



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 14, 2023 – 05:49 PM EDT

PDB ID : 1S3S  
Title : Crystal structure of AAA ATPase p97/VCP ND1 in complex with p47 C  
Authors : Dreveny, I.; Kondo, H.; Uchiyama, K.; Shaw, A.; Zhang, X.; Freemont, P.S.  
Deposited on : 2004-01-14  
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

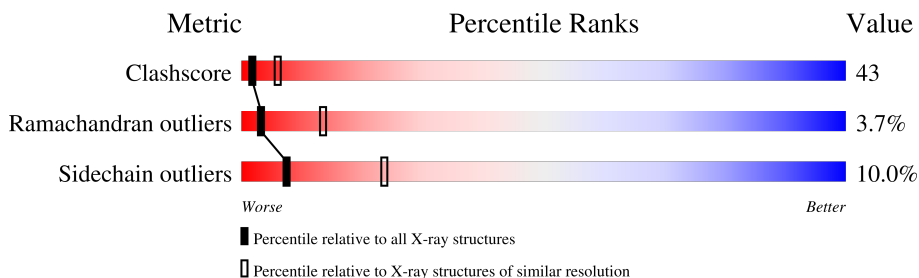
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)


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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	458	45% 44% 5% 5%
1	B	458	41% 44% 9% 5%
1	C	458	43% 45% 8% 5%
1	D	458	36% 53% 7% 5%
1	E	458	35% 54% 6% 5%
1	F	458	47% 41% 7% . .
2	G	127	39% 43% 9% . 7%
2	H	127	26% 47% 10% . 16%

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Mol	Chain	Length	Quality of chain
2	I	127	 12% 6% 81%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 22367 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transitional endoplasmic reticulum ATPase (TER ATPase) (15S Mg(2+)- ATPase p97 subunit) (Valosin containing protein) (VCP) [Contains: Valosin].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3398	2135	601	645	17			
1	B	436	Total	C	N	O	S	0	0	0
			3390	2130	598	645	17			
1	C	437	Total	C	N	O	S	0	0	0
			3405	2139	606	642	18			
1	D	436	Total	C	N	O	S	0	0	0
			3380	2124	598	640	18			
1	E	436	Total	C	N	O	S	0	0	0
			3399	2137	603	641	18			
1	F	441	Total	C	N	O	S	0	0	0
			3432	2157	609	648	18			

- Molecule 2 is a protein called p47 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	118	Total	C	N	O	S	0	0	0
			825	511	153	159	2			
2	H	107	Total	C	N	O	S	0	0	0
			758	474	140	142	2			
2	I	24	Total	C	N	O		0	0	0
			155	99	30	26				

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	F	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total 14	O 14	0	0
4	B	10	Total 10	O 10	0	0
4	C	6	Total 6	O 6	0	0
4	D	7	Total 7	O 7	0	0
4	E	6	Total 6	O 6	0	0
4	F	14	Total 14	O 14	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	G	2	Total O 2 2	0	0
4	H	3	Total O 3 3	0	0
4	I	1	Total O 1 1	0	0

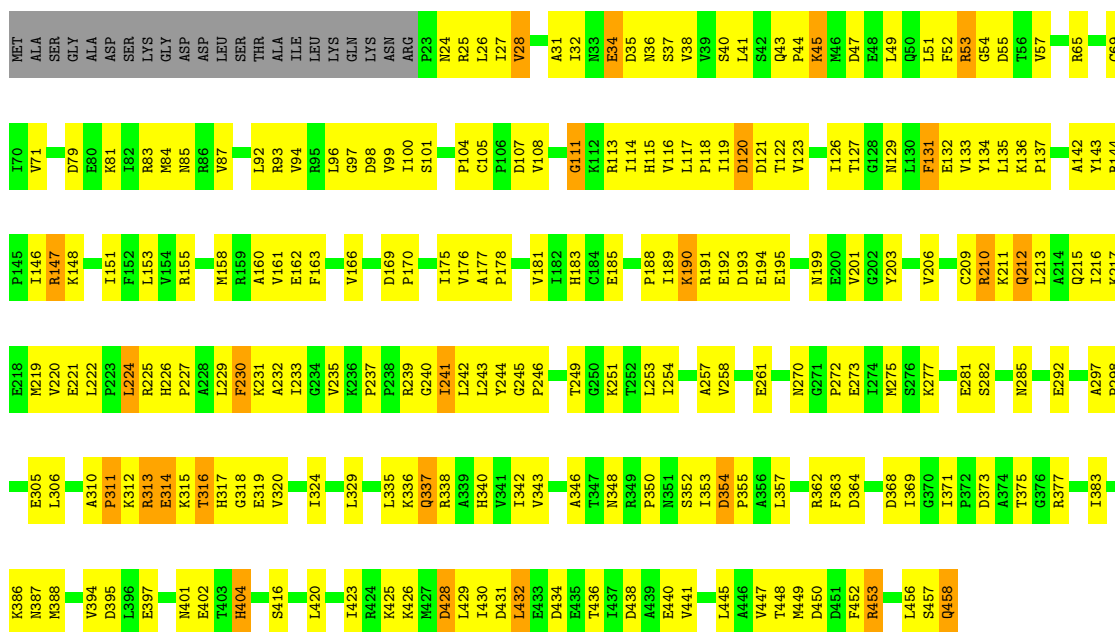
### 3 Residue-property plots

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

Note EDS was not executed.

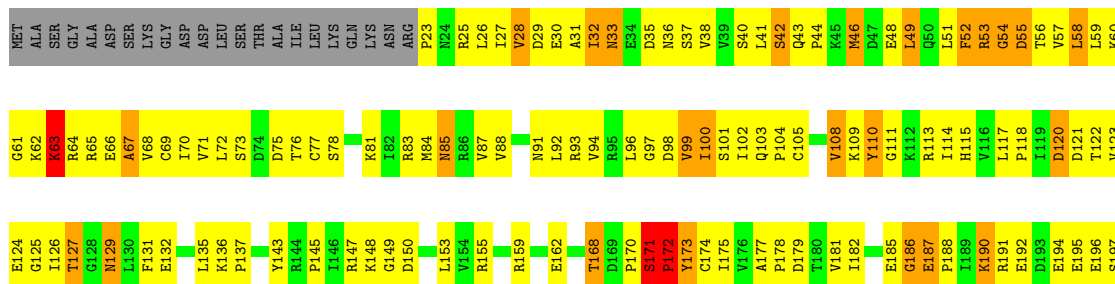
- Molecule 1: Transitional endoplasmic reticulum ATPase (TER ATPase) (15S Mg(2+)- ATPase p97 subunit) (Valosin containing protein) (VCP) [Contains: Valosin]

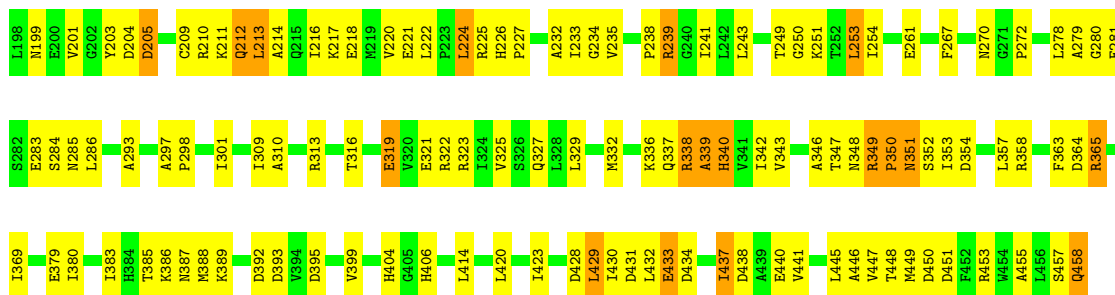
Chain A: 



- Molecule 1: Transitional endoplasmic reticulum ATPase (TER ATPase) (15S Mg(2+)- ATPase p97 subunit) (Valosin containing protein) (VCP) [Contains: Valosin]

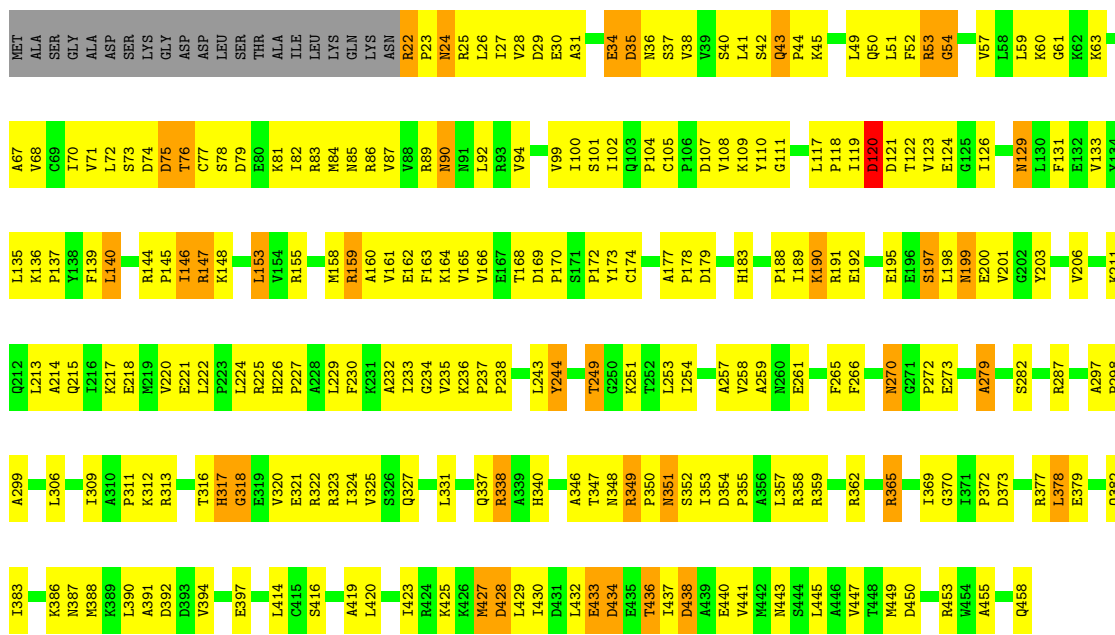
Chain B: 





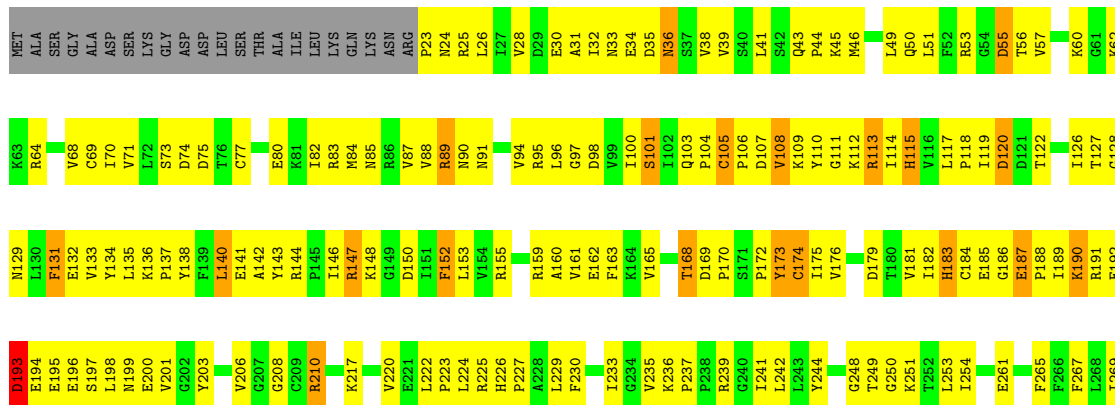
- Molecule 1: Transitional endoplasmic reticulum ATPase (TER ATPase) (15S Mg<sup>2+</sup>)- ATPase p97 subunit) (Valosin containing protein) (VCP) [Contains: Valosin]

Chain C: 43% 45% 8% 5%

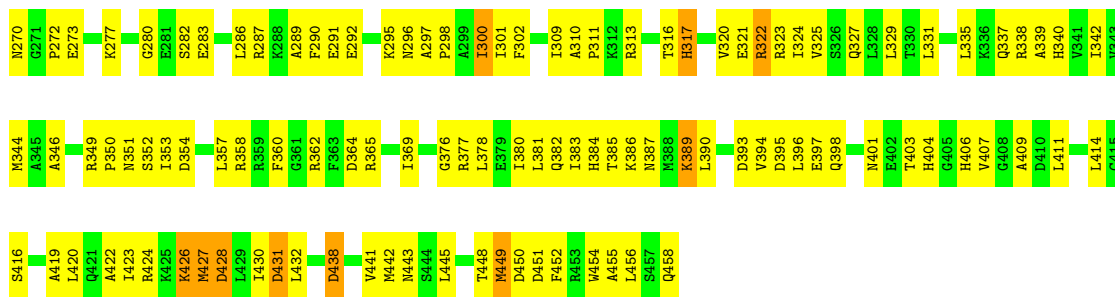


- Molecule 1: Transitional endoplasmic reticulum ATPase (TER ATPase) (15S Mg<sup>2+</sup>)- ATPase p97 subunit) (Valosin containing protein) (VCP) [Contains: Valosin]

Chain D: 36% 53% 7% 5%

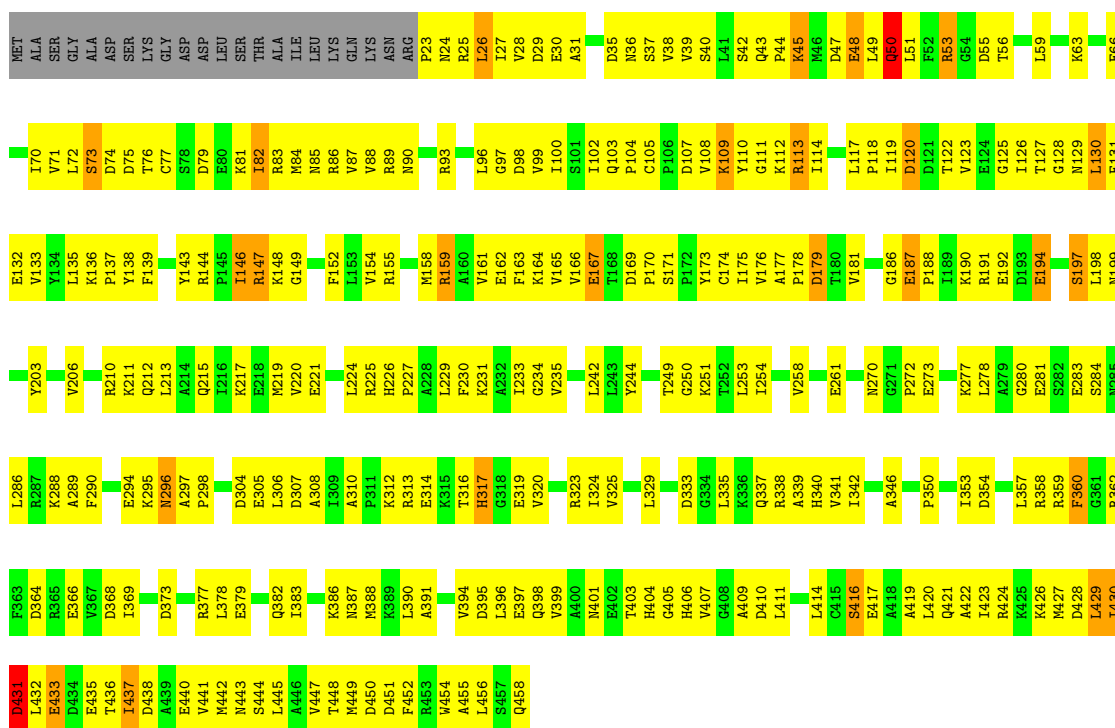






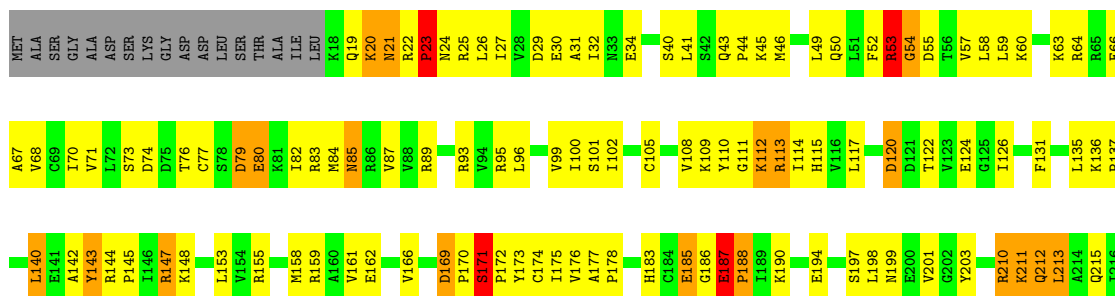
- Molecule 1: Transitional endoplasmic reticulum ATPase (TER ATPase) (15S Mg<sup>2+</sup>)- ATPase p97 subunit) (Valosin containing protein) (VCP) [Contains: Valosin]

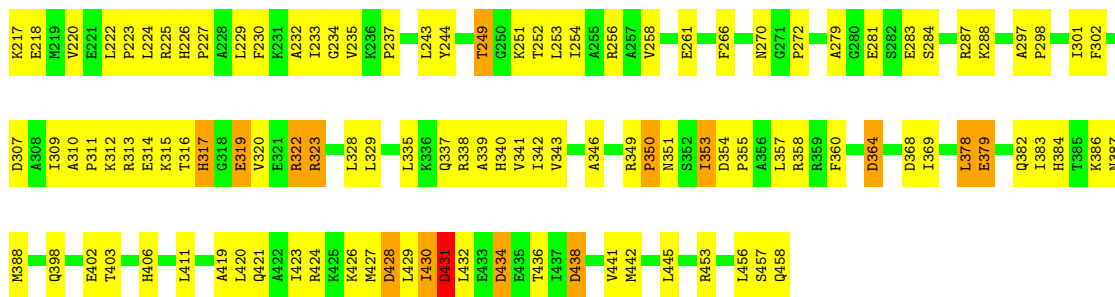
Chain E: 35% 54% 6% 5%



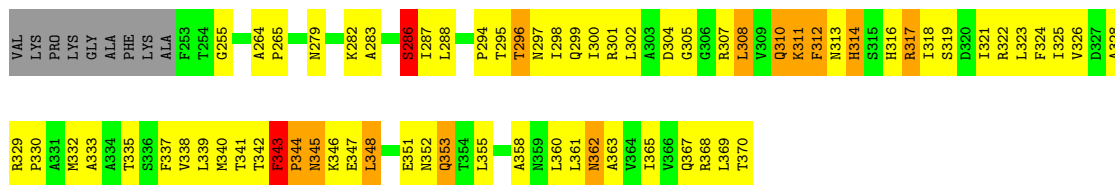
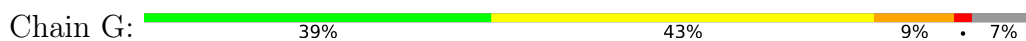
- Molecule 1: Transitional endoplasmic reticulum ATPase (TER ATPase) (15S Mg<sup>2+</sup>)- ATPase p97 subunit) (Valosin containing protein) (VCP) [Contains: Valosin]

Chain F: 47% 41% 7% 5%

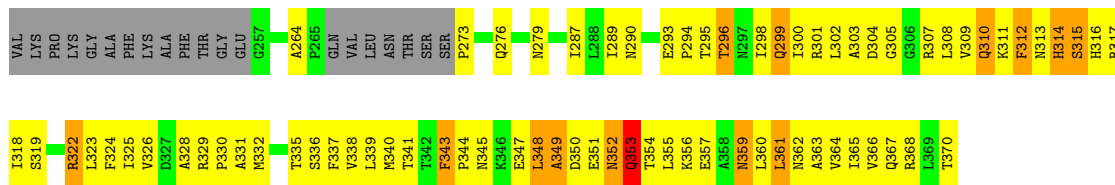




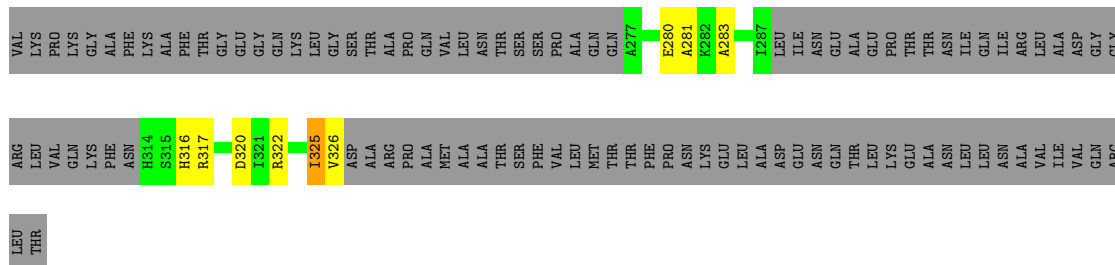
• Molecule 2: p47 protein



• Molecule 2: p47 protein



• Molecule 2: p47 protein



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.72Å 157.72Å 243.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.70 – 2.90	Depositor
% Data completeness (in resolution range)	96.3 (39.70-2.90)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.248 , 0.294	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	22367	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

## 5 Model quality [i](#)

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

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.43	0/3450	0.70	0/4662
1	B	0.43	0/3443	0.75	4/4656 (0.1%)
1	C	0.39	0/3458	0.64	0/4674
1	D	0.39	0/3433	0.67	0/4642
1	E	0.38	0/3452	0.65	2/4664 (0.0%)
1	F	0.46	0/3485	0.73	1/4709 (0.0%)
2	G	0.48	0/833	1.02	6/1135 (0.5%)
2	H	0.51	0/764	1.29	6/1037 (0.6%)
2	I	0.41	0/154	0.63	0/208
All	All	0.42	0/22472	0.73	19/30387 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	343	PHE	C-N-CD	-23.85	68.14	120.60
1	B	171	SER	C-N-CD	-16.94	83.33	120.60
2	G	343	PHE	C-N-CD	-14.94	87.73	120.60
2	H	343	PHE	C-N-CA	13.68	179.44	122.00
1	B	172	PRO	CA-N-CD	-7.27	101.32	111.50
1	F	171	SER	N-CA-C	7.09	130.15	111.00
2	H	314	HIS	N-CA-C	-6.73	92.83	111.00
1	E	186	GLY	N-CA-C	6.54	129.46	113.10
1	B	186	GLY	N-CA-C	6.21	128.63	113.10
2	H	296	THR	N-CA-CB	6.12	121.93	110.30
1	E	192	GLU	N-CA-C	-6.04	94.69	111.00
2	G	286	SER	N-CA-C	6.02	127.24	111.00
2	G	343	PHE	C-N-CA	5.79	146.33	122.00
2	H	353	GLN	N-CA-C	5.52	125.89	111.00
2	G	265	PRO	N-CA-CB	5.46	109.85	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	343	PHE	N-CA-C	5.38	125.54	111.00
2	H	273	PRO	N-CA-CB	5.38	109.76	103.30
1	B	437	ILE	N-CA-C	5.33	125.40	111.00
2	G	341	THR	N-CA-C	-5.05	97.37	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3398	0	3447	231	0
1	B	3390	0	3421	280	0
1	C	3405	0	3452	310	1
1	D	3380	0	3406	353	0
1	E	3399	0	3453	334	0
1	F	3432	0	3477	251	0
2	G	825	0	768	99	1
2	H	758	0	720	118	0
2	I	155	0	132	5	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	1	0
3	D	27	0	12	1	0
3	E	27	0	12	1	0
3	F	27	0	12	2	0
4	A	14	0	0	3	0
4	B	10	0	0	0	0
4	C	6	0	0	0	0
4	D	7	0	0	4	0
4	E	6	0	0	0	0
4	F	14	0	0	1	0
4	G	2	0	0	0	0
4	H	3	0	0	0	0
4	I	1	0	0	0	0
All	All	22367	0	22348	1924	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

