B	67	MET
1	B	69	GLU
1	B	70	SER
1	B	72	ARG
1	B	73	LYS
1	B	74	SER
1	B	75	SER
1	B	76	LYS
1	B	84	GLU
1	B	85	ASN
1	B	88	ILE
1	B	90	GLN
1	B	91	ILE
1	B	96	MET
1	B	103	ARG
1	B	106	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	110	ILE
1	B	113	LYS
1	B	118	THR
1	B	119	THR
1	B	120	CYS
1	B	121	ILE
1	B	122	VAL
1	B	127	LEU
1	B	129	ASP
1	B	132	LYS
1	B	133	ARG
1	B	136	LEU
1	B	139	MET
1	B	144	SER
1	B	148	ASP
1	B	151	ILE
1	B	154	CYS
1	B	155	GLN
1	B	158	MET
1	B	165	ILE
1	B	169	LEU
1	B	170	LEU
1	B	181	VAL
1	B	183	LEU
1	B	189	ASN
1	B	191	LYS
1	B	194	ARG
1	B	195	ASP
1	B	198	MET
1	B	199	VAL
1	B	202	LEU
1	B	204	HIS
1	B	206	THR
1	B	208	SER
1	B	210	LEU
1	B	212	GLU
1	B	213	LEU
1	B	214	GLU
1	B	215	LYS
1	B	217	THR
1	B	219	THR
1	B	220	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	223	GLU
1	B	226	LEU
1	B	234	ASP
1	B	242	VAL
1	B	247	ARG
1	B	248	LEU
1	B	253	MET
1	B	268	SER
1	B	275	GLN
1	B	281	GLN
1	B	290	ASP
1	B	297	SER
1	B	299	SER
1	B	304	GLU
1	B	306	TYR
1	B	313	LYS
1	B	315	MET
1	B	319	LEU
1	B	322	LEU
1	B	324	ILE
1	B	339	VAL
1	B	357	ASN
1	B	364	ASP
1	B	370	MET
1	B	372	VAL
1	B	375	SER
1	B	376	ILE
1	B	383	LEU
1	B	401	ARG
1	B	404	LYS
1	B	408	ARG
1	B	411	ASP
1	B	412	GLU
1	B	415	PHE
1	B	416	ILE
1	B	418	VAL
1	B	419	HIS
1	B	423	GLU
1	B	424	ILE
1	B	427	ILE
1	B	428	LEU
1	B	431	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	433	GLU
1	B	434	ASP
1	B	437	LEU
1	B	439	LYS
1	B	440	ILE
1	B	447	GLU
1	B	451	GLN
1	B	452	GLN
1	B	456	THR
1	B	459	ARG
1	B	462	LEU
1	B	466	ARG
1	B	468	THR
1	B	470	ARG
1	B	473	LYS
1	B	488	LEU
1	B	489	MET
1	B	494	LYS
1	B	497	VAL
1	B	499	ARG
1	B	501	GLU
1	B	502	MET
1	B	507	GLU
1	B	512	PHE
1	B	515	ARG
1	B	521	CYS
1	B	526	GLN
1	B	527	ILE
1	B	531	THR
1	B	532	GLU
1	B	539	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	102	ASN
1	A	125	ASN
1	A	189	ASN
1	A	220	GLN
1	A	231	ASN
1	A	233	ASN
1	A	281	GLN

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Mol	Chain	Res	Type
1	A	326	GLN
1	A	341	ASN
1	A	386	GLN
1	A	463	ASN
1	A	526	GLN
1	B	94	GLN
1	B	146	HIS
1	B	167	ASN
1	B	178	ASN
1	B	189	ASN
1	B	204	HIS
1	B	205	ASN
1	B	231	ASN
1	B	233	ASN
1	B	386	GLN
1	B	463	ASN
1	B	526	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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	CIU	A	1100	-	18,18,18	2.82	11 (61%)	23,23,23	2.03	4 (17%)
2	CIU	B	1200	-	18,18,18	2.83	11 (61%)	23,23,23	2.03	4 (17%)

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	CIU	A	1100	-	-	0/8/16/16	0/2/2/2
2	CIU	B	1200	-	-	0/8/16/16	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1200	CIU	C11-I4	6.73	2.27	2.10
2	A	1100	CIU	C11-I4	6.71	2.27	2.10
2	B	1200	CIU	C4-C3	3.96	1.61	1.52
2	A	1100	CIU	C4-C3	3.94	1.61	1.52
2	B	1200	CIU	C12-C11	3.86	1.47	1.38
2	A	1100	CIU	C12-C11	3.85	1.47	1.38
2	B	1200	CIU	C2-C3	3.49	1.60	1.52
2	A	1100	CIU	C2-C3	3.47	1.60	1.52
2	A	1100	CIU	C13-C8	2.92	1.44	1.39
2	B	1200	CIU	C13-C8	2.91	1.44	1.39
2	B	1200	CIU	C6-C5	2.67	1.62	1.51
2	A	1100	CIU	C6-C5	2.66	1.62	1.51
2	A	1100	CIU	C6-C1	2.50	1.61	1.51
2	A	1100	CIU	C5-C4	2.48	1.59	1.53
2	B	1200	CIU	C6-C1	2.48	1.61	1.51
2	B	1200	CIU	C5-C4	2.48	1.59	1.53
2	B	1200	CIU	C7-N1	-2.45	1.30	1.35
2	A	1100	CIU	C10-C11	2.45	1.44	1.38
2	B	1200	CIU	C10-C11	2.42	1.44	1.38
2	A	1100	CIU	C7-N1	-2.41	1.30	1.35
2	B	1200	CIU	C7-N2	-2.07	1.33	1.37
2	A	1100	CIU	C7-N2	-2.07	1.33	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1200	CIU	N2-C7-N1	5.36	121.25	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1100	CIU	N2-C7-N1	5.36	121.24	113.76
2	B	1200	CIU	C8-N2-C7	4.55	135.92	126.61
2	A	1100	CIU	O2-C7-N1	-4.55	114.34	122.62
2	A	1100	CIU	C8-N2-C7	4.53	135.89	126.61
2	B	1200	CIU	O2-C7-N1	-4.53	114.38	122.62
2	A	1100	CIU	C3-N1-C7	2.96	129.27	123.02
2	B	1200	CIU	C3-N1-C7	2.94	129.24	123.02

