Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2023 – 06:59 AM EDT

PDB ID	:	1I6V
Title	:	THERMUS AQUATICUS CORE RNA POLYMERASE-RIFAMPICIN COMPLEX
Authors	:	Campbell, E.A.; Korzheva, N.; Mustaev, A.; Murakami, K.; Goldfarb, A.; Darst, S.A.
Deposited on	:	2001-03-05
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

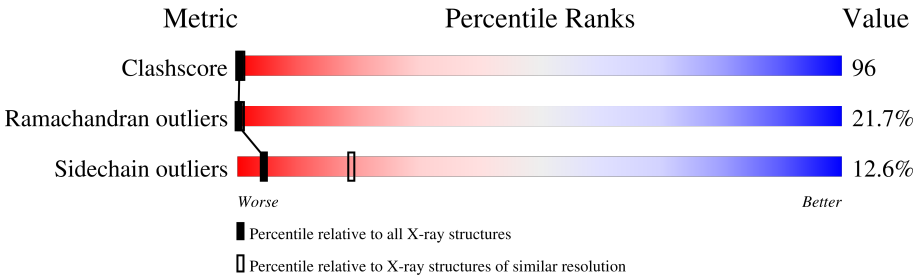
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	314	12% 40% 15% • 29%
1	B	314	11% 46% 16% • 27%
2	C	1118	14% 60% 24% •
3	D	1264	18% 52% 21% • 7%
4	E	99	19% 62% 18% •

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 21292 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 DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1741	1109	299	330	3			
1	B	230	Total	C	N	O	S	0	0	0
			1761	1122	299	337	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	VAL	GLY	conflict	UNP Q9KWU8
A	232	SER	LEU	conflict	UNP Q9KWU8
B	112	VAL	GLY	conflict	UNP Q9KWU8
B	232	SER	LEU	conflict	UNP Q9KWU8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1113	Total	C	N	O	S	12	0	0
			8508	5386	1514	1585	23			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	LYS	GLU	conflict	UNP Q9KWU7
C	?	-	GLU	deletion	UNP Q9KWU7
C	1111	VAL	ILE	conflict	UNP Q9KWU7

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1174	Total	C	N	O	S	17	0	0
			8502	5329	1550	1596	27			

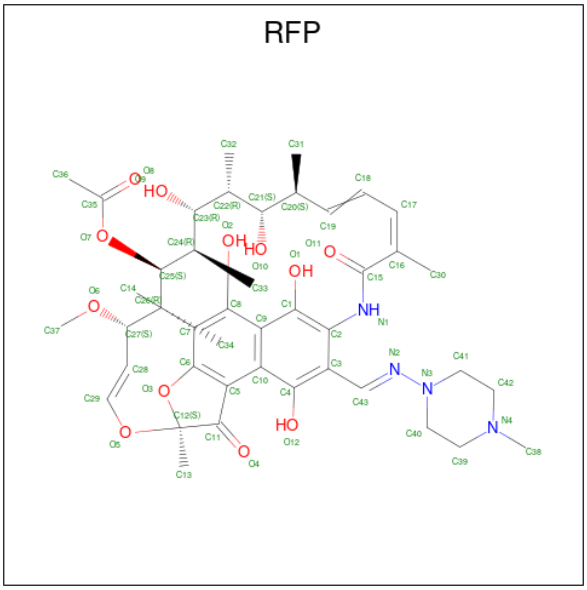
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	70	ALA	GLY	conflict	UNP Q9KWU6
D	77	ALA	GLY	conflict	UNP Q9KWU6
D	91	ALA	GLY	conflict	UNP Q9KWU6
D	113	ALA	GLY	conflict	UNP Q9KWU6
D	139	ALA	GLY	conflict	UNP Q9KWU6
D	144	ALA	GLY	conflict	UNP Q9KWU6
D	863	THR	VAL	conflict	UNP Q9KWU6
D	866	THR	VAL	conflict	UNP Q9KWU6
D	1009	ASN	LYS	conflict	UNP Q9KWU6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	98	Total	C	N	O	S	0	0	0
			719	453	132	130	4			

- Molecule 5 is RIFAMPICIN (three-letter code: RFP) (formula: $C_{43}H_{58}N_4O_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			59	43	4	12		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Mg 1 1	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total Zn 1 1	0	0

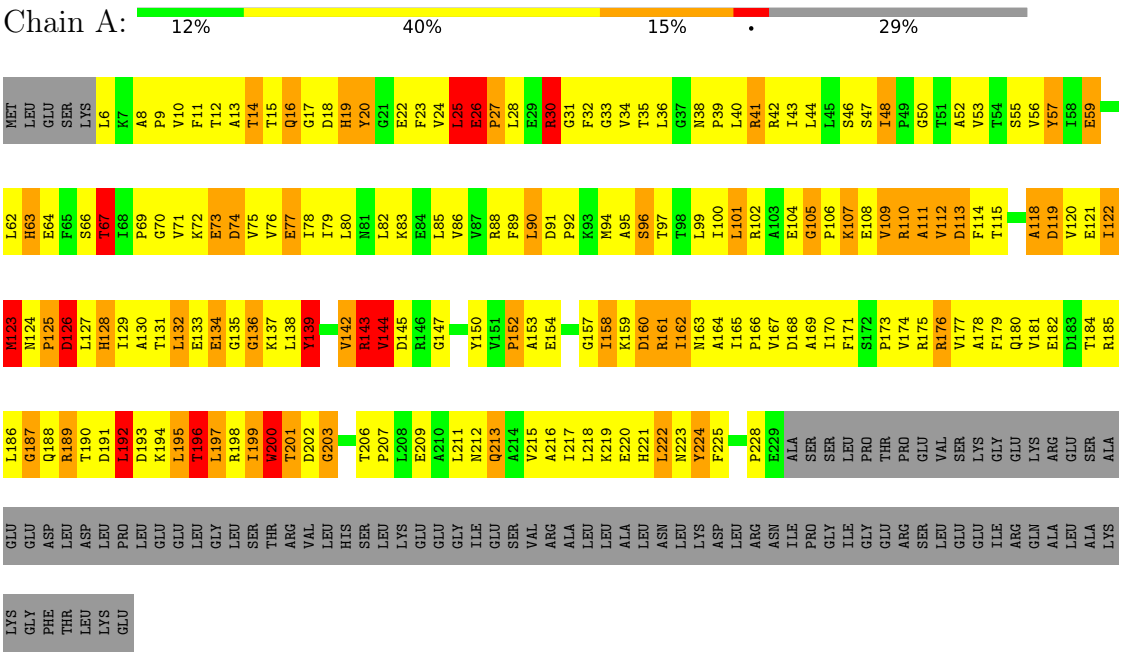
3 Residue-property plots (i)

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.

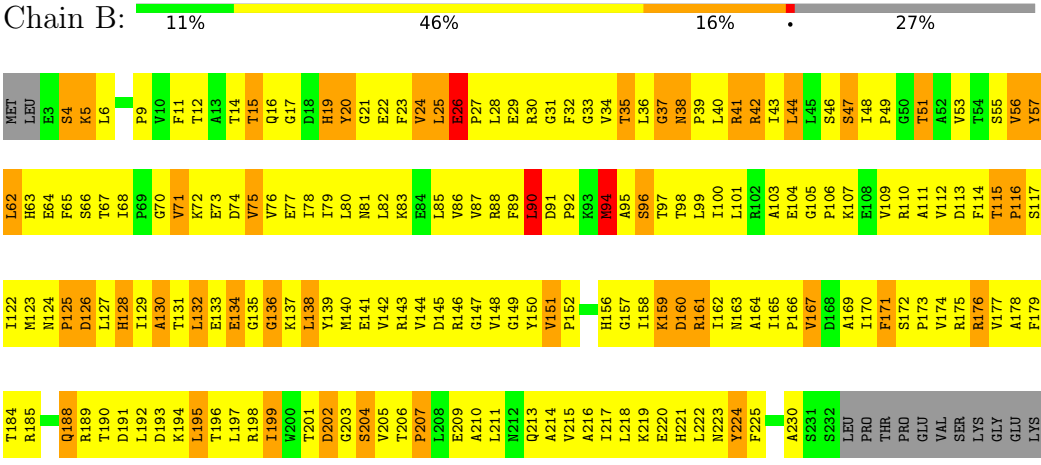
• Molecule 1: DNA-DIRECTED RNA POLYMERASE

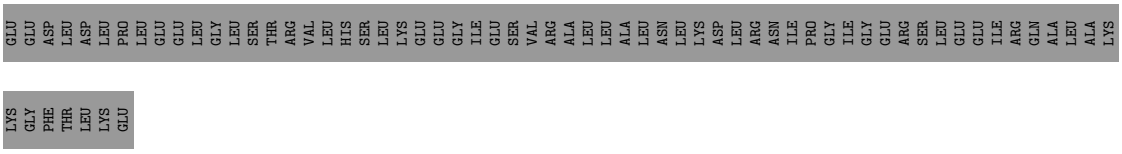
Chain A:



• Molecule 1: DNA-DIRECTED RNA POLYMERASE

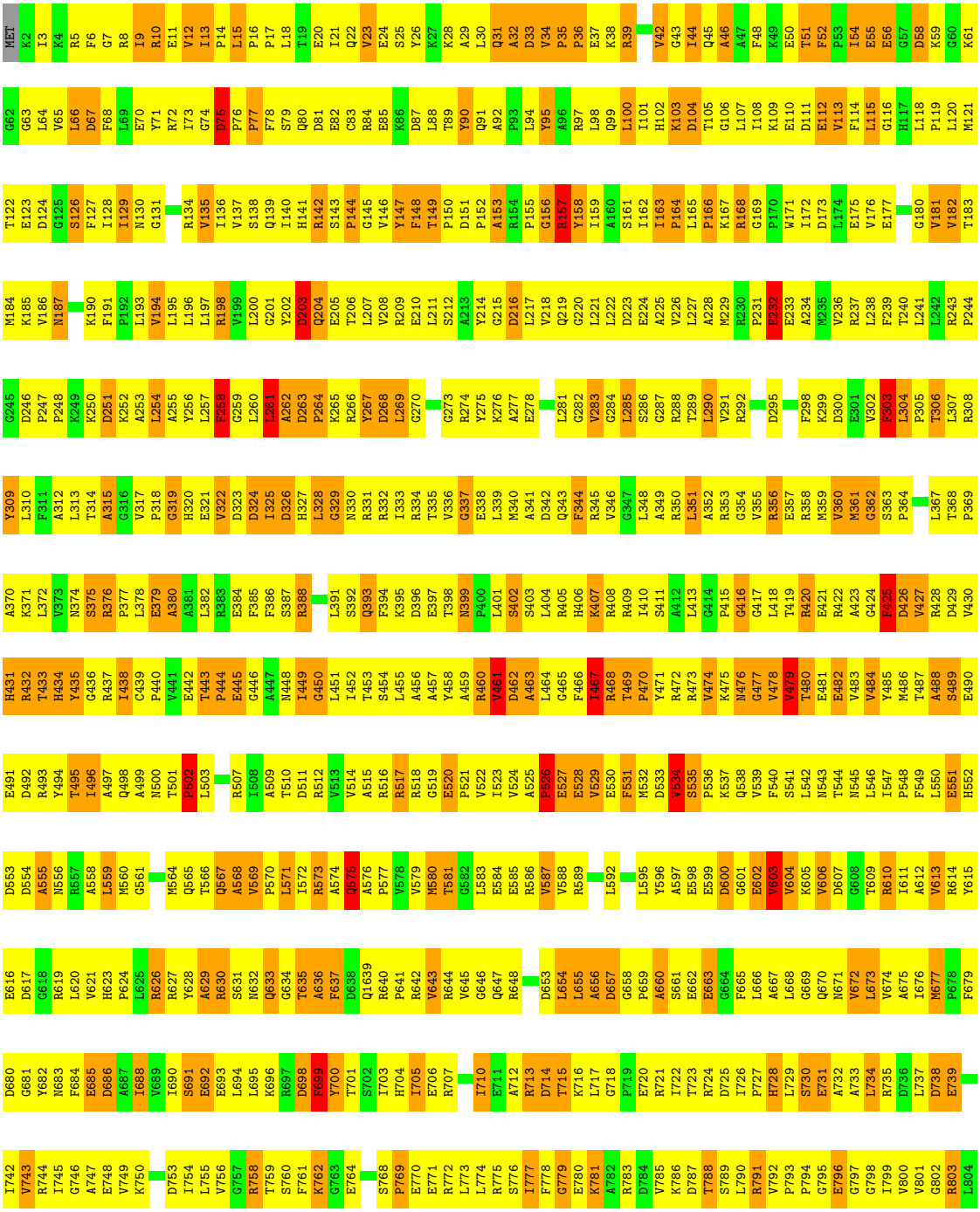
Chain B:

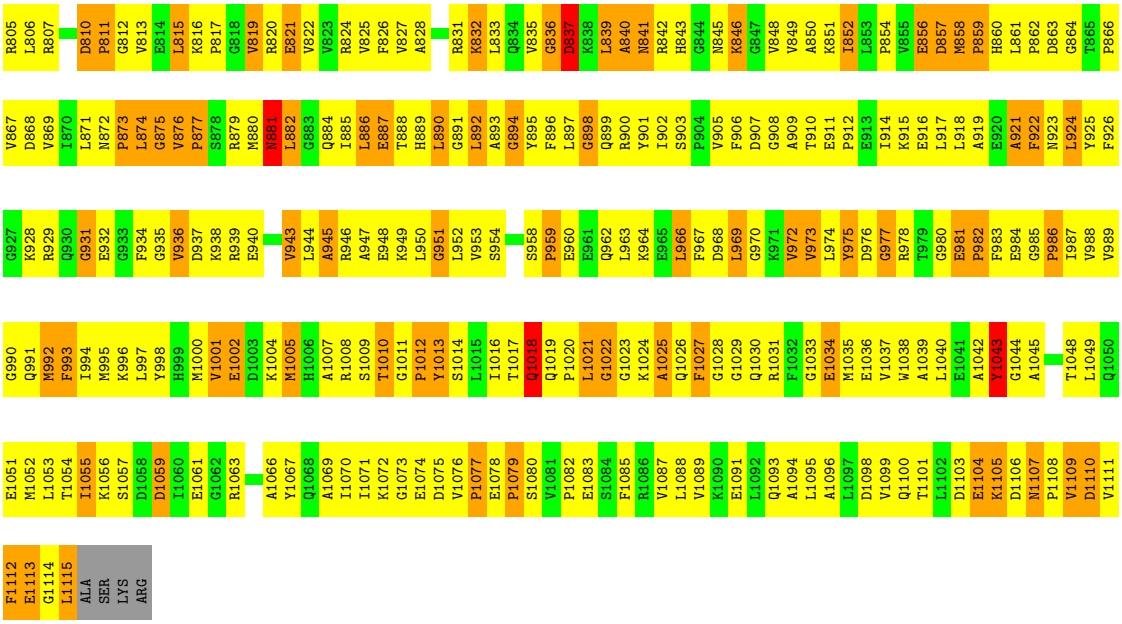




• Molecule 2: DNA-DIRECTED RNA POLYMERASE

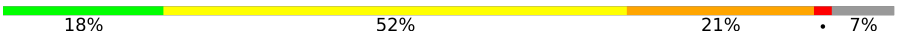
Chain C:

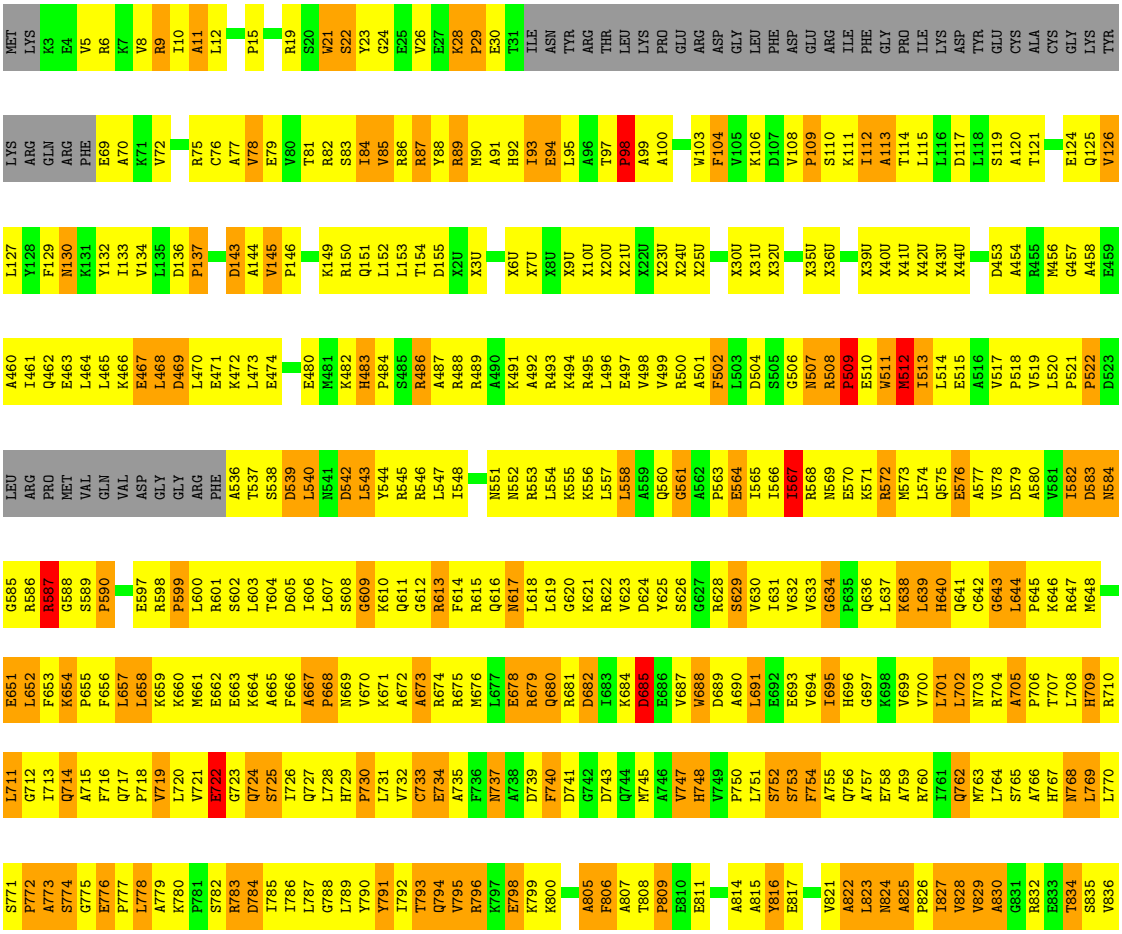


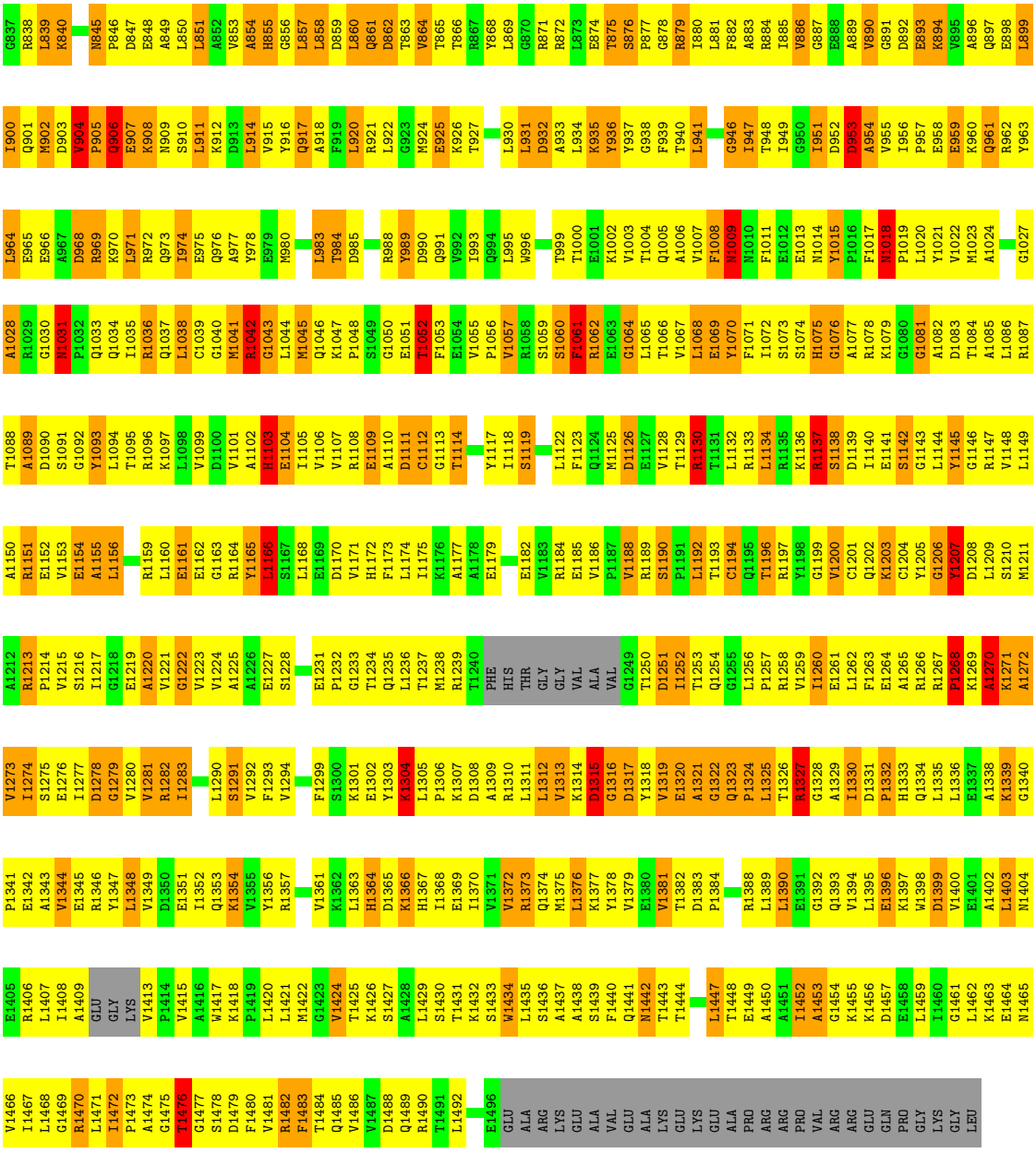


• Molecule 3: DNA-DIRECTED RNA POLYMERASE

Chain D:

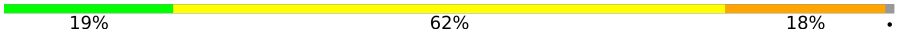


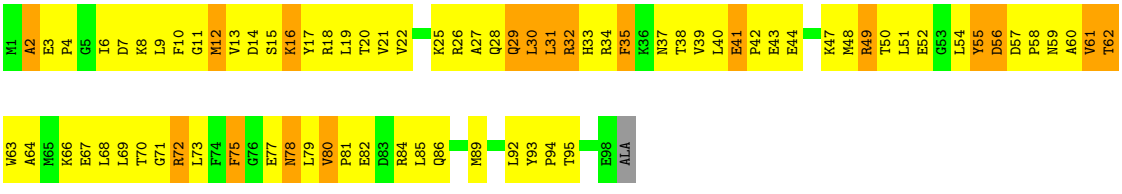




• Molecule 4: DNA-DIRECTED RNA POLYMERASE

Chain E:





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	199.45Å 199.45Å 289.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.30)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.276 , 0.359	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21292	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.43	0/1775	0.77	1/2417 (0.0%)
1	B	0.42	1/1795 (0.1%)	0.77	1/2447 (0.0%)
2	C	0.41	0/8672	0.80	7/11752 (0.1%)
3	D	0.44	1/8439 (0.0%)	0.84	19/11447 (0.2%)
4	E	0.37	0/730	0.71	0/991
All	All	0.42	2/21411 (0.0%)	0.81	28/29054 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	C	0	1
3	D	0	3
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1270	ALA	C-N	-12.09	1.06	1.34
1	B	94	MET	SD-CE	5.75	2.10	1.77

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1270	ALA	O-C-N	-19.05	92.23	122.70
3	D	1270	ALA	C-N-CA	13.67	155.87	121.70
3	D	1270	ALA	CA-C-N	12.08	143.77	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	580	MET	N-CA-C	6.98	129.85	111.00
3	D	1166	LEU	CA-CB-CG	6.22	129.61	115.30
3	D	508	ARG	N-CA-C	-6.00	94.79	111.00
1	A	25	LEU	N-CA-C	-5.91	95.05	111.00
3	D	954	ALA	N-CA-C	-5.87	95.16	111.00
2	C	836	GLY	N-CA-C	-5.82	98.55	113.10
3	D	137	PRO	N-CA-CB	5.80	110.26	103.30
3	D	775	GLY	N-CA-C	5.78	127.55	113.10
3	D	512	MET	N-CA-C	-5.73	95.53	111.00
3	D	834	THR	N-CA-C	-5.61	95.86	111.00
2	C	571	LEU	CA-CB-CG	5.57	128.10	115.30
1	B	26	GLU	N-CA-C	5.46	125.75	111.00
3	D	98	PRO	N-CA-CB	5.40	109.78	103.30
2	C	467	ILE	N-CA-C	5.38	125.54	111.00
3	D	29	PRO	N-CA-CB	5.33	109.69	103.30
3	D	1069	GLU	N-CA-C	-5.26	96.79	111.00
3	D	1042	ARG	N-CA-C	-5.24	96.86	111.00
2	C	329	GLY	N-CA-C	-5.23	100.02	113.10
3	D	826	PRO	N-CA-CB	5.23	109.57	103.30
3	D	146	PRO	N-CA-CB	5.17	109.50	103.30
3	D	109	PRO	N-CA-CB	5.16	109.50	103.30
2	C	379	GLU	N-CA-C	-5.14	97.13	111.00
3	D	1388	ARG	N-CA-C	5.12	124.82	111.00
2	C	655	LEU	CA-CB-CG	5.07	126.95	115.30
3	D	1018	ASN	C-N-CD	5.04	139.00	128.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	TYR	Sidechain
2	C	1013	TYR	Sidechain
3	D	1165	TYR	Sidechain
3	D	1268	PRO	Mainchain
3	D	1270	ALA	Mainchain

5.2 Too-close contacts (i)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1741	0	1747	348	0
1	B	1761	0	1754	316	0
2	C	8508	0	8421	1817	0
3	D	8502	0	8002	1671	0
4	E	719	0	685	138	0
5	C	59	0	56	6	0
6	D	1	0	0	0	0
7	D	1	0	0	0	0
All	All	21292	0	20665	4041	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 96.