All (1924) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:ARG:HG2	1:C:365:ARG:HH11	1.03	1.19
1:A:453:ARG:HH11	1:A:453:ARG:HG3	1.02	1.14
1:D:322:ARG:HG3	1:D:322:ARG:HH11	1.14	1.13
2:G:283:ALA:HB1	2:G:324:PHE:CE1	1.84	1.12
1:D:283:GLU:OE2	1:D:327:GLN:HB2	1.48	1.11
1:C:27:ILE:HB	1:C:81:LYS:HG2	1.31	1.10
2:G:301:ARG:HH12	2:G:308:LEU:HD22	1.13	1.10
2:G:317:ARG:HH11	2:G:317:ARG:HG3	1.15	1.08
1:A:311:PRO:HB2	1:A:315:LYS:HD2	1.08	1.08
1:A:316:THR:HG22	1:A:318:GLY:H	1.14	1.07
1:F:169:ASP:CB	1:F:170:PRO:HD3	1.83	1.07
1:E:244:TYR:HE2	1:E:366:GLU:HB3	1.15	1.07
1:B:51:LEU:HD21	1:B:104:PRO:HG3	1.26	1.06
1:C:230:PHE:HA	1:C:233:ILE:HG22	1.28	1.05
1:D:169:ASP:HB3	1:D:170:PRO:HD3	1.09	1.05
1:E:53:ARG:H	1:E:53:ARG:HD3	1.14	1.05
1:B:238:PRO:HB3	1:B:365:ARG:HD3	1.39	1.05
1:F:233:ILE:HG22	1:F:235:VAL:H	1.15	1.04
2:H:287:ILE:HD13	2:H:289:ILE:HG23	1.06	1.04
1:C:169:ASP:HB3	1:C:170:PRO:HD3	1.38	1.03
2:H:315:SER:OG	2:H:356:LYS:HE3	1.59	1.02
1:D:349:ARG:HE	1:D:351:ASN:HB2	1.23	1.02
1:C:427:MET:HA	1:C:430:ILE:HG22	1.41	1.01
1:D:169:ASP:HB3	1:D:170:PRO:CD	1.91	1.01
1:B:42:SER:HB3	1:B:44:PRO:HD2	1.43	1.00
1:B:52:PHE:H	1:B:52:PHE:HD2	1.03	1.00
1:E:131:PHE:HA	1:E:135:LEU:HD23	1.41	0.99
1:C:43:GLN:HG3	1:C:44:PRO:HD3	1.40	0.98
1:C:338:ARG:H	1:C:338:ARG:HD2	1.26	0.98
2:G:302:LEU:HD12	2:G:307:ARG:HB3	1.44	0.98
2:H:318:ILE:HB	2:H:351:GLU:O	1.64	0.98
1:C:36:ASN:HA	1:C:85:ASN:HD21	1.28	0.98
1:F:211:LYS:H	1:F:211:LYS:HD2	1.23	0.98
2:H:287:ILE:HD13	2:H:289:ILE:CG2	1.94	0.98
1:C:26:LEU:HD21	1:C:45:LYS:HE2	1.45	0.98
1:B:78:SER:HB2	1:B:81:LYS:HE3	1.42	0.97
1:C:203:TYR:CE2	1:C:261:GLU:HG2	1.99	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:VAL:HG22	1:E:173:TYR:CE1	2.00	0.97
1:C:279:ALA:CB	1:C:320:VAL:HG21	1.93	0.97
1:E:86:ARG:HD2	1:E:198:LEU:HD23	1.46	0.97
1:A:203:TYR:CE2	1:A:261:GLU:HG2	2.00	0.96
1:D:111:GLY:HA2	1:D:170:PRO:HG2	1.45	0.95
1:A:311:PRO:CB	1:A:315:LYS:HD2	1.95	0.95
1:A:27:ILE:HB	1:A:81:LYS:HG2	1.49	0.94
1:D:51:LEU:HD11	1:D:104:PRO:HG3	1.47	0.94
1:D:85:ASN:OD1	1:D:87:VAL:HG12	1.67	0.94
1:E:118:PRO:HB2	1:E:123:VAL:HG11	1.49	0.94
2:G:307:ARG:HH11	2:G:329:ARG:HH21	0.95	0.93
1:E:136:LYS:HB2	1:E:137:PRO:HD3	1.49	0.93
1:F:426:LYS:HD2	1:F:445:LEU:CD1	1.98	0.93
1:C:238:PRO:HB3	1:C:365:ARG:NH1	1.82	0.93
1:E:190:LYS:HG3	1:E:191:ARG:N	1.84	0.92
1:B:31:ALA:C	1:B:32:ILE:HD13	1.90	0.92
1:E:131:PHE:CZ	1:E:136:LYS:HE3	2.05	0.91
1:D:169:ASP:CB	1:D:170:PRO:HD3	2.00	0.91
1:F:210:ARG:HD2	1:F:211:LYS:HE3	1.52	0.91
1:C:353:ILE:HG23	1:C:357:LEU:HD12	1.52	0.91
1:E:135:LEU:HD22	1:E:135:LEU:H	1.35	0.91
1:B:127:THR:HG22	1:B:438:ASP:HA	1.52	0.90
1:E:169:ASP:HB3	1:E:170:PRO:HD3	1.51	0.90
1:E:113:ARG:HA	1:E:181:VAL:CG1	1.99	0.90
1:B:213:LEU:HD22	1:B:217:LYS:HE3	1.53	0.90
1:F:403:THR:HG21	1:F:411:LEU:HD21	1.50	0.90
1:A:316:THR:HG22	1:A:318:GLY:N	1.86	0.89
1:F:120:ASP:OD2	1:F:190:LYS:HA	1.72	0.89
1:E:244:TYR:CE2	1:E:366:GLU:HB3	2.06	0.89
2:G:301:ARG:NH1	2:G:308:LEU:HD22	1.86	0.89
2:G:307:ARG:NH1	2:G:329:ARG:HH21	1.70	0.89
1:B:36:ASN:HA	1:B:85:ASN:ND2	1.87	0.89
2:G:307:ARG:HH11	2:G:329:ARG:NH2	1.71	0.89
1:E:113:ARG:HA	1:E:181:VAL:HG12	1.54	0.88
1:B:51:LEU:HD21	1:B:104:PRO:CG	2.03	0.88
1:E:109:LYS:HE2	1:E:170:PRO:HB3	1.55	0.88
1:A:169:ASP:HB3	1:A:170:PRO:HD3	1.55	0.88
1:A:36:ASN:HD21	1:A:87:VAL:HG21	1.38	0.87
1:C:313:ARG:NH1	1:C:322:ARG:HG2	1.88	0.87
2:H:302:LEU:HD21	2:H:325:ILE:HG23	1.56	0.87
1:C:423:ILE:HG12	1:C:445:LEU:HD21	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:311:LYS:HG3	2:H:313:ASN:H	1.37	0.87
1:E:231:LYS:HD3	1:E:338:ARG:HH12	1.40	0.87
1:A:453:ARG:HG3	1:A:453:ARG:NH1	1.77	0.87
2:G:317:ARG:HG3	2:G:317:ARG:NH1	1.88	0.87
1:B:172:PRO:HB2	1:B:173:TYR:CD2	2.09	0.86
1:C:337:GLN:HG2	1:C:338:ARG:HE	1.38	0.86
1:D:427:MET:HG3	1:D:432:LEU:HD23	1.57	0.86
1:A:53:ARG:HG3	1:A:53:ARG:O	1.76	0.86
1:B:52:PHE:N	1:B:52:PHE:CD2	2.41	0.86
1:E:59:LEU:HD22	1:E:102:ILE:HG22	1.56	0.86
1:A:36:ASN:ND2	1:A:87:VAL:HG21	1.89	0.86
1:D:108:VAL:HG23	1:D:175:ILE:HD12	1.58	0.86
2:H:287:ILE:CD1	2:H:289:ILE:HG23	2.00	0.85
1:E:51:LEU:HD21	1:E:104:PRO:HG3	1.57	0.85
1:B:147:ARG:HD3	1:B:148:LYS:H	1.41	0.85
1:D:152:PHE:H	1:D:152:PHE:HD1	1.24	0.85
1:C:190:LYS:HE2	1:C:190:LYS:HA	1.58	0.85
1:F:203:TYR:CE2	1:F:261:GLU:HG2	2.12	0.85
1:C:153:LEU:HB2	1:C:198:LEU:HD12	1.57	0.85
1:F:53:ARG:HH11	1:F:53:ARG:CG	1.89	0.85
1:E:87:VAL:HG22	1:E:198:LEU:CD1	2.07	0.84
1:F:211:LYS:HD2	1:F:211:LYS:N	1.92	0.84
2:H:296:THR:CG2	2:H:361:LEU:HA	2.07	0.84
1:C:322:ARG:HH22	1:E:317:HIS:CD2	1.95	0.84
1:A:129:ASN:HD21	1:A:132:GLU:HG3	1.38	0.84
1:E:26:LEU:HD12	1:E:82:ILE:HB	1.59	0.84
1:E:53:ARG:H	1:E:53:ARG:CD	1.90	0.84
1:D:389:LYS:HB2	1:D:389:LYS:NZ	1.93	0.84
2:H:319:SER:O	2:H:323:LEU:HG	1.78	0.84
2:H:290:ASN:H	2:H:314:HIS:CE1	1.96	0.84
1:D:403:THR:HG21	1:D:411:LEU:HD21	1.60	0.84
1:A:111:GLY:HA2	1:A:170:PRO:HG2	1.58	0.83
1:C:59:LEU:HD23	1:C:102:ILE:HA	1.60	0.83
1:E:53:ARG:HD3	1:E:53:ARG:N	1.93	0.83
1:C:201:VAL:HG12	1:C:257:ALA:HB2	1.60	0.83
2:H:300:ILE:HB	2:H:309:VAL:HB	1.58	0.83
1:A:51:LEU:HD21	1:A:104:PRO:HG3	1.60	0.83
1:B:59:LEU:HD22	1:B:100:ILE:HD12	1.59	0.83
1:F:85:ASN:ND2	1:F:85:ASN:H	1.75	0.83
1:C:43:GLN:CG	1:C:44:PRO:HD3	2.08	0.83
1:F:229:LEU:HG	1:F:233:ILE:HD12	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:PHE:HA	1:C:233:ILE:CG2	2.08	0.82
2:H:298:ILE:H	2:H:311:LYS:HB3	1.43	0.82
1:D:322:ARG:HH11	1:D:322:ARG:CG	1.91	0.82
1:C:131:PHE:HA	1:C:135:LEU:HD23	1.61	0.82
1:C:365:ARG:HG2	1:C:365:ARG:NH1	1.84	0.82
1:A:453:ARG:HH11	1:A:453:ARG:CG	1.89	0.82
1:E:190:LYS:HG3	1:E:191:ARG:H	1.42	0.81
1:A:311:PRO:HB2	1:A:315:LYS:CD	2.02	0.81
1:B:173:TYR:CD2	1:B:173:TYR:N	2.48	0.81
1:C:279:ALA:HB1	1:C:320:VAL:HG21	1.59	0.81
1:D:389:LYS:HB2	1:D:389:LYS:HZ2	1.46	0.81
1:E:353:ILE:HG23	1:E:357:LEU:HD12	1.61	0.81
1:D:117:LEU:HD21	1:D:185:GLU:HB2	1.62	0.81
1:F:211:LYS:H	1:F:211:LYS:CD	1.93	0.81
1:A:388:MET:HE2	1:A:447:VAL:HG21	1.61	0.81
1:C:191:ARG:HD2	1:C:195:GLU:O	1.81	0.81
1:A:436:THR:HG22	1:A:441:VAL:HG21	1.61	0.81
1:C:59:LEU:HD21	1:C:102:ILE:HG13	1.63	0.81
1:C:233:ILE:HG13	1:C:235:VAL:H	1.45	0.81
1:D:51:LEU:HD21	1:D:104:PRO:CG	2.11	0.81
1:E:86:ARG:HD2	1:E:198:LEU:CD2	2.10	0.80
1:F:32:ILE:HG12	1:F:83:ARG:HD3	1.63	0.80
1:F:426:LYS:HD2	1:F:445:LEU:HD11	1.61	0.80
1:C:126:ILE:HG23	1:C:159:ARG:NH1	1.96	0.80
1:D:403:THR:CG2	1:D:406:HIS:HB2	2.10	0.80
1:F:430:ILE:O	1:F:432:LEU:HG	1.82	0.80
1:C:365:ARG:HH11	1:C:365:ARG:CG	1.91	0.80
1:B:48:GLU:C	1:B:49:LEU:HD23	2.03	0.80
1:F:26:LEU:HD21	1:F:45:LYS:HE2	1.64	0.79
1:F:105:CYS:SG	1:F:108:VAL:HG23	2.21	0.79
1:C:206:VAL:HG22	1:C:253:LEU:HD22	1.65	0.79
1:D:349:ARG:NE	1:D:351:ASN:HB2	1.96	0.79
1:A:28:VAL:HG12	1:A:98:ASP:O	1.82	0.79
1:D:111:GLY:HA2	1:D:170:PRO:CG	2.12	0.79
1:D:423:ILE:HD13	1:D:445:LEU:CD2	2.13	0.79
1:E:87:VAL:HG22	1:E:198:LEU:HD11	1.62	0.79
1:B:31:ALA:O	1:B:32:ILE:HD13	1.82	0.79
1:E:230:PHE:HA	1:E:233:ILE:HG22	1.64	0.79
1:C:279:ALA:HB2	1:C:320:VAL:HG21	1.63	0.79
1:F:147:ARG:HD3	1:F:148:LYS:N	1.97	0.79
1:A:129:ASN:ND2	1:A:132:GLU:HG3	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:394:VAL:HA	1:E:449:MET:HB2	1.63	0.79
2:H:311:LYS:HG3	2:H:312:PHE:H	1.48	0.79
1:B:423:ILE:HA	1:B:445:LEU:HD11	1.64	0.78
1:E:26:LEU:N	1:E:26:LEU:HD23	1.98	0.78
1:D:131:PHE:O	1:D:136:LYS:HG3	1.83	0.78
1:B:220:VAL:HB	1:B:224:LEU:HD22	1.64	0.78
1:C:353:ILE:CG2	1:C:357:LEU:HD12	2.12	0.78
1:D:398:GLN:HA	1:D:398:GLN:HE21	1.49	0.78
1:E:170:PRO:HB2	1:E:174:CYS:HB3	1.65	0.78
1:E:59:LEU:CD2	1:E:102:ILE:HG22	2.13	0.78
2:H:311:LYS:HE2	2:H:313:ASN:HD22	1.48	0.78
1:B:147:ARG:HD3	1:B:148:LYS:N	1.99	0.78
1:D:127:THR:HG22	1:D:128:GLY:H	1.49	0.78
1:F:64:ARG:HH11	1:F:64:ARG:HG3	1.49	0.78
1:F:319:GLU:O	1:F:323:ARG:HB2	1.82	0.78
1:B:449:MET:O	1:B:453:ARG:HG2	1.84	0.78
1:D:203:TYR:CE2	1:D:261:GLU:HG2	2.19	0.78
1:F:349:ARG:NH1	1:F:351:ASN:HB2	1.99	0.78
1:E:353:ILE:CG2	1:E:357:LEU:HD12	2.14	0.77
1:C:27:ILE:HD11	1:E:429:LEU:HD13	1.66	0.77
1:B:192:GLU:OE1	1:B:192:GLU:HA	1.84	0.77
1:E:30:GLU:HG3	1:E:96:LEU:HD21	1.65	0.77
2:H:289:ILE:HG13	2:H:289:ILE:O	1.83	0.77
2:H:350:ASP:HB3	2:H:352:ASN:HD21	1.48	0.77
1:A:26:LEU:HD21	1:A:45:LYS:HE2	1.64	0.77
1:D:50:GLN:O	1:D:51:LEU:HD23	1.84	0.77
1:B:172:PRO:HB2	1:B:173:TYR:CE2	2.20	0.77
1:C:135:LEU:HD22	1:C:135:LEU:H	1.48	0.77
2:H:299:GLN:OE1	2:H:308:LEU:HD11	1.84	0.77
1:D:186:GLY:O	1:D:187:GLU:HG2	1.85	0.77
1:D:270:ASN:OD1	1:D:272:PRO:HD2	1.85	0.77
1:F:27:ILE:HD13	1:F:99:VAL:HG12	1.67	0.77
1:F:426:LYS:HD2	1:F:445:LEU:HD12	1.67	0.76
2:G:326:VAL:HG13	2:G:333:ALA:HB2	1.66	0.76
1:D:122:THR:HG21	1:D:162:GLU:HB2	1.67	0.76
1:D:134:TYR:O	1:D:137:PRO:HD2	1.85	0.76
1:E:126:ILE:HD12	1:E:159:ARG:HD2	1.66	0.76
1:D:208:GLY:H	1:D:210:ARG:NH1	1.83	0.76
1:C:153:LEU:HD21	1:C:155:ARG:NH1	2.00	0.76
1:B:49:LEU:HD23	1:B:49:LEU:N	2.01	0.76
1:C:57:VAL:HG21	1:C:71:VAL:HG21	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:211:LYS:HD3	1:F:212:GLN:OE1	1.86	0.76
1:A:220:VAL:HB	1:A:224:LEU:HD22	1.67	0.76
1:B:349:ARG:HG3	1:B:350:PRO:HD2	1.66	0.75
1:C:27:ILE:CD1	1:E:429:LEU:HD13	2.16	0.75
1:F:53:ARG:HH11	1:F:53:ARG:HG3	1.49	0.75
2:G:283:ALA:HB1	2:G:324:PHE:CD1	2.20	0.75
1:D:147:ARG:HG3	1:D:147:ARG:HH11	1.51	0.75
1:D:441:VAL:HG23	1:D:442:MET:H	1.51	0.75
1:E:191:ARG:NH2	1:E:197:SER:HB2	2.01	0.75
1:E:227:PRO:HB3	1:E:340:HIS:CD2	2.21	0.75
1:F:52:PHE:HD2	2:G:362:ASN:O	1.69	0.75
1:B:120:ASP:OD2	1:B:190:LYS:HA	1.85	0.75
1:D:87:VAL:HG13	1:D:88:VAL:N	2.01	0.75
1:E:428:ASP:HA	1:E:433:GLU:OE2	1.86	0.75
1:F:186:GLY:O	1:F:187:GLU:HB2	1.85	0.75
2:H:302:LEU:HB2	2:H:307:ARG:HB2	1.68	0.75
2:H:350:ASP:HB2	2:H:353:GLN:HE22	1.50	0.75
1:C:338:ARG:H	1:C:338:ARG:CD	1.96	0.75
1:D:23:PRO:O	1:D:49:LEU:HD11	1.87	0.75
1:A:233:ILE:HG22	1:A:235:VAL:H	1.50	0.75
2:H:294:PRO:O	2:H:314:HIS:HB2	1.87	0.75
1:A:177:ALA:HB1	1:A:178:PRO:HD2	1.68	0.75
1:D:206:VAL:HG22	1:D:253:LEU:HD22	1.69	0.75
1:E:43:GLN:HB3	1:E:44:PRO:HD3	1.69	0.75
2:H:329:ARG:HB2	2:H:332:MET:HG2	1.68	0.75
1:B:250:GLY:O	1:B:254:ILE:HG13	1.87	0.74
1:E:53:ARG:CD	1:E:53:ARG:N	2.50	0.74
2:H:296:THR:HG21	2:H:361:LEU:HA	1.68	0.74
1:B:173:TYR:N	1:B:173:TYR:HD2	1.84	0.74
1:B:251:LYS:HD2	1:B:346:ALA:HB1	1.67	0.74
1:F:52:PHE:H	1:F:55:ASP:HB2	1.51	0.74
2:G:304:ASP:OD2	2:G:307:ARG:HB2	1.87	0.74
1:C:160:ALA:HB2	1:C:387:ASN:HD21	1.52	0.74
1:C:94:VAL:HG11	1:C:100:ILE:HD11	1.68	0.74
1:C:108:VAL:HG22	1:C:173:TYR:CD2	2.23	0.74
1:E:108:VAL:HG22	1:E:173:TYR:HE1	1.50	0.74
1:E:111:GLY:HA2	1:E:170:PRO:HG2	1.68	0.74
1:A:388:MET:CE	1:A:447:VAL:HG21	2.18	0.74
1:B:100:ILE:HD13	1:B:101:SER:N	2.03	0.74
1:D:322:ARG:HG3	1:D:322:ARG:NH1	1.95	0.74
1:E:29:ASP:HB2	1:E:81:LYS:HD3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:304:ASP:CG	2:G:307:ARG:HB2	2.08	0.74
2:G:337:PHE:HB3	2:G:369:LEU:HD23	1.70	0.73
1:D:118:PRO:HB3	1:D:163:PHE:CE1	2.23	0.73
1:D:283:GLU:OE2	1:D:327:GLN:CB	2.34	0.73
1:A:275:MET:HE3	1:A:324:ILE:HG21	1.70	0.73
1:A:127:THR:O	1:A:438:ASP:HA	1.88	0.73
1:D:242:LEU:HG	1:D:244:TYR:CE2	2.24	0.73
1:D:132:GLU:HA	1:D:136:LYS:CD	2.18	0.73
1:C:147:ARG:HD3	1:C:148:LYS:O	1.89	0.73
1:C:190:LYS:HE2	1:C:191:ARG:H	1.51	0.73
1:C:222:LEU:HD23	1:C:226:HIS:HD2	1.52	0.73
1:D:87:VAL:HG13	1:D:88:VAL:H	1.54	0.73
1:F:169:ASP:CB	1:F:170:PRO:CD	2.64	0.73
1:D:222:LEU:HD23	1:D:226:HIS:HD2	1.53	0.73
2:H:303:ALA:C	2:H:305:GLY:H	1.90	0.73
1:F:59:LEU:HD23	1:F:102:ILE:HA	1.71	0.72
2:G:304:ASP:OD1	2:G:307:ARG:HB2	1.88	0.72
1:D:51:LEU:HD21	1:D:104:PRO:HB3	1.71	0.72
1:F:279:ALA:HB2	1:F:320:VAL:HG13	1.71	0.72
1:C:279:ALA:HA	1:C:320:VAL:HG11	1.72	0.72
1:C:322:ARG:NH1	1:E:317:HIS:NE2	2.32	0.72
1:F:53:ARG:HG3	1:F:53:ARG:NH1	2.03	0.72
1:F:251:LYS:HD2	1:F:346:ALA:HB1	1.70	0.72
2:H:354:THR:HG22	2:H:357:GLU:HG3	1.71	0.71
1:A:201:VAL:HG12	1:A:257:ALA:HB2	1.72	0.71
1:A:436:THR:CG2	1:A:441:VAL:HG21	2.20	0.71
1:F:233:ILE:HG22	1:F:235:VAL:N	1.99	0.71
1:F:403:THR:HG22	1:F:403:THR:O	1.89	0.71
1:A:206:VAL:HG22	1:A:253:LEU:HD22	1.72	0.71
1:D:251:LYS:HD2	1:D:346:ALA:HB1	1.72	0.71
1:C:70:ILE:CD1	1:C:145:PRO:HG3	2.21	0.71
1:D:353:ILE:CG2	1:D:357:LEU:HD12	2.20	0.71
1:E:191:ARG:HH22	1:E:197:SER:HB2	1.56	0.71
1:E:432:LEU:HD12	1:E:441:VAL:HG21	1.72	0.71
1:C:423:ILE:HG12	1:C:445:LEU:CD2	2.20	0.71
1:D:193:ASP:OD1	1:D:193:ASP:N	2.24	0.71
1:E:290:PHE:O	1:E:294:GLU:HG3	1.91	0.71
1:A:96:LEU:O	1:A:225:ARG:NH2	2.24	0.71
1:B:111:GLY:HA2	1:B:170:PRO:HD2	1.72	0.71
1:C:433:GLU:HB3	1:C:436:THR:O	1.91	0.71
1:A:312:LYS:HB3	1:A:354:ASP:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:TYR:HE1	2:H:301:ARG:HE	1.36	0.71
1:E:108:VAL:HG11	1:E:175:ILE:HG13	1.73	0.71
1:F:201:VAL:HG11	1:F:253:LEU:HD12	1.71	0.71
1:D:136:LYS:HB2	1:D:137:PRO:HD3	1.70	0.71
1:E:312:LYS:HG2	1:E:313:ARG:N	2.04	0.71
2:H:355:LEU:CD2	2:H:360:LEU:HD12	2.21	0.70
1:C:60:LYS:O	1:C:100:ILE:HG23	1.89	0.70
1:C:359:ARG:HB3	1:C:362:ARG:HD2	1.72	0.70
1:A:371:ILE:HD12	1:A:371:ILE:H	1.57	0.70
1:F:337:GLN:O	1:F:339:ALA:N	2.24	0.70
2:G:300:ILE:O	2:G:308:LEU:HA	1.91	0.70
1:E:51:LEU:HD21	1:E:104:PRO:CG	2.22	0.70
1:A:131:PHE:HA	1:A:135:LEU:HD23	1.74	0.70
1:E:27:ILE:HB	1:E:81:LYS:HG2	1.72	0.70
1:F:349:ARG:HB2	1:F:350:PRO:HD2	1.74	0.70
2:H:340:MET:HG2	2:H:347:GLU:HG3	1.74	0.70
1:B:393:ASP:O	1:B:449:MET:HB2	1.92	0.70
1:E:403:THR:O	1:E:405:GLY:N	2.25	0.70
1:C:105:CYS:SG	1:C:108:VAL:HG23	2.31	0.70
1:F:66:GLU:HB2	1:F:147:ARG:NH1	2.07	0.70
1:C:57:VAL:HG21	1:C:71:VAL:CG2	2.21	0.70
1:E:84:MET:SD	1:E:88:VAL:HG23	2.32	0.70
1:F:424:ARG:O	1:F:428:ASP:HB3	1.91	0.70
2:H:355:LEU:HD22	2:H:360:LEU:HD12	1.73	0.70
2:G:301:ARG:HH11	2:G:308:LEU:HB3	1.57	0.70
1:B:52:PHE:O	1:B:54:GLY:N	2.25	0.70
1:B:437:ILE:HG22	1:B:438:ASP:N	2.05	0.70
2:H:296:THR:O	2:H:313:ASN:O	2.10	0.70
1:D:39:VAL:HG13	1:D:69:CYS:SG	2.32	0.69
1:A:371:ILE:HD12	1:A:371:ILE:N	2.07	0.69
1:C:251:LYS:HD2	1:C:346:ALA:HB1	1.74	0.69
1:F:95:ARG:HB2	1:F:225:ARG:HH12	1.57	0.69
1:A:94:VAL:HG13	1:A:98:ASP:HB2	1.73	0.69
1:A:237:PRO:HG2	1:A:337:GLN:NE2	2.06	0.69
1:C:313:ARG:HA	1:C:316:THR:HG22	1.74	0.69
1:D:51:LEU:CD1	1:D:104:PRO:HG3	2.23	0.69
1:D:349:ARG:HB2	1:D:350:PRO:HD2	1.75	0.69
1:E:113:ARG:H	1:E:169:ASP:HB2	1.56	0.69
2:H:287:ILE:HD12	2:H:287:ILE:C	2.13	0.69
2:H:301:ARG:HB3	2:H:366:VAL:HA	1.73	0.69
1:C:70:ILE:HD11	1:C:145:PRO:HG3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:310:ALA:HA	1:E:325:VAL:HG22	1.74	0.69
1:A:312:LYS:HG3	1:A:313:ARG:N	2.07	0.69
1:A:395:ASP:H	1:A:449:MET:HE2	1.58	0.69
1:E:424:ARG:O	1:E:428:ASP:HB3	1.93	0.69
1:E:313:ARG:O	1:E:316:THR:HG22	1.93	0.69
1:E:378:LEU:O	1:E:382:GLN:HG3	1.92	0.69
1:B:29:ASP:CG	1:B:30:GLU:H	1.93	0.69
2:H:296:THR:CG2	2:H:362:ASN:H	2.06	0.69
1:B:118:PRO:HB2	1:B:123:VAL:HG21	1.74	0.69
1:B:216:ILE:O	1:B:220:VAL:HG22	1.92	0.69
1:C:51:LEU:HD21	1:C:104:PRO:HB3	1.75	0.69
1:D:269:ILE:HD11	1:D:289:ALA:HB1	1.75	0.69
1:E:424:ARG:HA	1:E:428:ASP:HB2	1.74	0.69
1:F:114:ILE:HD11	1:F:174:CYS:SG	2.33	0.69
1:C:317:HIS:NE2	1:D:322:ARG:NH1	2.39	0.68
1:E:30:GLU:HG3	1:E:96:LEU:CD2	2.23	0.68
1:E:31:ALA:HA	1:E:83:ARG:HB3	1.74	0.68
2:H:311:LYS:HG3	2:H:312:PHE:N	2.09	0.68
1:C:351:ASN:HD22	1:C:351:ASN:N	1.89	0.68
1:A:432:LEU:HD12	1:E:27:ILE:HG12	1.75	0.68
1:B:171:SER:CB	1:B:172:PRO:HD3	2.22	0.68
1:D:248:GLY:HA3	1:D:409:ALA:HB2	1.75	0.68
1:A:114:ILE:HD13	1:A:146:ILE:HD11	1.75	0.68
1:E:158:MET:HE2	1:E:388:MET:HB3	1.74	0.68
1:C:313:ARG:HA	1:C:316:THR:CG2	2.24	0.68
1:D:320:VAL:O	1:D:324:ILE:HG13	1.93	0.68
1:D:397:GLU:O	1:D:401:ASN:ND2	2.27	0.68
1:D:423:ILE:HD13	1:D:445:LEU:HD21	1.75	0.68
1:E:112:LYS:HB2	1:E:169:ASP:HB3	1.74	0.68
1:D:51:LEU:HD21	1:D:104:PRO:CB	2.23	0.68
1:F:80:GLU:CD	1:F:80:GLU:H	1.97	0.68
1:D:190:LYS:HG3	1:D:191:ARG:N	2.09	0.68
1:F:112:LYS:NZ	1:F:113:ARG:HH11	1.92	0.68
1:B:203:TYR:CE2	1:B:261:GLU:HG2	2.29	0.68
1:A:136:LYS:HB3	1:A:137:PRO:HD3	1.74	0.67
2:H:350:ASP:HB3	2:H:352:ASN:ND2	2.09	0.67
1:A:210:ARG:H	1:A:210:ARG:HD2	1.58	0.67
1:B:135:LEU:H	1:B:135:LEU:HD22	1.60	0.67
1:E:225:ARG:C	1:E:227:PRO:HD3	2.15	0.67
1:E:109:LYS:HE2	1:E:170:PRO:CB	2.25	0.67
1:B:249:THR:HG21	1:B:369:ILE:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:424:ARG:O	1:D:428:ASP:HB2	1.94	0.67
2:G:338:VAL:HG12	2:G:339:LEU:N	2.10	0.67
1:B:105:CYS:SG	1:B:173:TYR:HE1	2.18	0.67
1:B:177:ALA:HB1	1:B:178:PRO:HD2	1.77	0.67
1:D:23:PRO:O	1:D:49:LEU:HD21	1.95	0.67
1:D:113:ARG:H	1:D:169:ASP:HB2	1.58	0.67
1:D:220:VAL:O	1:D:224:LEU:HB2	1.95	0.67
1:A:35:ASP:HB3	1:A:38:VAL:HG12	1.76	0.67
1:B:60:LYS:O	1:B:100:ILE:HG12	1.93	0.67
1:B:209:CYS:O	1:B:213:LEU:HB2	1.94	0.67
1:E:197:SER:OG	1:E:199:ASN:HB3	1.94	0.67
1:F:85:ASN:H	1:F:85:ASN:HD22	1.41	0.67
2:H:337:PHE:HB2	2:H:368:ARG:O	1.95	0.67
1:A:32:ILE:HG12	1:A:83:ARG:HD3	1.77	0.67
1:C:322:ARG:HH12	1:E:317:HIS:CE1	2.13	0.67
1:F:142:ALA:O	1:F:143:TYR:HB2	1.93	0.67
1:B:155:ARG:HD3	1:B:387:ASN:OD1	1.95	0.67
1:C:190:LYS:HE2	1:C:190:LYS:CA	2.24	0.67
1:E:109:LYS:CE	1:E:170:PRO:HB3	2.25	0.67
2:H:311:LYS:CE	2:H:313:ASN:HD22	2.08	0.66
1:C:126:ILE:CG2	1:C:159:ARG:NH1	2.58	0.66
2:G:311:LYS:O	2:G:312:PHE:HB2	1.95	0.66
1:B:100:ILE:HD13	1:B:101:SER:C	2.15	0.66
1:C:427:MET:SD	1:C:432:LEU:HD11	2.35	0.66
1:D:358:ARG:HG3	1:D:358:ARG:HH11	1.61	0.66
1:F:85:ASN:HD22	1:F:85:ASN:N	1.93	0.66
1:D:427:MET:HG3	1:D:432:LEU:CD2	2.26	0.66
1:D:41:LEU:HD23	1:D:82:ILE:HA	1.76	0.66
1:F:254:ILE:HD12	1:F:369:ILE:HD13	1.78	0.66
1:B:32:ILE:HG12	1:B:83:ARG:HD3	1.77	0.66
1:C:51:LEU:CD2	1:C:104:PRO:HB3	2.26	0.66
1:C:177:ALA:HB1	1:C:178:PRO:HD2	1.77	0.66
1:A:215:GLN:O	1:A:219:MET:HG3	1.96	0.66
1:C:229:LEU:HA	1:E:437:ILE:HD12	1.77	0.66
1:D:423:ILE:HD13	1:D:445:LEU:HD23	1.77	0.66
1:E:113:ARG:CG	1:E:169:ASP:HB2	2.26	0.66
2:H:296:THR:HG23	2:H:362:ASN:H	1.61	0.66
1:B:389:LYS:HD3	1:B:446:ALA:HB2	1.77	0.66
1:F:403:THR:HG21	1:F:411:LEU:CD2	2.26	0.66
1:B:322:ARG:HH12	1:D:317:HIS:CE1	2.14	0.65
1:D:242:LEU:HG	1:D:244:TYR:HE2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:THR:HG22	1:A:317:HIS:N	2.10	0.65
1:C:313:ARG:HH11	1:C:322:ARG:HG2	1.58	0.65
1:D:100:ILE:HD12	1:D:100:ILE:O	1.96	0.65
1:D:441:VAL:HG23	1:D:442:MET:N	2.10	0.65
1:E:203:TYR:CD2	1:E:217:LYS:HE2	2.30	0.65
1:B:35:ASP:HB3	1:B:38:VAL:HG12	1.78	0.65
1:B:113:ARG:HG2	1:B:181:VAL:HB	1.78	0.65
1:C:437:ILE:HG13	1:D:229:LEU:HA	1.77	0.65
1:D:43:GLN:HA	1:D:46:MET:HG3	1.77	0.65
1:A:153:LEU:HD11	1:A:160:ALA:HB1	1.75	0.65
1:E:129:ASN:O	1:E:133:VAL:HG22	1.97	0.65
2:G:313:ASN:ND2	2:G:314:HIS:H	1.94	0.65
1:B:211:LYS:O	1:B:214:ALA:HB3	1.97	0.65
1:B:293:ALA:CB	1:B:301:ILE:HD11	2.26	0.65
1:C:192:GLU:HB2	1:C:195:GLU:HG3	1.77	0.65
1:D:51:LEU:HD21	1:D:104:PRO:HG3	1.77	0.65
1:A:27:ILE:HD13	1:A:99:VAL:HG12	1.77	0.65
1:A:147:ARG:HD3	1:A:148:LYS:O	1.97	0.65
1:C:74:ASP:OD1	1:C:76:THR:HG23	1.95	0.65
1:D:112:LYS:HB2	1:D:169:ASP:OD2	1.95	0.65
1:D:120:ASP:N	1:D:188:PRO:HB3	2.12	0.65
1:E:72:LEU:HG	1:E:73:SER:H	1.61	0.65
2:G:348:LEU:HD21	2:G:360:LEU:HD21	1.78	0.65
1:B:254:ILE:HD12	1:B:369:ILE:HD13	1.79	0.65
1:A:317:HIS:CB	1:F:317:HIS:CD2	2.80	0.65
1:A:395:ASP:H	1:A:449:MET:CE	2.10	0.65
1:C:31:ALA:HB2	1:C:84:MET:C	2.17	0.65
1:E:215:GLN:O	1:E:219:MET:HG3	1.97	0.65
2:H:341:THR:O	2:H:345:ASN:HA	1.97	0.65
1:B:172:PRO:HB2	1:B:173:TYR:HD2	1.57	0.65
1:D:192:GLU:O	1:D:194:GLU:N	2.29	0.65
2:H:299:GLN:HG3	2:H:364:VAL:HG13	1.78	0.65
1:F:136:LYS:HB3	1:F:137:PRO:HD3	1.78	0.65
1:D:398:GLN:HA	1:D:398:GLN:NE2	2.12	0.64
1:E:278:LEU:HG	1:E:281:GLU:OE1	1.97	0.64
1:F:147:ARG:HH11	1:F:147:ARG:HG3	1.62	0.64
1:B:36:ASN:HA	1:B:85:ASN:HD21	1.61	0.64
1:F:108:VAL:HG11	1:F:175:ILE:HG13	1.78	0.64
1:C:75:ASP:OD1	1:C:75:ASP:N	2.26	0.64
1:C:337:GLN:HG2	1:C:338:ARG:NE	2.12	0.64
2:H:315:SER:HG	2:H:356:LYS:HE3	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:ILE:HD12	1:C:165:VAL:HG21	1.78	0.64
1:B:347:THR:HG21	1:B:353:ILE:HD11	1.79	0.64
1:E:390:LEU:HD23	1:E:447:VAL:CG1	2.28	0.64
1:B:27:ILE:HD13	1:B:99:VAL:HG23	1.80	0.64
1:B:388:MET:CE	1:B:447:VAL:HG21	2.28	0.64
1:D:55:ASP:O	1:D:71:VAL:HG12	1.97	0.64
1:F:438:ASP:HB3	1:F:441:VAL:HG23	1.78	0.64
2:H:322:ARG:O	2:H:326:VAL:HG23	1.97	0.64
1:B:105:CYS:SG	1:B:108:VAL:HG23	2.38	0.64
1:C:68:VAL:HG12	1:C:145:PRO:HB2	1.79	0.64
1:C:270:ASN:ND2	1:C:272:PRO:HD2	2.13	0.64
1:E:167:GLU:OE1	1:E:167:GLU:HA	1.98	0.64
2:H:299:GLN:HB3	2:H:364:VAL:HG22	1.80	0.64
1:C:201:VAL:HG11	1:C:253:LEU:HD23	1.80	0.63
1:D:132:GLU:HA	1:D:136:LYS:HD2	1.78	0.63
1:E:249:THR:CG2	1:E:369:ILE:HG22	2.29	0.63
1:F:233:ILE:CG2	1:F:235:VAL:H	2.01	0.63
1:F:403:THR:HG22	1:F:406:HIS:HB2	1.79	0.63
1:A:251:LYS:HD2	1:A:346:ALA:HB1	1.80	0.63
1:A:337:GLN:OE1	1:A:337:GLN:HA	1.98	0.63
1:B:319:GLU:HB3	1:B:323:ARG:HH21	1.63	0.63
1:D:249:THR:HG21	1:D:369:ILE:O	1.98	0.63
1:D:290:PHE:HA	1:D:301:ILE:HD11	1.81	0.63
1:F:108:VAL:CG1	1:F:175:ILE:HG13	2.28	0.63
1:F:126:ILE:HG21	1:F:159:ARG:HD2	1.81	0.63
1:F:135:LEU:HD22	1:F:135:LEU:H	1.63	0.63
1:C:229:LEU:HA	1:E:437:ILE:CD1	2.29	0.63
1:D:127:THR:HG22	1:D:128:GLY:N	2.13	0.63
1:E:312:LYS:HZ3	1:E:314:GLU:H	1.47	0.63
1:F:254:ILE:O	1:F:258:VAL:HG23	1.98	0.63
2:H:307:ARG:HD2	2:H:329:ARG:CZ	2.29	0.63
1:E:358:ARG:HH11	1:E:358:ARG:HG3	1.62	0.63
1:A:233:ILE:HD11	1:F:442:MET:HG3	1.78	0.63
1:B:55:ASP:O	1:B:71:VAL:HG12	1.98	0.63
1:B:105:CYS:SG	1:B:108:VAL:CG2	2.87	0.63
1:F:283:GLU:HB3	1:F:287:ARG:HH12	1.63	0.63
1:E:120:ASP:O	1:E:123:VAL:HG22	1.99	0.63
1:A:246:PRO:HG3	1:A:371:ILE:HD11	1.79	0.63
1:D:220:VAL:HB	1:D:224:LEU:HD22	1.81	0.63
1:E:312:LYS:NZ	1:E:314:GLU:H	1.97	0.63
1:B:58:LEU:HD13	1:B:59:LEU:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:VAL:HG11	1:C:102:ILE:HG12	1.80	0.63
1:E:270:ASN:OD1	1:E:272:PRO:HD2	1.98	0.63
1:F:122:THR:HG21	1:F:162:GLU:HB2	1.80	0.63
1:B:213:LEU:O	1:B:217:LYS:HG3	1.99	0.62
2:H:318:ILE:HD12	2:H:351:GLU:HA	1.81	0.62
1:F:187:GLU:OE1	1:F:187:GLU:HA	1.98	0.62
1:A:232:ALA:HB1	1:F:126:ILE:HG22	1.81	0.62
1:B:349:ARG:HD2	1:B:350:PRO:HD2	1.79	0.62
1:D:143:TYR:O	1:D:175:ILE:HG23	2.00	0.62
1:D:226:HIS:N	1:D:227:PRO:HD3	2.14	0.62
1:D:353:ILE:HG23	1:D:357:LEU:HD12	1.80	0.62
1:E:42:SER:OG	1:E:45:LYS:HB2	2.00	0.62
1:E:206:VAL:HG22	1:E:253:LEU:HD23	1.81	0.62
2:H:302:LEU:CB	2:H:307:ARG:HB2	2.29	0.62
1:D:118:PRO:O	1:D:188:PRO:HA	1.98	0.62
1:D:349:ARG:HG2	1:D:352:SER:OG	1.99	0.62
1:E:36:ASN:OD1	1:E:87:VAL:CG2	2.47	0.62
1:A:114:ILE:CD1	1:A:176:VAL:HG22	2.29	0.62
1:B:41:LEU:HD11	1:B:102:ILE:HD13	1.81	0.62
1:F:136:LYS:O	1:F:140:LEU:HB2	1.99	0.62
1:F:270:ASN:OD1	1:F:272:PRO:HD2	1.99	0.62
2:H:360:LEU:HD22	2:H:365:ILE:HD11	1.81	0.62
1:D:132:GLU:HA	1:D:136:LYS:HE3	1.82	0.62
1:D:135:LEU:H	1:D:135:LEU:HD22	1.63	0.62
1:D:338:ARG:HD2	1:D:338:ARG:O	2.00	0.62
1:E:136:LYS:HB2	1:E:137:PRO:CD	2.28	0.62
2:H:310:GLN:NE2	2:H:311:LYS:O	2.31	0.62
1:A:312:LYS:HG3	1:A:313:ARG:H	1.63	0.62
1:B:136:LYS:HB3	1:B:137:PRO:HD3	1.82	0.62
1:E:221:GLU:O	1:E:225:ARG:HB2	2.00	0.62
1:F:74:ASP:HB3	1:F:77:CYS:CB	2.29	0.62
2:H:354:THR:HG22	2:H:357:GLU:CG	2.30	0.62
1:A:100:ILE:O	1:A:100:ILE:HD12	1.99	0.62
1:A:239:ARG:HH11	1:A:335:LEU:HB2	1.64	0.62
1:F:45:LYS:O	1:F:45:LYS:HD3	2.00	0.62
2:H:296:THR:HG23	2:H:361:LEU:HA	1.82	0.62
1:B:58:LEU:HD13	1:B:59:LEU:N	2.15	0.61
1:B:353:ILE:HG22	1:B:354:ASP:N	2.15	0.61
1:E:373:ASP:O	1:E:377:ARG:HG3	2.00	0.61
1:F:213:LEU:O	1:F:217:LYS:HG3	2.00	0.61
1:B:349:ARG:CG	1:B:350:PRO:HD2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:LYS:O	1:E:181:VAL:HG12	2.00	0.61
1:A:233:ILE:CG2	1:A:235:VAL:HG23	2.30	0.61
1:B:53:ARG:NH1	1:B:72:LEU:HB3	2.15	0.61
1:B:127:THR:HG22	1:B:438:ASP:CA	2.29	0.61
1:C:169:ASP:HB3	1:C:170:PRO:CD	2.22	0.61
1:D:153:LEU:HD12	1:D:161:VAL:O	2.00	0.61
1:E:31:ALA:HB2	1:E:84:MET:C	2.20	0.61
2:H:287:ILE:HD12	2:H:287:ILE:O	2.00	0.61
2:H:296:THR:HG23	2:H:362:ASN:N	2.14	0.61
2:H:303:ALA:O	2:H:305:GLY:N	2.33	0.61
1:A:368:ASP:OD1	4:A:805:HOH:O	2.16	0.61
1:C:50:GLN:O	1:C:51:LEU:HD23	2.01	0.61
1:D:152:PHE:CD1	1:D:152:PHE:N	2.66	0.61
1:E:350:PRO:HB3	1:E:358:ARG:HH22	1.66	0.61
1:F:349:ARG:HH12	1:F:351:ASN:HB2	1.64	0.61
1:A:210:ARG:HG2	1:A:211:LYS:N	2.16	0.61
1:A:320:VAL:O	1:A:324:ILE:HG13	2.01	0.61
1:F:131:PHE:CZ	1:F:136:LYS:HD3	2.36	0.61
1:C:36:ASN:HA	1:C:85:ASN:ND2	2.09	0.61
1:C:92:LEU:O	1:C:94:VAL:HG13	2.01	0.61
1:C:213:LEU:O	1:C:217:LYS:HG3	2.00	0.61
1:D:249:THR:CG2	1:D:369:ILE:HG22	2.30	0.61
2:H:329:ARG:HB2	2:H:332:MET:CG	2.30	0.61
1:E:438:ASP:OD2	1:E:441:VAL:HG23	2.00	0.61
1:F:423:ILE:O	1:F:427:MET:HB3	2.00	0.61
1:D:119:ILE:HG23	1:D:189:ILE:O	2.01	0.61
1:E:113:ARG:HA	1:E:181:VAL:HG13	1.81	0.61
1:A:203:TYR:CD2	1:A:261:GLU:HG2	2.35	0.61
1:A:209:CYS:O	1:A:213:LEU:HB2	2.00	0.61
1:C:110:TYR:CD2	1:C:177:ALA:HB2	2.36	0.61
1:E:55:ASP:O	1:E:71:VAL:HG12	2.01	0.61
1:E:429:LEU:C	1:E:431:ASP:H	2.02	0.61
1:B:121:ASP:OD1	1:B:122:THR:HG23	2.01	0.61
1:C:190:LYS:CE	1:C:191:ARG:H	2.14	0.61
1:B:336:LYS:NZ	1:B:338:ARG:HG3	2.16	0.60
1:D:416:SER:O	1:D:420:LEU:HG	2.01	0.60
1:D:120:ASP:OD2	1:D:190:LYS:HA	2.02	0.60
1:D:152:PHE:HD1	1:D:152:PHE:N	1.98	0.60
1:E:97:GLY:HA3	1:E:225:ARG:NH2	2.16	0.60
1:F:256:ARG:HH11	1:F:266:PHE:HD2	1.49	0.60
1:B:239:ARG:HH21	1:B:340:HIS:HB3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ARG:HG3	1:B:350:PRO:CD	2.31	0.60
1:B:437:ILE:CG2	1:B:438:ASP:N	2.64	0.60
1:C:309:ILE:O	1:C:325:VAL:HG22	2.02	0.60
1:C:317:HIS:CD2	1:D:322:ARG:HH12	2.18	0.60
1:D:254:ILE:HD12	1:D:369:ILE:HD13	1.83	0.60
1:D:316:THR:O	1:D:322:ARG:NH2	2.34	0.60
2:G:283:ALA:CB	2:G:324:PHE:CE1	2.75	0.60
1:C:449:MET:O	1:C:453:ARG:HG3	2.01	0.60
1:E:132:GLU:HA	1:E:136:LYS:HG3	1.84	0.60
2:G:300:ILE:HD12	2:G:300:ILE:N	2.16	0.60
2:H:313:ASN:OD1	2:H:316:HIS:CB	2.49	0.60
2:H:315:SER:OG	2:H:356:LYS:CE	2.44	0.60
1:C:34:GLU:OE1	1:C:35:ASP:N	2.32	0.60
1:A:306:LEU:HD21	1:A:357:LEU:HD13	1.82	0.60
1:F:74:ASP:HB3	1:F:77:CYS:HB2	1.82	0.60
1:F:171:SER:HB3	1:F:172:PRO:CD	2.32	0.60
2:H:298:ILE:N	2:H:311:LYS:HB3	2.15	0.60
1:A:25:ARG:HE	1:A:99:VAL:HG21	1.66	0.60
1:C:427:MET:HG3	1:C:428:ASP:N	2.15	0.60
1:D:131:PHE:CE2	1:D:136:LYS:HG2	2.37	0.60
1:F:428:ASP:OD2	1:F:428:ASP:C	2.39	0.60
1:C:68:VAL:HG23	1:C:147:ARG:HB2	1.82	0.60
1:D:114:ILE:HD11	1:D:176:VAL:HG22	1.84	0.60
1:D:122:THR:HG21	1:D:162:GLU:CB	2.32	0.60
1:E:135:LEU:H	1:E:135:LEU:CD2	2.10	0.60
1:D:147:ARG:HG3	1:D:147:ARG:NH1	2.17	0.60
1:D:300:ILE:HD11	1:D:344:MET:HB2	1.84	0.60
1:E:45:LYS:HG3	1:E:79:ASP:O	2.02	0.60
1:A:394:VAL:HA	1:A:449:MET:HB2	1.84	0.60
1:B:58:LEU:HD22	1:B:68:VAL:HG22	1.83	0.60
1:B:349:ARG:HG2	1:B:351:ASN:ND2	2.17	0.60
1:C:147:ARG:HH11	1:C:147:ARG:HG3	1.67	0.60
1:C:423:ILE:CG1	1:C:445:LEU:HD21	2.30	0.60
1:F:131:PHE:HA	1:F:135:LEU:HD23	1.84	0.60
1:F:171:SER:HB3	1:F:172:PRO:HD3	1.84	0.60
1:C:373:ASP:O	1:C:377:ARG:HG3	2.02	0.59
1:E:452:PHE:O	1:E:456:LEU:HG	2.02	0.59
1:A:155:ARG:HD3	1:A:387:ASN:OD1	2.02	0.59
1:B:270:ASN:OD1	1:B:272:PRO:HD2	2.01	0.59
2:H:315:SER:CB	2:H:356:LYS:HE3	2.32	0.59
1:C:206:VAL:CG2	1:C:253:LEU:HD22	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:ILE:O	1:C:258:VAL:HG23	2.02	0.59
1:E:158:MET:HA	1:E:387:ASN:O	2.01	0.59
1:A:249:THR:HG21	1:A:369:ILE:O	2.03	0.59
1:D:135:LEU:H	1:D:135:LEU:CD2	2.15	0.59
1:E:319:GLU:OE1	1:E:323:ARG:NH2	2.36	0.59
1:F:113:ARG:H	1:F:169:ASP:CB	2.15	0.59
1:F:322:ARG:O	1:F:322:ARG:HG2	2.01	0.59
2:G:326:VAL:HG13	2:G:333:ALA:CB	2.32	0.59
1:C:348:ASN:C	1:C:349:ARG:HG2	2.22	0.59
1:D:250:GLY:O	1:D:254:ILE:HG13	2.02	0.59
1:B:114:ILE:HD11	1:B:182:ILE:HG12	1.85	0.59
1:B:239:ARG:HH11	1:B:239:ARG:HA	1.68	0.59
1:D:427:MET:SD	1:D:431:ASP:O	2.61	0.59
1:E:251:LYS:HD2	1:E:346:ALA:HB1	1.85	0.59
1:F:244:TYR:CZ	1:F:368:ASP:HB2	2.38	0.59
2:G:310:GLN:O	2:G:311:LYS:CB	2.49	0.59
1:A:28:VAL:HG13	1:A:97:GLY:H	1.67	0.59
1:C:59:LEU:CD2	1:C:102:ILE:HA	2.29	0.59
1:C:153:LEU:HD21	1:C:155:ARG:HH12	1.67	0.59
1:C:306:LEU:HG	1:C:353:ILE:HD12	1.84	0.59
1:D:87:VAL:CG1	1:D:88:VAL:H	2.15	0.59
1:D:147:ARG:HA	1:D:173:TYR:HB3	1.84	0.59
1:F:229:LEU:HG	1:F:233:ILE:CD1	2.32	0.59
1:A:229:LEU:O	1:A:231:LYS:N	2.35	0.59
1:B:53:ARG:NH1	1:B:73:SER:H	2.01	0.59
