



## wwPDB EM Map/Model Validation Report ⓘ

Jul 21, 2016 – 04:03 PM EDT

PDB ID : 5G5L  
EMDB ID: : EMD-3439  
Title : RNA polymerase I-Rrn3 complex at 4.8 Å resolution  
Authors : Engel, C.; Plitzko, J.; Cramer, P.  
Deposited on : 2016-05-26  
Resolution : 4.80 Å (reported)  
Based on PDB ID : 4C2M

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027790

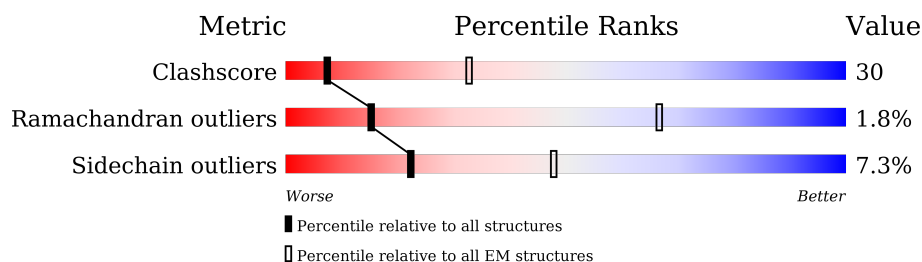
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.80 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1664	63% 23% . 11%
2	B	1203	69% 24% . .
3	C	335	61% 26% . . 9%
4	D	137	23% 18% .. 58%
5	E	215	77% 18% . .
6	F	155	53% 10% . 35%
7	G	326	39% 17% . 41%
8	H	146	72% 16% . 10%
9	I	125	54% 30% . 14%

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Mol	Chain	Length	Quality of chain
10	J	70	<div><div></div><div>79%17%...</div></div>
11	K	142	<div><div></div><div>51%19%•29%</div></div>
12	L	70	<div><div></div><div>29%27%6%39%</div></div>
13	M	415	<div><div></div><div>17%8%•75%</div></div>
14	N	233	<div><div></div><div>47%15%38%</div></div>
15	O	627	<div><div></div><div>25%40%8%•26%</div></div>

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 37349 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1480	Total	C	N	O	S	0	0
			11686	7384	2030	2211	61		

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1174	Total	C	N	O	S	0	0
			9327	5899	1635	1743	50		

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	305	Total	C	N	O	S	0	0
			2423	1539	416	460	8		

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	58	Total	C	N	O	0	0
			459	289	78	92		

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	212	Total	C	N	O	S	0	0
			1735	1102	306	316	11		

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	100	Total	C	N	O	S	0	0
			823	522	144	154	3		

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	193	Total	C	N	O	S	0	0
			1520	982	259	274	5		

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	131	Total	C	N	O	S	0	0
			1052	664	176	208	4		

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	107	Total	C	N	O	S	0	0
			820	511	138	162	9		

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			793	496	130	162	5		

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	43	Total	C	N	O	S	0	0
			340	211	66	59	4		

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	105	Total	C	N	O	0	0
			833	528	138	167		

- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	145	Total	C	N	O	S	0	0
			1151	735	188	224	4		

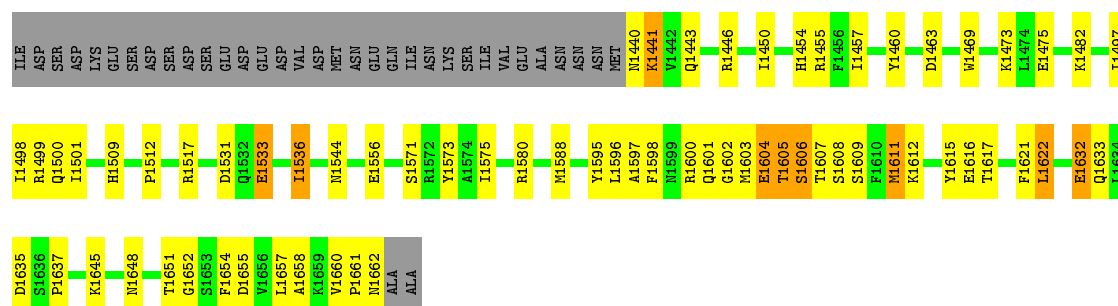
- Molecule 15 is a protein called RNA POLYMERASE I-SPECIFIC TRANSCRIPTION INITIATION FACTOR RRN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	463	Total	C	N	O	S	0	0
			3811	2473	623	694	21		

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

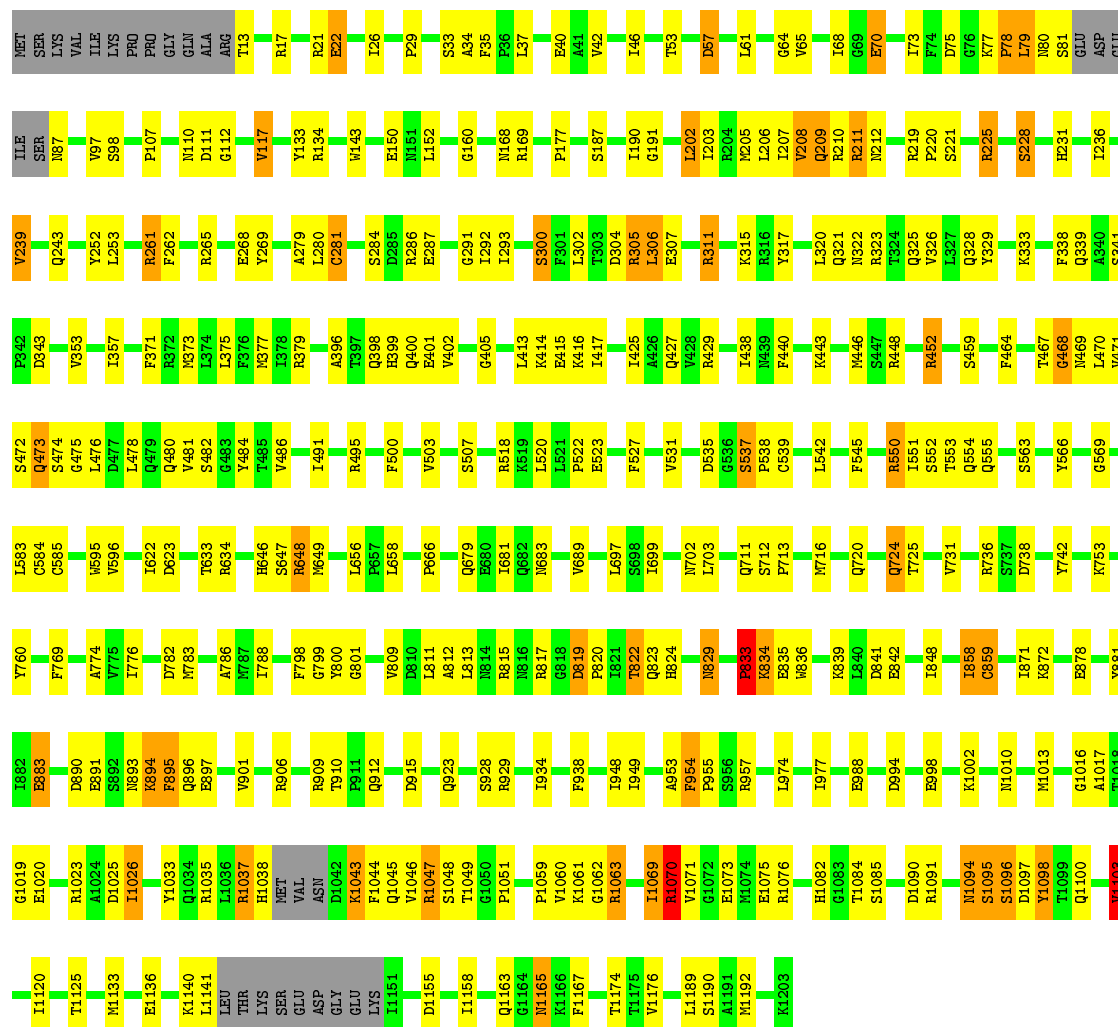
Mol	Chain	Residues	Atoms		AltConf
16	B	1	Total	Zn	0
			1	1	
16	A	2	Total	Zn	0
			2	2	
16	L	1	Total	Zn	0
			1	1	
16	J	1	Total	Zn	0
			1	1	
16	I	2	Total	Zn	0
			2	2	





• Molecule 2: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135

Chain B: 69% 24%

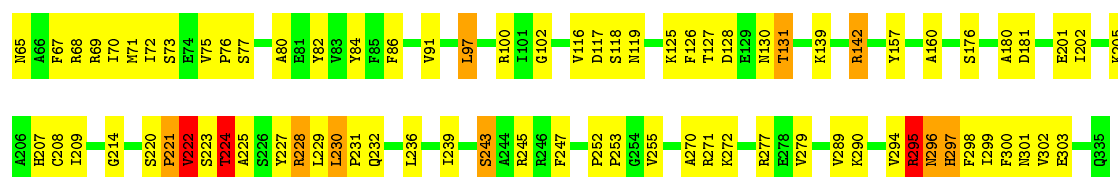


• Molecule 3: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1

Chain C: 61% 26% 9%

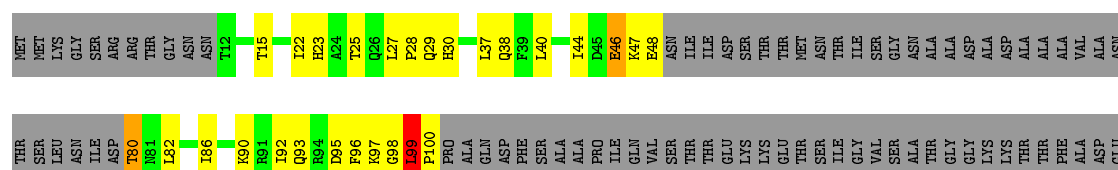






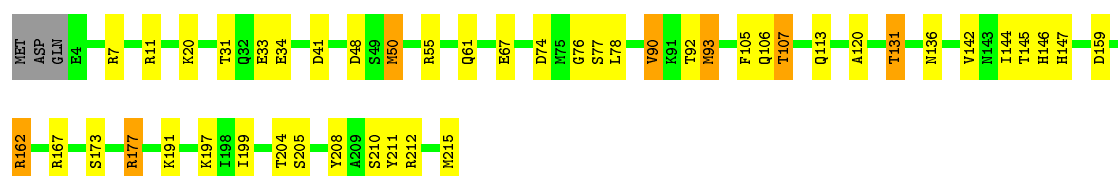
• Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14

Chain D: 23% 18% 58%



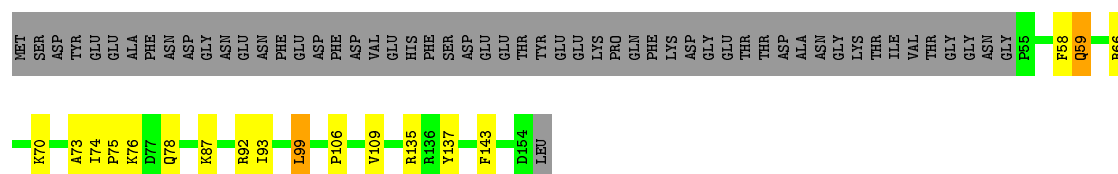
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain E: 77% 18%



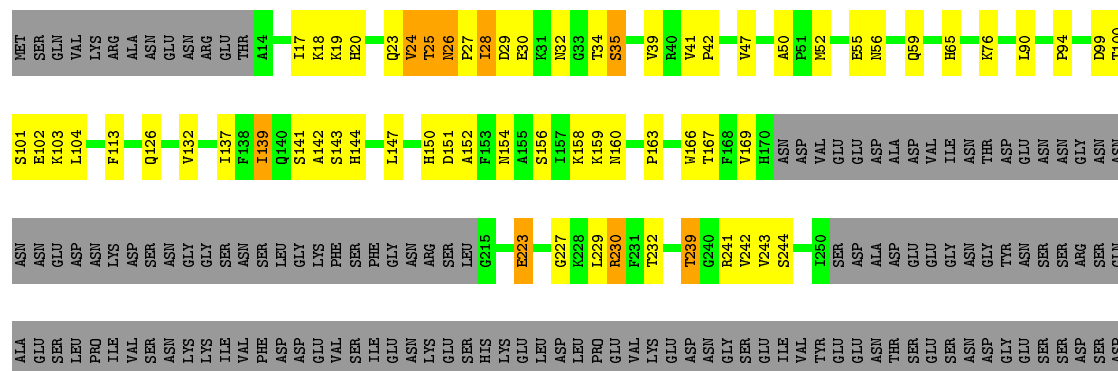
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F: 53% 10% 35%

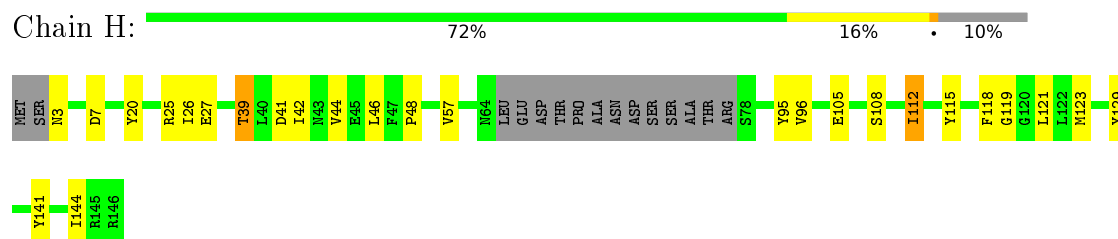


• Molecule 7: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43

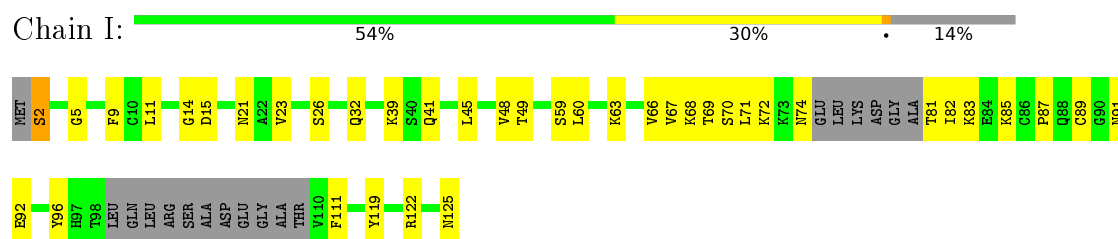
Chain G: 39% 17% 41%



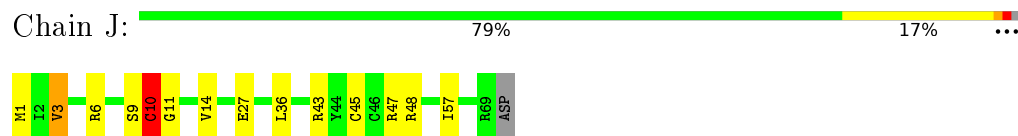
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3



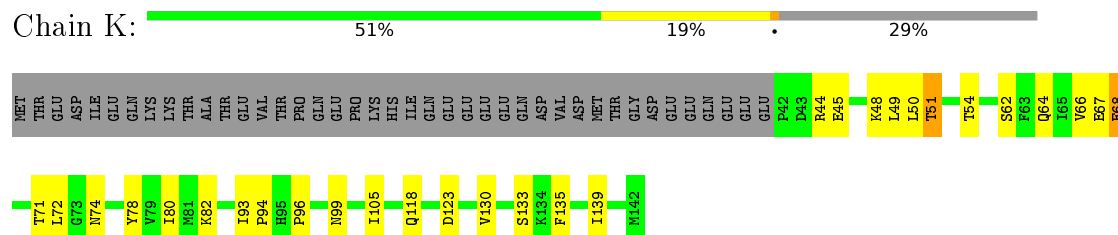
• Molecule 9: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12



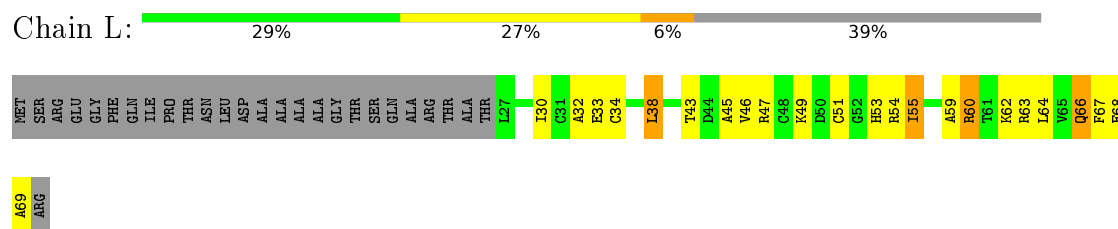
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



• Molecule 11: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2

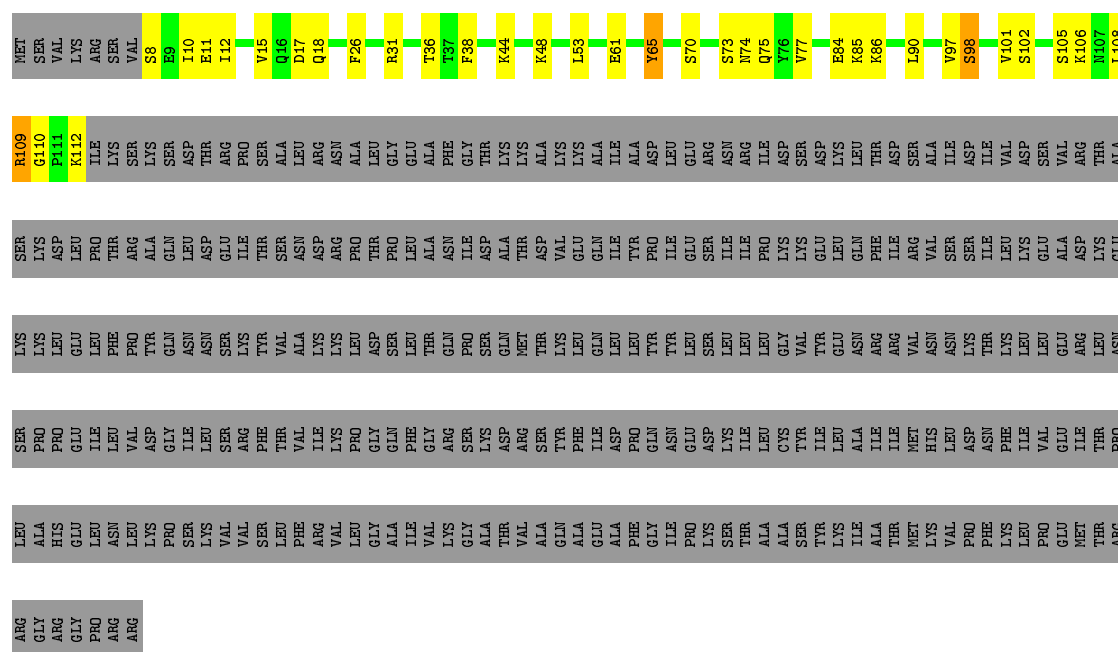


• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

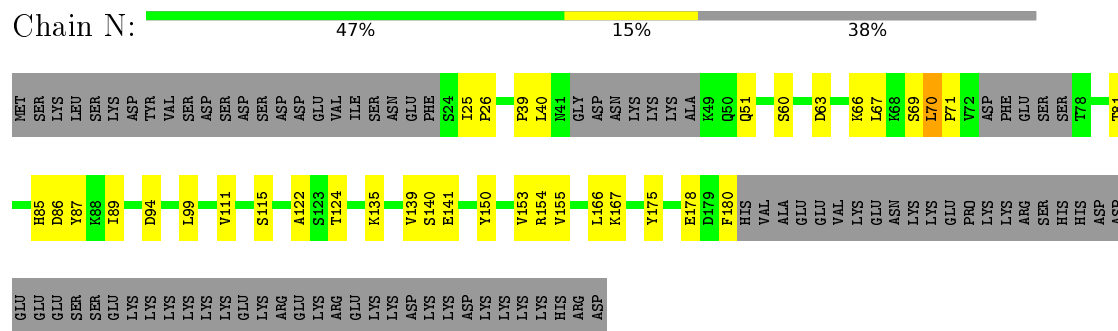


• Molecule 13: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49

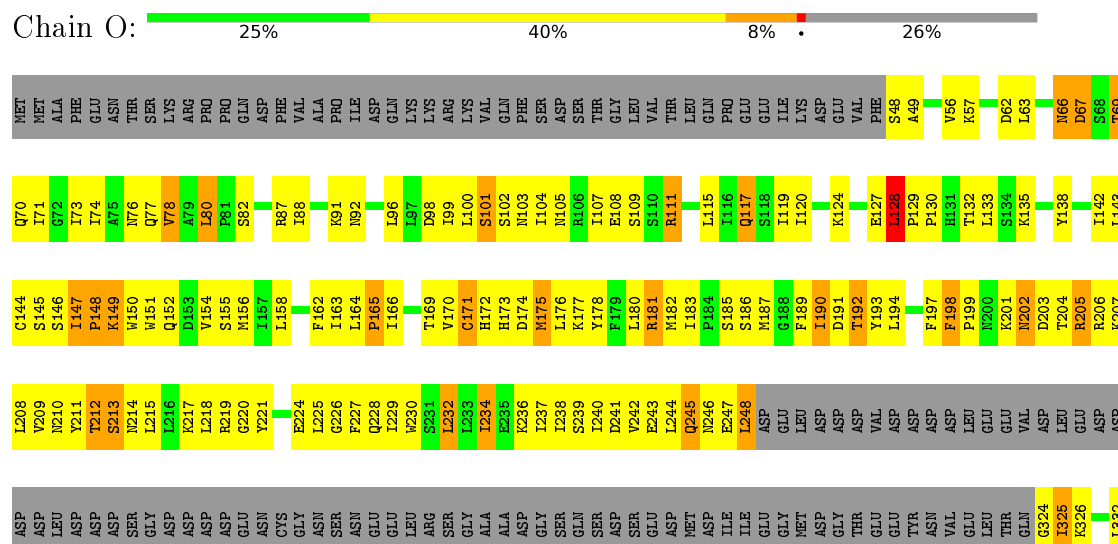




- Molecule 14: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34



● Molecule 15: RNA POLYMERASE I-SPECIFIC TRANSCRIPTION INITIATION FACTOR  
RRN3



I607	I531	D462	V401	L336
B608	V537	Q463	T402	T337
Y609	Q540	M467	I403	
I611	I543	E468	I404	T341
	N547	R469	D405	H342
	R551	F470	I406	V343
	LEU	K471	S407	
GLU	ARG	F472	F408	
ALA	ILE	H473	A409	
SER	GLY	Y474	V410	Q346
GLY	LEU	A475	T348	T347
TYR	ARG	E476	N411	P349
GLU	GLY	F477	E412	E350
ASP	ILE	Q478	A413	S351
GLY	ASP	A479	A414	L352
SER	GLY	L480	E415	E353
ASP	LYS	C481	K416	S354
ASP	ALA	Y482	K417	S355
	ASP	I483	I418	E356
	SER	F484	K419	G357
	ASP	C485	S420	V358
	LYS	F486	L421	G359
	LYS	R487	Q422	V360
	GLU	H488	Y423	F361
	ASN	R489	I424	I362
	SER	I490	G425	T363
	ALA	F491	S426	L364
	GLN		Y427	T365
	ALA	T494	I428	T366
	ASN	D495	A429	L367
	THR		R430	F368
	SER	E499	A431	K369
	SER	L502	K432	T370
	SER		K433	H371
	SER		L434	V372
	SER		S435	L373
	TRP	F505	R436	P374
	SER	F506	T437	T375
	LEU	Q507	Q438	T376
	ALA	R508	I439	Y377
			I440	T378
	T581	R582	F441	R379
	Q583	V510	V442	S380
	Q584	I511	A443	T381
	F585		S444	Q382
	I586	F514	Y445	V383
		N515	I446	L384
		P516	L447	V385
	Y591	L517	T447	F386
	F592	K518	S448	H387
	P593	P519	W449	V388
	Y594	C520	L450	S389
	D595	N521		Q390
	P596	E522	Y453	Q391
	L597	N523	V454	O392
	F598	Y524	R457	L395
	L599	N525	E458	H396
		L526	E459	D397
	Y602	F527	E460	S398
	M606	F528	V461	

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	RELION	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	37000	Depositor
Image detector	GATAN K2 SUMMIT (4K X 4K)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	A	0.48	0/11900	0.72	22/16073 (0.1%)
10	J	0.57	1/578 (0.2%)	0.59	0/775
11	K	0.46	0/804	0.79	3/1083 (0.3%)
12	L	0.38	0/342	0.55	0/454
13	M	0.42	0/849	0.56	1/1140 (0.1%)
14	N	0.40	0/1172	0.54	0/1580
15	O	0.38	1/3897 (0.0%)	0.58	3/5268 (0.1%)
2	B	0.49	1/9533 (0.0%)	0.77	25/12884 (0.2%)
3	C	0.43	0/2475	0.68	5/3354 (0.1%)
4	D	0.40	0/465	0.59	0/630
5	E	0.40	0/1771	0.66	3/2383 (0.1%)
6	F	0.45	0/838	0.58	0/1129
7	G	0.39	0/1558	0.60	3/2120 (0.1%)
8	H	0.42	0/1070	0.61	0/1449
9	I	0.42	0/831	0.57	0/1117
All	All	0.45	3/38083 (0.0%)	0.69	65/51439 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
15	O	0	5
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	10	CYS	CB-SG	7.64	1.95	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	198	PHE	C-N	-7.16	1.20	1.34
2	B	859	CYS	CB-SG	-6.12	1.71	1.82

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1023	ARG	NE-CZ-NH2	-13.90	113.35	120.30
2	B	452	ARG	NE-CZ-NH2	-13.35	113.63	120.30
1	A	397	ARG	NE-CZ-NH1	13.22	126.91	120.30
1	A	329	ARG	NE-CZ-NH2	-13.12	113.74	120.30
2	B	448	ARG	NE-CZ-NH2	-12.97	113.81	120.30
1	A	329	ARG	NE-CZ-NH1	12.94	126.77	120.30
2	B	429	ARG	NE-CZ-NH2	-12.81	113.89	120.30
1	A	59	ARG	NE-CZ-NH1	12.81	126.70	120.30
1	A	59	ARG	NE-CZ-NH2	-12.78	113.91	120.30
5	E	167	ARG	NE-CZ-NH1	12.52	126.56	120.30
5	E	167	ARG	NE-CZ-NH2	-12.50	114.05	120.30
1	A	416	ARG	NE-CZ-NH2	-12.41	114.09	120.30
11	K	44	ARG	NE-CZ-NH2	-12.29	114.15	120.30
2	B	448	ARG	NE-CZ-NH1	12.28	126.44	120.30
2	B	261	ARG	NE-CZ-NH1	12.22	126.41	120.30
2	B	452	ARG	NE-CZ-NH1	12.22	126.41	120.30
2	B	634	ARG	NE-CZ-NH2	-12.21	114.19	120.30
2	B	261	ARG	NE-CZ-NH2	-12.11	114.25	120.30
2	B	429	ARG	NE-CZ-NH1	12.07	126.33	120.30
11	K	44	ARG	NE-CZ-NH1	11.97	126.29	120.30
1	A	397	ARG	NE-CZ-NH2	-11.89	114.35	120.30
3	C	142	ARG	NE-CZ-NH2	-11.52	114.54	120.30
1	A	422	ARG	NE-CZ-NH2	-11.46	114.57	120.30
3	C	142	ARG	NE-CZ-NH1	11.44	126.02	120.30
1	A	342	ARG	NE-CZ-NH2	-11.35	114.62	120.30
1	A	422	ARG	NE-CZ-NH1	11.12	125.86	120.30
2	B	634	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	A	416	ARG	NE-CZ-NH1	11.00	125.80	120.30
1	A	230	ARG	NE-CZ-NH1	10.85	125.72	120.30
1	A	230	ARG	NE-CZ-NH2	-10.79	114.91	120.30
2	B	648	ARG	NE-CZ-NH2	-10.72	114.94	120.30
2	B	550	ARG	NE-CZ-NH2	-10.51	115.04	120.30
2	B	550	ARG	NE-CZ-NH1	9.88	125.24	120.30
2	B	1023	ARG	NE-CZ-NH1	9.57	125.08	120.30
1	A	342	ARG	NE-CZ-NH1	9.25	124.92	120.30
2	B	648	ARG	NE-CZ-NH1	9.09	124.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	460	GLU	N-CA-C	-7.44	90.91	111.00
2	B	261	ARG	CD-NE-CZ	6.91	133.28	123.60
1	A	397	ARG	CD-NE-CZ	6.90	133.25	123.60
15	O	598	PHE	N-CA-C	6.90	129.62	111.00
1	A	59	ARG	CD-NE-CZ	6.61	132.86	123.60
2	B	452	ARG	CD-NE-CZ	6.55	132.77	123.60
2	B	448	ARG	CD-NE-CZ	6.37	132.52	123.60
1	A	329	ARG	CD-NE-CZ	6.33	132.46	123.60
11	K	44	ARG	CD-NE-CZ	6.24	132.34	123.60
2	B	634	ARG	CD-NE-CZ	6.20	132.28	123.60
1	A	416	ARG	CD-NE-CZ	6.18	132.25	123.60
1	A	422	ARG	CD-NE-CZ	6.17	132.23	123.60
2	B	429	ARG	CD-NE-CZ	6.13	132.18	123.60
3	C	142	ARG	CD-NE-CZ	6.00	132.00	123.60
5	E	167	ARG	CD-NE-CZ	5.93	131.90	123.60
7	G	35	SER	O-C-N	5.92	132.17	122.70
1	A	1622	LEU	O-C-N	5.78	131.94	122.70
1	A	342	ARG	CD-NE-CZ	5.67	131.54	123.60
2	B	1103	VAL	CB-CA-C	-5.59	100.78	111.40
7	G	35	SER	CA-C-N	-5.54	105.02	117.20
2	B	550	ARG	CD-NE-CZ	5.45	131.23	123.60
2	B	648	ARG	CD-NE-CZ	5.39	131.15	123.60
2	B	1023	ARG	CD-NE-CZ	5.22	130.91	123.60
1	A	230	ARG	CD-NE-CZ	5.20	130.88	123.60
7	G	26	ASN	C-N-CD	5.12	139.16	128.40
15	O	128	LEU	C-N-CD	5.08	139.06	128.40
13	M	110	GLY	C-N-CD	5.06	139.03	128.40
3	C	220	SER	C-N-CD	5.05	139.00	128.40
3	C	230	LEU	C-N-CD	5.03	138.97	128.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1343	ASP	Peptide
15	O	374	PRO	Peptide
15	O	375	THR	Peptide
15	O	411	ASN	Peptide
15	O	598	PHE	Peptide
15	O	599	LEU	Peptide



## 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	11686	0	11770	682	0
2	B	9327	0	9214	482	0
3	C	2423	0	2409	283	0
4	D	459	0	461	103	0
5	E	1735	0	1764	40	0
6	F	823	0	840	64	0
7	G	1520	0	1529	162	0
8	H	1052	0	1021	15	0
9	I	820	0	805	71	0
10	J	569	0	585	6	0
11	K	793	0	790	36	0
12	L	340	0	361	47	0
13	M	833	0	826	32	0
14	N	1151	0	1169	44	0
15	O	3811	0	3800	754	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
All	All	37349	0	37344	2255	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 30.