All (4041) 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:B:94:MET:CE	1:B:94:MET:SD	2.10	1.39
2:C:690:ILE:HB	2:C:852:ILE:HG22	1.19	1.18
3:D:1280:VAL:HG12	3:D:1281:VAL:HG23	1.25	1.16
2:C:491:GLU:HA	2:C:531:PHE:HA	1.29	1.15
3:D:772:PRO:HG3	3:D:778:LEU:HB2	1.28	1.14
2:C:861:LEU:HG	2:C:862:PRO:HD2	1.23	1.14
3:D:1280:VAL:HG13	3:D:1315:ASP:HA	1.25	1.13
2:C:613:VAL:HG21	2:C:619:ARG:HG2	1.31	1.13
2:C:208:VAL:HG11	2:C:218:VAL:HG11	1.27	1.12
3:D:129:PHE:HA	3:D:454:ALA:HB1	1.24	1.12
1:A:96:SER:HB3	1:A:145:ASP:HA	1.16	1.11
3:D:890:VAL:HG12	3:D:891:GLY:H	1.12	1.10
3:D:1101:VAL:HG21	3:D:1424:VAL:HG22	1.33	1.10
3:D:1015:TYR:HB3	3:D:1019:PRO:HD3	1.33	1.10
3:D:483:HIS:H	3:D:484:PRO:HD2	1.00	1.09
2:C:17:PRO:HD2	2:C:20:GLU:HB2	1.32	1.09
2:C:261:LEU:HG	2:C:263:ASP:HB3	1.33	1.09
2:C:262:ALA:HB1	2:C:266:ARG:HD3	1.15	1.08
1:A:26:GLU:HB3	1:A:27:PRO:CD	1.81	1.08
2:C:129:ILE:HG21	2:C:387:SER:HB2	1.36	1.08
3:D:691:LEU:H	3:D:691:LEU:HD12	1.18	1.08
2:C:12:VAL:HG12	2:C:13:ILE:H	1.17	1.07
2:C:115:LEU:HD12	2:C:116:GLY:H	1.12	1.06
3:D:876:SER:H	3:D:879:ARG:HG3	1.20	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:399:ASN:C	2:C:399:ASN:HD22	1.59	1.06
3:D:772:PRO:CG	3:D:778:LEU:HB2	1.86	1.06
1:A:30:ARG:HD2	1:A:191:ASP:HB3	1.37	1.05
2:C:376:ARG:H	2:C:377:PRO:HD2	1.20	1.05
2:C:873:PRO:O	2:C:877:PRO:HD2	1.56	1.05
3:D:1019:PRO:HB2	3:D:1022:VAL:HG23	1.37	1.05
3:D:1154:GLU:HB3	3:D:1159:ARG:HG2	1.38	1.05
2:C:333:ILE:HD11	2:C:468:ARG:HE	1.20	1.05
2:C:474:VAL:HG22	2:C:530:GLU:HA	1.37	1.04
2:C:1008:ARG:HD3	2:C:1029:GLY:H	1.19	1.04
3:D:1273:VAL:HG23	3:D:1324:PRO:HG3	1.37	1.04
3:D:886:VAL:HG11	3:D:900:ILE:HD11	1.36	1.03
2:C:253:ALA:HA	2:C:256:TYR:HB2	1.36	1.03
3:D:811:GLU:HA	3:D:814:ALA:HB3	1.34	1.03
2:C:456:ALA:HB3	2:C:459:ALA:HB2	1.34	1.02
3:D:879:ARG:NH2	3:D:904:VAL:HA	1.75	1.02
2:C:710:ILE:HD11	2:C:790:LEU:HD22	1.05	1.02
1:B:195:LEU:HD11	1:B:197:LEU:HD13	1.42	1.02
2:C:140:ILE:HG22	2:C:333:ILE:HG12	1.40	1.01
1:B:26:GLU:HG3	1:B:194:LYS:HD2	1.38	1.01
1:A:26:GLU:HB3	1:A:27:PRO:HD3	1.43	1.01
1:B:97:THR:CG2	1:B:120:VAL:HG21	1.91	1.00
3:D:521:PRO:HG2	3:D:522:PRO:HD3	1.41	1.00
1:A:131:THR:HG23	2:C:644:ARG:HH21	1.24	1.00
1:A:158:ILE:HD11	1:A:161:ARG:HE	1.23	1.00
2:C:525:ALA:HB1	2:C:526:PRO:HD2	1.44	1.00
2:C:1045:ALA:HB1	2:C:1048:THR:HB	1.40	0.99
1:B:97:THR:HG21	1:B:120:VAL:HG21	1.42	0.99
2:C:72:ARG:HD3	2:C:112:GLU:OE1	1.62	0.99
3:D:772:PRO:HD2	3:D:776:GLU:O	1.62	0.99
3:D:1236:LEU:HB2	3:D:1256:LEU:HB2	1.45	0.99
2:C:755:LEU:HD12	2:C:790:LEU:HD23	1.41	0.99
3:D:1141:GLU:HA	3:D:1171:VAL:HG11	1.42	0.98
3:D:1353:GLN:HE21	3:D:1368:ILE:HD11	1.24	0.98
3:D:1092:GLY:HA2	3:D:1096:ARG:HE	1.29	0.98
3:D:860:LEU:HA	3:D:877:PRO:HG2	1.43	0.98
1:A:143:ARG:HE	1:A:159:LYS:HE2	1.24	0.98
2:C:110:GLU:HG2	2:C:369:PRO:HG2	1.44	0.98
3:D:483:HIS:H	3:D:484:PRO:CD	1.75	0.98
3:D:699:VAL:HB	3:D:716:PHE:O	1.63	0.97
3:D:721:VAL:HG12	3:D:722:GLU:H	1.28	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1055:ILE:H	2:C:1055:ILE:HD12	1.26	0.97
2:C:384:GLU:O	2:C:388:ARG:HB2	1.65	0.97
3:D:89:ARG:C	3:D:520:LEU:HD21	1.85	0.97
1:A:96:SER:CB	1:A:145:ASP:HA	1.95	0.97
2:C:567:GLN:HB2	2:C:997:LEU:HD22	1.44	0.96
2:C:946:ARG:HE	3:D:861:GLN:HE22	1.10	0.96
3:D:836:VAL:O	3:D:865:THR:HG23	1.65	0.96
1:B:106:PRO:HA	1:B:133:GLU:HA	1.46	0.96
2:C:159:ILE:HD11	2:C:310:LEU:HB2	1.48	0.96
2:C:195:LEU:HD13	2:C:227:LEU:HD13	1.48	0.96
2:C:497:ALA:HA	2:C:502:PRO:HG3	1.47	0.96
2:C:165:LEU:HD22	2:C:334:ARG:HD3	1.48	0.95
2:C:710:ILE:HG13	2:C:790:LEU:HD13	1.46	0.95
3:D:1310:ARG:HA	3:D:1323:GLN:O	1.66	0.94
3:D:483:HIS:HA	3:D:489:ARG:HG3	1.49	0.94
2:C:438:ILE:HD13	2:C:470:PRO:HD3	1.49	0.94
2:C:1001:VAL:HG11	3:D:724:GLN:HB3	1.49	0.94
3:D:1251:ASP:H	3:D:1269:LYS:HZ2	0.99	0.93
1:B:106:PRO:HB3	1:B:133:GLU:HG3	1.51	0.93
2:C:1038:TRP:NE1	3:D:1099:VAL:HG11	1.82	0.93
3:D:639:LEU:H	3:D:729:HIS:CD2	1.83	0.93
3:D:899:LEU:O	3:D:900:ILE:HG13	1.66	0.93
3:D:1336:LEU:HB2	3:D:1344:VAL:HG21	1.49	0.93
1:B:26:GLU:HB3	1:B:27:PRO:HD3	1.48	0.93
3:D:857:LEU:HD12	3:D:858:LEU:H	1.34	0.93
3:D:1118:ILE:HD13	3:D:1190:SER:HB3	1.51	0.93
2:C:585:GLU:HG2	2:C:665:PHE:HE2	1.33	0.92
2:C:710:ILE:HD11	2:C:790:LEU:CD2	1.97	0.92
2:C:115:LEU:HD12	2:C:116:GLY:N	1.83	0.92
1:A:30:ARG:H	1:A:30:ARG:HD3	1.35	0.92
2:C:690:ILE:CB	2:C:852:ILE:HG22	1.99	0.92
3:D:1236:LEU:HD11	3:D:1356:TYR:HE2	1.31	0.92
1:B:25:LEU:HD11	1:B:28:LEU:HD11	1.51	0.92
2:C:946:ARG:HE	3:D:861:GLN:NE2	1.67	0.92
2:C:613:VAL:HG13	2:C:620:LEU:H	1.33	0.92
3:D:806:PHE:H	3:D:827:ILE:HA	1.35	0.92
2:C:198:ARG:HG2	2:C:228:ALA:HA	1.52	0.92
2:C:585:GLU:HG2	2:C:665:PHE:CE2	2.05	0.91
1:A:38:ASN:ND2	2:C:980:GLY:HA2	1.84	0.91
3:D:699:VAL:H	3:D:756:GLN:NE2	1.68	0.91
3:D:900:ILE:HG22	3:D:902:MET:H	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:HB3	1:A:41:ARG:NH1	1.85	0.91
3:D:1382:THR:HG21	3:D:1418:LYS:HE3	1.52	0.91
1:A:197:LEU:HD23	1:A:197:LEU:H	1.35	0.91
3:D:1147:ARG:NH1	3:D:1190:SER:HB2	1.86	0.91
2:C:605:LYS:HG2	2:C:607:ASP:H	1.33	0.90
2:C:749:VAL:HG11	2:C:792:VAL:HG21	1.53	0.90
2:C:852:ILE:HD13	2:C:852:ILE:N	1.84	0.90
3:D:615:ARG:HA	3:D:618:LEU:HD12	1.52	0.90
3:D:728:LEU:HD22	3:D:745:MET:HE1	1.52	0.90
3:D:860:LEU:C	3:D:862:ASP:H	1.69	0.90
2:C:31:GLN:OE1	2:C:39:ARG:HB3	1.71	0.90
2:C:203:ASP:O	2:C:206:THR:HG22	1.72	0.90
3:D:483:HIS:N	3:D:484:PRO:HD2	1.86	0.90
2:C:564:MET:SD	2:C:840:ALA:HB1	2.12	0.90
3:D:552:ASN:HA	3:D:555:LYS:HB3	1.53	0.90
3:D:643:GLY:HA3	3:D:727:GLN:H	1.37	0.90
3:D:1278:ASP:HA	3:D:1318:TYR:HA	1.54	0.90
2:C:256:TYR:HA	2:C:260:LEU:HD13	1.54	0.89
4:E:31:LEU:HD12	4:E:35:PHE:HA	1.54	0.89
3:D:901:GLN:HB2	3:D:905:PRO:HG3	1.52	0.89
1:A:88:ARG:HD3	1:A:121:GLU:OE2	1.72	0.89
1:A:15:THR:HG22	1:B:230:ALA:HB1	1.53	0.89
1:A:160:ASP:O	1:A:162:ILE:HG22	1.72	0.89
3:D:1321:ALA:O	3:D:1323:GLN:N	2.05	0.89
2:C:99:GLN:HB3	2:C:109:LYS:HG2	1.54	0.89
3:D:1253:THR:HA	3:D:1258:ARG:HD2	1.53	0.89
2:C:246:ASP:HB3	2:C:247:PRO:HD2	1.54	0.89
2:C:1103:ASP:HB2	2:C:1108:PRO:HB2	1.55	0.89
3:D:1008:PHE:HE1	3:D:1035:ILE:HG13	1.37	0.89
3:D:1231:GLU:HB3	3:D:1232:PRO:HD3	1.53	0.89
2:C:1095:LEU:HD12	3:D:603:LEU:HD23	1.55	0.89
1:B:78:ILE:HG13	1:B:130:ALA:HB2	1.52	0.89
2:C:159:ILE:HD13	2:C:306:THR:HG23	1.55	0.89
2:C:260:LEU:O	2:C:261:LEU:HD23	1.73	0.89
3:D:631:ILE:HD13	3:D:745:MET:HE2	1.55	0.88
1:A:72:LYS:HA	2:C:607:ASP:HB3	1.55	0.88
3:D:1024:ALA:HA	3:D:1028:ALA:HB3	1.51	0.88
2:C:110:GLU:CG	2:C:369:PRO:HG2	2.03	0.88
2:C:701:THR:HG22	2:C:832:LYS:HA	1.56	0.88
2:C:1017:THR:O	2:C:1018:GLN:HB2	1.71	0.88
2:C:257:LEU:HD23	2:C:261:LEU:HD21	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:726:ILE:HD12	2:C:726:ILE:H	1.37	0.88
3:D:699:VAL:H	3:D:756:GLN:HE22	1.19	0.88
2:C:631:SER:HB2	2:C:635:THR:H	1.36	0.88
2:C:605:LYS:HA	2:C:612:ALA:HB3	1.53	0.88
2:C:32:ALA:HA	2:C:71:TYR:HE1	1.38	0.87
2:C:493:ARG:HH12	3:D:1069:GLU:HA	1.36	0.87
2:C:889:HIS:CE1	3:D:951:ILE:H	1.92	0.87
3:D:1015:TYR:CB	3:D:1019:PRO:HD3	2.05	0.87
2:C:588:VAL:O	2:C:588:VAL:HG12	1.74	0.87
3:D:1043:GLY:HA2	3:D:1057:VAL:HG23	1.54	0.87
2:C:290:LEU:HD11	2:C:298:PHE:HB3	1.56	0.87
3:D:704:ARG:HH12	3:D:743:ASP:CG	1.78	0.87
2:C:551:GLU:HA	2:C:906:PHE:HE2	1.39	0.87
2:C:762:LYS:HD2	2:C:786:LYS:HD2	1.56	0.87
4:E:78:ASN:OD1	4:E:79:LEU:HG	1.73	0.87
2:C:674:VAL:HB	2:C:869:VAL:HG13	1.56	0.87
2:C:1040:LEU:HD12	2:C:1045:ALA:HB3	1.57	0.87
3:D:783:ARG:O	3:D:784:ASP:HB2	1.71	0.87
1:A:79:ILE:HD11	1:A:165:ILE:HD12	1.57	0.87
1:B:211:LEU:O	1:B:215:VAL:HG23	1.74	0.86
2:C:892:LEU:H	2:C:892:LEU:CD2	1.88	0.86
3:D:1466:VAL:O	3:D:1469:GLY:N	2.08	0.86
2:C:15:LEU:HD11	2:C:461:VAL:HG21	1.57	0.86
2:C:396:ASP:OD1	2:C:402:SER:HB3	1.75	0.86
3:D:129:PHE:HA	3:D:454:ALA:CB	2.05	0.86
1:A:79:ILE:HD11	1:A:165:ILE:CD1	2.05	0.86
2:C:1008:ARG:HD3	2:C:1029:GLY:N	1.91	0.86
3:D:1019:PRO:C	3:D:1021:TYR:H	1.77	0.86
1:A:59:GLU:HG2	1:A:137:LYS:HE3	1.56	0.86
2:C:115:LEU:CD1	2:C:116:GLY:H	1.89	0.86
3:D:1194:CYS:HB3	3:D:1373:ARG:NH2	1.90	0.86
3:D:890:VAL:HG12	3:D:891:GLY:N	1.90	0.86
2:C:1052:MET:O	2:C:1053:LEU:HD13	1.74	0.86
2:C:569:VAL:HG13	2:C:569:VAL:O	1.73	0.86
2:C:9:ILE:HG22	2:C:10:ARG:N	1.89	0.85
1:A:131:THR:HG23	2:C:644:ARG:NH2	1.91	0.85
3:D:1043:GLY:HA3	3:D:1057:VAL:H	1.41	0.85
1:A:88:ARG:HB3	1:A:121:GLU:HB2	1.56	0.85
1:B:214:ALA:HA	1:B:217:ILE:HD12	1.55	0.85
2:C:959:PRO:HG2	2:C:960:GLU:H	1.41	0.85
3:D:876:SER:N	3:D:879:ARG:HG3	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:890:VAL:HG11	3:D:922:LEU:HD13	1.59	0.85
3:D:1132:LEU:HD13	3:D:1184:ARG:HH12	1.41	0.85
3:D:1261:GLU:CD	3:D:1268:PRO:HB3	1.97	0.85
2:C:323:ASP:C	2:C:325:ILE:H	1.79	0.85
2:C:642:ARG:HG2	2:C:643:VAL:HG23	1.56	0.85
3:D:113:ALA:HB2	3:D:495:ARG:HH22	1.38	0.85
3:D:855:HIS:H	3:D:855:HIS:CD2	1.93	0.85
2:C:443:THR:HG21	2:C:454:SER:HB2	1.56	0.84
3:D:1047:LYS:HA	3:D:1053:PHE:CE1	2.12	0.84
2:C:162:ILE:HG13	2:C:171:TRP:CZ3	2.11	0.84
2:C:613:VAL:CG2	2:C:619:ARG:HG2	2.06	0.84
3:D:1280:VAL:HG12	3:D:1281:VAL:CG2	2.08	0.84
2:C:12:VAL:HG12	2:C:13:ILE:N	1.90	0.84
3:D:502:PHE:HE1	3:D:1452:ILE:HG13	1.41	0.84
3:D:772:PRO:HG3	3:D:778:LEU:CB	2.07	0.84
3:D:1147:ARG:HH12	3:D:1190:SER:HB2	1.42	0.84
1:A:143:ARG:HE	1:A:159:LYS:CE	1.90	0.84
2:C:852:ILE:HD13	2:C:852:ILE:H	1.37	0.84
1:B:98:THR:HG22	1:B:99:LEU:N	1.92	0.84
2:C:882:LEU:N	2:C:882:LEU:HD23	1.91	0.84
2:C:89:THR:O	2:C:91:GLN:HG3	1.78	0.84
2:C:440:PRO:HB3	2:C:541:SER:HB3	1.58	0.84
2:C:843:HIS:CD2	2:C:884:GLN:HA	2.13	0.84
2:C:278:GLU:HG3	2:C:284:GLY:H	1.43	0.83
2:C:324:ASP:O	2:C:326:ASP:N	2.10	0.83
2:C:1008:ARG:CZ	2:C:1020:PRO:HB3	2.07	0.83
1:B:86:VAL:HG23	1:B:124:ASN:ND2	1.92	0.83
2:C:13:ILE:HG22	2:C:15:LEU:H	1.43	0.83
3:D:879:ARG:NE	3:D:904:VAL:HG22	1.94	0.83
2:C:198:ARG:CG	2:C:228:ALA:HA	2.08	0.83
2:C:333:ILE:HD11	2:C:468:ARG:NE	1.92	0.83
2:C:352:ALA:HA	2:C:355:VAL:HG12	1.59	0.83
2:C:1107:ASN:N	2:C:1108:PRO:HD3	1.93	0.83
3:D:879:ARG:CD	3:D:904:VAL:HG22	2.07	0.83
3:D:1450:ALA:HA	3:D:1455:LYS:HG3	1.61	0.83
2:C:58:ASP:CB	2:C:61:LYS:HG3	2.09	0.83
2:C:672:VAL:HG22	2:C:868:ASP:OD2	1.77	0.83
1:A:131:THR:O	1:A:131:THR:HG22	1.79	0.83
3:D:465:LEU:HD23	3:D:509:PRO:HB3	1.59	0.83
3:D:908:LYS:HG3	3:D:1027:GLY:CA	2.07	0.83
3:D:1015:TYR:HB3	3:D:1018:ASN:HB2	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:38:THR:HG22	4:E:40:LEU:H	1.43	0.83
2:C:1051:GLU:HG2	2:C:1056:LYS:HE2	1.58	0.83
3:D:590:PRO:HB3	3:D:599:PRO:HA	1.60	0.83
3:D:860:LEU:C	3:D:862:ASP:N	2.32	0.83
3:D:1011:PHE:HA	3:D:1014:ASN:O	1.76	0.83
4:E:9:LEU:HA	4:E:12:MET:HE2	1.59	0.83
3:D:511:TRP:O	3:D:512:MET:HG3	1.79	0.83
1:A:143:ARG:NE	1:A:159:LYS:HE2	1.94	0.82
2:C:875:GLY:HA2	2:C:879:ARG:HG3	1.61	0.82
3:D:1003:VAL:O	3:D:1007:VAL:HG12	1.79	0.82
3:D:1107:VAL:HG21	3:D:1215:VAL:HG11	1.61	0.82
3:D:1282:ARG:CG	3:D:1293:PHE:HB2	2.10	0.82
3:D:900:ILE:HG22	3:D:902:MET:N	1.94	0.82
3:D:1154:GLU:HA	3:D:1159:ARG:HA	1.61	0.82
2:C:924:LEU:N	2:C:924:LEU:HD23	1.94	0.82
2:C:1012:PRO:HB3	2:C:1023:GLY:HA3	1.58	0.82
3:D:792:ILE:HG21	3:D:881:LEU:HD23	1.60	0.82
1:B:25:LEU:HD11	1:B:28:LEU:HD21	1.59	0.82
3:D:1213:ARG:HG3	3:D:1214:PRO:N	1.95	0.82
1:B:103:ALA:HB3	1:B:137:LYS:O	1.80	0.82
3:D:521:PRO:CG	3:D:522:PRO:HD3	2.09	0.82
4:E:48:MET:HG2	4:E:49:ARG:H	1.45	0.82
2:C:110:GLU:H	2:C:369:PRO:HG3	1.44	0.82
3:D:1251:ASP:H	3:D:1269:LYS:NZ	1.76	0.82
3:D:1376:LEU:HD11	3:D:1421:LEU:HD12	1.62	0.82
3:D:1250:THR:HG23	3:D:1269:LYS:HD3	1.61	0.82
2:C:564:MET:SD	2:C:846:LYS:HB3	2.20	0.82
2:C:695:LEU:HD21	2:C:833:LEU:HB3	1.60	0.82
3:D:1403:LEU:HD21	3:D:1415:VAL:H	1.44	0.82
2:C:15:LEU:HD21	2:C:461:VAL:CG2	2.09	0.81
3:D:890:VAL:HG11	3:D:922:LEU:CD1	2.08	0.81
3:D:731:LEU:HD11	3:D:931:LEU:HD12	1.61	0.81
2:C:32:ALA:HA	2:C:71:TYR:CE1	2.14	0.81
3:D:1277:ILE:HD12	3:D:1294:VAL:HG12	1.61	0.81
1:B:151:VAL:HG23	1:B:169:ALA:HB3	1.62	0.81
2:C:604:VAL:HG11	2:C:619:ARG:NH2	1.94	0.81
2:C:1030:GLN:O	3:D:622:ARG:HA	1.79	0.81
2:C:1005:MET:O	2:C:1005:MET:HG3	1.80	0.81
3:D:1096:ARG:HH11	3:D:1096:ARG:HG3	1.42	0.81
2:C:260:LEU:HD23	2:C:261:LEU:N	1.95	0.81
2:C:836:GLY:HA3	2:C:1001:VAL:CG2	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1119:SER:HB3	3:D:1185:GLU:HB3	1.62	0.81
2:C:892:LEU:H	2:C:892:LEU:HD22	1.46	0.81
3:D:582:ILE:O	3:D:584:ASN:N	2.14	0.81
2:C:376:ARG:N	2:C:377:PRO:HD2	1.95	0.81
3:D:1037:GLN:HG3	3:D:1042:ARG:HG2	1.63	0.81
3:D:1403:LEU:O	3:D:1407:LEU:HB2	1.81	0.81
1:A:10:VAL:HB	1:A:26:GLU:CG	2.11	0.81
1:A:180:GLN:HE21	2:C:934:PHE:HB3	1.45	0.81
1:B:109:VAL:O	1:B:129:ILE:HB	1.80	0.81
2:C:467:ILE:CG2	2:C:484:VAL:HG21	2.11	0.81
2:C:589:ARG:HH21	2:C:654:LEU:HD12	1.45	0.81
3:D:1459:LEU:HB3	3:D:1465:ASN:HD22	1.46	0.81
2:C:1053:LEU:HD12	3:D:621:LYS:HD2	1.63	0.80
3:D:882:PHE:HA	3:D:885:ILE:HD12	1.63	0.80
3:D:1258:ARG:CZ	3:D:1262:LEU:HD11	2.11	0.80
2:C:136:ILE:HG21	2:C:336:VAL:HG13	1.60	0.80
3:D:969:ARG:HG3	3:D:970:LYS:N	1.95	0.80
2:C:969:LEU:HD11	3:D:952:ASP:H	1.42	0.80
1:A:158:ILE:HG23	1:A:159:LYS:H	1.45	0.80
1:B:26:GLU:HB3	1:B:27:PRO:CD	2.11	0.80
1:B:41:ARG:HD3	1:B:42:ARG:N	1.96	0.80
2:C:216:ASP:O	2:C:218:VAL:HG23	1.80	0.80
2:C:671:ASN:HA	2:C:993:PHE:HA	1.62	0.80
2:C:889:HIS:HE1	3:D:951:ILE:H	1.26	0.80
3:D:968:ASP:O	3:D:970:LYS:N	2.14	0.80
2:C:613:VAL:HG12	2:C:614:ARG:N	1.96	0.80
3:D:795:VAL:HG13	3:D:864:VAL:CG2	2.10	0.80
2:C:580:MET:HB2	2:C:584:GLU:OE1	1.81	0.80
2:C:261:LEU:CG	2:C:263:ASP:HB3	2.12	0.80
2:C:572:ILE:O	2:C:573:ARG:HB2	1.81	0.80
2:C:84:ARG:HA	2:C:131:GLY:HA2	1.64	0.80
2:C:108:ILE:HD13	2:C:368:THR:HG22	1.64	0.80
2:C:654:LEU:O	2:C:655:LEU:HB3	1.81	0.80
3:D:881:LEU:O	3:D:885:ILE:HG13	1.82	0.80
1:A:24:VAL:HG12	1:A:25:LEU:O	1.82	0.80
2:C:1005:MET:HB2	3:D:629:SER:HB2	1.63	0.80
3:D:1062:ARG:HH11	3:D:1062:ARG:HG3	1.45	0.80
3:D:1086:LEU:HD13	3:D:1238:MET:HB2	1.63	0.80
3:D:1351:GLU:OE1	3:D:1354:LYS:HD2	1.82	0.80
2:C:9:ILE:HG22	2:C:10:ARG:H	1.47	0.80
3:D:890:VAL:CG1	3:D:922:LEU:HD13	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1067:VAL:HG12	3:D:1069:GLU:HB2	1.64	0.80
2:C:149:THR:OG1	2:C:323:ASP:HA	1.82	0.79
2:C:460:ARG:NH1	2:C:464:LEU:HD21	1.97	0.79
2:C:631:SER:HB2	2:C:635:THR:N	1.96	0.79
3:D:772:PRO:HD3	3:D:778:LEU:H	1.47	0.79
3:D:886:VAL:CG1	3:D:900:ILE:HD11	2.12	0.79
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.63	0.79
2:C:147:TYR:O	2:C:322:VAL:HG13	1.83	0.79
3:D:876:SER:H	3:D:879:ARG:CG	1.95	0.79
2:C:290:LEU:HD12	2:C:291:VAL:H	1.45	0.79
3:D:1378:TYR:HE2	3:D:1431:THR:HB	1.45	0.79
2:C:149:THR:HB	2:C:158:TYR:HE1	1.46	0.79
2:C:440:PRO:HG3	2:C:454:SER:H	1.46	0.79
2:C:921:ALA:H	2:C:924:LEU:HD21	1.47	0.79
3:D:1459:LEU:CD1	3:D:1470:ARG:HH11	1.96	0.79
2:C:140:ILE:CG2	2:C:333:ILE:HG12	2.12	0.79
2:C:474:VAL:HG13	2:C:529:VAL:O	1.83	0.79
3:D:113:ALA:HB2	3:D:495:ARG:NH2	1.98	0.79
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.64	0.79
1:A:163:ASN:O	1:A:165:ILE:HG23	1.82	0.79
2:C:478:VAL:O	2:C:479:VAL:HG13	1.81	0.79
2:C:613:VAL:HG11	2:C:619:ARG:CG	2.12	0.79
2:C:452:ILE:HG21	5:C:1640:RFP:O11	1.82	0.79
2:C:807:ARG:O	2:C:810:ASP:HB2	1.83	0.79
3:D:721:VAL:HG12	3:D:722:GLU:N	1.98	0.79
2:C:839:LEU:HD12	2:C:994:ILE:CG2	2.12	0.79
3:D:1483:PHE:CZ	4:E:18:ARG:HG3	2.17	0.79
2:C:531:PHE:O	2:C:532:MET:HB2	1.82	0.79
2:C:163:ILE:HG22	2:C:164:PRO:HD2	1.65	0.78
2:C:577:PRO:HG2	2:C:580:MET:HB3	1.65	0.78
3:D:728:LEU:HD22	3:D:745:MET:CE	2.13	0.78
3:D:1207:TYR:HA	3:D:1213:ARG:O	1.82	0.78
2:C:873:PRO:HG2	2:C:874:LEU:H	1.46	0.78
2:C:862:PRO:HA	2:C:975:TYR:HE1	1.48	0.78
1:A:222:LEU:HD12	1:B:215:VAL:HG13	1.63	0.78
2:C:399:ASN:C	2:C:399:ASN:ND2	2.36	0.78
2:C:690:ILE:HB	2:C:852:ILE:CG2	2.08	0.78
2:C:952:LEU:HD23	2:C:966:LEU:HD11	1.65	0.78
3:D:1160:LEU:HD22	3:D:1164:ARG:NH1	1.98	0.78
3:D:1196:THR:HB	3:D:1199:GLY:O	1.84	0.78
1:B:44:LEU:O	1:B:174:VAL:HG21	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:225:ALA:O	2:C:229:MET:HG2	1.84	0.78
2:C:401:LEU:HD21	2:C:543:ASN:HB3	1.64	0.78
3:D:1019:PRO:HB2	3:D:1022:VAL:CG2	2.14	0.78
1:B:169:ALA:HB1	1:B:171:PHE:CZ	2.19	0.78
2:C:666:LEU:HD11	2:C:668:LEU:HD21	1.66	0.78
3:D:765:SER:O	3:D:769:LEU:HB2	1.83	0.78
3:D:947:ILE:O	3:D:947:ILE:HG13	1.83	0.78
3:D:948:THR:O	3:D:1020:LEU:HB2	1.84	0.78
2:C:533:ASP:HB3	2:C:538:GLN:NE2	1.99	0.78
2:C:602:GLU:H	2:C:647:GLN:HA	1.49	0.78
1:A:20:TYR:O	1:A:207:PRO:HG2	1.82	0.78
1:B:195:LEU:CD1	1:B:197:LEU:HD13	2.14	0.78
2:C:460:ARG:HH11	2:C:464:LEU:HD21	1.48	0.78
2:C:597:ALA:HA	2:C:614:ARG:HH11	1.48	0.78
3:D:1280:VAL:CG1	3:D:1281:VAL:HG23	2.11	0.78
3:D:1484:THR:O	3:D:1486:VAL:HG23	1.83	0.78
1:A:23:PHE:CD2	1:A:211:LEU:HD22	2.19	0.77
1:B:47:SER:O	1:B:48:ILE:HG13	1.84	0.77
3:D:905:PRO:O	3:D:906:GLN:HB2	1.84	0.77
3:D:1459:LEU:HD13	3:D:1470:ARG:HH11	1.47	0.77
2:C:474:VAL:HG22	2:C:530:GLU:CA	2.14	0.77
3:D:1007:VAL:HG21	3:D:1039:CYS:HB2	1.65	0.77
3:D:544:TYR:O	3:D:548:ILE:HG12	1.85	0.77
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.19	0.77
3:D:648:MET:O	3:D:652:LEU:HD23	1.85	0.77
3:D:1205:TYR:HD2	3:D:1215:VAL:HG21	1.49	0.77
2:C:256:TYR:O	2:C:261:LEU:HD22	1.85	0.77
2:C:376:ARG:H	2:C:377:PRO:CD	1.96	0.77
2:C:551:GLU:HA	2:C:906:PHE:CE2	2.18	0.77
2:C:813:VAL:HG12	2:C:815:LEU:HD11	1.64	0.77
3:D:1290:LEU:HB2	3:D:1305:LEU:O	1.85	0.77
1:A:195:LEU:HD23	1:A:196:THR:H	1.49	0.77
2:C:460:ARG:HD2	2:C:464:LEU:HD22	1.67	0.77
2:C:475:LYS:O	2:C:477:GLY:N	2.18	0.77
2:C:966:LEU:HD11	2:C:986:PRO:HG3	1.66	0.77
3:D:1282:ARG:HG2	3:D:1293:PHE:HB2	1.64	0.77
2:C:159:ILE:CG1	2:C:310:LEU:HD13	2.14	0.77
2:C:333:ILE:CD1	2:C:468:ARG:HE	1.97	0.77
2:C:944:LEU:HD21	2:C:963:LEU:HD22	1.66	0.77
3:D:547:LEU:HD13	3:D:577:ALA:O	1.85	0.77
1:A:109:VAL:HG23	1:A:130:ALA:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:13:ILE:CG2	2:C:15:LEU:H	1.98	0.77
2:C:493:ARG:NH1	3:D:1069:GLU:HA	2.00	0.77
2:C:1054:THR:HB	2:C:1055:ILE:HD12	1.67	0.77
3:D:731:LEU:CD1	3:D:931:LEU:HD12	2.15	0.77
1:A:173:PRO:O	1:A:202:ASP:HA	1.85	0.76
2:C:256:TYR:C	2:C:260:LEU:HB3	2.06	0.76
2:C:257:LEU:HD22	2:C:264:PRO:HG3	1.67	0.76
2:C:274:ARG:HE	2:C:275:TYR:HE1	1.31	0.76
2:C:810:ASP:OD1	2:C:811:PRO:HD2	1.85	0.76