1:B:131:PHE:HA	1:B:135:LEU:HD23	1.85	0.59
1:C:148:LYS:HE3	1:C:166:VAL:O	2.03	0.59
1:C:192:GLU:HG2	1:C:195:GLU:CD	2.22	0.59
1:C:203:TYR:CE2	1:C:217:LYS:HE2	2.38	0.59
1:D:146:ILE:O	1:D:173:TYR:HB2	2.02	0.59
1:F:210:ARG:HD2	1:F:211:LYS:CE	2.28	0.59
2:G:282:LYS:O	2:G:286:SER:N	2.33	0.59
1:E:203:TYR:CZ	1:E:261:GLU:HG2	2.37	0.59
1:E:379:GLU:O	1:E:383:ILE:HG13	2.03	0.59
2:G:264:ALA:HB2	2:G:370:THR:OXT	2.03	0.59
2:G:344:PRO:HD2	2:G:345:ASN:H	1.67	0.59
1:D:426:LYS:O	1:D:428:ASP:N	2.36	0.58
1:A:229:LEU:C	1:A:231:LYS:H	2.07	0.58
1:C:146:ILE:HD12	1:C:165:VAL:CG2	2.33	0.58
1:D:297:ALA:CB	1:D:339:ALA:O	2.51	0.58
1:E:131:PHE:HD1	1:E:135:LEU:HB2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:388:MET:HE3	1:E:447:VAL:HG11	1.84	0.58
1:B:92:LEU:O	1:B:94:VAL:HG13	2.03	0.58
1:D:120:ASP:HB3	1:D:188:PRO:HB2	1.85	0.58
1:D:419:ALA:O	1:D:423:ILE:HG12	2.03	0.58
1:E:297:ALA:HA	1:E:298:PRO:C	2.22	0.58
1:A:432:LEU:CD1	1:E:27:ILE:HG12	2.33	0.58
1:B:353:ILE:HG22	1:B:354:ASP:H	1.68	0.58
1:E:113:ARG:H	1:E:169:ASP:CB	2.16	0.58
1:B:192:GLU:OE1	1:B:192:GLU:CA	2.50	0.58
1:C:153:LEU:HD11	1:C:160:ALA:HB1	1.85	0.58
2:G:298:ILE:O	2:G:310:GLN:HA	2.03	0.58
1:B:388:MET:HE3	1:B:447:VAL:HG21	1.85	0.58
1:D:317:HIS:N	1:D:317:HIS:CD2	2.71	0.58
1:E:203:TYR:CE2	1:E:261:GLU:HG2	2.39	0.58
1:F:87:VAL:HG22	1:F:198:LEU:HD13	1.84	0.58
1:F:249:THR:HG23	1:F:369:ILE:HG22	1.84	0.58
2:H:318:ILE:HB	2:H:351:GLU:C	2.24	0.58
1:A:429:LEU:C	1:A:431:ASP:H	2.07	0.58
1:C:351:ASN:N	1:C:351:ASN:ND2	2.49	0.58
1:F:95:ARG:HB2	1:F:225:ARG:NH1	2.19	0.58
1:A:25:ARG:HH22	1:F:431:ASP:HB3	1.69	0.58
1:B:126:ILE:HG23	1:B:159:ARG:NH1	2.18	0.58
1:E:133:VAL:HG12	1:E:443:ASN:HD22	1.69	0.58
1:E:353:ILE:HG22	1:E:354:ASP:N	2.17	0.58
1:E:358:ARG:HG3	1:E:358:ARG:NH1	2.19	0.58
1:A:51:LEU:CD2	1:A:104:PRO:HG3	2.33	0.58
1:B:59:LEU:HD22	1:B:100:ILE:CD1	2.33	0.58
1:D:358:ARG:HG3	1:D:358:ARG:NH1	2.19	0.58
1:D:403:THR:HG23	1:D:406:HIS:HB2	1.86	0.58
1:F:185:GLU:OE1	1:F:185:GLU:N	2.37	0.58
2:G:322:ARG:O	2:G:326:VAL:HG23	2.03	0.58
1:B:316:THR:HG23	1:B:321:GLU:HB2	1.85	0.58
1:C:118:PRO:HB3	1:C:123:VAL:HG11	1.86	0.58
1:D:25:ARG:HA	1:D:100:ILE:O	2.03	0.58
2:G:279:ASN:HB3	2:G:328:ALA:O	2.03	0.58
2:G:297:ASN:O	2:G:362:ASN:HA	2.03	0.58
1:A:254:ILE:O	1:A:258:VAL:HG23	2.04	0.57
1:B:31:ALA:O	1:B:32:ILE:CD1	2.51	0.57
1:B:117:LEU:HD21	1:B:185:GLU:OE1	2.04	0.57
1:D:329:LEU:HD22	1:D:362:ARG:NH1	2.19	0.57
2:H:317:ARG:HB3	2:H:352:ASN:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:LYS:HG3	1:B:94:VAL:HG12	1.85	0.57
1:B:254:ILE:CD1	1:B:369:ILE:HD13	2.34	0.57
1:C:351:ASN:ND2	1:C:351:ASN:H	2.01	0.57
1:F:203:TYR:CD2	1:F:261:GLU:HG2	2.39	0.57
1:B:203:TYR:CD2	1:B:261:GLU:HG2	2.38	0.57
1:D:358:ARG:HG3	4:D:809:HOH:O	2.03	0.57
1:D:403:THR:HG23	1:D:406:HIS:CG	2.38	0.57
1:A:242:LEU:HD23	1:A:244:TYR:OH	2.04	0.57
1:C:119:ILE:HG13	1:C:162:GLU:O	2.05	0.57
1:D:34:GLU:HG3	1:D:34:GLU:O	2.04	0.57
1:D:394:VAL:HA	1:D:449:MET:HB2	1.87	0.57
1:F:64:ARG:HG3	1:F:64:ARG:NH1	2.13	0.57
1:B:115:HIS:ND1	1:B:185:GLU:OE2	2.38	0.57
1:D:135:LEU:HD22	1:D:135:LEU:N	2.19	0.57
1:D:185:GLU:OE2	4:D:806:HOH:O	2.17	0.57
1:E:155:ARG:CZ	1:E:386:LYS:HD2	2.34	0.57
1:E:442:MET:HA	1:E:445:LEU:HD12	1.87	0.57
1:D:113:ARG:HA	1:D:181:VAL:CG1	2.34	0.57
1:E:432:LEU:O	1:E:432:LEU:HD13	2.04	0.57
1:F:313:ARG:HG2	1:F:355:PRO:HD2	1.87	0.57
1:F:350:PRO:CB	1:F:358:ARG:NH2	2.67	0.57
2:G:308:LEU:HD23	2:G:308:LEU:H	1.70	0.57
1:C:318:GLY:HA2	1:C:322:ARG:CZ	2.35	0.57
1:D:117:LEU:HB2	1:D:189:ILE:HD11	1.87	0.57
1:F:177:ALA:HB1	1:F:178:PRO:HD2	1.86	0.57
1:C:222:LEU:HD23	1:C:226:HIS:CD2	2.38	0.57
1:D:115:HIS:C	1:D:115:HIS:CD2	2.77	0.57
1:E:297:ALA:HB1	1:E:340:HIS:HB2	1.87	0.57
1:F:283:GLU:HB3	1:F:287:ARG:NH1	2.20	0.57
1:A:55:ASP:O	1:A:71:VAL:HG12	2.05	0.57
1:A:310:ALA:CB	1:A:357:LEU:HD11	2.35	0.57
1:C:358:ARG:HG3	1:C:358:ARG:NH1	2.20	0.57
1:D:87:VAL:CG1	1:D:88:VAL:N	2.68	0.57
1:D:113:ARG:HA	1:D:181:VAL:HG12	1.87	0.57
1:D:147:ARG:HD3	1:D:148:LYS:N	2.19	0.57
1:E:72:LEU:HG	1:E:73:SER:N	2.20	0.57
1:E:350:PRO:HB3	1:E:358:ARG:NH2	2.20	0.57
1:F:353:ILE:HG23	1:F:357:LEU:HD12	1.87	0.57
1:D:230:PHE:CE1	1:D:237:PRO:HB3	2.40	0.56
1:F:249:THR:CG2	1:F:369:ILE:HG22	2.34	0.56
1:C:110:TYR:H	1:C:110:TYR:HD1	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:ASN:HB2	1:E:102:ILE:O	2.05	0.56
2:H:311:LYS:CG	2:H:313:ASN:HB2	2.35	0.56
1:A:297:ALA:HB1	1:A:340:HIS:HB2	1.87	0.56
1:B:78:SER:HB2	1:B:81:LYS:CE	2.26	0.56
1:B:227:PRO:HB3	1:B:340:HIS:NE2	2.21	0.56
1:C:192:GLU:CB	1:C:195:GLU:HG3	2.35	0.56
1:C:312:LYS:CG	1:C:355:PRO:HD3	2.36	0.56
1:D:340:HIS:ND1	4:D:805:HOH:O	2.22	0.56
1:E:131:PHE:CD1	1:E:135:LEU:HB2	2.40	0.56
1:F:100:ILE:HD12	1:F:100:ILE:O	2.04	0.56
2:I:325:ILE:O	2:I:325:ILE:HD13	2.03	0.56
1:A:123:VAL:HG12	1:A:126:ILE:HD11	1.87	0.56
1:B:336:LYS:HZ2	1:B:338:ARG:HG3	1.69	0.56
1:C:201:VAL:CG1	1:C:253:LEU:HD23	2.35	0.56
1:C:347:THR:C	1:C:348:ASN:HD22	2.09	0.56
1:E:312:LYS:HG2	1:E:313:ARG:H	1.70	0.56
1:A:134:TYR:O	1:A:137:PRO:HD2	2.04	0.56
1:A:147:ARG:HH11	1:A:147:ARG:HG3	1.71	0.56
1:A:210:ARG:HG2	1:A:211:LYS:H	1.71	0.56
1:B:428:ASP:C	1:B:430:ILE:H	2.09	0.56
1:D:35:ASP:HB3	1:D:38:VAL:HG12	1.88	0.56
1:E:233:ILE:HG23	1:E:235:VAL:H	1.71	0.56
2:H:276:GLN:HA	2:H:279:ASN:CB	2.36	0.56
1:A:129:ASN:O	1:A:133:VAL:HG23	2.06	0.56
1:B:43:GLN:N	1:B:44:PRO:CD	2.69	0.56
1:B:58:LEU:HB2	1:B:105:CYS:HB2	1.86	0.56
1:B:380:ILE:HA	1:B:383:ILE:HD12	1.87	0.56
1:C:159:ARG:O	1:C:387:ASN:ND2	2.38	0.56
1:E:249:THR:HG21	1:E:369:ILE:O	2.05	0.56
1:A:244:TYR:CZ	1:A:350:PRO:HG3	2.41	0.56
1:A:277:LYS:HB3	1:A:281:GLU:HG2	1.87	0.56
1:B:63:LYS:O	1:B:65:ARG:HG2	2.06	0.56
1:D:88:VAL:O	1:D:91:ASN:N	2.39	0.56
1:D:133:VAL:O	1:D:137:PRO:HG2	2.06	0.56
1:E:397:GLU:O	1:E:401:ASN:ND2	2.38	0.56
1:F:353:ILE:CG2	1:F:354:ASP:N	2.68	0.56
1:F:430:ILE:O	1:F:432:LEU:N	2.39	0.56
1:B:238:PRO:O	1:B:239:ARG:NH1	2.38	0.56
1:C:190:LYS:HE2	1:C:191:ARG:N	2.21	0.56
1:D:120:ASP:CA	1:D:188:PRO:HB3	2.36	0.56
1:D:132:GLU:HA	1:D:136:LYS:CE	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:TYR:C	1:D:137:PRO:HD2	2.26	0.56
1:D:236:LYS:HG2	1:D:337:GLN:HE21	1.70	0.56
1:E:113:ARG:HG3	1:E:169:ASP:HB2	1.88	0.56
1:E:249:THR:HG21	1:E:369:ILE:HG22	1.87	0.56
1:E:360:PHE:HA	1:E:364:ASP:HB3	1.88	0.56
2:H:303:ALA:C	2:H:305:GLY:N	2.60	0.56
1:B:41:LEU:HD11	1:B:102:ILE:CD1	2.35	0.56
1:C:27:ILE:CB	1:C:81:LYS:HG2	2.20	0.56
1:D:24:ASN:O	1:D:101:SER:HA	2.06	0.56
1:D:199:ASN:C	1:D:199:ASN:OD1	2.43	0.56
1:D:229:LEU:O	1:D:233:ILE:HG12	2.05	0.56
1:A:230:PHE:CZ	1:A:237:PRO:HB3	2.40	0.56
1:B:26:LEU:O	1:B:99:VAL:HA	2.05	0.56
1:B:48:GLU:HB2	1:B:49:LEU:HD23	1.86	0.56
1:B:348:ASN:HD22	1:B:348:ASN:N	2.03	0.56
1:D:57:VAL:O	1:D:68:VAL:HG13	2.05	0.56
2:G:308:LEU:HD23	2:G:308:LEU:N	2.20	0.56
1:A:371:ILE:H	1:A:371:ILE:CD1	2.16	0.55
1:B:222:LEU:HD23	1:B:226:HIS:HD2	1.71	0.55
1:C:119:ILE:HD12	1:C:162:GLU:HB3	1.88	0.55
1:C:338:ARG:HD2	1:C:338:ARG:N	2.08	0.55
1:A:313:ARG:HH11	1:A:313:ARG:HG2	1.69	0.55
1:D:89:ARG:NH2	1:D:261:GLU:OE2	2.39	0.55
1:D:297:ALA:HB1	1:D:339:ALA:O	2.06	0.55
1:F:105:CYS:SG	1:F:108:VAL:CG2	2.94	0.55
1:B:249:THR:CG2	1:B:369:ILE:HG22	2.36	0.55
1:F:110:TYR:CD2	1:F:177:ALA:HB2	2.41	0.55
1:F:230:PHE:CE1	1:F:237:PRO:HB3	2.42	0.55
1:C:87:VAL:HG22	1:C:198:LEU:HD11	1.88	0.55
1:C:214:ALA:O	1:C:217:LYS:HB2	2.06	0.55
1:A:312:LYS:HB3	1:A:354:ASP:CB	2.37	0.55
1:C:121:ASP:OD1	1:C:122:THR:HG23	2.07	0.55
1:A:120:ASP:OD2	1:A:190:LYS:HA	2.05	0.55
1:A:123:VAL:HG13	1:A:161:VAL:HG13	1.89	0.55
1:B:201:VAL:HG11	1:B:253:LEU:HD23	1.89	0.55
1:E:224:LEU:HD12	1:E:298:PRO:HB3	1.89	0.55
1:A:432:LEU:HD12	1:E:27:ILE:CD1	2.37	0.55
1:B:281:GLU:O	1:B:284:SER:HB3	2.06	0.55
1:B:316:THR:HG21	1:B:322:ARG:HD3	1.88	0.55
1:C:236:LYS:NZ	1:C:236:LYS:CB	2.70	0.55
1:E:424:ARG:HA	1:E:428:ASP:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:351:ASN:H	1:F:351:ASN:ND2	2.05	0.55
2:G:358:ALA:CB	2:G:360:LEU:HG	2.37	0.55
1:C:230:PHE:CA	1:C:233:ILE:HG22	2.19	0.55
1:D:147:ARG:HB3	1:D:150:ASP:OD2	2.06	0.55
1:E:31:ALA:HB2	1:E:84:MET:CA	2.37	0.55
1:F:40:SER:O	1:F:41:LEU:HD23	2.07	0.55
1:F:74:ASP:OD1	1:F:76:THR:HG22	2.07	0.55
1:B:431:ASP:O	1:B:433:GLU:N	2.39	0.55
1:C:358:ARG:HG3	1:C:358:ARG:HH11	1.72	0.55
1:F:117:LEU:HD12	1:F:166:VAL:HG21	1.89	0.55
1:F:313:ARG:HD3	1:F:355:PRO:HG2	1.89	0.55
1:A:220:VAL:HG12	1:A:342:ILE:HD13	1.89	0.55
1:B:108:VAL:HG12	1:B:175:ILE:HG13	1.88	0.55
1:B:172:PRO:C	1:B:173:TYR:HD2	2.10	0.55
1:C:236:LYS:NZ	1:C:236:LYS:HB3	2.21	0.55
1:D:111:GLY:HA3	1:D:174:CYS:SG	2.47	0.55
1:D:248:GLY:CA	1:D:409:ALA:HB2	2.37	0.55
1:D:316:THR:HB	1:D:322:ARG:NE	2.22	0.55
1:E:131:PHE:CE2	1:E:136:LYS:HE3	2.41	0.55
1:F:25:ARG:HH11	1:F:101:SER:HB3	1.72	0.55
1:B:23:PRO:HB2	1:B:25:ARG:HG3	1.89	0.54
1:B:123:VAL:HG13	1:B:126:ILE:CG1	2.37	0.54
1:C:38:VAL:HG21	1:C:72:LEU:HD12	1.89	0.54
1:C:379:GLU:O	1:C:383:ILE:HG13	2.06	0.54
1:D:140:LEU:HD12	1:D:141:GLU:CG	2.37	0.54
1:E:97:GLY:C	1:E:225:ARG:HH22	2.10	0.54
1:E:114:ILE:CD1	1:E:176:VAL:HG22	2.38	0.54
1:E:147:ARG:HH11	1:E:147:ARG:HG3	1.71	0.54
1:B:46:MET:CE	1:B:73:SER:HB2	2.37	0.54
1:D:26:LEU:HA	1:D:80:GLU:OE1	2.07	0.54
1:D:265:PHE:CD2	1:D:296:ASN:HB2	2.43	0.54
1:F:297:ALA:HA	1:F:298:PRO:C	2.27	0.54
1:F:337:GLN:C	1:F:339:ALA:N	2.60	0.54
2:G:326:VAL:CG1	2:G:333:ALA:HB2	2.34	0.54
1:B:297:ALA:HA	1:B:298:PRO:C	2.27	0.54
1:C:265:PHE:HB3	1:C:299:ALA:HB2	1.88	0.54
1:A:100:ILE:HD12	1:A:100:ILE:C	2.27	0.54
1:D:140:LEU:HD12	1:D:141:GLU:HG3	1.88	0.54
1:E:203:TYR:CE2	1:E:217:LYS:HE2	2.42	0.54
1:F:210:ARG:H	1:F:211:LYS:HD2	1.72	0.54
1:A:206:VAL:CG2	1:A:253:LEU:HD22	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ILE:O	1:A:241:ILE:HG13	2.07	0.54
1:D:57:VAL:HG22	1:D:69:CYS:O	2.08	0.54
1:E:36:ASN:OD1	1:E:87:VAL:HG21	2.07	0.54
1:E:108:VAL:CG1	1:E:175:ILE:HG13	2.37	0.54
1:E:429:LEU:C	1:E:431:ASP:N	2.60	0.54
1:C:348:ASN:HD22	1:C:348:ASN:N	2.05	0.54
1:D:452:PHE:O	1:D:456:LEU:HG	2.08	0.54
1:E:26:LEU:HD12	1:E:82:ILE:CB	2.33	0.54
1:E:231:LYS:HG3	1:E:338:ARG:HH22	1.72	0.54
1:F:337:GLN:C	1:F:339:ALA:H	2.10	0.54
1:F:421:GLN:OE1	1:F:421:GLN:HA	2.07	0.54
2:I:281:ALA:C	2:I:283:ALA:H	2.11	0.54
1:B:129:ASN:HB3	1:B:132:GLU:OE1	2.08	0.54
1:B:241:ILE:HD12	1:B:342:ILE:CG2	2.38	0.54
1:E:447:VAL:HG21	1:E:452:PHE:HE1	1.72	0.54
1:F:120:ASP:OD2	1:F:190:LYS:HD2	2.08	0.54
1:A:315:LYS:O	1:A:316:THR:OG1	2.24	0.54
1:B:28:VAL:HG23	1:B:96:LEU:HA	1.90	0.54
1:B:336:LYS:NZ	1:B:338:ARG:HE	2.06	0.54
1:B:423:ILE:HG12	1:B:445:LEU:HD13	1.89	0.54
1:C:57:VAL:CG2	1:C:71:VAL:CG2	2.86	0.54
1:D:117:LEU:HB2	1:D:189:ILE:CD1	2.38	0.54
1:E:40:SER:HB3	1:E:83:ARG:HB2	1.90	0.54
1:F:312:LYS:HE3	1:F:313:ARG:HG3	1.90	0.54
1:A:26:LEU:CD2	1:A:45:LYS:HE2	2.36	0.54
1:A:337:GLN:OE1	1:A:337:GLN:CA	2.55	0.54
1:A:432:LEU:HD12	1:E:27:ILE:CG1	2.38	0.54
1:D:186:GLY:O	1:D:187:GLU:CG	2.53	0.54
1:D:349:ARG:HE	1:D:351:ASN:CB	2.07	0.54
1:C:297:ALA:HB1	1:C:340:HIS:HB2	1.90	0.54
1:E:63:LYS:NZ	1:E:194:GLU:CD	2.61	0.54
1:E:270:ASN:O	1:E:273:GLU:HB3	2.08	0.54
1:E:417:GLU:OE1	1:E:417:GLU:HA	2.08	0.54
1:B:249:THR:O	1:B:249:THR:HG22	2.08	0.53
1:B:430:ILE:O	1:B:430:ILE:HG22	2.08	0.53
1:C:49:LEU:HD23	1:C:102:ILE:HG21	1.90	0.53
1:C:126:ILE:CG2	1:C:159:ARG:HH11	2.22	0.53
1:D:132:GLU:CA	1:D:136:LYS:HE3	2.38	0.53
1:D:170:PRO:HD2	1:D:174:CYS:HB3	1.91	0.53
1:F:112:LYS:HB2	1:F:169:ASP:CB	2.38	0.53
1:A:316:THR:CG2	1:A:317:HIS:N	2.70	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ARG:HH12	1:C:322:ARG:HG2	1.73	0.53
1:D:36:ASN:HD22	1:D:36:ASN:N	2.05	0.53
1:F:23:PRO:O	1:F:49:LEU:HD11	2.09	0.53
1:F:43:GLN:NE2	1:F:73:SER:HB3	2.23	0.53
1:A:34:GLU:OE1	1:A:34:GLU:N	2.41	0.53
1:B:108:VAL:O	2:H:301:ARG:NH2	2.40	0.53
1:B:120:ASP:OD2	1:B:190:LYS:HD2	2.08	0.53
1:C:67:ALA:HB3	1:C:92:LEU:HD21	1.91	0.53
1:E:26:LEU:HD21	1:E:102:ILE:HG23	1.91	0.53
1:E:249:THR:O	1:E:249:THR:HG22	2.08	0.53
1:E:313:ARG:HA	1:E:316:THR:HG22	1.90	0.53
1:A:131:PHE:C	1:A:131:PHE:CD1	2.81	0.53
1:D:310:ALA:HA	1:D:325:VAL:HG22	1.90	0.53
1:D:403:THR:HG22	1:D:406:HIS:HB2	1.90	0.53
1:E:82:ILE:HG21	1:E:100:ILE:HD11	1.90	0.53
1:E:158:MET:HE1	1:E:419:ALA:HB1	1.90	0.53
1:F:112:LYS:HZ1	1:F:113:ARG:HH11	1.57	0.53
1:F:249:THR:HG21	1:F:369:ILE:O	2.08	0.53
1:F:383:ILE:O	1:F:386:LYS:HG2	2.08	0.53
2:H:301:ARG:NH1	2:H:308:LEU:HD13	2.23	0.53
1:C:203:TYR:CD2	1:C:261:GLU:HG2	2.41	0.53
1:E:213:LEU:HD22	1:E:217:LYS:HE3	1.90	0.53
2:H:354:THR:CG2	2:H:357:GLU:HG3	2.39	0.53
1:D:95:ARG:HB2	1:D:225:ARG:NH1	2.23	0.53
1:E:138:TYR:CE2	1:E:152:PHE:CD2	2.96	0.53
1:F:313:ARG:O	1:F:316:THR:HG23	2.07	0.53
2:H:295:THR:HA	2:H:314:HIS:HA	1.91	0.53
2:G:287:ILE:HG22	2:G:288:LEU:N	2.22	0.53
1:E:378:LEU:HD23	1:E:397:GLU:HA	1.90	0.53
1:F:43:GLN:N	1:F:44:PRO:HD2	2.24	0.53
1:B:358:ARG:HG3	1:B:358:ARG:NH1	2.24	0.53
1:B:383:ILE:O	1:B:386:LYS:HG2	2.09	0.53
1:E:169:ASP:HB3	1:E:170:PRO:CD	2.31	0.53
1:E:231:LYS:HG3	1:E:338:ARG:NH2	2.23	0.53
1:E:360:PHE:O	1:E:364:ASP:OD2	2.27	0.53
1:E:447:VAL:CG2	1:E:452:PHE:HE1	2.22	0.53
2:G:344:PRO:HB2	2:G:346:LYS:HE2	1.90	0.53
1:C:49:LEU:CD2	1:C:102:ILE:HG21	2.39	0.53
1:C:378:LEU:HD12	1:C:382:GLN:OE1	2.09	0.53
1:C:449:MET:O	1:C:449:MET:HG3	2.07	0.53
1:D:131:PHE:CD2	1:D:136:LYS:HE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:307:ARG:CD	2:G:329:ARG:NH2	2.72	0.53
2:H:302:LEU:HB2	2:H:307:ARG:CB	2.36	0.53
1:A:318:GLY:O	1:A:320:VAL:N	2.39	0.52
1:A:383:ILE:O	1:A:386:LYS:HG2	2.09	0.52
1:C:40:SER:HB2	1:C:83:ARG:HB2	1.92	0.52
1:C:320:VAL:HG12	1:C:324:ILE:CD1	2.39	0.52
1:C:369:ILE:O	1:C:369:ILE:HG22	2.08	0.52
1:E:48:GLU:CG	1:E:49:LEU:N	2.71	0.52
1:E:166:VAL:O	1:E:167:GLU:HB2	2.09	0.52
1:F:147:ARG:HD3	1:F:148:LYS:O	2.08	0.52
1:F:419:ALA:O	1:F:423:ILE:HG13	2.08	0.52
1:A:24:ASN:OD1	1:A:24:ASN:N	2.42	0.52
1:B:233:ILE:HG22	1:B:235:VAL:HG23	1.91	0.52
1:B:349:ARG:CD	1:B:350:PRO:HD2	2.38	0.52
1:C:153:LEU:CD1	1:C:160:ALA:HB1	2.39	0.52
1:E:109:LYS:CD	1:E:170:PRO:HB3	2.39	0.52
2:H:299:GLN:HG2	2:H:364:VAL:HG22	1.91	0.52
1:B:62:LYS:HG3	1:B:93:ARG:O	2.09	0.52
1:C:78:SER:OG	1:C:81:LYS:HE2	2.10	0.52
1:D:31:ALA:HB2	1:D:84:MET:C	2.28	0.52
1:D:74:ASP:OD1	1:D:77:CYS:N	2.43	0.52
1:E:329:LEU:HD22	1:E:362:ARG:NH1	2.24	0.52
2:H:307:ARG:HD2	2:H:329:ARG:NH2	2.25	0.52
1:A:135:LEU:H	1:A:135:LEU:HD22	1.74	0.52
1:B:445:LEU:HD23	1:B:445:LEU:C	2.29	0.52
1:B:457:SER:O	1:B:458:GLN:NE2	2.42	0.52
1:C:120:ASP:O	1:C:124:GLU:HG3	2.09	0.52
1:C:312:LYS:HG2	1:C:355:PRO:HD3	1.91	0.52
1:D:126:ILE:HG21	1:D:159:ARG:HD2	1.92	0.52
1:E:125:GLY:O	1:E:436:THR:CG2	2.58	0.52
1:E:226:HIS:N	1:E:227:PRO:HD3	2.24	0.52
1:E:395:ASP:O	1:E:398:GLN:N	2.41	0.52
1:F:233:ILE:HG22	1:F:234:GLY:N	2.24	0.52
1:C:168:THR:HB	1:C:174:CYS:SG	2.50	0.52
1:D:290:PHE:HA	1:D:301:ILE:CD1	2.39	0.52
1:D:322:ARG:CG	1:D:322:ARG:NH1	2.58	0.52
1:F:53:ARG:HH11	1:F:53:ARG:HG2	1.74	0.52
1:C:164:LYS:HB3	1:C:189:ILE:HD11	1.92	0.52
2:G:279:ASN:O	2:G:328:ALA:HA	2.09	0.52
1:C:233:ILE:HD11	1:E:158:MET:CB	2.40	0.52
1:E:36:ASN:CG	1:E:87:VAL:HG21	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:338:VAL:CG1	2:G:339:LEU:N	2.72	0.52
1:D:131:PHE:CE2	1:D:136:LYS:HE2	2.44	0.52
1:E:42:SER:OG	1:E:79:ASP:HA	2.10	0.52
1:E:84:MET:HB2	1:E:88:VAL:HG21	1.90	0.52
1:E:135:LEU:HD22	1:E:135:LEU:N	2.17	0.52
1:F:220:VAL:HB	1:F:224:LEU:HD12	1.92	0.52
1:C:35:ASP:O	1:C:38:VAL:HG12	2.09	0.52
1:D:28:VAL:HG12	1:D:98:ASP:O	2.10	0.52
1:E:48:GLU:HG2	1:E:49:LEU:N	2.25	0.52
1:E:147:ARG:HD3	1:E:148:LYS:O	2.10	0.52
1:E:231:LYS:HD3	1:E:338:ARG:NH1	2.19	0.52
1:F:87:VAL:HG22	1:F:198:LEU:CD1	2.40	0.52
1:B:76:THR:O	1:B:76:THR:HG22	2.10	0.52
1:C:57:VAL:CG2	1:C:71:VAL:HG23	2.40	0.52
1:C:388:MET:CE	1:C:447:VAL:HG21	2.40	0.52
1:F:279:ALA:HB2	1:F:320:VAL:CG1	2.40	0.52
2:H:305:GLY:C	2:H:307:ARG:H	2.13	0.52
2:H:311:LYS:HG2	2:H:313:ASN:HB2	1.92	0.52
1:B:53:ARG:CZ	1:B:73:SER:HB3	2.40	0.51
1:B:110:TYR:HD1	1:B:110:TYR:H	1.58	0.51
1:D:131:PHE:HE2	1:D:136:LYS:HG2	1.74	0.51
1:D:190:LYS:HE2	1:D:191:ARG:H	1.75	0.51
1:E:383:ILE:O	1:E:386:LYS:HG2	2.09	0.51
1:F:297:ALA:HB1	1:F:340:HIS:HB2	1.92	0.51
2:G:304:ASP:OD1	2:G:307:ARG:CB	2.57	0.51
2:G:338:VAL:HG12	2:G:339:LEU:H	1.76	0.51
1:A:169:ASP:HB3	1:A:170:PRO:CD	2.36	0.51
1:E:414:LEU:HD12	1:E:455:ALA:HB1	1.92	0.51
1:A:43:GLN:HB3	1:A:44:PRO:HD3	1.92	0.51
1:C:254:ILE:HD12	1:C:369:ILE:HD13	1.93	0.51
1:D:140:LEU:HD12	1:D:140:LEU:C	2.31	0.51
1:E:74:ASP:OD1	1:E:76:THR:N	2.43	0.51
1:E:108:VAL:HG22	1:E:173:TYR:CD1	2.44	0.51
1:D:138:TYR:CZ	1:D:144:ARG:HD3	2.46	0.51
1:D:186:GLY:O	1:D:187:GLU:CB	2.58	0.51
1:D:280:GLY:HA2	1:D:323:ARG:HH21	1.75	0.51
1:D:383:ILE:O	1:D:386:LYS:HE3	2.11	0.51
1:E:40:SER:OG	1:E:74:ASP:HB2	2.10	0.51
1:E:229:LEU:O	1:E:233:ILE:HB	2.10	0.51
1:F:112:LYS:NZ	1:F:113:ARG:NH1	2.57	0.51
1:C:41:LEU:HD21	1:C:82:ILE:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:ASN:O	1:F:22:ARG:HG2	2.10	0.51
1:A:35:ASP:HB3	1:A:38:VAL:CG1	2.40	0.51
1:A:212:GLN:H	1:A:212:GLN:CD	2.13	0.51
1:A:353:ILE:HG23	1:A:357:LEU:HD12	1.92	0.51
1:A:457:SER:O	1:A:458:GLN:NE2	2.44	0.51
1:D:153:LEU:HD22	1:D:198:LEU:HB3	1.91	0.51
1:D:364:ASP:OD2	1:D:364:ASP:N	2.42	0.51
1:F:70:ILE:CD1	2:G:343:PHE:CE1	2.94	0.51
2:H:311:LYS:CG	2:H:312:PHE:H	2.19	0.51
2:H:316:HIS:O	2:H:355:LEU:HG	2.10	0.51
1:C:232:ALA:HB2	1:E:125:GLY:O	2.09	0.51
1:C:287:ARG:HH11	1:C:327:GLN:NE2	2.07	0.51
1:A:249:THR:HG23	1:A:369:ILE:HG22	1.93	0.51
1:D:155:ARG:HG2	1:D:160:ALA:HB2	1.92	0.51
1:D:422:ALA:HB2	1:D:451:ASP:OD2	2.09	0.51
1:D:430:ILE:HG22	1:D:430:ILE:O	2.09	0.51
1:A:275:MET:CE	1:A:324:ILE:HG21	2.41	0.51
1:A:329:LEU:HD22	1:A:362:ARG:NH1	2.26	0.51
1:D:43:GLN:HB2	1:D:44:PRO:HD3	1.93	0.51
1:D:438:ASP:O	1:D:441:VAL:HG22	2.11	0.51
2:H:295:THR:HA	2:H:314:HIS:HB2	1.91	0.51
2:H:299:GLN:CB	2:H:364:VAL:HG22	2.40	0.51
1:A:108:VAL:CG1	1:A:175:ILE:HG13	2.40	0.51
1:C:100:ILE:HG22	1:C:101:SER:N	2.26	0.51
1:C:311:PRO:HA	1:C:352:SER:O	2.10	0.51
1:C:350:PRO:HB3	1:C:358:ARG:NH2	2.26	0.51
1:C:388:MET:HE3	1:C:447:VAL:HG21	1.93	0.51
1:D:309:ILE:C	1:D:311:PRO:HD3	2.32	0.51
1:F:243:LEU:O	1:F:346:ALA:HA	2.11	0.51
1:F:311:PRO:HB2	1:F:315:LYS:HB2	1.93	0.51
1:A:237:PRO:HD2	1:A:337:GLN:HE21	1.75	0.50
1:B:36:ASN:CG	1:B:87:VAL:HG21	2.31	0.50
1:C:122:THR:HG21	1:C:162:GLU:HB2	1.93	0.50
1:C:438:ASP:HB3	1:C:441:VAL:HG23	1.93	0.50
1:D:230:PHE:CZ	1:D:237:PRO:HB3	2.46	0.50
1:E:429:LEU:O	1:E:431:ASP:N	2.44	0.50
1:A:213:LEU:O	1:A:217:LYS:HG3	2.12	0.50
1:A:241:ILE:HD11	1:A:243:LEU:CD1	2.41	0.50
1:A:313:ARG:HG2	1:A:313:ARG:NH1	2.27	0.50
1:A:353:ILE:HG22	1:A:354:ASP:N	2.27	0.50
1:A:428:ASP:OD1	1:A:429:LEU:HG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:LEU:HD23	1:B:105:CYS:SG	2.51	0.50
1:B:135:LEU:HD22	1:B:135:LEU:N	2.25	0.50
1:B:283:GLU:HB3	1:B:327:GLN:HE21	1.76	0.50
1:C:40:SER:O	1:C:41:LEU:HD23	2.11	0.50
1:C:197:SER:OG	1:C:199:ASN:N	2.41	0.50
1:D:84:MET:HG3	1:D:89:ARG:HG3	1.93	0.50
1:E:206:VAL:HG22	1:E:253:LEU:CD2	2.42	0.50
1:F:222:LEU:HB2	1:F:223:PRO:HD3	1.93	0.50
1:A:122:THR:HG21	1:A:162:GLU:HB2	1.93	0.50
1:A:314:GLU:O	1:A:314:GLU:HG2	2.10	0.50
1:D:71:VAL:O	1:D:71:VAL:HG13	2.11	0.50
2:H:347:GLU:O	2:H:349:ALA:N	2.44	0.50
1:A:377:ARG:CZ	1:A:404:HIS:HA	2.42	0.50
1:B:233:ILE:HG22	1:B:234:GLY:N	2.26	0.50
1:C:22:ARG:HB2	1:C:24:ASN:OD1	2.12	0.50
1:D:377:ARG:HD2	1:D:403:THR:CG2	2.42	0.50
1:E:39:VAL:HG22	1:E:70:ILE:O	2.10	0.50
1:B:338:ARG:O	1:B:339:ALA:HB3	2.11	0.50
1:C:229:LEU:O	1:C:233:ILE:HG22	2.11	0.50
1:C:338:ARG:CD	1:C:338:ARG:N	2.68	0.50
1:D:113:ARG:NH1	4:D:806:HOH:O	2.43	0.50
1:D:201:VAL:HG11	1:D:253:LEU:HD23	1.93	0.50
1:D:203:TYR:CE2	1:D:217:LYS:HE2	2.47	0.50
1:E:126:ILE:CD1	1:E:159:ARG:HD2	2.37	0.50
1:C:133:VAL:HG13	1:C:443:ASN:ND2	2.26	0.50
1:C:211:LYS:O	1:C:214:ALA:HB3	2.11	0.50
1:C:279:ALA:HB1	1:C:320:VAL:CG2	2.36	0.50
1:E:88:VAL:HG23	1:E:89:ARG:N	2.27	0.50
1:F:46:MET:O	1:F:50:GLN:N	2.45	0.50
2:G:301:ARG:NH1	2:G:308:LEU:HB3	2.25	0.50
2:H:360:LEU:O	2:H:361:LEU:C	2.49	0.50
1:A:115:HIS:HE1	1:A:185:GLU:H	1.60	0.50
1:A:191:ARG:HD3	1:A:195:GLU:O	2.12	0.50
1:B:118:PRO:HB2	1:B:123:VAL:CG2	2.42	0.50
1:D:138:TYR:CE2	1:D:152:PHE:HD2	2.29	0.50
1:D:310:ALA:CB	1:D:357:LEU:HD11	2.41	0.50
1:E:50:GLN:O	1:E:51:LEU:HD23	2.11	0.50
2:G:344:PRO:CB	2:G:346:LYS:HE2	2.41	0.50
1:B:78:SER:CB	1:B:81:LYS:HE3	2.30	0.50
1:B:329:LEU:HD23	1:B:357:LEU:HD23	1.93	0.50
1:B:358:ARG:HG3	1:B:358:ARG:HH11	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:PRO:HB2	1:C:377:ARG:HG2	1.94	0.50
1:D:84:MET:HG3	1:D:89:ARG:CG	2.42	0.50
1:D:381:LEU:HB3	1:D:396:LEU:HD22	1.94	0.50
1:D:430:ILE:O	1:D:431:ASP:OD1	2.30	0.50
1:E:131:PHE:CE1	1:E:136:LYS:HE3	2.45	0.50
1:E:250:GLY:O	1:E:253:LEU:HB3	2.12	0.50
1:F:82:ILE:HG21	1:F:100:ILE:HD11	1.92	0.50
1:F:82:ILE:O	1:F:82:ILE:HG23	2.12	0.50
1:A:120:ASP:OD1	1:A:121:ASP:N	2.41	0.50
1:A:357:LEU:O	1:A:363:PHE:HB2	2.12	0.50
1:A:423:ILE:HA	1:A:445:LEU:HD11	1.94	0.50
1:A:429:LEU:O	1:A:431:ASP:N	2.45	0.50
1:B:239:ARG:HH21	1:B:340:HIS:CB	2.25	0.50
1:B:241:ILE:CD1	1:B:342:ILE:HG21	2.42	0.50
1:C:423:ILE:HD13	1:D:229:LEU:HD11	1.93	0.50
1:E:30:GLU:OE2	1:E:203:TYR:HD2	1.95	0.50
1:A:52:PHE:O	1:A:54:GLY:N	2.42	0.49
1:B:37:SER:O	1:B:69:CYS:HB3	2.12	0.49
1:B:349:ARG:HG2	1:B:351:ASN:HD21	1.75	0.49
1:B:440:GLU:C	1:B:440:GLU:CD	2.70	0.49
1:D:283:GLU:OE2	1:D:323:ARG:O	2.29	0.49
1:D:309:ILE:O	1:D:311:PRO:HD3	2.12	0.49
1:E:48:GLU:HG2	1:E:49:LEU:HG	1.92	0.49
1:E:143:TYR:CE1	1:E:178:PRO:HD3	2.47	0.49
1:F:115:HIS:HA	1:F:183:HIS:O	2.12	0.49
1:F:398:GLN:OE1	1:F:398:GLN:HA	2.10	0.49
1:F:456:LEU:C	1:F:458:GLN:H	2.14	0.49
2:H:317:ARG:HG2	2:H:352:ASN:O	2.12	0.49
1:B:32:ILE:HD11	1:B:83:ARG:NH1	2.27	0.49
1:E:31:ALA:HB2	1:E:84:MET:N	2.27	0.49
1:F:21:ASN:O	1:F:22:ARG:CG	2.60	0.49
1:F:68:VAL:HG12	1:F:145:PRO:HB2	1.94	0.49
2:G:311:LYS:O	2:G:312:PHE:CB	2.59	0.49
1:A:192:GLU:HB2	1:A:195:GLU:HG3	1.94	0.49
1:B:110:TYR:CD2	1:B:177:ALA:HB2	2.46	0.49
1:B:171:SER:HB2	1:B:172:PRO:HD3	1.93	0.49
1:D:32:ILE:HB	1:D:83:ARG:HD3	1.94	0.49
1:D:398:GLN:HE21	1:D:398:GLN:CA	2.16	0.49
1:E:26:LEU:N	1:E:26:LEU:CD2	2.69	0.49
1:E:242:LEU:HD23	1:E:244:TYR:OH	2.13	0.49
1:E:422:ALA:HA	1:E:426:LYS:HZ2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ARG:C	1:A:227:PRO:HD3	2.33	0.49
1:A:447:VAL:CG1	1:A:452:PHE:HE1	2.25	0.49
1:C:244:TYR:CD2	1:C:244:TYR:N	2.80	0.49
1:D:426:LYS:CG	1:D:427:MET:H	2.24	0.49
1:E:74:ASP:OD1	1:E:75:ASP:N	2.45	0.49
1:E:83:ARG:HG2	1:E:83:ARG:HH11	1.77	0.49
1:E:147:ARG:HD3	1:E:147:ARG:C	2.33	0.49
1:F:70:ILE:HD12	2:G:343:PHE:CE1	2.47	0.49
1:F:379:GLU:O	1:F:383:ILE:HG13	2.11	0.49
2:G:294:PRO:O	2:G:314:HIS:HA	2.11	0.49
1:B:297:ALA:HB1	1:B:340:HIS:O	2.12	0.49
1:C:24:ASN:O	1:C:101:SER:HA	2.13	0.49
1:F:384:HIS:HE1	3:F:805:ADP:N3	2.10	0.49
1:A:32:ILE:HG12	1:A:83:ARG:CD	2.41	0.49
1:D:407:VAL:HG23	1:D:409:ALA:H	1.78	0.49
1:E:119:ILE:HG12	1:E:162:GLU:O	2.13	0.49
1:E:383:ILE:O	1:E:386:LYS:HE3	2.13	0.49
1:F:215:GLN:O	1:F:218:GLU:HG2	2.12	0.49
1:F:350:PRO:HB3	1:F:358:ARG:NH2	2.28	0.49
1:F:428:ASP:OD2	1:F:429:LEU:N	2.46	0.49
2:G:307:ARG:CD	2:G:329:ARG:HH21	2.25	0.49
2:G:368:ARG:HH11	2:G:368:ARG:HG3	1.77	0.49
2:H:330:PRO:HG2	2:H:331:ALA:H	1.78	0.49
1:C:192:GLU:HB2	1:C:195:GLU:CG	2.40	0.49
1:D:292:GLU:O	1:D:295:LYS:HB3	2.12	0.49
1:D:317:HIS:O	1:D:321:GLU:HG3	2.13	0.49
1:F:24:ASN:HB2	1:F:102:ILE:O	2.11	0.49
1:F:53:ARG:HB2	2:G:363:ALA:CB	2.43	0.49
1:F:312:LYS:HG3	1:F:313:ARG:N	2.28	0.49
1:A:26:LEU:O	1:A:99:VAL:HA	2.13	0.49
1:A:368:ASP:CG	4:A:805:HOH:O	2.50	0.49
1:C:135:LEU:H	1:C:135:LEU:CD2	2.22	0.49
1:E:117:LEU:HD22	1:E:187:GLU:O	2.12	0.49
1:F:233:ILE:CG2	1:F:234:GLY:N	2.76	0.49
1:B:148:LYS:C	1:B:150:ASP:H	2.16	0.49
1:F:52:PHE:CD2	2:G:362:ASN:O	2.59	0.49
2:H:302:LEU:O	2:H:305:GLY:O	2.29	0.49
1:D:136:LYS:O	1:D:140:LEU:HB2	2.13	0.49
1:F:70:ILE:HG13	1:F:145:PRO:HG3	1.94	0.49
1:B:53:ARG:NH2	1:B:73:SER:HB3	2.28	0.48
1:B:60:LYS:HG2	1:B:61:GLY:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:LYS:CB	1:B:137:PRO:HD3	2.43	0.48
1:B:285:ASN:O	1:B:286:LEU:C	2.52	0.48
1:D:100:ILE:HD12	1:D:100:ILE:C	2.33	0.48
1:D:353:ILE:HG22	1:D:354:ASP:N	2.28	0.48
1:E:169:ASP:CB	1:E:170:PRO:HD3	2.29	0.48
1:E:230:PHE:HA	1:E:233:ILE:CG2	2.39	0.48
1:E:421:GLN:OE1	1:E:421:GLN:HA	2.13	0.48
2:G:358:ALA:HB3	2:G:360:LEU:HG	1.95	0.48
2:H:290:ASN:O	2:H:293:GLU:N	2.46	0.48
2:H:299:GLN:CG	2:H:364:VAL:HG13	2.43	0.48
1:A:71:VAL:HG13	1:A:71:VAL:O	2.13	0.48
1:A:226:HIS:N	1:A:227:PRO:HD3	2.27	0.48
1:B:28:VAL:CG2	1:B:96:LEU:HA	2.42	0.48
1:B:197:SER:OG	1:B:199:ASN:HB3	2.12	0.48
1:B:309:ILE:O	1:B:325:VAL:HG22	2.12	0.48
1:B:448:THR:O	1:B:451:ASP:HB2	2.13	0.48
1:C:243:LEU:O	1:C:346:ALA:HA	2.12	0.48
1:C:428:ASP:OD1	1:C:429:LEU:HG	2.12	0.48
1:E:159:ARG:C	1:E:387:ASN:ND2	2.66	0.48
1:F:27:ILE:CD1	1:F:99:VAL:HG12	2.41	0.48
2:G:352:ASN:O	2:G:353:GLN:C	2.51	0.48
1:B:348:ASN:O	1:B:349:ARG:HB2	2.13	0.48
1:C:57:VAL:HG11	1:C:102:ILE:CG1	2.42	0.48
1:D:206:VAL:CG2	1:D:253:LEU:HD22	2.42	0.48
1:D:441:VAL:CG2	1:D:442:MET:H	2.23	0.48
2:G:318:ILE:HB	2:G:351:GLU:O	2.13	0.48
1:B:31:ALA:HB2	1:B:84:MET:O	2.13	0.48
1:B:353:ILE:CG2	1:B:357:LEU:HD12	2.42	0.48
1:C:99:VAL:O	1:C:100:ILE:HD13	2.13	0.48
1:C:172:PRO:HG2	1:C:173:TYR:CD1	2.48	0.48
1:C:318:GLY:CA	1:C:322:ARG:NH2	2.76	0.48
1:D:222:LEU:HD23	1:D:226:HIS:CD2	2.40	0.48
1:E:159:ARG:O	1:E:387:ASN:ND2	2.46	0.48
1:F:114:ILE:CD1	1:F:176:VAL:HG22	2.43	0.48
1:F:115:HIS:HE1	1:F:117:LEU:HD21	1.78	0.48
2:G:287:ILE:CG2	2:G:288:LEU:N	2.76	0.48
2:H:355:LEU:HD23	2:H:360:LEU:HD12	1.94	0.48
2:I:281:ALA:C	2:I:283:ALA:N	2.66	0.48
1:D:185:GLU:OE1	1:D:185:GLU:N	2.47	0.48
1:B:26:LEU:HD13	1:B:41:LEU:HD22	1.96	0.48
1:C:37:SER:OG	1:C:144:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ASP:H	1:D:188:PRO:HB3	1.75	0.48
1:D:248:GLY:HA3	1:D:409:ALA:CB	2.43	0.48
1:F:21:ASN:C	1:F:22:ARG:HG2	2.34	0.48
1:A:313:ARG:HD3	1:A:313:ARG:HA	1.59	0.48
1:C:146:ILE:HG13	1:C:146:ILE:O	2.09	0.48
1:E:179:ASP:N	1:E:179:ASP:OD1	2.46	0.48
2:G:343:PHE:N	2:G:344:PRO:CD	2.75	0.48
1:B:62:LYS:HB2	1:B:93:ARG:HB2	1.95	0.48
1:B:84:MET:SD	1:B:88:VAL:HB	2.54	0.48
1:C:133:VAL:HG13	1:C:443:ASN:HD22	1.79	0.48
1:C:423:ILE:O	1:C:427:MET:HB3	2.14	0.48
1:D:378:LEU:O	1:D:382:GLN:HG3	2.14	0.48
1:D:427:MET:CG	1:D:432:LEU:HD23	2.37	0.48
1:A:45:LYS:HG3	1:A:79:ASP:O	2.14	0.48
1:C:27:ILE:HB	1:C:81:LYS:CG	2.23	0.48
1:D:120:ASP:HA	1:D:188:PRO:HB3	1.96	0.48
1:E:125:GLY:O	1:E:436:THR:HG23	2.14	0.48
1:E:398:GLN:O	1:E:401:ASN:HB2	2.14	0.48
1:E:426:LYS:O	1:E:430:ILE:HD13	2.13	0.48
1:E:438:ASP:HB2	1:E:440:GLU:OE1	2.14	0.48
1:F:144:ARG:HH11	1:F:144:ARG:HG2	1.78	0.48
2:G:304:ASP:HB2	2:G:329:ARG:HH12	1.79	0.48
1:A:143:TYR:HE2	4:A:813:HOH:O	1.97	0.48
1:B:29:ASP:CG	1:B:30:GLU:N	2.65	0.48
1:B:192:GLU:HB2	1:B:195:GLU:HG3	1.94	0.48
1:C:68:VAL:CG1	1:C:145:PRO:HB2	2.43	0.48
1:C:226:HIS:CE1	1:E:433:GLU:HG3	2.49	0.48
1:C:233:ILE:HD11	1:E:158:MET:HB3	1.95	0.48
1:C:287:ARG:HG3	1:C:327:GLN:NE2	2.29	0.48
1:D:414:LEU:HD12	1:D:455:ALA:HB1	1.95	0.48
1:F:52:PHE:N	1:F:55:ASP:HB2	2.25	0.48
1:F:135:LEU:HD22	1:F:135:LEU:N	2.28	0.48
1:A:193:ASP:OD1	1:A:194:GLU:N	2.46	0.47
1:A:237:PRO:HD2	1:A:337:GLN:HG3	1.95	0.47
1:B:102:ILE:HG23	1:B:102:ILE:O	2.14	0.47
1:C:158:MET:HE1	1:C:419:ALA:HB1	1.96	0.47
1:C:427:MET:SD	1:C:432:LEU:CD1	3.01	0.47
1:E:83:ARG:HG2	1:E:83:ARG:NH1	2.29	0.47
1:E:144:ARG:HG2	1:E:144:ARG:HH11	1.79	0.47
1:F:31:ALA:HB2	1:F:84:MET:C	2.33	0.47
2:G:313:ASN:ND2	2:G:314:HIS:N	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:294:PRO:HG3	2:H:356:LYS:HZ3	1.78	0.47
2:H:361:LEU:O	2:H:362:ASN:HB2	2.13	0.47
1:E:23:PRO:HD2	1:E:48:GLU:OE2	2.14	0.47
1:F:197:SER:C	1:F:199:ASN:H	2.18	0.47
3:F:805:ADP:H5'1	3:F:805:ADP:H8	1.79	0.47
2:G:313:ASN:HD22	2:G:314:HIS:H	1.59	0.47
1:A:181:VAL:HG12	1:A:183:HIS:CD2	2.49	0.47
1:B:28:VAL:HG22	1:B:97:GLY:H	1.78	0.47
1:B:322:ARG:NH1	1:D:317:HIS:CE1	2.81	0.47
1:C:26:LEU:O	1:C:99:VAL:HA	2.14	0.47
1:C:414:LEU:HD12	1:C:455:ALA:HB1	1.96	0.47
1:D:51:LEU:CD2	1:D:104:PRO:HB3	2.43	0.47
1:A:438:ASP:HB3	1:A:440:GLU:CD	2.34	0.47