All (2255) 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)
3:C:75:VAL:HG11	3:C:221:PRO:CG	1.33	1.52
1:A:478:TYR:HA	2:B:1048:SER:CA	1.42	1.50
1:A:436:ALA:CB	1:A:443:ALA:HB2	1.43	1.46
1:A:83:VAL:HG21	1:A:427:PHE:CZ	1.50	1.46
15:O:458:GLU:HA	15:O:461:VAL:CG2	1.26	1.44
15:O:458:GLU:CA	15:O:461:VAL:HG23	1.28	1.41
15:O:454:VAL:CB	15:O:514:PHE:HE2	1.30	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:TYR:CA	2:B:1048:SER:HA	1.53	1.38
2:B:207:ILE:HG13	2:B:503:VAL:CG2	1.54	1.37
15:O:408:PHE:CZ	15:O:446:LEU:CD1	2.06	1.37
15:O:408:PHE:CZ	15:O:446:LEU:HD11	1.59	1.37
1:A:436:ALA:HB2	1:A:443:ALA:CB	1.54	1.37
15:O:471:LYS:HB2	15:O:585:PHE:CE1	1.58	1.37
1:A:83:VAL:HG11	1:A:427:PHE:CE2	1.59	1.36
15:O:138:TYR:CE2	15:O:142:ILE:HD11	1.56	1.36
3:C:31:TRP:CB	11:K:82:LYS:HD2	1.54	1.35
15:O:454:VAL:HB	15:O:514:PHE:CE2	1.61	1.35
1:A:437:PHE:CZ	1:A:456:VAL:HG23	1.62	1.35
7:G:242:VAL:HG11	15:O:185:SER:OG	1.22	1.35
1:A:437:PHE:CZ	1:A:456:VAL:CG2	2.11	1.34
2:B:42:VAL:CG1	2:B:46:ILE:HD11	1.57	1.33
3:C:75:VAL:HG11	3:C:221:PRO:CD	1.59	1.32
3:C:75:VAL:CG1	3:C:221:PRO:CG	2.07	1.31
3:C:54:PHE:CE2	3:C:300:PHE:HB2	1.66	1.30
3:C:55:ASP:CG	3:C:299:ILE:HG12	1.51	1.29
1:A:477:ASN:OD1	2:B:1059:PRO:HG3	1.13	1.29
3:C:84:TYR:HE2	12:L:66:GLN:OE1	1.16	1.29
15:O:198:PHE:CD2	15:O:232:LEU:HG	1.65	1.29
4:D:30:HIS:NE2	7:G:26:ASN:OD1	1.66	1.27
15:O:432:LYS:HG2	15:O:608:GLU:O	1.23	1.27
4:D:25:THR:CG2	6:F:59:GLN:HE21	1.45	1.27
3:C:84:TYR:CE2	12:L:66:GLN:OE1	1.87	1.26
3:C:75:VAL:CG1	3:C:221:PRO:CD	2.14	1.26
1:A:478:TYR:N	2:B:1048:SER:O	1.66	1.25
1:A:1008:ASP:OD2	1:A:1202:LEU:HD13	1.37	1.24
15:O:431:ALA:CB	15:O:434:LEU:HD11	1.63	1.24
3:C:54:PHE:CE2	3:C:300:PHE:CB	2.20	1.24
1:A:1348:VAL:HB	2:B:268:GLU:O	1.35	1.24
15:O:237:ILE:CB	15:O:381:ILE:HD12	1.68	1.24
7:G:158:LYS:CG	15:O:105:ASN:OD1	1.86	1.23
15:O:432:LYS:HB3	15:O:609:TYR:CA	1.69	1.23
1:A:756:LYS:HD3	9:I:85:LYS:NZ	1.51	1.23
15:O:432:LYS:CG	15:O:608:GLU:O	1.88	1.22
2:B:769:PHE:CE1	2:B:798:PHE:CE1	2.26	1.22
4:D:30:HIS:CE1	7:G:26:ASN:OD1	1.92	1.22
2:B:769:PHE:CE1	2:B:798:PHE:HE1	1.56	1.22
3:C:230:LEU:CD2	3:C:294:VAL:HG21	1.67	1.22
1:A:1605:THR:O	1:A:1606:SER:O	1.57	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:454:VAL:CB	15:O:514:PHE:CE2	2.17	1.22
3:C:54:PHE:CZ	3:C:300:PHE:HB3	1.73	1.22
3:C:131:THR:HG23	3:C:209:ILE:CG2	1.69	1.21
15:O:352:LEU:HD23	15:O:358:VAL:CG2	1.69	1.21
15:O:373:LEU:HD11	15:O:416:LYS:CG	1.69	1.21
15:O:352:LEU:CD2	15:O:358:VAL:HG22	1.71	1.20
3:C:31:TRP:CD1	11:K:82:LYS:NZ	2.10	1.20
15:O:432:LYS:CB	15:O:609:TYR:HA	1.71	1.20
1:A:477:ASN:OD1	2:B:1059:PRO:CG	1.90	1.20
3:C:62:SER:HB2	11:K:74:ASN:ND2	1.51	1.20
15:O:426:SER:OG	15:O:594:TYR:HB2	1.42	1.19
1:A:1050:TYR:CE1	1:A:1185:VAL:HG11	1.76	1.19
15:O:247:GLU:OE1	15:O:325:ILE:HG12	1.42	1.19
15:O:390:GLN:O	15:O:609:TYR:CE1	1.94	1.19
3:C:55:ASP:HA	3:C:299:ILE:HA	1.20	1.18
3:C:54:PHE:O	3:C:300:PHE:N	1.76	1.18
15:O:237:ILE:CG2	15:O:381:ILE:HD12	1.73	1.18
1:A:1008:ASP:OD1	1:A:1202:LEU:HD22	1.43	1.18
7:G:141:SER:CB	15:O:138:TYR:OH	1.92	1.17
15:O:162:PHE:O	15:O:210:ASN:O	1.61	1.17
15:O:237:ILE:HB	15:O:381:ILE:HD12	1.22	1.17
1:A:437:PHE:CE1	1:A:456:VAL:HG23	1.78	1.17
2:B:207:ILE:CG1	2:B:503:VAL:CG2	2.22	1.17
1:A:1006:LEU:CD1	2:B:716:MET:SD	2.32	1.17
2:B:207:ILE:CG1	2:B:503:VAL:HG21	1.73	1.17
1:A:1006:LEU:HD11	2:B:716:MET:SD	1.85	1.16
1:A:83:VAL:HG21	1:A:427:PHE:CE2	1.78	1.16
7:G:158:LYS:CD	15:O:105:ASN:OD1	1.91	1.16
15:O:430:ARG:NH2	15:O:596:PRO:HD3	1.60	1.16
1:A:1048:PHE:CZ	5:E:211:TYR:HD1	1.64	1.16
1:A:1011:VAL:HG11	1:A:1201:THR:C	1.63	1.16
2:B:207:ILE:HG13	2:B:503:VAL:HG22	1.26	1.16
1:A:756:LYS:CD	9:I:85:LYS:NZ	2.07	1.16
3:C:59:ILE:HG23	3:C:298:PHE:CE1	1.79	1.15
4:D:92:ILE:HG12	7:G:152:ALA:HB2	1.29	1.15
7:G:158:LYS:HG2	15:O:105:ASN:OD1	1.43	1.15
1:A:1344:ILE:HD12	2:B:329:TYR:HE2	1.10	1.14
1:A:556:ALA:HB2	15:O:246:ASN:ND2	1.63	1.14
15:O:219:ARG:NH2	15:O:360:VAL:HG21	1.63	1.14
15:O:408:PHE:CE2	15:O:446:LEU:HD11	1.83	1.14
15:O:408:PHE:CZ	15:O:446:LEU:HD13	1.81	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:143:SER:HB2	15:O:104:ILE:H	1.06	1.13
15:O:454:VAL:HA	15:O:514:PHE:CZ	1.83	1.12
2:B:42:VAL:HB	2:B:46:ILE:CD1	1.77	1.12
7:G:28:ILE:HG22	7:G:29:ASP:H	1.02	1.12
1:A:1348:VAL:CB	2:B:268:GLU:O	1.97	1.12
15:O:247:GLU:OE1	15:O:325:ILE:CG1	1.97	1.12
3:C:58:ASN:HA	3:C:296:ASN:CB	1.79	1.11
2:B:42:VAL:CG1	2:B:46:ILE:CD1	2.26	1.11
3:C:54:PHE:CD2	3:C:300:PHE:HB2	1.85	1.11
15:O:370:THR:O	15:O:374:PRO:HD3	1.51	1.11
15:O:598:PHE:HB3	15:O:599:LEU:HD13	1.12	1.11
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.12	1.11
15:O:156:MET:HG3	15:O:197:PHE:CE2	1.83	1.11
15:O:454:VAL:CG2	15:O:514:PHE:HE2	1.62	1.11
13:M:101:VAL:CG1	13:M:106:LYS:HG3	1.81	1.10
2:B:42:VAL:CB	2:B:46:ILE:CD1	2.29	1.10
7:G:158:LYS:HB3	15:O:105:ASN:ND2	1.65	1.10
1:A:1226:VAL:O	1:A:1598:PHE:HD2	1.34	1.10
15:O:129:PRO:HD2	15:O:132:THR:HB	1.32	1.10
15:O:156:MET:SD	15:O:197:PHE:CZ	2.45	1.10
15:O:446:LEU:O	15:O:449:TRP:HB3	1.51	1.10
1:A:83:VAL:CG1	1:A:427:PHE:CE2	2.34	1.10
1:A:480:ALA:HB2	2:B:1046:VAL:HG23	1.23	1.10
15:O:240:ILE:HG21	15:O:332:LEU:HB2	1.24	1.10
4:D:25:THR:HG22	6:F:59:GLN:HE21	1.07	1.10
3:C:31:TRP:CE3	11:K:82:LYS:HG3	1.86	1.10
7:G:158:LYS:CB	15:O:105:ASN:ND2	2.15	1.10
1:A:1011:VAL:HG11	1:A:1201:THR:O	1.51	1.10
3:C:58:ASN:CA	3:C:296:ASN:HB2	1.81	1.10
3:C:59:ILE:CG2	3:C:298:PHE:CD1	2.35	1.09
1:A:475:ARG:HD2	2:B:1059:PRO:O	1.51	1.09
15:O:425:GLY:HA2	15:O:483:ILE:HD11	1.34	1.09
3:C:55:ASP:OD1	3:C:299:ILE:HG12	1.53	1.09
7:G:158:LYS:HA	15:O:105:ASN:HD21	1.08	1.09
15:O:447:THR:O	15:O:450:LEU:HB2	1.50	1.09
3:C:56:LEU:HB2	3:C:298:PHE:HB2	1.35	1.09
3:C:230:LEU:HD23	3:C:294:VAL:CG2	1.83	1.09
3:C:31:TRP:HB3	11:K:82:LYS:HD2	1.17	1.09
1:A:436:ALA:CB	1:A:443:ALA:CB	2.21	1.08
3:C:230:LEU:HD12	3:C:231:PRO:CD	1.84	1.08
1:A:475:ARG:CD	2:B:1059:PRO:O	2.00	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:28:PRO:HG2	7:G:24:VAL:HG11	1.28	1.08
15:O:138:TYR:CE2	15:O:142:ILE:CD1	2.35	1.08
15:O:201:LYS:HD2	15:O:239:SER:OG	1.54	1.08
1:A:1011:VAL:CG1	1:A:1201:THR:O	2.00	1.08
1:A:478:TYR:CZ	2:B:1049:THR:HG23	1.88	1.08
2:B:42:VAL:CB	2:B:46:ILE:HD11	1.84	1.08
4:D:25:THR:HA	6:F:59:GLN:HG2	1.32	1.08
15:O:129:PRO:CD	15:O:132:THR:HB	1.83	1.08
3:C:75:VAL:HB	3:C:221:PRO:HD3	1.36	1.07
3:C:57:ILE:HA	3:C:297:HIS:HA	1.14	1.07
15:O:156:MET:SD	15:O:197:PHE:HZ	1.78	1.07
1:A:478:TYR:CZ	2:B:1049:THR:CG2	2.38	1.07
3:C:230:LEU:HD12	3:C:231:PRO:HD3	1.36	1.07
15:O:138:TYR:CZ	15:O:142:ILE:HD11	1.89	1.07
13:M:101:VAL:HG11	13:M:106:LYS:HG3	1.27	1.06
1:A:1008:ASP:O	1:A:1011:VAL:HG23	1.53	1.06
1:A:475:ARG:NH2	2:B:1061:LYS:HB2	1.70	1.06
15:O:245:GLN:HG3	15:O:378:THR:HA	1.15	1.06
4:D:80:THR:OG1	15:O:227:PHE:CG	2.08	1.06
15:O:431:ALA:HB3	15:O:434:LEU:HD11	1.37	1.06
2:B:42:VAL:HG12	2:B:46:ILE:CD1	1.84	1.06
15:O:240:ILE:HG22	15:O:332:LEU:HD22	1.08	1.06
3:C:41:GLU:HB3	3:C:57:ILE:CG2	1.83	1.06
15:O:198:PHE:CD1	15:O:236:LYS:HE3	1.90	1.06
1:A:1053:ASP:OD2	1:A:1580:ARG:NH2	1.88	1.06
3:C:75:VAL:HG11	3:C:221:PRO:HG2	1.06	1.05
15:O:162:PHE:CA	15:O:214:ASN:CB	2.33	1.05
1:A:408:LYS:HA	1:A:411:VAL:CG1	1.85	1.05
15:O:152:GLN:HG2	15:O:193:TYR:OH	1.52	1.05
15:O:431:ALA:HB1	15:O:434:LEU:HD11	1.34	1.05
15:O:240:ILE:CG2	15:O:332:LEU:HD22	1.87	1.05
1:A:1179:ILE:HD11	1:A:1183:GLU:HG3	1.33	1.05
1:A:1048:PHE:CZ	5:E:211:TYR:CD1	2.44	1.05
15:O:198:PHE:CZ	15:O:236:LYS:HG3	1.92	1.05
3:C:75:VAL:CB	3:C:221:PRO:CD	2.35	1.04
15:O:488:HIS:CG	15:O:489:ASN:H	1.74	1.04
15:O:390:GLN:NE2	15:O:432:LYS:H	1.54	1.04
3:C:131:THR:HG23	3:C:209:ILE:HG22	1.08	1.04
7:G:241:ARG:CB	15:O:189:PHE:CE2	2.39	1.04
15:O:152:GLN:CG	15:O:193:TYR:OH	2.04	1.04
1:A:83:VAL:HG11	1:A:427:PHE:CD2	1.90	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:ALA:HB1	1:A:581:ILE:CG2	1.87	1.04
7:G:141:SER:HB2	15:O:138:TYR:OH	1.53	1.04
15:O:174:ASP:HA	15:O:177:LYS:HE2	1.40	1.03
15:O:435:SER:HB3	15:O:438:GLN:HG3	1.37	1.03
4:D:25:THR:CG2	6:F:59:GLN:NE2	2.21	1.03
15:O:237:ILE:HB	15:O:381:ILE:CD1	1.88	1.03
12:L:68:GLU:HG2	12:L:69:ALA:H	1.23	1.03
1:A:1003:ARG:NE	2:B:520:LEU:HB2	1.74	1.03
1:A:1050:TYR:CE1	1:A:1185:VAL:CG1	2.42	1.02
1:A:782:ASP:OD2	1:A:931:SER:O	1.78	1.02
3:C:59:ILE:CG2	3:C:298:PHE:CE1	2.43	1.02
2:B:472:SER:CB	2:B:476:LEU:HD12	1.88	1.02
2:B:1155:ASP:OD2	7:G:239:THR:OG1	1.76	1.02
1:A:413:LEU:HB3	1:A:417:ARG:NH2	1.75	1.02
15:O:241:ASP:OD1	15:O:378:THR:HG22	1.58	1.02
1:A:909:SER:OG	9:I:83:LYS:CE	2.08	1.01
3:C:51:GLU:HB3	3:C:303:GLU:HG2	1.42	1.01
15:O:369:LYS:O	15:O:373:LEU:N	1.91	1.01
1:A:392:THR:CG2	1:A:430:ILE:HB	1.88	1.01
7:G:158:LYS:HB3	15:O:105:ASN:CG	1.79	1.01
1:A:480:ALA:CB	2:B:1046:VAL:HG23	1.90	1.01
3:C:56:LEU:CD1	3:C:300:PHE:CE1	2.44	1.01
15:O:201:LYS:CD	15:O:239:SER:OG	2.09	1.01
2:B:42:VAL:C	2:B:46:ILE:HD12	1.82	1.00
15:O:428:ILE:HG23	15:O:439:ILE:HG21	1.38	1.00
7:G:158:LYS:CA	15:O:105:ASN:HD21	1.75	1.00
3:C:45:SER:HB2	3:C:271:ARG:NH2	1.76	1.00
7:G:158:LYS:HZ3	15:O:108:GLU:CG	1.27	1.00
15:O:348:THR:HG22	15:O:351:SER:HB3	1.42	1.00
1:A:799:GLU:HG3	1:A:1062:HIS:CG	1.95	1.00
1:A:408:LYS:HA	1:A:411:VAL:HG12	1.40	1.00
15:O:352:LEU:HA	15:O:358:VAL:HG23	1.44	1.00
1:A:782:ASP:OD1	1:A:783:LYS:N	1.93	1.00
1:A:756:LYS:CD	9:I:85:LYS:HZ2	1.70	1.00
15:O:240:ILE:HG21	15:O:332:LEU:CB	1.92	1.00
15:O:352:LEU:HD23	15:O:358:VAL:HG22	1.00	1.00
15:O:428:ILE:HD12	15:O:439:ILE:HG23	1.44	1.00
15:O:471:LYS:CB	15:O:585:PHE:CE1	2.45	0.99
2:B:75:ASP:HB3	2:B:440:PHE:CE2	1.97	0.99
1:A:1055:ILE:HD12	1:A:1063:MET:CE	1.91	0.99
15:O:454:VAL:CG2	15:O:514:PHE:CE2	2.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:143:SER:CB	15:O:104:ILE:H	1.75	0.99
15:O:158:LEU:HD23	15:O:172:HIS:HD2	1.25	0.99
1:A:1006:LEU:HD12	2:B:716:MET:SD	2.01	0.99
7:G:158:LYS:CA	15:O:105:ASN:ND2	2.25	0.99
1:A:1344:ILE:HD12	2:B:329:TYR:CE2	1.97	0.98
2:B:70:GLU:CB	2:B:98:SER:HB3	1.93	0.98
2:B:1019:GLY:HA3	3:C:65:ASN:HB2	1.45	0.98
3:C:54:PHE:CZ	3:C:300:PHE:CB	2.41	0.98
3:C:84:TYR:CD2	12:L:66:GLN:HB2	1.99	0.98
2:B:70:GLU:HB3	2:B:98:SER:HB3	0.99	0.98
15:O:240:ILE:CG2	15:O:332:LEU:HD13	1.93	0.98
15:O:373:LEU:HD11	15:O:416:LYS:HG3	1.43	0.98
7:G:241:ARG:CB	15:O:189:PHE:HE2	1.76	0.98
15:O:598:PHE:CB	15:O:599:LEU:HD13	1.92	0.98
1:A:392:THR:HG21	1:A:430:ILE:CB	1.94	0.98
6:F:75:PRO:HG2	6:F:78:GLN:CB	1.92	0.98
1:A:909:SER:OG	9:I:83:LYS:HE2	1.62	0.97
1:A:83:VAL:CG2	1:A:427:PHE:CZ	2.47	0.97
4:D:96:PHE:HE1	7:G:150:HIS:HB3	1.28	0.97
15:O:423:TYR:HD1	15:O:594:TYR:CE2	1.82	0.97
13:M:105:SER:HA	13:M:108:LEU:HG	1.46	0.97
1:A:392:THR:HG21	1:A:430:ILE:HB	0.98	0.97
1:A:509:GLU:OE2	1:A:579:ARG:NE	1.97	0.97
1:A:953:GLU:HG2	1:A:1205:PHE:CE2	2.00	0.97
2:B:70:GLU:HB3	2:B:98:SER:CB	1.93	0.97
15:O:454:VAL:HB	15:O:514:PHE:HE2	0.99	0.96
1:A:480:ALA:HB2	2:B:1046:VAL:CG2	1.95	0.96
1:A:476:VAL:HG11	2:B:1071:VAL:HG23	1.47	0.96
1:A:1660:VAL:O	7:G:102:GLU:HA	1.65	0.96
3:C:59:ILE:HG22	3:C:298:PHE:CD1	1.98	0.96
1:A:83:VAL:CG2	1:A:427:PHE:CE2	2.48	0.96
1:A:966:LEU:HD22	1:A:997:PHE:CZ	2.00	0.96
2:B:769:PHE:CD1	2:B:798:PHE:HE1	1.83	0.96
15:O:156:MET:CG	15:O:197:PHE:CE2	2.48	0.96
1:A:1055:ILE:HG21	1:A:1060:GLU:HG3	1.47	0.95
1:A:502:ALA:HB1	1:A:581:ILE:HG21	1.46	0.95
1:A:1:MET:HG2	2:B:1098:TYR:CZ	2.01	0.95
7:G:158:LYS:HD3	15:O:105:ASN:OD1	1.66	0.95
1:A:516:ILE:HG12	15:O:376:TYR:CE2	2.01	0.95
15:O:440:ILE:HG23	15:O:491:PHE:HE1	1.27	0.95
15:O:408:PHE:HZ	15:O:446:LEU:HD11	1.25	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:ALA:CB	1:A:581:ILE:HG21	1.97	0.95
2:B:1090:ASP:OD1	2:B:1095:SER:OG	1.85	0.95
15:O:454:VAL:HG23	15:O:514:PHE:CE2	2.01	0.95
1:A:1344:ILE:CD1	2:B:329:TYR:HE2	1.78	0.94
2:B:77:LYS:NZ	2:B:438:ILE:O	1.99	0.94
15:O:63:LEU:HD12	15:O:71:ILE:HG13	1.47	0.94
15:O:374:PRO:O	15:O:419:LYS:NZ	2.01	0.94
1:A:401:ASP:OD2	1:A:405:LYS:HE3	1.67	0.94
15:O:234:ILE:CG2	15:O:371:HIS:HD2	1.81	0.94
7:G:158:LYS:HD3	15:O:105:ASN:CG	1.88	0.94
3:C:75:VAL:HB	3:C:221:PRO:CD	1.94	0.94
1:A:799:GLU:HG3	1:A:1062:HIS:ND1	1.83	0.93
1:A:990:ILE:HA	1:A:994:GLU:OE1	1.69	0.93
2:B:894:LYS:H	12:L:54:ARG:NH2	1.66	0.93
15:O:342:HIS:CD2	15:O:346:GLN:HE21	1.85	0.93
15:O:417:LYS:HD2	15:O:472:HIS:CE1	2.02	0.93
1:A:878:ARG:HG2	9:I:67:VAL:HG11	1.48	0.93
15:O:241:ASP:CG	15:O:378:THR:HG22	1.88	0.93
2:B:209:GLN:HG2	2:B:210:ARG:H	1.31	0.93
2:B:211:ARG:HG2	2:B:401:GLU:OE1	1.68	0.93
3:C:57:ILE:HD12	3:C:297:HIS:ND1	1.82	0.93
15:O:198:PHE:HD2	15:O:232:LEU:HG	1.05	0.93
3:C:62:SER:CB	11:K:74:ASN:ND2	2.32	0.93
7:G:242:VAL:HG11	15:O:185:SER:HG	1.32	0.93
15:O:342:HIS:O	15:O:346:GLN:HG2	1.68	0.93
3:C:75:VAL:CG1	3:C:221:PRO:HG2	1.89	0.93
4:D:80:THR:OG1	15:O:227:PHE:CD2	2.20	0.93
15:O:358:VAL:O	15:O:362:ASN:ND2	2.00	0.93
1:A:413:LEU:HB3	1:A:417:ARG:HH21	1.29	0.93
4:D:92:ILE:HG22	4:D:96:PHE:CZ	2.03	0.93
7:G:158:LYS:CB	15:O:105:ASN:CG	2.35	0.93
7:G:158:LYS:CG	15:O:105:ASN:CG	2.37	0.93
3:C:75:VAL:CB	3:C:221:PRO:HD2	1.97	0.92
15:O:598:PHE:HB3	15:O:599:LEU:CD1	1.99	0.92
3:C:131:THR:CG2	3:C:209:ILE:HG22	1.98	0.92
7:G:154:ASN:HD21	15:O:182:MET:CE	1.82	0.92
1:A:83:VAL:HG21	1:A:427:PHE:HZ	1.13	0.92
15:O:224:GLU:N	15:O:224:GLU:OE1	2.02	0.92
1:A:756:LYS:HD3	9:I:85:LYS:HZ1	1.19	0.92
3:C:71:MET:SD	3:C:225:ALA:HB1	2.10	0.92
15:O:147:ILE:O	15:O:149:LYS:N	2.03	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:85:HIS:HE1	14:N:141:GLU:CD	1.72	0.92
15:O:390:GLN:O	15:O:609:TYR:HE1	1.52	0.92
15:O:386:PHE:HD2	15:O:606:MET:CE	1.83	0.92
15:O:435:SER:CB	15:O:438:GLN:HG3	1.98	0.92
1:A:1658:ALA:O	7:G:104:LEU:HA	1.70	0.91
15:O:240:ILE:HG22	15:O:332:LEU:CD2	1.98	0.91
6:F:74:ILE:HG23	6:F:75:PRO:HD2	1.51	0.91
7:G:28:ILE:HG22	7:G:29:ASP:N	1.81	0.91
2:B:894:LYS:H	12:L:54:ARG:HH21	0.92	0.91
15:O:219:ARG:NH2	15:O:360:VAL:CG2	2.32	0.91
15:O:408:PHE:HZ	15:O:446:LEU:CD1	1.74	0.91
3:C:253:PRO:HB2	14:N:180:PHE:CD1	2.06	0.91
3:C:52:ALA:O	3:C:301:ASN:HA	1.69	0.91
15:O:390:GLN:NE2	15:O:609:TYR:HB3	1.86	0.91
1:A:478:TYR:C	2:B:1047:ARG:O	2.08	0.91
15:O:240:ILE:HG21	15:O:332:LEU:HD13	1.51	0.91
1:A:1036:ASN:O	1:A:1049:MET:HA	1.71	0.91
15:O:478:GLN:HE21	15:O:592:PHE:HZ	1.19	0.91
1:A:412:SER:O	1:A:416:ARG:N	2.03	0.90
2:B:42:VAL:HG11	2:B:46:ILE:HD11	1.52	0.90
2:B:894:LYS:N	12:L:54:ARG:HH21	1.69	0.90
2:B:472:SER:OG	2:B:476:LEU:HD12	1.71	0.90
3:C:230:LEU:HD23	3:C:294:VAL:HG21	0.91	0.90
15:O:342:HIS:CE1	15:O:346:GLN:HG3	2.05	0.90
15:O:426:SER:OG	15:O:594:TYR:CB	2.18	0.90
1:A:1055:ILE:HD11	1:A:1174:TYR:CE2	2.06	0.90
15:O:240:ILE:CG2	15:O:332:LEU:HB2	2.01	0.90
4:D:25:THR:HA	6:F:59:GLN:CG	1.99	0.90
15:O:454:VAL:HA	15:O:514:PHE:HZ	1.34	0.90
1:A:1048:PHE:HE2	5:E:211:TYR:H	1.11	0.90
1:A:756:LYS:CD	9:I:85:LYS:HZ1	1.76	0.90
15:O:471:LYS:HB2	15:O:585:PHE:HE1	1.00	0.90
1:A:516:ILE:HG21	15:O:376:TYR:OH	1.72	0.90
3:C:41:GLU:HB3	3:C:57:ILE:HG21	1.53	0.90
4:D:28:PRO:HG2	7:G:24:VAL:CG1	2.01	0.90
1:A:413:LEU:O	1:A:417:ARG:NE	2.05	0.90
3:C:75:VAL:HG11	3:C:221:PRO:HD2	1.54	0.90
15:O:158:LEU:HD23	15:O:172:HIS:CD2	2.07	0.90
15:O:426:SER:CB	15:O:594:TYR:HB2	2.01	0.90
15:O:432:LYS:HB2	15:O:609:TYR:C	1.93	0.90
3:C:31:TRP:CG	11:K:82:LYS:HD2	2.06	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:86:PHE:CE1	12:L:64:LEU:HD13	2.07	0.89
15:O:198:PHE:CG	15:O:236:LYS:HE3	2.06	0.89
1:A:1226:VAL:O	1:A:1598:PHE:CD2	2.24	0.89
7:G:158:LYS:HA	15:O:105:ASN:ND2	1.85	0.89
15:O:194:LEU:O	15:O:232:LEU:HD21	1.72	0.89
15:O:421:LEU:HD13	15:O:476:ALA:HB2	1.54	0.89
2:B:478:LEU:HD13	2:B:484:TYR:CE1	2.06	0.89
4:D:96:PHE:CE1	7:G:150:HIS:HB3	2.07	0.89
1:A:1050:TYR:HE1	1:A:1185:VAL:CG1	1.83	0.89
1:A:1179:ILE:HD11	1:A:1183:GLU:CG	2.01	0.89
15:O:129:PRO:CG	15:O:132:THR:HB	2.01	0.89
4:D:80:THR:HG21	15:O:227:PHE:HB3	1.53	0.89
3:C:37:LYS:HD2	11:K:130:VAL:HG22	1.54	0.89
2:B:42:VAL:CB	2:B:46:ILE:HD12	2.00	0.89
15:O:432:LYS:CB	15:O:609:TYR:CA	2.41	0.89
15:O:457:ARG:HA	15:O:460:GLU:HB2	1.54	0.89
15:O:219:ARG:HH21	15:O:360:VAL:CG2	1.85	0.89
1:A:891:ILE:CD1	9:I:71:LEU:HB2	2.03	0.89
13:M:102:SER:O	13:M:106:LYS:HB2	1.73	0.89
1:A:406:LEU:CD1	1:A:411:VAL:HB	2.03	0.88
6:F:66:ARG:CZ	7:G:90:LEU:HD13	2.02	0.88
2:B:894:LYS:HG2	12:L:47:ARG:CD	2.04	0.88
3:C:58:ASN:H	3:C:296:ASN:C	1.75	0.88
1:A:401:ASP:O	1:A:405:LYS:HB2	1.74	0.88
3:C:56:LEU:HD11	3:C:300:PHE:CE1	2.08	0.88
4:D:28:PRO:CG	7:G:24:VAL:HG11	2.03	0.88
1:A:1348:VAL:CG2	2:B:268:GLU:O	2.21	0.88
1:A:83:VAL:CG1	1:A:427:PHE:HE2	1.80	0.88
1:A:1038:ILE:HG12	1:A:1049:MET:O	1.74	0.88
15:O:521:ASN:HD22	15:O:524:VAL:H	1.22	0.88
3:C:230:LEU:CD1	3:C:231:PRO:CD	2.52	0.88
1:A:556:ALA:HB2	15:O:246:ASN:HD22	1.38	0.88
2:B:769:PHE:CE1	2:B:798:PHE:CZ	2.61	0.88
15:O:488:HIS:ND1	15:O:489:ASN:N	2.21	0.88
15:O:488:HIS:O	15:O:490:ILE:N	2.06	0.88
15:O:459:GLU:O	15:O:463:GLN:HG3	1.73	0.87
3:C:75:VAL:CB	3:C:221:PRO:HD3	2.01	0.87
3:C:230:LEU:CD1	3:C:231:PRO:HD2	2.04	0.87
1:A:1662:ASN:HA	7:G:101:SER:HB2	1.57	0.87
15:O:417:LYS:CD	15:O:472:HIS:CE1	2.57	0.87
1:A:756:LYS:HD2	9:I:85:LYS:NZ	1.86	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:198:PHE:HD2	15:O:232:LEU:CG	1.86	0.87
3:C:131:THR:CG2	3:C:209:ILE:CG2	2.51	0.87
1:A:1055:ILE:HD12	1:A:1063:MET:SD	2.14	0.87
1:A:475:ARG:HD3	2:B:1059:PRO:O	1.73	0.87
7:G:158:LYS:HZ3	15:O:108:GLU:HG2	1.39	0.87
1:A:862:THR:O	9:I:67:VAL:HG12	1.73	0.87
1:A:1:MET:HA	2:B:1098:TYR:CD1	2.10	0.87
3:C:75:VAL:CG1	3:C:221:PRO:HG3	2.03	0.87
3:C:70:ILE:HD11	11:K:71:THR:CG2	2.04	0.87
1:A:1660:VAL:HG22	7:G:103:LYS:O	1.75	0.86
4:D:25:THR:O	6:F:59:GLN:HG3	1.75	0.86
4:D:80:THR:CB	15:O:227:PHE:CD2	2.58	0.86
1:A:1600:ARG:CD	1:A:1616:GLU:OE1	2.24	0.86
1:A:636:HIS:ND1	2:B:1091:ARG:NH2	2.22	0.86
11:K:66:VAL:HG12	11:K:67:GLU:HG2	1.57	0.86
1:A:1348:VAL:HB	2:B:268:GLU:C	1.95	0.86
3:C:56:LEU:HG	3:C:300:PHE:CD1	2.10	0.86
1:A:408:LYS:CA	1:A:411:VAL:HG12	2.04	0.86
7:G:143:SER:HB2	15:O:104:ILE:N	1.89	0.86
3:C:31:TRP:CD2	11:K:82:LYS:HG3	2.10	0.86
1:A:475:ARG:HH22	2:B:1061:LYS:HB2	1.36	0.86
3:C:59:ILE:HG22	3:C:298:PHE:HD1	1.38	0.86
1:A:878:ARG:HE	9:I:67:VAL:CG1	1.87	0.86
1:A:1003:ARG:CZ	2:B:520:LEU:HB2	2.04	0.86
3:C:31:TRP:HB3	11:K:82:LYS:CD	2.03	0.86
15:O:366:THR:O	15:O:370:THR:HG23	1.75	0.86
15:O:417:LYS:HB3	15:O:472:HIS:NE2	1.91	0.86
1:A:620:ASN:OD1	1:A:667:ARG:NH2	2.07	0.86
4:D:80:THR:CG2	15:O:227:PHE:HB3	2.06	0.86
1:A:468:ARG:NE	1:A:1021:ARG:NH1	2.23	0.86
7:G:141:SER:CA	15:O:138:TYR:OH	2.24	0.86
15:O:521:ASN:ND2	15:O:523:ASN:H	1.74	0.86
15:O:457:ARG:O	15:O:460:GLU:HB2	1.76	0.85
15:O:458:GLU:CA	15:O:461:VAL:CG2	2.08	0.85
1:A:1008:ASP:OD1	1:A:1202:LEU:CD2	2.24	0.85
15:O:396:MET:HE1	15:O:434:LEU:HD12	1.57	0.85
15:O:181:ARG:HH11	15:O:181:ARG:CB	1.89	0.85
15:O:163:ILE:HG22	15:O:211:TYR:HB2	1.58	0.85
1:A:1661:PRO:C	7:G:101:SER:O	2.13	0.85
3:C:64:ALA:C	3:C:227:TYR:HE2	1.80	0.85
15:O:408:PHE:CE2	15:O:446:LEU:CD1	2.50	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1060:GLU:HA	1:A:1063:MET:HG3	1.55	0.84
15:O:369:LYS:HZ3	15:O:369:LYS:HB3	1.37	0.84
1:A:392:THR:HB	1:A:430:ILE:HD13	1.59	0.84
2:B:472:SER:HB3	2:B:476:LEU:HD12	1.57	0.84
7:G:25:THR:HG22	7:G:26:ASN:H	1.40	0.84
15:O:181:ARG:HB2	15:O:181:ARG:HH11	1.41	0.84
15:O:237:ILE:HG22	15:O:381:ILE:HD12	1.60	0.84
15:O:361:PHE:O	15:O:365:THR:HG23	1.78	0.84
15:O:386:PHE:HD2	15:O:606:MET:HE1	1.41	0.84
1:A:1055:ILE:HG23	1:A:1063:MET:SD	2.17	0.84
3:C:253:PRO:HB2	14:N:180:PHE:HD1	1.41	0.84
15:O:243:GLU:HA	15:O:246:ASN:ND2	1.90	0.84
15:O:447:THR:HG22	15:O:480:LEU:HD22	1.58	0.84
1:A:1019:LEU:HD12	1:A:1227:MET:HG3	1.58	0.84
1:A:1600:ARG:HD2	1:A:1616:GLU:OE1	1.77	0.84
1:A:436:ALA:HB2	1:A:443:ALA:HB2	0.86	0.84
1:A:413:LEU:C	1:A:417:ARG:HH21	1.81	0.84
2:B:472:SER:CB	2:B:476:LEU:CD1	2.54	0.84
15:O:240:ILE:CB	15:O:332:LEU:HD13	2.07	0.84
2:B:42:VAL:O	2:B:46:ILE:HD12	1.76	0.84
2:B:37:LEU:HD13	2:B:760:TYR:CZ	2.12	0.84
6:F:74:ILE:CG2	6:F:75:PRO:HD2	2.08	0.84
4:D:96:PHE:HE1	7:G:150:HIS:CB	1.91	0.84
15:O:422:GLN:NE2	15:O:592:PHE:CE2	2.45	0.84
7:G:242:VAL:HG12	15:O:185:SER:OG	1.77	0.83
1:A:1008:ASP:CG	1:A:1202:LEU:HD13	1.98	0.83
2:B:894:LYS:O	2:B:896:GLN:N	2.11	0.83
15:O:398:SER:O	15:O:401:VAL:HG12	1.79	0.83
15:O:467:MET:HG3	15:O:519:PHE:CZ	2.13	0.83
1:A:436:ALA:CA	1:A:443:ALA:HB2	2.09	0.83
3:C:86:PHE:HE1	12:L:64:LEU:HD13	1.42	0.83
1:A:863:ASN:ND2	9:I:68:LYS:N	2.25	0.83
15:O:359:GLY:HA2	15:O:362:ASN:HD22	1.43	0.83