2:C:969:LEU:HD21	3:D:952:ASP:HB2	1.66	0.76
3:D:465:LEU:HD22	3:D:512:MET:SD	2.26	0.76
3:D:822:ALA:HA	3:D:832:ARG:HB3	1.65	0.76
2:C:163:ILE:H	2:C:163:ILE:HD12	1.47	0.76
2:C:890:LEU:O	2:C:890:LEU:HG	1.85	0.76
3:D:855:HIS:H	3:D:855:HIS:HD2	1.30	0.76
1:B:98:THR:CG2	1:B:99:LEU:N	2.48	0.76
2:C:437:ARG:HB3	3:D:1071:PHE:CE1	2.20	0.76
2:C:963:LEU:HD12	2:C:972:VAL:HG22	1.65	0.76
3:D:1043:GLY:CA	3:D:1057:VAL:HG23	2.15	0.76
3:D:1376:LEU:CD1	3:D:1421:LEU:HD12	2.16	0.76
3:D:1481:VAL:O	3:D:1482:ARG:HG3	1.85	0.76
2:C:79:SER:OG	2:C:82:GLU:HB2	1.86	0.76
2:C:139:GLN:CD	2:C:334:ARG:HH21	1.88	0.76
3:D:767:HIS:CE1	4:E:6:ILE:HG13	2.20	0.76
3:D:795:VAL:H	3:D:862:ASP:CB	1.99	0.76
3:D:1252:ILE:O	3:D:1258:ARG:HB2	1.85	0.76
2:C:181:VAL:HG12	2:C:182:VAL:HG23	1.67	0.76
2:C:398:THR:OG1	2:C:633:GLN:HG3	1.86	0.76
2:C:1016:ILE:HD12	3:D:536:ALA:HA	1.66	0.76
1:A:41:ARG:NE	2:C:860:HIS:NE2	2.34	0.76
2:C:605:LYS:CA	2:C:612:ALA:HB3	2.16	0.76
3:D:1103:HIS:C	3:D:1105:ILE:H	1.89	0.76
3:D:1273:VAL:H	3:D:1324:PRO:HG3	1.51	0.76
3:D:1273:VAL:N	3:D:1324:PRO:HG3	2.01	0.76
3:D:1378:TYR:CD1	3:D:1422:MET:HG3	2.20	0.76
1:A:215:VAL:O	1:A:219:LYS:HG3	1.85	0.76
2:C:348:LEU:HD12	2:C:378:LEU:HD11	1.67	0.76
3:D:691:LEU:H	3:D:691:LEU:CD1	1.98	0.76
3:D:806:PHE:HA	3:D:827:ILE:O	1.86	0.76
3:D:1156:LEU:HD12	3:D:1177:ALA:HA	1.68	0.76
2:C:208:VAL:CG1	2:C:218:VAL:HG11	2.12	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:387:SER:O	2:C:388:ARG:HG3	1.85	0.75
3:D:1126:ASP:OD1	3:D:1128:VAL:HB	1.86	0.75
3:D:1443:THR:HG22	3:D:1447:LEU:HD22	1.67	0.75
1:A:197:LEU:H	1:A:197:LEU:CD2	1.98	0.75
2:C:80:GLN:O	2:C:81:ASP:HB2	1.84	0.75
3:D:506:GLY:O	3:D:507:ASN:HB3	1.86	0.75
3:D:518:PRO:HB3	3:D:544:TYR:CE1	2.21	0.75
3:D:790:TYR:CE2	3:D:906:GLN:HB3	2.22	0.75
3:D:1235:GLN:O	3:D:1236:LEU:HD23	1.87	0.75
1:A:35:THR:HG21	1:B:43:ILE:HD11	1.67	0.75
1:A:72:LYS:CA	2:C:607:ASP:HB3	2.17	0.75
1:B:103:ALA:HB1	1:B:132:LEU:HD11	1.67	0.75
1:B:199:ILE:HG23	1:B:201:THR:HG23	1.68	0.75
2:C:710:ILE:N	2:C:710:ILE:HD12	2.01	0.75
2:C:1053:LEU:CD1	3:D:621:LYS:HD2	2.15	0.75
2:C:440:PRO:HD3	2:C:455:LEU:N	2.02	0.75
3:D:865:THR:HG22	3:D:866:THR:N	2.01	0.75
1:A:39:PRO:O	1:A:43:ILE:HG12	1.86	0.75
1:B:100:ILE:HG23	1:B:141:GLU:HG2	1.69	0.75
2:C:239:PHE:CE1	2:C:254:LEU:HD23	2.22	0.75
2:C:659:PRO:O	2:C:660:ALA:HB2	1.85	0.75
2:C:748:GLU:HA	2:C:799:ILE:HA	1.66	0.75
3:D:1481:VAL:CG1	4:E:21:VAL:HG21	2.17	0.75
1:B:78:ILE:CG1	1:B:130:ALA:HB2	2.16	0.75
2:C:730:SER:HA	2:C:734:LEU:HD11	1.67	0.75
3:D:626:SER:HA	3:D:652:LEU:HD11	1.68	0.75
3:D:881:LEU:HG	3:D:885:ILE:HD11	1.68	0.75
3:D:1283:ILE:HG12	3:D:1292:VAL:HG22	1.69	0.75
4:E:40:LEU:C	4:E:42:PRO:HD2	2.06	0.75
2:C:251:ASP:O	2:C:252:LYS:HB3	1.84	0.75
2:C:438:ILE:HD12	2:C:484:VAL:HG22	1.69	0.75
2:C:705:ILE:H	2:C:705:ILE:HD12	1.51	0.75
3:D:855:HIS:O	3:D:857:LEU:N	2.20	0.75
1:B:33:GLY:O	1:B:195:LEU:HD23	1.87	0.75
3:D:100:ALA:HB1	3:D:579:ASP:OD1	1.87	0.75
3:D:968:ASP:O	3:D:971:LEU:N	2.19	0.75
1:B:214:ALA:HA	1:B:217:ILE:CD1	2.17	0.75
2:C:17:PRO:O	2:C:18:LEU:HB2	1.86	0.75
3:D:1047:LYS:HB3	3:D:1048:PRO:HD2	1.69	0.75
1:B:98:THR:HG23	1:B:142:VAL:O	1.87	0.74
3:D:1069:GLU:HG3	3:D:1072:ILE:HD13	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1280:VAL:HG12	3:D:1281:VAL:N	2.02	0.74
3:D:1282:ARG:O	3:D:1283:ILE:HG13	1.87	0.74
1:A:101:LEU:HD12	1:A:102:ARG:N	2.01	0.74
2:C:958:SER:O	2:C:962:GLN:HG3	1.85	0.74
3:D:1092:GLY:HA2	3:D:1096:ARG:NE	2.01	0.74
2:C:168:ARG:NH2	2:C:266:ARG:HG2	2.03	0.74
3:D:827:ILE:O	3:D:828:VAL:HG23	1.87	0.74
3:D:1031:ASN:O	3:D:1035:ILE:HG12	1.88	0.74
3:D:1322:GLY:O	3:D:1323:GLN:HB2	1.86	0.74
1:B:178:ALA:HB3	1:B:198:ARG:HE	1.52	0.74
2:C:106:GLY:O	2:C:107:LEU:HD23	1.86	0.74
2:C:260:LEU:HD23	2:C:261:LEU:HB3	1.68	0.74
2:C:571:LEU:HD22	2:C:670:GLN:HG3	1.70	0.74
3:D:1150:ALA:HB2	3:D:1189:ARG:HG2	1.67	0.74
3:D:1459:LEU:HB3	3:D:1465:ASN:ND2	2.01	0.74
2:C:401:LEU:HD21	2:C:543:ASN:CB	2.16	0.74
3:D:675:ARG:HA	3:D:678:GLU:HB2	1.69	0.74
3:D:752:SER:O	3:D:754:PHE:N	2.21	0.74
1:A:89:PHE:O	1:A:119:ASP:HB3	1.86	0.74
1:A:94:MET:CE	1:A:119:ASP:HB2	2.17	0.74
2:C:148:PHE:O	2:C:149:THR:HB	1.87	0.74
2:C:305:PRO:O	2:C:308:ARG:HB3	1.88	0.74
2:C:861:LEU:CG	2:C:862:PRO:HD2	2.10	0.74
2:C:911:GLU:O	2:C:915:LYS:HG2	1.85	0.74
2:C:922:PHE:C	2:C:924:LEU:H	1.89	0.74
1:B:25:LEU:HD11	1:B:28:LEU:CD1	2.16	0.74
2:C:290:LEU:HA	2:C:300:ASP:HA	1.68	0.74
2:C:328:LEU:O	2:C:467:ILE:HD13	1.87	0.74
2:C:1030:GLN:HE22	3:D:628:ARG:HD3	1.52	0.74
2:C:256:TYR:O	2:C:260:LEU:HD22	1.87	0.74
3:D:1042:ARG:HG3	3:D:1042:ARG:O	1.87	0.74
3:D:1060:SER:O	3:D:1062:ARG:N	2.19	0.74
3:D:1364:HIS:CG	3:D:1365:ASP:H	2.06	0.74
2:C:710:ILE:CG1	2:C:790:LEU:HD13	2.18	0.74
3:D:795:VAL:HG23	3:D:904:VAL:HG11	1.68	0.74
2:C:34:VAL:HG11	2:C:39:ARG:HG2	1.69	0.74
3:D:639:LEU:N	3:D:729:HIS:CD2	2.56	0.74
3:D:1109:GLU:HG3	3:D:1110:ALA:N	2.02	0.74
2:C:262:ALA:HB1	2:C:266:ARG:CD	2.09	0.73
2:C:290:LEU:HD21	2:C:298:PHE:HD2	1.53	0.73
2:C:355:VAL:HG23	2:C:372:LEU:HB3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:10:ILE:HG13	3:D:11:ALA:H	1.52	0.73
1:A:165:ILE:O	1:A:165:ILE:HG13	1.87	0.73
1:B:174:VAL:HG12	1:B:201:THR:HG21	1.69	0.73
2:C:492:ASP:H	2:C:532:MET:H	1.36	0.73
2:C:755:LEU:HD12	2:C:790:LEU:CD2	2.18	0.73
3:D:519:VAL:HG12	3:D:520:LEU:H	1.50	0.73
3:D:1118:ILE:CD1	3:D:1190:SER:HB3	2.18	0.73
3:D:1275:SER:H	3:D:1322:GLY:HA2	1.52	0.73
2:C:285:LEU:HD23	2:C:286:SER:H	1.53	0.73
2:C:291:VAL:HB	2:C:299:LYS:HG3	1.71	0.73
2:C:613:VAL:HG11	2:C:619:ARG:HG2	1.70	0.73
2:C:727:PRO:HG3	2:C:785:VAL:HG12	1.69	0.73
3:D:1045:MET:HA	3:D:1045:MET:CE	2.18	0.73
1:A:83:LYS:HE2	1:A:168:ASP:HB2	1.70	0.73
2:C:256:TYR:O	2:C:260:LEU:HB3	1.88	0.73
3:D:630:VAL:O	3:D:725:SER:HA	1.86	0.73
1:A:184:THR:O	1:A:185:ARG:HD3	1.89	0.73
2:C:285:LEU:HD11	2:C:302:VAL:HG21	1.70	0.73
2:C:391:LEU:HD22	2:C:415:PRO:CD	2.17	0.73
2:C:753:ASP:O	2:C:791:ARG:HA	1.89	0.73
3:D:1106:VAL:HG21	3:D:1474:ALA:HB2	1.71	0.73
3:D:1281:VAL:HG12	3:D:1282:ARG:N	2.04	0.73
3:D:1338:ALA:O	3:D:1339:LYS:HB2	1.87	0.73
3:D:1481:VAL:HG11	4:E:21:VAL:HG21	1.69	0.73
2:C:129:ILE:CG2	2:C:387:SER:HB2	2.17	0.73
2:C:629:ALA:O	2:C:630:ARG:HD3	1.88	0.73
3:D:1314:LYS:O	3:D:1315:ASP:O	2.07	0.73
3:D:1483:PHE:CE1	4:E:22:VAL:HG23	2.24	0.73
3:D:508:ARG:O	3:D:510:GLU:N	2.21	0.73
2:C:66:LEU:HA	2:C:100:LEU:HA	1.70	0.73
2:C:110:GLU:CB	2:C:369:PRO:HG2	2.19	0.73
2:C:552:HIS:CE1	3:D:1064:GLY:H	2.07	0.73
2:C:553:ASP:OD2	2:C:843:HIS:ND1	2.20	0.73
2:C:1094:ALA:HB1	3:D:603:LEU:HD21	1.71	0.73
3:D:578:VAL:C	3:D:580:ALA:H	1.91	0.73
3:D:790:TYR:CD2	3:D:906:GLN:HB3	2.24	0.73
3:D:879:ARG:HD2	3:D:904:VAL:HG22	1.69	0.73
3:D:1145:TYR:HD2	3:D:1145:TYR:C	1.90	0.73
2:C:363:SER:O	2:C:367:LEU:HG	1.89	0.72
2:C:267:TYR:CD2	2:C:267:TYR:N	2.56	0.72
2:C:795:GLY:O	2:C:797:GLY:N	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1147:ARG:HB3	3:D:1188:VAL:CG2	2.18	0.72
3:D:580:ALA:O	3:D:584:ASN:HB2	1.89	0.72
1:A:90:LEU:HB2	1:A:119:ASP:HB3	1.70	0.72
2:C:676:ILE:O	2:C:677:MET:HB3	1.89	0.72
3:D:893:GLU:O	3:D:894:LYS:HB2	1.88	0.72
1:A:12:THR:HB	1:A:24:VAL:HB	1.71	0.72
2:C:597:ALA:HB2	2:C:655:LEU:HD13	1.69	0.72
2:C:277:ALA:HB1	2:C:281:LEU:HD12	1.70	0.72
2:C:559:LEU:HD12	2:C:560:MET:N	2.04	0.72
2:C:775:ARG:O	2:C:780:GLU:N	2.22	0.72
3:D:879:ARG:CZ	3:D:904:VAL:HA	2.19	0.72
1:A:142:VAL:HG22	1:A:142:VAL:O	1.89	0.72
2:C:421:GLU:HG3	2:C:423:ALA:H	1.54	0.72
2:C:801:VAL:CG2	2:C:828:ALA:HB2	2.18	0.72
1:A:143:ARG:O	1:A:144:VAL:HG13	1.89	0.72
2:C:399:ASN:ND2	2:C:401:LEU:N	2.38	0.72
2:C:897:LEU:HD23	2:C:899:GLN:OE1	1.89	0.72
3:D:865:THR:HG22	3:D:866:THR:H	1.53	0.72
3:D:1281:VAL:CG1	3:D:1282:ARG:H	2.01	0.72
3:D:1402:ALA:HB1	3:D:1415:VAL:HG11	1.72	0.72
1:A:41:ARG:HB3	1:A:41:ARG:HH11	1.54	0.72
1:B:55:SER:HA	1:B:166:PRO:HA	1.70	0.72
2:C:139:GLN:HE22	2:C:416:GLY:HA3	1.53	0.72
2:C:946:ARG:NE	2:C:984:GLU:HB2	2.05	0.72
3:D:1033:GLN:HA	3:D:1036:ARG:HD3	1.72	0.72
3:D:1205:TYR:CD2	3:D:1215:VAL:HG21	2.25	0.72
1:A:42:ARG:HH21	1:B:34:VAL:HB	1.55	0.72
1:A:90:LEU:HD12	1:A:119:ASP:HA	1.69	0.72
3:D:609:GLY:HA2	3:D:615:ARG:CZ	2.19	0.72
3:D:668:PRO:HG2	3:D:672:ALA:CB	2.19	0.72
3:D:1034:GLN:O	3:D:1037:GLN:HB3	1.90	0.72
1:A:162:ILE:HG23	1:A:163:ASN:N	2.05	0.71
2:C:688:ILE:HG23	2:C:871:LEU:HD12	1.70	0.71
2:C:877:PRO:HA	2:C:882:LEU:HD21	1.72	0.71
3:D:1094:LEU:HD22	3:D:1256:LEU:HD11	1.72	0.71
1:B:66:SER:OG	1:B:67:THR:N	2.19	0.71
2:C:710:ILE:CD1	2:C:790:LEU:HD22	2.02	0.71
1:A:212:ASN:O	1:A:215:VAL:HG22	1.89	0.71
2:C:80:GLN:HE22	2:C:122:THR:HG23	1.55	0.71
2:C:253:ALA:O	2:C:254:LEU:HB3	1.90	0.71
2:C:469:THR:HG22	2:C:483:VAL:HA	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1356:TYR:HB3	3:D:1361:VAL:HB	1.70	0.71
2:C:775:ARG:HA	2:C:780:GLU:CB	2.20	0.71
2:C:1012:PRO:CB	2:C:1023:GLY:HA3	2.21	0.71
3:D:756:GLN:O	3:D:760:ARG:HG2	1.90	0.71
3:D:1443:THR:CG2	3:D:1447:LEU:HD22	2.20	0.71
1:A:10:VAL:H	1:A:26:GLU:HB2	1.55	0.71
1:B:174:VAL:HA	1:B:201:THR:HG22	1.72	0.71
2:C:262:ALA:CB	2:C:266:ARG:HD3	2.08	0.71
2:C:921:ALA:N	2:C:924:LEU:HD21	2.05	0.71
2:C:940:GLU:HG2	2:C:973:VAL:HG21	1.73	0.71
3:D:564:GLU:HG3	3:D:568:ARG:HE	1.55	0.71
1:B:82:LEU:HD21	1:B:142:VAL:HG21	1.72	0.71
2:C:166:PRO:HB3	2:C:417:GLY:H	1.56	0.71
2:C:399:ASN:HD21	2:C:401:LEU:HB3	1.56	0.71
2:C:523:ILE:O	2:C:525:ALA:N	2.23	0.71
2:C:525:ALA:CB	2:C:526:PRO:HD2	2.20	0.71
2:C:570:PRO:HB3	2:C:659:PRO:O	1.90	0.71
3:D:705:ALA:HB3	3:D:706:PRO:CD	2.21	0.71
3:D:728:LEU:HD13	3:D:745:MET:HE3	1.73	0.71
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.72	0.71
1:A:75:VAL:HA	1:A:78:ILE:HD12	1.71	0.71
2:C:51:THR:OG1	2:C:348:LEU:HD23	1.91	0.71
2:C:910:THR:HG22	2:C:912:PRO:HD2	1.72	0.71
3:D:691:LEU:HD12	3:D:691:LEU:N	1.98	0.71
3:D:899:LEU:HD13	3:D:899:LEU:N	2.06	0.71
3:D:1486:VAL:HG21	4:E:25:LYS:HZ1	1.55	0.71
1:A:110:ARG:HB2	1:A:126:ASP:O	1.90	0.71
1:B:213:GLN:O	1:B:217:ILE:HG13	1.90	0.71
3:D:688:TRP:O	3:D:690:ALA:N	2.24	0.71
3:D:699:VAL:CB	3:D:716:PHE:O	2.36	0.71
2:C:144:PRO:HA	2:C:162:ILE:CG2	2.21	0.71
2:C:877:PRO:O	2:C:881:ASN:N	2.22	0.71
2:C:939:ARG:HD3	2:C:975:TYR:HE2	1.55	0.71
2:C:1066:ALA:O	2:C:1070:ILE:HD13	1.90	0.71
3:D:486:ARG:HG3	3:D:487:ALA:H	1.55	0.71
3:D:586:ARG:O	3:D:588:GLY:N	2.23	0.71
1:A:47:SER:O	1:A:48:ILE:HG13	1.88	0.70
1:A:112:VAL:O	1:A:114:PHE:N	2.24	0.70
2:C:467:ILE:HG21	2:C:484:VAL:HG21	1.71	0.70
2:C:630:ARG:HA	2:C:705:ILE:HD13	1.73	0.70
3:D:460:ALA:O	3:D:463:GLU:HB3	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1311:LEU:HB2	3:D:1323:GLN:OE1	1.91	0.70
1:A:85:LEU:HA	1:A:124:ASN:HD21	1.55	0.70
1:A:106:PRO:O	1:A:107:LYS:HB3	1.91	0.70
1:B:26:GLU:CB	1:B:27:PRO:HD3	2.20	0.70
2:C:196:LEU:O	2:C:200:LEU:HG	1.91	0.70
2:C:564:MET:HG3	2:C:997:LEU:HD11	1.72	0.70
3:D:571:LYS:C	3:D:573:MET:H	1.94	0.70
3:D:631:ILE:CD1	3:D:745:MET:HE2	2.21	0.70
1:A:30:ARG:HD2	1:A:191:ASP:CB	2.19	0.70
3:D:645:PRO:HD2	3:D:648:MET:SD	2.30	0.70
3:D:899:LEU:HD11	3:D:921:ARG:HD2	1.73	0.70
3:D:1402:ALA:CB	3:D:1415:VAL:HG11	2.22	0.70
3:D:1457:ASP:CG	3:D:1459:LEU:HD23	2.11	0.70
2:C:613:VAL:HG22	2:C:620:LEU:C	2.12	0.70
2:C:801:VAL:HG21	2:C:828:ALA:HB2	1.74	0.70
2:C:922:PHE:HA	2:C:925:TYR:HB3	1.73	0.70
2:C:943:VAL:HG21	2:C:973:VAL:HG13	1.73	0.70
3:D:502:PHE:HE2	3:D:509:PRO:HG3	1.56	0.70
3:D:1281:VAL:HG12	3:D:1282:ARG:H	1.55	0.70
3:D:1432:LYS:HG3	3:D:1433:SER:H	1.55	0.70
2:C:90:TYR:CE2	2:C:120:LEU:HB2	2.27	0.70
3:D:590:PRO:O	3:D:600:LEU:HD11	1.92	0.70
3:D:1145:TYR:C	3:D:1145:TYR:CD2	2.63	0.70
3:D:1273:VAL:CG2	3:D:1324:PRO:HG3	2.18	0.70
2:C:841:ASN:C	2:C:841:ASN:HD22	1.94	0.70
1:A:30:ARG:NH1	1:A:191:ASP:HB2	2.06	0.70
2:C:148:PHE:CZ	2:C:309:TYR:HD2	2.10	0.70
2:C:197:LEU:HD22	2:C:202:TYR:HD1	1.54	0.70
2:C:1099:VAL:HG22	3:D:10:ILE:HD12	1.73	0.70
3:D:688:TRP:C	3:D:690:ALA:H	1.94	0.70
2:C:142:ARG:HG2	2:C:147:TYR:CZ	2.26	0.70
2:C:874:LEU:HD13	3:D:787:LEU:HD22	1.73	0.70
3:D:890:VAL:CG1	3:D:891:GLY:H	1.97	0.70
3:D:890:VAL:HG13	3:D:926:LYS:HE2	1.74	0.70
3:D:1104:GLU:HG2	3:D:1104:GLU:O	1.91	0.70
3:D:1265:ALA:O	3:D:1266:ARG:HG3	1.91	0.70
1:A:66:SER:HB2	1:A:75:VAL:HG21	1.72	0.70
1:B:25:LEU:HD11	1:B:28:LEU:CD2	2.22	0.70
2:C:565:GLN:HG3	2:C:995:MET:CE	2.21	0.70
3:D:1211:MET:CE	4:E:16:LYS:HD2	2.21	0.70
3:D:1431:THR:O	3:D:1432:LYS:HG2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:291:VAL:HG11	2:C:299:LYS:HE2	1.74	0.70
2:C:674:VAL:HG22	2:C:675:ALA:N	2.07	0.70
4:E:26:ARG:NE	4:E:67:GLU:OE2	2.25	0.70
2:C:588:VAL:HG23	2:C:666:LEU:HB2	1.74	0.69
3:D:657:LEU:O	3:D:660:LYS:N	2.24	0.69
3:D:1019:PRO:CB	3:D:1022:VAL:HG23	2.19	0.69
3:D:1403:LEU:HG	3:D:1415:VAL:HB	1.73	0.69
1:B:25:LEU:HD11	1:B:28:LEU:CG	2.23	0.69
1:B:199:ILE:HG23	1:B:201:THR:CG2	2.22	0.69
2:C:177:GLU:HG2	2:C:181:VAL:H	1.55	0.69
2:C:498:GLN:H	2:C:502:PRO:HD3	1.56	0.69
2:C:862:PRO:HA	2:C:975:TYR:CE1	2.27	0.69
2:C:950:LEU:O	3:D:1018:ASN:OD1	2.10	0.69
3:D:587:ARG:HG2	3:D:588:GLY:N	2.07	0.69
3:D:836:VAL:HG11	3:D:858:LEU:HG	1.72	0.69
2:C:312:ALA:HB1	2:C:318:PRO:CG	2.22	0.69
2:C:391:LEU:HD22	2:C:415:PRO:HD2	1.74	0.69
2:C:500:ASN:C	2:C:502:PRO:HD2	2.12	0.69
2:C:536:PRO:HB3	3:D:1068:LEU:HD11	1.75	0.69
3:D:1107:VAL:HG21	3:D:1215:VAL:CG1	2.21	0.69
3:D:1202:GLN:O	3:D:1203:LYS:HB2	1.92	0.69
1:A:206:THR:HB	1:A:209:GLU:HG3	1.75	0.69
2:C:666:LEU:HD11	2:C:668:LEU:CD2	2.22	0.69
1:A:109:VAL:O	1:A:129:ILE:HB	1.93	0.69
2:C:142:ARG:HA	2:C:330:ASN:O	1.91	0.69
2:C:299:LYS:HG3	2:C:299:LYS:O	1.91	0.69
3:D:701:LEU:HD12	3:D:715:ALA:HB2	1.75	0.69
3:D:1108:ARG:O	3:D:1109:GLU:HG2	1.92	0.69
2:C:352:ALA:O	2:C:355:VAL:HG12	1.92	0.69
3:D:552:ASN:HA	3:D:555:LYS:CB	2.22	0.69
3:D:1145:TYR:HD2	3:D:1146:GLY:N	1.91	0.69
1:A:6:LEU:C	1:A:8:ALA:H	1.94	0.69
1:B:179:PHE:HB2	1:B:197:LEU:HD12	1.73	0.69
2:C:889:HIS:C	2:C:891:GLY:H	1.95	0.69
3:D:1270:ALA:CB	3:D:1328:GLY:HA3	2.22	0.69
2:C:126:SER:HB3	2:C:135:VAL:HG13	1.73	0.69
2:C:726:ILE:HD12	2:C:726:ILE:N	2.07	0.69
2:C:796:GLU:HG2	3:D:681:ARG:HH12	1.57	0.69
2:C:1052:MET:HG2	3:D:623:VAL:HG22	1.75	0.69
3:D:42(U):UNK:O	3:D:43(U):UNK:O	2.10	0.69
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1144:LEU:O	3:D:1147:ARG:HG2	1.92	0.69
4:E:59:ASN:ND2	4:E:61:VAL:HG23	2.08	0.69
1:B:59:GLU:O	1:B:60:ASP:HB2	1.93	0.69
2:C:42:VAL:N	2:C:46:ALA:HB2	2.08	0.69
2:C:323:ASP:C	2:C:325:ILE:N	2.47	0.69
2:C:333:ILE:HG21	2:C:460:ARG:HH22	1.58	0.69
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.74	0.69
2:C:683:ASN:HB2	2:C:872:ASN:HB2	1.74	0.69
2:C:1005:MET:HA	3:D:628:ARG:O	1.92	0.69
3:D:1147:ARG:HB3	3:D:1188:VAL:HG22	1.74	0.69
3:D:1251:ASP:C	3:D:1253:THR:H	1.95	0.69
2:C:469:THR:HB	2:C:482:GLU:O	1.93	0.69
3:D:456:MET:HG2	3:D:457:GLY:N	2.08	0.69
3:D:493:ARG:O	3:D:496:LEU:HB3	1.93	0.69
3:D:808:THR:N	3:D:809:PRO:HD3	2.08	0.69
3:D:886:VAL:HG11	3:D:900:ILE:CD1	2.18	0.69
3:D:1201:CYS:SG	3:D:1202:GLN:N	2.65	0.69
4:E:50:THR:O	4:E:52:GLU:N	2.26	0.69
1:A:72:LYS:HG3	2:C:607:ASP:OD1	1.92	0.68
1:B:44:LEU:HG	1:B:199:ILE:HD11	1.74	0.68
2:C:613:VAL:HG21	2:C:619:ARG:CG	2.17	0.68
3:D:115:LEU:C	3:D:117:ASP:H	1.93	0.68
3:D:1104:GLU:HB2	3:D:1461:GLY:HA2	1.75	0.68
4:E:30:LEU:C	4:E:32:ARG:H	1.97	0.68
1:A:105:GLY:N	1:A:136:GLY:HA3	2.07	0.68
2:C:211:LEU:HD22	2:C:304:LEU:HD12	1.75	0.68
2:C:837:ASP:OD2	2:C:837:ASP:N	2.24	0.68
3:D:1014:ASN:O	3:D:1015:TYR:CG	2.47	0.68
3:D:1105:ILE:HD11	3:D:1374:GLN:NE2	2.07	0.68
3:D:1160:LEU:HD22	3:D:1164:ARG:HH12	1.58	0.68
2:C:54:ILE:HD11	2:C:356:ARG:HB2	1.75	0.68
2:C:64:LEU:HD11	2:C:367:LEU:HD12	1.73	0.68
2:C:545:ASN:HB3	2:C:583:LEU:HD12	1.75	0.68
2:C:569:VAL:HG12	2:C:996:LYS:O	1.94	0.68
3:D:765:SER:HB2	3:D:769:LEU:HD12	1.76	0.68
2:C:139:GLN:NE2	2:C:334:ARG:HH21	1.91	0.68
2:C:759:THR:HB	2:C:785:VAL:CG1	2.23	0.68
2:C:881:ASN:N	2:C:881:ASN:ND2	2.42	0.68
2:C:1052:MET:C	2:C:1053:LEU:HD22	2.14	0.68
3:D:1062:ARG:HG3	3:D:1062:ARG:NH1	2.08	0.68
2:C:22:GLN:HE21	2:C:336:VAL:CG2	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:401:LEU:HD13	2:C:587:VAL:HG11	1.74	0.68
2:C:502:PRO:O	2:C:507:ARG:NH2	2.26	0.68
2:C:613:VAL:HG12	2:C:614:ARG:H	1.58	0.68
2:C:660:ALA:O	2:C:667:ALA:N	2.24	0.68
2:C:816:LYS:HD2	2:C:817:PRO:HD2	1.74	0.68
3:D:750:PRO:HG2	3:D:756:GLN:OE1	1.93	0.68
1:A:175:ARG:HB2	1:A:201:THR:HB	1.76	0.68
2:C:142:ARG:NE	2:C:324:ASP:HA	2.08	0.68
2:C:261:LEU:C	2:C:263:ASP:H	1.97	0.68
2:C:852:ILE:N	2:C:852:ILE:CD1	2.57	0.68
2:C:939:ARG:HD3	2:C:975:TYR:CE2	2.29	0.68
2:C:193:LEU:HD13	2:C:193:LEU:O	1.94	0.68
2:C:313:LEU:HD13	2:C:319:GLY:O	1.94	0.68
2:C:770:GLU:O	2:C:774:LEU:HG	1.94	0.68
2:C:1089:VAL:O	2:C:1093:GLN:HG3	1.94	0.68
3:D:112:ILE:O	3:D:114:THR:N	2.26	0.68
3:D:836:VAL:HG11	3:D:858:LEU:CG	2.22	0.68
3:D:859:ASP:O	3:D:860:LEU:HB3	1.94	0.68
1:B:147:GLY:HA3	1:B:171:PHE:CD1	2.29	0.68
2:C:54:ILE:HG12	2:C:355:VAL:HG13	1.76	0.68
2:C:99:GLN:CB	2:C:109:LYS:HG2	2.22	0.68
2:C:836:GLY:HA3	2:C:1001:VAL:HG21	1.76	0.68
2:C:924:LEU:O	2:C:928:LYS:HG3	1.94	0.68
4:E:81:PRO:HG3	4:E:84:ARG:HD2	1.76	0.68
1:A:157:GLY:HA3	1:A:166:PRO:HB3	1.76	0.68
2:C:204:GLN:HG3	2:C:205:GLU:HG2	1.75	0.68
2:C:1054:THR:O	2:C:1056:LYS:N	2.27	0.68
3:D:662:GLU:HB2	3:D:670:VAL:HG22	1.75	0.68
3:D:770:LEU:H	3:D:770:LEU:HD12	1.59	0.68
3:D:789:LEU:HD13	3:D:882:PHE:HE1	1.58	0.68
1:B:49:PRO:HB3	1:B:146:ARG:NH2	2.10	0.68
2:C:145:GLY:O	2:C:146:VAL:HG23	1.93	0.68
2:C:147:TYR:O	2:C:148:PHE:HB2	1.93	0.68
1:B:56:VAL:O	1:B:164:ALA:O	2.12	0.67
2:C:410:ILE:HG12	2:C:468:ARG:HH21	1.58	0.67
2:C:635:THR:O	2:C:636:ALA:HB3	1.94	0.67
2:C:754:ILE:CD1	2:C:791:ARG:HE	2.07	0.67
2:C:755:LEU:HD23	2:C:792:VAL:CG2	2.24	0.67
3:D:509:PRO:HA	3:D:511:TRP:NE1	2.09	0.67
3:D:721:VAL:CG1	3:D:722:GLU:H	2.06	0.67
3:D:1123:PHE:CE2	3:D:1184:ARG:HG2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:285:LEU:HD11	2:C:302:VAL:CG2	2.24	0.67
2:C:729:LEU:HB2	2:C:787:ASP:OD2	1.93	0.67
3:D:26:VAL:C	3:D:28:LYS:H	1.95	0.67
3:D:126:VAL:H	3:D:456:MET:HE2	1.58	0.67
3:D:502:PHE:CE1	3:D:1452:ILE:HG13	2.28	0.67
3:D:631:ILE:HG21	3:D:745:MET:HE2	1.77	0.67
3:D:709:HIS:HD2	3:D:711:LEU:HB2	1.59	0.67
3:D:1106:VAL:O	3:D:1108:ARG:HG3	1.94	0.67