1:B:115:HIS:HB3	1:B:185:GLU:OE2	2.14	0.47
1:C:119:ILE:HD12	1:C:162:GLU:CB	2.45	0.47
1:D:208:GLY:N	1:D:210:ARG:NH1	2.56	0.47
1:E:419:ALA:O	1:E:423:ILE:HG13	2.14	0.47
2:G:342:THR:O	2:G:344:PRO:HD3	2.14	0.47
2:H:311:LYS:HG3	2:H:313:ASN:N	2.17	0.47
1:A:115:HIS:CE1	1:A:185:GLU:HB2	2.50	0.47
1:A:155:ARG:CD	1:A:387:ASN:OD1	2.62	0.47
1:B:162:GLU:CD	1:B:191:ARG:HH22	2.17	0.47
1:C:70:ILE:HD13	1:C:145:PRO:HG3	1.95	0.47
1:D:60:LYS:HE3	1:D:103:GLN:OE1	2.13	0.47
1:E:86:ARG:O	1:E:90:ASN:ND2	2.48	0.47
1:B:65:ARG:HH21	1:B:93:ARG:HH12	1.61	0.47
1:C:43:GLN:HG3	1:C:44:PRO:CD	2.28	0.47
1:C:87:VAL:HG22	1:C:198:LEU:CD1	2.44	0.47
1:D:34:GLU:O	1:D:34:GLU:CG	2.63	0.47
1:E:131:PHE:O	1:E:136:LYS:HG2	2.15	0.47
1:F:110:TYR:HD1	1:F:110:TYR:H	1.61	0.47
1:F:111:GLY:HA2	1:F:170:PRO:HG2	1.96	0.47
2:G:304:ASP:OD2	2:G:307:ARG:CB	2.60	0.47
2:H:311:LYS:CG	2:H:312:PHE:N	2.77	0.47
1:B:53:ARG:HH12	1:B:72:LEU:HB3	1.80	0.47
1:C:378:LEU:CD2	1:C:397:GLU:HA	2.44	0.47
1:D:35:ASP:HB3	1:D:38:VAL:CG1	2.45	0.47
1:D:107:ASP:OD1	1:D:109:LYS:HE3	2.14	0.47
1:D:143:TYR:HA	1:D:176:VAL:O	2.15	0.47
1:E:220:VAL:HB	1:E:224:LEU:HD22	1.97	0.47
1:E:233:ILE:HG23	1:E:234:GLY:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:GLY:HA2	3:E:804:ADP:O1A	2.15	0.47
1:E:421:GLN:NE2	1:E:454:TRP:CE2	2.82	0.47
1:F:52:PHE:O	1:F:54:GLY:N	2.47	0.47
1:F:113:ARG:O	1:F:114:ILE:HG13	2.15	0.47
1:F:171:SER:HB2	4:F:811:HOH:O	2.14	0.47
1:A:105:CYS:SG	1:A:108:VAL:HG23	2.55	0.47
1:A:232:ALA:O	1:A:233:ILE:HD13	2.15	0.47
1:B:35:ASP:HB3	1:B:38:VAL:CG1	2.42	0.47
1:B:147:ARG:CD	1:B:148:LYS:H	2.18	0.47
1:B:204:ASP:OD2	1:B:205:ASP:OD1	2.33	0.47
1:C:236:LYS:HB3	1:C:236:LYS:HZ3	1.78	0.47
1:D:122:THR:HG21	1:D:162:GLU:CG	2.45	0.47
1:D:127:THR:CG2	1:D:128:GLY:H	2.24	0.47
1:D:270:ASN:HB3	1:D:273:GLU:HB3	1.96	0.47
1:E:82:ILE:HD13	1:E:100:ILE:HD11	1.97	0.47
1:E:249:THR:HG22	1:E:369:ILE:HG22	1.95	0.47
1:F:25:ARG:O	1:F:26:LEU:HD23	2.15	0.47
1:F:74:ASP:HB3	1:F:77:CYS:HB3	1.96	0.47
1:F:100:ILE:HD12	1:F:100:ILE:C	2.35	0.47
1:F:309:ILE:C	1:F:311:PRO:HD3	2.36	0.47
1:C:136:LYS:O	1:C:140:LEU:HB2	2.15	0.47
1:E:353:ILE:CG2	1:E:354:ASP:N	2.77	0.47
1:B:293:ALA:HB3	1:B:301:ILE:HD11	1.95	0.47
1:C:432:LEU:O	1:C:437:ILE:HD13	2.15	0.47
1:D:197:SER:O	1:D:200:GLU:HG3	2.14	0.47
1:D:448:THR:C	1:D:450:ASP:N	2.68	0.47
1:E:105:CYS:SG	1:E:173:TYR:CZ	3.08	0.47
1:E:430:ILE:N	1:E:430:ILE:CD1	2.77	0.47
1:F:335:LEU:HD11	1:F:341:VAL:HB	1.97	0.47
2:H:350:ASP:HB2	2:H:353:GLN:NE2	2.26	0.47
1:A:113:ARG:HG2	1:A:169:ASP:HB2	1.97	0.46
1:C:313:ARG:HA	1:C:316:THR:HG21	1.98	0.46
1:D:38:VAL:HG22	1:D:39:VAL:N	2.29	0.46
1:D:87:VAL:HG13	1:D:88:VAL:HG23	1.97	0.46
2:H:299:GLN:CD	2:H:308:LEU:HD11	2.35	0.46
2:H:340:MET:CG	2:H:347:GLU:HG3	2.44	0.46
1:B:279:ALA:HB2	1:F:319:GLU:OE2	2.15	0.46
1:B:348:ASN:N	1:B:348:ASN:ND2	2.63	0.46
1:C:31:ALA:HB2	1:C:85:ASN:N	2.30	0.46
1:D:56:THR:HG21	1:D:175:ILE:HD11	1.96	0.46
1:D:203:TYR:CD2	1:D:261:GLU:HG2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:391:ALA:HB3	1:E:448:THR:HA	1.97	0.46
1:F:60:LYS:HB2	1:F:101:SER:OG	2.15	0.46
1:F:350:PRO:CB	1:F:358:ARG:HH22	2.26	0.46
2:G:301:ARG:HD2	2:G:301:ARG:HA	1.72	0.46
2:H:365:ILE:N	2:H:365:ILE:HD12	2.30	0.46
1:A:94:VAL:CG1	1:A:98:ASP:HB2	2.45	0.46
1:B:62:LYS:CG	1:B:94:VAL:HG12	2.45	0.46
1:B:218:GLU:OE1	1:D:454:TRP:HZ2	1.98	0.46
1:C:52:PHE:O	1:C:54:GLY:N	2.47	0.46
1:D:36:ASN:CB	1:D:87:VAL:HG11	2.46	0.46
1:D:267:PHE:C	1:D:267:PHE:CD1	2.89	0.46
1:E:146:ILE:CG2	1:E:176:VAL:HG23	2.46	0.46
2:G:307:ARG:HD3	2:G:329:ARG:NH2	2.30	0.46
2:H:303:ALA:HB2	2:H:367:GLN:O	2.15	0.46
1:A:117:LEU:HD12	1:A:166:VAL:HG21	1.98	0.46
1:A:270:ASN:O	1:A:273:GLU:HB3	2.16	0.46
1:B:59:LEU:HD23	1:B:102:ILE:HA	1.98	0.46
1:B:388:MET:HE1	1:B:447:VAL:HG21	1.97	0.46
1:D:183:HIS:HB3	1:D:185:GLU:OE2	2.15	0.46
1:E:63:LYS:HZ3	1:E:194:GLU:CD	2.17	0.46
1:E:233:ILE:HG13	1:E:234:GLY:H	1.80	0.46
1:E:395:ASP:O	1:E:398:GLN:HB3	2.15	0.46
1:F:430:ILE:O	1:F:432:LEU:CG	2.59	0.46
1:F:434:ASP:C	1:F:436:THR:H	2.17	0.46
2:H:359:ASN:O	2:H:359:ASN:ND2	2.40	0.46
1:A:383:ILE:O	1:A:386:LYS:HE3	2.15	0.46
1:B:65:ARG:HG3	1:B:93:ARG:CG	2.45	0.46
1:C:394:VAL:HA	1:C:449:MET:HB2	1.98	0.46
1:C:433:GLU:O	1:C:434:ASP:C	2.54	0.46
1:D:187:GLU:HA	1:D:188:PRO:HD3	1.76	0.46
1:D:287:ARG:HH11	1:D:287:ARG:HG3	1.80	0.46
1:D:385:THR:HB	1:D:390:LEU:HD11	1.96	0.46
1:E:23:PRO:O	1:E:49:LEU:HD21	2.16	0.46
2:G:338:VAL:CG1	2:G:339:LEU:H	2.28	0.46
2:H:354:THR:CG2	2:H:357:GLU:CG	2.94	0.46
1:A:108:VAL:HG12	1:A:175:ILE:HG13	1.98	0.46
1:B:53:ARG:NH2	1:B:73:SER:O	2.48	0.46
1:C:86:ARG:O	1:C:90:ASN:HB2	2.15	0.46
1:D:280:GLY:HA2	1:D:323:ARG:NH2	2.31	0.46
1:E:136:LYS:CB	1:E:137:PRO:HD3	2.32	0.46
1:E:147:ARG:HD3	1:E:148:LYS:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:PHE:C	1:F:54:GLY:H	2.18	0.46
1:C:233:ILE:CD1	1:E:158:MET:HB2	2.45	0.46
1:C:388:MET:HG3	1:C:390:LEU:CD2	2.46	0.46
1:D:114:ILE:CD1	1:D:176:VAL:HG22	2.46	0.46
1:D:208:GLY:H	1:D:210:ARG:HH12	1.57	0.46
1:A:297:ALA:HA	1:A:298:PRO:C	2.36	0.46
1:D:62:LYS:HD2	1:D:94:VAL:HG12	1.98	0.46
1:D:329:LEU:HD23	1:D:357:LEU:HD23	1.98	0.46
1:E:120:ASP:HA	1:E:188:PRO:HB2	1.97	0.46
1:E:422:ALA:O	1:E:426:LYS:HD2	2.16	0.46
1:F:41:LEU:HD11	1:F:102:ILE:HD13	1.98	0.46
1:A:353:ILE:CG2	1:A:357:LEU:HD12	2.46	0.46
1:B:30:GLU:O	1:B:83:ARG:HB3	2.16	0.46
1:B:233:ILE:CG2	1:B:235:VAL:HG23	2.46	0.46
1:C:53:ARG:CZ	1:C:73:SER:OG	2.64	0.46
1:C:158:MET:HE3	1:C:388:MET:HB3	1.98	0.46
1:C:164:LYS:HB3	1:C:189:ILE:CD1	2.46	0.46
1:C:249:THR:HG23	1:C:369:ILE:CG2	2.46	0.46
1:D:316:THR:HB	1:D:322:ARG:HE	1.81	0.46
1:D:376:GLY:O	1:D:380:ILE:HG13	2.15	0.46
1:E:430:ILE:O	1:E:430:ILE:HG22	2.16	0.46
1:F:32:ILE:HG12	1:F:83:ARG:CD	2.37	0.46
1:F:226:HIS:N	1:F:227:PRO:HD3	2.30	0.46
1:F:314:GLU:O	1:F:315:LYS:HD3	2.16	0.46
1:F:403:THR:CG2	1:F:406:HIS:HB2	2.43	0.46
1:B:40:SER:HB2	1:B:83:ARG:HB2	1.96	0.46
1:B:232:ALA:O	1:B:233:ILE:HD13	2.16	0.46
1:C:191:ARG:NH1	1:C:197:SER:HA	2.31	0.46
1:C:230:PHE:CE2	1:C:237:PRO:HB3	2.51	0.46
1:D:117:LEU:CD2	1:D:185:GLU:HB2	2.41	0.46
1:E:320:VAL:O	1:E:324:ILE:HG13	2.15	0.46
1:F:20:LYS:O	1:F:20:LYS:HG2	2.15	0.46
2:G:344:PRO:CD	2:G:345:ASN:H	2.25	0.46
1:B:66:GLU:O	1:B:67:ALA:HB2	2.16	0.45
1:B:105:CYS:SG	1:B:173:TYR:CE1	3.05	0.45
1:B:428:ASP:C	1:B:430:ILE:N	2.69	0.45
1:B:437:ILE:CG2	1:B:438:ASP:H	2.28	0.45
1:C:221:GLU:O	1:C:225:ARG:HB2	2.17	0.45
1:D:239:ARG:NH2	1:D:335:LEU:O	2.49	0.45
1:E:131:PHE:CD1	1:E:136:LYS:HG2	2.51	0.45
1:A:254:ILE:HD12	1:A:369:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:LYS:HB3	1:A:354:ASP:CG	2.36	0.45
1:C:309:ILE:O	1:C:309:ILE:HG22	2.16	0.45
1:D:51:LEU:CD2	1:D:104:PRO:HG3	2.44	0.45
1:D:106:PRO:O	1:D:108:VAL:HG12	2.16	0.45
1:D:201:VAL:CG1	1:D:253:LEU:HD23	2.46	0.45
1:D:350:PRO:HG2	1:D:351:ASN:H	1.81	0.45
2:G:339:LEU:HB2	2:G:348:LEU:HB2	1.99	0.45
2:H:299:GLN:CG	2:H:364:VAL:HG22	2.45	0.45
1:A:210:ARG:H	1:A:210:ARG:CD	2.25	0.45
1:C:42:SER:HB3	1:C:79:ASP:OD1	2.16	0.45
1:C:251:LYS:CD	1:C:346:ALA:HB1	2.46	0.45
1:D:131:PHE:HE1	1:D:182:ILE:O	2.00	0.45
1:D:159:ARG:N	1:D:387:ASN:HB3	2.31	0.45
1:D:423:ILE:HA	1:D:445:LEU:HD21	1.98	0.45
1:E:305:GLU:O	1:E:308:ALA:HB3	2.16	0.45
1:E:416:SER:O	1:E:420:LEU:HG	2.17	0.45
1:C:155:ARG:HG2	1:C:160:ALA:HB2	1.99	0.45
1:D:50:GLN:O	1:D:51:LEU:CD2	2.60	0.45
1:F:117:LEU:CD1	1:F:166:VAL:HG21	2.46	0.45
1:A:25:ARG:O	1:A:26:LEU:HD23	2.17	0.45
1:A:249:THR:CG2	1:A:369:ILE:HG22	2.47	0.45
1:B:212:GLN:H	1:B:212:GLN:CD	2.19	0.45
1:B:455:ALA:O	1:B:458:GLN:HB2	2.17	0.45
1:C:59:LEU:CD2	1:C:102:ILE:HG13	2.38	0.45
1:D:43:GLN:N	1:D:44:PRO:CD	2.79	0.45
1:D:131:PHE:HA	1:D:135:LEU:HB2	1.97	0.45
1:F:22:ARG:CG	1:F:25:ARG:HG2	2.47	0.45
1:F:26:LEU:HB2	1:F:100:ILE:HD11	1.97	0.45
2:G:316:HIS:C	2:G:317:ARG:HG2	2.37	0.45
1:A:429:LEU:C	1:A:431:ASP:N	2.70	0.45
1:B:117:LEU:HD11	1:B:185:GLU:O	2.16	0.45
1:B:125:GLY:C	1:F:232:ALA:HB2	2.37	0.45
1:C:153:LEU:HB2	1:C:198:LEU:CD1	2.40	0.45
1:D:111:GLY:HA2	1:D:170:PRO:CD	2.46	0.45
1:D:152:PHE:CD1	1:D:163:PHE:O	2.70	0.45
1:E:35:ASP:O	1:E:85:ASN:ND2	2.50	0.45
1:E:51:LEU:CD2	1:E:104:PRO:HG3	2.39	0.45
1:E:407:VAL:HG23	1:E:409:ALA:H	1.82	0.45
1:F:378:LEU:O	1:F:382:GLN:HG3	2.16	0.45
1:B:278:LEU:HD12	1:B:279:ALA:H	1.82	0.45
1:C:225:ARG:C	1:C:227:PRO:HD3	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:PHE:CD2	1:D:136:LYS:CE	3.00	0.45
1:D:432:LEU:HD23	1:D:432:LEU:HA	1.77	0.45
1:E:441:VAL:O	1:E:444:SER:OG	2.29	0.45
1:F:158:MET:HA	1:F:387:ASN:O	2.16	0.45
1:F:187:GLU:HA	1:F:188:PRO:HD3	1.58	0.45
2:H:300:ILE:HB	2:H:309:VAL:CB	2.40	0.45
1:A:28:VAL:HG11	1:A:94:VAL:CG1	2.47	0.45
1:B:143:TYR:HE2	2:H:340:MET:HE1	1.81	0.45
1:C:118:PRO:HG3	1:C:163:PHE:HE1	1.82	0.45
1:D:39:VAL:HG22	1:D:70:ILE:O	2.16	0.45
1:D:249:THR:O	1:D:249:THR:HG22	2.16	0.45
1:F:423:ILE:HG12	1:F:445:LEU:CD2	2.47	0.45
1:A:235:VAL:HG11	1:F:420:LEU:HG	1.99	0.45
1:A:270:ASN:OD1	1:A:272:PRO:HG2	2.17	0.45
1:B:135:LEU:H	1:B:135:LEU:CD2	2.28	0.45
1:C:133:VAL:CG1	1:C:443:ASN:HD22	2.30	0.45
1:C:233:ILE:HD12	1:C:234:GLY:H	1.82	0.45
1:D:172:PRO:O	1:D:173:TYR:HB3	2.17	0.45
1:D:192:GLU:O	1:D:195:GLU:N	2.50	0.45
2:G:298:ILE:CG2	2:G:365:ILE:HD12	2.47	0.45
2:I:280:GLU:O	2:I:283:ALA:HB3	2.17	0.45
1:A:43:GLN:N	1:A:44:PRO:CD	2.80	0.45
1:B:40:SER:O	1:B:41:LEU:HD23	2.16	0.45
1:B:136:LYS:HB3	1:B:136:LYS:HE2	1.71	0.45
1:C:321:GLU:O	1:C:325:VAL:HG23	2.17	0.45
1:D:140:LEU:CD1	1:D:141:GLU:HG3	2.47	0.45
1:E:341:VAL:HG12	1:E:342:ILE:N	2.32	0.45
1:E:406:HIS:HB3	1:E:410:ASP:HB2	1.99	0.45
1:F:430:ILE:O	1:F:431:ASP:C	2.54	0.45
2:H:294:PRO:HG3	2:H:356:LYS:NZ	2.32	0.45
1:B:32:ILE:HD13	1:B:32:ILE:N	2.30	0.44
1:B:145:PRO:HA	1:B:175:ILE:HA	1.99	0.44
1:C:74:ASP:HB3	1:C:77:CYS:HB2	1.98	0.44
1:C:324:ILE:O	1:C:327:GLN:HB3	2.16	0.44
1:F:220:VAL:HB	1:F:224:LEU:CD1	2.47	0.44
2:G:332:MET:HG2	2:G:367:GLN:HE22	1.82	0.44
1:A:142:ALA:CB	1:A:144:ARG:HG3	2.48	0.44
1:A:245:GLY:O	1:A:348:ASN:HA	2.16	0.44
1:A:336:LYS:HZ2	1:A:338:ARG:HG3	1.81	0.44
1:B:44:PRO:O	1:B:48:GLU:HG3	2.17	0.44
1:D:30:GLU:HG2	1:D:96:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:VAL:HG22	1:E:198:LEU:HD13	1.94	0.44
1:F:29:ASP:OD1	1:F:30:GLU:N	2.51	0.44
1:F:252:THR:HA	1:F:302:PHE:CE2	2.53	0.44
1:F:329:LEU:HD23	1:F:357:LEU:HD23	1.99	0.44
1:F:430:ILE:O	1:F:430:ILE:HG22	2.16	0.44
2:H:318:ILE:CG2	2:H:351:GLU:HB3	2.48	0.44
1:C:313:ARG:CA	1:C:316:THR:HG22	2.45	0.44
1:A:395:ASP:OD1	1:A:397:GLU:HB3	2.17	0.44
1:B:171:SER:O	1:B:173:TYR:N	2.48	0.44
1:B:353:ILE:HG22	1:B:357:LEU:HD12	1.99	0.44
1:E:93:ARG:HG2	1:E:93:ARG:HH11	1.81	0.44
1:E:114:ILE:HD11	1:E:176:VAL:HG22	1.98	0.44
1:E:212:GLN:NE2	1:E:368:ASP:O	2.51	0.44
2:G:319:SER:HB3	2:G:351:GLU:HG3	1.98	0.44
2:H:301:ARG:HH11	2:H:308:LEU:HD13	1.81	0.44
1:A:348:ASN:HD22	1:A:348:ASN:N	2.15	0.44
1:C:323:ARG:HD3	1:E:277:LYS:O	2.17	0.44
1:C:358:ARG:O	1:C:359:ARG:C	2.54	0.44
1:D:210:ARG:N	1:D:210:ARG:HD3	2.32	0.44
1:E:390:LEU:HD11	1:E:396:LEU:HD11	2.00	0.44
1:F:53:ARG:NH1	2:G:361:LEU:O	2.50	0.44
1:F:63:LYS:HD2	1:F:93:ARG:HG3	1.98	0.44
1:F:70:ILE:HD13	2:G:343:PHE:HE1	1.83	0.44
1:F:155:ARG:CZ	1:F:386:LYS:HD2	2.48	0.44
1:F:430:ILE:HD13	1:F:430:ILE:N	2.32	0.44
2:H:293:GLU:HB3	2:H:294:PRO:HD2	1.98	0.44
2:H:313:ASN:HD21	2:H:316:HIS:CB	2.31	0.44
1:C:117:LEU:HA	1:C:118:PRO:HD3	1.79	0.44
1:C:306:LEU:HD21	1:C:357:LEU:HD13	1.99	0.44
1:D:113:ARG:O	1:D:114:ILE:HG13	2.18	0.44
1:D:297:ALA:HA	1:D:298:PRO:C	2.38	0.44
1:D:441:VAL:CG2	1:D:442:MET:N	2.79	0.44
2:H:355:LEU:HD22	2:H:360:LEU:CD1	2.42	0.44
1:A:92:LEU:O	1:A:93:ARG:HB2	2.17	0.44
1:B:27:ILE:HA	1:B:98:ASP:O	2.17	0.44
1:B:57:VAL:CG1	1:B:71:VAL:HG11	2.48	0.44
1:C:61:GLY:CA	1:C:100:ILE:HD12	2.47	0.44
1:C:270:ASN:O	1:C:273:GLU:HB3	2.17	0.44
1:C:312:LYS:HG3	1:C:355:PRO:HD3	1.99	0.44
1:D:105:CYS:C	1:D:107:ASP:H	2.20	0.44
1:D:310:ALA:HB3	1:D:357:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:TYR:HE1	1:E:258:VAL:HA	1.82	0.44
2:G:329:ARG:HA	2:G:330:PRO:HD3	1.69	0.44
2:H:287:ILE:CD1	2:H:287:ILE:C	2.79	0.44
1:A:230:PHE:CD1	1:A:237:PRO:HD3	2.53	0.44
1:A:243:LEU:HD23	1:A:251:LYS:HB3	2.00	0.44
1:D:43:GLN:HA	1:D:46:MET:CG	2.48	0.44
1:D:119:ILE:HA	1:D:189:ILE:O	2.18	0.44
1:F:153:LEU:HD12	1:F:161:VAL:O	2.17	0.44
2:G:339:LEU:O	2:G:340:MET:HG3	2.18	0.44
2:H:290:ASN:CB	2:H:293:GLU:HG3	2.48	0.44
1:B:71:VAL:O	1:B:71:VAL:HG13	2.18	0.44
1:B:438:ASP:OD1	1:B:441:VAL:HG23	2.18	0.44
1:D:230:PHE:CD1	1:D:233:ILE:HD11	2.53	0.44
1:D:287:ARG:O	1:D:291:GLU:HB2	2.18	0.44
1:F:108:VAL:HG22	1:F:173:TYR:CD1	2.53	0.44
1:B:203:TYR:CZ	1:B:261:GLU:HG2	2.53	0.43
1:C:22:ARG:N	1:C:22:ARG:HD2	2.33	0.43
1:C:35:ASP:CB	1:C:38:VAL:HG12	2.47	0.43
1:D:226:HIS:N	1:D:227:PRO:CD	2.79	0.43
1:F:310:ALA:CB	1:F:357:LEU:HD11	2.48	0.43
1:A:44:PRO:O	1:A:47:ASP:HB2	2.18	0.43
1:B:58:LEU:O	1:B:59:LEU:HD23	2.18	0.43
1:D:131:PHE:CD2	1:D:131:PHE:C	2.92	0.43
1:D:140:LEU:HD12	1:D:141:GLU:N	2.33	0.43
1:E:105:CYS:SG	1:E:105:CYS:O	2.75	0.43
1:E:295:LYS:HB3	1:E:296:ASN:ND2	2.33	0.43
1:E:394:VAL:CA	1:E:449:MET:HB2	2.43	0.43
1:F:201:VAL:HG11	1:F:253:LEU:CD1	2.46	0.43
2:G:282:LYS:O	2:G:286:SER:HB2	2.18	0.43
1:B:57:VAL:HG13	1:B:71:VAL:CG1	2.48	0.43
1:B:171:SER:CB	1:B:172:PRO:CD	2.94	0.43
1:C:110:TYR:HD1	1:C:110:TYR:N	2.16	0.43
1:C:320:VAL:HG12	1:C:324:ILE:HD11	2.01	0.43
1:C:353:ILE:HG22	1:C:354:ASP:N	2.33	0.43
1:D:349:ARG:CB	1:D:350:PRO:HD2	2.47	0.43
1:F:70:ILE:CD1	2:G:343:PHE:HE1	2.31	0.43
1:F:110:TYR:N	1:F:110:TYR:CD1	2.86	0.43
1:A:436:THR:C	1:A:438:ASP:H	2.21	0.43
1:B:267:PHE:CD1	1:B:267:PHE:C	2.92	0.43
1:D:168:THR:CG2	1:D:174:CYS:HB3	2.48	0.43
1:D:239:ARG:NH1	1:D:335:LEU:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:TYR:CD2	1:E:177:ALA:CB	3.01	0.43
1:B:343:VAL:HG12	1:B:363:PHE:CE1	2.54	0.43
1:C:51:LEU:HD22	1:C:104:PRO:HB3	2.01	0.43
1:C:146:ILE:O	1:C:146:ILE:CG1	2.66	0.43
1:C:147:ARG:HG3	1:C:147:ARG:NH1	2.33	0.43
1:C:298:PRO:HA	1:C:340:HIS:O	2.19	0.43
1:D:236:LYS:HG2	1:D:337:GLN:NE2	2.33	0.43
1:D:296:ASN:HD22	1:D:296:ASN:N	2.15	0.43
1:E:42:SER:HB3	1:E:77:CYS:O	2.19	0.43
1:E:110:TYR:CD2	1:E:177:ALA:HB2	2.53	0.43
1:A:315:LYS:HE2	1:A:352:SER:O	2.19	0.43
1:B:77:CYS:SG	1:B:81:LYS:O	2.77	0.43
1:B:343:VAL:HG12	1:B:363:PHE:HE1	1.83	0.43
1:D:136:LYS:HB2	1:D:137:PRO:CD	2.45	0.43
1:D:317:HIS:N	1:D:317:HIS:HD2	2.16	0.43
1:F:52:PHE:CD1	2:G:299:GLN:OE1	2.72	0.43
1:C:159:ARG:C	1:C:387:ASN:ND2	2.72	0.43
1:C:416:SER:HA	1:D:235:VAL:HG13	1.99	0.43
1:D:403:THR:HG23	1:D:406:HIS:CB	2.48	0.43
1:E:143:TYR:CE1	1:E:178:PRO:CD	3.02	0.43
1:E:148:LYS:HA	1:E:165:VAL:CG1	2.48	0.43
2:H:360:LEU:O	2:H:363:ALA:N	2.50	0.43
1:A:158:MET:HA	1:A:387:ASN:O	2.18	0.43
1:A:237:PRO:CD	1:A:337:GLN:HE21	2.32	0.43
1:A:354:ASP:OD1	1:A:355:PRO:HD2	2.19	0.43
1:B:58:LEU:CD2	1:B:68:VAL:HG22	2.47	0.43
1:C:136:LYS:HB3	1:C:137:PRO:CD	2.48	0.43
1:E:110:TYR:HD1	1:E:110:TYR:H	1.65	0.43
1:E:448:THR:C	1:E:450:ASP:H	2.22	0.43
2:G:296:THR:CG2	2:G:297:ASN:N	2.81	0.43
1:A:220:VAL:O	1:A:224:LEU:HB2	2.19	0.43
1:B:172:PRO:CB	1:B:173:TYR:HD2	2.29	0.43
1:C:220:VAL:HG13	1:C:224:LEU:HD22	2.01	0.43
1:C:383:ILE:O	1:C:386:LYS:HG2	2.19	0.43
1:D:152:PHE:CE1	1:D:163:PHE:HB3	2.54	0.43
1:E:430:ILE:N	1:E:430:ILE:HD12	2.32	0.43
1:F:31:ALA:HB2	1:F:85:ASN:N	2.33	0.43
2:H:353:GLN:HE21	2:H:353:GLN:HB3	1.58	0.43
1:A:416:SER:O	1:A:420:LEU:HG	2.19	0.43
1:B:70:ILE:HG13	2:H:343:PHE:CE1	2.53	0.43
1:B:123:VAL:O	1:B:126:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:PRO:O	1:C:25:ARG:N	2.52	0.43
1:C:126:ILE:HG21	1:C:159:ARG:HH11	1.84	0.43
1:D:300:ILE:HA	1:D:342:ILE:O	2.18	0.43
1:E:110:TYR:N	1:E:110:TYR:CD1	2.87	0.43
1:E:112:LYS:HD3	1:E:112:LYS:HA	1.79	0.43
1:E:139:PHE:CE1	1:E:176:VAL:HG21	2.54	0.43
1:F:187:GLU:OE1	1:F:187:GLU:CA	2.64	0.43
1:F:360:PHE:O	1:F:364:ASP:OD2	2.37	0.43
1:A:57:VAL:HG22	1:A:69:CYS:O	2.19	0.42
1:B:383:ILE:O	1:B:386:LYS:HE3	2.19	0.42
1:C:57:VAL:CG1	1:C:102:ILE:HG12	2.46	0.42
1:C:89:ARG:HG2	1:C:94:VAL:HG23	2.01	0.42
1:C:191:ARG:NH2	1:C:197:SER:HB2	2.34	0.42
1:C:265:PHE:HB3	1:C:299:ALA:CB	2.49	0.42
1:C:279:ALA:O	1:C:282:SER:HB3	2.19	0.42
1:C:437:ILE:CG1	1:D:229:LEU:HA	2.45	0.42
1:D:51:LEU:CG	1:D:104:PRO:HG3	2.48	0.42
1:E:427:MET:HA	1:E:430:ILE:HB	2.01	0.42
1:F:301:ILE:HB	1:F:343:VAL:HG22	2.00	0.42
1:F:350:PRO:HB3	1:F:358:ARG:HH22	1.84	0.42
2:G:335:THR:HG21	2:G:369:LEU:HD22	2.01	0.42
1:B:364:ASP:OD1	1:B:365:ARG:HG2	2.19	0.42
1:B:429:LEU:HB2	1:B:431:ASP:OD1	2.19	0.42
1:D:297:ALA:HB2	1:D:339:ALA:O	2.19	0.42
1:D:414:LEU:HD12	1:D:455:ALA:CB	2.48	0.42
1:E:306:LEU:HG	1:E:353:ILE:HD12	2.01	0.42
1:F:328:LEU:HD23	1:F:357:LEU:HD21	2.00	0.42
2:G:335:THR:CG2	2:G:369:LEU:HD22	2.48	0.42
2:H:295:THR:HA	2:H:314:HIS:CB	2.49	0.42
1:A:305:GLU:OE2	1:E:359:ARG:NH1	2.52	0.42
1:A:312:LYS:CG	1:A:313:ARG:N	2.81	0.42
1:A:315:LYS:O	1:A:316:THR:CB	2.67	0.42
1:B:108:VAL:HG22	1:B:173:TYR:CD1	2.54	0.42
1:B:123:VAL:O	1:B:124:GLU:C	2.56	0.42
1:D:230:PHE:HA	1:D:233:ILE:HG12	2.01	0.42
1:E:430:ILE:CD1	1:E:430:ILE:H	2.32	0.42
1:F:225:ARG:C	1:F:227:PRO:HD3	2.39	0.42
2:G:286:SER:O	2:G:287:ILE:HD13	2.19	0.42
1:A:129:ASN:O	1:A:133:VAL:CG2	2.67	0.42
1:B:127:THR:HB	1:B:437:ILE:O	2.20	0.42
1:B:241:ILE:HA	1:B:365:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:MET:HE1	1:B:363:PHE:CZ	2.55	0.42
1:C:158:MET:HA	1:C:387:ASN:O	2.19	0.42
1:E:74:ASP:OD1	1:E:76:THR:HG23	2.19	0.42
1:E:122:THR:O	1:E:161:VAL:HG22	2.19	0.42
1:E:286:LEU:O	1:E:289:ALA:HB3	2.19	0.42
1:F:70:ILE:HD13	2:G:343:PHE:CE1	2.55	0.42
2:G:296:THR:HG21	2:G:355:LEU:HD13	2.00	0.42
2:H:309:VAL:HG11	2:H:324:PHE:HE2	1.85	0.42
1:A:447:VAL:CG1	1:A:452:PHE:CE1	3.03	0.42
1:A:448:THR:C	1:A:450:ASP:N	2.72	0.42
1:B:65:ARG:CZ	1:B:91:ASN:O	2.67	0.42
1:B:241:ILE:HD12	1:B:342:ILE:HG21	2.01	0.42
1:B:336:LYS:HZ1	1:B:338:ARG:HE	1.68	0.42
1:C:29:ASP:CG	1:C:30:GLU:H	2.22	0.42
1:C:378:LEU:HD23	1:C:397:GLU:HA	2.02	0.42
1:D:35:ASP:O	1:D:38:VAL:HG12	2.19	0.42
1:E:35:ASP:HB3	1:E:38:VAL:HG23	2.02	0.42
1:E:152:PHE:CE1	1:E:163:PHE:HB2	2.55	0.42
1:E:233:ILE:HD12	1:E:233:ILE:HA	1.83	0.42
2:G:298:ILE:HG21	2:G:365:ILE:HD12	2.01	0.42
2:H:337:PHE:HA	2:H:370:THR:H	1.84	0.42
1:C:27:ILE:O	1:C:81:LYS:HB3	2.19	0.42
1:C:30:GLU:OE2	1:C:217:LYS:NZ	2.46	0.42
1:C:243:LEU:HD12	1:C:243:LEU:N	2.34	0.42
1:D:49:LEU:O	1:D:51:LEU:HG	2.19	0.42
1:D:109:LYS:NZ	1:D:172:PRO:HD2	2.35	0.42
1:D:111:GLY:CA	1:D:170:PRO:HG2	2.31	0.42
1:D:138:TYR:CE2	1:D:152:PHE:CD2	3.07	0.42
1:E:26:LEU:HD12	1:E:82:ILE:CG2	2.49	0.42
1:E:447:VAL:HG21	1:E:452:PHE:CE1	2.52	0.42
1:A:116:VAL:CG1	1:A:163:PHE:HB3	2.49	0.42
1:A:242:LEU:HD13	1:A:363:PHE:CD1	2.54	0.42
1:B:48:GLU:HB2	1:B:49:LEU:CD2	2.48	0.42
1:C:110:TYR:N	1:C:110:TYR:CD1	2.85	0.42
1:D:395:ASP:O	1:D:398:GLN:HB3	2.19	0.42
1:E:254:ILE:HD12	1:E:369:ILE:HD13	2.01	0.42
2:G:311:LYS:O	2:G:312:PHE:CD1	2.72	0.42
2:H:287:ILE:HG21	2:H:312:PHE:CE1	2.54	0.42
1:A:237:PRO:CG	1:A:337:GLN:NE2	2.81	0.42
1:A:240:GLY:HA2	1:A:343:VAL:O	2.20	0.42
1:A:317:HIS:CB	1:F:317:HIS:HD2	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:GLU:O	1:B:383:ILE:HG13	2.20	0.42
1:C:311:PRO:O	1:C:354:ASP:HB2	2.20	0.42
1:D:152:PHE:CE1	1:D:163:PHE:CB	3.03	0.42
1:D:302:PHE:HA	1:D:344:MET:O	2.20	0.42
1:E:158:MET:CE	1:E:419:ALA:HB1	2.49	0.42
1:E:280:GLY:CA	1:E:283:GLU:OE2	2.67	0.42
1:E:312:LYS:HG2	1:E:312:LYS:HZ3	1.71	0.42
1:E:378:LEU:C	1:E:378:LEU:HD13	2.39	0.42
1:E:429:LEU:HD22	1:E:429:LEU:HA	1.90	0.42
1:F:115:HIS:NE2	1:F:185:GLU:HB2	2.34	0.42
2:G:300:ILE:N	2:G:300:ILE:CD1	2.83	0.42
2:G:307:ARG:HD2	2:G:329:ARG:NH2	2.33	0.42
2:H:318:ILE:CD1	2:H:351:GLU:HA	2.48	0.42
1:B:33:ASN:ND2	1:B:38:VAL:HG11	2.35	0.42
1:B:52:PHE:HB3	2:H:362:ASN:O	2.19	0.42
1:B:65:ARG:HE	1:B:93:ARG:NH1	2.17	0.42
1:B:225:ARG:C	1:B:227:PRO:HD3	2.40	0.42
1:B:243:LEU:HD12	1:B:243:LEU:N	2.35	0.42
1:C:158:MET:CE	1:C:419:ALA:HB1	2.49	0.42
1:C:190:LYS:NZ	1:C:191:ARG:HB3	2.35	0.42
1:C:416:SER:O	1:C:420:LEU:HG	2.20	0.42
1:D:88:VAL:O	1:D:90:ASN:N	2.52	0.42
1:B:25:ARG:HA	1:B:100:ILE:O	2.20	0.42
1:B:168:THR:CG2	1:B:174:CYS:SG	3.08	0.42
1:B:220:VAL:O	1:B:224:LEU:HB2	2.20	0.42
1:C:322:ARG:NH1	1:E:317:HIS:CE1	2.83	0.42
1:D:110:TYR:CE2	1:D:143:TYR:CE2	3.08	0.42
1:F:89:ARG:CZ	1:F:96:LEU:HD21	2.50	0.42
1:F:144:ARG:HG2	1:F:144:ARG:NH1	2.35	0.42
2:G:304:ASP:CG	2:G:307:ARG:CB	2.85	0.42
2:H:338:VAL:HG12	2:H:339:LEU:N	2.35	0.42
1:A:131:PHE:HA	1:A:135:LEU:HB2	2.02	0.41
1:C:36:ASN:CA	1:C:85:ASN:HD21	2.12	0.41
1:D:41:LEU:HD21	1:D:82:ILE:HB	2.02	0.41
1:D:111:GLY:N	1:D:174:CYS:HB2	2.34	0.41
1:D:222:LEU:N	1:D:223:PRO:HD2	2.35	0.41
1:E:25:ARG:C	1:E:26:LEU:HD23	2.39	0.41
1:E:296:ASN:ND2	1:E:296:ASN:N	2.67	0.41
1:E:333:ASP:C	1:E:335:LEU:H	2.24	0.41
1:F:108:VAL:O	2:G:301:ARG:NH2	2.53	0.41
1:A:329:LEU:HD23	1:A:357:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:VAL:HG11	1:A:452:PHE:CE1	2.55	0.41
1:C:139:PHE:O	1:C:140:LEU:C	2.59	0.41
1:D:147:ARG:NH1	1:D:147:ARG:CG	2.83	0.41
1:E:35:ASP:HB3	1:E:38:VAL:CG2	2.50	0.41
1:E:113:ARG:HG3	1:E:169:ASP:H	1.85	0.41
1:E:148:LYS:HG2	1:E:149:GLY:N	2.35	0.41
1:E:399:VAL:O	1:E:403:THR:HG23	2.20	0.41
1:E:448:THR:C	1:E:450:ASP:N	2.72	0.41
1:F:249:THR:CG2	1:F:249:THR:O	2.67	0.41
2:H:339:LEU:O	2:H:348:LEU:N	2.53	0.41
1:B:56:THR:HG22	1:B:70:ILE:CD1	2.50	0.41
1:C:233:ILE:HD11	1:E:158:MET:HB2	2.01	0.41
1:D:112:LYS:O	1:D:181:VAL:HG12	2.21	0.41
1:E:28:VAL:HG13	1:E:96:LEU:HA	2.02	0.41
1:E:47:ASP:O	1:E:50:GLN:HG2	2.20	0.41
1:E:130:LEU:N	1:E:130:LEU:HD23	2.35	0.41
1:B:125:GLY:O	1:B:437:ILE:HB	2.21	0.41
1:C:388:MET:HG3	1:C:390:LEU:HD21	2.01	0.41
1:D:31:ALA:CB	1:D:85:ASN:HB3	2.50	0.41
1:D:36:ASN:HA	1:D:87:VAL:HG11	2.02	0.41
1:D:286:LEU:HD23	1:D:286:LEU:HA	1.84	0.41
1:D:296:ASN:N	1:D:296:ASN:ND2	2.68	0.41
1:D:448:THR:C	1:D:450:ASP:H	2.24	0.41
1:F:66:GLU:HB2	1:F:147:ARG:HH12	1.79	0.41
1:F:313:ARG:HB2	1:F:314:GLU:OE2	2.20	0.41
2:G:317:ARG:NH1	2:G:317:ARG:CG	2.66	0.41
1:A:40:SER:O	1:A:41:LEU:HD23	2.20	0.41
1:A:115:HIS:CE1	1:A:185:GLU:H	2.39	0.41
1:C:111:GLY:HA2	1:C:170:PRO:HG2	2.02	0.41
1:C:287:ARG:HH11	1:C:327:GLN:HE22	1.66	0.41
1:C:365:ARG:NH1	1:C:365:ARG:CG	2.61	0.41
1:D:153:LEU:HD22	1:D:198:LEU:CB	2.50	0.41
1:F:155:ARG:NE	1:F:386:LYS:HD2	2.36	0.41
2:I:322:ARG:O	2:I:326:VAL:HG23	2.21	0.41
1:A:94:VAL:HG13	1:A:98:ASP:OD2	2.20	0.41
1:A:221:GLU:O	1:A:225:ARG:HB2	2.21	0.41
1:A:432:LEU:HD11	1:E:27:ILE:HG23	2.03	0.41
1:B:437:ILE:HG13	1:F:232:ALA:HB3	2.03	0.41
1:C:82:ILE:O	1:C:82:ILE:HG23	2.20	0.41
1:C:243:LEU:N	1:C:243:LEU:CD1	2.84	0.41
1:C:249:THR:HG23	1:C:369:ILE:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:LEU:HG	1:C:353:ILE:CD1	2.48	0.41
1:D:131:PHE:C	1:D:131:PHE:HD2	2.24	0.41
1:D:241:ILE:HA	1:D:365:ARG:O	2.20	0.41
1:E:27:ILE:HA	1:E:98:ASP:O	2.21	0.41
1:E:66:GLU:HB2	1:E:147:ARG:NH1	2.35	0.41
1:E:391:ALA:CB	1:E:448:THR:HA	2.50	0.41
1:E:432:LEU:HD22	1:E:432:LEU:HA	1.88	0.41
1:F:220:VAL:HG12	1:F:342:ILE:HD13	2.02	0.41
2:G:358:ALA:HB1	2:G:360:LEU:HG	2.03	0.41
1:A:37:SER:O	1:A:69:CYS:HB3	2.21	0.41
1:A:118:PRO:HG2	1:A:188:PRO:HG3	2.01	0.41
1:A:119:ILE:HD11	1:A:151:ILE:HD13	2.03	0.41
1:B:423:ILE:HG12	1:B:445:LEU:CD1	2.49	0.41
1:C:190:LYS:HG3	1:C:191:ARG:N	2.35	0.41
1:D:111:GLY:CA	1:D:174:CYS:HB2	2.51	0.41
1:D:146:ILE:HD12	1:D:165:VAL:HG21	2.03	0.41
1:E:105:CYS:SG	1:E:173:TYR:OH	2.71	0.41
1:E:143:TYR:O	1:E:175:ILE:HG23	2.21	0.41
1:A:28:VAL:HG13	1:A:97:GLY:N	2.33	0.41
1:B:51:LEU:HD23	1:B:51:LEU:HA	1.82	0.41
1:B:177:ALA:C	1:B:179:ASP:H	2.24	0.41
1:D:28:VAL:HG13	1:D:97:GLY:H	1.85	0.41
1:D:142:ALA:CB	1:D:144:ARG:HG3	2.51	0.41
1:D:168:THR:HG21	1:D:173:TYR:C	2.40	0.41
1:E:166:VAL:O	1:E:166:VAL:HG12	2.21	0.41
1:E:339:ALA:O	1:E:340:HIS:HB2	2.21	0.41
1:A:212:GLN:O	1:A:216:ILE:HG13	2.21	0.41
1:B:109:LYS:O	1:B:110:TYR:C	2.59	0.41
1:B:310:ALA:HA	1:B:325:VAL:HG22	2.03	0.41
1:B:433:GLU:O	1:B:434:ASP:CB	2.68	0.41
1:C:135:LEU:HD22	1:C:135:LEU:N	2.25	0.41
1:C:254:ILE:HD12	1:C:369:ILE:CD1	2.51	0.41
1:C:259:ALA:HB1	1:C:266:PHE:HB2	2.03	0.41
1:D:112:LYS:O	1:D:181:VAL:N	2.50	0.41
1:E:56:THR:O	1:E:56:THR:HG23	2.20	0.41
1:E:112:LYS:HB2	1:E:169:ASP:CB	2.47	0.41
1:F:26:LEU:HD22	1:F:80:GLU:O	2.21	0.41
1:F:281:GLU:O	1:F:284:SER:HB3	2.21	0.41
1:F:438:ASP:HB3	1:F:441:VAL:CG2	2.46	0.41
2:G:294:PRO:O	2:G:314:HIS:CB	2.69	0.41
2:G:321:ILE:O	2:G:325:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:344:PRO:HD2	2:G:345:ASN:N	2.35	0.41
2:H:340:MET:HG2	2:H:347:GLU:CG	2.48	0.41
1:A:229:LEU:C	1:A:231:LYS:N	2.72	0.41
1:C:153:LEU:CB	1:C:198:LEU:HD12	2.41	0.41
1:C:320:VAL:HG12	1:C:320:VAL:O	2.21	0.41
1:D:389:LYS:HE2	1:D:443:ASN:OD1	2.21	0.41
1:E:110:TYR:HD1	1:E:110:TYR:N	2.19	0.41
1:F:57:VAL:HG11	1:F:71:VAL:HG21	2.02	0.41
1:F:58:LEU:HD12	1:F:67:ALA:O	2.21	0.41
1:A:121:ASP:OD1	1:A:122:THR:HG23	2.21	0.40
1:A:285:ASN:N	1:A:285:ASN:HD22	2.18	0.40
1:B:187:GLU:HA	1:B:188:PRO:HD3	1.86	0.40
1:B:349:ARG:HG3	1:B:350:PRO:N	2.36	0.40
1:B:353:ILE:H	1:B:353:ILE:HG13	1.63	0.40
1:B:385:THR:HA	1:B:388:MET:HG2	2.02	0.40
1:B:428:ASP:O	1:B:430:ILE:N	2.54	0.40
1:C:331:LEU:HA	1:C:331:LEU:HD23	1.90	0.40
1:C:419:ALA:O	1:C:423:ILE:HG13	2.22	0.40
1:D:85:ASN:C	1:D:89:ARG:HD3	2.41	0.40
1:D:113:ARG:C	1:D:114:ILE:HG13	2.42	0.40
1:D:426:LYS:HG3	1:D:427:MET:H	1.87	0.40
1:F:24:ASN:O	1:F:101:SER:HA	2.21	0.40
2:H:303:ALA:H	2:H:367:GLN:HB3	1.86	0.40
1:A:142:ALA:HB1	1:A:144:ARG:HG3	2.02	0.40
1:A:181:VAL:HG12	1:A:183:HIS:NE2	2.36	0.40
1:A:199:ASN:O	1:A:199:ASN:ND2	2.54	0.40
1:D:31:ALA:HB2	1:D:85:ASN:N	2.35	0.40
1:D:41:LEU:CD2	1:D:82:ILE:HA	2.50	0.40
1:D:286:LEU:HB3	1:D:331:LEU:CD1	2.51	0.40
1:D:383:ILE:O	1:D:386:LYS:HG2	2.21	0.40
1:E:82:ILE:HD13	1:E:100:ILE:CD1	2.52	0.40
1:E:127:THR:HG22	1:E:128:GLY:N	2.37	0.40
1:E:152:PHE:CZ	1:E:163:PHE:HB2	2.56	0.40
1:E:178:PRO:HG2	1:E:179:ASP:OD1	2.21	0.40
1:E:281:GLU:O	1:E:284:SER:HB3	2.21	0.40
1:F:110:TYR:HD1	1:F:110:TYR:N	2.18	0.40
1:F:147:ARG:NH1	1:F:147:ARG:HG3	2.32	0.40
1:F:307:ASP:HA	1:F:353:ILE:CD1	2.52	0.40
1:F:313:ARG:HG2	1:F:355:PRO:CD	2.50	0.40
1:A:31:ALA:HB2	1:A:84:MET:C	2.42	0.40
1:A:222:LEU:HD23	1:A:226:HIS:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:VAL:HG21	1:E:319:GLU:HG3	2.02	0.40
1:A:452:PHE:O	1:A:456:LEU:HG	2.21	0.40
1:B:233:ILE:CG2	1:B:234:GLY:N	2.84	0.40
1:B:440:GLU:OE2	1:B:440:GLU:O	2.39	0.40
1:C:35:ASP:HB3	1:C:38:VAL:HG12	2.03	0.40
1:D:107:ASP:O	1:D:109:LYS:HG3	2.22	0.40
1:D:111:GLY:H	1:D:174:CYS:HB2	1.87	0.40
1:D:120:ASP:H	1:D:188:PRO:CB	2.34	0.40
1:D:227:PRO:HB3	1:D:340:HIS:CD2	2.57	0.40
1:D:277:LYS:HB2	1:D:282:SER:OG	2.22	0.40
1:D:384:HIS:HE1	3:D:803:ADP:N3	2.19	0.40
1:D:427:MET:HA	1:D:430:ILE:HB	2.03	0.40
1:E:407:VAL:O	1:E:411:LEU:HG	2.21	0.40
2:G:344:PRO:CD	2:G:345:ASN:N	2.85	0.40
1:A:373:ASP:OD1	1:A:375:THR:N	2.54	0.40
1:B:36:ASN:ND2	1:B:87:VAL:HG21	2.35	0.40
1:B:49:LEU:N	1:B:49:LEU:CD2	2.73	0.40
1:C:129:ASN:HD22	1:C:129:ASN:HA	1.70	0.40
1:C:136:LYS:HB3	1:C:137:PRO:HD3	2.03	0.40
1:C:215:GLN:O	1:C:218:GLU:HG2	2.21	0.40
1:C:238:PRO:HB3	1:C:365:ARG:HH12	1.77	0.40
1:C:425:LYS:O	1:C:428:ASP:OD1	2.39	0.40
1:E:87:VAL:CG2	1:E:198:LEU:CD1	2.91	0.40
1:F:353:ILE:HG22	1:F:354:ASP:N	2.37	0.40
1:A:394:VAL:HG22	1:A:449:MET:N	2.36	0.40
1:A:447:VAL:HG11	1:A:452:PHE:HE1	1.87	0.40
1:B:153:LEU:HD13	1:B:162:GLU:HG2	2.03	0.40
1:B:395:ASP:O	1:B:399:VAL:HG23	2.22	0.40
1:B:414:LEU:HD12	1:B:455:ALA:HB1	2.03	0.40
1:B:420:LEU:HG	1:F:235:VAL:HG11	2.04	0.40
1:C:100:ILE:CG2	1:C:101:SER:N	2.84	0.40
1:C:161:VAL:HG12	1:C:162:GLU:N	2.36	0.40
1:C:229:LEU:HA	1:E:437:ILE:HD11	2.03	0.40
1:C:253:LEU:HD12	3:C:802:ADP:H2'	2.04	0.40
1:D:393:ASP:O	1:D:449:MET:HB2	2.22	0.40
1:E:152:PHE:CE1	1:E:163:PHE:CB	3.04	0.40
1:E:198:LEU:HD23	1:E:198:LEU:HA	1.95	0.40
1:E:422:ALA:HB1	1:E:426:LYS:HZ3	1.87	0.40
1:F:249:THR:HG23	1:F:249:THR:O	2.22	0.40
1:F:279:ALA:CB	1:F:320:VAL:HG13	2.44	0.40
1:F:403:THR:CG2	1:F:411:LEU:HD21	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:300:ILE:HG21	2:G:325:ILE:CD1	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:HIS:CE1	2:G:255:GLY:O[1_445]	2.17	0.03