1:A:990:ILE:HB	1:A:994:GLU:HB2	1.61	0.83
1:A:990:ILE:CA	1:A:994:GLU:OE1	2.26	0.83
3:C:51:GLU:HB3	3:C:303:GLU:CG	2.08	0.83
15:O:240:ILE:HG21	15:O:332:LEU:CD1	2.08	0.83
15:O:156:MET:CG	15:O:197:PHE:CZ	2.61	0.83
15:O:370:THR:O	15:O:374:PRO:CD	2.25	0.83
2:B:207:ILE:HG12	2:B:503:VAL:HG21	1.59	0.83
15:O:242:VAL:HA	15:O:378:THR:HG21	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:390:GLN:NE2	15:O:432:LYS:N	2.25	0.83
1:A:1026:GLN:OE1	1:A:1603:MET:HB2	1.78	0.83
4:D:25:THR:CA	6:F:59:GLN:HG2	2.07	0.83
15:O:428:ILE:CG2	15:O:439:ILE:HG21	2.09	0.83
15:O:457:ARG:CA	15:O:460:GLU:HB2	2.09	0.83
1:A:1:MET:HA	2:B:1098:TYR:CE1	2.13	0.83
1:A:556:ALA:CB	15:O:246:ASN:HD22	1.90	0.83
15:O:454:VAL:CA	15:O:514:PHE:CE2	2.62	0.83
1:A:1654:PHE:CZ	6:F:92:ARG:HD3	2.14	0.83
3:C:253:PRO:HG2	14:N:180:PHE:HB3	1.61	0.83
1:A:1179:ILE:CD1	1:A:1183:GLU:HG3	2.09	0.83
1:A:1603:MET:HE2	1:A:1615:TYR:CD2	2.14	0.83
15:O:352:LEU:O	15:O:358:VAL:HG21	1.77	0.83
15:O:488:HIS:CG	15:O:489:ASN:N	2.40	0.83
1:A:1575:ILE:CG1	9:I:122:ARG:HH12	1.92	0.82
15:O:242:VAL:N	15:O:378:THR:HG21	1.94	0.82
15:O:440:ILE:HG23	15:O:491:PHE:CE1	2.13	0.82
3:C:31:TRP:CG	11:K:82:LYS:NZ	2.44	0.82
1:A:406:LEU:HD13	1:A:411:VAL:HB	1.60	0.82
15:O:246:ASN:OD1	15:O:247:GLU:N	2.11	0.82
3:C:55:ASP:HA	3:C:299:ILE:CA	2.07	0.82
7:G:158:LYS:HD3	15:O:105:ASN:CB	2.09	0.82
1:A:437:PHE:CZ	1:A:456:VAL:HG21	2.14	0.82
4:D:25:THR:HB	6:F:59:GLN:NE2	1.94	0.82
3:C:55:ASP:CA	3:C:299:ILE:HA	2.08	0.82
1:A:1:MET:HG2	2:B:1098:TYR:CE2	2.12	0.82
1:A:556:ALA:CB	15:O:246:ASN:ND2	2.41	0.82
4:D:95:ASP:OD2	7:G:150:HIS:HA	1.80	0.82
15:O:245:GLN:HG3	15:O:378:THR:CA	2.05	0.82
4:D:25:THR:CA	6:F:59:GLN:CG	2.57	0.82
7:G:158:LYS:NZ	15:O:108:GLU:HG2	1.95	0.82
4:D:25:THR:HB	6:F:59:GLN:CD	2.00	0.81
1:A:863:ASN:HD22	9:I:67:VAL:HA	1.45	0.81
15:O:386:PHE:CD2	15:O:606:MET:CE	2.62	0.81
15:O:457:ARG:C	15:O:460:GLU:HB2	2.01	0.81
2:B:472:SER:HB3	2:B:476:LEU:CD1	2.11	0.81
2:B:776:ILE:HB	2:B:1026:ILE:HD13	1.60	0.81
15:O:162:PHE:HA	15:O:214:ASN:CB	2.09	0.81
15:O:383:TYR:CD2	15:O:597:LEU:HD22	2.15	0.81
1:A:50:TYR:HE1	1:A:368:ARG:O	1.64	0.81
15:O:237:ILE:CG2	15:O:381:ILE:CD1	2.57	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:454:VAL:HA	15:O:514:PHE:CE2	2.15	0.81
1:A:1011:VAL:HG13	1:A:1201:THR:O	1.80	0.81
1:A:782:ASP:CG	1:A:931:SER:O	2.18	0.81
1:A:1316:VAL:HG21	1:A:1498:ILE:HA	1.63	0.81
4:D:80:THR:HG21	15:O:227:PHE:CD2	2.16	0.81
3:C:253:PRO:O	14:N:180:PHE:CD1	2.34	0.81
15:O:369:LYS:HE2	15:O:370:THR:CG2	2.10	0.81
3:C:75:VAL:HG12	3:C:221:PRO:CG	2.11	0.81
15:O:458:GLU:HA	15:O:461:VAL:HG21	1.59	0.81
15:O:243:GLU:HA	15:O:246:ASN:HD21	1.46	0.80
1:A:564:PRO:HG2	15:O:371:HIS:ND1	1.97	0.80
1:A:966:LEU:HD22	1:A:997:PHE:HZ	1.44	0.80
12:L:34:CYS:HB3	12:L:51:CYS:SG	2.21	0.80
15:O:387:HIS:HB2	15:O:606:MET:SD	2.21	0.80
1:A:1004:GLU:HA	1:A:1007:ILE:HD12	1.64	0.80
2:B:208:VAL:HG23	2:B:401:GLU:HG2	1.64	0.80
3:C:57:ILE:HA	3:C:297:HIS:CA	2.05	0.80
4:D:92:ILE:CG2	4:D:96:PHE:CZ	2.63	0.80
1:A:1000:MET:HG2	2:B:520:LEU:HD23	1.62	0.80
3:C:56:LEU:HD12	3:C:300:PHE:HE1	1.46	0.80
4:D:28:PRO:HD2	7:G:24:VAL:HG13	1.62	0.80
3:C:37:LYS:HD2	11:K:130:VAL:CG2	2.11	0.80
15:O:240:ILE:HG21	15:O:332:LEU:CG	2.11	0.80
7:G:141:SER:HA	15:O:138:TYR:OH	1.82	0.80
7:G:158:LYS:CD	15:O:105:ASN:CG	2.48	0.80
3:C:75:VAL:HG21	3:C:221:PRO:HD2	1.64	0.80
15:O:166:ILE:CD1	15:O:213:SER:OG	2.30	0.80
6:F:75:PRO:CG	6:F:78:GLN:HB2	2.05	0.79
1:A:996:TYR:O	1:A:1000:MET:HG3	1.83	0.79
1:A:478:TYR:CE1	2:B:1049:THR:HG23	2.16	0.79
3:C:71:MET:HE1	3:C:302:VAL:HG22	1.64	0.79
1:A:1655:ASP:HB2	6:F:135:ARG:HB3	1.65	0.79
3:C:31:TRP:HB2	11:K:82:LYS:HD2	1.59	0.79
1:A:403:LEU:CD1	1:A:419:ILE:HG21	2.12	0.79
15:O:234:ILE:HG21	15:O:371:HIS:CD2	2.18	0.79
4:D:25:THR:CB	6:F:59:GLN:NE2	2.46	0.79
15:O:436:ARG:O	15:O:440:ILE:HG13	1.82	0.79
1:A:401:ASP:O	1:A:405:LYS:CB	2.31	0.79
1:A:401:ASP:OD2	1:A:405:LYS:CE	2.31	0.79
15:O:129:PRO:HG2	15:O:132:THR:HB	1.63	0.79
2:B:480:GLN:N	2:B:480:GLN:OE1	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:584:GLN:OE1	15:O:584:GLN:N	2.11	0.78
1:A:953:GLU:HA	1:A:1205:PHE:CD2	2.18	0.78
1:A:638:PRO:HA	2:B:1090:ASP:OD2	1.82	0.78
2:B:42:VAL:HG12	2:B:46:ILE:CG1	2.14	0.78
3:C:253:PRO:CB	14:N:180:PHE:HD1	1.95	0.78
2:B:566:TYR:HD2	13:M:73:SER:OG	1.66	0.78
15:O:243:GLU:O	15:O:246:ASN:OD1	1.99	0.78
15:O:372:VAL:C	15:O:374:PRO:HD2	2.04	0.78
15:O:478:GLN:NE2	15:O:592:PHE:HZ	1.81	0.78
1:A:249:THR:OG1	1:A:435:ASN:ND2	2.16	0.78
2:B:75:ASP:HB3	2:B:440:PHE:CZ	2.17	0.78
1:A:1348:VAL:HG11	2:B:268:GLU:HB2	1.66	0.78
15:O:174:ASP:CA	15:O:177:LYS:HE2	2.12	0.78
3:C:50:ARG:O	3:C:303:GLU:HA	1.84	0.78
1:A:1344:ILE:HG22	2:B:333:LYS:HB3	1.66	0.78
3:C:75:VAL:CG2	3:C:221:PRO:HD2	2.14	0.78
4:D:23:HIS:CD2	6:F:58:PHE:CE2	2.71	0.78
15:O:242:VAL:CA	15:O:378:THR:HG21	2.14	0.78
15:O:373:LEU:CD1	15:O:416:LYS:HG3	2.13	0.78
1:A:1604:GLU:O	1:A:1612:LYS:HE2	1.83	0.78
2:B:934:ILE:HG22	3:C:72:ILE:HB	1.66	0.78
15:O:129:PRO:HG2	15:O:132:THR:CB	2.14	0.78
15:O:430:ARG:NH2	15:O:596:PRO:CD	2.44	0.78
4:D:28:PRO:CG	7:G:24:VAL:CG1	2.62	0.77
2:B:68:ILE:HD11	2:B:414:LYS:HG3	1.66	0.77
2:B:1043:LYS:HD3	2:B:1063:ARG:NH2	1.97	0.77
1:A:1344:ILE:HG22	2:B:333:LYS:CB	2.15	0.77
7:G:154:ASN:HD21	15:O:182:MET:HE3	1.48	0.77
1:A:1:MET:HB2	2:B:1098:TYR:CG	2.19	0.77
1:A:475:ARG:CZ	2:B:1061:LYS:HB2	2.14	0.77
2:B:467:THR:HB	2:B:469:ASN:ND2	2.00	0.77
15:O:186:SER:O	15:O:190:ILE:HG22	1.84	0.77
15:O:414:ALA:O	15:O:418:ILE:HD12	1.85	0.77
1:A:1028:GLU:HG3	1:A:1029:GLY:N	2.00	0.77
15:O:234:ILE:CG2	15:O:371:HIS:CD2	2.66	0.77
15:O:386:PHE:CD2	15:O:606:MET:HE1	2.20	0.77
1:A:1603:MET:CE	1:A:1615:TYR:CD2	2.68	0.76
1:A:1662:ASN:CA	7:G:101:SER:HB2	2.13	0.76
3:C:75:VAL:HG12	3:C:221:PRO:HG3	1.63	0.76
9:I:60:LEU:HA	9:I:63:LYS:HG3	1.65	0.76
15:O:359:GLY:O	15:O:363:THR:HG22	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:425:GLY:HA2	15:O:483:ILE:CD1	2.13	0.76
2:B:878:GLU:OE2	2:B:909:ARG:NH1	2.17	0.76
15:O:174:ASP:O	15:O:177:LYS:HG2	1.85	0.76
15:O:240:ILE:HB	15:O:332:LEU:HD13	1.66	0.76
1:A:437:PHE:HZ	1:A:456:VAL:CG2	1.98	0.76
3:C:56:LEU:CD1	3:C:300:PHE:HE1	1.95	0.76
15:O:360:VAL:O	15:O:364:LEU:HG	1.83	0.76
3:C:75:VAL:CG1	3:C:221:PRO:HD3	2.10	0.76
2:B:328:GLN:HE22	13:M:109:ARG:HH21	1.31	0.76
15:O:62:ASP:HB3	15:O:67:ASP:OD2	1.86	0.76
1:A:438:ILE:HG23	2:B:1192:MET:HG2	1.68	0.76
3:C:55:ASP:OD1	3:C:299:ILE:CG1	2.34	0.76
15:O:432:LYS:CB	15:O:609:TYR:C	2.54	0.76
15:O:484:PHE:CE1	15:O:502:LEU:CD1	2.69	0.76
1:A:502:ALA:HB1	1:A:581:ILE:HG22	1.64	0.76
2:B:1069:ILE:HG22	2:B:1070:ARG:H	1.50	0.76
1:A:641:GLU:HB2	6:F:99:LEU:HD13	1.68	0.76
15:O:158:LEU:CD2	15:O:172:HIS:CD2	2.67	0.76
1:A:478:TYR:CE2	2:B:1049:THR:CG2	2.68	0.76
15:O:454:VAL:CA	15:O:514:PHE:CZ	2.67	0.76
3:C:131:THR:HG23	3:C:209:ILE:HG23	1.68	0.76
7:G:159:LYS:H	15:O:105:ASN:HD22	1.32	0.76
1:A:1055:ILE:CG2	1:A:1060:GLU:HG3	2.16	0.76
3:C:70:ILE:HD11	11:K:71:THR:HG21	1.67	0.76
7:G:154:ASN:OD1	15:O:183:ILE:HG12	1.85	0.76
1:A:1052:GLY:O	5:E:205:SER:HB2	1.85	0.76
1:A:1050:TYR:CD1	1:A:1185:VAL:HG11	2.20	0.75
1:A:878:ARG:NE	9:I:67:VAL:CG1	2.48	0.75
2:B:769:PHE:HE1	2:B:798:PHE:CZ	2.03	0.75
15:O:219:ARG:HH22	15:O:360:VAL:HG21	1.47	0.75
15:O:371:HIS:C	15:O:374:PRO:HD2	2.06	0.75
6:F:66:ARG:NH2	7:G:90:LEU:HD13	2.01	0.75
15:O:359:GLY:HA2	15:O:362:ASN:ND2	2.01	0.75
1:A:1019:LEU:CD1	1:A:1227:MET:HG3	2.17	0.75
15:O:166:ILE:HD13	15:O:213:SER:OG	1.86	0.75
1:A:891:ILE:HD13	9:I:71:LEU:HB2	1.68	0.75
1:A:1048:PHE:HE2	5:E:211:TYR:N	1.83	0.75
15:O:428:ILE:HD12	15:O:439:ILE:CG2	2.16	0.75
1:A:1048:PHE:CE2	5:E:211:TYR:N	2.53	0.75
2:B:42:VAL:HB	2:B:46:ILE:HD11	1.51	0.75
2:B:207:ILE:CG1	2:B:503:VAL:HG22	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:131:THR:HG22	3:C:208:CYS:O	1.86	0.75
4:D:44:ILE:HG21	4:D:90:LYS:HE3	1.69	0.75
15:O:230:TRP:CE2	15:O:364:LEU:HD21	2.20	0.75
7:G:154:ASN:HD21	15:O:182:MET:HE1	1.51	0.75
15:O:198:PHE:CE2	15:O:232:LEU:HG	2.22	0.75
15:O:342:HIS:NE2	15:O:346:GLN:NE2	2.34	0.75
3:C:31:TRP:CB	11:K:82:LYS:CD	2.51	0.74
1:A:437:PHE:CE1	1:A:456:VAL:CG2	2.58	0.74
15:O:101:SER:HB3	15:O:142:ILE:HD12	1.69	0.74
15:O:484:PHE:CE1	15:O:502:LEU:HD12	2.21	0.74
15:O:440:ILE:CG2	15:O:491:PHE:HE1	2.01	0.74
1:A:1348:VAL:CG1	2:B:268:GLU:HB2	2.18	0.74
3:C:45:SER:CB	3:C:271:ARG:NH2	2.49	0.74
4:D:96:PHE:HE1	7:G:150:HIS:CG	2.04	0.74
1:A:1575:ILE:HG12	9:I:122:ARG:HH12	1.52	0.74
15:O:241:ASP:OD1	15:O:378:THR:CG2	2.33	0.74
1:A:556:ALA:HB1	15:O:243:GLU:OE2	1.88	0.74
3:C:64:ALA:O	3:C:227:TYR:HE2	1.69	0.74
15:O:369:LYS:HE2	15:O:370:THR:HG23	1.67	0.74
4:D:25:THR:HG22	6:F:59:GLN:NE2	1.93	0.74
15:O:143:LEU:HD11	15:O:150:TRP:CD1	2.22	0.74
15:O:374:PRO:HG2	15:O:375:THR:HG23	1.69	0.74
15:O:484:PHE:HE1	15:O:502:LEU:HD12	1.52	0.74
3:C:82:TYR:CD1	12:L:68:GLU:HG3	2.22	0.74
15:O:238:ILE:HD11	15:O:371:HIS:HB3	1.70	0.74
15:O:390:GLN:HE22	15:O:432:LYS:N	1.86	0.74
15:O:421:LEU:CD1	15:O:476:ALA:HB2	2.18	0.74
2:B:401:GLU:HG3	2:B:402:VAL:N	2.03	0.74
15:O:407:SER:HB2	15:O:408:PHE:CD1	2.22	0.74
1:A:411:VAL:HG22	1:A:412:SER:H	1.52	0.73
2:B:42:VAL:HB	2:B:46:ILE:HD12	1.59	0.73
2:B:518:ARG:NH2	2:B:537:SER:O	2.21	0.73
15:O:371:HIS:O	15:O:374:PRO:HD2	1.88	0.73
4:D:37:LEU:HD22	4:D:97:LYS:HE3	1.70	0.73
1:A:1048:PHE:HB2	5:E:208:TYR:OH	1.89	0.73
15:O:245:GLN:HA	15:O:245:GLN:HE21	1.51	0.73
15:O:423:TYR:CD1	15:O:594:TYR:CE2	2.72	0.73
1:A:527:PRO:O	1:A:580:HIS:CE1	2.41	0.73
3:C:64:ALA:C	3:C:227:TYR:CE2	2.60	0.73
4:D:25:THR:HB	6:F:59:GLN:CG	2.19	0.73
15:O:432:LYS:HG2	15:O:608:GLU:C	2.07	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:478:LEU:HD13	2:B:484:TYR:HE1	1.50	0.73
3:C:55:ASP:OD1	3:C:299:ILE:HG23	1.88	0.73
2:B:1020:GLU:HG2	3:C:61:THR:HG21	1.70	0.73
3:C:253:PRO:O	14:N:180:PHE:CE1	2.41	0.73
7:G:143:SER:OG	15:O:101:SER:O	2.06	0.73
7:G:144:HIS:NE2	15:O:145:SER:CB	2.51	0.73
15:O:120:ILE:CD1	15:O:150:TRP:CE3	2.71	0.73
15:O:194:LEU:CD2	15:O:225:LEU:HD11	2.19	0.73
7:G:28:ILE:CG2	7:G:29:ASP:H	1.89	0.73
15:O:201:LYS:HD3	15:O:239:SER:OG	1.88	0.73
15:O:241:ASP:C	15:O:378:THR:HG21	2.08	0.73
15:O:373:LEU:HD11	15:O:416:LYS:HG2	1.65	0.73
15:O:237:ILE:HG22	15:O:381:ILE:HB	1.71	0.73
15:O:356:GLU:O	15:O:360:VAL:HG23	1.88	0.73
3:C:56:LEU:HG	3:C:300:PHE:HD1	1.53	0.73
4:D:92:ILE:HG12	7:G:152:ALA:CB	2.16	0.73
1:A:1305:GLU:OE2	9:I:63:LYS:NZ	2.16	0.72
2:B:552:SER:O	2:B:647:SER:N	2.21	0.72
15:O:152:GLN:HG3	15:O:193:TYR:OH	1.89	0.72
15:O:156:MET:SD	15:O:197:PHE:CE2	2.82	0.72
15:O:348:THR:CG2	15:O:351:SER:HB3	2.19	0.72
1:A:50:TYR:CE1	1:A:368:ARG:O	2.42	0.72
15:O:162:PHE:O	15:O:210:ASN:C	2.27	0.72
15:O:234:ILE:HG22	15:O:371:HIS:HD2	1.53	0.72
15:O:447:THR:O	15:O:450:LEU:CB	2.33	0.72
15:O:390:GLN:HE21	15:O:432:LYS:H	1.38	0.72
1:A:509:GLU:CD	1:A:579:ARG:HE	1.92	0.72
2:B:207:ILE:CD1	2:B:503:VAL:CG2	2.68	0.72
15:O:352:LEU:CA	15:O:358:VAL:HG23	2.19	0.72
4:D:23:HIS:CD2	6:F:58:PHE:CZ	2.78	0.72
1:A:413:LEU:CB	1:A:417:ARG:HH21	2.03	0.72
14:N:85:HIS:CE1	14:N:141:GLU:CD	2.60	0.72
15:O:488:HIS:CD2	15:O:489:ASN:OD1	2.42	0.72
1:A:1056:ASP:OD1	1:A:1179:ILE:HD13	1.90	0.72
2:B:938:PHE:CE1	3:C:68:ARG:CZ	2.73	0.72
2:B:938:PHE:CZ	3:C:68:ARG:HD2	2.24	0.72
1:A:878:ARG:HE	9:I:67:VAL:HG12	1.53	0.72
2:B:207:ILE:CD1	2:B:503:VAL:HG21	2.20	0.72
3:C:56:LEU:CB	3:C:298:PHE:HB2	2.17	0.72
4:D:23:HIS:HD2	6:F:58:PHE:CZ	2.07	0.72
15:O:225:LEU:HD13	15:O:225:LEU:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:TYR:CA	2:B:1048:SER:CA	2.34	0.71
3:C:45:SER:CB	3:C:271:ARG:HH22	2.03	0.71
12:L:68:GLU:HG2	12:L:69:ALA:N	2.01	0.71
15:O:432:LYS:HB3	15:O:609:TYR:HA	0.81	0.71
1:A:1055:ILE:CD1	1:A:1063:MET:CE	2.67	0.71
2:B:152:LEU:HD13	2:B:443:LYS:HG3	1.71	0.71
3:C:54:PHE:O	3:C:299:ILE:HA	1.90	0.71
15:O:158:LEU:HD22	15:O:172:HIS:HA	1.71	0.71
1:A:411:VAL:HG22	1:A:412:SER:N	2.05	0.71
1:A:1003:ARG:HD2	2:B:520:LEU:H	1.56	0.71
1:A:527:PRO:O	1:A:580:HIS:HE1	1.73	0.71
2:B:1069:ILE:HD12	2:B:1069:ILE:N	2.05	0.71
2:B:281:CYS:HA	2:B:323:ARG:HD2	1.72	0.71
15:O:361:PHE:CE1	15:O:365:THR:HG21	2.24	0.71
1:A:524:ILE:O	1:A:554:ARG:NH1	2.23	0.71
2:B:1069:ILE:HG22	2:B:1070:ARG:N	2.03	0.71
3:C:52:ALA:O	3:C:301:ASN:OD1	2.07	0.71
1:A:478:TYR:CD1	2:B:1048:SER:HB2	2.25	0.71
1:A:1048:PHE:CD2	5:E:210:SER:HA	2.26	0.71
4:D:92:ILE:CG1	7:G:152:ALA:HB2	2.16	0.71
15:O:128:LEU:HB3	15:O:129:PRO:CD	2.21	0.71
15:O:163:ILE:HA	15:O:211:TYR:N	1.97	0.71
1:A:468:ARG:NE	1:A:1021:ARG:HH12	1.89	0.71
1:A:1038:ILE:HD11	1:A:1050:TYR:HA	1.71	0.71
3:C:62:SER:HB2	11:K:74:ASN:CG	2.10	0.71
1:A:83:VAL:CG2	1:A:427:PHE:HE2	2.03	0.71
2:B:211:ARG:NH2	2:B:239:VAL:HG21	2.06	0.71
3:C:31:TRP:CE3	11:K:82:LYS:CG	2.69	0.71
3:C:70:ILE:HD11	11:K:71:THR:HG23	1.71	0.71
6:F:106:PRO:HG2	7:G:55:GLU:HG3	1.73	0.71
15:O:352:LEU:O	15:O:358:VAL:CG2	2.39	0.71
1:A:990:ILE:HB	1:A:994:GLU:CB	2.21	0.70
2:B:1165:ASN:N	2:B:1165:ASN:OD1	2.24	0.70
2:B:470:LEU:HB2	2:B:484:TYR:CE2	2.26	0.70
3:C:54:PHE:CE2	3:C:300:PHE:CG	2.78	0.70
15:O:198:PHE:CE1	15:O:236:LYS:HG3	2.25	0.70
15:O:152:GLN:HG2	15:O:193:TYR:HH	1.53	0.70
15:O:459:GLU:O	15:O:463:GLN:CG	2.37	0.70
3:C:64:ALA:CB	3:C:298:PHE:CE2	2.73	0.70
9:I:2:SER:HB2	9:I:11:LEU:HD21	1.72	0.70
15:O:373:LEU:N	15:O:374:PRO:CD	2.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:447:THR:CG2	15:O:480:LEU:HD22	2.21	0.70
1:A:891:ILE:HD12	9:I:71:LEU:HB2	1.71	0.70
3:C:71:MET:HE1	3:C:225:ALA:CB	2.21	0.70
7:G:158:LYS:HD3	15:O:105:ASN:HB3	1.72	0.70
1:A:438:ILE:HG23	2:B:1192:MET:HE3	1.73	0.70
2:B:894:LYS:N	12:L:54:ARG:NH2	2.34	0.70
7:G:159:LYS:H	15:O:105:ASN:ND2	1.89	0.70
15:O:225:LEU:O	15:O:227:PHE:N	2.24	0.70
4:D:80:THR:HG21	15:O:227:PHE:HD2	1.56	0.70
15:O:428:ILE:O	15:O:487:ARG:NE	2.24	0.70
1:A:1246:VAL:O	1:A:1517:ARG:NH2	2.25	0.70
15:O:373:LEU:O	15:O:373:LEU:HD12	1.91	0.70
1:A:436:ALA:HB1	1:A:443:ALA:CB	2.19	0.70
1:A:478:TYR:CE2	2:B:1049:THR:HG22	2.27	0.70
15:O:426:SER:HG	15:O:594:TYR:HB2	1.54	0.70
3:C:223:SER:O	3:C:224:THR:HB	1.92	0.70
2:B:291:GLY:HA3	2:B:375:LEU:HD13	1.74	0.70
1:A:1055:ILE:CD1	1:A:1063:MET:HE3	2.20	0.69
1:A:436:ALA:O	1:A:440:SER:HA	1.91	0.69
2:B:64:GLY:O	2:B:68:ILE:HG13	1.92	0.69
3:C:54:PHE:N	3:C:300:PHE:O	2.21	0.69
13:M:38:PHE:HB3	13:M:53:LEU:HD11	1.73	0.69
15:O:369:LYS:HB3	15:O:369:LYS:NZ	2.04	0.69
1:A:1348:VAL:HG23	2:B:268:GLU:O	1.91	0.69
1:A:406:LEU:CD1	1:A:411:VAL:CB	2.71	0.69
1:A:438:ILE:CG2	2:B:1192:MET:HG2	2.23	0.69
1:A:782:ASP:OD1	1:A:931:SER:O	2.10	0.69
1:A:1049:MET:HG2	1:A:1050:TYR:H	1.55	0.69
2:B:211:ARG:CG	2:B:401:GLU:OE1	2.39	0.69
2:B:42:VAL:HG12	2:B:46:ILE:HG13	1.73	0.69
1:A:99:ARG:O	1:A:109:ARG:NH2	2.24	0.69
2:B:300:SER:OG	9:I:49:THR:HG22	1.92	0.69
7:G:156:SER:CB	15:O:146:SER:HA	2.22	0.69
15:O:220:GLY:O	15:O:221:TYR:CD1	2.46	0.69
1:A:1:MET:CA	2:B:1098:TYR:CD1	2.75	0.69
4:D:99:LEU:HB3	4:D:100:PRO:CD	2.22	0.69
15:O:369:LYS:O	15:O:373:LEU:CB	2.41	0.69
3:C:31:TRP:CG	11:K:82:LYS:CD	2.76	0.69
1:A:478:TYR:CA	2:B:1047:ARG:O	2.41	0.69
3:C:41:GLU:HB3	3:C:57:ILE:HG22	1.74	0.69
3:C:253:PRO:HB2	14:N:180:PHE:CB	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:VAL:HG13	1:A:994:GLU:OE2	1.92	0.69
1:A:1573:TYR:O	9:I:122:ARG:NH2	2.26	0.69
15:O:417:LYS:HD3	15:O:472:HIS:HE1	1.57	0.69
1:A:1348:VAL:HG23	2:B:269:TYR:HA	1.75	0.68
4:D:48:GLU:CG	4:D:86:ILE:CD1	2.71	0.68
2:B:1002:LYS:HD2	14:N:166:LEU:HB2	1.74	0.68
2:B:769:PHE:CD1	2:B:798:PHE:CE1	2.68	0.68
4:D:25:THR:CB	6:F:59:GLN:CG	2.71	0.68
15:O:174:ASP:HA	15:O:177:LYS:CE	2.22	0.68
2:B:566:TYR:HB3	13:M:74:ASN:OD1	1.94	0.68
15:O:390:GLN:CB	15:O:609:TYR:CD1	2.76	0.68
1:A:432:ASN:HD21	1:A:444:GLN:H	1.38	0.68
3:C:71:MET:CE	3:C:225:ALA:CB	2.71	0.68
3:C:64:ALA:HB1	3:C:227:TYR:CE2	2.29	0.68
15:O:430:ARG:HH21	15:O:596:PRO:HD3	1.55	0.68
2:B:934:ILE:CG2	3:C:73:SER:HB3	2.24	0.68
3:C:55:ASP:HB3	3:C:297:HIS:CD2	2.28	0.68
2:B:1043:LYS:HG3	2:B:1063:ARG:NE	2.09	0.68
4:D:80:THR:CG2	15:O:227:PHE:CD2	2.76	0.68
15:O:241:ASP:CG	15:O:380:SER:HB2	2.14	0.68
15:O:430:ARG:HH22	15:O:596:PRO:HD3	1.58	0.68
1:A:35:PRO:HA	1:A:390:LEU:CD1	2.24	0.68
3:C:54:PHE:O	3:C:299:ILE:C	2.32	0.68
1:A:209:THR:HG21	5:E:173:SER:OG	1.93	0.68
15:O:343:VAL:CG1	15:O:388:VAL:CG2	2.71	0.68
2:B:207:ILE:HD11	2:B:503:VAL:CG1	2.25	0.68
3:C:52:ALA:O	3:C:301:ASN:CG	2.31	0.68
15:O:237:ILE:CB	15:O:381:ILE:CD1	2.57	0.68
2:B:938:PHE:CE1	3:C:68:ARG:NE	2.61	0.67
1:A:572:THR:HA	7:G:52:MET:CE	2.23	0.67
15:O:368:PHE:O	15:O:372:VAL:HG23	1.94	0.67
3:C:57:ILE:HD12	3:C:297:HIS:CE1	2.29	0.67
15:O:474:TYR:HB3	15:O:520:CYS:SG	2.33	0.67
2:B:566:TYR:CE2	13:M:70:SER:HA	2.30	0.67
3:C:57:ILE:CD1	3:C:297:HIS:ND1	2.56	0.67
5:E:76:GLY:HA3	5:E:106:GLN:HB2	1.76	0.67
15:O:458:GLU:HG3	15:O:514:PHE:CZ	2.28	0.67
3:C:71:MET:HE1	3:C:225:ALA:HB2	1.75	0.67
15:O:66:ASN:N	15:O:66:ASN:HD22	1.89	0.67
1:A:436:ALA:HB2	1:A:443:ALA:HB1	1.66	0.67
1:A:381:SER:HB2	1:A:453:ILE:CG2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1043:LYS:CG	2:B:1063:ARG:CZ	2.68	0.67
15:O:241:ASP:C	15:O:378:THR:CG2	2.63	0.67
15:O:431:ALA:HB1	15:O:434:LEU:CD1	2.20	0.67
1:A:81:LEU:HB2	1:A:358:ASP:O	1.94	0.67
4:D:48:GLU:HG2	4:D:86:ILE:HD11	1.76	0.67
1:A:1006:LEU:HB3	2:B:539:CYS:SG	2.34	0.67
15:O:471:LYS:HB2	15:O:585:PHE:CZ	2.25	0.67
1:A:1344:ILE:HG21	2:B:333:LYS:HG3	1.76	0.67
3:C:71:MET:O	3:C:222:VAL:HG21	1.94	0.67
1:A:1556:GLU:OE2	5:E:212:ARG:NH1	2.28	0.67
15:O:371:HIS:O	15:O:374:PRO:HG2	1.95	0.67
1:A:1011:VAL:C	1:A:1201:THR:HG21	2.15	0.67
1:A:356:PHE:C	1:A:357:MET:HG3	2.14	0.67
1:A:406:LEU:HD12	1:A:406:LEU:O	1.94	0.67
3:C:84:TYR:HD2	12:L:66:GLN:HB2	1.59	0.67
15:O:108:GLU:HB2	15:O:147:ILE:HD11	1.76	0.67
1:A:1027:LEU:O	1:A:1028:GLU:HG2	1.95	0.66
2:B:470:LEU:HD22	2:B:484:TYR:OH	1.95	0.66
3:C:253:PRO:CG	14:N:180:PHE:HB3	2.25	0.66
3:C:86:PHE:HE1	12:L:64:LEU:CD1	2.08	0.66
15:O:371:HIS:O	15:O:374:PRO:CG	2.43	0.66
2:B:207:ILE:HD11	2:B:503:VAL:HG11	1.76	0.66
15:O:240:ILE:CG2	15:O:332:LEU:CD1	2.67	0.66
15:O:390:GLN:CD	15:O:609:TYR:HB3	2.15	0.66
1:A:1050:TYR:CE1	1:A:1185:VAL:HG12	2.29	0.66
3:C:131:THR:CG2	3:C:209:ILE:HG23	2.25	0.66
4:D:25:THR:CA	6:F:59:GLN:HG3	2.24	0.66
13:M:101:VAL:HG12	13:M:106:LYS:HG3	1.72	0.66
15:O:390:GLN:HB3	15:O:609:TYR:CD1	2.30	0.66
1:A:113:VAL:HG21	1:A:178:LEU:HD13	1.77	0.66
3:C:223:SER:HB2	3:C:303:GLU:HB3	1.76	0.66
4:D:96:PHE:CE1	7:G:150:HIS:CG	2.83	0.66
1:A:863:ASN:HD22	9:I:67:VAL:CA	2.07	0.66
15:O:240:ILE:CG2	15:O:332:LEU:CD2	2.63	0.66
1:A:437:PHE:O	1:A:455:GLY:HA3	1.96	0.66
7:G:242:VAL:HG21	15:O:183:ILE:CG2	2.26	0.66
15:O:434:LEU:HD12	15:O:434:LEU:N	2.10	0.66
1:A:403:LEU:HD12	1:A:419:ILE:HG21	1.77	0.66
15:O:428:ILE:HG23	15:O:439:ILE:CG2	2.23	0.66
1:A:1000:MET:CG	2:B:520:LEU:HD23	2.26	0.66
1:A:1344:ILE:CG2	2:B:333:LYS:HG3	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ARG:NH1	1:A:230:ARG:O	2.29	0.66
15:O:454:VAL:HG23	15:O:458:GLU:HG3	1.77	0.66
1:A:403:LEU:CD1	1:A:419:ILE:CG2	2.74	0.66
15:O:247:GLU:OE1	15:O:325:ILE:HG13	1.95	0.66
2:B:209:GLN:HG2	2:B:210:ARG:N	2.07	0.65
2:B:209:GLN:O	2:B:401:GLU:N	2.27	0.65
1:A:1000:MET:HG2	2:B:520:LEU:CD2	2.25	0.65
3:C:52:ALA:O	3:C:301:ASN:CA	2.42	0.65
15:O:422:GLN:NE2	15:O:592:PHE:CD2	2.65	0.65
1:A:756:LYS:HD3	9:I:85:LYS:HZ2	1.32	0.65
1:A:478:TYR:CA	2:B:1048:SER:O	2.44	0.65
2:B:300:SER:OG	9:I:49:THR:CG2	2.44	0.65
2:B:711:GLN:HG2	2:B:713:PRO:HD2	1.78	0.65
3:C:230:LEU:CG	3:C:294:VAL:HG21	2.26	0.65
15:O:108:GLU:O	15:O:108:GLU:HG3	1.96	0.65
15:O:146:SER:O	15:O:148:PRO:HD3	1.95	0.65
15:O:219:ARG:HH21	15:O:360:VAL:HG22	1.60	0.65
4:D:48:GLU:HG3	4:D:86:ILE:HD12	1.78	0.65
2:B:891:GLU:HA	12:L:54:ARG:NE	2.12	0.65
3:C:272:LYS:HG2	14:N:175:TYR:CD1	2.32	0.65
15:O:458:GLU:CG	15:O:514:PHE:CZ	2.79	0.65
1:A:1034:TYR:CD1	1:A:1181:PRO:HG2	2.32	0.65
1:A:799:GLU:HG3	1:A:1062:HIS:CE1	2.32	0.65
2:B:566:TYR:CD2	13:M:73:SER:OG	2.48	0.65
2:B:938:PHE:CZ	3:C:68:ARG:CD	2.80	0.65
4:D:99:LEU:HB3	4:D:100:PRO:HD3	1.78	0.65
15:O:343:VAL:CG1	15:O:388:VAL:HG23	2.27	0.65
1:A:406:LEU:CD1	1:A:411:VAL:CG2	2.74	0.65
2:B:341:SER:OG	2:B:343:ASP:OD1	2.13	0.65
4:D:25:THR:HG21	6:F:59:GLN:NE2	2.12	0.65
1:A:502:ALA:CB	1:A:581:ILE:CG2	2.63	0.65
3:C:222:VAL:C	3:C:224:THR:N	2.49	0.65
15:O:241:ASP:CB	15:O:380:SER:HB2	2.26	0.65
15:O:488:HIS:NE2	15:O:489:ASN:OD1	2.29	0.65
1:A:1651:THR:OG1	2:B:1085:SER:OG	2.14	0.65
1:A:782:ASP:CG	1:A:783:LYS:N	2.50	0.65