4:E:29:GLN:N	4:E:32:ARG:HG2	2.10	0.67
1:B:16:GLN:HB3	1:B:19:HIS:O	1.93	0.67
1:B:26:GLU:O	1:B:28:LEU:HG	1.95	0.67
2:C:35:PRO:O	2:C:37:GLU:N	2.27	0.67
2:C:328:LEU:O	2:C:467:ILE:HG21	1.94	0.67
2:C:903:SER:HB2	2:C:909:ALA:HB2	1.77	0.67
3:D:578:VAL:O	3:D:582:ILE:HG13	1.94	0.67
3:D:957:PRO:HB2	3:D:959:GLU:HG2	1.76	0.67
3:D:1033:GLN:O	3:D:1036:ARG:HG2	1.94	0.67
3:D:1153:VAL:HG12	3:D:1153:VAL:O	1.95	0.67
3:D:1207:TYR:HA	3:D:1214:PRO:HA	1.76	0.67
1:B:72:LYS:N	1:B:131:THR:O	2.27	0.67
2:C:257:LEU:O	2:C:259:GLY:N	2.28	0.67
2:C:285:LEU:CD2	2:C:286:SER:H	2.06	0.67
2:C:605:LYS:HD3	2:C:607:ASP:HA	1.76	0.67
2:C:674:VAL:CG2	2:C:675:ALA:N	2.57	0.67
2:C:892:LEU:HD23	2:C:893:ALA:H	1.60	0.67
3:D:551:ASN:O	3:D:555:LYS:HB2	1.93	0.67
3:D:639:LEU:H	3:D:729:HIS:HD2	1.38	0.67
3:D:1327:ARG:NH1	3:D:1327:ARG:HB3	2.10	0.67
1:B:202:ASP:C	1:B:204:SER:H	1.98	0.67
2:C:246:ASP:HB3	2:C:247:PRO:CD	2.25	0.67
2:C:423:ALA:HA	2:C:427:VAL:HG21	1.77	0.67
2:C:159:ILE:O	2:C:173:ASP:HA	1.93	0.67
2:C:440:PRO:HD3	2:C:455:LEU:CA	2.24	0.67
2:C:579:VAL:HG21	2:C:887:GLU:HG3	1.75	0.67
3:D:612:GLY:O	3:D:614:PHE:N	2.27	0.67
4:E:48:MET:HG2	4:E:49:ARG:N	2.10	0.67
2:C:164:PRO:HD3	2:C:267:TYR:CD2	2.30	0.67
2:C:673:LEU:O	2:C:868:ASP:HB2	1.95	0.67
2:C:1034:GLU:CD	3:D:1096:ARG:HH12	1.98	0.67
3:D:465:LEU:HD22	3:D:512:MET:CE	2.25	0.67
3:D:553:ARG:O	3:D:554:LEU:HD23	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:699:VAL:HG22	3:D:756:GLN:NE2	2.10	0.67
3:D:709:HIS:CD2	3:D:711:LEU:HB2	2.30	0.67
3:D:947:ILE:HD12	3:D:1020:LEU:HB3	1.77	0.67
3:D:1125:MET:HB2	3:D:1132:LEU:HD23	1.75	0.67
4:E:82:GLU:O	4:E:85:LEU:HB3	1.95	0.67
1:B:76:VAL:HB	3:D:872:ARG:HH22	1.58	0.67
2:C:640:ARG:HH11	2:C:640:ARG:HG3	1.60	0.67
3:D:906:GLN:OE1	3:D:906:GLN:N	2.28	0.67
3:D:1043:GLY:O	3:D:1056:PRO:HA	1.95	0.67
3:D:1103:HIS:HB2	3:D:1462:LEU:HD12	1.77	0.67
1:A:44:LEU:HD13	1:A:199:ILE:HG13	1.75	0.67
1:A:180:GLN:HG3	2:C:934:PHE:CD2	2.30	0.67
1:B:25:LEU:C	1:B:25:LEU:HD12	2.15	0.67
1:B:30:ARG:HA	1:B:193:ASP:OD1	1.95	0.67
3:D:557:LEU:HD11	3:D:563:PRO:HD2	1.77	0.67
3:D:891:GLY:N	3:D:926:LYS:HZ1	1.92	0.67
1:A:194:LYS:O	1:A:196:THR:HG22	1.94	0.67
1:A:197:LEU:HD23	1:A:197:LEU:N	2.08	0.67
2:C:605:LYS:HA	2:C:612:ALA:CB	2.24	0.67
3:D:100:ALA:CB	3:D:575:GLN:HG3	2.25	0.67
3:D:795:VAL:HG13	3:D:864:VAL:HG22	1.77	0.67
3:D:1136:LYS:O	3:D:1138:SER:N	2.28	0.67
3:D:1252:ILE:C	3:D:1254:GLN:H	1.96	0.67
4:E:29:GLN:CA	4:E:32:ARG:HG2	2.25	0.67
2:C:882:LEU:N	2:C:882:LEU:CD2	2.59	0.66
3:D:705:ALA:CB	3:D:706:PRO:CD	2.73	0.66
3:D:760:ARG:HH12	4:E:59:ASN:HD21	1.42	0.66
3:D:777:PRO:HG2	3:D:912:LYS:HG3	1.76	0.66
3:D:947:ILE:HB	3:D:1020:LEU:HD22	1.76	0.66
4:E:25:LYS:HA	4:E:28:GLN:HB3	1.77	0.66
2:C:438:ILE:CD1	2:C:484:VAL:HG22	2.25	0.66
2:C:676:ILE:CG2	2:C:873:PRO:HB3	2.25	0.66
2:C:929:ARG:C	2:C:931:GLY:H	1.98	0.66
3:D:103:TRP:O	3:D:104:PHE:CB	2.43	0.66
3:D:510:GLU:O	3:D:512:MET:N	2.28	0.66
1:A:62:LEU:HD13	2:C:745:ILE:HB	1.78	0.66
2:C:266:ARG:NE	2:C:268:ASP:HB3	2.10	0.66
2:C:323:ASP:O	2:C:325:ILE:N	2.24	0.66
2:C:440:PRO:HG3	2:C:454:SER:N	2.10	0.66
2:C:755:LEU:CD1	2:C:790:LEU:HD23	2.23	0.66
2:C:876:VAL:HB	2:C:877:PRO:CD	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1018:GLN:OE1	2:C:1018:GLN:HA	1.95	0.66
3:D:764:LEU:HG	3:D:766:ALA:H	1.60	0.66
3:D:1304:LYS:HD3	3:D:1304:LYS:N	2.10	0.66
1:A:195:LEU:HD23	1:A:196:THR:N	2.11	0.66
1:B:25:LEU:CD1	1:B:28:LEU:HD21	2.25	0.66
2:C:148:PHE:O	2:C:149:THR:CB	2.42	0.66
2:C:710:ILE:HG12	2:C:790:LEU:HB2	1.77	0.66
3:D:91:ALA:O	3:D:517:VAL:HG13	1.96	0.66
3:D:108:VAL:N	3:D:511:TRP:HH2	1.94	0.66
3:D:849:ALA:O	3:D:853:VAL:HG23	1.95	0.66
3:D:1141:GLU:HA	3:D:1171:VAL:CG1	2.22	0.66
1:A:41:ARG:HG2	1:A:177:VAL:CG1	2.25	0.66
1:B:106:PRO:CA	1:B:133:GLU:HA	2.24	0.66
2:C:712:ALA:HB2	2:C:722:ILE:HD12	1.78	0.66
3:D:1486:VAL:HG21	4:E:25:LYS:NZ	2.11	0.66
2:C:881:ASN:N	2:C:881:ASN:HD22	1.92	0.66
2:C:922:PHE:C	2:C:924:LEU:N	2.49	0.66
3:D:546:ARG:HH12	3:D:589:SER:HB2	1.59	0.66
3:D:879:ARG:NH2	3:D:905:PRO:HD2	2.11	0.66
3:D:904:VAL:HG12	3:D:906:GLN:OE1	1.95	0.66
3:D:1236:LEU:HD11	3:D:1356:TYR:CE2	2.22	0.66
3:D:1396:GLU:O	3:D:1400:VAL:HG23	1.95	0.66
1:A:211:LEU:O	1:A:215:VAL:HG13	1.95	0.66
1:A:217:ILE:HG22	1:A:221:HIS:CD2	2.31	0.66
2:C:862:PRO:HG3	2:C:925:TYR:OH	1.96	0.66
2:C:892:LEU:CD2	2:C:892:LEU:N	2.54	0.66
2:C:953:VAL:HG11	2:C:962:GLN:HB3	1.78	0.66
2:C:839:LEU:HD12	2:C:994:ILE:HG22	1.77	0.66
3:D:91:ALA:HB3	3:D:518:PRO:HG2	1.76	0.66
3:D:1142:SER:O	3:D:1365:ASP:HB2	1.95	0.66
2:C:502:PRO:HB2	2:C:507:ARG:HH12	1.59	0.66
3:D:772:PRO:HG3	3:D:778:LEU:CD2	2.26	0.66
3:D:792:ILE:O	3:D:792:ILE:HG22	1.95	0.66
3:D:908:LYS:HG3	3:D:1027:GLY:HA3	1.77	0.66
2:C:163:ILE:HG23	2:C:265:LYS:NZ	2.11	0.65
2:C:626:ARG:NE	2:C:637:PHE:HZ	1.94	0.65
4:E:40:LEU:HB3	4:E:44:GLU:O	1.96	0.65
1:B:30:ARG:HG3	1:B:30:ARG:O	1.95	0.65
2:C:336:VAL:HA	2:C:339:LEU:HD12	1.78	0.65
2:C:958:SER:HB2	2:C:959:PRO:HD2	1.78	0.65
3:D:772:PRO:HD3	3:D:778:LEU:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1112:CYS:SG	3:D:1113:GLY:N	2.69	0.65
3:D:1273:VAL:HG23	3:D:1324:PRO:CG	2.19	0.65
2:C:721:ARG:O	2:C:758:ARG:HB2	1.95	0.65
3:D:90:MET:N	3:D:520:LEU:HD21	2.10	0.65
3:D:91:ALA:HB3	3:D:518:PRO:HD2	1.78	0.65
1:B:150:TYR:CE1	1:B:170:ILE:HG22	2.31	0.65
2:C:613:VAL:CG1	2:C:620:LEU:H	2.05	0.65
2:C:648:ARG:HG2	2:C:648:ARG:HH11	1.61	0.65
2:C:943:VAL:O	2:C:946:ARG:N	2.28	0.65
2:C:1045:ALA:HB1	2:C:1048:THR:CB	2.23	0.65
3:D:681:ARG:O	3:D:682:ASP:HB2	1.97	0.65
3:D:1069:GLU:O	3:D:1072:ILE:N	2.28	0.65
1:A:162:ILE:HG12	1:A:163:ASN:OD1	1.95	0.65
1:B:58:ILE:HG23	1:B:140:MET:HG2	1.77	0.65
1:B:174:VAL:HG12	1:B:201:THR:CG2	2.26	0.65
2:C:142:ARG:HH12	2:C:171:TRP:HH2	1.45	0.65
2:C:159:ILE:HG12	2:C:310:LEU:HD13	1.76	0.65
2:C:410:ILE:HG12	2:C:468:ARG:NH2	2.11	0.65
2:C:576:ALA:H	2:C:662:GLU:HG2	1.62	0.65
2:C:1034:GLU:HB3	3:D:618:LEU:O	1.96	0.65
3:D:754:PHE:O	3:D:758:GLU:HG2	1.96	0.65
3:D:789:LEU:HD11	3:D:934:LEU:HD22	1.78	0.65
1:A:35:THR:HG22	1:B:218:LEU:HD13	1.77	0.65
1:B:94:MET:CE	1:B:94:MET:HB2	2.27	0.65
2:C:796:GLU:HG2	3:D:681:ARG:HH22	1.62	0.65
2:C:857:ASP:O	2:C:858:MET:HB2	1.95	0.65
2:C:1020:PRO:HD2	3:D:622:ARG:O	1.96	0.65
3:D:860:LEU:HA	3:D:877:PRO:CG	2.21	0.65
2:C:404:LEU:HD23	2:C:587:VAL:HG13	1.79	0.65
2:C:467:ILE:HG22	2:C:484:VAL:HG21	1.77	0.65
2:C:564:MET:CG	2:C:997:LEU:HD11	2.26	0.65
2:C:575:GLN:O	2:C:667:ALA:HB1	1.96	0.65
2:C:604:VAL:HG11	2:C:619:ARG:HH22	1.61	0.65
2:C:1008:ARG:HB2	2:C:1028:GLY:HA3	1.77	0.65
1:A:213:GLN:O	1:A:216:ALA:HB3	1.97	0.65
2:C:813:VAL:CG1	2:C:815:LEU:HD11	2.26	0.65
2:C:953:VAL:CG2	2:C:966:LEU:HD13	2.27	0.65
3:D:129:PHE:CA	3:D:454:ALA:HB1	2.15	0.65
3:D:916:TYR:C	3:D:916:TYR:CD2	2.71	0.65
2:C:439:CYS:SG	2:C:440:PRO:HD2	2.37	0.65
2:C:631:SER:OG	2:C:635:THR:HG22	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1017:PHE:HA	3:D:1023:MET:SD	2.37	0.65
2:C:94:LEU:O	2:C:115:LEU:HB3	1.97	0.65
2:C:360:VAL:O	2:C:361:MET:C	2.35	0.65
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.79	0.65
2:C:495:THR:HG22	2:C:496:ILE:H	1.61	0.65
2:C:688:ILE:CG2	2:C:871:LEU:HD12	2.27	0.65
2:C:813:VAL:HG12	2:C:815:LEU:CD1	2.27	0.65
2:C:910:THR:C	2:C:912:PRO:HD2	2.17	0.65
2:C:1008:ARG:CD	2:C:1029:GLY:H	2.02	0.65
3:D:670:VAL:O	3:D:673:ALA:HB3	1.97	0.65
3:D:877:PRO:O	3:D:880:ILE:HB	1.95	0.65
2:C:184:MET:HB3	2:C:191:PHE:CZ	2.32	0.64
2:C:1063:ARG:O	2:C:1066:ALA:HB3	1.97	0.64
3:D:657:LEU:O	3:D:658:LEU:C	2.35	0.64
1:A:23:PHE:HZ	1:A:207:PRO:HB2	1.63	0.64
2:C:163:ILE:HG21	2:C:169:GLY:HA3	1.79	0.64
2:C:605:LYS:CG	2:C:607:ASP:H	2.10	0.64
2:C:573:ARG:HH11	2:C:573:ARG:HG3	1.62	0.64
3:D:978:TYR:C	3:D:980:MET:H	2.01	0.64
3:D:1093:TYR:HE2	3:D:1097:LYS:NZ	1.96	0.64
3:D:1277:ILE:HG22	3:D:1279:GLY:H	1.62	0.64
3:D:1364:HIS:O	3:D:1365:ASP:HB3	1.97	0.64
3:D:1457:ASP:OD1	3:D:1459:LEU:HD23	1.96	0.64
2:C:839:LEU:HD23	2:C:849:VAL:HG22	1.80	0.64
3:D:1118:ILE:N	3:D:1118:ILE:HD12	2.11	0.64
3:D:1136:LYS:HE3	3:D:1139:ASP:OD1	1.96	0.64
3:D:1348:LEU:O	3:D:1352:ILE:HG13	1.97	0.64
2:C:1019:GLN:HB3	2:C:1057:SER:OG	1.96	0.64
2:C:1113:GLU:O	2:C:1115:LEU:HD23	1.98	0.64
3:D:578:VAL:HG12	3:D:582:ILE:HD11	1.79	0.64
3:D:641:GLN:HB3	3:D:719:VAL:HG21	1.79	0.64
3:D:1093:TYR:HE2	3:D:1097:LYS:HZ2	1.45	0.64
2:C:34:VAL:CG1	2:C:38:LYS:HG3	2.27	0.64
2:C:151:ASP:H	2:C:157:ARG:HA	1.63	0.64
2:C:331:ARG:O	2:C:467:ILE:HG12	1.96	0.64
3:D:764:LEU:HD23	3:D:767:HIS:NE2	2.12	0.64
3:D:793:THR:HG22	3:D:879:ARG:HH22	1.61	0.64
3:D:1282:ARG:CB	3:D:1293:PHE:HB2	2.26	0.64
3:D:1381:VAL:HG12	3:D:1382:THR:H	1.62	0.64
2:C:304:LEU:N	2:C:305:PRO:CD	2.61	0.64
2:C:589:ARG:NH2	2:C:654:LEU:HA	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:768:SER:HB2	2:C:769:PRO:HD2	1.79	0.64
2:C:859:PRO:O	2:C:867:VAL:HG23	1.98	0.64
3:D:968:ASP:O	3:D:969:ARG:C	2.36	0.64
3:D:996:TRP:HA	3:D:999:THR:HG22	1.78	0.64
3:D:1037:GLN:HG3	3:D:1042:ARG:CG	2.26	0.64
3:D:1323:GLN:N	3:D:1324:PRO:CD	2.61	0.64
2:C:12:VAL:HG21	2:C:479:VAL:HG11	1.79	0.64
2:C:256:TYR:CA	2:C:260:LEU:HD13	2.28	0.64
3:D:886:VAL:HG21	3:D:914:LEU:HD11	1.79	0.64
3:D:1086:LEU:O	3:D:1089:ALA:HB3	1.98	0.64
3:D:1142:SER:O	3:D:1364:HIS:HD2	1.80	0.64
2:C:946:ARG:HH11	2:C:946:ARG:HG2	1.63	0.64
4:E:59:ASN:HD22	4:E:62:THR:HG1	1.46	0.64
3:D:626:SER:HB2	3:D:748:HIS:HA	1.80	0.64
3:D:1378:TYR:CE2	3:D:1431:THR:HB	2.30	0.64
3:D:1433:SER:HB3	3:D:1464:GLU:OE2	1.98	0.64
4:E:59:ASN:HD21	4:E:61:VAL:HG23	1.63	0.64
1:B:14:THR:CB	1:B:22:GLU:HB3	2.27	0.63
3:D:606:ILE:H	3:D:606:ILE:HD12	1.63	0.63
3:D:840:LYS:CB	3:D:846:PRO:HA	2.28	0.63
3:D:1326:THR:O	3:D:1327:ARG:HB3	1.97	0.63
3:D:1484:THR:HG21	4:E:79:LEU:HB2	1.79	0.63
4:E:47:LYS:HD3	4:E:54:LEU:HD23	1.80	0.63
1:A:88:ARG:HB2	1:A:123:MET:SD	2.38	0.63
1:B:23:PHE:HD1	1:B:211:LEU:HD22	1.63	0.63
1:B:76:VAL:HB	3:D:872:ARG:NH2	2.13	0.63
2:C:831:ARG:HH12	2:C:1002:GLU:HB2	1.63	0.63
3:D:1280:VAL:HG12	3:D:1281:VAL:H	1.63	0.63
1:A:115:THR:HG23	1:A:115:THR:O	1.98	0.63
2:C:66:LEU:HD11	2:C:98:LEU:CB	2.27	0.63
2:C:1087:VAL:HG12	2:C:1091:GLU:OE2	1.97	0.63
3:D:496:LEU:HD12	3:D:500:ARG:HG2	1.81	0.63
3:D:723:GLY:O	3:D:724:GLN:HB2	1.98	0.63
3:D:965:GLU:O	3:D:968:ASP:HB2	1.97	0.63
3:D:969:ARG:HG3	3:D:970:LYS:H	1.60	0.63
3:D:1096:ARG:HG3	3:D:1096:ARG:NH1	2.10	0.63
2:C:303:PHE:H	2:C:305:PRO:HD2	1.63	0.63
3:D:580:ALA:HB2	3:D:587:ARG:HH22	1.63	0.63
3:D:769:LEU:HD22	3:D:779:ALA:HB2	1.80	0.63
3:D:788:GLY:O	3:D:792:ILE:HD13	1.97	0.63
3:D:1043:GLY:HA2	3:D:1057:VAL:CG2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1282:ARG:HB3	3:D:1293:PHE:HB2	1.80	0.63
2:C:38:LYS:O	2:C:39:ARG:HB2	1.98	0.63
2:C:66:LEU:CA	2:C:100:LEU:HA	2.28	0.63
2:C:129:ILE:CD1	2:C:386:PHE:HB3	2.29	0.63
2:C:408:ARG:NH2	2:C:456:ALA:O	2.28	0.63
2:C:475:LYS:C	2:C:477:GLY:H	2.02	0.63
2:C:580:MET:HB2	2:C:584:GLU:CD	2.19	0.63
2:C:602:GLU:O	2:C:603:VAL:HG13	1.99	0.63
2:C:1089:VAL:HG13	2:C:1099:VAL:HB	1.80	0.63
3:D:976:GLN:C	3:D:978:TYR:H	2.02	0.63
3:D:1103:HIS:C	3:D:1105:ILE:N	2.50	0.63
1:A:131:THR:CG2	2:C:644:ARG:HE	2.12	0.63
2:C:87:ASP:OD2	2:C:824:ARG:NH2	2.31	0.63
2:C:202:TYR:CE1	2:C:304:LEU:HB3	2.32	0.63
2:C:401:LEU:O	2:C:404:LEU:HB3	1.99	0.63
2:C:588:VAL:O	2:C:588:VAL:CG1	2.46	0.63
2:C:685:GLU:OE1	2:C:685:GLU:HA	1.99	0.63
2:C:874:LEU:O	2:C:876:VAL:HG23	1.98	0.63
3:D:89:ARG:O	3:D:520:LEU:HD11	1.97	0.63
3:D:643:GLY:HA2	3:D:721:VAL:HG21	1.80	0.63
3:D:880:ILE:O	3:D:883:ALA:HB3	1.98	0.63
3:D:972:ARG:O	3:D:976:GLN:HB2	1.99	0.63
3:D:1403:LEU:HD12	3:D:1417:TRP:HZ3	1.64	0.63
1:B:87:VAL:HG12	1:B:88:ARG:N	2.14	0.63
1:B:174:VAL:HA	1:B:201:THR:CB	2.28	0.63
3:D:1139:ASP:O	3:D:1143:GLY:N	2.32	0.63
3:D:1304:LYS:HD3	3:D:1304:LYS:H	1.61	0.63
1:A:46:SER:OG	2:C:856:GLU:HG2	1.98	0.63
1:B:90:LEU:HB2	1:B:119:ASP:HA	1.80	0.63
2:C:26:TYR:O	2:C:30:LEU:N	2.29	0.63
2:C:492:ASP:O	2:C:532:MET:HA	1.98	0.63
3:D:35(U):UNK:O	3:D:36(U):UNK:CB	2.47	0.63
3:D:456:MET:HG2	3:D:457:GLY:H	1.64	0.63
3:D:519:VAL:HG12	3:D:520:LEU:N	2.13	0.63
3:D:679:ARG:O	3:D:681:ARG:N	2.32	0.63
3:D:1154:GLU:O	3:D:1155:ALA:HB2	1.98	0.63
4:E:14:ASP:CG	4:E:15:SER:N	2.51	0.63
1:A:86:VAL:HG12	1:A:124:ASN:CG	2.18	0.63
2:C:202:TYR:HB3	2:C:207:LEU:HD13	1.80	0.63
2:C:257:LEU:CD2	2:C:264:PRO:HG3	2.29	0.63
2:C:268:ASP:O	2:C:270:GLY:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:816:LYS:HD2	2:C:817:PRO:CD	2.28	0.63
3:D:678:GLU:C	3:D:680:GLN:H	2.02	0.63
3:D:908:LYS:HD3	3:D:909:ASN:HB2	1.81	0.63
3:D:1236:LEU:HD12	3:D:1256:LEU:HD13	1.81	0.63
3:D:1324:PRO:HG2	3:D:1325:LEU:N	2.14	0.63
1:A:217:ILE:HG22	1:A:221:HIS:NE2	2.14	0.62
1:B:98:THR:CG2	1:B:99:LEU:H	2.12	0.62
1:B:115:THR:O	1:B:117:SER:N	2.32	0.62
2:C:110:GLU:HB2	2:C:369:PRO:HG2	1.80	0.62
2:C:787:ASP:O	2:C:787:ASP:OD1	2.17	0.62
2:C:66:LEU:HD11	2:C:98:LEU:HB3	1.80	0.62
2:C:676:ILE:O	2:C:677:MET:CB	2.47	0.62
2:C:722:ILE:HA	2:C:758:ARG:CB	2.29	0.62
2:C:1107:ASN:N	2:C:1108:PRO:CD	2.62	0.62
3:D:502:PHE:CE2	3:D:509:PRO:HG3	2.33	0.62
2:C:603:VAL:HG21	2:C:646:GLY:H	1.65	0.62
2:C:1012:PRO:HB3	2:C:1023:GLY:CA	2.29	0.62
2:C:1034:GLU:HA	2:C:1037:VAL:HG23	1.81	0.62
3:D:767:HIS:HE1	4:E:2:ALA:HB1	1.64	0.62
3:D:1083:ASP:O	3:D:1086:LEU:HB2	1.99	0.62
2:C:208:VAL:HG12	2:C:209:ARG:HG3	1.80	0.62
2:C:324:ASP:C	2:C:326:ASP:H	2.02	0.62
3:D:554:LEU:O	3:D:558:LEU:HD12	1.99	0.62
3:D:770:LEU:H	3:D:770:LEU:CD1	2.11	0.62
1:A:28:LEU:HD12	1:A:195:LEU:HB2	1.81	0.62
1:A:173:PRO:O	1:A:203:GLY:N	2.31	0.62
2:C:100:LEU:HD11	2:C:369:PRO:HD3	1.81	0.62
2:C:911:GLU:HA	2:C:914:ILE:HD12	1.81	0.62
2:C:1001:VAL:O	2:C:1004:LYS:N	2.27	0.62
3:D:688:TRP:HA	3:D:688:TRP:CE3	2.34	0.62
1:B:76:VAL:O	1:B:80:LEU:HG	1.98	0.62
2:C:595:LEU:HD21	2:C:623:HIS:HB3	1.82	0.62
2:C:946:ARG:NE	3:D:861:GLN:HE22	1.89	0.62
2:C:1038:TRP:CD1	3:D:1099:VAL:HG11	2.34	0.62
3:D:558:LEU:CD2	3:D:567:ILE:HG13	2.30	0.62
3:D:1291:SER:HA	3:D:1303:TYR:O	1.99	0.62
3:D:1462:LEU:HD23	3:D:1473:PRO:HG2	1.80	0.62
1:B:53:VAL:HG11	1:B:82:LEU:HG	1.82	0.62
1:B:174:VAL:HA	1:B:201:THR:CG2	2.29	0.62
2:C:502:PRO:HB2	2:C:507:ARG:NH1	2.14	0.62
3:D:3(U):UNK:O	3:D:39(U):UNK:O	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:639:LEU:HD23	3:D:729:HIS:CD2	2.35	0.62
3:D:793:THR:CG2	3:D:879:ARG:HH22	2.12	0.62
3:D:795:VAL:HG12	3:D:796:ARG:N	2.15	0.62
3:D:1019:PRO:C	3:D:1021:TYR:N	2.48	0.62
2:C:565:GLN:HG3	2:C:995:MET:HE1	1.81	0.62
2:C:635:THR:HG22	2:C:636:ALA:N	2.14	0.62
2:C:1052:MET:HE1	3:D:748:HIS:HB3	1.82	0.62
3:D:1075:HIS:O	3:D:1077:ALA:N	2.32	0.62
3:D:1266:ARG:O	3:D:1268:PRO:HD3	2.00	0.62
1:B:49:PRO:HD2	1:B:213:GLN:NE2	2.15	0.62
1:B:80:LEU:O	1:B:83:LYS:HB2	2.00	0.62
2:C:168:ARG:HH21	2:C:266:ARG:HG2	1.64	0.62
3:D:637:LEU:O	3:D:638:LYS:O	2.17	0.62
3:D:658:LEU:HA	3:D:661:MET:HE2	1.81	0.62
3:D:903:ASP:OD1	3:D:903:ASP:O	2.18	0.62
3:D:952:ASP:C	3:D:954:ALA:H	2.03	0.62
2:C:379:GLU:O	2:C:380:ALA:HB3	1.99	0.62
2:C:629:ALA:C	2:C:630:ARG:HD3	2.21	0.62
2:C:1113:GLU:C	2:C:1115:LEU:H	2.02	0.62
3:D:793:THR:CG2	3:D:879:ARG:HH12	2.13	0.62
3:D:863:THR:N	3:D:876:SER:OG	2.33	0.62
3:D:1059:SER:O	3:D:1061:PHE:N	2.33	0.62
3:D:1304:LYS:O	3:D:1304:LYS:HG2	2.00	0.62
3:D:1394:VAL:HG12	3:D:1395:LEU:N	2.15	0.62
3:D:1403:LEU:CD2	3:D:1415:VAL:H	2.11	0.62
1:A:110:ARG:HD3	1:A:113:ASP:OD2	2.00	0.61
1:A:224:TYR:CD1	1:B:9:PRO:HD2	2.35	0.61
2:C:22:GLN:HE21	2:C:336:VAL:HG21	1.64	0.61
2:C:22:GLN:O	2:C:24:GLU:N	2.32	0.61
2:C:559:LEU:HD12	2:C:559:LEU:C	2.21	0.61
3:D:10:ILE:HG21	3:D:1450:ALA:HB1	1.82	0.61
3:D:757:ALA:HB2	4:E:61:VAL:CG1	2.30	0.61
3:D:1263:PHE:CE2	3:D:1352:ILE:HD13	2.35	0.61
1:A:15:THR:OG1	1:A:16:GLN:N	2.32	0.61
1:A:35:THR:HG21	1:B:43:ILE:CD1	2.30	0.61
2:C:159:ILE:HG21	2:C:306:THR:CG2	2.30	0.61
2:C:438:ILE:HG23	2:C:470:PRO:HB3	1.81	0.61
2:C:613:VAL:CG1	2:C:614:ARG:N	2.64	0.61
2:C:946:ARG:NE	3:D:861:GLN:NE2	2.43	0.61
3:D:1262:LEU:HD21	3:D:1351:GLU:HG3	1.81	0.61
3:D:1264:GLU:HG2	3:D:1266:ARG:NH2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:GLN:CG	3:D:688:TRP:HD1	2.13	0.61
2:C:14:PRO:O	2:C:15:LEU:HB3	1.99	0.61
2:C:686:ASP:OD2	3:D:739:ASP:OD2	2.18	0.61
3:D:518:PRO:CB	3:D:544:TYR:CE1	2.82	0.61
3:D:770:LEU:HD12	3:D:770:LEU:N	2.15	0.61
3:D:891:GLY:N	3:D:926:LYS:NZ	2.47	0.61
3:D:921:ARG:O	3:D:922:LEU:HD23	2.00	0.61
3:D:1103:HIS:O	3:D:1104:GLU:HB3	2.01	0.61
3:D:1270:ALA:HB3	3:D:1328:GLY:HA3	1.82	0.61
3:D:1333:HIS:CE1	3:D:1421:LEU:HB3	2.35	0.61
1:A:86:VAL:HG21	1:A:203:GLY:C	2.20	0.61
1:A:142:VAL:O	1:A:143:ARG:O	2.18	0.61
2:C:614:ARG:O	2:C:616:GLU:N	2.30	0.61
3:D:633:VAL:HG22	3:D:634:GLY:N	2.15	0.61
3:D:638:LYS:HA	3:D:729:HIS:CG	2.35	0.61
3:D:699:VAL:HG12	3:D:717:GLN:CG	2.30	0.61
3:D:1045:MET:HA	3:D:1045:MET:HE2	1.82	0.61
1:A:31:GLY:H	1:A:193:ASP:CG	2.03	0.61
1:A:169:ALA:O	1:A:170:ILE:HD13	2.01	0.61
2:C:184:MET:HB3	2:C:191:PHE:CE1	2.36	0.61
2:C:348:LEU:CD1	2:C:378:LEU:HD11	2.30	0.61
2:C:588:VAL:CG2	2:C:666:LEU:HB2	2.29	0.61
2:C:605:LYS:HA	2:C:612:ALA:H	1.65	0.61
2:C:729:LEU:O	2:C:731:GLU:N	2.33	0.61
3:D:1036:ARG:O	3:D:1040:GLY:O	2.18	0.61
3:D:1150:ALA:HB2	3:D:1189:ARG:CG	2.29	0.61
1:A:10:VAL:HB	1:A:26:GLU:HG3	1.82	0.61
1:B:125:PRO:HG2	1:B:126:ASP:H	1.65	0.61
2:C:9:ILE:CG2	2:C:10:ARG:N	2.61	0.61
2:C:342:ASP:O	2:C:345:ARG:HB2	2.01	0.61
2:C:466:PHE:CE1	2:C:467:ILE:HD12	2.35	0.61
2:C:1005:MET:HB2	3:D:629:SER:CB	2.29	0.61
3:D:760:ARG:NH1	4:E:59:ASN:HD21	1.98	0.61
3:D:792:ILE:N	3:D:792:ILE:HD12	2.16	0.61
2:C:491:GLU:O	2:C:509:ALA:HB1	2.01	0.61
2:C:1101:THR:O	2:C:1110:ASP:N	2.33	0.61
3:D:607:LEU:O	3:D:608:SER:HB2	2.00	0.61
3:D:1372:VAL:HG22	3:D:1375:MET:HE3	1.80	0.61
2:C:1067:TYR:CG	2:C:1067:TYR:O	2.54	0.61
3:D:509:PRO:HA	3:D:511:TRP:HE1	1.64	0.61
3:D:590:PRO:HA	3:D:600:LEU:HG	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:985:ASP:O	3:D:988:ARG:HB3	2.00	0.61
3:D:1017:PHE:HA	3:D:1023:MET:HE1	1.81	0.61
3:D:1278:ASP:HA	3:D:1317:ASP:O	2.01	0.61
3:D:1379:VAL:O	3:D:1393:GLN:HA	2.01	0.61
1:A:175:ARG:O	1:A:176:ARG:HB2	2.01	0.61
1:A:180:GLN:HE21	2:C:934:PHE:CB	2.12	0.61
1:B:26:GLU:HG3	1:B:194:LYS:CD	2.22	0.61
2:C:327:HIS:C	2:C:329:GLY:H	2.03	0.61