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	434/458 (95%)	379 (87%)	43 (10%)	12 (3%)	5	19
1	B	434/458 (95%)	362 (83%)	51 (12%)	21 (5%)	2	8
1	C	435/458 (95%)	374 (86%)	50 (12%)	11 (2%)	5	21
1	D	434/458 (95%)	372 (86%)	50 (12%)	12 (3%)	5	19
1	E	434/458 (95%)	365 (84%)	57 (13%)	12 (3%)	5	19
1	F	439/458 (96%)	378 (86%)	43 (10%)	18 (4%)	3	11
2	G	116/127 (91%)	94 (81%)	13 (11%)	9 (8%)	1	2
2	H	103/127 (81%)	82 (80%)	13 (13%)	8 (8%)	1	2
2	I	20/127 (16%)	18 (90%)	1 (5%)	1 (5%)	2	7
All	All	2849/3129 (91%)	2424 (85%)	321 (11%)	104 (4%)	3	13

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	120	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	230	PHE
1	A	314	GLU
1	A	316	THR
1	A	319	GLU
1	A	402	GLU
1	B	53	ARG
1	B	63	LYS
1	B	172	PRO
1	B	404	HIS
1	B	432	LEU
1	C	24	ASN
1	C	53	ARG
1	C	318	GLY
1	C	434	ASP
1	D	108	VAL
1	D	120	ASP
1	D	187	GLU
1	D	193	ASP
1	D	360	PHE
1	D	426	LYS
1	D	427	MET
1	E	120	ASP
1	E	404	HIS
1	E	437	ILE
1	F	21	ASN
1	F	23	PRO
1	F	53	ARG
1	F	171	SER
1	F	187	GLU
1	F	338	ARG
1	F	431	ASP
2	G	286	SER
2	G	311	LYS
2	G	312	PHE
2	G	314	HIS
2	G	343	PHE
2	G	344	PRO
2	H	264	ALA
2	H	304	ASP
2	H	315	SER
2	H	344	PRO
1	A	111	GLY