3:C:59:ILE:HG23	3:C:298:PHE:HE1	1.54	0.65
7:G:144:HIS:NE2	15:O:145:SER:HB2	2.12	0.65
15:O:241:ASP:HA	15:O:380:SER:HB2	1.78	0.65
1:A:1053:ASP:O	1:A:1054:ALA:HB3	1.97	0.65
1:A:406:LEU:HD11	1:A:411:VAL:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ILE:HG23	2:B:1192:MET:CE	2.26	0.65
2:B:915:ASP:OD1	2:B:1038:HIS:HD2	1.78	0.65
2:B:923:GLN:NE2	2:B:953:ALA:O	2.30	0.65
15:O:343:VAL:HG11	15:O:388:VAL:CG2	2.27	0.65
1:A:953:GLU:C	1:A:1205:PHE:CB	2.66	0.64
7:G:156:SER:HB2	15:O:146:SER:HA	1.78	0.64
15:O:417:LYS:CD	15:O:472:HIS:HE1	2.10	0.64
15:O:428:ILE:HD12	15:O:439:ILE:HD12	1.79	0.64
1:A:1575:ILE:HG13	9:I:122:ARG:HH12	1.60	0.64
15:O:374:PRO:CG	15:O:375:THR:HG23	2.27	0.64
1:A:1262:LEU:CD2	1:A:1497:ILE:HG12	2.28	0.64
1:A:834:ARG:NH2	2:B:994:ASP:OD1	2.30	0.64
3:C:54:PHE:CE1	3:C:300:PHE:HB3	2.31	0.64
7:G:159:LYS:HB3	15:O:103:ASN:OD1	1.98	0.64
2:B:1120:ILE:HD12	15:O:117:GLN:HE22	1.63	0.64
15:O:510:VAL:HG13	15:O:517:LEU:HD11	1.79	0.64
2:B:623:ASP:O	2:B:648:ARG:NH1	2.25	0.64
1:A:1344:ILE:CD1	2:B:329:TYR:CE2	2.71	0.64
1:A:1023:LEU:HD23	1:A:1598:PHE:CD1	2.32	0.64
2:B:469:ASN:HA	2:B:481:VAL:O	1.97	0.64
3:C:86:PHE:CE1	12:L:64:LEU:CD1	2.79	0.64
1:A:1036:ASN:HB3	1:A:1049:MET:HG3	1.78	0.64
1:A:413:LEU:O	1:A:417:ARG:NH2	2.30	0.64
1:A:83:VAL:CB	1:A:427:PHE:CE2	2.81	0.64
1:A:480:ALA:CB	2:B:1046:VAL:CG2	2.63	0.64
7:G:144:HIS:NE2	15:O:145:SER:HB3	2.13	0.64
3:C:82:TYR:HE1	12:L:68:GLU:OE1	1.80	0.64
1:A:1038:ILE:CG1	1:A:1049:MET:O	2.44	0.64
1:A:1273:THR:HG23	9:I:48:VAL:HG22	1.79	0.64
2:B:699:ILE:HD13	2:B:760:TYR:CE1	2.32	0.64
15:O:240:ILE:CG2	15:O:332:LEU:CG	2.76	0.64
1:A:1055:ILE:CG2	1:A:1063:MET:SD	2.85	0.64
1:A:995:TYR:O	1:A:999:CYS:HB2	1.98	0.64
3:C:73:SER:O	3:C:214:GLY:N	2.31	0.64
5:E:20:LYS:HE2	5:E:34:GLU:HG2	1.80	0.64
15:O:170:VAL:HG13	15:O:171:CYS:N	2.12	0.64
1:A:478:TYR:OH	2:B:1049:THR:HG21	1.97	0.64
3:C:54:PHE:O	3:C:299:ILE:CA	2.45	0.64
1:A:399:LEU:CD2	1:A:423:LEU:HA	2.28	0.64
1:A:953:GLU:C	1:A:1205:PHE:HB3	2.18	0.64
1:A:1021:ARG:HD3	2:B:1073:GLU:OE1	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:368:PHE:CE2	15:O:382:GLN:HA	2.33	0.64
15:O:383:TYR:CE2	15:O:597:LEU:HD22	2.33	0.64
1:A:1055:ILE:HD12	1:A:1063:MET:HE3	1.74	0.63
4:D:25:THR:CB	6:F:59:GLN:HE21	2.06	0.63
1:A:1322:ILE:HD12	1:A:1457:ILE:HD11	1.79	0.63
8:H:44:VAL:HG22	8:H:48:PRO:HA	1.81	0.63
15:O:454:VAL:HG23	15:O:458:GLU:CG	2.28	0.63
1:A:476:VAL:HG11	2:B:1071:VAL:CG2	2.25	0.63
1:A:478:TYR:N	2:B:1048:SER:C	2.52	0.63
3:C:41:GLU:CB	3:C:57:ILE:CG2	2.70	0.63
1:A:1654:PHE:CE2	6:F:92:ARG:HD3	2.33	0.63
15:O:392:GLN:HB2	15:O:395:LEU:HD22	1.79	0.63
15:O:426:SER:OG	15:O:594:TYR:CA	2.46	0.63
1:A:1026:GLN:HE22	1:A:1603:MET:HA	1.61	0.63
15:O:454:VAL:HG23	15:O:458:GLU:OE2	1.98	0.63
2:B:281:CYS:HA	2:B:323:ARG:CD	2.29	0.63
3:C:75:VAL:CG1	3:C:221:PRO:HD2	2.06	0.63
7:G:141:SER:CB	15:O:138:TYR:CZ	2.81	0.63
1:A:1600:ARG:NE	1:A:1616:GLU:OE1	2.30	0.63
1:A:888:LYS:HE2	9:I:69:THR:HG22	1.79	0.63
2:B:475:GLY:O	2:B:476:LEU:HB2	1.98	0.63
15:O:155:SER:HA	15:O:158:LEU:HD12	1.81	0.63
15:O:379:ARG:CB	15:O:382:GLN:HE22	2.12	0.63
1:A:402:ASP:O	1:A:406:LEU:HD23	1.99	0.63
1:A:401:ASP:OD2	1:A:405:LYS:NZ	2.32	0.63
1:A:408:LYS:HA	1:A:411:VAL:HG11	1.79	0.63
4:D:80:THR:CG2	15:O:227:PHE:CB	2.75	0.63
1:A:1655:ASP:N	6:F:135:ARG:O	2.28	0.63
6:F:70:LYS:HG3	7:G:94:PRO:HB2	1.80	0.63
15:O:373:LEU:N	15:O:374:PRO:HD2	2.14	0.63
1:A:1060:GLU:O	1:A:1060:GLU:HG2	1.98	0.63
4:D:23:HIS:HD2	6:F:58:PHE:CE2	2.16	0.63
7:G:158:LYS:CE	15:O:105:ASN:OD1	2.47	0.63
15:O:245:GLN:HA	15:O:245:GLN:NE2	2.14	0.63
15:O:471:LYS:HG3	15:O:472:HIS:N	2.14	0.63
1:A:436:ALA:O	1:A:440:SER:CA	2.46	0.62
1:A:509:GLU:HG2	1:A:579:ARG:HG2	1.81	0.62
3:C:75:VAL:HG12	3:C:76:PRO:O	1.98	0.62
7:G:142:ALA:O	15:O:102:SER:O	2.16	0.62
12:L:68:GLU:CG	12:L:69:ALA:H	2.05	0.62
1:A:83:VAL:CG2	1:A:427:PHE:HZ	2.01	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:991:LYS:N	1:A:994:GLU:OE1	2.31	0.62
15:O:181:ARG:HH11	15:O:181:ARG:CG	2.12	0.62
1:A:1050:TYR:HB2	1:A:1179:ILE:HG21	1.81	0.62
2:B:42:VAL:CA	2:B:46:ILE:HD12	2.29	0.62
15:O:151:TRP:CZ2	15:O:176:LEU:HD23	2.35	0.62
1:A:572:THR:HA	7:G:52:MET:HE1	1.80	0.62
3:C:41:GLU:O	3:C:57:ILE:HG22	1.99	0.62
15:O:386:PHE:CD2	15:O:606:MET:HE2	2.34	0.62
15:O:98:ASP:OD2	15:O:135:LYS:HD3	1.99	0.62
15:O:225:LEU:C	15:O:225:LEU:HD13	2.19	0.62
15:O:457:ARG:HA	15:O:460:GLU:CB	2.30	0.62
2:B:40:GLU:OE1	2:B:550:ARG:NH2	2.32	0.62
7:G:142:ALA:C	15:O:102:SER:O	2.38	0.62
15:O:447:THR:HA	15:O:450:LEU:HD12	1.80	0.62
1:A:1011:VAL:C	1:A:1201:THR:CG2	2.68	0.62
1:A:406:LEU:HD12	1:A:411:VAL:HB	1.82	0.62
5:E:197:LYS:HD3	5:E:199:ILE:HD11	1.79	0.62
1:A:1028:GLU:CG	1:A:1029:GLY:N	2.62	0.62
1:A:1657:LEU:HD21	6:F:135:ARG:CZ	2.30	0.62
2:B:1043:LYS:HG3	2:B:1063:ARG:CD	2.29	0.62
2:B:554:GLN:HA	2:B:646:HIS:CD2	2.34	0.62
3:C:58:ASN:N	3:C:296:ASN:O	2.30	0.62
15:O:460:GLU:O	15:O:469:ARG:NH1	2.32	0.62
1:A:891:ILE:CD1	9:I:71:LEU:CB	2.77	0.62
3:C:222:VAL:C	3:C:224:THR:H	2.03	0.62
3:C:59:ILE:O	3:C:298:PHE:HE1	1.83	0.62
15:O:343:VAL:HG12	15:O:388:VAL:HG23	1.82	0.62
15:O:435:SER:HB3	15:O:438:GLN:CG	2.23	0.62
3:C:62:SER:CB	11:K:74:ASN:HD21	2.12	0.62
15:O:368:PHE:CE2	15:O:385:MET:HB2	2.34	0.62
15:O:581:THR:HA	15:O:584:GLN:NE2	2.15	0.62
2:B:934:ILE:HG23	3:C:73:SER:HB3	1.82	0.61
3:C:55:ASP:OD2	3:C:299:ILE:HG12	1.97	0.61
4:D:47:LYS:HD2	4:D:82:LEU:HD21	1.82	0.61
15:O:100:LEU:HD22	15:O:107:ILE:HD11	1.82	0.61
15:O:144:CYS:O	15:O:148:PRO:HG3	2.00	0.61
12:L:30:ILE:CD1	12:L:59:ALA:HB2	2.29	0.61
15:O:431:ALA:HB3	15:O:434:LEU:CD1	2.23	0.61
15:O:447:THR:CG2	15:O:480:LEU:CD2	2.79	0.61
15:O:450:LEU:O	15:O:454:VAL:HG12	1.99	0.61
3:C:131:THR:CG2	3:C:208:CYS:O	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:71:MET:CE	3:C:302:VAL:HG22	2.29	0.61
15:O:158:LEU:HB3	15:O:172:HIS:HB3	1.82	0.61
1:A:1025:LYS:HZ2	2:B:1076:ARG:NH1	1.98	0.61
1:A:406:LEU:HD13	1:A:411:VAL:CB	2.27	0.61
2:B:481:VAL:HG12	2:B:481:VAL:O	2.01	0.61
2:B:769:PHE:HE1	2:B:798:PHE:HZ	1.48	0.61
1:A:1662:ASN:N	7:G:101:SER:O	2.32	0.61
7:G:141:SER:HB3	15:O:138:TYR:OH	1.95	0.61
15:O:447:THR:HG22	15:O:480:LEU:CD2	2.28	0.61
1:A:413:LEU:O	1:A:417:ARG:CZ	2.47	0.61
1:A:478:TYR:H	2:B:1048:SER:C	2.03	0.61
2:B:1069:ILE:O	2:B:1070:ARG:HB2	2.00	0.61
6:F:73:ALA:HB2	6:F:143:PHE:CZ	2.36	0.61
15:O:181:ARG:HB2	15:O:181:ARG:NH1	2.12	0.61
15:O:369:LYS:HG3	15:O:406:ILE:HD11	1.83	0.61
15:O:396:MET:SD	15:O:434:LEU:HA	2.41	0.61
1:A:1050:TYR:CB	1:A:1179:ILE:HG21	2.31	0.61
2:B:923:GLN:NE2	2:B:957:ARG:HD2	2.16	0.61
3:C:71:MET:CE	3:C:225:ALA:HB1	2.30	0.61
12:L:30:ILE:HD11	12:L:59:ALA:HB2	1.82	0.61
15:O:67:ASP:OD1	15:O:69:THR:HB	2.00	0.61
1:A:1660:VAL:CG2	7:G:103:LYS:HB2	2.30	0.61
1:A:509:GLU:HG3	1:A:579:ARG:HD3	1.81	0.61
3:C:71:MET:SD	3:C:225:ALA:CB	2.88	0.61
4:D:44:ILE:HD13	4:D:90:LYS:HG3	1.82	0.61
15:O:408:PHE:CE1	15:O:446:LEU:HD13	2.35	0.61
15:O:454:VAL:HG23	15:O:458:GLU:CD	2.20	0.61
1:A:564:PRO:HB2	15:O:371:HIS:CE1	2.36	0.61
15:O:371:HIS:O	15:O:374:PRO:CD	2.49	0.61
15:O:56:VAL:HG21	15:O:99:ILE:HD12	1.82	0.61
1:A:479:ALA:HB2	2:B:1091:ARG:HH22	1.65	0.60
2:B:552:SER:OG	2:B:647:SER:N	2.35	0.60
8:H:25:ARG:NH1	8:H:27:GLU:OE2	2.34	0.60
15:O:457:ARG:O	15:O:460:GLU:CB	2.47	0.60
15:O:467:MET:HG3	15:O:519:PHE:CE2	2.36	0.60
15:O:582:ARG:O	15:O:586:ILE:HG13	2.01	0.60
1:A:932:GLY:O	9:I:125:ASN:ND2	2.34	0.60
1:A:1651:THR:OG1	2:B:1085:SER:CB	2.49	0.60
1:A:1344:ILE:HG22	2:B:333:LYS:CG	2.31	0.60
1:A:1052:GLY:O	5:E:205:SER:CB	2.48	0.60
5:E:93:MET:HG3	5:E:120:ALA:HB1	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:487:ARG:HH11	15:O:487:ARG:CG	2.14	0.60
1:A:799:GLU:OE2	1:A:1062:HIS:HB2	2.01	0.60
2:B:938:PHE:CD1	3:C:68:ARG:CZ	2.83	0.60
1:A:1261:VAL:HG13	1:A:1265:GLU:CD	2.22	0.60
1:A:1261:VAL:HG13	1:A:1265:GLU:OE1	2.01	0.60
2:B:1020:GLU:CG	3:C:61:THR:HG21	2.32	0.60
4:D:80:THR:HG21	15:O:227:PHE:CB	2.28	0.60
3:C:272:LYS:CG	14:N:175:TYR:CE1	2.83	0.60
7:G:143:SER:CB	15:O:101:SER:O	2.48	0.60
1:A:1034:TYR:HA	1:A:1181:PRO:CG	2.32	0.60
2:B:1090:ASP:O	2:B:1095:SER:N	2.34	0.60
1:A:1226:VAL:HG12	1:A:1227:MET:HG2	1.83	0.60
1:A:246:ASP:HB3	1:A:248:PHE:H	1.66	0.60
1:A:996:TYR:HE1	1:A:1000:MET:CE	2.14	0.60
1:A:449:GLY:O	1:A:451:VAL:N	2.34	0.60
2:B:228:SER:HB2	2:B:253:LEU:HD23	1.84	0.60
15:O:241:ASP:OD1	15:O:379:ARG:C	2.39	0.60
1:A:84:PRO:HG2	1:A:318:THR:HG22	1.84	0.60
1:A:477:ASN:O	1:A:478:TYR:HB2	2.01	0.60
2:B:699:ILE:CD1	2:B:760:TYR:CE1	2.85	0.60
1:A:87:ASN:HB2	1:A:357:MET:SD	2.42	0.60
15:O:98:ASP:OD2	15:O:135:LYS:NZ	2.35	0.60
1:A:1026:GLN:OE1	1:A:1603:MET:CB	2.48	0.59
3:C:55:ASP:HB3	3:C:297:HIS:NE2	2.17	0.59
1:A:1008:ASP:O	1:A:1011:VAL:CG2	2.41	0.59
1:A:1034:TYR:HA	1:A:1181:PRO:HG3	1.84	0.59
1:A:1054:ALA:O	1:A:1178:LEU:HD23	2.02	0.59
2:B:1019:GLY:HA3	3:C:65:ASN:CB	2.27	0.59
15:O:198:PHE:CD1	15:O:236:LYS:CE	2.78	0.59
1:A:406:LEU:HD13	1:A:411:VAL:CG2	2.31	0.59
6:F:106:PRO:HG2	7:G:55:GLU:CG	2.30	0.59
1:A:699:CYS:O	1:A:815:ARG:NH1	2.35	0.59
2:B:207:ILE:O	2:B:207:ILE:HG22	2.02	0.59
1:A:1027:LEU:HD21	1:A:1588:MET:HG2	1.84	0.59
1:A:35:PRO:HA	1:A:390:LEU:HD12	1.84	0.59
1:A:878:ARG:HG2	9:I:67:VAL:CG1	2.29	0.59
2:B:211:ARG:HB3	2:B:239:VAL:CG1	2.32	0.59
2:B:551:ILE:HA	2:B:648:ARG:O	2.02	0.59
2:B:566:TYR:HB2	13:M:73:SER:OG	2.03	0.59
4:D:80:THR:OG1	15:O:227:PHE:CD1	2.55	0.59
5:E:55:ARG:NH2	5:E:113:GLN:OE1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:PHE:CE2	8:H:141:TYR:HE2	2.21	0.59
15:O:374:PRO:HB2	15:O:375:THR:HG23	1.85	0.59
15:O:390:GLN:HB2	15:O:609:TYR:CD1	2.37	0.59
1:A:509:GLU:O	1:A:576:LYS:HA	2.03	0.59
1:A:863:ASN:ND2	9:I:68:LYS:H	2.01	0.59
15:O:101:SER:HB3	15:O:142:ILE:CD1	2.33	0.59
1:A:516:ILE:HG21	15:O:376:TYR:CZ	2.38	0.59
1:A:581:ILE:HG13	1:A:582:LYS:H	1.68	0.59
2:B:829:ASN:N	2:B:829:ASN:OD1	2.36	0.59
2:B:328:GLN:NE2	13:M:109:ARG:HH21	1.99	0.59
2:B:110:ASN:O	2:B:112:GLY:N	2.35	0.59
2:B:209:GLN:O	2:B:401:GLU:HG2	2.03	0.59
3:C:231:PRO:HG2	3:C:270:ALA:HB1	1.83	0.59
2:B:563:SER:CB	13:M:73:SER:HB3	2.33	0.59
3:C:272:LYS:HG2	14:N:175:TYR:CE1	2.38	0.59
15:O:369:LYS:HD3	15:O:373:LEU:HD22	1.85	0.59
15:O:428:ILE:CD1	15:O:439:ILE:HD12	2.33	0.59
1:A:990:ILE:CB	1:A:994:GLU:OE1	2.51	0.58
2:B:538:PRO:HB2	2:B:542:LEU:HG	1.84	0.58
15:O:348:THR:HG23	15:O:351:SER:H	1.67	0.58
15:O:241:ASP:O	15:O:378:THR:CG2	2.51	0.58
15:O:607:LYS:HG3	15:O:608:GLU:N	2.17	0.58
3:C:253:PRO:CB	14:N:180:PHE:HB3	2.33	0.58
1:A:1048:PHE:HZ	5:E:211:TYR:CD1	2.18	0.58
7:G:159:LYS:N	15:O:105:ASN:HD22	2.01	0.58
1:A:827:THR:OG1	1:A:828:CYS:N	2.36	0.58
7:G:30:GLU:HA	7:G:32:ASN:N	2.18	0.58
15:O:129:PRO:CG	15:O:132:THR:CB	2.74	0.58
15:O:164:LEU:O	15:O:165:PRO:O	2.20	0.58
15:O:369:LYS:CE	15:O:370:THR:HG22	2.33	0.58
1:A:1074:TYR:HE2	1:A:1159:ASP:HB3	1.68	0.58
1:A:1055:ILE:HD11	1:A:1174:TYR:CD2	2.39	0.58
1:A:1660:VAL:HG23	7:G:103:LYS:HB2	1.85	0.58
1:A:415:ASP:HA	1:A:418:VAL:HG12	1.84	0.58
2:B:415:GLU:OE2	2:B:474:SER:OG	2.21	0.58
2:B:328:GLN:HE22	13:M:109:ARG:NH2	1.99	0.58
1:A:437:PHE:CZ	1:A:456:VAL:HG22	2.28	0.58
4:D:48:GLU:HG3	4:D:86:ILE:CD1	2.32	0.58
11:K:68:GLU:HG2	11:K:72:LEU:HD23	1.86	0.58
15:O:454:VAL:CG2	15:O:458:GLU:OE2	2.51	0.58
1:A:468:ARG:HE	1:A:1021:ARG:NH1	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:221:PRO:O	3:C:222:VAL:HG13	2.04	0.58
2:B:1019:GLY:CA	3:C:65:ASN:HB2	2.28	0.58
4:D:27:LEU:HD22	7:G:23:GLN:O	2.03	0.58
4:D:25:THR:HG21	6:F:59:GLN:HE21	1.57	0.58
3:C:253:PRO:HB2	14:N:180:PHE:HB3	1.85	0.58
15:O:386:PHE:HD2	15:O:606:MET:HE2	1.62	0.58
15:O:484:PHE:CD1	15:O:502:LEU:HD13	2.38	0.58
7:G:159:LYS:N	15:O:105:ASN:ND2	2.51	0.58
2:B:1016:GLY:O	3:C:69:ARG:HD2	2.04	0.58
2:B:923:GLN:HG2	2:B:949:ILE:HD11	1.84	0.58
13:M:10:ILE:HB	14:N:70:LEU:HB3	1.86	0.58
1:A:406:LEU:CD1	1:A:411:VAL:HG21	2.34	0.58
2:B:117:VAL:HG13	2:B:117:VAL:O	2.03	0.58
4:D:48:GLU:OE1	4:D:90:LYS:NZ	2.37	0.58
4:D:25:THR:C	6:F:59:GLN:HG3	2.24	0.58
12:L:38:LEU:HD12	12:L:49:LYS:HG3	1.85	0.58
15:O:421:LEU:HD13	15:O:476:ALA:CB	2.31	0.58
15:O:423:TYR:HD1	15:O:594:TYR:CZ	2.20	0.58
12:L:33:GLU:HG3	12:L:53:HIS:CE1	2.39	0.57
14:N:69:SER:OG	14:N:70:LEU:N	2.37	0.57
15:O:174:ASP:O	15:O:177:LYS:CG	2.52	0.57
1:A:407:GLN:O	1:A:411:VAL:HG12	2.04	0.57
1:A:581:ILE:HG13	1:A:582:LYS:N	2.19	0.57
14:N:89:ILE:HG12	14:N:139:VAL:HG22	1.85	0.57
3:C:56:LEU:CG	3:C:300:PHE:CD1	2.86	0.57
15:O:369:LYS:O	15:O:373:LEU:HB3	2.04	0.57
1:A:1055:ILE:HG22	1:A:1060:GLU:HB2	1.87	0.57
1:A:476:VAL:CG1	2:B:1071:VAL:HG23	2.30	0.57
2:B:467:THR:C	2:B:469:ASN:H	2.07	0.57
15:O:247:GLU:HB3	15:O:325:ILE:HD11	1.86	0.57
15:O:471:LYS:CB	15:O:585:PHE:HE1	1.94	0.57
3:C:51:GLU:CB	3:C:303:GLU:CG	2.80	0.57
2:B:848:ILE:HB	12:L:60:ARG:HG3	1.86	0.57
15:O:487:ARG:O	15:O:490:ILE:HB	2.03	0.57
1:A:953:GLU:HA	1:A:1205:PHE:CG	2.40	0.57
1:A:493:ASN:HB3	1:A:654:ASP:OD1	2.04	0.57
1:A:782:ASP:O	1:A:784:SER:N	2.38	0.57
2:B:207:ILE:HD11	2:B:503:VAL:CG2	2.34	0.57
2:B:893:ASN:HA	12:L:54:ARG:NH2	2.20	0.57
6:F:66:ARG:CZ	7:G:90:LEU:CD1	2.80	0.57
7:G:143:SER:HB3	15:O:103:ASN:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:173:HIS:CD2	15:O:217:LYS:HG2	2.39	0.57
15:O:391:GLN:OE1	15:O:609:TYR:OH	2.23	0.57
1:A:1003:ARG:NE	2:B:520:LEU:CB	2.61	0.57
1:A:1348:VAL:CG2	2:B:268:GLU:C	2.72	0.57
15:O:128:LEU:HD22	15:O:129:PRO:HD3	1.86	0.57
15:O:190:ILE:HA	15:O:193:TYR:CD2	2.39	0.57
15:O:417:LYS:HB3	15:O:472:HIS:CE1	2.39	0.57
15:O:484:PHE:CE1	15:O:502:LEU:HD13	2.39	0.57
1:A:1235:THR:O	1:A:1544:ASN:ND2	2.38	0.57
1:A:468:ARG:NE	1:A:1021:ARG:CZ	2.63	0.57
2:B:833:PRO:HG2	2:B:836:TRP:CE2	2.40	0.57
15:O:230:TRP:CZ2	15:O:364:LEU:HD11	2.39	0.57
15:O:422:GLN:NE2	15:O:592:PHE:CZ	2.69	0.57
1:A:18:ILE:HD12	1:A:354:SER:HB3	1.85	0.57
1:A:478:TYR:HA	2:B:1048:SER:C	2.18	0.57
1:A:988:SER:HB2	2:B:988:GLU:HG2	1.87	0.57
2:B:1043:LYS:HG3	2:B:1063:ARG:HD2	1.85	0.57
1:A:727:THR:HG21	8:H:119:GLY:O	2.05	0.57
1:A:1048:PHE:O	1:A:1049:MET:HB2	2.04	0.57
3:C:56:LEU:CG	3:C:300:PHE:CE1	2.88	0.57
4:D:48:GLU:CG	4:D:86:ILE:HD11	2.35	0.57
15:O:158:LEU:HD22	15:O:172:HIS:CB	2.35	0.57
1:A:563:THR:HA	15:O:375:THR:HG21	1.87	0.56
2:B:1020:GLU:CG	3:C:61:THR:OG1	2.53	0.56
2:B:894:LYS:HG2	12:L:47:ARG:HD2	1.86	0.56
2:B:894:LYS:HG2	12:L:47:ARG:NE	2.19	0.56
15:O:154:VAL:O	15:O:158:LEU:HG	2.04	0.56
1:A:412:SER:HB3	1:A:414:GLU:H	1.70	0.56
1:A:799:GLU:CD	1:A:1062:HIS:HB2	2.25	0.56
2:B:207:ILE:HD11	2:B:503:VAL:HG21	1.87	0.56
2:B:800:TYR:CD1	2:B:801:GLY:N	2.73	0.56
4:D:28:PRO:HD2	7:G:24:VAL:CG1	2.35	0.56
5:E:145:THR:C	5:E:147:HIS:H	2.08	0.56
6:F:75:PRO:HG2	6:F:78:GLN:CG	2.34	0.56
7:G:20:HIS:O	7:G:20:HIS:ND1	2.38	0.56
3:C:82:TYR:CE1	12:L:68:GLU:OE1	2.58	0.56
1:A:1050:TYR:CG	1:A:1179:ILE:HG21	2.40	0.56
2:B:1013:MET:SD	2:B:1026:ILE:HG12	2.45	0.56
2:B:338:PHE:HZ	2:B:357:ILE:HD12	1.70	0.56
3:C:223:SER:HB2	3:C:303:GLU:CB	2.35	0.56
7:G:143:SER:CB	15:O:104:ILE:N	2.57	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:109:SER:OG	15:O:111:ARG:HG3	2.05	0.56
15:O:66:ASN:N	15:O:66:ASN:ND2	2.53	0.56
2:B:890:ASP:O	12:L:54:ARG:NE	2.38	0.56
5:E:90:VAL:HG13	5:E:120:ALA:HA	1.88	0.56
7:G:56:ASN:HB3	7:G:59:GLN:HB3	1.86	0.56
1:A:966:LEU:CD2	1:A:997:PHE:CZ	2.83	0.56
3:C:56:LEU:HD12	3:C:300:PHE:CE1	2.23	0.56
11:K:49:LEU:HD23	11:K:51:THR:HG23	1.86	0.56
15:O:458:GLU:HG2	15:O:514:PHE:CZ	2.40	0.56
2:B:1020:GLU:HG2	3:C:61:THR:OG1	2.06	0.56
3:C:86:PHE:HE2	3:C:205:LYS:HG3	1.69	0.56
12:L:63:ARG:HG3	12:L:64:LEU:H	1.69	0.56
1:A:477:ASN:OD1	2:B:1047:ARG:NH1	2.39	0.56
2:B:208:VAL:HG23	2:B:401:GLU:CG	2.35	0.56
2:B:554:GLN:CA	2:B:646:HIS:CD2	2.89	0.56
7:G:141:SER:HB3	15:O:138:TYR:CZ	2.41	0.56
15:O:396:MET:HE1	15:O:434:LEU:CD1	2.32	0.56
15:O:447:THR:HA	15:O:450:LEU:CG	2.35	0.56
15:O:432:LYS:HG3	15:O:608:GLU:O	1.96	0.56
15:O:98:ASP:CG	15:O:135:LYS:HD3	2.26	0.56
1:A:990:ILE:HB	1:A:994:GLU:OE1	2.06	0.56
15:O:191:ASP:O	15:O:194:LEU:HB2	2.06	0.56
15:O:205:ARG:O	15:O:209:VAL:HG12	2.05	0.56
2:B:480:GLN:HB3	2:B:507:SER:OG	2.05	0.56
3:C:71:MET:CE	3:C:225:ALA:HB2	2.33	0.56
13:M:15:VAL:HG22	13:M:90:LEU:HB2	1.88	0.56
15:O:63:LEU:HD23	15:O:111:ARG:HD2	1.87	0.56
1:A:1655:ASP:CG	6:F:137:TYR:CE2	2.76	0.56
1:A:35:PRO:HA	1:A:390:LEU:HD13	1.88	0.56
1:A:797:LEU:HD13	1:A:809:VAL:HG21	1.87	0.56
15:O:129:PRO:HG2	15:O:132:THR:OG1	2.06	0.56
15:O:447:THR:C	15:O:450:LEU:H	2.09	0.56
15:O:458:GLU:CB	15:O:461:VAL:CG2	2.80	0.56
15:O:484:PHE:CD1	15:O:502:LEU:CD1	2.89	0.56
15:O:440:ILE:CG2	15:O:491:PHE:CE1	2.82	0.56
1:A:468:ARG:CZ	1:A:1021:ARG:NH1	2.65	0.56
1:A:1482:LYS:HE2	2:B:304:ASP:CG	2.26	0.56
2:B:470:LEU:HB3	2:B:481:VAL:HG13	1.87	0.56
3:C:64:ALA:CB	3:C:298:PHE:CD2	2.89	0.56
1:A:1655:ASP:CB	6:F:135:ARG:HB3	2.36	0.56
1:A:87:ASN:CB	1:A:357:MET:SD	2.94	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:TYR:OH	2:B:1049:THR:CG2	2.51	0.55
2:B:1020:GLU:HG2	3:C:61:THR:CG2	2.34	0.55
1:A:1:MET:CG	2:B:1098:TYR:CE2	2.88	0.55
2:B:470:LEU:HB2	2:B:484:TYR:HE2	1.66	0.55
15:O:166:ILE:HD11	15:O:213:SER:OG	2.06	0.55
15:O:369:LYS:HE2	15:O:370:THR:HG22	1.87	0.55
15:O:343:VAL:CG1	15:O:388:VAL:HG21	2.36	0.55
1:A:1162:ASN:HD21	1:A:1164:LYS:HB2	1.71	0.55
1:A:1038:ILE:HG12	1:A:1049:MET:C	2.27	0.55
1:A:1049:MET:C	1:A:1051:GLY:H	2.09	0.55
1:A:1575:ILE:HG13	9:I:122:ARG:HH22	1.71	0.55
1:A:916:THR:O	1:A:919:LYS:NZ	2.40	0.55
2:B:236:ILE:HD13	2:B:377:MET:HE1	1.88	0.55
2:B:934:ILE:CG2	3:C:72:ILE:HB	2.35	0.55
3:C:84:TYR:CE2	12:L:66:GLN:CD	2.77	0.55
15:O:359:GLY:CA	15:O:362:ASN:HD22	2.16	0.55
15:O:447:THR:HA	15:O:450:LEU:HG	1.88	0.55
15:O:447:THR:O	15:O:450:LEU:N	2.39	0.55
1:A:1050:TYR:CD2	1:A:1179:ILE:HG21	2.41	0.55
1:A:1348:VAL:N	2:B:268:GLU:O	2.37	0.55
1:A:389:VAL:HA	1:A:430:ILE:HD11	1.88	0.55
2:B:859:CYS:HB3	2:B:872:LYS:HB2	1.88	0.55
10:J:10:CYS:HB3	10:J:43:ARG:NH1	2.21	0.55
13:M:11:GLU:N	13:M:86:LYS:O	2.36	0.55
15:O:432:LYS:HB2	15:O:610:TYR:N	2.20	0.55
1:A:437:PHE:CE2	1:A:456:VAL:CG2	2.85	0.55
3:C:139:LYS:HG2	3:C:201:GLU:HB3	1.89	0.55
5:E:144:ILE:O	5:E:147:HIS:HB2	2.07	0.55
1:A:1657:LEU:HD22	7:G:104:LEU:HD13	1.89	0.55
15:O:343:VAL:HG11	15:O:388:VAL:HG21	1.89	0.55
15:O:447:THR:HA	15:O:450:LEU:CD1	2.36	0.55
15:O:517:LEU:HD12	15:O:543:ILE:HG21	1.88	0.55
1:A:405:LYS:O	1:A:405:LYS:HG2	2.07	0.55
5:E:159:ASP:OD1	5:E:162:ARG:NH1	2.38	0.55
7:G:143:SER:HB3	15:O:101:SER:O	2.06	0.55
1:A:1024:THR:O	1:A:1028:GLU:HB3	2.07	0.55
1:A:1162:ASN:HD22	1:A:1165:LYS:HG3	1.71	0.55
2:B:322:ASN:HB3	2:B:325:GLN:H	1.71	0.55
3:C:56:LEU:HG	3:C:300:PHE:CE1	2.41	0.55
15:O:164:LEU:HB3	15:O:165:PRO:HD2	1.89	0.55
15:O:432:LYS:CB	15:O:608:GLU:O	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:25:THR:HG22	7:G:26:ASN:N	2.17	0.55
7:G:28:ILE:CG2	7:G:29:ASP:N	2.56	0.55
1:A:1596:LEU:HD22	1:A:1602:GLY:HA2	1.89	0.55
2:B:373:MET:O	2:B:377:MET:HG3	2.08	0.55
3:C:57:ILE:CG1	3:C:297:HIS:ND1	2.70	0.55
3:C:45:SER:HB2	3:C:271:ARG:CZ	2.35	0.55
15:O:158:LEU:HD22	15:O:172:HIS:CA	2.36	0.55
15:O:369:LYS:HD2	15:O:369:LYS:C	2.27	0.55
1:A:863:ASN:HD21	9:I:68:LYS:N	2.05	0.54
15:O:147:ILE:HG22	15:O:147:ILE:O	2.07	0.54
1:A:996:TYR:CE1	1:A:1000:MET:CE	2.90	0.54
2:B:42:VAL:HG21	2:B:190:ILE:HB	1.89	0.54
7:G:143:SER:HA	15:O:103:ASN:HA	1.90	0.54
1:A:800:VAL:HG23	1:A:1068:PHE:CZ	2.41	0.54
1:A:479:ALA:HB2	2:B:1091:ARG:NH2	2.22	0.54
3:C:253:PRO:HB2	14:N:180:PHE:CG	2.42	0.54
1:A:412:SER:C	1:A:414:GLU:N	2.56	0.54
15:O:158:LEU:CD2	15:O:172:HIS:HD2	2.01	0.54
15:O:488:HIS:C	15:O:490:ILE:H	2.10	0.54
15:O:487:ARG:NH2	15:O:611:ILE:HD12	2.22	0.54
1:A:402:ASP:HA	1:A:405:LYS:HB3	1.88	0.54
1:A:399:LEU:HD11	1:A:423:LEU:HG	1.89	0.54
2:B:401:GLU:HG3	2:B:402:VAL:H	1.69	0.54
2:B:799:GLY:O	2:B:1035:ARG:NH1	2.39	0.54
4:D:48:GLU:HG2	4:D:86:ILE:CD1	2.36	0.54
7:G:229:LEU:HD12	7:G:230:ARG:H	1.72	0.54
7:G:158:LYS:HZ2	15:O:108:GLU:CG	2.03	0.54
15:O:360:VAL:O	15:O:363:THR:HG23	2.06	0.54
15:O:372:VAL:C	15:O:374:PRO:CD	2.76	0.54
15:O:241:ASP:CA	15:O:380:SER:HB2	2.38	0.54
1:A:1008:ASP:OD1	1:A:1202:LEU:HB3	2.07	0.54
1:A:1446:ARG:O	1:A:1450:ILE:HG13	2.08	0.54
1:A:478:TYR:CA	2:B:1048:SER:C	2.74	0.54
2:B:284:SER:OG	2:B:287:GLU:HG3	2.07	0.54
3:C:58:ASN:HA	3:C:296:ASN:HB2	0.84	0.54
3:C:253:PRO:CA	14:N:180:PHE:HD1	2.20	0.54
1:A:589:MET:HE1	1:A:614:LEU:HD13	1.89	0.54
1:A:878:ARG:CZ	9:I:66:VAL:HG23	2.38	0.54
1:A:1347:ALA:HA	2:B:269:TYR:CE1	2.43	0.54
3:C:59:ILE:HG22	3:C:298:PHE:CE1	2.31	0.54