2:C:482:GLU:HA	2:C:486:MET:CE	2.31	0.61
2:C:552:HIS:CE1	3:D:1064:GLY:N	2.69	0.61
3:D:545:ARG:HG3	3:D:546:ARG:N	2.15	0.61
1:B:175:ARG:O	1:B:176:ARG:HB2	2.01	0.60
2:C:8:ARG:HH11	2:C:495:THR:HG23	1.65	0.60
2:C:569:VAL:O	2:C:569:VAL:CG1	2.44	0.60
2:C:963:LEU:CD1	2:C:972:VAL:HG22	2.30	0.60
3:D:857:LEU:O	3:D:858:LEU:C	2.39	0.60
3:D:916:TYR:HD2	3:D:917:GLN:N	1.99	0.60
3:D:1192:LEU:HD13	3:D:1345:GLU:OE1	2.01	0.60
3:D:1356:TYR:HD1	3:D:1363:LEU:HD21	1.65	0.60
3:D:1485:GLN:CB	4:E:22:VAL:HG22	2.31	0.60
1:B:86:VAL:HG23	1:B:124:ASN:CG	2.22	0.60
1:B:143:ARG:HD2	1:B:159:LYS:CG	2.31	0.60
2:C:475:LYS:CB	2:C:527:GLU:H	2.14	0.60
2:C:491:GLU:HG3	2:C:510:THR:HB	1.81	0.60
2:C:589:ARG:NH1	2:C:596:TYR:HB3	2.16	0.60
2:C:598:GLU:OE2	2:C:614:ARG:NH2	2.33	0.60
3:D:638:LYS:C	3:D:639:LEU:O	2.38	0.60
3:D:747:VAL:O	3:D:747:VAL:HG22	2.01	0.60
3:D:1324:PRO:HG2	3:D:1325:LEU:H	1.67	0.60
1:B:42:ARG:HG3	1:B:42:ARG:HH11	1.65	0.60
2:C:342:ASP:O	2:C:346:VAL:HG23	2.01	0.60
2:C:588:VAL:HG11	2:C:661:SER:HB3	1.81	0.60
2:C:729:LEU:HB3	2:C:734:LEU:HD21	1.83	0.60
2:C:1055:ILE:H	2:C:1055:ILE:CD1	2.02	0.60
3:D:948:THR:H	3:D:1020:LEU:HD13	1.66	0.60
1:B:148:VAL:HG23	1:B:149:GLY:N	2.16	0.60
2:C:165:LEU:HD13	2:C:342:ASP:OD2	2.01	0.60
3:D:100:ALA:HB2	3:D:575:GLN:HG3	1.83	0.60
3:D:566:ILE:C	3:D:570:GLU:HG3	2.21	0.60
3:D:1003:VAL:O	3:D:1006:ALA:HB3	2.02	0.60
3:D:1272:ALA:CB	3:D:1325:LEU:HA	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1346:ARG:HH12	3:D:1349:VAL:HG11	1.66	0.60
3:D:1364:HIS:CD2	3:D:1365:ASP:H	2.19	0.60
4:E:29:GLN:HA	4:E:32:ARG:HG2	1.84	0.60
1:B:51:THR:HG21	1:B:87:VAL:O	2.01	0.60
2:C:317:VAL:H	2:C:318:PRO:HD2	1.66	0.60
2:C:706:GLU:HG3	2:C:707:ARG:N	2.15	0.60
2:C:875:GLY:HA3	2:C:879:ARG:HD2	1.84	0.60
3:D:10:ILE:HG13	3:D:11:ALA:N	2.17	0.60
3:D:609:GLY:HA2	3:D:615:ARG:NH2	2.15	0.60
3:D:1236:LEU:CB	3:D:1256:LEU:HB2	2.27	0.60
1:A:30:ARG:HH11	1:A:191:ASP:HB2	1.66	0.60
2:C:110:GLU:HB2	2:C:369:PRO:CG	2.32	0.60
2:C:391:LEU:HD22	2:C:415:PRO:HD3	1.82	0.60
2:C:519:GLY:C	2:C:521:PRO:HD3	2.22	0.60
2:C:636:ALA:HB2	2:C:705:ILE:HD11	1.82	0.60
3:D:465:LEU:HD22	3:D:512:MET:HE1	1.83	0.60
3:D:932:ASP:O	3:D:933:ALA:C	2.40	0.60
1:A:16:GLN:HG3	1:A:20:TYR:HB2	1.83	0.60
2:C:152:PRO:HD2	2:C:158:TYR:CE2	2.35	0.60
2:C:184:MET:HE1	2:C:303:PHE:CZ	2.37	0.60
2:C:440:PRO:CG	2:C:454:SER:H	2.15	0.60
2:C:460:ARG:HD2	2:C:464:LEU:CD2	2.30	0.60
2:C:730:SER:O	2:C:731:GLU:C	2.40	0.60
2:C:1033:GLY:O	2:C:1035:MET:N	2.35	0.60
3:D:88:TYR:O	3:D:520:LEU:HD13	2.01	0.60
3:D:566:ILE:HG22	3:D:566:ILE:O	2.01	0.60
3:D:969:ARG:CG	3:D:970:LYS:N	2.62	0.60
3:D:1194:CYS:SG	3:D:1201:CYS:HB2	2.41	0.60
4:E:30:LEU:O	4:E:32:ARG:N	2.31	0.60
1:A:41:ARG:HH11	1:A:41:ARG:C	2.04	0.60
2:C:572:ILE:O	2:C:573:ARG:CB	2.49	0.60
2:C:743:VAL:HG11	2:C:800:VAL:HG21	1.83	0.60
3:D:91:ALA:HB3	3:D:518:PRO:CG	2.31	0.60
4:E:14:ASP:CG	4:E:15:SER:H	2.05	0.60
1:A:44:LEU:O	1:A:174:VAL:HG21	2.01	0.60
2:C:253:ALA:CA	2:C:256:TYR:HB2	2.22	0.60
2:C:613:VAL:HG11	2:C:619:ARG:HA	1.83	0.60
2:C:712:ALA:HB1	2:C:720:GLU:O	2.02	0.60
2:C:815:LEU:HD12	2:C:815:LEU:N	2.16	0.60
2:C:1054:THR:CB	2:C:1055:ILE:HD12	2.32	0.60
3:D:587:ARG:HG2	3:D:588:GLY:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:901:GLN:CB	3:D:905:PRO:HG3	2.28	0.60
3:D:969:ARG:CG	3:D:970:LYS:H	2.14	0.60
2:C:77:PRO:HD3	2:C:92:ALA:HA	1.83	0.60
2:C:261:LEU:O	2:C:263:ASP:N	2.35	0.60
2:C:423:ALA:HA	2:C:427:VAL:CG2	2.32	0.60
2:C:759:THR:HB	2:C:785:VAL:HG13	1.83	0.60
3:D:637:LEU:CB	3:D:641:GLN:HG3	2.32	0.60
3:D:1192:LEU:HD13	3:D:1345:GLU:HB3	1.83	0.60
3:D:1219:GLU:O	3:D:1221:VAL:N	2.33	0.60
1:A:158:ILE:HD11	1:A:161:ARG:NE	2.06	0.59
2:C:8:ARG:NH1	2:C:495:THR:HG23	2.17	0.59
2:C:80:GLN:NE2	2:C:122:THR:HG23	2.17	0.59
2:C:721:ARG:C	2:C:758:ARG:HB2	2.22	0.59
3:D:854:ALA:O	3:D:855:HIS:C	2.41	0.59
3:D:1382:THR:HG21	3:D:1418:LYS:CE	2.29	0.59
2:C:1054:THR:CG2	2:C:1055:ILE:HD12	2.32	0.59
2:C:1085:PHE:CE1	3:D:1468:LEU:HD13	2.36	0.59
3:D:638:LYS:HA	3:D:729:HIS:CD2	2.37	0.59
3:D:1435:LEU:HD21	3:D:1468:LEU:HD21	1.85	0.59
3:D:1435:LEU:O	3:D:1438:ALA:HB3	2.02	0.59
1:A:30:ARG:CD	1:A:191:ASP:HB3	2.23	0.59
1:A:57:TYR:C	1:A:57:TYR:CD2	2.74	0.59
1:B:37:GLY:HA3	1:B:195:LEU:HD21	1.82	0.59
2:C:149:THR:HG23	2:C:150:PRO:HD2	1.84	0.59
3:D:21:TRP:O	3:D:23:TYR:N	2.35	0.59
3:D:1275:SER:H	3:D:1322:GLY:CA	2.14	0.59
1:A:100:ILE:HG22	1:A:101:LEU:N	2.17	0.59
2:C:31:GLN:O	2:C:33:ASP:N	2.36	0.59
2:C:89:THR:HG23	2:C:129:ILE:HA	1.84	0.59
2:C:850:ALA:HA	3:D:632:VAL:HG11	1.84	0.59
3:D:24(U):UNK:O	3:D:25(U):UNK:CB	2.50	0.59
3:D:767:HIS:CE1	4:E:2:ALA:HB1	2.38	0.59
3:D:860:LEU:O	3:D:862:ASP:N	2.34	0.59
1:A:162:ILE:HG23	1:A:163:ASN:H	1.67	0.59
2:C:369:PRO:O	2:C:370:ALA:HB3	2.02	0.59
2:C:539:VAL:O	2:C:539:VAL:HG12	2.02	0.59
2:C:981:GLU:HB3	2:C:982:PRO:HD2	1.85	0.59
3:D:466:LYS:O	3:D:468:LEU:N	2.35	0.59
3:D:612:GLY:C	3:D:614:PHE:H	2.05	0.59
3:D:1014:ASN:O	3:D:1015:TYR:CD2	2.54	0.59
4:E:68:LEU:CD1	4:E:73:LEU:HD12	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:9:ILE:N	2:C:9:ILE:HD12	2.18	0.59
2:C:679:PHE:O	2:C:681:GLY:N	2.35	0.59
2:C:861:LEU:HG	2:C:862:PRO:CD	2.16	0.59
3:D:701:LEU:HD12	3:D:715:ALA:CB	2.33	0.59
3:D:964:LEU:O	3:D:966:GLU:N	2.33	0.59
3:D:1222:GLY:O	3:D:1225:ALA:HB3	2.02	0.59
3:D:1364:HIS:CG	3:D:1365:ASP:N	2.69	0.59
1:B:79:ILE:HG23	1:B:167:VAL:HG12	1.85	0.59
2:C:480:THR:HG23	2:C:480:THR:O	2.03	0.59
2:C:527:GLU:O	2:C:528:GLU:C	2.41	0.59
2:C:564:MET:SD	2:C:840:ALA:CB	2.87	0.59
2:C:577:PRO:HA	2:C:671:ASN:HD22	1.67	0.59
2:C:769:PRO:O	2:C:771:GLU:N	2.34	0.59
2:C:1034:GLU:HA	2:C:1037:VAL:CG2	2.33	0.59
3:D:518:PRO:HB3	3:D:544:TYR:CZ	2.38	0.59
3:D:719:VAL:O	3:D:721:VAL:HG23	2.02	0.59
3:D:850:LEU:HA	3:D:853:VAL:HB	1.85	0.59
3:D:978:TYR:CG	3:D:988:ARG:HD2	2.37	0.59
3:D:1017:PHE:HA	3:D:1023:MET:CE	2.33	0.59
3:D:1107:VAL:HG13	3:D:1202:GLN:HA	1.84	0.59
3:D:1109:GLU:HG3	3:D:1110:ALA:H	1.67	0.59
1:B:42:ARG:HG3	1:B:42:ARG:NH1	2.18	0.59
1:B:214:ALA:HA	1:B:217:ILE:CG1	2.32	0.59
1:B:223:ASN:O	1:B:225:PHE:N	2.36	0.59
2:C:11:GLU:OE1	2:C:473:ARG:HG3	2.03	0.59
2:C:367:LEU:HD13	2:C:372:LEU:HD21	1.85	0.59
2:C:439:CYS:HB2	2:C:468:ARG:NH1	2.17	0.59
2:C:882:LEU:HD11	2:C:884:GLN:HE21	1.67	0.59
2:C:950:LEU:HB3	3:D:1018:ASN:OD1	2.03	0.59
3:D:795:VAL:HG21	3:D:904:VAL:HG21	1.85	0.59
3:D:1431:THR:C	3:D:1432:LYS:HG2	2.23	0.59
1:B:199:ILE:O	1:B:199:ILE:HG22	2.03	0.59
2:C:972:VAL:O	2:C:974:LEU:N	2.35	0.59
3:D:7(U):UNK:O	3:D:35(U):UNK:N	2.36	0.59
3:D:590:PRO:CB	3:D:599:PRO:HA	2.33	0.59
3:D:916:TYR:C	3:D:918:ALA:H	2.05	0.59
3:D:927:THR:HG22	3:D:931:LEU:HD23	1.84	0.59
3:D:961:GLN:O	3:D:962:ARG:C	2.40	0.59
1:A:101:LEU:HD12	1:A:101:LEU:C	2.22	0.59
1:B:149:GLY:HA2	1:B:172:SER:OG	2.03	0.59
2:C:181:VAL:HG21	2:C:220:GLY:HA3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:368:THR:HB	2:C:369:PRO:HD2	1.85	0.59
2:C:461:VAL:O	2:C:462:ASP:CB	2.51	0.59
2:C:467:ILE:O	2:C:469:THR:HG23	2.03	0.59
2:C:525:ALA:O	2:C:526:PRO:C	2.40	0.59
2:C:568:ALA:O	2:C:569:VAL:HB	2.03	0.59
2:C:613:VAL:CG1	2:C:614:ARG:H	2.16	0.59
2:C:1021:LEU:HG	3:D:622:ARG:HD2	1.84	0.59
2:C:1103:ASP:HB2	2:C:1108:PRO:CB	2.30	0.59
3:D:126:VAL:H	3:D:456:MET:CE	2.15	0.59
3:D:1147:ARG:CB	3:D:1188:VAL:HG21	2.32	0.59
4:E:86:GLN:O	4:E:89:MET:HB2	2.03	0.59
1:A:185:ARG:HH21	1:A:194:LYS:HE3	1.68	0.58
1:A:221:HIS:HA	1:A:224:TYR:CD2	2.38	0.58
2:C:162:ILE:CG2	2:C:163:ILE:N	2.66	0.58
2:C:440:PRO:HG3	2:C:454:SER:HB3	1.85	0.58
2:C:755:LEU:O	2:C:755:LEU:HD13	2.03	0.58
2:C:882:LEU:HD23	2:C:882:LEU:H	1.68	0.58
2:C:989:VAL:HG12	2:C:990:GLY:N	2.16	0.58
3:D:762:GLN:NE2	4:E:20:THR:HG21	2.18	0.58
3:D:948:THR:N	3:D:1020:LEU:HD13	2.18	0.58
2:C:164:PRO:HG2	2:C:168:ARG:HG2	1.84	0.58
2:C:839:LEU:O	2:C:995:MET:O	2.21	0.58
3:D:879:ARG:HG2	3:D:879:ARG:HH11	1.68	0.58
3:D:1273:VAL:N	3:D:1324:PRO:CG	2.67	0.58
1:B:14:THR:OG1	1:B:22:GLU:HB3	2.03	0.58
1:B:80:LEU:HD13	3:D:839:LEU:CB	2.33	0.58
1:B:101:LEU:HD13	1:B:114:PHE:HA	1.85	0.58
2:C:110:GLU:H	2:C:369:PRO:CG	2.16	0.58
2:C:483:VAL:O	2:C:486:MET:N	2.36	0.58
2:C:603:VAL:CG2	2:C:646:GLY:H	2.16	0.58
2:C:841:ASN:ND2	2:C:845:ASN:H	2.00	0.58
3:D:701:LEU:HD11	3:D:759:ALA:HB1	1.85	0.58
3:D:757:ALA:HB2	4:E:61:VAL:HG11	1.86	0.58
3:D:1165:TYR:CZ	3:D:1214:PRO:HB3	2.38	0.58
1:A:224:TYR:CE1	1:B:9:PRO:HD2	2.39	0.58
2:C:11:GLU:OE2	2:C:473:ARG:NE	2.36	0.58
2:C:348:LEU:C	2:C:350:ARG:H	2.06	0.58
2:C:636:ALA:CB	2:C:705:ILE:HD11	2.33	0.58
2:C:850:ALA:HA	3:D:632:VAL:CG1	2.34	0.58
2:C:885:ILE:O	2:C:887:GLU:N	2.37	0.58
3:D:1125:MET:HG2	3:D:1126:ASP:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1200:VAL:HA	3:D:1373:ARG:HH12	1.69	0.58
2:C:483:VAL:O	2:C:486:MET:HB2	2.03	0.58
2:C:501:THR:O	2:C:502:PRO:C	2.42	0.58
2:C:565:GLN:HG3	2:C:995:MET:HE3	1.85	0.58
2:C:945:ALA:O	2:C:949:LYS:HG3	2.03	0.58
2:C:1098:ASP:OD1	2:C:1100:GLN:HG3	2.02	0.58
3:D:129:PHE:O	3:D:130:ASN:CB	2.50	0.58
3:D:599:PRO:O	3:D:600:LEU:HD23	2.04	0.58
3:D:798:GLU:HG3	3:D:821:VAL:CB	2.32	0.58
3:D:907:GLU:HB3	3:D:911:LEU:HD22	1.86	0.58
3:D:948:THR:H	3:D:1020:LEU:CD1	2.16	0.58
3:D:1353:GLN:HE21	3:D:1368:ILE:CD1	2.07	0.58
2:C:419:THR:O	2:C:420:ARG:C	2.42	0.58
2:C:987:ILE:HD11	3:D:946:GLY:C	2.23	0.58
3:D:699:VAL:HA	3:D:717:GLN:HA	1.84	0.58
3:D:1211:MET:HE2	4:E:16:LYS:HD2	1.84	0.58
1:A:131:THR:HG23	2:C:644:ARG:HE	1.68	0.58
1:B:94:MET:HE1	1:B:119:ASP:HB2	1.86	0.58
2:C:198:ARG:NH1	2:C:231:PRO:HD3	2.19	0.58
2:C:312:ALA:HB1	2:C:318:PRO:HG3	1.85	0.58
2:C:613:VAL:CG1	2:C:619:ARG:HG2	2.33	0.58
2:C:1052:MET:HE3	2:C:1056:LYS:HZ1	1.69	0.58
2:C:1100:GLN:O	3:D:8:VAL:O	2.22	0.58
3:D:551:ASN:HA	3:D:574:LEU:HD13	1.84	0.58
3:D:582:ILE:HG22	3:D:583:ASP:H	1.68	0.58
3:D:1035:ILE:C	3:D:1037:GLN:H	2.05	0.58
1:A:90:LEU:HB2	1:A:119:ASP:CB	2.34	0.58
1:A:143:ARG:HD3	1:A:145:ASP:OD1	2.04	0.58
1:A:158:ILE:HG13	1:A:161:ARG:HG2	1.86	0.58
1:A:181:VAL:O	1:A:181:VAL:HG12	2.04	0.58
1:B:36:LEU:O	1:B:39:PRO:HD2	2.03	0.58
1:B:55:SER:OG	1:B:157:GLY:HA3	2.03	0.58
2:C:395:LYS:HG3	2:C:397:GLU:HG3	1.85	0.58
3:D:642:CYS:SG	3:D:702:LEU:HD23	2.43	0.58
3:D:704:ARG:NH1	3:D:743:ASP:CG	2.53	0.58
3:D:898:GLU:C	3:D:899:LEU:HD13	2.24	0.58
3:D:959:GLU:O	3:D:963:TYR:CD1	2.56	0.58
1:A:198:ARG:HH12	2:C:932:GLU:HB3	1.68	0.58
2:C:386:PHE:O	2:C:392:SER:OG	2.15	0.58
2:C:487:THR:O	2:C:489:SER:N	2.37	0.58
2:C:684:PHE:CD2	2:C:685:GLU:HG2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1008:ARG:NH2	2:C:1020:PRO:HB3	2.18	0.58
3:D:1008:PHE:CE1	3:D:1035:ILE:HG13	2.28	0.58
3:D:1014:ASN:C	3:D:1015:TYR:CG	2.76	0.58
3:D:1194:CYS:HB3	3:D:1373:ARG:HH22	1.66	0.58
3:D:1281:VAL:HA	3:D:1314:LYS:HA	1.85	0.58
3:D:1452:ILE:HG22	3:D:1453:ALA:N	2.19	0.58
3:D:1486:VAL:O	4:E:79:LEU:HD12	2.04	0.58
2:C:128:ILE:HD12	2:C:128:ILE:N	2.19	0.58
2:C:758:ARG:HH11	2:C:758:ARG:HG3	1.68	0.58
2:C:1082:PRO:HG2	2:C:1085:PHE:CB	2.34	0.58
3:D:1059:SER:O	3:D:1060:SER:C	2.38	0.58
3:D:1234:THR:HG22	3:D:1234:THR:O	2.04	0.58
3:D:1261:GLU:OE1	3:D:1268:PRO:HB3	2.02	0.58
1:A:124:ASN:O	1:A:125:PRO:O	2.22	0.57
2:C:281:LEU:HD21	2:C:306:THR:OG1	2.04	0.57
2:C:349:ALA:C	2:C:350:ARG:HG3	2.23	0.57
2:C:579:VAL:CG2	2:C:887:GLU:HG3	2.34	0.57
2:C:635:THR:O	2:C:636:ALA:CB	2.51	0.57
3:D:789:LEU:HD13	3:D:882:PHE:CE1	2.39	0.57
3:D:794:GLN:O	3:D:795:VAL:HB	2.03	0.57
3:D:1031:ASN:OD1	3:D:1033:GLN:HG2	2.04	0.57
3:D:1059:SER:C	3:D:1061:PHE:N	2.56	0.57
4:E:68:LEU:HD13	4:E:73:LEU:HD12	1.84	0.57
2:C:136:ILE:CG2	2:C:336:VAL:HG13	2.33	0.57
2:C:137:VAL:CG1	2:C:411:SER:HB2	2.34	0.57
2:C:695:LEU:O	2:C:698:ASP:N	2.35	0.57
2:C:926:PHE:CE1	2:C:929:ARG:HD2	2.39	0.57
2:C:946:ARG:O	2:C:950:LEU:HG	2.04	0.57
3:D:959:GLU:O	3:D:963:TYR:HD1	1.87	0.57
1:A:106:PRO:O	1:A:107:LYS:CB	2.52	0.57
2:C:26:TYR:CE2	2:C:30:LEU:HD22	2.39	0.57
2:C:399:ASN:ND2	2:C:401:LEU:H	2.01	0.57
2:C:551:GLU:HG3	2:C:906:PHE:CD2	2.39	0.57
2:C:742:ILE:HG23	2:C:756:VAL:HG22	1.86	0.57
3:D:969:ARG:HG3	3:D:970:LYS:HG3	1.85	0.57
3:D:1076:GLY:O	3:D:1079:LYS:HG2	2.04	0.57
3:D:1103:HIS:H	3:D:1222:GLY:HA3	1.70	0.57
3:D:1109:GLU:O	3:D:1217:ILE:HD11	2.03	0.57
1:A:71:VAL:HG13	1:A:132:LEU:HB3	1.85	0.57
1:A:178:ALA:O	1:A:179:PHE:HB3	2.04	0.57
1:A:222:LEU:HD12	1:B:215:VAL:CG1	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLU:N	1:B:73:GLU:OE2	2.38	0.57
2:C:64:LEU:CD1	2:C:367:LEU:HD12	2.34	0.57
2:C:157:ARG:HG3	2:C:313:LEU:HG	1.85	0.57
2:C:466:PHE:CD1	2:C:467:ILE:HG13	2.39	0.57
3:D:772:PRO:CD	3:D:778:LEU:HB2	2.34	0.57
3:D:1204:CYS:C	3:D:1206:GLY:H	2.08	0.57
1:A:228:PRO:HA	1:B:11:PHE:O	2.05	0.57
1:B:95:ALA:O	1:B:96:SER:HB3	2.05	0.57
2:C:34:VAL:HG11	2:C:38:LYS:HG3	1.86	0.57
3:D:639:LEU:HD23	3:D:729:HIS:HD2	1.68	0.57
3:D:829:VAL:O	3:D:830:ALA:HB3	2.05	0.57
3:D:1084:THR:C	3:D:1086:LEU:H	2.07	0.57
3:D:1275:SER:N	3:D:1322:GLY:HA2	2.18	0.57
3:D:1280:VAL:HG13	3:D:1315:ASP:CA	2.18	0.57
3:D:1280:VAL:CG1	3:D:1281:VAL:N	2.68	0.57
3:D:1353:GLN:HB3	3:D:1357:ARG:CD	2.34	0.57
4:E:38:THR:HG22	4:E:39:VAL:N	2.20	0.57
1:B:19:HIS:HB3	1:B:201:THR:O	2.04	0.57
2:C:3:ILE:CG2	2:C:902:ILE:HD13	2.35	0.57
2:C:142:ARG:CD	2:C:324:ASP:HA	2.34	0.57
2:C:662:GLU:O	2:C:663:GLU:HB2	2.04	0.57
2:C:1054:THR:C	2:C:1056:LYS:H	2.08	0.57
3:D:758:GLU:O	3:D:762:GLN:HG3	2.04	0.57
3:D:1430:SER:O	3:D:1431:THR:HB	2.05	0.57
4:E:17:TYR:O	4:E:21:VAL:HG23	2.05	0.57
1:A:56:VAL:HB	1:A:142:VAL:HB	1.86	0.57
2:C:202:TYR:CD1	2:C:304:LEU:HD13	2.39	0.57
2:C:374:ASN:O	2:C:376:ARG:N	2.38	0.57
2:C:747:ALA:O	2:C:749:VAL:HG23	2.05	0.57
2:C:760:SER:O	2:C:785:VAL:HG22	2.05	0.57
3:D:558:LEU:HD21	3:D:567:ILE:HG13	1.86	0.57
3:D:890:VAL:HG11	3:D:922:LEU:HD11	1.87	0.57
4:E:79:LEU:O	4:E:81:PRO:HD2	2.04	0.57
1:A:41:ARG:HG2	1:A:177:VAL:HB	1.85	0.57
1:A:225:PHE:CZ	1:B:25:LEU:HD23	2.40	0.57
1:B:25:LEU:CD1	1:B:28:LEU:HD11	2.29	0.57
2:C:149:THR:HB	2:C:158:TYR:CE1	2.34	0.57
2:C:162:ILE:HG22	2:C:163:ILE:N	2.20	0.57
2:C:211:LEU:HD22	2:C:304:LEU:CD1	2.34	0.57
2:C:410:ILE:HG21	2:C:468:ARG:NH2	2.19	0.57
2:C:1052:MET:HE2	3:D:623:VAL:HG11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1014:ASN:O	3:D:1015:TYR:CB	2.53	0.57
2:C:51:THR:HG1	2:C:348:LEU:HD23	1.70	0.57
2:C:260:LEU:HD12	2:C:292:ARG:CB	2.35	0.57
2:C:988:VAL:HG12	3:D:948:THR:OG1	2.04	0.57
3:D:480:GLU:HA	3:D:493:ARG:NH1	2.19	0.57
3:D:853:VAL:HG21	3:D:877:PRO:CB	2.35	0.57
3:D:1312:LEU:O	3:D:1313:VAL:CB	2.53	0.57
3:D:1479:ASP:C	3:D:1481:VAL:H	2.07	0.57
1:B:26:GLU:CB	1:B:27:PRO:CD	2.79	0.57
1:B:129:ILE:O	1:B:130:ALA:HB2	2.04	0.57
2:C:12:VAL:O	2:C:13:ILE:HD12	2.05	0.57
2:C:545:ASN:CB	2:C:583:LEU:HD12	2.35	0.57
2:C:659:PRO:O	2:C:660:ALA:CB	2.52	0.57
3:D:69:GLU:O	3:D:70:ALA:HB3	2.05	0.57
3:D:626:SER:HA	3:D:652:LEU:CD1	2.35	0.57
3:D:1023:MET:SD	3:D:1023:MET:N	2.77	0.57
3:D:1250:THR:HG21	3:D:1270:ALA:HB2	1.86	0.57
4:E:3:GLU:HB3	4:E:4:PRO:CD	2.35	0.57
1:A:72:LYS:N	2:C:607:ASP:HB3	2.20	0.56
1:A:101:LEU:HD21	1:A:109:VAL:HG11	1.85	0.56
1:B:150:TYR:CD1	1:B:170:ILE:HG22	2.40	0.56
2:C:468:ARG:O	2:C:469:THR:O	2.23	0.56
2:C:597:ALA:HA	2:C:614:ARG:NH1	2.19	0.56
2:C:728:HIS:CD2	2:C:783:ARG:HH11	2.22	0.56
2:C:843:HIS:HD2	2:C:884:GLN:HA	1.66	0.56
2:C:874:LEU:CD2	3:D:784:ASP:HA	2.35	0.56
2:C:892:LEU:HD23	2:C:892:LEU:N	2.19	0.56
2:C:1077:PRO:O	2:C:1079:PRO:HD3	2.05	0.56
3:D:663:GLU:C	3:D:665:ALA:H	2.09	0.56
3:D:777:PRO:CG	3:D:912:LYS:HG3	2.34	0.56
3:D:934:LEU:O	3:D:935:LYS:C	2.44	0.56
3:D:1277:ILE:HG22	3:D:1278:ASP:N	2.20	0.56
3:D:1379:VAL:HG22	3:D:1394:VAL:O	2.04	0.56
1:B:53:VAL:HG12	1:B:167:VAL:HG21	1.86	0.56
1:B:72:LYS:HB3	1:B:131:THR:HB	1.87	0.56
2:C:100:LEU:HD21	2:C:368:THR:CA	2.36	0.56
2:C:129:ILE:HD12	2:C:386:PHE:HB3	1.85	0.56
2:C:142:ARG:HE	2:C:324:ASP:HA	1.69	0.56
2:C:163:ILE:CG2	2:C:164:PRO:HD2	2.34	0.56
2:C:317:VAL:N	2:C:318:PRO:HD2	2.20	0.56
2:C:568:ALA:O	2:C:569:VAL:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1055:ILE:CG2	2:C:1066:ALA:HB2	2.34	0.56
3:D:461:ILE:HG22	3:D:465:LEU:CD1	2.35	0.56
3:D:580:ALA:HB2	3:D:587:ARG:NH2	2.21	0.56
3:D:702:LEU:HD12	3:D:745:MET:SD	2.45	0.56
3:D:957:PRO:HG3	3:D:1007:VAL:HB	1.87	0.56
1:A:52:ALA:HB3	1:A:171:PHE:CE1	2.39	0.56
1:B:77:GLU:OE1	1:B:77:GLU:HA	2.05	0.56
1:B:100:ILE:HA	1:B:141:GLU:HA	1.86	0.56
1:B:126:ASP:O	1:B:127:LEU:HB3	2.05	0.56
2:C:159:ILE:HD11	2:C:310:LEU:CB	2.29	0.56
2:C:169:GLY:HA2	2:C:264:PRO:O	2.06	0.56
2:C:640:ARG:HG3	2:C:640:ARG:NH1	2.20	0.56
2:C:726:ILE:H	2:C:726:ILE:CD1	2.14	0.56
2:C:735:ARG:HA	2:C:737:LEU:O	2.04	0.56
2:C:873:PRO:HG2	2:C:874:LEU:N	2.18	0.56
2:C:989:VAL:CG1	2:C:990:GLY:N	2.68	0.56
3:D:88:TYR:O	3:D:89:ARG:CB	2.53	0.56
3:D:88:TYR:C	3:D:520:LEU:HD13	2.25	0.56
3:D:91:ALA:CB	3:D:518:PRO:HG2	2.36	0.56
3:D:811:GLU:CA	3:D:814:ALA:HB3	2.24	0.56
3:D:1154:GLU:CB	3:D:1159:ARG:HG2	2.25	0.56
3:D:1381:VAL:HG12	3:D:1382:THR:N	2.20	0.56
3:D:1475:GLY:C	3:D:1477:GLY:N	2.59	0.56
1:A:26:GLU:OE2	1:A:185:ARG:CZ	2.53	0.56
1:A:99:LEU:O	1:A:100:ILE:HD13	2.06	0.56
2:C:100:LEU:HD21	2:C:368:THR:HA	1.87	0.56
2:C:493:ARG:HH12	3:D:1069:GLU:CD	2.08	0.56
2:C:873:PRO:CG	2:C:874:LEU:H	2.18	0.56
2:C:940:GLU:HA	2:C:973:VAL:HG21	1.87	0.56
3:D:20(U):UNK:O	3:D:21(U):UNK:CB	2.53	0.56
3:D:898:GLU:OE1	3:D:921:ARG:NH1	2.38	0.56
3:D:1062:ARG:C	3:D:1062:ARG:HD3	2.25	0.56
3:D:1208:ASP:HA	3:D:1215:VAL:HG22	1.87	0.56
3:D:1376:LEU:HD11	3:D:1421:LEU:CD1	2.32	0.56
3:D:1463:LYS:O	3:D:1467:ILE:HG13	2.05	0.56
3:D:1483:PHE:HE2	4:E:18:ARG:NE	2.03	0.56
1:A:199:ILE:HG22	1:A:199:ILE:O	2.05	0.56
2:C:443:THR:N	2:C:444:PRO:CD	2.69	0.56
2:C:456:ALA:HB3	2:C:459:ALA:CB	2.24	0.56
2:C:918:LEU:HD13	2:C:968:ASP:HA	1.87	0.56
2:C:944:LEU:C	2:C:946:ARG:H	2.07	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1076:VAL:HG21	3:D:753:SER:HB3	1.88	0.56
2:C:1087:VAL:HG12	2:C:1087:VAL:O	2.06	0.56
3:D:87:ARG:CB	3:D:522:PRO:HG2	2.36	0.56
3:D:616:GLN:O	3:D:617:ASN:HB2	2.04	0.56
1:A:159:LYS:C	1:A:161:ARG:H	2.09	0.56
1:A:185:ARG:NH2	1:A:194:LYS:HE3	2.20	0.56
1:B:188:GLN:HG2	3:D:688:TRP:CD1	2.40	0.56
2:C:151:ASP:HB2	2:C:156:GLY:O	2.04	0.56
2:C:314:THR:O	2:C:315:ALA:CB	2.53	0.56
2:C:681:GLY:HA2	3:D:939:PHE:CE2	2.40	0.56