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	430	ILE
1	B	110	TYR
1	B	120	ASP
1	B	221	GLU
1	B	406	HIS
1	B	433	GLU
1	C	120	ASP
1	C	279	ALA
1	D	53	ARG
1	D	313	ARG
1	D	404	HIS
1	E	159	ARG
1	E	431	ASP
2	G	353	GLN
2	H	348	LEU
2	H	361	LEU
1	B	339	ALA
1	C	140	LEU
1	C	370	GLY
1	D	89	ARG
1	E	50	GLN
1	E	317	HIS
1	F	19	GLN
1	F	143	TYR
1	F	188	PRO
1	F	319	GLU
1	F	457	SER
2	G	348	LEU
2	H	328	ALA
2	H	349	ALA
1	A	311	PRO
1	B	429	LEU
1	E	167	GLU
1	E	304	ASP
1	E	360	PHE
1	F	20	LYS
2	I	316	HIS
1	A	404	HIS
1	A	425	LYS
1	B	186	GLY
1	B	280	GLY
1	C	391	ALA

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Mol	Chain	Res	Type
1	D	173	TYR
1	E	430	ILE
1	E	435	GLU
1	F	79	ASP
1	B	67	ALA
1	B	171	SER
1	B	313	ARG
1	B	352	SER
1	C	188	PRO
1	F	54	GLY
1	F	169	ASP
1	B	108	VAL
1	C	54	GLY
1	B	149	GLY
1	F	430	ILE
1	B	54	GLY
2	G	305	GLY
1	F	350	PRO