15:O:169:THR:HA	15:O:172:HIS:ND1	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:426:SER:HB3	15:O:594:TYR:HD2	1.72	0.54
1:A:1344:ILE:CG2	2:B:333:LYS:CG	2.86	0.54
9:I:71:LEU:HG	9:I:72:LYS:O	2.08	0.54
1:A:1651:THR:OG1	2:B:1085:SER:HB2	2.07	0.54
3:C:253:PRO:CB	14:N:180:PHE:CD1	2.79	0.54
15:O:100:LEU:HD22	15:O:107:ILE:CD1	2.38	0.54
15:O:423:TYR:CD1	15:O:594:TYR:CZ	2.95	0.54
2:B:1043:LYS:CG	2:B:1063:ARG:NE	2.70	0.54
2:B:21:ARG:NH1	2:B:22:GLU:OE1	2.40	0.54
7:G:132:VAL:HG22	7:G:232:THR:HG22	1.90	0.54
1:A:556:ALA:CA	15:O:246:ASN:HD22	2.20	0.54
15:O:391:GLN:NE2	15:O:609:TYR:CE2	2.76	0.54
2:B:788:ILE:HB	2:B:948:ILE:HB	1.89	0.53
1:A:1136:VAL:HG22	1:A:1174:TYR:CG	2.44	0.53
1:A:413:LEU:C	1:A:417:ARG:NH2	2.56	0.53
1:A:389:VAL:HA	1:A:430:ILE:CD1	2.38	0.53
3:C:55:ASP:CB	3:C:297:HIS:HE2	2.21	0.53
3:C:97:LEU:HD11	3:C:202:ILE:HD13	1.90	0.53
15:O:368:PHE:CZ	15:O:385:MET:HB2	2.43	0.53
1:A:641:GLU:HB2	6:F:99:LEU:CD1	2.36	0.53
3:C:55:ASP:OD1	3:C:299:ILE:CG2	2.56	0.53
1:A:1660:VAL:HG22	7:G:103:LYS:C	2.28	0.53
9:I:96:TYR:HA	9:I:111:PHE:O	2.09	0.53
15:O:69:THR:O	15:O:73:ILE:HG13	2.07	0.53
1:A:572:THR:HA	7:G:52:MET:HE3	1.90	0.53
2:B:398:GLN:O	2:B:398:GLN:HG2	2.06	0.53
15:O:147:ILE:HG22	15:O:149:LYS:HB3	1.90	0.53
1:A:1655:ASP:HB2	6:F:135:ARG:CB	2.38	0.53
1:A:91:PHE:CD2	1:A:249:THR:HG22	2.43	0.53
1:A:1482:LYS:HE2	2:B:304:ASP:OD2	2.08	0.53
2:B:470:LEU:O	2:B:481:VAL:CG1	2.56	0.53
4:D:37:LEU:CD2	4:D:97:LYS:HE3	2.38	0.53
13:M:75:GLN:HB2	14:N:60:SER:HA	1.91	0.53
15:O:342:HIS:O	15:O:346:GLN:CG	2.51	0.53
15:O:63:LEU:CD2	15:O:111:ARG:HD2	2.38	0.53
1:A:1008:ASP:OD1	1:A:1202:LEU:CG	2.56	0.53
2:B:563:SER:HA	13:M:73:SER:OG	2.08	0.53
3:C:67:PHE:O	3:C:71:MET:HG3	2.08	0.53
2:B:934:ILE:HG21	3:C:73:SER:HB3	1.91	0.53
15:O:156:MET:HE2	15:O:193:TYR:CE1	2.44	0.53
15:O:218:LEU:HD23	15:O:229:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:238:ILE:CD1	15:O:371:HIS:HB3	2.37	0.53
15:O:390:GLN:HB2	15:O:609:TYR:CG	2.43	0.53
1:A:1289:SER:HB3	1:A:1475:GLU:HG2	1.91	0.53
1:A:1344:ILE:CG2	2:B:333:LYS:CB	2.86	0.53
1:A:248:PHE:CD1	1:A:442:LYS:O	2.62	0.53
2:B:317:TYR:HB3	2:B:320:LEU:HD12	1.89	0.53
4:D:28:PRO:CD	7:G:24:VAL:HG13	2.35	0.53
4:D:92:ILE:HG22	4:D:96:PHE:CE2	2.41	0.53
11:K:48:LYS:HE2	11:K:64:GLN:NE2	2.23	0.53
15:O:374:PRO:CB	15:O:375:THR:HG23	2.39	0.53
1:A:408:LYS:C	1:A:411:VAL:HG12	2.29	0.53
2:B:472:SER:O	2:B:474:SER:N	2.41	0.53
3:C:131:THR:HG21	3:C:207:HIS:HB3	1.91	0.53
4:D:23:HIS:CD2	6:F:58:PHE:CD2	2.97	0.53
7:G:30:GLU:HA	7:G:32:ASN:H	1.74	0.53
13:M:12:ILE:HD12	14:N:67:LEU:HB2	1.90	0.53
15:O:189:PHE:CD1	15:O:190:ILE:N	2.76	0.53
15:O:520:CYS:O	15:O:521:ASN:O	2.27	0.53
1:A:1317:ILE:HA	1:A:1321:PHE:HB3	1.90	0.53
2:B:207:ILE:CD1	2:B:503:VAL:HG22	2.36	0.53
2:B:211:ARG:NH2	2:B:243:GLN:OE1	2.42	0.53
2:B:566:TYR:HD2	13:M:73:SER:HG	1.56	0.53
3:C:272:LYS:HG3	14:N:175:TYR:CE1	2.44	0.53
2:B:555:GLN:HB2	2:B:646:HIS:CE1	2.44	0.52
1:A:800:VAL:HG23	1:A:1068:PHE:HZ	1.73	0.52
1:A:477:ASN:OD1	2:B:1059:PRO:HG2	1.99	0.52
2:B:894:LYS:HG2	12:L:47:ARG:HD3	1.89	0.52
3:C:64:ALA:CB	3:C:227:TYR:CE2	2.92	0.52
15:O:459:GLU:C	15:O:461:VAL:N	2.61	0.52
2:B:33:SER:C	2:B:35:PHE:H	2.12	0.52
3:C:64:ALA:HB3	3:C:298:PHE:CE2	2.44	0.52
15:O:371:HIS:C	15:O:374:PRO:CD	2.78	0.52
15:O:499:GLU:O	15:O:502:LEU:HG	2.09	0.52
3:C:127:THR:H	3:C:130:ASN:HB2	1.74	0.52
7:G:142:ALA:HB3	15:O:102:SER:HA	1.91	0.52
9:I:59:SER:O	9:I:63:LYS:HG3	2.09	0.52
15:O:337:THR:O	15:O:341:THR:OG1	2.27	0.52
2:B:22:GLU:O	2:B:26:ILE:HG13	2.10	0.52
7:G:242:VAL:HG21	15:O:183:ILE:HG21	1.91	0.52
9:I:59:SER:O	9:I:63:LYS:CG	2.57	0.52
1:A:509:GLU:HG3	1:A:579:ARG:CD	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:969:PHE:CE2	1:A:978:ALA:HA	2.44	0.52
2:B:915:ASP:OD1	2:B:1038:HIS:CD2	2.61	0.52
2:B:527:PHE:CE1	2:B:666:PRO:HG3	2.45	0.52
15:O:348:THR:HG22	15:O:351:SER:CB	2.26	0.52
2:B:833:PRO:O	2:B:834:LYS:HB3	2.10	0.52
3:C:82:TYR:CE1	12:L:68:GLU:HG3	2.44	0.52
15:O:156:MET:HG3	15:O:197:PHE:HE2	1.60	0.52
15:O:155:SER:HB2	15:O:176:LEU:HD21	1.91	0.52
15:O:373:LEU:CD1	15:O:416:LYS:CG	2.62	0.52
1:A:441:THR:HG22	1:A:441:THR:O	2.10	0.52
2:B:134:ARG:HD2	2:B:160:GLY:HA3	1.91	0.52
2:B:42:VAL:O	2:B:46:ILE:CD1	2.52	0.52
4:D:37:LEU:HD22	4:D:97:LYS:CE	2.39	0.52
13:M:105:SER:HA	13:M:108:LEU:CG	2.29	0.52
15:O:175:MET:HA	15:O:175:MET:HE2	1.92	0.52
15:O:206:ARG:HA	15:O:209:VAL:HG12	1.90	0.52
15:O:402:THR:O	15:O:406:ILE:HG13	2.10	0.52
15:O:458:GLU:CG	15:O:514:PHE:CE2	2.92	0.52
3:C:51:GLU:CB	3:C:303:GLU:HG3	2.40	0.52
7:G:26:ASN:HD21	7:G:126:GLN:HE21	1.56	0.52
15:O:459:GLU:HG3	15:O:460:GLU:N	2.25	0.52
1:A:497:VAL:HG21	1:A:605:VAL:HG13	1.92	0.51
1:A:722:PRO:HG2	8:H:46:LEU:HD13	1.90	0.51
2:B:37:LEU:CD1	2:B:760:TYR:CZ	2.90	0.51
15:O:415:GLU:O	15:O:419:LYS:HG3	2.10	0.51
15:O:518:LYS:HD3	15:O:519:PHE:CZ	2.45	0.51
1:A:636:HIS:CE1	2:B:1091:ARG:HH21	2.28	0.51
2:B:1069:ILE:CD1	2:B:1069:ILE:N	2.73	0.51
2:B:307:GLU:OE2	2:B:311:ARG:NH1	2.43	0.51
2:B:938:PHE:CD1	3:C:68:ARG:NE	2.78	0.51
3:C:47:LEU:HD23	3:C:48:ASP:N	2.25	0.51
2:B:1120:ILE:CD1	15:O:117:GLN:HE22	2.23	0.51
15:O:241:ASP:O	15:O:378:THR:HG23	2.10	0.51
15:O:478:GLN:OE1	15:O:521:ASN:HB2	2.10	0.51
15:O:426:SER:HB3	15:O:594:TYR:HB2	1.88	0.51
15:O:377:TYR:O	15:O:378:THR:OG1	2.20	0.51
1:A:87:ASN:HA	1:A:357:MET:SD	2.50	0.51
15:O:457:ARG:O	15:O:461:VAL:HG23	2.10	0.51
15:O:98:ASP:OD2	15:O:135:LYS:CE	2.58	0.51
1:A:1003:ARG:CD	2:B:520:LEU:N	2.73	0.51
1:A:1603:MET:HE1	1:A:1615:TYR:CD2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1657:LEU:HB3	7:G:104:LEU:HB3	1.93	0.51
2:B:1047:ARG:NH2	2:B:1051:PRO:O	2.43	0.51
3:C:64:ALA:O	3:C:227:TYR:CE2	2.58	0.51
15:O:158:LEU:HD22	15:O:172:HIS:CD2	2.46	0.51
15:O:383:TYR:CZ	15:O:597:LEU:HB2	2.46	0.51
1:A:392:THR:CB	1:A:430:ILE:HD13	2.37	0.51
2:B:527:PHE:CD1	2:B:666:PRO:HG3	2.46	0.51
4:D:95:ASP:OD2	7:G:150:HIS:CA	2.56	0.51
15:O:151:TRP:HZ2	15:O:176:LEU:HA	1.76	0.51
15:O:379:ARG:CB	15:O:382:GLN:NE2	2.74	0.51
15:O:487:ARG:CG	15:O:487:ARG:NH1	2.73	0.51
1:A:1028:GLU:CG	1:A:1029:GLY:H	2.24	0.51
1:A:1056:ASP:OD2	1:A:1179:ILE:HA	2.11	0.51
1:A:401:ASP:O	1:A:405:LYS:HB3	2.09	0.51
2:B:472:SER:O	2:B:473:GLN:C	2.48	0.51
3:C:31:TRP:CD2	11:K:82:LYS:CG	2.91	0.51
15:O:247:GLU:OE1	15:O:325:ILE:CD1	2.57	0.51
1:A:954:GLY:N	1:A:1205:PHE:HB3	2.25	0.51
2:B:819:ASP:CG	2:B:820:PRO:HD2	2.31	0.51
3:C:229:LEU:HD22	3:C:295:ARG:O	2.11	0.51
1:A:1655:ASP:CG	6:F:137:TYR:HE2	2.14	0.51
2:B:300:SER:CB	9:I:49:THR:HG22	2.41	0.51
15:O:369:LYS:CE	15:O:370:THR:CG2	2.86	0.51
1:A:475:ARG:HB3	2:B:1059:PRO:HB2	1.90	0.51
1:A:840:ASN:O	1:A:844:THR:HG23	2.11	0.51
2:B:769:PHE:CZ	2:B:798:PHE:CE1	2.91	0.51
3:C:131:THR:HG22	3:C:208:CYS:N	2.26	0.51
7:G:244:SER:HB2	15:O:148:PRO:HD2	1.91	0.51
15:O:198:PHE:CD2	15:O:232:LEU:CG	2.60	0.51
1:A:1003:ARG:CD	2:B:520:LEU:H	2.23	0.51
1:A:1450:ILE:HD12	1:A:1460:TYR:CD2	2.46	0.51
1:A:527:PRO:C	1:A:580:HIS:HE1	2.14	0.51
2:B:934:ILE:HG21	3:C:69:ARG:O	2.10	0.51
15:O:248:LEU:HD23	15:O:248:LEU:O	2.10	0.51
1:A:509:GLU:OE2	1:A:579:ARG:CZ	2.58	0.50
1:A:991:LYS:HB3	1:A:993:GLN:OE1	2.11	0.50
1:A:880:GLN:OE1	2:B:633:THR:O	2.27	0.50
2:B:934:ILE:HG21	3:C:73:SER:CB	2.41	0.50
3:C:296:ASN:O	3:C:297:HIS:HB2	2.11	0.50
3:C:57:ILE:O	3:C:58:ASN:HB2	2.12	0.50
1:A:1048:PHE:CE2	5:E:211:TYR:HD1	2.21	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1660:VAL:O	7:G:103:LYS:N	2.39	0.50
4:D:28:PRO:CD	7:G:24:VAL:CG1	2.89	0.50
15:O:444:SER:O	15:O:447:THR:OG1	2.23	0.50
15:O:446:LEU:O	15:O:449:TRP:CB	2.42	0.50
1:A:478:TYR:HD1	2:B:1048:SER:HB2	1.76	0.50
1:A:1660:VAL:N	7:G:103:LYS:O	2.41	0.50
10:J:1:MET:HG2	10:J:57:ILE:HB	1.93	0.50
4:D:80:THR:HG23	15:O:227:PHE:HB3	1.88	0.50
1:A:564:PRO:HB2	15:O:371:HIS:HE1	1.76	0.50
1:A:1326:GLU:OE2	1:A:1454:HIS:HB3	2.11	0.50
2:B:1010:ASN:HB3	2:B:1025:ASP:HB3	1.93	0.50
2:B:894:LYS:HD3	12:L:47:ARG:NH1	2.26	0.50
15:O:591:TYR:CE2	15:O:593:PRO:HG3	2.46	0.50
1:A:970:LYS:HG2	1:A:973:GLU:HG2	1.92	0.50
2:B:469:ASN:CA	2:B:481:VAL:O	2.60	0.50
6:F:74:ILE:CG2	6:F:75:PRO:CD	2.87	0.50
2:B:1002:LYS:CD	14:N:166:LEU:HB2	2.40	0.50
1:A:437:PHE:CE2	1:A:456:VAL:HG23	2.36	0.50
2:B:293:ILE:HG12	2:B:306:LEU:HD13	1.94	0.50
2:B:472:SER:HB3	2:B:476:LEU:HD11	1.92	0.50
1:A:1003:ARG:CD	2:B:520:LEU:HB2	2.41	0.50
2:B:68:ILE:HD11	2:B:414:LYS:CG	2.39	0.50
8:H:26:ILE:HD12	8:H:42:ILE:HD12	1.93	0.50
15:O:242:VAL:HA	15:O:378:THR:CG2	2.37	0.50
15:O:352:LEU:HD22	15:O:358:VAL:HG22	1.81	0.50
2:B:203:ILE:HG21	2:B:405:GLY:HA2	1.93	0.50
2:B:284:SER:HB2	9:I:14:GLY:HA3	1.93	0.50
3:C:230:LEU:HD11	3:C:231:PRO:HD2	1.92	0.50
4:D:44:ILE:CG2	4:D:90:LYS:HE3	2.40	0.50
5:E:145:THR:C	5:E:147:HIS:N	2.65	0.50
14:N:87:TYR:CE1	14:N:141:GLU:OE1	2.64	0.50
15:O:359:GLY:CA	15:O:362:ASN:ND2	2.73	0.50
15:O:488:HIS:O	15:O:491:PHE:N	2.37	0.50
1:A:505:LEU:HD12	1:A:581:ILE:HD13	1.93	0.50
3:C:100:ARG:NH2	10:J:3:VAL:O	2.44	0.50
15:O:208:LEU:O	15:O:212:THR:HG23	2.12	0.50
1:A:953:GLU:CA	1:A:1205:PHE:CG	2.95	0.50
3:C:222:VAL:O	3:C:224:THR:N	2.44	0.50
3:C:231:PRO:HG2	3:C:270:ALA:CB	2.42	0.50
3:C:47:LEU:HD23	3:C:48:ASP:H	1.77	0.50
2:B:328:GLN:NE2	13:M:109:ARG:NH2	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1025:LYS:NZ	2:B:1076:ARG:NH1	2.59	0.50
1:A:1048:PHE:CE2	5:E:210:SER:HA	2.46	0.50
1:A:1056:ASP:HB2	1:A:1177:SER:O	2.11	0.50
2:B:858:ILE:HD13	2:B:872:LYS:O	2.11	0.50
15:O:352:LEU:CA	15:O:358:VAL:CG2	2.90	0.50
1:A:863:ASN:HD22	9:I:67:VAL:C	2.15	0.49
1:A:1003:ARG:HD2	2:B:520:LEU:N	2.23	0.49
7:G:47:VAL:HB	7:G:65:HIS:CD2	2.47	0.49
14:N:85:HIS:CE1	14:N:141:GLU:OE1	2.64	0.49
15:O:368:PHE:C	15:O:368:PHE:CD1	2.85	0.49
15:O:453:TYR:CE1	15:O:473:PHE:HB2	2.47	0.49
1:A:1006:LEU:HD21	2:B:535:ASP:CB	2.42	0.49
7:G:143:SER:HB3	15:O:103:ASN:CA	2.42	0.49
15:O:324:GLY:O	15:O:326:LYS:N	2.44	0.49
15:O:368:PHE:CD2	15:O:385:MET:HG2	2.47	0.49
15:O:468:GLU:C	15:O:470:PHE:N	2.65	0.49
1:A:381:SER:HB2	1:A:453:ILE:HG21	1.93	0.49
2:B:1019:GLY:CA	3:C:65:ASN:CG	2.81	0.49
2:B:338:PHE:CE1	2:B:353:VAL:HG22	2.47	0.49
4:D:23:HIS:CG	6:F:58:PHE:CD2	3.00	0.49
7:G:242:VAL:HG21	15:O:183:ILE:HG23	1.93	0.49
9:I:91:ASN:OD1	9:I:92:GLU:N	2.45	0.49
1:A:1622:LEU:HD21	2:B:1189:LEU:HD22	1.94	0.49
1:A:412:SER:H	1:A:415:ASP:HB2	1.76	0.49
1:A:507:TYR:HB2	1:A:637:PHE:CE2	2.47	0.49
2:B:1043:LYS:HE2	2:B:1063:ARG:CD	2.42	0.49
3:C:71:MET:HE1	3:C:225:ALA:HB1	1.90	0.49
3:C:71:MET:CE	3:C:302:VAL:CG2	2.90	0.49
1:A:1053:ASP:HB2	5:E:204:THR:CG2	2.43	0.49
2:B:1120:ILE:HD12	15:O:117:GLN:NE2	2.27	0.49
15:O:430:ARG:O	15:O:431:ALA:O	2.31	0.49
1:A:1148:LEU:HD22	1:A:1163:GLU:HG3	1.92	0.49
1:A:995:TYR:O	1:A:999:CYS:N	2.35	0.49
2:B:211:ARG:HH11	2:B:211:ARG:HG2	1.77	0.49
4:D:30:HIS:HE2	7:G:26:ASN:CG	2.11	0.49
12:L:45:ALA:O	12:L:47:ARG:N	2.46	0.49
15:O:173:HIS:CE1	15:O:217:LYS:HB3	2.47	0.49
1:A:1034:TYR:HA	1:A:1181:PRO:HB3	1.95	0.49
1:A:1500:GLN:HG2	1:A:1501:ILE:N	2.28	0.49
15:O:173:HIS:CD2	15:O:217:LYS:CG	2.95	0.49
15:O:488:HIS:C	15:O:490:ILE:N	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:488:HIS:CE1	15:O:489:ASN:H	2.27	0.49
1:A:1026:GLN:NE2	1:A:1603:MET:HA	2.26	0.49
15:O:177:LYS:HG3	15:O:178:TYR:N	2.26	0.49
15:O:443:ALA:O	15:O:447:THR:HG23	2.12	0.49
2:B:211:ARG:NH1	2:B:211:ARG:HG2	2.28	0.49
6:F:75:PRO:HG3	6:F:78:GLN:NE2	2.27	0.49
15:O:361:PHE:CD1	15:O:361:PHE:C	2.86	0.49
15:O:507:GLN:O	15:O:511:ILE:HG23	2.12	0.49
1:A:795:HIS:NE2	1:A:1062:HIS:HE1	2.11	0.49
1:A:1661:PRO:CA	7:G:101:SER:O	2.61	0.49
1:A:249:THR:HG1	1:A:435:ASN:HD21	1.58	0.49
1:A:476:VAL:O	2:B:1059:PRO:HG2	2.13	0.49
1:A:982:VAL:HG13	1:A:994:GLU:CD	2.33	0.49
2:B:252:TYR:OH	2:B:305:ARG:NH1	2.44	0.49
2:B:262:PHE:CD1	2:B:357:ILE:HD13	2.48	0.49
13:M:65:TYR:CE1	13:M:97:VAL:HB	2.48	0.49
15:O:234:ILE:O	15:O:238:ILE:HG13	2.12	0.49
1:A:582:LYS:O	1:A:585:ASP:HB2	2.12	0.49
1:A:91:PHE:CZ	1:A:249:THR:HA	2.46	0.49
1:A:1662:ASN:N	7:G:101:SER:HB2	2.28	0.49
15:O:163:ILE:HG22	15:O:207:LYS:O	2.12	0.49
15:O:434:LEU:CD1	15:O:434:LEU:N	2.75	0.49
2:B:281:CYS:HA	2:B:323:ARG:NE	2.28	0.48
1:A:1053:ASP:HB2	5:E:204:THR:HG22	1.95	0.48
15:O:396:MET:HE1	15:O:433:LYS:C	2.34	0.48
15:O:468:GLU:C	15:O:470:PHE:H	2.15	0.48
15:O:390:GLN:C	15:O:609:TYR:CE1	2.81	0.48
1:A:475:ARG:NH1	2:B:1061:LYS:HB2	2.28	0.48
2:B:225:ARG:NH2	2:B:261:ARG:HD3	2.27	0.48
4:D:95:ASP:OD1	7:G:151:ASP:HB2	2.12	0.48
7:G:137:ILE:HG13	7:G:227:GLY:O	2.13	0.48
8:H:112:ILE:HD12	8:H:129:TYR:HB2	1.93	0.48
15:O:591:TYR:HE2	15:O:593:PRO:HG3	1.77	0.48
1:A:996:TYR:HE1	1:A:1000:MET:HE1	1.78	0.48
1:A:1050:TYR:HE1	1:A:1185:VAL:HG12	1.67	0.48
1:A:1055:ILE:CG2	1:A:1060:GLU:HB2	2.43	0.48
1:A:1260:LYS:HE2	1:A:1262:LEU:HD11	1.95	0.48
2:B:1043:LYS:HG3	2:B:1063:ARG:CZ	2.43	0.48
2:B:209:GLN:CG	2:B:210:ARG:H	2.08	0.48
15:O:391:GLN:HE22	15:O:609:TYR:HE2	1.61	0.48
1:A:440:SER:C	1:A:442:LYS:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:TYR:CD1	1:A:365:THR:HG23	2.47	0.48
5:E:145:THR:O	5:E:147:HIS:N	2.46	0.48
15:O:597:LEU:HD12	15:O:598:PHE:H	1.77	0.48
15:O:383:TYR:CG	15:O:597:LEU:HD22	2.47	0.48
15:O:91:LYS:HG3	15:O:92:ASN:N	2.28	0.48
1:A:1606:SER:HB3	1:A:1611:MET:HE2	1.96	0.48
2:B:471:VAL:O	2:B:471:VAL:HG12	2.13	0.48
2:B:929:ARG:HH22	11:K:96:PRO:HB2	1.77	0.48
15:O:199:PRO:HB2	15:O:208:LEU:HD23	1.95	0.48
1:A:365:THR:O	1:A:368:ARG:N	2.37	0.48
1:A:413:LEU:CA	1:A:417:ARG:HH21	2.27	0.48
1:A:721:LYS:HB3	8:H:96:VAL:HB	1.95	0.48
2:B:550:ARG:O	2:B:649:MET:HA	2.14	0.48
2:B:800:TYR:CD1	2:B:800:TYR:C	2.87	0.48
4:D:48:GLU:CD	4:D:90:LYS:NZ	2.66	0.48
1:A:932:GLY:C	9:I:125:ASN:HD21	2.16	0.48
14:N:111:VAL:HG13	14:N:122:ALA:HB2	1.96	0.48
15:O:241:ASP:OD1	15:O:380:SER:HB2	2.13	0.48
15:O:408:PHE:CD2	15:O:449:TRP:CE2	3.02	0.48
15:O:484:PHE:O	15:O:488:HIS:HB3	2.14	0.48
15:O:440:ILE:HD13	15:O:491:PHE:CD1	2.48	0.48
1:A:399:LEU:HD22	1:A:423:LEU:HA	1.95	0.48
1:A:597:LYS:HB2	2:B:1082:HIS:CE1	2.48	0.48
1:A:1003:ARG:HD2	2:B:520:LEU:CB	2.43	0.48
1:A:40:ASN:OD1	1:A:40:ASN:N	2.44	0.48
1:A:747:ILE:HD13	1:A:748:ASN:H	1.77	0.48
1:A:480:ALA:CA	2:B:1046:VAL:HG23	2.42	0.48
3:C:157:TYR:HB2	3:C:160:ALA:HB2	1.94	0.48
4:D:92:ILE:CD1	7:G:152:ALA:CB	2.92	0.48
5:E:61:GLN:HE21	5:E:105:PHE:HE1	1.61	0.48
1:A:684:ASP:OD1	8:H:20:TYR:HB3	2.13	0.48
15:O:369:LYS:HE2	15:O:370:THR:N	2.28	0.48
15:O:477:PHE:CE2	15:O:481:CYS:SG	3.07	0.48
1:A:1006:LEU:CD2	2:B:535:ASP:HB2	2.43	0.48
1:A:1023:LEU:CD2	1:A:1598:PHE:CD1	2.97	0.48
1:A:1162:ASN:ND2	1:A:1165:LYS:HG3	2.29	0.48
1:A:869:PRO:HG2	1:A:872:ASP:HB2	1.96	0.48
2:B:1133:MET:CE	7:G:17:ILE:HD13	2.44	0.48
2:B:552:SER:O	2:B:647:SER:CA	2.61	0.48
15:O:369:LYS:HD2	15:O:370:THR:HA	1.95	0.48
15:O:446:LEU:C	15:O:449:TRP:HB3	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:ILE:CG2	1:A:1060:GLU:CG	2.90	0.48
1:A:1312:GLU:O	1:A:1316:VAL:HG23	2.13	0.48
2:B:1045:GLN:HB3	2:B:1063:ARG:HG3	1.95	0.48
2:B:894:LYS:HD3	12:L:47:ARG:CZ	2.44	0.48
2:B:70:GLU:CB	2:B:97:VAL:O	2.62	0.48
15:O:146:SER:C	15:O:148:PRO:HD3	2.34	0.48
1:A:747:ILE:HD13	1:A:748:ASN:N	2.29	0.47
4:D:92:ILE:HD11	7:G:152:ALA:HB1	1.95	0.47
7:G:158:LYS:HE2	15:O:105:ASN:OD1	2.14	0.47
15:O:151:TRP:CZ2	15:O:176:LEU:HA	2.49	0.47
15:O:225:LEU:HD12	15:O:229:ILE:HG13	1.96	0.47
1:A:960:MET:SD	2:B:522:PRO:HB2	2.54	0.47
1:A:959:VAL:HG22	1:A:965:THR:HG22	1.95	0.47
2:B:73:ILE:HB	2:B:425:ILE:HD12	1.96	0.47
4:D:80:THR:HG21	15:O:227:PHE:CG	2.48	0.47
15:O:369:LYS:O	15:O:373:LEU:CA	2.60	0.47
15:O:478:GLN:NE2	15:O:592:PHE:CZ	2.69	0.47
2:B:208:VAL:CG2	2:B:401:GLU:CG	2.92	0.47
2:B:73:ILE:HD12	2:B:425:ILE:HG23	1.95	0.47
3:C:230:LEU:CG	3:C:294:VAL:CG2	2.92	0.47
15:O:120:ILE:HD13	15:O:150:TRP:CE3	2.49	0.47
1:A:1348:VAL:HB	2:B:268:GLU:CA	2.43	0.47
2:B:552:SER:O	2:B:647:SER:HA	2.14	0.47
2:B:584:CYS:HB3	2:B:596:VAL:HG23	1.95	0.47
10:J:6:ARG:HD2	10:J:11:GLY:O	2.13	0.47
1:A:1261:VAL:HG12	1:A:1262:LEU:N	2.28	0.47
1:A:1605:THR:C	1:A:1606:SER:O	2.37	0.47
1:A:1482:LYS:HE2	2:B:304:ASP:OD1	2.15	0.47
1:A:1048:PHE:CE1	5:E:211:TYR:CD1	3.01	0.47
5:E:48:ASP:OD1	5:E:50:MET:HB3	2.13	0.47
1:A:258:GLU:HA	1:A:261:ILE:HD12	1.97	0.47
2:B:338:PHE:CZ	2:B:357:ILE:HD12	2.49	0.47
2:B:470:LEU:O	2:B:481:VAL:HG13	2.15	0.47
15:O:107:ILE:O	15:O:109:SER:N	2.46	0.47
1:A:439:ASP:HB3	1:A:442:LYS:HD2	1.96	0.47
1:A:741:PRO:HA	1:A:742:PRO:HD3	1.68	0.47
2:B:1020:GLU:HG2	3:C:61:THR:CB	2.44	0.47
15:O:460:GLU:O	15:O:469:ARG:NH2	2.47	0.47
15:O:521:ASN:ND2	15:O:523:ASN:N	2.54	0.47
2:B:812:ALA:HA	2:B:815:ARG:HD3	1.95	0.47
3:C:126:PHE:HD1	3:C:131:THR:HG1	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1573:TYR:HB3	9:I:122:ARG:NH2	2.30	0.47
15:O:237:ILE:CG2	15:O:381:ILE:CG1	2.93	0.47
15:O:471:LYS:CG	15:O:472:HIS:N	2.75	0.47
1:A:19:LEU:HD11	2:B:1190:SER:HB2	1.96	0.47
2:B:396:ALA:HB1	2:B:523:GLU:HG3	1.96	0.47
3:C:247:PHE:HE1	3:C:289:VAL:HG21	1.80	0.47
1:A:479:ALA:HB2	1:A:636:HIS:ND1	2.29	0.47
3:C:86:PHE:CD1	12:L:64:LEU:HD13	2.46	0.47
3:C:31:TRP:NE1	11:K:82:LYS:NZ	2.54	0.47
13:M:109:ARG:HH22	13:M:112:LYS:HG3	1.79	0.47
15:O:170:VAL:CG1	15:O:171:CYS:N	2.78	0.47
15:O:176:LEU:HD13	15:O:218:LEU:HD13	1.96	0.47
1:A:55:GLY:HA2	1:A:62:CYS:SG	2.56	0.47
2:B:413:LEU:O	2:B:417:ILE:HG13	2.14	0.47
15:O:129:PRO:O	15:O:133:LEU:CB	2.62	0.47
15:O:602:TYR:O	15:O:606:MET:HG2	2.15	0.47
2:B:1103:VAL:HG22	2:B:1176:VAL:HG22	1.97	0.46
2:B:203:ILE:CG2	2:B:405:GLY:HA2	2.45	0.46
2:B:470:LEU:N	2:B:481:VAL:O	2.47	0.46
2:B:569:GLY:HA2	14:N:140:SER:OG	2.15	0.46
3:C:231:PRO:CG	3:C:270:ALA:O	2.62	0.46
3:C:239:ILE:HG23	3:C:243:SER:HB3	1.96	0.46
1:A:863:ASN:HD22	9:I:68:LYS:N	2.08	0.46
15:O:138:TYR:CD2	15:O:142:ILE:CD1	2.92	0.46
15:O:488:HIS:O	15:O:489:ASN:C	2.54	0.46
1:A:1320:GLN:HB2	1:A:1320:GLN:HE21	1.56	0.46
1:A:364:PRO:HB2	1:A:367:PHE:CD2	2.51	0.46
1:A:403:LEU:CD2	1:A:423:LEU:HD11	2.45	0.46
2:B:681:ILE:O	14:N:154:ARG:NE	2.36	0.46
2:B:736:ARG:HD3	2:B:738:ASP:OD2	2.15	0.46
4:D:46:GLU:OE1	4:D:47:LYS:HE2	2.15	0.46
4:D:95:ASP:HB2	7:G:151:ASP:HB3	1.97	0.46
15:O:170:VAL:HG13	15:O:171:CYS:H	1.79	0.46
15:O:206:ARG:HA	15:O:209:VAL:CG1	2.44	0.46
15:O:388:VAL:HG13	15:O:389:SER:N	2.31	0.46
1:A:1053:ASP:O	1:A:1054:ALA:CB	2.62	0.46
1:A:1060:GLU:HA	1:A:1063:MET:CG	2.37	0.46
1:A:1258:ILE:HB	1:A:1501:ILE:HD12	1.97	0.46
1:A:1440:ASN:HA	1:A:1443:GLN:HB2	1.96	0.46
1:A:412:SER:C	1:A:414:GLU:H	2.17	0.46
1:A:492:THR:HG23	1:A:811:SER:OG	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:996:TYR:CE1	1:A:1000:MET:HE3	2.51	0.46
3:C:231:PRO:HG3	3:C:270:ALA:O	2.16	0.46
15:O:181:ARG:NH1	15:O:181:ARG:CG	2.77	0.46
2:B:679:GLN:HG3	14:N:155:VAL:O	2.14	0.46
3:C:71:MET:HE1	3:C:302:VAL:CG2	2.40	0.46
9:I:23:VAL:O	9:I:39:LYS:NZ	2.48	0.46
11:K:93:ILE:HA	11:K:94:PRO:HD2	1.75	0.46
15:O:148:PRO:HB3	15:O:183:ILE:HD13	1.98	0.46
15:O:433:LYS:HG3	15:O:433:LYS:O	2.16	0.46
15:O:74:ILE:O	15:O:78:VAL:HG13	2.16	0.46
2:B:280:LEU:HD13	2:B:371:PHE:N	2.30	0.46
4:D:95:ASP:HB2	7:G:151:ASP:CB	2.46	0.46
1:A:211:THR:HG23	5:E:177:ARG:CZ	2.45	0.46
15:O:506:PHE:HD2	15:O:537:VAL:CG1	2.28	0.46
1:A:411:VAL:CG2	1:A:412:SER:N	2.76	0.46
1:A:507:TYR:HB2	1:A:637:PHE:CZ	2.51	0.46
2:B:467:THR:O	2:B:469:ASN:N	2.49	0.46
7:G:141:SER:HB2	15:O:138:TYR:CZ	2.43	0.46
7:G:143:SER:HB3	15:O:102:SER:C	2.35	0.46
15:O:352:LEU:HA	15:O:358:VAL:CG2	2.31	0.46
1:A:1028:GLU:HG3	1:A:1637:PRO:HG2	1.97	0.46
1:A:94:LEU:HD11	1:A:356:PHE:CZ	2.51	0.46
2:B:265:ARG:NH2	2:B:339:GLN:OE1	2.48	0.46
1:A:1003:ARG:CD	2:B:520:LEU:CB	2.93	0.46
2:B:822:THR:HB	2:B:823:GLN:HG3	1.98	0.46
4:D:48:GLU:CG	4:D:86:ILE:HD12	2.39	0.46
2:B:202:LEU:HD13	2:B:500:PHE:CE1	2.51	0.46
3:C:57:ILE:CA	3:C:297:HIS:HA	2.09	0.46
3:C:50:ARG:O	3:C:303:GLU:CA	2.58	0.46
4:D:25:THR:CB	6:F:59:GLN:HG2	2.39	0.46
15:O:459:GLU:O	15:O:463:GLN:CB	2.63	0.46
15:O:447:THR:HB	15:O:505:PHE:CE2	2.51	0.46
1:A:1575:ILE:HG13	9:I:122:ARG:NH1	2.29	0.46
1:A:184:LYS:HA	1:A:187:GLU:HG2	1.98	0.46
1:A:5:LYS:HE2	1:A:5:LYS:HB3	1.68	0.46
2:B:774:ALA:HB1	2:B:1026:ILE:HD11	1.97	0.46
2:B:1120:ILE:CD1	15:O:117:GLN:NE2	2.79	0.46
1:A:438:ILE:CG2	2:B:1192:MET:CE	2.92	0.46
2:B:890:ASP:HB3	2:B:896:GLN:OE1	2.15	0.46
3:C:31:TRP:NE1	11:K:78:TYR:OH	2.46	0.46
5:E:131:THR:HG21	5:E:191:LYS:CE	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:239:SER:O	15:O:243:GLU:HG2	2.16	0.46
1:A:412:SER:HB3	1:A:414:GLU:HB3	1.96	0.46
2:B:293:ILE:CD1	2:B:302:LEU:HB3	2.46	0.46
2:B:554:GLN:C	2:B:646:HIS:CD2	2.90	0.46