3:D:502:PHE:CD1	3:D:1452:ILE:HG23	2.40	0.56
3:D:1079:LYS:C	3:D:1081:GLY:H	2.07	0.56
3:D:1266:ARG:O	3:D:1268:PRO:CD	2.54	0.56
1:A:157:GLY:CA	1:A:166:PRO:HB3	2.35	0.56
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.41	0.56
1:B:94:MET:SD	1:B:97:THR:HG22	2.45	0.56
2:C:100:LEU:CD1	2:C:108:ILE:HB	2.35	0.56
2:C:260:LEU:CD2	2:C:261:LEU:HB3	2.34	0.56
2:C:325:ILE:C	2:C:327:HIS:H	2.07	0.56
2:C:328:LEU:C	2:C:467:ILE:HD13	2.26	0.56
2:C:337:GLY:O	2:C:341:ALA:HB2	2.06	0.56
2:C:605:LYS:HG3	2:C:611:ILE:HA	1.88	0.56
2:C:693:GLU:OE1	2:C:693:GLU:HA	2.06	0.56
3:D:554:LEU:HD11	3:D:571:LYS:HA	1.87	0.56
3:D:795:VAL:N	3:D:862:ASP:CB	2.67	0.56
3:D:1030:GLY:O	3:D:1031:ASN:HB3	2.06	0.56
3:D:1194:CYS:HB3	3:D:1373:ARG:HH21	1.70	0.56
3:D:1381:VAL:HB	3:D:1390:LEU:O	2.06	0.56
4:E:10:PHE:CE2	4:E:16:LYS:HG3	2.41	0.56
1:A:41:ARG:HH21	2:C:860:HIS:CD2	2.24	0.56
1:A:198:ARG:O	1:A:199:ILE:C	2.44	0.56
1:B:78:ILE:HA	1:B:81:ASN:HD22	1.71	0.56
2:C:31:GLN:HG2	2:C:39:ARG:HD2	1.86	0.56
2:C:144:PRO:HA	2:C:162:ILE:HG21	1.87	0.56
2:C:440:PRO:HG2	2:C:453:THR:OG1	2.06	0.56
2:C:498:GLN:H	2:C:502:PRO:CD	2.18	0.56
2:C:1008:ARG:NE	2:C:1010:THR:O	2.39	0.56
3:D:897:GLN:HE21	3:D:897:GLN:HA	1.71	0.56
2:C:183:THR:HG21	2:C:190:LYS:HG3	1.88	0.56
2:C:233:GLU:O	2:C:237:ARG:HG2	2.06	0.56
2:C:263:ASP:OD2	2:C:264:PRO:HD3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:352:ALA:CA	2:C:355:VAL:HG12	2.32	0.56
2:C:395:LYS:CE	2:C:403:SER:HB2	2.35	0.56
2:C:750:LYS:HE3	3:D:680:GLN:HE22	1.71	0.56
2:C:1008:ARG:HH12	2:C:1021:LEU:N	2.04	0.56
3:D:978:TYR:C	3:D:980:MET:N	2.59	0.56
3:D:1280:VAL:CG1	3:D:1281:VAL:H	2.18	0.56
3:D:1353:GLN:HB3	3:D:1357:ARG:HD2	1.87	0.56
3:D:1450:ALA:CA	3:D:1455:LYS:HG3	2.33	0.56
1:B:103:ALA:HB1	1:B:132:LEU:CD1	2.36	0.56
2:C:166:PRO:CB	2:C:417:GLY:H	2.19	0.56
2:C:203:ASP:N	2:C:207:LEU:HB2	2.21	0.56
2:C:731:GLU:O	2:C:733:ALA:N	2.38	0.56
2:C:841:ASN:C	2:C:841:ASN:ND2	2.59	0.56
3:D:699:VAL:HG12	3:D:717:GLN:HG2	1.87	0.56
3:D:808:THR:N	3:D:809:PRO:CD	2.69	0.56
3:D:971:LEU:O	3:D:974:ILE:N	2.36	0.56
3:D:1015:TYR:CB	3:D:1018:ASN:HB2	2.34	0.56
3:D:1031:ASN:HD21	3:D:1034:GLN:HB2	1.71	0.56
1:A:121:GLU:O	1:A:123:MET:N	2.31	0.55
1:A:143:ARG:HG3	1:A:159:LYS:HG3	1.88	0.55
2:C:208:VAL:HG21	2:C:218:VAL:HG13	1.87	0.55
2:C:343:GLN:HG2	2:C:385:PHE:CB	2.36	0.55
2:C:567:GLN:O	2:C:997:LEU:HA	2.06	0.55
2:C:605:LYS:CD	2:C:607:ASP:HA	2.35	0.55
2:C:867:VAL:HG12	2:C:868:ASP:H	1.70	0.55
3:D:99:ALA:HB3	3:D:458:ALA:HB1	1.87	0.55
3:D:603:LEU:HA	3:D:606:ILE:HD13	1.87	0.55
3:D:659:LYS:C	3:D:659:LYS:HD3	2.27	0.55
3:D:904:VAL:HG12	3:D:906:GLN:CD	2.26	0.55
3:D:936:TYR:O	3:D:940:THR:HG22	2.05	0.55
3:D:1437:ALA:HA	3:D:1440:PHE:HD1	1.71	0.55
3:D:1483:PHE:HE1	4:E:22:VAL:HG23	1.72	0.55
1:A:131:THR:HG23	2:C:644:ARG:CZ	2.37	0.55
1:B:94:MET:CE	1:B:94:MET:CB	2.84	0.55
2:C:21:ILE:O	2:C:25:SER:HB2	2.06	0.55
2:C:31:GLN:HG2	2:C:39:ARG:CD	2.35	0.55
2:C:355:VAL:HG13	2:C:356:ARG:N	2.21	0.55
2:C:360:VAL:HG12	2:C:361:MET:N	2.20	0.55
2:C:501:THR:N	2:C:502:PRO:HD2	2.20	0.55
2:C:580:MET:O	2:C:581:THR:HB	2.07	0.55
2:C:595:LEU:HG	2:C:655:LEU:CD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:665:PHE:O	2:C:666:LEU:C	2.44	0.55
2:C:845:ASN:ND2	2:C:884:GLN:OE1	2.36	0.55
3:D:25(U):UNK:HA	3:D:40(U):UNK:O	2.06	0.55
3:D:1008:PHE:CD2	3:D:1008:PHE:O	2.59	0.55
3:D:1109:GLU:CG	3:D:1110:ALA:N	2.68	0.55
3:D:1335:LEU:HD23	3:D:1344:VAL:HG22	1.88	0.55
2:C:549:PHE:HE1	2:C:579:VAL:HG11	1.71	0.55
2:C:603:VAL:HG21	2:C:645:VAL:HA	1.87	0.55
2:C:755:LEU:HB3	2:C:790:LEU:HD23	1.86	0.55
2:C:831:ARG:O	2:C:832:LYS:O	2.25	0.55
3:D:857:LEU:CD1	3:D:858:LEU:H	2.14	0.55
3:D:865:THR:CG2	3:D:866:THR:N	2.69	0.55
3:D:1141:GLU:CA	3:D:1171:VAL:HG11	2.27	0.55
3:D:1429:LEU:HD12	3:D:1429:LEU:O	2.07	0.55
3:D:1475:GLY:C	3:D:1477:GLY:H	2.08	0.55
1:A:198:ARG:NH1	2:C:934:PHE:CE1	2.74	0.55
2:C:30:LEU:O	2:C:32:ALA:N	2.40	0.55
2:C:163:ILE:HG23	2:C:265:LYS:HZ1	1.72	0.55
2:C:177:GLU:CG	2:C:181:VAL:H	2.19	0.55
2:C:304:LEU:HD23	2:C:305:PRO:CD	2.37	0.55
2:C:313:LEU:HD13	2:C:319:GLY:C	2.27	0.55
2:C:796:GLU:HA	3:D:681:ARG:HH22	1.72	0.55
2:C:837:ASP:H	2:C:1001:VAL:HG23	1.71	0.55
3:D:100:ALA:HA	3:D:575:GLN:OE1	2.06	0.55
3:D:502:PHE:CD2	3:D:507:ASN:ND2	2.73	0.55
3:D:675:ARG:HA	3:D:678:GLU:CB	2.37	0.55
3:D:807:ALA:C	3:D:809:PRO:HD3	2.27	0.55
3:D:865:THR:CG2	3:D:866:THR:H	2.18	0.55
3:D:907:GLU:CG	3:D:911:LEU:HD13	2.37	0.55
3:D:1402:ALA:C	3:D:1404:ASN:H	2.10	0.55
1:A:16:GLN:HG3	1:A:20:TYR:CB	2.36	0.55
1:A:122:ILE:O	1:A:122:ILE:HG22	2.06	0.55
1:A:131:THR:O	1:A:131:THR:CG2	2.52	0.55
1:B:173:PRO:HG3	1:B:204:SER:OG	2.06	0.55
2:C:142:ARG:HG2	2:C:147:TYR:OH	2.07	0.55
2:C:754:ILE:HD13	2:C:791:ARG:HE	1.71	0.55
2:C:1009:SER:HB2	3:D:651:GLU:O	2.07	0.55
3:D:681:ARG:O	3:D:682:ASP:CB	2.55	0.55
3:D:728:LEU:HD13	3:D:745:MET:CE	2.36	0.55
3:D:772:PRO:HG2	3:D:772:PRO:O	2.06	0.55
2:C:15:LEU:HD21	2:C:461:VAL:HG21	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:803:ARG:HB3	2:C:825:VAL:HG22	1.88	0.55
2:C:852:ILE:O	2:C:852:ILE:HG12	2.06	0.55
2:C:1073:GLY:HA2	3:D:659:LYS:HE3	1.88	0.55
3:D:648:MET:CE	3:D:747:VAL:HG11	2.36	0.55
3:D:793:THR:HG21	3:D:907:GLU:OE1	2.06	0.55
3:D:864:VAL:H	3:D:876:SER:HG	1.51	0.55
3:D:1069:GLU:HG3	3:D:1072:ILE:CD1	2.35	0.55
3:D:1083:ASP:O	3:D:1086:LEU:N	2.37	0.55
3:D:1283:ILE:HD12	3:D:1312:LEU:HA	1.89	0.55
3:D:1324:PRO:CG	3:D:1325:LEU:H	2.20	0.55
3:D:1459:LEU:CD1	3:D:1470:ARG:NH1	2.69	0.55
3:D:1471:LEU:HG	3:D:1471:LEU:O	2.06	0.55
2:C:881:ASN:ND2	3:D:1034:GLN:CD	2.60	0.55
2:C:1020:PRO:O	2:C:1021:LEU:HG	2.06	0.55
1:B:12:THR:HB	1:B:24:VAL:HB	1.88	0.55
2:C:44:ILE:H	2:C:44:ILE:HD12	1.71	0.55
2:C:327:HIS:O	2:C:329:GLY:N	2.36	0.55
2:C:479:VAL:O	2:C:480:THR:O	2.25	0.55
2:C:688:ILE:HG22	2:C:869:VAL:HG23	1.89	0.55
2:C:816:LYS:HG3	2:C:819:VAL:HG23	1.89	0.55
2:C:1012:PRO:CG	2:C:1023:GLY:HA3	2.37	0.55
3:D:30(U):UNK:O	3:D:31(U):UNK:CB	2.55	0.55
3:D:616:GLN:O	3:D:617:ASN:CB	2.54	0.55
3:D:965:GLU:O	3:D:968:ASP:N	2.40	0.55
1:A:56:VAL:O	1:A:165:ILE:HG12	2.07	0.55
1:A:95:ALA:O	1:A:96:SER:HB3	2.06	0.55
1:B:104:GLU:O	1:B:136:GLY:HA3	2.06	0.55
1:B:143:ARG:HG2	1:B:144:VAL:N	2.21	0.55
2:C:601:GLY:O	2:C:602:GLU:CB	2.54	0.55
2:C:613:VAL:HG11	2:C:619:ARG:HG3	1.87	0.55
2:C:676:ILE:HG21	2:C:873:PRO:HB3	1.87	0.55
2:C:831:ARG:HG2	2:C:1002:GLU:OE2	2.06	0.55
2:C:839:LEU:O	2:C:840:ALA:O	2.25	0.55
2:C:924:LEU:N	2:C:924:LEU:CD2	2.66	0.55
2:C:1005:MET:HG2	3:D:724:GLN:HG3	1.88	0.55
3:D:1281:VAL:HG13	3:D:1314:LYS:CB	2.36	0.55
3:D:1402:ALA:O	3:D:1406:ARG:HB2	2.06	0.55
1:B:62:LEU:HD23	1:B:163:ASN:OD1	2.07	0.55
1:B:78:ILE:HG13	1:B:129:ILE:O	2.07	0.55
2:C:291:VAL:O	2:C:299:LYS:N	2.38	0.55
2:C:552:HIS:CE1	3:D:1064:GLY:HA2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:672:VAL:HG22	2:C:673:LEU:H	1.71	0.55
2:C:700:TYR:HB2	2:C:833:LEU:HD22	1.89	0.55
3:D:666:PHE:O	3:D:667:ALA:HB3	2.06	0.55
3:D:669:ASN:O	3:D:672:ALA:HB3	2.06	0.55
3:D:970:LYS:HA	3:D:973:GLN:HB2	1.87	0.55
3:D:1148:VAL:HG23	3:D:1165:TYR:CD2	2.42	0.55
3:D:1407:LEU:C	3:D:1409:ALA:H	2.10	0.55
3:D:1436:SER:HB3	3:D:1464:GLU:HG2	1.88	0.55
1:B:100:ILE:HA	1:B:140:MET:O	2.06	0.54
1:B:151:VAL:HG23	1:B:169:ALA:CB	2.32	0.54
2:C:5:ARG:HH22	2:C:10:ARG:NH1	2.05	0.54
2:C:163:ILE:HD12	2:C:163:ILE:N	2.20	0.54
2:C:200:LEU:HD22	2:C:290:LEU:HD13	1.88	0.54
2:C:203:ASP:O	2:C:204:GLN:O	2.25	0.54
2:C:257:LEU:O	2:C:258:PHE:C	2.46	0.54
2:C:440:PRO:HG3	2:C:454:SER:CB	2.36	0.54
2:C:472:ARG:HG2	2:C:472:ARG:HH11	1.73	0.54
2:C:495:THR:HG22	2:C:496:ILE:N	2.21	0.54
2:C:780:GLU:O	2:C:781:LYS:C	2.46	0.54
2:C:889:HIS:C	2:C:891:GLY:N	2.60	0.54
3:D:26:VAL:C	3:D:28:LYS:N	2.60	0.54
3:D:660:LYS:O	3:D:664:LYS:HB2	2.06	0.54
3:D:762:GLN:O	3:D:768:ASN:HB2	2.07	0.54
3:D:1142:SER:O	3:D:1364:HIS:CD2	2.59	0.54
3:D:1324:PRO:CG	3:D:1325:LEU:N	2.70	0.54
3:D:1434:TRP:CD1	3:D:1447:LEU:HD12	2.43	0.54
4:E:27:ALA:HB1	4:E:60:ALA:HB1	1.89	0.54
1:A:72:LYS:HA	2:C:607:ASP:CB	2.32	0.54
2:C:17:PRO:HD2	2:C:20:GLU:CB	2.23	0.54
2:C:202:TYR:HE1	2:C:304:LEU:HB3	1.73	0.54
2:C:291:VAL:HB	2:C:299:LYS:CG	2.37	0.54
2:C:410:ILE:HB	2:C:453:THR:HG23	1.89	0.54
2:C:1111:VAL:O	2:C:1111:VAL:HG12	2.07	0.54
3:D:104:PHE:O	3:D:511:TRP:HZ3	1.90	0.54
3:D:564:GLU:CG	3:D:568:ARG:HE	2.20	0.54
4:E:38:THR:HG22	4:E:40:LEU:N	2.18	0.54
1:A:26:GLU:CB	1:A:27:PRO:CD	2.72	0.54
1:B:147:GLY:HA3	1:B:171:PHE:CG	2.43	0.54
1:B:170:ILE:HD12	1:B:170:ILE:O	2.07	0.54
1:B:173:PRO:O	1:B:201:THR:HB	2.07	0.54
2:C:101:ILE:HG22	2:C:102:HIS:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:439:CYS:HB2	2:C:468:ARG:HH11	1.72	0.54
2:C:1052:MET:HG2	3:D:623:VAL:CG2	2.37	0.54
3:D:91:ALA:HB3	3:D:518:PRO:CD	2.36	0.54
3:D:461:ILE:HG22	3:D:465:LEU:HD13	1.89	0.54
3:D:542:ASP:O	3:D:543:LEU:C	2.45	0.54
3:D:629:SER:HB3	3:D:726:ILE:HD12	1.88	0.54
3:D:699:VAL:CA	3:D:716:PHE:O	2.55	0.54
3:D:905:PRO:O	3:D:906:GLN:CB	2.54	0.54
3:D:952:ASP:O	3:D:954:ALA:N	2.41	0.54
3:D:1105:ILE:HG23	3:D:1200:VAL:CB	2.37	0.54
3:D:1444:THR:O	3:D:1448:THR:N	2.35	0.54
1:B:73:GLU:OE1	1:B:128:HIS:CE1	2.60	0.54
2:C:470:PRO:HG3	2:C:472:ARG:NH2	2.23	0.54
2:C:492:ASP:HA	2:C:509:ALA:CB	2.37	0.54
2:C:1038:TRP:HE1	3:D:1463:LYS:HE3	1.73	0.54
3:D:573:MET:HA	3:D:576:GLU:HB2	1.88	0.54
3:D:688:TRP:C	3:D:690:ALA:N	2.60	0.54
3:D:897:GLN:HA	3:D:897:GLN:NE2	2.22	0.54
3:D:965:GLU:HA	3:D:968:ASP:HB2	1.89	0.54
3:D:1118:ILE:HD11	3:D:1193:THR:HG22	1.90	0.54
3:D:1236:LEU:CD1	3:D:1259:VAL:HG21	2.37	0.54
4:E:42:PRO:HG2	4:E:44:GLU:HG2	1.89	0.54
1:A:162:ILE:HG23	1:A:163:ASN:ND2	2.22	0.54
2:C:159:ILE:HG21	2:C:306:THR:HG23	1.88	0.54
2:C:238:LEU:O	2:C:241:LEU:HB2	2.07	0.54
2:C:328:LEU:CB	2:C:484:VAL:HG11	2.38	0.54
2:C:574:ALA:C	2:C:575:GLN:HG3	2.28	0.54
2:C:692:GLU:OE1	2:C:696:LYS:HE3	2.07	0.54
2:C:881:ASN:OD1	3:D:1034:GLN:NE2	2.40	0.54
2:C:1052:MET:HG3	2:C:1056:LYS:HE3	1.89	0.54
3:D:772:PRO:CB	3:D:778:LEU:HB2	2.36	0.54
3:D:911:LEU:O	3:D:915:VAL:HG23	2.08	0.54
3:D:953:ASP:OD1	3:D:1020:LEU:HG	2.06	0.54
3:D:1148:VAL:O	3:D:1148:VAL:HG12	2.08	0.54
3:D:1271:LYS:O	3:D:1272:ALA:C	2.46	0.54
1:A:104:GLU:C	1:A:136:GLY:HA3	2.27	0.54
1:B:118:ALA:O	1:B:120:VAL:N	2.41	0.54
1:B:143:ARG:HD2	1:B:159:LYS:HG2	1.90	0.54
2:C:266:ARG:C	2:C:268:ASP:H	2.11	0.54
3:D:480:GLU:O	3:D:493:ARG:NH2	2.39	0.54
4:E:26:ARG:NH2	4:E:30:LEU:CD1	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PRO:HG3	1:B:224:TYR:CG	2.43	0.54
1:A:128:HIS:CE1	1:A:131:THR:OG1	2.61	0.54
1:B:188:GLN:CG	3:D:688:TRP:CD1	2.91	0.54
2:C:603:VAL:O	2:C:604:VAL:HG23	2.07	0.54
2:C:908:GLY:O	2:C:909:ALA:HB3	2.07	0.54
3:D:969:ARG:NH2	3:D:970:LYS:HE3	2.22	0.54
3:D:1069:GLU:O	3:D:1071:PHE:N	2.41	0.54
3:D:1331:ASP:O	3:D:1333:HIS:N	2.40	0.54
1:A:157:GLY:N	1:A:166:PRO:HB3	2.23	0.54
1:A:175:ARG:O	1:A:176:ARG:CB	2.56	0.54
2:C:231:PRO:O	2:C:233:GLU:N	2.40	0.54
2:C:328:LEU:C	2:C:484:VAL:HG11	2.28	0.54
2:C:745:ILE:HD12	2:C:802:GLY:HA2	1.90	0.54
2:C:831:ARG:O	2:C:832:LYS:C	2.46	0.54
2:C:958:SER:C	2:C:962:GLN:HE21	2.10	0.54
3:D:654:LYS:O	3:D:657:LEU:HB3	2.08	0.54
3:D:703:ASN:OD1	3:D:704:ARG:N	2.41	0.54
3:D:957:PRO:CD	3:D:1007:VAL:HB	2.38	0.54
3:D:1031:ASN:ND2	3:D:1034:GLN:HB2	2.23	0.54
1:B:47:SER:O	1:B:48:ILE:CG1	2.55	0.54
1:B:76:VAL:HA	1:B:79:ILE:HB	1.90	0.54
2:C:148:PHE:HE2	2:C:310:LEU:HA	1.73	0.54
2:C:289:THR:O	2:C:290:LEU:O	2.26	0.54
2:C:1001:VAL:HG11	3:D:724:GLN:CB	2.32	0.54
3:D:28:LYS:CB	3:D:548:ILE:HG23	2.38	0.54
3:D:497:GLU:HG2	3:D:1389:LEU:HD21	1.88	0.54
1:A:83:LYS:CE	1:A:168:ASP:HB2	2.38	0.54
1:B:220:GLU:O	1:B:223:ASN:HB2	2.08	0.54
1:B:221:HIS:HA	1:B:224:TYR:CE1	2.43	0.54
2:C:31:GLN:HG2	2:C:39:ARG:NE	2.23	0.54
2:C:115:LEU:HA	2:C:375:SER:OG	2.08	0.54
2:C:198:ARG:HG3	2:C:228:ALA:HA	1.89	0.54
2:C:586:ARG:O	2:C:588:VAL:N	2.40	0.54
2:C:722:ILE:HA	2:C:758:ARG:HB2	1.90	0.54
2:C:949:LYS:C	2:C:951:GLY:H	2.11	0.54
2:C:1115:LEU:HD23	2:C:1115:LEU:N	2.23	0.54
3:D:82:ARG:O	3:D:84:ILE:N	2.41	0.54
3:D:558:LEU:HD11	3:D:567:ILE:HD11	1.90	0.54
3:D:760:ARG:HH12	4:E:59:ASN:ND2	2.06	0.54
3:D:832:ARG:O	3:D:832:ARG:HG2	2.07	0.54
3:D:1213:ARG:HG3	3:D:1214:PRO:CD	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:VAL:HG13	1:B:199:ILE:HD12	1.90	0.53
2:C:640:ARG:HG3	2:C:641:PRO:HD2	1.89	0.53
2:C:915:LYS:O	2:C:919:ALA:N	2.41	0.53
3:D:117:ASP:C	3:D:119:SER:H	2.10	0.53
3:D:149:LYS:O	3:D:151:GLN:N	2.41	0.53
3:D:723:GLY:C	3:D:724:GLN:HE21	2.12	0.53
3:D:1009:ASN:OD1	3:D:1009:ASN:O	2.25	0.53
3:D:1264:GLU:O	3:D:1265:ALA:HB3	2.08	0.53
2:C:520:GLU:N	2:C:521:PRO:HD3	2.22	0.53
2:C:555:ALA:O	2:C:558:ALA:HB3	2.08	0.53
2:C:959:PRO:HG2	2:C:960:GLU:N	2.18	0.53
3:D:876:SER:O	3:D:877:PRO:C	2.46	0.53
3:D:879:ARG:HE	3:D:904:VAL:H	1.56	0.53
3:D:1479:ASP:C	3:D:1481:VAL:N	2.61	0.53
1:A:22:GLU:HA	1:A:198:ARG:HA	1.89	0.53
1:B:53:VAL:HG23	1:B:85:LEU:HD23	1.90	0.53
1:B:101:LEU:HD23	1:B:140:MET:HE2	1.89	0.53
2:C:13:ILE:HG23	2:C:14:PRO:CD	2.38	0.53
2:C:363:SER:OG	2:C:364:PRO:HD2	2.08	0.53
2:C:466:PHE:HD1	2:C:467:ILE:CG1	2.22	0.53
2:C:493:ARG:NH1	3:D:1069:GLU:CD	2.62	0.53
2:C:566:THR:C	2:C:568:ALA:H	2.12	0.53
2:C:598:GLU:N	2:C:614:ARG:NH1	2.56	0.53
2:C:854:PRO:HB2	2:C:856:GLU:HG3	1.91	0.53
2:C:901:TYR:C	2:C:902:ILE:HD12	2.29	0.53
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.43	0.53
3:D:8:VAL:HG12	3:D:1434:TRP:HH2	1.72	0.53
3:D:702:LEU:O	3:D:713:ILE:O	2.26	0.53
3:D:882:PHE:HA	3:D:885:ILE:CD1	2.35	0.53
3:D:951:ILE:HG22	3:D:952:ASP:N	2.23	0.53
3:D:1033:GLN:HG3	3:D:1034:GLN:N	2.24	0.53
3:D:1156:LEU:CD1	3:D:1177:ALA:HA	2.38	0.53
3:D:1281:VAL:HG22	3:D:1315:ASP:H	1.73	0.53
3:D:1363:LEU:O	3:D:1364:HIS:HB2	2.08	0.53
3:D:1409:ALA:O	3:D:1413:VAL:N	2.40	0.53
3:D:1465:ASN:HD21	3:D:1470:ARG:NH1	2.06	0.53
1:A:138:LEU:O	1:A:139:TYR:C	2.47	0.53
1:B:71:VAL:HA	1:B:132:LEU:HA	1.91	0.53
1:B:124:ASN:OD1	1:B:124:ASN:N	2.41	0.53
2:C:243:ARG:HG3	2:C:244:PRO:HA	1.89	0.53
2:C:399:ASN:ND2	2:C:402:SER:H	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:478:VAL:C	2:C:479:VAL:HG22	2.29	0.53
2:C:613:VAL:HG22	2:C:620:LEU:N	2.24	0.53
2:C:801:VAL:HG23	2:C:828:ALA:HB2	1.88	0.53
2:C:882:LEU:HD11	2:C:884:GLN:NE2	2.23	0.53
3:D:989:TYR:CZ	3:D:993:ILE:HG13	2.44	0.53
3:D:1043:GLY:CA	3:D:1057:VAL:H	2.17	0.53
3:D:1224:VAL:O	3:D:1224:VAL:HG12	2.08	0.53
3:D:1420:LEU:HD12	3:D:1421:LEU:H	1.72	0.53
3:D:1434:TRP:HD1	3:D:1447:LEU:HD12	1.74	0.53
3:D:1459:LEU:HD12	3:D:1470:ARG:NH1	2.24	0.53
4:E:41:GLU:N	4:E:42:PRO:HD2	2.23	0.53
1:A:6:LEU:C	1:A:8:ALA:N	2.62	0.53
1:B:109:VAL:HG21	1:B:138:LEU:HD23	1.91	0.53
2:C:100:LEU:HD23	2:C:372:LEU:HD12	1.90	0.53
2:C:466:PHE:HD1	2:C:467:ILE:HG13	1.72	0.53
2:C:580:MET:O	2:C:581:THR:O	2.27	0.53
2:C:628:TYR:O	2:C:629:ALA:O	2.26	0.53
2:C:672:VAL:O	2:C:991:GLN:HA	2.08	0.53
2:C:1076:VAL:HG21	3:D:753:SER:CB	2.38	0.53
3:D:571:LYS:C	3:D:573:MET:N	2.62	0.53
3:D:715:ALA:O	3:D:764:LEU:HD12	2.07	0.53
3:D:916:TYR:CD2	3:D:917:GLN:N	2.76	0.53
3:D:949:ILE:O	3:D:949:ILE:HG22	2.08	0.53
3:D:1041:MET:HG2	3:D:1042:ARG:N	2.24	0.53
1:A:31:GLY:N	1:A:193:ASP:OD2	2.37	0.53
1:B:33:GLY:HA3	1:B:181:VAL:HG21	1.90	0.53
2:C:102:HIS:HD2	2:C:106:GLY:HA3	1.72	0.53
2:C:118:LEU:HD23	2:C:118:LEU:C	2.28	0.53
2:C:376:ARG:N	2:C:377:PRO:CD	2.62	0.53
2:C:440:PRO:HG3	2:C:454:SER:CA	2.38	0.53
2:C:449:ILE:O	2:C:451:LEU:N	2.41	0.53
2:C:839:LEU:O	2:C:994:ILE:HG22	2.08	0.53
2:C:892:LEU:HD23	2:C:893:ALA:N	2.22	0.53
2:C:1103:ASP:O	2:C:1104:GLU:C	2.47	0.53
3:D:643:GLY:CA	3:D:727:GLN:HB2	2.39	0.53
3:D:792:ILE:HG12	3:D:941:LEU:HG	1.91	0.53
3:D:879:ARG:NE	3:D:904:VAL:H	2.06	0.53
3:D:1311:LEU:H	3:D:1311:LEU:HD12	1.73	0.53
3:D:1393:GLN:HE21	3:D:1420:LEU:HD21	1.74	0.53
1:A:131:THR:HG23	2:C:644:ARG:NE	2.23	0.53
2:C:443:THR:H	2:C:444:PRO:CD	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:589:ARG:HH12	2:C:596:TYR:CB	2.22	0.53
2:C:718:GLY:HA3	2:C:761:PHE:CG	2.43	0.53
2:C:1019:GLN:HB2	3:D:622:ARG:HB2	1.91	0.53
3:D:89:ARG:O	3:D:520:LEU:HD21	2.07	0.53
3:D:542:ASP:O	3:D:544:TYR:N	2.42	0.53
3:D:634:GLY:O	3:D:636:GLN:N	2.42	0.53
3:D:876:SER:CA	3:D:879:ARG:HG3	2.38	0.53
3:D:1231:GLU:HB3	3:D:1232:PRO:CD	2.32	0.53
4:E:63:TRP:O	4:E:66:LYS:N	2.40	0.53
1:B:207:PRO:O	1:B:210:ALA:N	2.42	0.53
2:C:144:PRO:HA	2:C:162:ILE:HG22	1.89	0.53
2:C:240:THR:O	2:C:240:THR:HG22	2.09	0.53
2:C:759:THR:HB	2:C:785:VAL:HG11	1.89	0.53
2:C:841:ASN:HD21	2:C:845:ASN:H	1.55	0.53
2:C:987:ILE:HD11	3:D:946:GLY:CA	2.38	0.53
3:D:563:PRO:O	3:D:565:ILE:N	2.42	0.53
3:D:578:VAL:C	3:D:580:ALA:N	2.62	0.53
3:D:910:SER:O	3:D:911:LEU:C	2.46	0.53
2:C:111:ASP:O	2:C:113:VAL:N	2.34	0.53
2:C:218:VAL:O	2:C:221:LEU:N	2.42	0.53
2:C:336:VAL:O	2:C:339:LEU:N	2.41	0.53
2:C:552:HIS:CE1	3:D:1064:GLY:CA	2.92	0.53
2:C:811:PRO:O	2:C:813:VAL:N	2.41	0.53
2:C:840:ALA:HB2	2:C:846:LYS:HA	1.91	0.53
3:D:468:LEU:O	3:D:471:GLU:HG2	2.09	0.53
3:D:809:PRO:C	3:D:811:GLU:N	2.62	0.53
3:D:1402:ALA:O	3:D:1404:ASN:N	2.42	0.53
1:A:41:ARG:HH11	1:A:41:ARG:CB	2.21	0.53
1:A:41:ARG:HE	2:C:860:HIS:CE1	2.26	0.53
1:A:52:ALA:HB3	1:A:171:PHE:CD1	2.44	0.53
1:A:225:PHE:HE1	1:B:36:LEU:HD13	1.73	0.53
1:B:53:VAL:CG2	1:B:85:LEU:HD23	2.40	0.53
1:B:58:ILE:HA	1:B:139:TYR:O	2.09	0.53
1:B:174:VAL:HA	1:B:201:THR:HB	1.90	0.53
2:C:17:PRO:O	2:C:18:LEU:CB	2.56	0.53
2:C:257:LEU:O	2:C:260:LEU:N	2.41	0.53
2:C:290:LEU:HD12	2:C:291:VAL:N	2.21	0.53
2:C:308:ARG:O	2:C:310:LEU:N	2.42	0.53
2:C:564:MET:CE	2:C:846:LYS:HB3	2.39	0.53
2:C:577:PRO:HG2	2:C:580:MET:CB	2.38	0.53
2:C:1017:THR:O	2:C:1018:GLN:CB	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1095:LEU:HD11	3:D:603:LEU:HB3	1.91	0.53
3:D:811:GLU:HA	3:D:814:ALA:CB	2.24	0.53
3:D:971:LEU:O	3:D:974:ILE:HG22	2.09	0.53
3:D:1015:TYR:HA	3:D:1018:ASN:HD22	1.74	0.53
3:D:1260:ILE:HG22	3:D:1261:GLU:N	2.23	0.53
1:A:26:GLU:OE2	1:A:185:ARG:NH2	2.42	0.52
1:A:74:ASP:C	1:A:74:ASP:OD1	2.46	0.52
1:B:14:THR:HB	1:B:22:GLU:HB3	1.90	0.52
1:B:179:PHE:CB	1:B:197:LEU:HD12	2.39	0.52
2:C:163:ILE:HG21	2:C:169:GLY:CA	2.39	0.52
2:C:921:ALA:HA	2:C:924:LEU:HG	1.92	0.52
3:D:509:PRO:HA	3:D:511:TRP:CD1	2.44	0.52
3:D:542:ASP:O	3:D:545:ARG:N	2.41	0.52
3:D:638:LYS:CB	3:D:932:ASP:OD1	2.57	0.52