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/390 (95%)	340 (92%)	29 (8%)	12	34
1	B	367/390 (94%)	325 (89%)	42 (11%)	5	17
1	C	369/390 (95%)	329 (89%)	40 (11%)	6	20
1	D	364/390 (93%)	330 (91%)	34 (9%)	9	27
1	E	369/390 (95%)	334 (90%)	35 (10%)	8	26
1	F	371/390 (95%)	335 (90%)	36 (10%)	8	25
2	G	75/105 (71%)	66 (88%)	9 (12%)	5	15
2	H	68/105 (65%)	59 (87%)	9 (13%)	4	12
2	I	10/105 (10%)	7 (70%)	3 (30%)	0	1
All	All	2362/2655 (89%)	2125 (90%)	237 (10%)	7	23



All (237) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	34	GLU
1	A	45	LYS
1	A	49	LEU
1	A	65	ARG
1	A	85	ASN
1	A	101	SER
1	A	107	ASP
1	A	131	PHE
1	A	147	ARG
1	A	189	ILE
1	A	190	LYS
1	A	210	ARG
1	A	212	GLN
1	A	224	LEU
1	A	241	ILE
1	A	282	SER
1	A	292	GLU
1	A	313	ARG
1	A	337	GLN
1	A	354	ASP
1	A	364	ASP
1	A	401	ASN
1	A	426	LYS
1	A	428	ASP
1	A	432	LEU
1	A	434	ASP
1	A	453	ARG
1	A	458	GLN
1	B	28	VAL
1	B	32	ILE
1	B	33	ASN
1	B	42	SER
1	B	46	MET
1	B	49	LEU
1	B	52	PHE
1	B	55	ASP
1	B	58	LEU
1	B	63	LYS
1	B	64	ARG
1	B	75	ASP
1	B	85	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	99	VAL
1	B	100	ILE
1	B	103	GLN
1	B	127	THR
1	B	129	ASN
1	B	168	THR
1	B	173	TYR
1	B	187	GLU
1	B	190	LYS
1	B	194	GLU
1	B	196	GLU
1	B	205	ASP
1	B	210	ARG
1	B	212	GLN
1	B	213	LEU
1	B	224	LEU
1	B	239	ARG
1	B	253	LEU
1	B	319	GLU
1	B	337	GLN
1	B	338	ARG
1	B	340	HIS
1	B	349	ARG
1	B	350	PRO
1	B	351	ASN
1	B	365	ARG
1	B	392	ASP
1	B	450	ASP
1	B	458	GLN
1	C	22	ARG
1	C	28	VAL
1	C	34	GLU
1	C	35	ASP
1	C	43	GLN
1	C	63	LYS
1	C	75	ASP
1	C	76	THR
1	C	90	ASN
1	C	107	ASP
1	C	109	LYS
1	C	120	ASP
1	C	129	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	146	ILE
1	C	147	ARG
1	C	153	LEU
1	C	159	ARG
1	C	179	ASP
1	C	190	LYS
1	C	197	SER
1	C	199	ASN
1	C	200	GLU
1	C	244	TYR
1	C	249	THR
1	C	270	ASN
1	C	317	HIS
1	C	338	ARG
1	C	349	ARG
1	C	351	ASN
1	C	365	ARG
1	C	378	LEU
1	C	392	ASP
1	C	427	MET
1	C	428	ASP
1	C	433	GLU
1	C	436	THR
1	C	438	ASP
1	C	440	GLU
1	C	450	ASP
1	C	458	GLN
1	D	33	ASN
1	D	36	ASN
1	D	45	LYS
1	D	55	ASP
1	D	64	ARG
1	D	73	SER
1	D	75	ASP
1	D	101	SER
1	D	105	CYS
1	D	113	ARG
1	D	115	HIS
1	D	129	ASN
1	D	131	PHE
1	D	140	LEU
1	D	147	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	152	PHE
1	D	168	THR
1	D	174	CYS
1	D	179	ASP
1	D	183	HIS
1	D	184	CYS
1	D	190	LYS
1	D	193	ASP
1	D	196	GLU
1	D	210	ARG
1	D	300	ILE
1	D	317	HIS
1	D	322	ARG
1	D	389	LYS
1	D	428	ASP
1	D	431	ASP
1	D	438	ASP
1	D	449	MET
1	D	458	GLN
1	E	26	LEU
1	E	37	SER
1	E	45	LYS
1	E	48	GLU
1	E	50	GLN
1	E	53	ARG
1	E	73	SER
1	E	82	ILE
1	E	99	VAL
1	E	103	GLN
1	E	107	ASP
1	E	109	LYS
1	E	113	ARG
1	E	130	LEU
1	E	146	ILE
1	E	147	ARG
1	E	154	VAL
1	E	164	LYS
1	E	171	SER
1	E	179	ASP
1	E	187	GLU
1	E	194	GLU
1	E	197	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	210	ARG
1	E	211	LYS
1	E	288	LYS
1	E	296	ASN
1	E	307	ASP
1	E	337	GLN
1	E	416	SER
1	E	429	LEU
1	E	431	ASP
1	E	433	GLU
1	E	451	ASP
1	E	458	GLN
1	F	23	PRO
1	F	34	GLU
1	F	53	ARG
1	F	79	ASP
1	F	80	GLU
1	F	85	ASN
1	F	109	LYS
1	F	112	LYS
1	F	113	ARG
1	F	120	ASP
1	F	124	GLU
1	F	140	LEU
1	F	147	ARG
1	F	185	GLU
1	F	187	GLU
1	F	194	GLU
1	F	210	ARG
1	F	211	LYS
1	F	212	GLN
1	F	213	LEU
1	F	249	THR
1	F	288	LYS
1	F	317	HIS
1	F	322	ARG
1	F	323	ARG
1	F	353	ILE
1	F	364	ASP
1	F	378	LEU
1	F	379	GLU
1	F	388	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	402	GLU
1	F	428	ASP
1	F	431	ASP
1	F	434	ASP
1	F	438	ASP
1	F	453	ARG
2	G	295	THR
2	G	296	THR
2	G	308	LEU
2	G	310	GLN
2	G	317	ARG
2	G	323	LEU
2	G	345	ASN
2	G	347	GLU
2	G	362	ASN
2	H	299	GLN
2	H	310	GLN
2	H	312	PHE
2	H	322	ARG
2	H	335	THR
2	H	336	SER
2	H	352	ASN
2	H	353	GLN
2	H	359	ASN
2	I	317	ARG
2	I	320	ASP
2	I	325	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	36	ASN
1	A	43	GLN
1	A	90	ASN
1	A	115	HIS
1	A	199	ASN
1	A	226	HIS
1	A	285	ASN
1	A	348	ASN
1	A	404	HIS
1	A	458	GLN
1	B	33	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	36	ASN
1	B	50	GLN
1	B	90	ASN
1	B	103	GLN
1	B	129	ASN
1	B	226	HIS
1	B	285	ASN
1	B	348	ASN
1	B	351	ASN
1	B	382	GLN
1	B	401	ASN
1	B	458	GLN
1	C	85	ASN
1	C	91	ASN
1	C	103	GLN
1	C	115	HIS
1	C	129	ASN
1	C	183	HIS
1	C	199	ASN
1	C	226	HIS
1	C	270	ASN
1	C	327	GLN
1	C	348	ASN
1	C	351	ASN
1	C	384	HIS
1	C	387	ASN
1	C	443	ASN
1	C	458	GLN
1	D	33	ASN
1	D	36	ASN
1	D	90	ASN
1	D	129	ASN
1	D	226	HIS
1	D	285	ASN
1	D	296	ASN
1	D	317	HIS
1	D	337	GLN
1	D	348	ASN
1	D	384	HIS
1	D	387	ASN
1	D	398	GLN
1	D	401	ASN