There are no chirality outliers.

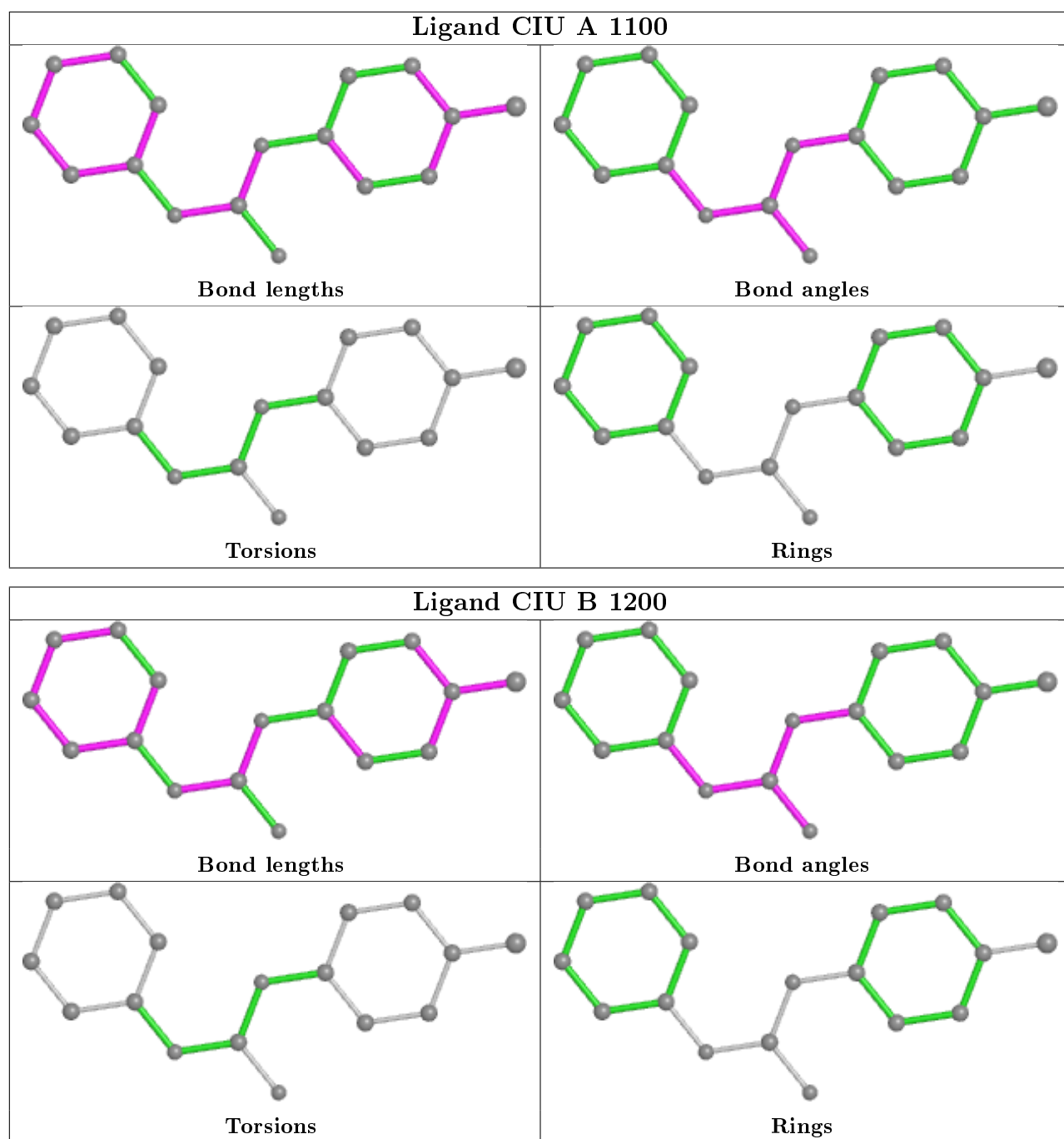
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1100	CIU	2	0
2	B	1200	CIU	5	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.



## 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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.