3:D:705:ALA:HB3	3:D:706:PRO:HD2	1.91	0.52
3:D:965:GLU:C	3:D:968:ASP:H	2.13	0.52
3:D:1043:GLY:O	3:D:1057:VAL:HG23	2.08	0.52
3:D:1192:LEU:CD2	3:D:1369:GLU:HB3	2.39	0.52
4:E:3:GLU:HG3	4:E:6:ILE:HD11	1.91	0.52
1:A:162:ILE:HG12	1:A:163:ASN:CG	2.30	0.52
1:A:186:LEU:O	1:A:187:GLY:C	2.46	0.52
1:B:79:ILE:HG23	1:B:167:VAL:CG1	2.40	0.52
1:B:203:GLY:O	1:B:204:SER:CB	2.58	0.52
2:C:232:GLU:C	2:C:234:ALA:N	2.61	0.52
2:C:501:THR:N	2:C:502:PRO:CD	2.73	0.52
2:C:507:ARG:O	2:C:518:ARG:HA	2.09	0.52
2:C:552:HIS:NE2	2:C:886:LEU:HD12	2.24	0.52
2:C:600:ASP:C	2:C:648:ARG:HB2	2.28	0.52
3:D:502:PHE:HE1	3:D:1452:ILE:CG1	2.17	0.52
3:D:890:VAL:HG13	3:D:922:LEU:HD13	1.90	0.52
3:D:1082:ALA:O	3:D:1085:ALA:HB3	2.09	0.52
3:D:1119:SER:HA	3:D:1186:VAL:O	2.09	0.52
3:D:1216:SER:OG	4:E:16:LYS:N	2.42	0.52
3:D:1223:VAL:O	3:D:1227:GLU:HG3	2.10	0.52
3:D:1439:SER:OG	3:D:1467:ILE:HD11	2.09	0.52
4:E:25:LYS:O	4:E:25:LYS:HD3	2.08	0.52
2:C:874:LEU:O	2:C:876:VAL:N	2.42	0.52
3:D:115:LEU:C	3:D:117:ASP:N	2.59	0.52
3:D:569:ASN:O	3:D:572:ARG:HG2	2.10	0.52
3:D:764:LEU:HD21	3:D:766:ALA:HB3	1.92	0.52
3:D:1274:ILE:HD11	3:D:1334:GLN:NE2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1365:ASP:C	3:D:1366:LYS:HG3	2.29	0.52
1:A:76:VAL:HG21	2:C:628:TYR:OH	2.09	0.52
1:A:101:LEU:O	1:A:139:TYR:HA	2.09	0.52
1:A:121:GLU:HB3	1:A:123:MET:HE3	1.91	0.52
2:C:68:PHE:CD2	2:C:98:LEU:HD22	2.43	0.52
2:C:603:VAL:O	2:C:604:VAL:CB	2.58	0.52
2:C:642:ARG:O	2:C:643:VAL:HB	2.09	0.52
2:C:922:PHE:CD2	2:C:964:LYS:HG3	2.45	0.52
2:C:953:VAL:HG23	2:C:966:LEU:HD13	1.91	0.52
2:C:1045:ALA:CB	2:C:1048:THR:HB	2.28	0.52
3:D:494:LYS:O	3:D:497:GLU:HB2	2.08	0.52
3:D:495:ARG:O	3:D:499:VAL:N	2.28	0.52
3:D:885:ILE:HG12	3:D:937:TYR:CE2	2.44	0.52
3:D:1202:GLN:O	3:D:1203:LYS:CB	2.57	0.52
3:D:1251:ASP:O	3:D:1253:THR:N	2.40	0.52
4:E:9:LEU:HD23	4:E:69:LEU:HD13	1.90	0.52
1:A:9:PRO:HA	1:A:27:PRO:HD2	1.91	0.52
1:A:16:GLN:HA	1:A:16:GLN:HE21	1.75	0.52
1:B:199:ILE:HG22	1:B:207:PRO:HB3	1.90	0.52
2:C:146:VAL:HG22	2:C:161:SER:HA	1.91	0.52
2:C:552:HIS:ND1	3:D:1064:GLY:HA2	2.25	0.52
2:C:626:ARG:NE	2:C:637:PHE:CZ	2.76	0.52
2:C:820:ARG:O	2:C:821:GLU:O	2.27	0.52
2:C:959:PRO:CG	2:C:960:GLU:H	2.18	0.52
3:D:545:ARG:CG	3:D:546:ARG:N	2.72	0.52
3:D:658:LEU:HA	3:D:661:MET:CE	2.39	0.52
3:D:863:THR:C	3:D:864:VAL:HG23	2.30	0.52
3:D:927:THR:O	3:D:931:LEU:HD23	2.09	0.52
3:D:1399:ASP:OD2	3:D:1417:TRP:HB3	2.10	0.52
1:B:148:VAL:HG23	1:B:149:GLY:H	1.74	0.52
2:C:445:GLU:HG3	5:C:1640:RFP:H303	1.90	0.52
2:C:568:ALA:O	2:C:569:VAL:HG12	2.10	0.52
3:D:783:ARG:O	3:D:784:ASP:CB	2.49	0.52
3:D:1292:VAL:HG23	3:D:1305:LEU:HD23	1.91	0.52
3:D:1437:ALA:HA	3:D:1440:PHE:CD1	2.45	0.52
1:A:56:VAL:HG13	1:A:167:VAL:CG2	2.40	0.52
1:B:59:GLU:O	1:B:60:ASP:CB	2.58	0.52
1:B:132:LEU:N	1:B:132:LEU:CD2	2.73	0.52
2:C:141:HIS:HE1	2:C:334:ARG:HG3	1.75	0.52
2:C:613:VAL:HG22	2:C:621:VAL:N	2.24	0.52
2:C:671:ASN:HB3	2:C:993:PHE:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:911:GLU:N	2:C:912:PRO:HD2	2.25	0.52
3:D:691:LEU:C	3:D:693:GLU:N	2.63	0.52
3:D:774:SER:HA	3:D:1209:LEU:HD21	1.92	0.52
3:D:1110:ALA:O	3:D:1112:CYS:N	2.42	0.52
3:D:1462:LEU:HD23	3:D:1473:PRO:CG	2.40	0.52
1:A:53:VAL:HG21	1:A:82:LEU:O	2.09	0.52
1:A:105:GLY:HA2	1:A:136:GLY:H	1.75	0.52
1:A:134:GLU:CB	2:C:606:VAL:HG23	2.40	0.52
1:B:38:ASN:HB3	1:B:39:PRO:CD	2.35	0.52
2:C:713:ARG:HB2	2:C:720:GLU:OE1	2.09	0.52
3:D:699:VAL:HG12	3:D:717:GLN:HG3	1.92	0.52
3:D:885:ILE:HD13	3:D:937:TYR:HD2	1.75	0.52
3:D:1147:ARG:HB3	3:D:1188:VAL:HG21	1.89	0.52
3:D:1221:VAL:O	3:D:1222:GLY:C	2.46	0.52
3:D:1304:LYS:H	3:D:1304:LYS:CD	2.23	0.52
3:D:1365:ASP:O	3:D:1366:LYS:HB2	2.09	0.52
1:A:28:LEU:CD1	1:A:195:LEU:HB2	2.40	0.52
1:B:74:ASP:O	1:B:75:VAL:C	2.48	0.52
2:C:84:ARG:HA	2:C:131:GLY:CA	2.38	0.52
2:C:137:VAL:HG21	2:C:393:GLN:CD	2.29	0.52
3:D:599:PRO:C	3:D:600:LEU:HD23	2.30	0.52
3:D:759:ALA:HA	3:D:763:MET:HG2	1.92	0.52
3:D:968:ASP:O	3:D:971:LEU:HB2	2.09	0.52
3:D:1365:ASP:O	3:D:1366:LYS:CB	2.58	0.52
1:A:122:ILE:O	1:A:124:ASN:N	2.43	0.52
1:A:124:ASN:ND2	1:A:127:LEU:HD22	2.25	0.52
1:A:222:LEU:O	1:A:225:PHE:HD1	1.92	0.52
2:C:16:PRO:HB3	2:C:586:ARG:HH21	1.75	0.52
2:C:52:PHE:O	2:C:52:PHE:HD1	1.93	0.52
2:C:65:VAL:HB	2:C:101:ILE:HG12	1.91	0.52
2:C:215:GLY:O	2:C:217:LEU:HG	2.10	0.52
2:C:369:PRO:C	2:C:371:LYS:H	2.12	0.52
2:C:613:VAL:HG21	2:C:619:ARG:HE	1.75	0.52
3:D:518:PRO:HA	3:D:544:TYR:OH	2.09	0.52
3:D:1335:LEU:HD23	3:D:1344:VAL:CG2	2.40	0.52
3:D:1486:VAL:O	4:E:79:LEU:CD1	2.58	0.52
1:A:108:GLU:HG2	2:C:644:ARG:NH2	2.24	0.51
2:C:325:ILE:O	2:C:327:HIS:N	2.43	0.51
2:C:399:ASN:OD1	2:C:668:LEU:HD22	2.11	0.51
2:C:586:ARG:O	2:C:589:ARG:N	2.43	0.51
2:C:845:ASN:HD21	2:C:876:VAL:HG11	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:552:ASN:C	3:D:554:LEU:H	2.13	0.51
3:D:823:LEU:O	3:D:824:ASN:CB	2.58	0.51
3:D:1237:THR:O	3:D:1257:PRO:HD3	2.11	0.51
3:D:1443:THR:O	3:D:1447:LEU:HB2	2.09	0.51
1:A:59:GLU:HG2	1:A:137:LYS:CE	2.34	0.51
1:A:125:PRO:O	1:A:127:LEU:N	2.43	0.51
2:C:73:ILE:HG22	2:C:74:GLY:N	2.26	0.51
2:C:610:ARG:HA	2:C:623:HIS:O	2.11	0.51
2:C:662:GLU:O	2:C:662:GLU:HG3	2.10	0.51
2:C:690:ILE:O	2:C:852:ILE:HA	2.10	0.51
3:D:643:GLY:HA3	3:D:727:GLN:N	2.16	0.51
3:D:962:ARG:O	3:D:966:GLU:HG3	2.10	0.51
1:B:56:VAL:HG13	1:B:142:VAL:HB	1.92	0.51
2:C:184:MET:CG	2:C:193:LEU:HD23	2.40	0.51
2:C:601:GLY:HA3	2:C:647:GLN:C	2.31	0.51
2:C:603:VAL:O	2:C:604:VAL:HB	2.11	0.51
2:C:873:PRO:O	2:C:874:LEU:C	2.47	0.51
2:C:950:LEU:O	2:C:951:GLY:C	2.49	0.51
3:D:617:ASN:OD1	3:D:621:LYS:HE3	2.11	0.51
3:D:1377:LYS:HG2	3:D:1378:TYR:CE1	2.45	0.51
3:D:1403:LEU:HD12	3:D:1417:TRP:CZ3	2.43	0.51
4:E:30:LEU:C	4:E:32:ARG:N	2.64	0.51
1:B:38:ASN:ND2	1:B:41:ARG:HD2	2.25	0.51
2:C:163:ILE:CB	2:C:164:PRO:HD2	2.41	0.51
2:C:236:VAL:HG13	2:C:248:PRO:O	2.10	0.51
2:C:282:GLY:O	2:C:283:VAL:HB	2.10	0.51
2:C:283:VAL:CG1	2:C:284:GLY:N	2.73	0.51
2:C:577:PRO:HB3	2:C:993:PHE:CE2	2.44	0.51
2:C:874:LEU:HD21	3:D:784:ASP:N	2.25	0.51
3:D:104:PHE:O	3:D:511:TRP:CZ3	2.62	0.51
3:D:639:LEU:O	3:D:641:GLN:N	2.41	0.51
3:D:916:TYR:O	3:D:918:ALA:N	2.43	0.51
3:D:1475:GLY:O	3:D:1477:GLY:N	2.43	0.51
4:E:13:VAL:HG21	4:E:19:LEU:HB2	1.92	0.51
1:A:225:PHE:CE2	1:B:25:LEU:HD23	2.46	0.51
2:C:3:ILE:HD13	2:C:900:ARG:HB2	1.91	0.51
2:C:13:ILE:HG23	2:C:14:PRO:HD2	1.91	0.51
2:C:193:LEU:HD11	2:C:307:LEU:HD22	1.93	0.51
2:C:243:ARG:CG	2:C:244:PRO:HA	2.41	0.51
2:C:270:GLY:O	2:C:274:ARG:HG2	2.09	0.51
2:C:937:ASP:OD1	2:C:939:ARG:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:729:HIS:O	3:D:731:LEU:N	2.44	0.51
3:D:808:THR:HG22	3:D:808:THR:O	2.09	0.51
3:D:1330:ILE:O	3:D:1331:ASP:C	2.49	0.51
1:B:118:ALA:C	1:B:120:VAL:H	2.13	0.51
2:C:8:ARG:O	2:C:494:TYR:OH	2.27	0.51
2:C:15:LEU:HD21	2:C:461:VAL:CB	2.41	0.51
2:C:443:THR:H	2:C:444:PRO:HD3	1.76	0.51
2:C:460:ARG:HG3	2:C:461:VAL:N	2.26	0.51
2:C:548:PRO:HG3	2:C:842:ARG:NH2	2.25	0.51
2:C:631:SER:OG	2:C:636:ALA:N	2.31	0.51
2:C:699:PHE:O	2:C:701:THR:N	2.43	0.51
2:C:713:ARG:HH12	2:C:816:LYS:HG2	1.74	0.51
2:C:1034:GLU:O	2:C:1037:VAL:N	2.43	0.51
3:D:486:ARG:CG	3:D:487:ALA:H	2.22	0.51
3:D:1038:LEU:O	3:D:1060:SER:O	2.28	0.51
3:D:1397:LYS:HD2	3:D:1400:VAL:HB	1.92	0.51
1:A:196:THR:O	1:A:196:THR:OG1	2.26	0.51
2:C:282:GLY:O	2:C:283:VAL:CB	2.59	0.51
2:C:310:LEU:O	2:C:313:LEU:HB3	2.10	0.51
2:C:430:VAL:O	2:C:431:HIS:C	2.49	0.51
2:C:874:LEU:CD2	3:D:784:ASP:CA	2.88	0.51
2:C:976:ASP:O	2:C:978:ARG:N	2.44	0.51
3:D:999:THR:HG23	3:D:1000:THR:N	2.26	0.51
3:D:1088:THR:O	3:D:1091:SER:HB3	2.10	0.51
3:D:1110:ALA:HA	3:D:1202:GLN:O	2.10	0.51
3:D:1166:LEU:HD22	3:D:1166:LEU:H	1.75	0.51
1:B:205:VAL:HG12	1:B:206:THR:N	2.26	0.51
2:C:758:ARG:HG3	2:C:758:ARG:NH1	2.25	0.51
2:C:1034:GLU:OE2	3:D:1096:ARG:NH1	2.44	0.51
3:D:542:ASP:O	3:D:545:ARG:HG2	2.10	0.51
3:D:879:ARG:CZ	3:D:904:VAL:CA	2.88	0.51
3:D:1251:ASP:C	3:D:1253:THR:N	2.62	0.51
4:E:41:GLU:N	4:E:42:PRO:CD	2.74	0.51
1:A:105:GLY:O	1:A:133:GLU:HA	2.10	0.51
1:A:158:ILE:HG13	1:A:161:ARG:CG	2.41	0.51
2:C:333:ILE:HG21	2:C:460:ARG:NH2	2.26	0.51
2:C:401:LEU:HD21	2:C:543:ASN:HB2	1.92	0.51
2:C:676:ILE:HG22	2:C:677:MET:N	2.25	0.51
2:C:729:LEU:HD21	2:C:754:ILE:CD1	2.40	0.51
2:C:755:LEU:HD13	2:C:755:LEU:C	2.31	0.51
2:C:925:TYR:OH	2:C:972:VAL:HG21	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:981:GLU:HB3	2:C:982:PRO:CD	2.41	0.51
2:C:1101:THR:HB	2:C:1110:ASP:CB	2.41	0.51
3:D:489:ARG:O	3:D:493:ARG:HG2	2.11	0.51
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.92	0.51
3:D:645:PRO:HB3	3:D:724:GLN:H	1.76	0.51
3:D:1150:ALA:O	3:D:1151:ARG:HB2	2.10	0.51
3:D:1228:SER:O	3:D:1232:PRO:HD2	2.11	0.51
1:A:72:LYS:O	1:A:73:GLU:O	2.29	0.51
1:B:64:GLU:HA	1:B:75:VAL:HG11	1.93	0.51
1:B:97:THR:HG21	1:B:120:VAL:CG2	2.30	0.51
2:C:115:LEU:CG	2:C:116:GLY:H	2.24	0.51
2:C:254:LEU:C	2:C:256:TYR:H	2.12	0.51
2:C:428:ARG:O	2:C:429:ASP:CB	2.59	0.51
2:C:564:MET:HG3	2:C:997:LEU:CD1	2.39	0.51
2:C:796:GLU:CG	3:D:681:ARG:HH22	2.24	0.51
2:C:943:VAL:O	2:C:944:LEU:C	2.49	0.51
2:C:950:LEU:C	3:D:1018:ASN:HD21	2.14	0.51
2:C:1008:ARG:O	3:D:652:LEU:HD13	2.11	0.51
2:C:1059:ASP:HA	2:C:1083:GLU:CB	2.41	0.51
3:D:905:PRO:HG2	3:D:906:GLN:N	2.26	0.51
3:D:1277:ILE:CG2	3:D:1279:GLY:H	2.24	0.51
3:D:1457:ASP:C	3:D:1459:LEU:H	2.14	0.51
4:E:17:TYR:N	4:E:17:TYR:CD1	2.77	0.51
1:A:42:ARG:HD3	2:C:977:GLY:O	2.12	0.50
1:B:114:PHE:O	1:B:116:PRO:N	2.44	0.50
2:C:139:GLN:NE2	2:C:334:ARG:NH2	2.59	0.50
2:C:183:THR:CG2	2:C:190:LYS:HG3	2.40	0.50
2:C:201:GLY:O	2:C:203:ASP:OD2	2.29	0.50
2:C:354:GLY:O	2:C:357:GLU:HB3	2.11	0.50
2:C:637:PHE:HB2	2:C:659:PRO:CB	2.41	0.50
3:D:117:ASP:C	3:D:119:SER:N	2.65	0.50
3:D:521:PRO:N	3:D:522:PRO:CD	2.73	0.50
3:D:729:HIS:HE1	3:D:935:LYS:HD3	1.75	0.50
3:D:795:VAL:HG12	3:D:796:ARG:H	1.75	0.50
3:D:1105:ILE:HG21	3:D:1370:ILE:HG23	1.92	0.50
3:D:1107:VAL:HG12	3:D:1217:ILE:HD13	1.92	0.50
3:D:1353:GLN:O	3:D:1356:TYR:N	2.43	0.50
3:D:1483:PHE:CE2	4:E:18:ARG:NE	2.79	0.50
4:E:77:GLU:OE1	4:E:77:GLU:HA	2.11	0.50
1:A:6:LEU:O	1:A:8:ALA:N	2.45	0.50
2:C:148:PHE:HE2	2:C:310:LEU:CA	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:377:PRO:O	2:C:379:GLU:O	2.27	0.50
2:C:743:VAL:HG13	2:C:744:ARG:N	2.26	0.50
2:C:796:GLU:HG2	3:D:681:ARG:NH1	2.25	0.50
3:D:690:ALA:O	3:D:694:VAL:HG23	2.11	0.50
3:D:968:ASP:HA	3:D:971:LEU:HB2	1.94	0.50
4:E:28:GLN:O	4:E:28:GLN:HG2	2.11	0.50
4:E:48:MET:O	4:E:49:ARG:HG3	2.12	0.50
2:C:15:LEU:HD22	2:C:471:TYR:OH	2.11	0.50
2:C:35:PRO:C	2:C:37:GLU:H	2.12	0.50
2:C:66:LEU:HD11	2:C:98:LEU:HB2	1.94	0.50
2:C:137:VAL:HG12	2:C:411:SER:HB2	1.93	0.50
2:C:415:PRO:O	2:C:416:GLY:O	2.29	0.50
2:C:1082:PRO:HG2	2:C:1085:PHE:HB3	1.93	0.50
3:D:1252:ILE:C	3:D:1254:GLN:N	2.64	0.50
3:D:1273:VAL:H	3:D:1324:PRO:CG	2.22	0.50
3:D:1459:LEU:HD12	3:D:1470:ARG:HH11	1.76	0.50
4:E:27:ALA:HB1	4:E:60:ALA:CB	2.41	0.50
1:A:56:VAL:HG13	1:A:167:VAL:HG23	1.94	0.50
1:B:58:ILE:HG23	1:B:140:MET:CG	2.42	0.50
1:B:58:ILE:O	1:B:59:GLU:C	2.49	0.50
1:B:68:ILE:N	1:B:68:ILE:HD12	2.27	0.50
2:C:118:LEU:HD23	2:C:119:PRO:O	2.10	0.50
2:C:186:VAL:HG11	2:C:258:PHE:CD2	2.47	0.50
2:C:263:ASP:CG	2:C:264:PRO:HD3	2.31	0.50
2:C:348:LEU:HA	2:C:351:LEU:HB3	1.93	0.50
2:C:407:LYS:C	2:C:409:ARG:H	2.13	0.50
2:C:492:ASP:H	2:C:532:MET:N	2.08	0.50
2:C:492:ASP:N	2:C:532:MET:H	2.05	0.50
2:C:613:VAL:CB	2:C:619:ARG:HG2	2.41	0.50
3:D:492:ALA:O	3:D:495:ARG:HB2	2.11	0.50
3:D:824:ASN:O	3:D:825:ALA:C	2.50	0.50
3:D:908:LYS:HG3	3:D:1027:GLY:HA2	1.90	0.50
3:D:1008:PHE:HE1	3:D:1035:ILE:CG1	2.18	0.50
3:D:1118:ILE:CD1	3:D:1190:SER:H	2.24	0.50
3:D:1322:GLY:O	3:D:1323:GLN:CB	2.58	0.50
1:A:34:VAL:O	1:A:35:THR:C	2.48	0.50
1:B:49:PRO:HD2	1:B:213:GLN:HE21	1.76	0.50
1:B:144:VAL:HG12	1:B:145:ASP:H	1.76	0.50
1:B:199:ILE:O	1:B:199:ILE:CG2	2.59	0.50
2:C:7:GLY:O	2:C:8:ARG:HG3	2.12	0.50
2:C:393:GLN:HE22	5:C:1640:RFP:C8	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:502:PRO:O	2:C:507:ARG:CZ	2.59	0.50
3:D:506:GLY:O	3:D:507:ASN:CB	2.59	0.50
3:D:795:VAL:HA	3:D:862:ASP:CB	2.41	0.50
3:D:879:ARG:NH2	3:D:904:VAL:CA	2.63	0.50
3:D:1118:ILE:HD11	3:D:1190:SER:H	1.76	0.50
3:D:1363:LEU:O	3:D:1363:LEU:HD23	2.11	0.50
3:D:1381:VAL:O	3:D:1382:THR:HG23	2.11	0.50
3:D:1449:GLU:O	3:D:1450:ALA:C	2.50	0.50
1:A:218:LEU:O	1:A:222:LEU:HD23	2.12	0.50
1:B:40:LEU:O	1:B:44:LEU:HB2	2.11	0.50
1:B:151:VAL:CG2	1:B:169:ALA:HB3	2.36	0.50
1:B:202:ASP:C	1:B:204:SER:N	2.64	0.50
2:C:65:VAL:HB	2:C:101:ILE:CG1	2.42	0.50
2:C:342:ASP:N	2:C:345:ARG:HH11	2.10	0.50
2:C:352:ALA:HA	2:C:355:VAL:CG1	2.37	0.50
2:C:902:ILE:O	2:C:902:ILE:HG22	2.10	0.50
2:C:1106:ASP:C	2:C:1108:PRO:HD3	2.32	0.50
3:D:612:GLY:C	3:D:614:PHE:N	2.63	0.50
3:D:853:VAL:HG11	3:D:860:LEU:HB2	1.93	0.50
3:D:885:ILE:CD1	3:D:937:TYR:HD2	2.24	0.50
3:D:1004:THR:HG22	3:D:1005:GLN:N	2.27	0.50
3:D:1007:VAL:HG13	3:D:1008:PHE:N	2.26	0.50
3:D:1276:GLU:CD	3:D:1301:LYS:HE2	2.32	0.50
3:D:1347:TYR:CZ	3:D:1351:GLU:HG2	2.46	0.50
1:A:67:THR:O	1:A:69:PRO:HD3	2.12	0.50
1:A:108:GLU:HG3	2:C:644:ARG:HH22	1.77	0.50
1:B:23:PHE:CD1	1:B:211:LEU:HD22	2.47	0.50
2:C:148:PHE:CE2	2:C:310:LEU:HA	2.47	0.50
2:C:220:GLY:HA2	2:C:223:ASP:OD2	2.10	0.50
2:C:277:ALA:O	2:C:281:LEU:N	2.36	0.50
2:C:482:GLU:HA	2:C:486:MET:HE1	1.94	0.50
2:C:662:GLU:O	2:C:663:GLU:CB	2.58	0.50
2:C:710:ILE:HG21	2:C:758:ARG:HD2	1.92	0.50
2:C:755:LEU:HD23	2:C:792:VAL:HG23	1.92	0.50
2:C:798:GLY:O	2:C:827:VAL:HG13	2.12	0.50
3:D:1250:THR:HG23	3:D:1269:LYS:CD	2.39	0.50
3:D:1347:TYR:OH	3:D:1351:GLU:HG2	2.11	0.50
3:D:1436:SER:CB	3:D:1464:GLU:HG2	2.41	0.50
3:D:1490:ARG:C	3:D:1492:LEU:H	2.15	0.50
1:A:41:ARG:HB3	1:A:41:ARG:CZ	2.40	0.50
1:A:157:GLY:O	1:A:158:ILE:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:PRO:HA	1:B:132:LEU:O	2.12	0.50
2:C:42:VAL:H	2:C:46:ALA:HB2	1.77	0.50
2:C:180:GLY:O	2:C:181:VAL:HB	2.12	0.50
2:C:250:LYS:HG3	2:C:250:LYS:O	2.12	0.50
2:C:705:ILE:HG23	2:C:828:ALA:HA	1.94	0.50
2:C:722:ILE:O	2:C:722:ILE:HG22	2.12	0.50
3:D:1051:GLU:O	3:D:1052:THR:C	2.50	0.50
3:D:1434:TRP:HB2	3:D:1450:ALA:HB2	1.94	0.50
3:D:1465:ASN:OD1	3:D:1470:ARG:HB3	2.11	0.50
1:A:158:ILE:HG12	1:A:159:LYS:N	2.27	0.50
1:B:4:SER:O	1:B:5:LYS:CB	2.59	0.50
2:C:159:ILE:HG13	2:C:310:LEU:HD13	1.89	0.50
2:C:352:ALA:O	2:C:353:ARG:C	2.50	0.50
2:C:354:GLY:O	2:C:358:ARG:HG2	2.12	0.50
2:C:434:HIS:O	2:C:436:GLY:N	2.45	0.50
2:C:635:THR:CG2	2:C:636:ALA:N	2.74	0.50
2:C:704:HIS:ND1	2:C:831:ARG:HD2	2.26	0.50
2:C:712:ALA:HB3	2:C:820:ARG:O	2.12	0.50
2:C:768:SER:O	2:C:769:PRO:O	2.30	0.50
3:D:1205:TYR:CD1	3:D:1366:LYS:HD2	2.47	0.50
3:D:1236:LEU:HD13	3:D:1259:VAL:HG21	1.92	0.50
1:A:127:LEU:HG	1:A:129:ILE:HD11	1.94	0.49
1:A:178:ALA:HB2	2:C:864:GLY:HA3	1.94	0.49
1:A:188:GLN:O	1:A:189:ARG:HB3	2.12	0.49
2:C:9:ILE:CG2	2:C:10:ARG:H	2.13	0.49
2:C:222:LEU:O	2:C:225:ALA:N	2.43	0.49
2:C:257:LEU:HB2	2:C:258:PHE:HD1	1.77	0.49
2:C:261:LEU:C	2:C:263:ASP:N	2.64	0.49
2:C:755:LEU:HD11	2:C:825:VAL:HB	1.94	0.49
2:C:845:ASN:HD22	2:C:884:GLN:CD	2.15	0.49
2:C:1043:TYR:CE2	3:D:710:ARG:HD3	2.47	0.49
3:D:10:ILE:HG21	3:D:1450:ALA:CB	2.42	0.49
3:D:110:SER:C	3:D:112:ILE:H	2.15	0.49
3:D:935:LYS:HG3	3:D:939:PHE:HE1	1.77	0.49
3:D:1403:LEU:HD21	3:D:1415:VAL:N	2.20	0.49
1:A:41:ARG:HH11	1:A:42:ARG:N	2.10	0.49
1:A:108:GLU:CG	2:C:644:ARG:NH2	2.75	0.49
1:A:167:VAL:HG12	1:A:168:ASP:N	2.27	0.49
2:C:551:GLU:HG2	2:C:906:PHE:HA	1.94	0.49
2:C:712:ALA:HB2	2:C:722:ILE:CD1	2.41	0.49
2:C:1054:THR:HG22	2:C:1055:ILE:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:40(U):UNK:O	3:D:41(U):UNK:O	2.30	0.49
3:D:502:PHE:HD1	3:D:1452:ILE:HG23	1.77	0.49
3:D:732:VAL:O	3:D:733:CYS:C	2.49	0.49
3:D:936:TYR:C	3:D:936:TYR:CD2	2.86	0.49
3:D:1353:GLN:NE2	3:D:1368:ILE:HD11	2.08	0.49
1:A:77:GLU:O	1:A:80:LEU:N	2.45	0.49
1:B:132:LEU:HD23	1:B:132:LEU:H	1.77	0.49
2:C:181:VAL:CG1	2:C:182:VAL:HG23	2.40	0.49
2:C:226:VAL:HG23	2:C:227:LEU:N	2.27	0.49
2:C:474:VAL:HG22	2:C:530:GLU:CB	2.43	0.49
2:C:483:VAL:O	2:C:485:TYR:N	2.46	0.49
2:C:571:LEU:CD2	2:C:670:GLN:HG3	2.40	0.49
2:C:691:SER:O	2:C:692:GLU:C	2.49	0.49
2:C:747:ALA:O	2:C:800:VAL:HG23	2.12	0.49
3:D:9(U):UNK:O	3:D:10(U):UNK:CB	2.60	0.49
3:D:935:LYS:HG3	3:D:939:PHE:CE1	2.48	0.49
3:D:1321:ALA:O	3:D:1324:PRO:HD2	2.12	0.49
1:A:150:TYR:HB2	2:C:696:LYS:HE2	1.93	0.49
2:C:163:ILE:HG21	2:C:169:GLY:C	2.33	0.49
2:C:198:ARG:C	2:C:198:ARG:HD3	2.32	0.49
2:C:263:ASP:CB	2:C:264:PRO:HD3	2.42	0.49
2:C:598:GLU:HG3	2:C:614:ARG:NH2	2.28	0.49
2:C:727:PRO:C	2:C:729:LEU:H	2.14	0.49
2:C:872:ASN:HD21	2:C:874:LEU:HB3	1.77	0.49
3:D:633:VAL:HA	3:D:740:PHE:CZ	2.47	0.49
3:D:684:LYS:HE2	3:D:685:ASP:OD2	2.12	0.49
3:D:973:GLN:O	3:D:977:ALA:HB2	2.13	0.49
3:D:996:TRP:HA	3:D:999:THR:CG2	2.42	0.49
1:A:111:ALA:HB2	1:A:127:LEU:HB3	1.93	0.49
2:C:44:ILE:HG22	2:C:45:GLN:N	2.27	0.49
2:C:45:GLN:O	2:C:48:PHE:HB2	2.12	0.49
2:C:164:PRO:HD3	2:C:267:TYR:CE2	2.48	0.49
2:C:328:LEU:O	2:C:484:VAL:HG11	2.12	0.49
3:D:1327:ARG:CB	3:D:1327:ARG:HH11	2.25	0.49
3:D:1331:ASP:O	3:D:1334:GLN:N	2.28	0.49
1:A:38:ASN:HB3	1:A:39:PRO:HD3	1.95	0.49
1:B:14:THR:HG22	1:B:14:THR:O	2.12	0.49
2:C:910:THR:CG2	2:C:912:PRO:HD2	2.40	0.49
3:D:687:VAL:O	3:D:690:ALA:CB	2.60	0.49
3:D:739:ASP:O	3:D:741:ASP:N	2.46	0.49
3:D:764:LEU:HB3	3:D:767:HIS:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:864:VAL:HG12	3:D:874:GLU:O	2.13	0.49
3:D:879:ARG:HH22	3:D:905:PRO:HD2	1.78	0.49
3:D:1017:PHE:O	3:D:1019:PRO:N	2.46	0.49
1:A:77:GLU:OE2	2:C:640:ARG:NH1	2.46	0.49
1:B:80:LEU:HB3	3:D:839:LEU:CB	2.42	0.49
2:C:12:VAL:HG21	2:C:479:VAL:CG1	2.43	0.49
2:C:89:THR:HG23	2:C:129:ILE:HG23	1.94	0.49
2:C:100:LEU:CD1	2:C:369:PRO:HD3	2.42	0.49
2:C:142:ARG:HG2	2:C:147:TYR:CE1	2.47	0.49
2:C:344:PHE:HE2	2:C:378:LEU:HD23	1.77	0.49
2:C:636:ALA:HB2	2:C:705:ILE:CD1	2.42	0.49
2:C:676:ILE:C	3:D:948:THR:HG22	2.32	0.49
2:C:969:LEU:CD2	3:D:952:ASP:HB2	2.40	0.49
2:C:1053:LEU:HD13	3:D:621:LYS:HD2	1.94	0.49
3:D:97:THR:O	3:D:571:LYS:HE3	2.13	0.49
3:D:552:ASN:C	3:D:554:LEU:N	2.66	0.49
3:D:1156:LEU:HB3	3:D:1173:PHE:HE1	1.77	0.49
3:D:1429:LEU:HD13	3:D:1440:PHE:CD2	2.47	0.49
1:A:41:ARG:HG2	1:A:177:VAL:CB	2.43	0.49