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Mol	Chain	Res	Type
1	E	90	ASN
1	E	212	GLN
1	E	215	GLN
1	E	296	ASN
1	E	327	GLN
1	E	348	ASN
1	E	387	ASN
1	E	406	HIS
1	E	443	ASN
1	E	458	GLN
1	F	36	ASN
1	F	43	GLN
1	F	85	ASN
1	F	90	ASN
1	F	226	HIS
1	F	348	ASN
1	F	351	ASN
1	F	384	HIS
1	F	443	ASN
2	G	299	GLN
2	G	313	ASN
2	H	299	GLN
2	H	310	GLN
2	H	314	HIS
2	H	352	ASN
2	H	353	GLN
2	H	362	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 5.6 Ligand geometry

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ADP	C	802	-	24,29,29	1.40	4 (16%)	29,45,45	1.67	3 (10%)
3	ADP	A	800	-	24,29,29	1.41	4 (16%)	29,45,45	1.58	1 (3%)
3	ADP	F	805	-	24,29,29	1.58	6 (25%)	29,45,45	1.57	1 (3%)
3	ADP	B	801	-	24,29,29	1.51	6 (25%)	29,45,45	1.60	1 (3%)
3	ADP	D	803	-	24,29,29	1.48	4 (16%)	29,45,45	1.60	2 (6%)
3	ADP	E	804	-	24,29,29	1.41	4 (16%)	29,45,45	1.62	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	C	802	-	-	6/12/32/32	0/3/3/3
3	ADP	A	800	-	-	8/12/32/32	0/3/3/3
3	ADP	F	805	-	-	8/12/32/32	0/3/3/3
3	ADP	B	801	-	-	5/12/32/32	0/3/3/3
3	ADP	D	803	-	-	8/12/32/32	0/3/3/3
3	ADP	E	804	-	-	8/12/32/32	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	805	ADP	O4'-C1'	3.19	1.45	1.41
3	D	803	ADP	O4'-C1'	3.09	1.45	1.41
3	A	800	ADP	O4'-C1'	2.98	1.45	1.41
3	D	803	ADP	C2-N3	2.90	1.36	1.32
3	F	805	ADP	C5-N7	-2.83	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	ADP	C5-N7	-2.74	1.29	1.39
3	E	804	ADP	C5-N7	-2.74	1.29	1.39
3	B	801	ADP	C2-N3	2.70	1.36	1.32
3	B	801	ADP	O4'-C1'	2.67	1.44	1.41
3	C	802	ADP	C5-N7	-2.59	1.30	1.39
3	F	805	ADP	C8-N7	-2.58	1.30	1.34
3	F	805	ADP	C2-N3	2.54	1.36	1.32
3	D	803	ADP	C5-N7	-2.53	1.30	1.39
3	E	804	ADP	C2-N3	2.53	1.36	1.32
3	B	801	ADP	C4-N3	2.52	1.39	1.35
3	A	800	ADP	C5-N7	-2.49	1.30	1.39
3	C	802	ADP	C2-N3	2.31	1.35	1.32
3	C	802	ADP	O4'-C1'	2.30	1.44	1.41
3	F	805	ADP	PB-O3B	-2.26	1.46	1.54
3	E	804	ADP	O4'-C1'	2.24	1.44	1.41
3	B	801	ADP	C8-N7	-2.12	1.30	1.34
3	A	800	ADP	C2-N3	2.11	1.35	1.32
3	C	802	ADP	PA-O2A	-2.10	1.45	1.55
3	A	800	ADP	PA-O2A	-2.10	1.45	1.55
3	F	805	ADP	PA-O2A	-2.04	1.45	1.55
3	E	804	ADP	PA-O2A	-2.04	1.45	1.55
3	B	801	ADP	PA-O2A	-2.02	1.45	1.55
3	D	803	ADP	PA-O2A	-2.01	1.45	1.55

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	ADP	N3-C2-N1	-6.89	117.91	128.68
3	A	800	ADP	N3-C2-N1	-6.68	118.25	128.68
3	F	805	ADP	N3-C2-N1	-6.66	118.27	128.68
3	C	802	ADP	N3-C2-N1	-6.63	118.31	128.68
3	D	803	ADP	N3-C2-N1	-6.56	118.42	128.68
3	E	804	ADP	N3-C2-N1	-6.45	118.60	128.68
3	C	802	ADP	C2'-C3'-C4'	2.68	107.86	102.64
3	E	804	ADP	C2'-C3'-C4'	2.50	107.50	102.64
3	D	803	ADP	C2'-C3'-C4'	2.30	107.12	102.64
3	E	804	ADP	C3'-C2'-C1'	2.14	104.20	100.98
3	C	802	ADP	O5'-C5'-C4'	-2.04	101.96	108.99

There are no chirality outliers.

All (43) torsion outliers are listed below:

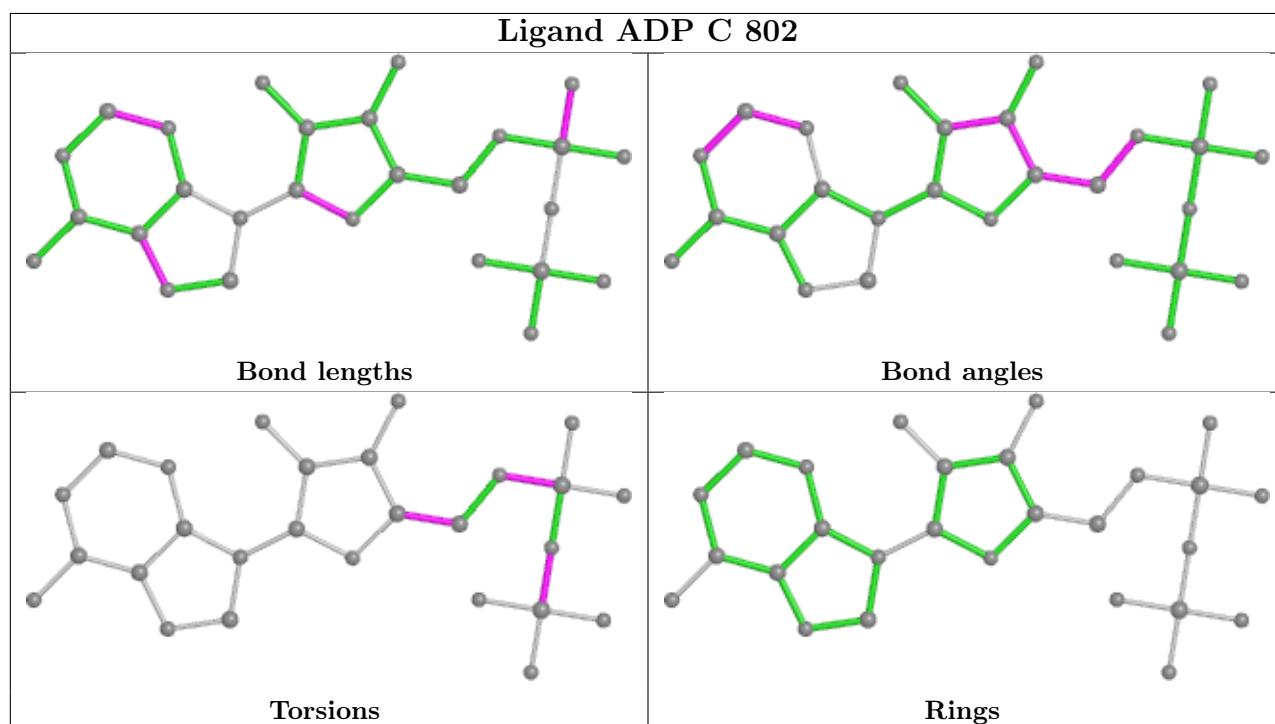
Mol	Chain	Res	Type	Atoms
3	A	800	ADP	C5'-O5'-PA-O1A
3	A	800	ADP	C5'-O5'-PA-O2A
3	A	800	ADP	C5'-O5'-PA-O3A
3	B	801	ADP	PA-O3A-PB-O2B
3	B	801	ADP	C5'-O5'-PA-O1A
3	B	801	ADP	C5'-O5'-PA-O2A
3	B	801	ADP	C5'-O5'-PA-O3A
3	B	801	ADP	O4'-C4'-C5'-O5'
3	C	802	ADP	C5'-O5'-PA-O1A
3	C	802	ADP	C5'-O5'-PA-O2A
3	C	802	ADP	C5'-O5'-PA-O3A
3	D	803	ADP	C5'-O5'-PA-O1A
3	D	803	ADP	C5'-O5'-PA-O2A
3	D	803	ADP	C5'-O5'-PA-O3A
3	E	804	ADP	C5'-O5'-PA-O1A
3	E	804	ADP	C5'-O5'-PA-O2A
3	E	804	ADP	C5'-O5'-PA-O3A
3	F	805	ADP	C5'-O5'-PA-O1A
3	F	805	ADP	C5'-O5'-PA-O2A
3	F	805	ADP	C5'-O5'-PA-O3A
3	A	800	ADP	O4'-C4'-C5'-O5'
3	C	802	ADP	O4'-C4'-C5'-O5'
3	D	803	ADP	O4'-C4'-C5'-O5'
3	E	804	ADP	O4'-C4'-C5'-O5'
3	F	805	ADP	O4'-C4'-C5'-O5'
3	E	804	ADP	C3'-C4'-C5'-O5'
3	D	803	ADP	C3'-C4'-C5'-O5'
3	C	802	ADP	C3'-C4'-C5'-O5'
3	D	803	ADP	PA-O3A-PB-O1B
3	F	805	ADP	PA-O3A-PB-O1B
3	A	800	ADP	C3'-C4'-C5'-O5'
3	A	800	ADP	PA-O3A-PB-O1B
3	A	800	ADP	PA-O3A-PB-O2B
3	A	800	ADP	PA-O3A-PB-O3B
3	C	802	ADP	PA-O3A-PB-O2B
3	D	803	ADP	PA-O3A-PB-O2B
3	D	803	ADP	PA-O3A-PB-O3B
3	E	804	ADP	PA-O3A-PB-O2B
3	E	804	ADP	PA-O3A-PB-O3B
3	F	805	ADP	PA-O3A-PB-O2B
3	F	805	ADP	PA-O3A-PB-O3B
3	F	805	ADP	C3'-C4'-C5'-O5'
3	E	804	ADP	PA-O3A-PB-O1B

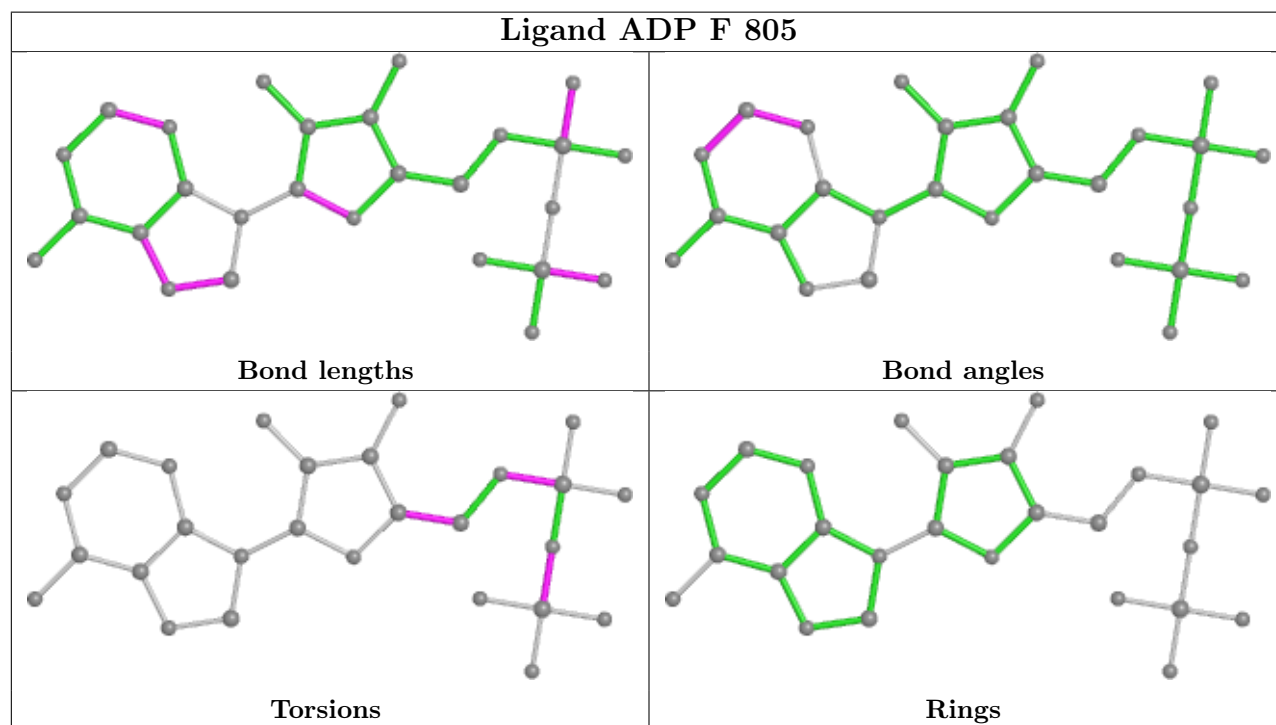
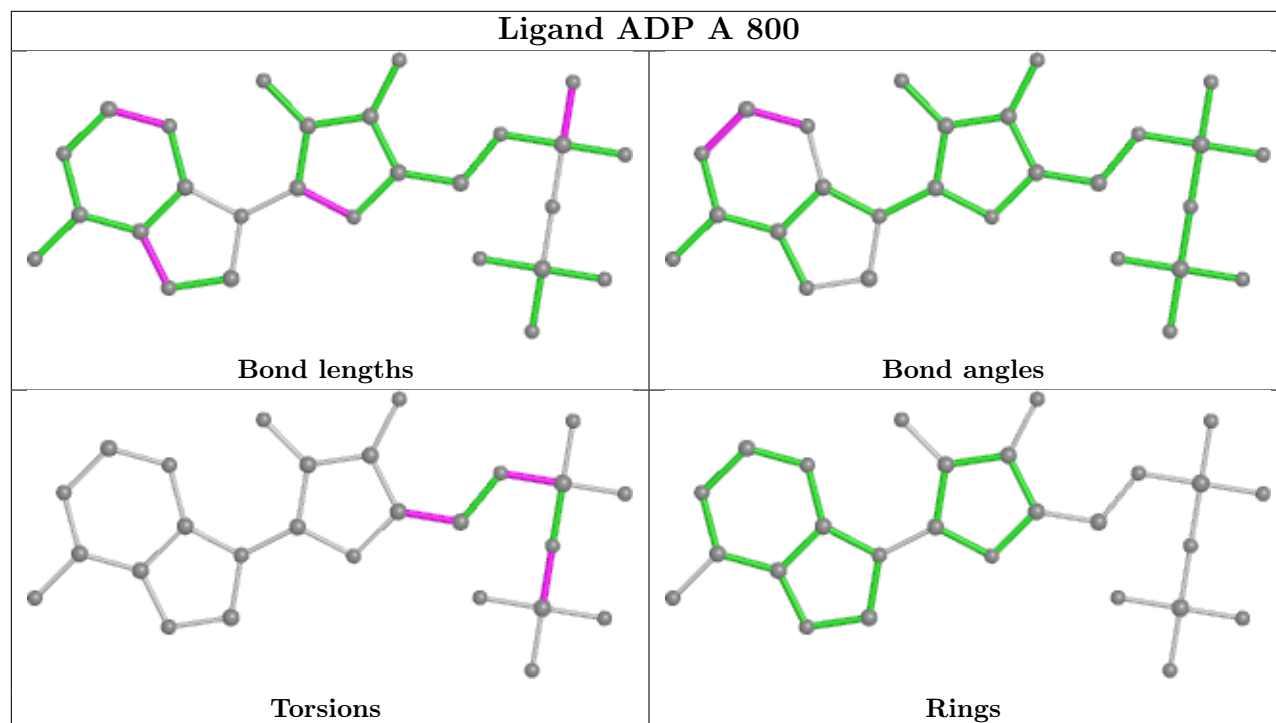
There are no ring outliers.

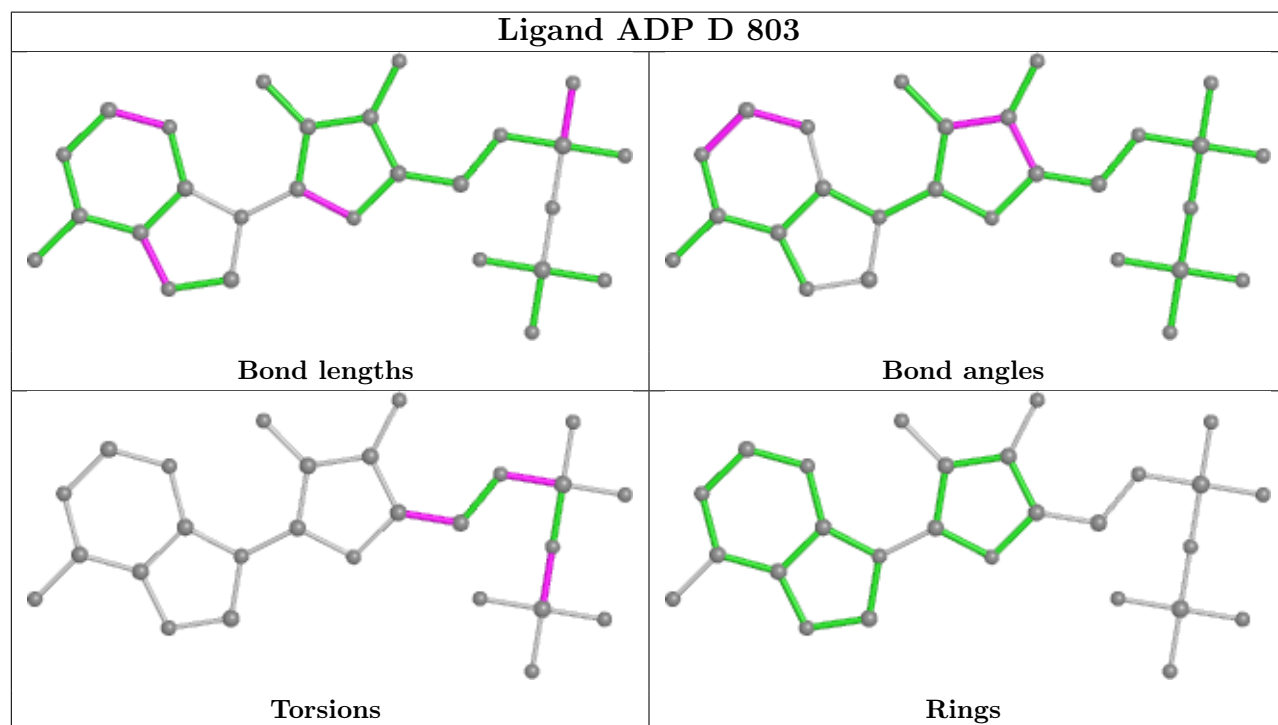
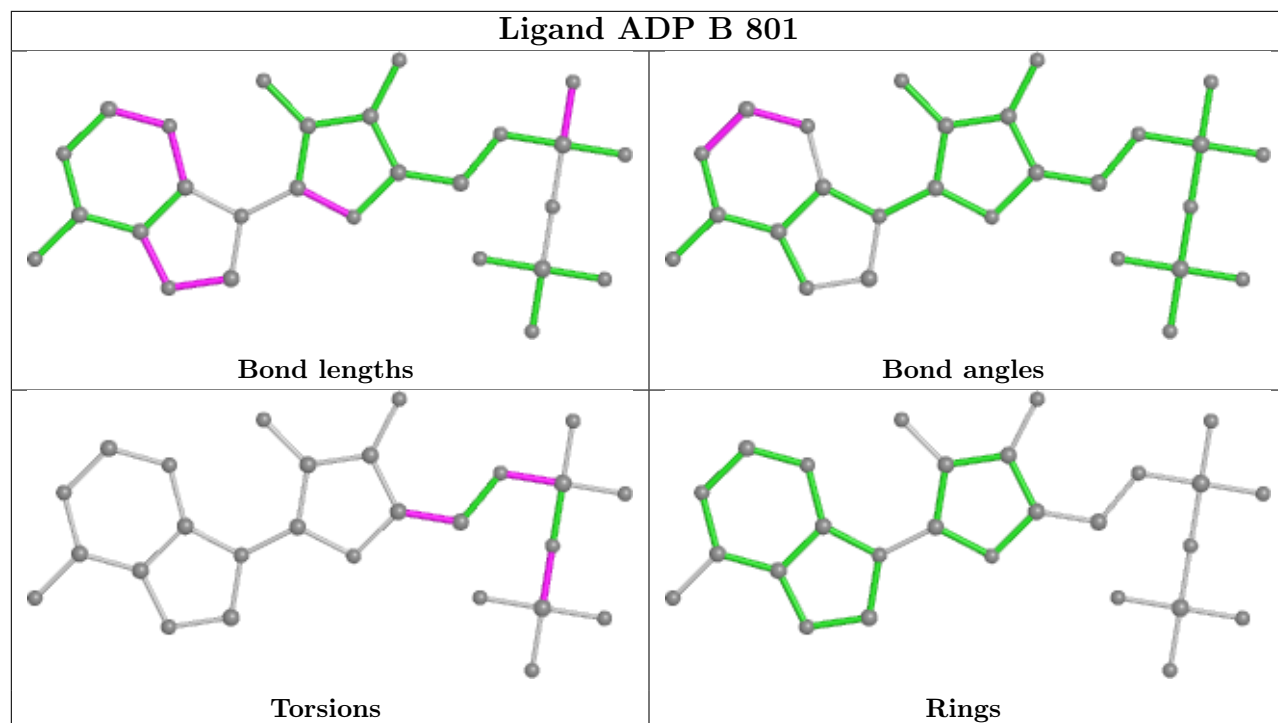
4 monomers are involved in 5 short contacts:

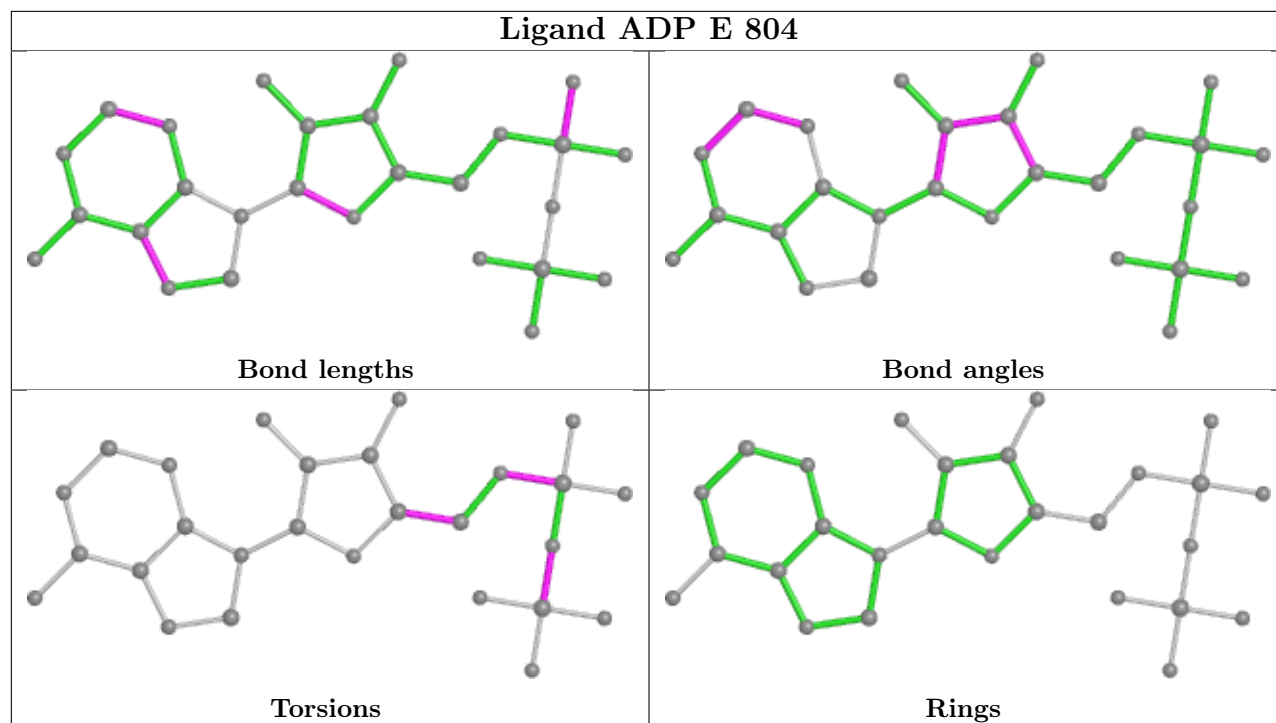
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	802	ADP	1	0
3	F	805	ADP	2	0
3	D	803	ADP	1	0
3	E	804	ADP	1	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.