1:A:618:TYR:CE1	2:B:783:MET:HB2	2.50	0.46
4:D:92:ILE:CD1	7:G:152:ALA:HB1	2.45	0.46
15:O:467:MET:HE1	15:O:470:PHE:HE2	1.81	0.46
1:A:1019:LEU:CD1	1:A:1227:MET:CG	2.91	0.45
1:A:1608:SER:OG	1:A:1632:GLU:OE2	2.20	0.45
2:B:724:GLN:O	2:B:1037:ARG:HG3	2.17	0.45
2:B:292:ILE:HB	2:B:306:LEU:HD11	1.98	0.45
4:D:28:PRO:CB	7:G:24:VAL:HG11	2.46	0.45
13:M:26:PHE:CE1	13:M:98:SER:HB2	2.51	0.45
15:O:428:ILE:CG2	15:O:439:ILE:CG2	2.86	0.45
15:O:506:PHE:CG	15:O:528:PHE:HZ	2.34	0.45
1:A:954:GLY:N	1:A:1205:PHE:CB	2.79	0.45
1:A:436:ALA:O	1:A:440:SER:N	2.49	0.45
2:B:552:SER:C	2:B:647:SER:H	2.16	0.45
4:D:40:LEU:HD13	4:D:93:GLN:HB2	1.98	0.45
9:I:89:CYS:SG	9:I:91:ASN:HB2	2.56	0.45
11:K:80:ILE:HD13	11:K:105:ILE:HD11	1.98	0.45
15:O:485:CYS:SG	15:O:531:ILE:HD12	2.56	0.45
15:O:458:GLU:HG3	15:O:514:PHE:CE2	2.51	0.45
2:B:68:ILE:CD1	2:B:414:LYS:HG3	2.41	0.45
2:B:480:GLN:CB	2:B:507:SER:OG	2.64	0.45
3:C:228:ARG:HG3	3:C:299:ILE:HB	1.98	0.45
3:C:54:PHE:CD1	3:C:300:PHE:O	2.69	0.45
15:O:190:ILE:HD13	15:O:190:ILE:C	2.37	0.45
15:O:245:GLN:O	15:O:248:LEU:N	2.39	0.45
15:O:370:THR:O	15:O:374:PRO:CG	2.63	0.45
15:O:459:GLU:O	15:O:463:GLN:N	2.50	0.45
15:O:69:THR:HG22	15:O:70:GLN:N	2.31	0.45
1:A:1237:GLN:H	1:A:1544:ASN:HB2	1.81	0.45
2:B:841:ASP:OD1	2:B:842:GLU:N	2.40	0.45
3:C:294:VAL:HG12	3:C:294:VAL:O	2.15	0.45
3:C:295:ARG:HD3	3:C:295:ARG:HA	1.66	0.45
2:B:1020:GLU:HG3	3:C:61:THR:OG1	2.17	0.45
7:G:143:SER:CB	15:O:103:ASN:HA	2.46	0.45
15:O:169:THR:O	15:O:170:VAL:C	2.54	0.45
1:A:1006:LEU:HD21	2:B:535:ASP:HB2	1.98	0.45
1:A:1657:LEU:HD22	7:G:104:LEU:CD1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:ASP:O	1:A:785:GLN:N	2.27	0.45
1:A:863:ASN:ND2	9:I:67:VAL:C	2.70	0.45
1:A:953:GLU:HG2	1:A:1205:PHE:CD2	2.50	0.45
2:B:61:LEU:HA	2:B:61:LEU:HD23	1.76	0.45
2:B:646:HIS:O	2:B:647:SER:HB2	2.16	0.45
1:A:1048:PHE:HZ	5:E:211:TYR:HB2	1.81	0.45
7:G:242:VAL:HG12	15:O:185:SER:CB	2.46	0.45
15:O:372:VAL:CG1	15:O:423:TYR:OH	2.64	0.45
1:A:1348:VAL:CA	2:B:268:GLU:O	2.63	0.45
2:B:585:CYS:HB2	2:B:595:TRP:CZ3	2.51	0.45
4:D:80:THR:CG2	15:O:227:PHE:CG	2.99	0.45
6:F:75:PRO:HG3	6:F:78:GLN:CD	2.37	0.45
1:A:891:ILE:CD1	9:I:71:LEU:N	2.80	0.45
15:O:148:PRO:HB3	15:O:183:ILE:CD1	2.46	0.45
15:O:407:SER:CB	15:O:408:PHE:CD1	2.95	0.45
15:O:521:ASN:HD22	15:O:523:ASN:H	1.59	0.45
1:A:799:GLU:CG	1:A:1062:HIS:CG	2.85	0.45
1:A:799:GLU:CG	1:A:1062:HIS:ND1	2.69	0.45
1:A:1154:LEU:O	1:A:1158:SER:HB2	2.17	0.45
1:A:1291:VAL:HG22	1:A:1473:LYS:HG3	1.99	0.45
1:A:1657:LEU:HD11	6:F:135:ARG:HB2	1.98	0.45
2:B:205:MET:HE1	2:B:500:PHE:O	2.16	0.45
3:C:117:ASP:OD1	3:C:119:ASN:ND2	2.44	0.45
3:C:176:SER:O	3:C:180:ALA:HB2	2.16	0.45
13:M:65:TYR:HE1	13:M:97:VAL:HB	1.81	0.45
15:O:369:LYS:HE3	15:O:370:THR:HG22	1.99	0.45
15:O:384:ILE:HA	15:O:602:TYR:OH	2.16	0.45
15:O:408:PHE:HZ	15:O:446:LEU:CD2	2.30	0.45
15:O:468:GLU:O	15:O:470:PHE:N	2.49	0.45
1:A:878:ARG:NE	9:I:67:VAL:HG13	2.30	0.45
2:B:1158:ILE:HA	2:B:1167:PHE:O	2.17	0.45
5:E:7:ARG:O	5:E:11:ARG:HG3	2.17	0.45
15:O:237:ILE:HG22	15:O:381:ILE:CB	2.44	0.45
15:O:98:ASP:OD2	15:O:135:LYS:CD	2.64	0.45
1:A:1463:ASP:HB2	1:A:1469:TRP:CE2	2.52	0.45
3:C:57:ILE:HG13	3:C:296:ASN:O	2.17	0.45
11:K:49:LEU:HG	11:K:54:THR:HG21	1.98	0.45
3:C:71:MET:CB	3:C:225:ALA:HB3	2.47	0.45
5:E:144:ILE:HG13	5:E:145:THR:N	2.32	0.45
4:D:22:ILE:O	7:G:76:LYS:HG2	2.17	0.45
13:M:61:GLU:OE2	13:M:106:LYS:NZ	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1054:ALA:HB1	1:A:1178:LEU:HD22	1.98	0.44
3:C:231:PRO:HG2	3:C:270:ALA:C	2.37	0.44
7:G:163:PRO:HG2	7:G:166:TRP:CD1	2.53	0.44
1:A:878:ARG:NH2	9:I:66:VAL:HG23	2.32	0.44
15:O:426:SER:HB3	15:O:594:TYR:CD2	2.50	0.44
15:O:426:SER:OG	15:O:594:TYR:C	2.54	0.44
1:A:54:LEU:HD13	1:A:368:ARG:NH2	2.33	0.44
1:A:799:GLU:HG3	1:A:1062:HIS:CD2	2.49	0.44
2:B:470:LEU:HD22	2:B:478:LEU:HD12	1.99	0.44
2:B:683:ASN:HA	14:N:150:TYR:CZ	2.53	0.44
15:O:143:LEU:HD11	15:O:150:TRP:HD1	1.77	0.44
15:O:156:MET:CE	15:O:193:TYR:CE1	3.00	0.44
1:A:437:PHE:CE2	1:A:456:VAL:HG21	2.52	0.44
1:A:480:ALA:HA	2:B:1046:VAL:HA	1.97	0.44
2:B:833:PRO:HG2	2:B:836:TRP:CZ2	2.52	0.44
5:E:78:LEU:HD13	5:E:107:THR:HB	1.98	0.44
5:E:177:ARG:HD3	5:E:215:MET:HB2	1.99	0.44
7:G:154:ASN:ND2	15:O:182:MET:HE1	2.26	0.44
15:O:488:HIS:CE1	15:O:489:ASN:OD1	2.71	0.44
1:A:1441:LYS:HB3	1:A:1441:LYS:HE2	1.75	0.44
1:A:257:ASN:OD1	1:A:258:GLU:N	2.51	0.44
1:A:35:PRO:CA	1:A:390:LEU:HD13	2.47	0.44
2:B:107:PRO:HG2	2:B:133:TYR:CZ	2.52	0.44
2:B:468:GLY:O	2:B:484:TYR:HD2	2.01	0.44
2:B:786:ALA:HB1	2:B:928:SER:HB2	1.98	0.44
3:C:131:THR:HG22	3:C:208:CYS:C	2.35	0.44
3:C:230:LEU:CG	3:C:231:PRO:HD2	2.48	0.44
2:B:1020:GLU:OE2	3:C:61:THR:HG21	2.18	0.44
3:C:272:LYS:HA	14:N:175:TYR:CE2	2.53	0.44
1:A:1229:ALA:HB3	1:A:1597:ALA:HB2	1.99	0.44
1:A:1600:ARG:NH2	1:A:1617:THR:OG1	2.48	0.44
1:A:37:VAL:HG12	1:A:38:LEU:HG	2.00	0.44
1:A:891:ILE:HD13	9:I:71:LEU:CB	2.44	0.44
1:A:920:PHE:CD1	1:A:921:PRO:HA	2.52	0.44
2:B:399:HIS:C	2:B:400:GLN:CG	2.86	0.44
3:C:252:PRO:HD2	3:C:255:VAL:HG21	1.99	0.44
4:D:48:GLU:OE2	4:D:90:LYS:NZ	2.51	0.44
10:J:36:LEU:HD13	10:J:47:ARG:HB3	1.98	0.44
15:O:163:ILE:CG2	15:O:211:TYR:HB2	2.38	0.44
15:O:368:PHE:HE2	15:O:382:GLN:HA	1.81	0.44
15:O:391:GLN:CD	15:O:609:TYR:OH	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1313:LEU:O	1:A:1317:ILE:HD12	2.18	0.44
1:A:1654:PHE:HA	6:F:135:ARG:O	2.17	0.44
2:B:190:ILE:HG13	2:B:191:GLY:N	2.32	0.44
2:B:910:THR:OG1	2:B:912:GLN:NE2	2.51	0.44
2:B:954:PHE:H	2:B:955:PRO:HD2	1.83	0.44
2:B:974:LEU:O	10:J:47:ARG:NH1	2.50	0.44
12:L:63:ARG:HD2	12:L:63:ARG:HA	1.74	0.44
15:O:158:LEU:HD22	15:O:172:HIS:CG	2.52	0.44
15:O:237:ILE:HG22	15:O:381:ILE:CD1	2.34	0.44
15:O:581:THR:HA	15:O:584:GLN:CD	2.37	0.44
1:A:1023:LEU:CD2	1:A:1598:PHE:CE1	3.01	0.44
1:A:509:GLU:CG	1:A:579:ARG:HE	2.31	0.44
1:A:1:MET:CB	2:B:1098:TYR:CG	2.98	0.44
2:B:938:PHE:CD1	3:C:68:ARG:NH2	2.86	0.44
4:D:28:PRO:HB2	7:G:24:VAL:CG1	2.47	0.44
5:E:93:MET:CG	5:E:120:ALA:HB1	2.46	0.44
15:O:78:VAL:HA	15:O:88:ILE:HG22	2.00	0.44
1:A:1660:VAL:O	7:G:102:GLU:CA	2.50	0.44
1:A:782:ASP:O	1:A:783:LYS:C	2.56	0.44
2:B:78:PRO:O	2:B:79:LEU:HB3	2.17	0.44
15:O:128:LEU:HB3	15:O:129:PRO:HD2	1.97	0.44
15:O:237:ILE:HD13	15:O:384:ILE:HD11	2.00	0.44
1:A:507:TYR:CD2	1:A:508:PRO:O	2.70	0.44
3:C:55:ASP:CG	3:C:299:ILE:CG1	2.47	0.44
15:O:412:GLU:OE1	15:O:412:GLU:HA	2.18	0.44
15:O:458:GLU:CB	15:O:461:VAL:HG21	2.47	0.44
15:O:515:ASN:N	15:O:516:PRO:HD3	2.33	0.44
15:O:76:ASN:O	15:O:80:LEU:HD13	2.18	0.44
1:A:1:MET:CB	2:B:1098:TYR:CD1	3.01	0.43
1:A:34:ASN:C	1:A:390:LEU:HD13	2.38	0.43
1:A:509:GLU:OE2	1:A:579:ARG:NH2	2.51	0.43
1:A:677:GLY:HA3	1:A:786:TYR:OH	2.18	0.43
3:C:230:LEU:CG	3:C:231:PRO:CD	2.96	0.43
6:F:76:LYS:C	6:F:78:GLN:H	2.22	0.43
6:F:75:PRO:CG	6:F:78:GLN:CD	2.87	0.43
4:D:96:PHE:CE1	7:G:150:HIS:CD2	3.06	0.43
15:O:174:ASP:C	15:O:177:LYS:HG2	2.36	0.43
15:O:607:LYS:HE2	15:O:607:LYS:HB2	1.88	0.43
15:O:56:VAL:CG2	15:O:99:ILE:HD12	2.48	0.43
1:A:1028:GLU:HA	1:A:1187:ILE:HG12	2.00	0.43
1:A:1261:VAL:HG21	1:A:1306:TYR:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:26:SER:O	9:I:39:LYS:HB2	2.18	0.43
2:B:563:SER:HB2	13:M:73:SER:HB3	2.00	0.43
15:O:194:LEU:HD21	15:O:225:LEU:HD11	1.96	0.43
15:O:458:GLU:HA	15:O:461:VAL:HG23	0.48	0.43
1:A:36:THR:HG22	1:A:45:VAL:HG21	2.00	0.43
1:A:403:LEU:HA	1:A:403:LEU:HD12	1.79	0.43
1:A:436:ALA:HA	1:A:443:ALA:HB2	1.99	0.43
1:A:509:GLU:HA	1:A:509:GLU:OE1	2.18	0.43
1:A:782:ASP:C	1:A:784:SER:N	2.71	0.43
2:B:1069:ILE:CG2	2:B:1070:ARG:N	2.73	0.43
2:B:203:ILE:HB	2:B:405:GLY:HA3	2.00	0.43
1:A:718:THR:HG21	8:H:118:PHE:O	2.18	0.43
14:N:87:TYR:CD1	14:N:141:GLU:HA	2.53	0.43
15:O:413:ALA:HB1	15:O:415:GLU:OE1	2.18	0.43
1:A:535:GLN:HA	1:A:546:LEU:HG	1.99	0.43
3:C:64:ALA:HB2	3:C:298:PHE:CE2	2.51	0.43
15:O:245:GLN:CG	15:O:378:THR:HG23	2.48	0.43
15:O:383:TYR:O	15:O:386:PHE:N	2.51	0.43
15:O:460:GLU:O	15:O:469:ARG:CZ	2.66	0.43
1:A:1606:SER:HB3	1:A:1611:MET:CE	2.47	0.43
2:B:209:GLN:CG	2:B:210:ARG:N	2.76	0.43
3:C:84:TYR:CZ	12:L:66:GLN:OE1	2.60	0.43
13:M:8:SER:O	14:N:71:PRO:HA	2.19	0.43
14:N:40:LEU:HD12	14:N:40:LEU:HA	1.84	0.43
14:N:94:ASP:HB3	14:N:99:LEU:HG	2.00	0.43
15:O:173:HIS:HE1	15:O:214:ASN:O	2.02	0.43
15:O:431:ALA:HB3	15:O:434:LEU:HD21	2.00	0.43
15:O:434:LEU:HD23	15:O:439:ILE:HG13	2.00	0.43
2:B:236:ILE:HG21	2:B:377:MET:HE1	1.99	0.43
2:B:893:ASN:O	2:B:895:PHE:HD1	2.01	0.43
15:O:66:ASN:CG	15:O:111:ARG:NH1	2.72	0.43
15:O:189:PHE:HA	15:O:192:THR:HG23	1.99	0.43
15:O:232:LEU:HA	15:O:232:LEU:HD12	1.74	0.43
15:O:352:LEU:HD23	15:O:358:VAL:HG23	1.85	0.43
1:A:399:LEU:CD1	1:A:423:LEU:HG	2.44	0.43
15:O:377:TYR:CD2	15:O:377:TYR:O	2.70	0.43
1:A:1600:ARG:NH2	1:A:1621:PHE:CE2	2.86	0.43
2:B:29:PRO:O	2:B:177:PRO:HD2	2.18	0.43
2:B:699:ILE:O	2:B:703:LEU:HG	2.19	0.43
2:B:923:GLN:HG2	2:B:949:ILE:CD1	2.47	0.43
7:G:29:ASP:OD1	7:G:30:GLU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:356:GLU:HA	15:O:356:GLU:OE1	2.19	0.43
15:O:412:GLU:O	15:O:413:ALA:C	2.57	0.43
15:O:487:ARG:HG3	15:O:487:ARG:NH1	2.34	0.43
1:A:1305:GLU:CD	9:I:63:LYS:HE3	2.39	0.43
2:B:399:HIS:O	2:B:400:GLN:HG2	2.18	0.43
2:B:555:GLN:N	2:B:646:HIS:NE2	2.67	0.43
2:B:1017:ALA:C	3:C:65:ASN:ND2	2.72	0.43
15:O:169:THR:O	15:O:172:HIS:N	2.52	0.43
4:D:80:THR:HB	15:O:227:PHE:CD2	2.50	0.43
15:O:48:SER:O	15:O:49:ALA:C	2.57	0.43
1:A:1575:ILE:HG12	9:I:122:ARG:NH1	2.28	0.43
1:A:407:GLN:HB3	1:A:409:ASP:OD2	2.19	0.43
2:B:742:TYR:CE2	2:B:1037:ARG:HD3	2.54	0.43
1:A:1657:LEU:HD21	6:F:135:ARG:NH2	2.34	0.43
15:O:124:LYS:O	15:O:127:GLU:HB2	2.18	0.43
15:O:225:LEU:CD1	15:O:225:LEU:C	2.86	0.43
1:A:1070:LEU:C	1:A:1072:ASN:H	2.21	0.42
1:A:1172:LEU:O	1:A:1176:ARG:HG2	2.19	0.42
2:B:883:GLU:HG3	2:B:906:ARG:HB2	2.01	0.42
14:N:63:ASP:OD2	14:N:66:LYS:NZ	2.35	0.42
15:O:390:GLN:NE2	15:O:431:ALA:HA	2.34	0.42
2:B:550:ARG:HD3	2:B:550:ARG:HA	1.80	0.42
6:F:66:ARG:NH1	7:G:90:LEU:CD1	2.82	0.42
12:L:32:ALA:HB3	12:L:55:ILE:HG23	2.01	0.42
15:O:156:MET:HG2	15:O:197:PHE:CZ	2.53	0.42
15:O:199:PRO:HD3	15:O:211:TYR:CG	2.54	0.42
15:O:457:ARG:HA	15:O:460:GLU:CG	2.49	0.42
15:O:96:LEU:O	15:O:100:LEU:HG	2.20	0.42
1:A:953:GLU:CA	1:A:1205:PHE:CD2	2.97	0.42
1:A:550:SER:OG	1:A:553:GLN:HG3	2.19	0.42
1:A:938:VAL:HG22	9:I:82:ILE:HD13	2.00	0.42
2:B:300:SER:OG	9:I:49:THR:HG23	2.17	0.42
2:B:569:GLY:CA	14:N:140:SER:OG	2.66	0.42
3:C:55:ASP:HB3	3:C:297:HIS:HE2	1.80	0.42
15:O:173:HIS:NE2	15:O:217:LYS:HB3	2.35	0.42
15:O:336:LEU:HD11	15:O:380:SER:O	2.19	0.42
1:A:1034:TYR:HA	1:A:1181:PRO:CB	2.49	0.42
1:A:998:HIS:NE2	2:B:712:SER:N	2.55	0.42
3:C:57:ILE:HB	3:C:297:HIS:CE1	2.55	0.42
6:F:93:ILE:HA	6:F:93:ILE:HD13	1.70	0.42
14:N:70:LEU:HA	14:N:71:PRO:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:404:ILE:CD1	15:O:442:VAL:HG11	2.49	0.42
15:O:430:ARG:HH22	15:O:596:PRO:CD	2.25	0.42
15:O:515:ASN:HD21	15:O:547:ASN:HD21	1.67	0.42
2:B:1082:HIS:HB3	2:B:1084:THR:HG23	2.01	0.42
2:B:211:ARG:CB	2:B:239:VAL:CG1	2.98	0.42
2:B:809:VAL:HG13	2:B:901:VAL:HB	2.01	0.42
3:C:31:TRP:CE3	11:K:82:LYS:CB	3.02	0.42
4:D:44:ILE:HG21	4:D:90:LYS:CE	2.45	0.42
7:G:160:ASN:OD1	7:G:160:ASN:N	2.52	0.42
9:I:60:LEU:CA	9:I:63:LYS:HG3	2.45	0.42
15:O:369:LYS:CD	15:O:369:LYS:C	2.86	0.42
1:A:990:ILE:CB	1:A:994:GLU:HB2	2.41	0.42
1:A:475:ARG:NH1	2:B:1061:LYS:HA	2.35	0.42
2:B:399:HIS:C	2:B:400:GLN:HG3	2.40	0.42
2:B:57:ASP:N	2:B:57:ASP:OD1	2.52	0.42
1:A:1655:ASP:HB2	6:F:135:ARG:CG	2.49	0.42
2:B:890:ASP:O	12:L:54:ARG:CD	2.68	0.42
15:O:124:LYS:HD3	15:O:127:GLU:OE2	2.20	0.42
15:O:202:ASN:N	15:O:202:ASN:OD1	2.52	0.42
15:O:234:ILE:HD13	15:O:234:ILE:HA	1.74	0.42
15:O:468:GLU:HG2	15:O:469:ARG:N	2.33	0.42
1:A:999:CYS:SG	2:B:531:VAL:HG22	2.59	0.42
11:K:50:LEU:O	11:K:54:THR:HG23	2.20	0.42
13:M:102:SER:O	13:M:106:LYS:CB	2.56	0.42
7:G:159:LYS:HD2	15:O:103:ASN:CG	2.39	0.42
15:O:413:ALA:C	15:O:415:GLU:N	2.72	0.42
1:A:1003:ARG:HD2	2:B:520:LEU:HB3	2.02	0.42
1:A:478:TYR:HA	2:B:1048:SER:HA	0.57	0.42
2:B:469:ASN:HA	2:B:482:SER:HA	2.00	0.42
2:B:478:LEU:HB3	2:B:484:TYR:OH	2.20	0.42
2:B:697:LEU:HB2	2:B:702:ASN:ND2	2.35	0.42
2:B:938:PHE:CE2	3:C:68:ARG:HD2	2.54	0.42
1:A:1575:ILE:CG1	9:I:122:ARG:HH22	2.32	0.42
15:O:447:THR:HG21	15:O:480:LEU:HD21	2.02	0.42
15:O:447:THR:HB	15:O:505:PHE:CZ	2.55	0.42
1:A:660:PRO:O	1:A:1057:ILE:HG21	2.20	0.42
3:C:116:VAL:HG11	3:C:125:LYS:HE3	2.01	0.42
2:B:881:TYR:CZ	12:L:67:PHE:HE1	2.37	0.42
15:O:66:ASN:ND2	15:O:111:ARG:CZ	2.83	0.42
15:O:129:PRO:HD2	15:O:132:THR:CB	2.25	0.42
15:O:409:ALA:O	15:O:417:LYS:HE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:467:MET:CG	15:O:519:PHE:CZ	2.96	0.42
15:O:77:GLN:HG2	15:O:88:ILE:HB	2.01	0.42
1:A:953:GLU:C	1:A:1205:PHE:CG	2.94	0.42
2:B:1017:ALA:O	3:C:65:ASN:ND2	2.53	0.42
3:C:57:ILE:HG13	3:C:297:HIS:HB2	2.02	0.42
2:B:938:PHE:CE1	3:C:68:ARG:CD	3.03	0.42
5:E:67:GLU:CD	5:E:67:GLU:H	2.23	0.42
4:D:28:PRO:CB	7:G:24:VAL:CG1	2.98	0.42
15:O:370:THR:O	15:O:374:PRO:HG3	2.19	0.42
1:A:1648:ASN:O	1:A:1652:GLY:O	2.38	0.41
1:A:365:THR:C	1:A:367:PHE:N	2.73	0.41
1:A:692:TYR:O	1:A:696:ILE:HG12	2.19	0.41
1:A:478:TYR:O	2:B:1047:ARG:O	2.37	0.41
2:B:211:ARG:HH21	2:B:239:VAL:HG21	1.81	0.41
3:C:236:LEU:HD11	3:C:290:LYS:HG3	2.02	0.41
15:O:173:HIS:CG	15:O:217:LYS:HG3	2.55	0.41
15:O:417:LYS:HD3	15:O:472:HIS:CE1	2.33	0.41
1:A:385:LEU:HD23	1:A:385:LEU:HA	1.88	0.41
1:A:437:PHE:C	1:A:439:ASP:H	2.22	0.41
1:A:507:TYR:CE2	1:A:508:PRO:O	2.73	0.41
1:A:874:GLU:OE2	1:A:878:ARG:HD2	2.20	0.41
2:B:1090:ASP:HA	2:B:1094:ASN:HB2	2.02	0.41
2:B:1020:GLU:CD	3:C:61:THR:HG21	2.40	0.41
8:H:105:GLU:HG2	8:H:115:TYR:HE1	1.84	0.41
14:N:81:THR:HG22	14:N:86:ASP:HB3	2.01	0.41
15:O:56:VAL:HG23	15:O:57:LYS:N	2.35	0.41
15:O:430:ARG:O	15:O:610:TYR:HA	2.20	0.41
1:A:451:VAL:HA	1:A:452:PRO:HD3	1.95	0.41
1:A:680:LEU:O	1:A:728:GLY:HA3	2.21	0.41
2:B:478:LEU:CB	2:B:484:TYR:OH	2.69	0.41
2:B:656:LEU:HD21	2:B:689:VAL:HG12	2.01	0.41
3:C:64:ALA:HB1	3:C:298:PHE:CD2	2.56	0.41
15:O:150:TRP:O	15:O:154:VAL:HG23	2.21	0.41
15:O:234:ILE:HG22	15:O:371:HIS:CD2	2.42	0.41
15:O:458:GLU:HG2	15:O:461:VAL:HG21	2.02	0.41
15:O:592:PHE:HA	15:O:593:PRO:HD3	1.91	0.41
1:A:1248:ASP:OD1	1:A:1517:ARG:NH1	2.49	0.41
1:A:1499:ARG:HG2	1:A:1500:GLN:N	2.35	0.41
1:A:854:GLY:HA3	1:A:974:THR:O	2.21	0.41
1:A:891:ILE:HD12	9:I:71:LEU:N	2.35	0.41
2:B:1094:ASN:O	2:B:1096:SER:N	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:321:GLN:HB3	9:I:32:GLN:HE21	1.84	0.41
2:B:401:GLU:C	2:B:402:VAL:HG23	2.41	0.41
2:B:143:TRP:CE3	2:B:446:MET:HG3	2.54	0.41
2:B:553:THR:C	2:B:646:HIS:HD2	2.23	0.41
3:C:41:GLU:C	3:C:57:ILE:HG22	2.41	0.41
7:G:223:GLU:HG3	7:G:223:GLU:H	1.71	0.41
15:O:108:GLU:HB2	15:O:147:ILE:CD1	2.47	0.41
15:O:201:LYS:HG3	15:O:201:LYS:H	1.59	0.41
15:O:352:LEU:CD2	15:O:358:VAL:CG2	2.56	0.41
15:O:423:TYR:CE1	15:O:593:PRO:HB2	2.55	0.41
1:A:1348:VAL:HA	1:A:1349:PRO:HD3	1.93	0.41
1:A:1242:ILE:HG22	1:A:1536:ILE:HG22	2.01	0.41
2:B:464:PHE:O	2:B:468:GLY:N	2.49	0.41
3:C:84:TYR:HD2	12:L:66:GLN:CB	2.30	0.41
4:D:82:LEU:O	4:D:86:ILE:HG23	2.20	0.41
7:G:24:VAL:O	7:G:25:THR:O	2.39	0.41
3:C:84:TYR:CE2	12:L:66:GLN:HB2	2.47	0.41
7:G:154:ASN:ND2	15:O:182:MET:HE3	2.27	0.41
1:A:1056:ASP:HB3	1:A:1059:LYS:HB2	2.02	0.41
1:A:1:MET:HB2	2:B:1098:TYR:CD2	2.54	0.41
1:A:248:PHE:HD1	1:A:442:LYS:O	2.01	0.41
2:B:211:ARG:O	2:B:212:ASN:HB2	2.21	0.41
2:B:286:ARG:HD2	2:B:286:ARG:HA	1.88	0.41
7:G:139:ILE:CD1	15:O:178:TYR:OH	2.68	0.41
1:A:1305:GLU:HG3	9:I:60:LEU:HG	2.03	0.41
3:C:272:LYS:HG3	14:N:175:TYR:CZ	2.55	0.41
14:N:25:ILE:HA	14:N:26:PRO:HD3	1.84	0.41
1:A:1063:MET:HB3	1:A:1063:MET:HE2	1.85	0.41
2:B:206:LEU:HD23	2:B:206:LEU:HA	1.81	0.41
3:C:80:ALA:HB3	3:C:102:GLY:HA2	2.03	0.41
7:G:28:ILE:HG23	7:G:34:THR:O	2.20	0.41
8:H:95:TYR:HD2	8:H:144:ILE:HD12	1.86	0.41
12:L:33:GLU:HG3	12:L:53:HIS:ND1	2.36	0.41
15:O:241:ASP:HA	15:O:380:SER:CB	2.46	0.41
1:A:1049:MET:C	1:A:1051:GLY:N	2.74	0.41
1:A:1179:ILE:HD11	1:A:1183:GLU:CD	2.40	0.41
3:C:57:ILE:HB	3:C:297:HIS:ND1	2.35	0.41
4:D:23:HIS:CD2	6:F:58:PHE:CE1	3.08	0.41
11:K:54:THR:HG22	11:K:62:SER:H	1.86	0.41
15:O:107:ILE:CG2	15:O:107:ILE:O	2.69	0.41
15:O:115:LEU:O	15:O:119:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:237:ILE:HG21	15:O:381:ILE:CG1	2.51	0.41
1:A:1195:GLU:HB3	1:A:1196:PRO:HD3	2.03	0.41
1:A:1317:ILE:O	1:A:1322:ILE:HG12	2.21	0.41
1:A:1262:LEU:HD22	1:A:1497:ILE:HG12	2.03	0.41
1:A:1575:ILE:HG13	9:I:122:ARG:NH2	2.36	0.41
2:B:1043:LYS:HE2	2:B:1063:ARG:HD2	2.01	0.41
2:B:262:PHE:CE1	2:B:357:ILE:HD13	2.56	0.41
2:B:527:PHE:CE2	2:B:666:PRO:HA	2.55	0.41
8:H:41:ASP:HB2	8:H:121:LEU:HB3	2.02	0.41
9:I:2:SER:HA	9:I:9:PHE:O	2.21	0.41
15:O:107:ILE:CD1	15:O:115:LEU:HD23	2.51	0.41
15:O:147:ILE:HG22	15:O:149:LYS:CB	2.51	0.41
15:O:163:ILE:HD12	15:O:207:LYS:HG2	2.02	0.41
1:A:1074:TYR:CE2	1:A:1159:ASP:HB3	2.54	0.41
1:A:315:ILE:HG13	1:A:319:GLU:HB2	2.03	0.41
1:A:440:SER:C	1:A:442:LYS:N	2.74	0.41
1:A:509:GLU:CG	1:A:579:ARG:CD	2.99	0.41
2:B:1094:ASN:C	2:B:1096:SER:H	2.24	0.41
2:B:279:ALA:HB2	2:B:326:VAL:HG12	2.03	0.41
2:B:545:PHE:CZ	2:B:551:ILE:HD11	2.56	0.41
7:G:50:ALA:HA	7:G:113:PHE:CD2	2.56	0.41
15:O:369:LYS:CB	15:O:369:LYS:HZ3	2.21	0.41
1:A:1037:SER:HA	1:A:1049:MET:HA	2.03	0.41
1:A:700:ILE:HA	1:A:700:ILE:HD13	1.81	0.41
1:A:964:LYS:HE2	1:A:964:LYS:HB3	1.83	0.41
2:B:1069:ILE:CG2	2:B:1070:ARG:H	2.20	0.41
2:B:371:PHE:CE2	2:B:375:LEU:HD11	2.56	0.41
2:B:401:GLU:CG	2:B:402:VAL:N	2.73	0.41
2:B:42:VAL:O	2:B:46:ILE:CG1	2.69	0.41
2:B:699:ILE:HD13	2:B:760:TYR:CD1	2.55	0.41
2:B:736:ARG:NH1	2:B:738:ASP:OD1	2.54	0.41
15:O:194:LEU:O	15:O:232:LEU:CD2	2.57	0.41
15:O:447:THR:O	15:O:450:LEU:CA	2.68	0.41
1:A:411:VAL:CG2	1:A:412:SER:H	2.26	0.40
2:B:416:LYS:HD3	2:B:416:LYS:HA	1.87	0.40
1:A:1006:LEU:CD2	2:B:535:ASP:CB	2.99	0.40
15:O:198:PHE:HD2	15:O:232:LEU:CD2	2.32	0.40
1:A:1055:ILE:HG21	1:A:1060:GLU:CG	2.34	0.40
1:A:1229:ALA:HB1	1:A:1595:TYR:CE2	2.56	0.40
1:A:356:PHE:C	1:A:357:MET:CG	2.86	0.40
1:A:365:THR:O	1:A:367:PHE:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:ILE:HG12	15:O:376:TYR:HE2	1.73	0.40
1:A:556:ALA:HA	15:O:246:ASN:HD22	1.85	0.40
2:B:219:ARG:HA	2:B:220:PRO:HD2	1.73	0.40
2:B:427:GLN:OE1	2:B:452:ARG:NH1	2.54	0.40
2:B:555:GLN:CB	2:B:646:HIS:CE1	3.04	0.40
7:G:41:VAL:HA	7:G:42:PRO:HD3	1.92	0.40
8:H:7:ASP:HA	8:H:57:VAL:O	2.21	0.40
11:K:135:PHE:CE2	11:K:139:ILE:HD11	2.56	0.40
12:L:68:GLU:CG	12:L:69:ALA:N	2.73	0.40
15:O:128:LEU:HD13	15:O:132:THR:HG22	2.02	0.40
15:O:244:LEU:O	15:O:244:LEU:HD23	2.20	0.40
1:A:1008:ASP:OD1	1:A:1202:LEU:HD13	2.19	0.40
1:A:1661:PRO:HA	7:G:101:SER:O	2.21	0.40
1:A:487:ASP:HB2	1:A:615:ARG:HB3	2.02	0.40
3:C:128:ASP:OD1	3:C:128:ASP:N	2.54	0.40
4:D:25:THR:HB	6:F:59:GLN:HG3	2.02	0.40
1:A:756:LYS:HD2	9:I:85:LYS:HZ2	1.61	0.40
15:O:505:PHE:O	15:O:509:MET:HG2	2.21	0.40
1:A:601:MET:HE1	1:A:656:GLN:HB2	2.03	0.40
2:B:467:THR:HB	2:B:469:ASN:HD21	1.81	0.40
2:B:491:ILE:HB	2:B:495:ARG:HD2	2.03	0.40
3:C:45:SER:HB3	3:C:271:ARG:HH22	1.80	0.40
15:O:237:ILE:HB	15:O:381:ILE:HD11	1.92	0.40
15:O:422:GLN:HB3	15:O:593:PRO:HD3	2.02	0.40
1:A:389:VAL:O	1:A:393:SER:HB2	2.22	0.40
1:A:498:PRO:HA	1:A:499:PRO:HD3	1.81	0.40
2:B:168:ASN:O	2:B:169:ARG:HD3	2.21	0.40
4:D:23:HIS:CB	6:F:58:PHE:CD2	3.04	0.40
1:A:1048:PHE:HD2	5:E:210:SER:HG	1.69	0.40
7:G:17:ILE:C	7:G:19:LYS:H	2.25	0.40
8:H:39:THR:O	8:H:123:MET:HA	2.22	0.40
9:I:87:PRO:HG2	9:I:119:TYR:CE2	2.56	0.40
15:O:342:HIS:NE2	15:O:346:GLN:HG3	2.34	0.40
15:O:376:TYR:O	15:O:377:TYR:HB3	2.22	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1464/1664 (88%)	1370 (94%)	82 (6%)	12 (1%)	24	69
2	B	1166/1203 (97%)	1086 (93%)	56 (5%)	24 (2%)	9	51
3	C	303/335 (90%)	278 (92%)	18 (6%)	7 (2%)	8	49
4	D	54/137 (39%)	50 (93%)	2 (4%)	2 (4%)	4	39
5	E	210/215 (98%)	197 (94%)	11 (5%)	2 (1%)	19	65
6	F	98/155 (63%)	94 (96%)	4 (4%)	0	100	100
7	G	189/326 (58%)	171 (90%)	13 (7%)	5 (3%)	7	46
8	H	127/146 (87%)	121 (95%)	6 (5%)	0	100	100
9	I	101/125 (81%)	89 (88%)	9 (9%)	3 (3%)	5	44
10	J	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
11	K	99/142 (70%)	92 (93%)	7 (7%)	0	100	100
12	L	41/70 (59%)	32 (78%)	6 (15%)	3 (7%)	1	21
13	M	103/415 (25%)	93 (90%)	8 (8%)	2 (2%)	10	53
14	N	139/233 (60%)	123 (88%)	13 (9%)	3 (2%)	8	50
15	O	457/627 (73%)	400 (88%)	38 (8%)	19 (4%)	3	35
All	All	4618/5863 (79%)	4259 (92%)	277 (6%)	82 (2%)	15	54

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1606	SER
2	B	111	ASP
2	B	117	VAL
2	B	895	PHE
2	B	1069	ILE
3	C	224	THR
4	D	99	LEU
7	G	25	THR

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Mol	Chain	Res	Type
9	I	41	GLN
15	O	165	PRO
15	O	226	GLY
15	O	325	ILE
15	O	380	SER
15	O	431	ALA
15	O	489	ASN
15	O	521	ASN
1	A	448	SER
1	A	783	LYS
1	A	1533	GLU
2	B	473	GLN
2	B	817	ARG
2	B	1140	LYS
4	D	98	GLY
5	E	50	MET
7	G	27	PRO
9	I	5	GLY
12	L	62	LYS
15	O	374	PRO
15	O	488	HIS
15	O	540	CYS
1	A	450	LYS
1	A	1050	TYR
2	B	34	ALA
2	B	78	PRO
2	B	208	VAL
2	B	209	GLN
2	B	1044	PHE
2	B	1070	ARG
2	B	1095	SER
2	B	1098	TYR
3	C	297	HIS
5	E	146	HIS
7	G	99	ASP
9	I	21	ASN
12	L	46	VAL
13	M	85	LYS
15	O	82	SER
15	O	130	PRO
15	O	457	ARG
15	O	469	ARG

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Mol	Chain	Res	Type
2	B	834	LYS
2	B	1094	ASN
3	C	295	ARG
7	G	100	THR
12	L	43	THR
13	M	36	THR
14	N	115	SER
15	O	148	PRO
15	O	187	MET
1	A	439	ASP
1	A	451	VAL
1	A	564	PRO
1	A	581	ILE
1	A	1049	MET
2	B	80	ASN
2	B	1062	GLY
2	B	1096	SER
3	C	32	ASN
3	C	296	ASN
15	O	377	TYR
1	A	1512	PRO
2	B	1063	ARG
3	C	222	VAL
15	O	147	ILE
3	C	221	PRO
14	N	70	LEU
15	O	128	LEU
2	B	468	GLY
14	N	39	PRO
7	G	28	ILE
2	B	833	PRO
2	B	954	PHE

### 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 PDB entries followed by that with respect to all EM entries.

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	1307/1465 (89%)	1221 (93%)	86 (7%)	21	59
2	B	1027/1053 (98%)	956 (93%)	71 (7%)	19	58
3	C	269/296 (91%)	249 (93%)	20 (7%)	17	55
4	D	55/116 (47%)	49 (89%)	6 (11%)	8	37
5	E	194/197 (98%)	180 (93%)	14 (7%)	18	57
6	F	90/137 (66%)	86 (96%)	4 (4%)	35	70
7	G	170/291 (58%)	158 (93%)	12 (7%)	18	57
8	H	115/128 (90%)	111 (96%)	4 (4%)	43	76
9	I	97/110 (88%)	91 (94%)	6 (6%)	23	61
10	J	64/65 (98%)	57 (89%)	7 (11%)	8	37
11	K	91/130 (70%)	84 (92%)	7 (8%)	16	54
12	L	38/57 (67%)	34 (90%)	4 (10%)	8	39
13	M	95/371 (26%)	85 (90%)	10 (10%)	8	39
14	N	135/220 (61%)	129 (96%)	6 (4%)	35	70
15	O	427/576 (74%)	378 (88%)	49 (12%)	7	35
All	All	4174/5212 (80%)	3868 (93%)	306 (7%)	22	56

All (306) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	40	ASN
1	A	83	VAL
1	A	90	PHE
1	A	117	ARG
1	A	136	LEU
1	A	174	SER
1	A	186	SER
1	A	202	THR
1	A	230	ARG
1	A	257	ASN
1	A	271	ARG
1	A	272	GLN
1	A	273	ASP
1	A	312	SER
1	A	315	ILE
1	A	346	SER
1	A	357	MET

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Mol	Chain	Res	Type
1	A	373	LEU
1	A	379	GLU
1	A	393	SER
1	A	409	ASP
1	A	412	SER
1	A	413	LEU
1	A	439	ASP
1	A	446	ARG
1	A	447	THR
1	A	451	VAL
1	A	503	VAL
1	A	555	LYS
1	A	582	LYS
1	A	611	GLU
1	A	627	ASP
1	A	656	GLN
1	A	661	THR
1	A	666	VAL
1	A	670	ILE
1	A	684	ASP
1	A	708	THR
1	A	709	ARG
1	A	739	VAL
1	A	747	ILE
1	A	758	GLU
1	A	783	LYS
1	A	957	VAL
1	A	966	LEU
1	A	988	SER
1	A	999	CYS
1	A	1004	GLU
1	A	1026	GLN
1	A	1033	SER
1	A	1056	ASP
1	A	1085	LEU
1	A	1098	SER
1	A	1118	VAL
1	A	1123	VAL
1	A	1131	LYS
1	A	1159	ASP
1	A	1162	ASN
1	A	1204	THR

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Mol	Chain	Res	Type
1	A	1215	VAL
1	A	1226	VAL
1	A	1273	THR
1	A	1275	THR
1	A	1276	THR
1	A	1304	GLU
1	A	1310	LYS
1	A	1314	GLN
1	A	1320	GLN
1	A	1441	LYS
1	A	1455	ARG
1	A	1509	HIS
1	A	1531	ASP
1	A	1533	GLU
1	A	1536	ILE
1	A	1571	SER
1	A	1601	GLN
1	A	1604	GLU
1	A	1605	THR
1	A	1607	THR
1	A	1609	SER
1	A	1611	MET
1	A	1632	GLU
1	A	1633	GLN
1	A	1635	ASP
1	A	1645	LYS
2	B	13	THR
2	B	17	ARG
2	B	22	GLU
2	B	53	THR
2	B	57	ASP
2	B	65	VAL
2	B	70	GLU
2	B	79	LEU
2	B	81	SER
2	B	87	ASN
2	B	150	GLU
2	B	187	SER
2	B	202	LEU
2	B	211	ARG
2	B	221	SER
2	B	225	ARG

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Mol	Chain	Res	Type
2	B	228	SER
2	B	231	HIS
2	B	239	VAL
2	B	281	CYS
2	B	300	SER
2	B	305	ARG
2	B	306	LEU
2	B	311	ARG
2	B	315	LYS
2	B	379	ARG
2	B	459	SER
2	B	486	VAL
2	B	537	SER
2	B	583	LEU
2	B	622	ILE
2	B	658	LEU
2	B	720	GLN
2	B	724	GLN
2	B	725	THR
2	B	731	VAL
2	B	753	LYS
2	B	782	ASP
2	B	811	LEU
2	B	813	LEU
2	B	819	ASP
2	B	822	THR
2	B	824	HIS
2	B	829	ASN
2	B	833	PRO
2	B	835	GLU
2	B	839	LYS
2	B	858	ILE
2	B	871	ILE
2	B	883	GLU
2	B	894	LYS
2	B	897	GLU
2	B	977	ILE
2	B	998	GLU
2	B	1026	ILE
2	B	1033	TYR
2	B	1037	ARG
2	B	1043	LYS

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Mol	Chain	Res	Type
2	B	1047	ARG
2	B	1060	VAL
2	B	1070	ARG
2	B	1075	GLU
2	B	1097	ASP
2	B	1100	GLN
2	B	1103	VAL
2	B	1125	THR
2	B	1136	GLU
2	B	1141	LEU
2	B	1163	GLN
2	B	1165	ASN
2	B	1174	THR
3	C	38	LYS
3	C	43	ASN
3	C	50	ARG
3	C	61	THR
3	C	77	SER
3	C	91	VAL
3	C	97	LEU
3	C	118	SER
3	C	131	THR
3	C	142	ARG
3	C	181	ASP
3	C	222	VAL
3	C	224	THR
3	C	228	ARG
3	C	232	GLN
3	C	243	SER
3	C	245	ARG
3	C	277	ARG
3	C	279	VAL
3	C	295	ARG
4	D	15	THR
4	D	29	GLN
4	D	38	GLN
4	D	46	GLU
4	D	80	THR
4	D	99	LEU
5	E	31	THR
5	E	33	GLU
5	E	41	ASP

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Mol	Chain	Res	Type
5	E	74	ASP
5	E	77	SER
5	E	90	VAL
5	E	92	THR
5	E	93	MET
5	E	107	THR
5	E	131	THR
5	E	136	ASN
5	E	142	VAL
5	E	162	ARG
5	E	177	ARG
6	F	59	GLN
6	F	87	LYS
6	F	99	LEU
6	F	109	VAL
7	G	18	LYS
7	G	24	VAL
7	G	35	SER
7	G	39	VAL
7	G	139	ILE
7	G	147	LEU
7	G	167	THR
7	G	169	VAL
7	G	223	GLU
7	G	230	ARG
7	G	239	THR
7	G	243	VAL
8	H	3	ASN
8	H	39	THR
8	H	108	SER
8	H	112	ILE
9	I	2	SER
9	I	15	ASP
9	I	45	LEU
9	I	70	SER
9	I	74	ASN
9	I	81	THR
10	J	3	VAL
10	J	9	SER
10	J	10	CYS
10	J	14	VAL
10	J	27	GLU

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Mol	Chain	Res	Type
10	J	45	CYS
10	J	48	ARG
11	K	45	GLU
11	K	51	THR
11	K	68	GLU
11	K	99	ASN
11	K	118	GLN
11	K	123	ASP
11	K	133	SER
12	L	38	LEU
12	L	55	ILE
12	L	60	ARG
12	L	66	GLN
13	M	17	ASP
13	M	18	GLN
13	M	31	ARG
13	M	44	LYS
13	M	48	LYS
13	M	65	TYR
13	M	77	VAL
13	M	84	GLU
13	M	98	SER
13	M	109	ARG
14	N	51	GLN
14	N	124	THR
14	N	135	LYS
14	N	153	VAL
14	N	167	LYS
14	N	178	GLU
15	O	66	ASN
15	O	67	ASP
15	O	69	THR
15	O	78	VAL
15	O	80	LEU
15	O	87	ARG
15	O	101	SER
15	O	111	ARG
15	O	117	GLN
15	O	149	LYS
15	O	171	CYS
15	O	175	MET
15	O	180	LEU

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Mol	Chain	Res	Type
15	O	181	ARG
15	O	190	ILE
15	O	192	THR
15	O	202	ASN
15	O	203	ASP
15	O	204	THR
15	O	205	ARG
15	O	212	THR
15	O	213	SER
15	O	215	LEU
15	O	228	GLN
15	O	232	LEU
15	O	234	ILE
15	O	245	GLN
15	O	248	LEU
15	O	341	THR
15	O	350	GLU
15	O	354	SER
15	O	363	THR
15	O	368	PHE
15	O	369	LYS
15	O	395	LEU
15	O	437	THR
15	O	454	VAL
15	O	457	ARG
15	O	487	ARG
15	O	489	ASN
15	O	494	THR
15	O	495	ASP
15	O	522	GLU
15	O	526	LEU
15	O	540	CYS
15	O	581	THR
15	O	584	GLN
15	O	597	LEU
15	O	602	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	432	ASN
1	A	580	HIS

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Mol	Chain	Res	Type
1	A	863	ASN
1	A	1162	ASN
2	B	328	GLN
2	B	462	GLN
2	B	646	HIS
2	B	912	GLN
2	B	1038	HIS
2	B	1163	GLN
4	D	23	HIS
4	D	93	GLN
6	F	59	GLN
6	F	78	GLN
7	G	126	GLN
7	G	150	HIS
7	G	154	ASN
9	I	32	GLN
12	L	66	GLN
14	N	85	HIS
15	O	66	ASN
15	O	70	GLN
15	O	105	ASN
15	O	117	GLN
15	O	172	HIS
15	O	173	HIS
15	O	245	GLN
15	O	346	GLN
15	O	362	ASN
15	O	371	HIS
15	O	390	GLN
15	O	472	HIS
15	O	497	ASN
15	O	507	GLN
15	O	521	ASN
15	O	547	ASN
15	O	549	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.