1:A:41:ARG:NH2	2:C:860:HIS:CD2	2.81	0.49
1:B:46:SER:O	1:B:47:SER:C	2.50	0.49
1:B:94:MET:HE1	1:B:119:ASP:O	2.13	0.49
2:C:149:THR:HG23	2:C:323:ASP:CB	2.42	0.49
2:C:173:ASP:HB3	2:C:185:LYS:HE3	1.95	0.49
2:C:559:LEU:C	2:C:559:LEU:CD1	2.80	0.49
2:C:875:GLY:HA2	2:C:879:ARG:CG	2.39	0.49
2:C:889:HIS:HE1	3:D:951:ILE:N	2.03	0.49
2:C:1030:GLN:NE2	3:D:628:ARG:HD3	2.25	0.49
3:D:583:ASP:O	3:D:585:GLY:N	2.46	0.49
3:D:1034:GLN:HE22	3:D:1037:GLN:NE2	2.11	0.49
3:D:1324:PRO:CD	3:D:1325:LEU:H	2.25	0.49
3:D:1394:VAL:CG1	3:D:1395:LEU:N	2.75	0.49
1:A:9:PRO:HB2	1:A:25:LEU:HD13	1.93	0.49
1:A:15:THR:HG22	1:B:230:ALA:CB	2.34	0.49
1:B:57:TYR:CD2	1:B:58:ILE:N	2.81	0.49
2:C:286:SER:O	2:C:288:ARG:N	2.46	0.49
2:C:325:ILE:C	2:C:327:HIS:N	2.66	0.49
2:C:421:GLU:O	2:C:422:ARG:C	2.50	0.49
2:C:551:GLU:O	3:D:1065:LEU:HB3	2.13	0.49
2:C:691:SER:O	2:C:693:GLU:N	2.45	0.49
2:C:705:ILE:HD12	2:C:705:ILE:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:803:ARG:H	2:C:803:ARG:HD2	1.78	0.49
3:D:648:MET:HE2	3:D:747:VAL:HG11	1.95	0.49
3:D:794:GLN:OE1	3:D:794:GLN:HA	2.12	0.49
3:D:1171:VAL:O	3:D:1171:VAL:HG12	2.12	0.49
1:A:16:GLN:OE1	1:A:19:HIS:HE1	1.96	0.49
1:B:143:ARG:CG	1:B:144:VAL:N	2.76	0.49
2:C:129:ILE:HG22	2:C:130:ASN:ND2	2.28	0.49
2:C:159:ILE:HG21	2:C:306:THR:HG21	1.95	0.49
2:C:556:ASN:O	2:C:559:LEU:HG	2.12	0.49
2:C:745:ILE:HG22	2:C:746:GLY:N	2.28	0.49
2:C:1020:PRO:HD3	2:C:1057:SER:HA	1.94	0.49
2:C:1091:GLU:OE1	3:D:613:ARG:HG3	2.13	0.49
3:D:482:LYS:HE2	3:D:488:ARG:HB3	1.95	0.49
3:D:552:ASN:O	3:D:555:LYS:N	2.44	0.49
3:D:709:HIS:HA	3:D:1227:GLU:HB3	1.95	0.49
3:D:1027:GLY:O	3:D:1028:ALA:HB2	2.13	0.49
3:D:1272:ALA:HB1	3:D:1325:LEU:HA	1.95	0.49
1:A:10:VAL:HB	1:A:26:GLU:HG2	1.90	0.48
1:B:77:GLU:O	1:B:81:ASN:ND2	2.46	0.48
2:C:115:LEU:HD13	2:C:375:SER:OG	2.13	0.48
2:C:256:TYR:CG	2:C:260:LEU:HD13	2.48	0.48
2:C:307:LEU:O	2:C:310:LEU:HB3	2.13	0.48
2:C:473:ARG:HE	2:C:476:ASN:HA	1.77	0.48
2:C:487:THR:O	2:C:488:ALA:C	2.51	0.48
2:C:569:VAL:O	2:C:571:LEU:HD12	2.13	0.48
2:C:845:ASN:O	2:C:845:ASN:OD1	2.30	0.48
3:D:664:LYS:O	3:D:665:ALA:HB3	2.13	0.48
3:D:1065:LEU:C	3:D:1067:VAL:H	2.15	0.48
3:D:1071:PHE:CE2	3:D:1075:HIS:NE2	2.78	0.48
3:D:1164:ARG:HG2	3:D:1165:TYR:N	2.28	0.48
3:D:1425:THR:C	3:D:1427:SER:H	2.15	0.48
3:D:1483:PHE:HZ	4:E:18:ARG:HG3	1.76	0.48
4:E:79:LEU:O	4:E:81:PRO:CD	2.61	0.48
1:A:55:SER:HG	1:A:164:ALA:HB1	1.78	0.48
1:A:162:ILE:CG2	1:A:163:ASN:N	2.73	0.48
1:A:195:LEU:CD2	1:A:196:THR:N	2.76	0.48
1:A:198:ARG:NH1	2:C:934:PHE:HE1	2.11	0.48
2:C:342:ASP:HA	2:C:345:ARG:HD2	1.94	0.48
2:C:465:GLY:O	2:C:466:PHE:HB3	2.13	0.48
2:C:479:VAL:O	2:C:480:THR:C	2.52	0.48
2:C:489:SER:O	2:C:490:GLU:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:836:GLY:O	2:C:837:ASP:O	2.31	0.48
3:D:1277:ILE:HG22	3:D:1278:ASP:H	1.76	0.48
1:A:62:LEU:CD1	2:C:745:ILE:HB	2.43	0.48
2:C:725:ASP:OD1	2:C:725:ASP:O	2.31	0.48
2:C:839:LEU:HD23	2:C:849:VAL:CG2	2.42	0.48
2:C:872:ASN:HD21	2:C:874:LEU:CB	2.26	0.48
2:C:900:ARG:C	2:C:901:TYR:CD1	2.86	0.48
2:C:946:ARG:HG2	2:C:946:ARG:NH1	2.29	0.48
3:D:28:LYS:O	3:D:548:ILE:HG21	2.13	0.48
3:D:626:SER:OG	3:D:748:HIS:N	2.46	0.48
3:D:961:GLN:O	3:D:964:LEU:O	2.30	0.48
3:D:1008:PHE:O	3:D:1008:PHE:HD2	1.96	0.48
3:D:1223:VAL:C	3:D:1225:ALA:H	2.16	0.48
2:C:134:ARG:HB3	2:C:393:GLN:O	2.14	0.48
3:D:552:ASN:C	3:D:555:LYS:H	2.16	0.48
3:D:669:ASN:OD1	3:D:670:VAL:N	2.47	0.48
3:D:853:VAL:HG13	3:D:858:LEU:O	2.13	0.48
3:D:935:LYS:O	3:D:936:TYR:C	2.52	0.48
3:D:1102:ALA:O	3:D:1103:HIS:O	2.31	0.48
3:D:1476:THR:HG22	4:E:21:VAL:CG2	2.43	0.48
1:A:80:LEU:HD11	2:C:572:ILE:HG21	1.96	0.48
1:A:152:PRO:O	1:A:154:GLU:N	2.44	0.48
1:A:158:ILE:HG23	1:A:159:LYS:N	2.22	0.48
1:B:128:HIS:O	1:B:129:ILE:HB	2.13	0.48
1:B:185:ARG:CB	1:B:190:THR:HA	2.43	0.48
2:C:142:ARG:HD2	2:C:324:ASP:HA	1.95	0.48
2:C:278:GLU:HG3	2:C:284:GLY:N	2.22	0.48
2:C:304:LEU:H	2:C:305:PRO:CD	2.26	0.48
2:C:324:ASP:C	2:C:326:ASP:N	2.66	0.48
2:C:493:ARG:NH1	3:D:1069:GLU:OE2	2.47	0.48
2:C:674:VAL:CG2	2:C:675:ALA:H	2.26	0.48
2:C:800:VAL:O	2:C:800:VAL:HG12	2.12	0.48
2:C:816:LYS:HB3	2:C:819:VAL:HG21	1.96	0.48
2:C:1059:ASP:HA	2:C:1083:GLU:OE1	2.13	0.48
3:D:646:LYS:HB3	3:D:720:LEU:HD23	1.96	0.48
3:D:699:VAL:N	3:D:756:GLN:HE22	1.99	0.48
3:D:1278:ASP:HA	3:D:1318:TYR:CA	2.36	0.48
3:D:1311:LEU:O	3:D:1323:GLN:OE1	2.30	0.48
3:D:1316:GLY:O	3:D:1317:ASP:CB	2.61	0.48
1:B:44:LEU:HG	1:B:199:ILE:CD1	2.40	0.48
1:B:44:LEU:CD2	1:B:199:ILE:HD11	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:GLY:HA3	1:B:166:PRO:HB3	1.95	0.48
1:B:184:THR:HG21	1:B:194:LYS:HD3	1.96	0.48
2:C:208:VAL:HG12	2:C:209:ARG:N	2.29	0.48
2:C:208:VAL:HG21	2:C:218:VAL:CG1	2.43	0.48
2:C:255:ALA:O	2:C:298:PHE:HE2	1.97	0.48
2:C:476:ASN:O	2:C:477:GLY:C	2.51	0.48
2:C:573:ARG:O	2:C:670:GLN:HG2	2.13	0.48
2:C:574:ALA:O	2:C:575:GLN:HG3	2.14	0.48
2:C:648:ARG:O	2:C:653:ASP:HB2	2.14	0.48
2:C:705:ILE:HA	2:C:827:VAL:O	2.13	0.48
2:C:860:HIS:HD2	2:C:977:GLY:HA3	1.77	0.48
2:C:948:GLU:HA	2:C:953:VAL:H	1.77	0.48
2:C:1054:THR:C	2:C:1056:LYS:N	2.64	0.48
3:D:669:ASN:OD1	3:D:671:LYS:HG2	2.13	0.48
3:D:793:THR:HG22	3:D:879:ARG:HH12	1.77	0.48
3:D:1129:THR:O	3:D:1130:ARG:C	2.52	0.48
3:D:1250:THR:HA	3:D:1269:LYS:HZ3	1.77	0.48
3:D:1341:PRO:HD2	3:D:1342:GLU:OE1	2.14	0.48
1:A:198:ARG:HH12	2:C:932:GLU:CD	2.17	0.48
2:C:87:ASP:CG	2:C:824:ARG:HH22	2.16	0.48
2:C:95:TYR:HB3	2:C:114:PHE:HA	1.95	0.48
2:C:172:ILE:HD13	2:C:184:MET:SD	2.54	0.48
2:C:466:PHE:CD1	2:C:467:ILE:CG1	2.96	0.48
2:C:1109:VAL:O	2:C:1109:VAL:HG13	2.13	0.48
3:D:795:VAL:CG2	3:D:904:VAL:HG21	2.44	0.48
3:D:1045:MET:HG2	3:D:1073:SER:HB3	1.94	0.48
3:D:1105:ILE:CG2	3:D:1200:VAL:CB	2.92	0.48
3:D:1147:ARG:O	3:D:1165:TYR:HA	2.14	0.48
3:D:1253:THR:CA	3:D:1258:ARG:HD2	2.36	0.48
3:D:1434:TRP:HZ3	3:D:1457:ASP:H	1.62	0.48
4:E:8:LYS:CE	4:E:69:LEU:HD21	2.43	0.48
1:A:121:GLU:C	1:A:123:MET:H	2.16	0.48
1:A:128:HIS:C	1:A:128:HIS:CD2	2.86	0.48
1:A:131:THR:CG2	2:C:644:ARG:HH21	2.11	0.48
1:B:203:GLY:O	1:B:204:SER:HB3	2.14	0.48
2:C:14:PRO:HA	2:C:458:TYR:CE1	2.49	0.48
2:C:91:GLN:HA	2:C:119:PRO:HA	1.96	0.48
2:C:427:VAL:O	2:C:430:VAL:HB	2.14	0.48
2:C:745:ILE:C	2:C:747:ALA:H	2.16	0.48
2:C:761:PHE:O	2:C:762:LYS:O	2.31	0.48
2:C:892:LEU:C	2:C:894:GLY:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:953:VAL:HG11	2:C:962:GLN:CB	2.42	0.48
2:C:1020:PRO:O	2:C:1021:LEU:CB	2.62	0.48
2:C:1023:GLY:C	2:C:1024:LYS:HG3	2.34	0.48
2:C:1106:ASP:N	2:C:1108:PRO:HD3	2.29	0.48
3:D:8:VAL:CG1	3:D:1434:TRP:HH2	2.27	0.48
3:D:647:ARG:HD2	3:D:647:ARG:HA	1.63	0.48
3:D:716:PHE:CE2	3:D:765:SER:HB3	2.48	0.48
3:D:1336:LEU:HA	3:D:1340:GLY:O	2.14	0.48
3:D:1393:GLN:HE21	3:D:1420:LEU:CD2	2.27	0.48
1:B:25:LEU:HD12	1:B:26:GLU:N	2.28	0.48
1:B:31:GLY:O	1:B:35:THR:OG1	2.31	0.48
2:C:13:ILE:HG13	2:C:14:PRO:HD2	1.96	0.48
2:C:44:ILE:H	2:C:44:ILE:CD1	2.26	0.48
2:C:254:LEU:O	2:C:257:LEU:HD12	2.14	0.48
2:C:328:LEU:HD23	2:C:468:ARG:HD2	1.95	0.48
2:C:501:THR:O	2:C:501:THR:HG22	2.14	0.48
2:C:735:ARG:C	2:C:737:LEU:N	2.66	0.48
2:C:880:MET:C	2:C:881:ASN:ND2	2.67	0.48
3:D:124:GLU:HA	3:D:456:MET:SD	2.54	0.48
3:D:632:VAL:HG12	3:D:633:VAL:O	2.13	0.48
3:D:836:VAL:HG11	3:D:858:LEU:CD1	2.44	0.48
3:D:905:PRO:HG2	3:D:906:GLN:H	1.78	0.48
3:D:1103:HIS:H	3:D:1222:GLY:CA	2.27	0.48
3:D:1238:MET:HG3	3:D:1238:MET:O	2.13	0.48
1:A:43:ILE:CD1	1:B:32:PHE:CE1	2.97	0.48
1:A:133:GLU:C	1:A:135:GLY:H	2.16	0.48
2:C:74:GLY:O	2:C:76:PRO:N	2.47	0.48
2:C:156:GLY:O	2:C:157:ARG:O	2.32	0.48
2:C:613:VAL:CG1	2:C:619:ARG:HA	2.44	0.48
2:C:668:LEU:HB2	2:C:995:MET:HE2	1.95	0.48
2:C:929:ARG:C	2:C:931:GLY:N	2.66	0.48
3:D:468:LEU:C	3:D:470:LEU:N	2.67	0.48
3:D:500:ARG:O	3:D:504:ASP:HB2	2.14	0.48
3:D:724:GLN:O	3:D:725:SER:O	2.31	0.48
3:D:848:GLU:HA	3:D:851:LEU:HB3	1.96	0.48
3:D:1015:TYR:HB3	3:D:1018:ASN:CB	2.40	0.48
3:D:1071:PHE:HA	3:D:1074:SER:HB3	1.96	0.48
3:D:1076:GLY:HA2	3:D:1079:LYS:HE2	1.96	0.48
3:D:1086:LEU:HD12	3:D:1089:ALA:CB	2.44	0.48
3:D:1101:VAL:HG21	3:D:1424:VAL:CG2	2.24	0.48
1:A:13:ALA:O	1:A:15:THR:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LYS:HB3	1:A:73:GLU:OE2	2.14	0.47
1:A:112:VAL:C	1:A:114:PHE:H	2.17	0.47
1:B:26:GLU:O	1:B:27:PRO:C	2.53	0.47
2:C:173:ASP:CB	2:C:185:LYS:HE3	2.44	0.47
2:C:425:PHE:O	2:C:426:ASP:HB3	2.14	0.47
2:C:495:THR:O	2:C:496:ILE:CB	2.61	0.47
2:C:831:ARG:HH12	2:C:1002:GLU:CB	2.27	0.47
2:C:1103:ASP:O	2:C:1106:ASP:N	2.44	0.47
3:D:690:ALA:O	3:D:694:VAL:N	2.47	0.47
3:D:716:PHE:CE2	3:D:765:SER:CB	2.97	0.47
3:D:815:ALA:O	3:D:817:GLU:N	2.47	0.47
3:D:879:ARG:HG2	3:D:879:ARG:NH1	2.29	0.47
3:D:1140:ILE:HD13	3:D:1175:ILE:HG12	1.95	0.47
3:D:1274:ILE:H	3:D:1274:ILE:HD12	1.77	0.47
3:D:1344:VAL:O	3:D:1348:LEU:N	2.44	0.47
4:E:8:LYS:NZ	4:E:69:LEU:HD21	2.29	0.47
4:E:25:LYS:O	4:E:28:GLN:C	2.52	0.47
1:A:225:PHE:CE1	1:B:36:LEU:HD13	2.50	0.47
1:B:164:ALA:O	1:B:165:ILE:C	2.52	0.47
2:C:6:PHE:HD2	2:C:909:ALA:H	1.61	0.47
2:C:21:ILE:HD11	2:C:455:LEU:HD21	1.97	0.47
2:C:73:ILE:HD12	2:C:94:LEU:HD13	1.96	0.47
2:C:328:LEU:HD21	2:C:468:ARG:NH1	2.29	0.47
2:C:399:ASN:HD21	2:C:401:LEU:N	2.10	0.47
2:C:564:MET:CE	2:C:846:LYS:HG2	2.45	0.47
2:C:589:ARG:NH2	2:C:654:LEU:HD12	2.23	0.47
2:C:679:PHE:N	2:C:683:ASN:OD1	2.43	0.47
2:C:831:ARG:NH1	2:C:1002:GLU:CD	2.67	0.47
2:C:1008:ARG:HH12	2:C:1021:LEU:H	1.61	0.47
2:C:1059:ASP:CG	2:C:1083:GLU:HB2	2.35	0.47
2:C:1082:PRO:HG2	2:C:1085:PHE:HB2	1.96	0.47
3:D:643:GLY:O	3:D:644:LEU:HB2	2.13	0.47
3:D:800:LYS:CB	3:D:821:VAL:H	2.26	0.47
3:D:1384:PRO:HG3	3:D:1389:LEU:O	2.14	0.47
4:E:26:ARG:HH22	4:E:37:ASN:HB3	1.77	0.47
1:B:81:ASN:O	1:B:82:LEU:C	2.51	0.47
1:B:132:LEU:CD2	1:B:132:LEU:H	2.27	0.47
2:C:7:GLY:HA2	2:C:907:ASP:OD1	2.14	0.47
2:C:13:ILE:HG22	2:C:15:LEU:N	2.21	0.47
2:C:14:PRO:HA	2:C:458:TYR:CD1	2.48	0.47
2:C:184:MET:CE	2:C:191:PHE:HZ	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:790:LEU:O	2:C:791:ARG:O	2.32	0.47
2:C:831:ARG:NH1	2:C:1002:GLU:OE2	2.48	0.47
2:C:993:PHE:CD1	2:C:993:PHE:O	2.67	0.47
3:D:21:TRP:C	3:D:23:TYR:H	2.18	0.47
3:D:575:GLN:NE2	3:D:579:ASP:OD2	2.47	0.47
3:D:1065:LEU:C	3:D:1067:VAL:N	2.67	0.47
3:D:1481:VAL:O	3:D:1482:ARG:CG	2.60	0.47
1:A:10:VAL:O	1:A:12:THR:N	2.43	0.47
1:B:44:LEU:HG	1:B:199:ILE:CG1	2.44	0.47
2:C:83:CYS:SG	2:C:88:LEU:HB2	2.55	0.47
2:C:184:MET:HE3	2:C:191:PHE:HZ	1.79	0.47
2:C:261:LEU:O	2:C:264:PRO:HD2	2.14	0.47
2:C:274:ARG:CG	2:C:275:TYR:N	2.78	0.47
2:C:405:ARG:HD2	2:C:543:ASN:ND2	2.29	0.47
2:C:601:GLY:HA3	2:C:648:ARG:N	2.30	0.47
2:C:657:ASP:OD1	2:C:663:GLU:HA	2.14	0.47
3:D:654:LYS:O	3:D:657:LEU:N	2.47	0.47
3:D:707:THR:C	3:D:708:LEU:HG	2.34	0.47
3:D:1053:PHE:CD1	3:D:1072:ILE:HG23	2.49	0.47
3:D:1274:ILE:HA	3:D:1322:GLY:N	2.30	0.47
1:A:18:ASP:O	1:A:19:HIS:HB3	2.15	0.47
1:A:79:ILE:CD1	1:A:165:ILE:HD12	2.38	0.47
1:A:88:ARG:CB	1:A:121:GLU:HB2	2.38	0.47
1:A:108:GLU:CG	2:C:644:ARG:HH22	2.27	0.47
1:B:87:VAL:CG1	1:B:88:ARG:N	2.77	0.47
1:B:118:ALA:C	1:B:120:VAL:N	2.68	0.47
1:B:219:LYS:O	1:B:222:LEU:HB2	2.14	0.47
2:C:23:VAL:HG12	2:C:24:GLU:N	2.30	0.47
2:C:46:ALA:O	2:C:50:GLU:N	2.31	0.47
2:C:159:ILE:CD1	2:C:310:LEU:HB2	2.34	0.47
2:C:195:LEU:HD13	2:C:227:LEU:CD1	2.31	0.47
2:C:333:ILE:CG2	2:C:460:ARG:HH22	2.25	0.47
2:C:408:ARG:NH1	2:C:455:LEU:HD23	2.29	0.47
2:C:425:PHE:O	2:C:426:ASP:CB	2.62	0.47
2:C:449:ILE:HG22	2:C:450:GLY:N	2.29	0.47
2:C:637:PHE:HE1	2:C:1639:GLN:HE21	1.61	0.47
2:C:768:SER:CB	2:C:769:PRO:HD2	2.42	0.47
2:C:778:PHE:N	2:C:778:PHE:CD1	2.82	0.47
2:C:966:LEU:CD1	2:C:986:PRO:HG3	2.40	0.47
2:C:985:GLY:O	2:C:986:PRO:O	2.32	0.47
2:C:1036:GLU:O	2:C:1039:ALA:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1095:LEU:CD1	3:D:603:LEU:HD23	2.35	0.47
3:D:564:GLU:O	3:D:565:ILE:C	2.53	0.47
3:D:836:VAL:CG1	3:D:858:LEU:HD11	2.45	0.47
3:D:1035:ILE:C	3:D:1037:GLN:N	2.68	0.47
3:D:1155:ALA:O	3:D:1156:LEU:C	2.53	0.47
3:D:1277:ILE:HG22	3:D:1279:GLY:N	2.27	0.47
3:D:1336:LEU:HD13	3:D:1340:GLY:C	2.35	0.47
4:E:8:LYS:HB3	4:E:69:LEU:HD11	1.96	0.47
1:A:35:THR:HG21	1:B:43:ILE:CG1	2.45	0.47
1:A:41:ARG:HH12	1:A:42:ARG:HG2	1.80	0.47
1:B:111:ALA:O	1:B:114:PHE:CD1	2.68	0.47
1:B:119:ASP:C	1:B:120:VAL:HG23	2.35	0.47
1:B:181:VAL:O	1:B:181:VAL:HG13	2.14	0.47
2:C:1007:ALA:HB1	3:D:652:LEU:CD2	2.44	0.47
3:D:464:LEU:O	3:D:468:LEU:CB	2.63	0.47
3:D:497:GLU:HG2	3:D:1389:LEU:HD11	1.96	0.47
3:D:705:ALA:CB	3:D:706:PRO:HD3	2.44	0.47
3:D:859:ASP:OD1	3:D:861:GLN:NE2	2.48	0.47
3:D:897:GLN:HE21	3:D:897:GLN:CA	2.27	0.47
3:D:899:LEU:HD22	3:D:899:LEU:H	1.79	0.47
3:D:1071:PHE:O	3:D:1074:SER:N	2.46	0.47
1:A:152:PRO:C	1:A:154:GLU:H	2.18	0.47
1:B:26:GLU:OE1	1:B:27:PRO:HD3	2.15	0.47
1:B:113:ASP:O	1:B:114:PHE:C	2.53	0.47
2:C:15:LEU:HD21	2:C:461:VAL:HB	1.96	0.47
2:C:30:LEU:HD12	2:C:44:ILE:HG12	1.97	0.47
2:C:78:PHE:HB3	2:C:82:GLU:OE2	2.15	0.47
2:C:327:HIS:C	2:C:329:GLY:N	2.68	0.47
2:C:397:GLU:OE2	2:C:632:ASN:ND2	2.47	0.47
2:C:460:ARG:HB2	2:C:468:ARG:HA	1.97	0.47
2:C:547:ILE:HG23	2:C:843:HIS:CE1	2.50	0.47
2:C:747:ALA:O	2:C:748:GLU:C	2.52	0.47
2:C:749:VAL:HG23	2:C:800:VAL:HG23	1.96	0.47
2:C:875:GLY:O	2:C:876:VAL:C	2.53	0.47
2:C:881:ASN:CG	3:D:1034:GLN:CD	2.73	0.47
2:C:1034:GLU:OE2	3:D:1096:ARG:NH2	2.47	0.47
2:C:1067:TYR:O	2:C:1071:ILE:HD13	2.15	0.47
2:C:1073:GLY:CA	3:D:659:LYS:HE3	2.44	0.47
3:D:602:SER:O	3:D:606:ILE:HD12	2.15	0.47
3:D:708:LEU:O	3:D:709:HIS:O	2.33	0.47
3:D:962:ARG:O	3:D:966:GLU:CG	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1055:VAL:O	3:D:1055:VAL:HG12	2.13	0.47
3:D:1095:THR:O	3:D:1099:VAL:HG23	2.13	0.47
3:D:1132:LEU:CD1	3:D:1184:ARG:HH12	2.20	0.47
3:D:1136:LYS:CG	3:D:1139:ASP:OD2	2.62	0.47
3:D:1465:ASN:O	3:D:1470:ARG:HB2	2.15	0.47
2:C:97:ARG:HG2	2:C:112:GLU:H	1.79	0.47
2:C:198:ARG:CZ	2:C:203:ASP:OD2	2.63	0.47
2:C:554:ASP:O	2:C:555:ALA:C	2.53	0.47
2:C:774:LEU:O	2:C:778:PHE:N	2.47	0.47
2:C:944:LEU:HD11	2:C:963:LEU:CD2	2.45	0.47
2:C:987:ILE:HG22	2:C:987:ILE:O	2.14	0.47
2:C:1034:GLU:O	2:C:1037:VAL:HB	2.15	0.47
2:C:1056:LYS:O	3:D:624:ASP:HB2	2.14	0.47
3:D:537:THR:O	3:D:537:THR:HG22	2.15	0.47
3:D:687:VAL:O	3:D:690:ALA:HB3	2.15	0.47
3:D:764:LEU:CD2	3:D:766:ALA:HB3	2.45	0.47
3:D:947:ILE:CA	3:D:1020:LEU:HD13	2.43	0.47
3:D:1005:GLN:O	3:D:1009:ASN:HB3	2.15	0.47
3:D:1311:LEU:HD12	3:D:1311:LEU:N	2.30	0.47
1:A:111:ALA:O	1:A:112:VAL:C	2.53	0.47
1:A:199:ILE:HD12	1:A:199:ILE:N	2.30	0.47
1:A:223:ASN:O	1:A:225:PHE:N	2.48	0.47
1:B:32:PHE:HA	1:B:35:THR:OG1	2.15	0.47
2:C:26:TYR:HE2	2:C:30:LEU:HD22	1.80	0.47
2:C:208:VAL:O	2:C:209:ARG:HB2	2.14	0.47
2:C:216:ASP:C	2:C:218:VAL:N	2.67	0.47
2:C:252:LYS:HE3	2:C:298:PHE:HE1	1.80	0.47
2:C:730:SER:O	2:C:731:GLU:O	2.33	0.47
2:C:794:PRO:HG2	2:C:1027:PHE:HB2	1.97	0.47
2:C:876:VAL:HB	2:C:877:PRO:HD3	1.94	0.47
2:C:890:LEU:HD11	2:C:917:LEU:HD13	1.97	0.47
2:C:1055:ILE:HD12	2:C:1055:ILE:N	2.11	0.47
2:C:1091:GLU:OE1	3:D:606:ILE:HG22	2.15	0.47
3:D:120:ALA:HB1	3:D:126:VAL:CB	2.45	0.47
3:D:793:THR:HA	3:D:879:ARG:HH12	1.80	0.47
3:D:1134:LEU:N	3:D:1134:LEU:HD23	2.29	0.47
3:D:1231:GLU:C	3:D:1233:GLY:N	2.67	0.47
3:D:1327:ARG:NH1	3:D:1327:ARG:CB	2.76	0.47
1:A:34:VAL:C	1:A:36:LEU:N	2.67	0.47
1:A:222:LEU:CD1	1:B:215:VAL:HG13	2.40	0.47
1:B:11:PHE:HA	1:B:25:LEU:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ARG:CZ	2:C:854:PRO:HB3	2.45	0.47
2:C:20:GLU:OE2	2:C:461:VAL:HG23	2.15	0.47
2:C:78:PHE:HB3	2:C:82:GLU:CD	2.36	0.47
2:C:78:PHE:HD2	2:C:82:GLU:OE2	1.98	0.47
2:C:101:ILE:HG22	2:C:102:HIS:N	2.29	0.47
2:C:175:GLU:O	2:C:182:VAL:HA	2.15	0.47
2:C:304:LEU:HD23	2:C:305:PRO:N	2.30	0.47
2:C:314:THR:O	2:C:315:ALA:HB3	2.15	0.47
2:C:706:GLU:O	2:C:826:PHE:HA	2.15	0.47
2:C:862:PRO:HG2	2:C:863:ASP:H	1.80	0.47
3:D:99:ALA:O	3:D:575:GLN:HB2	2.14	0.47
3:D:507:ASN:O	3:D:508:ARG:HG2	2.15	0.47
3:D:553:ARG:C	3:D:554:LEU:HD23	2.36	0.47
3:D:706:PRO:HG2	3:D:706:PRO:O	2.15	0.47
3:D:937:TYR:O	3:D:941:LEU:HB2	2.14	0.47
3:D:1081:GLY:HA2	3:D:1084:THR:HG23	1.97	0.47
3:D:1205:TYR:O	3:D:1206:GLY:O	2.32	0.47
3:D:1236:LEU:HB3	3:D:1256:LEU:N	2.30	0.47
4:E:13:VAL:HG21	4:E:19:LEU:CB	2.45	0.47
1:A:134:GLU:HB3	2:C:606:VAL:HG23	1.96	0.46
1:A:195:LEU:C	1:A:196:THR:HG22	2.34	0.46
1:A:199:ILE:HG21	1:A:207:PRO:HA	1.97	0.46
1:B:24:VAL:HG12	1:B:24:VAL:O	2.13	0.46
2:C:115:LEU:HA	2:C:375:SER:CB	2.45	0.46
2:C:127:PHE:N	2:C:127:PHE:CD1	2.83	0.46
2:C:149:THR:CB	2:C:158:TYR:HE1	2.22	0.46
2:C:358:ARG:O	2:C:359:MET:C	2.53	0.46
2:C:595:LEU:HG	2:C:655:LEU:HD23	1.97	0.46
2:C:674:VAL:HG23	2:C:869:VAL:O	2.15	0.46
2:C:796:GLU:HG2	3:D:681:ARG:NH2	2.28	0.46
2:C:846:LYS:HD2	2:C:846:LYS:O	2.16	0.46
2:C:890:LEU:HD11	2:C:901:TYR:CE2	2.50	0.46
2:C:1052:MET:HE1	3:D:748:HIS:CB	2.43	0.46
3:D:149:LYS:C	3:D:151:GLN:N	2.68	0.46
3:D:789:LEU:CD1	3:D:934:LEU:HD22	2.44	0.46
3:D:1075:HIS:H	3:D:1075:HIS:CD2	2.33	0.46
3:D:1094:LEU:O	3:D:1095:THR:C	2.53	0.46
3:D:1101:VAL:CG2	3:D:1424:VAL:HG22	2.24	0.46
3:D:1251:ASP:O	3:D:1252:ILE:HB	2.15	0.46
3:D:1340:GLY:HA3	3:D:1342:GLU:OE1	2.15	0.46
1:A:70:GLY:HA2	2:C:606:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:HH12	2:C:932:GLU:CB	2.27	0.46
2:C:65:VAL:HB	2:C:101:ILE:HB	1.97	0.46
2:C:166:PRO:HB3	2:C:417:GLY:N	2.27	0.46
2:C:215:GLY:O	2:C:216:ASP:O	2.34	0.46
2:C:434:HIS:C	2:C:436:GLY:N	2.69	0.46
2:C:613:VAL:HG13	2:C:620:LEU:N	2.15	0.46
2:C:691:SER:HB2	2:C:858:MET:CE	2.45	0.46
2:C:728:HIS:CD2	2:C:783:ARG:NH1	2.83	0.46
2:C:928:LYS:O	2:C:931:GLY:N	2.48	0.46
3:D:1083:ASP:C	3:D:1085:ALA:N	2.69	0.46
4:E:55:TYR:O	4:E:56:ASP:C	2.54	0.46
4:E:86:GLN:HA	4:E:89:MET:HG2	1.97	0.46
1:B:188:GLN:NE2	1:B:188:GLN:C	2.69	0.46
2:C:72:ARG:HH11	2:C:112:GLU:CD	2.17	0.46
2:C:308:ARG:C	2:C:310:LEU:N	2.68	0.46
2:C:308:ARG:C	2:C:310:LEU:H	2.19	0.46
2:C:545:ASN:HA	2:C:905:VAL:HG21	1.98	0.46
2:C:609:THR:O	2:C:609:THR:HG23	2.14	0.46
2:C:1099:VAL:HG22	3:D:10:ILE:CD1	2.42	0.46
3:D:149:LYS:O	3:D:152:LEU:N	2.48	0.46
3:D:560:GLN:O	3:D:561:GLY:C	2.54	0.46
3:D:631:ILE:HD11	3:D:743:ASP:CB	2.45	0.46
3:D:638:LYS:CB	3:D:729:HIS:NE2	2.78	0.46
3:D:752:SER:O	3:D:753:SER:C	2.54	0.46
3:D:794:GLN:HB3	3:D:1017:PHE:CZ	2.49	0.46
3:D:1339:LYS:HD2	3:D:1339:LYS:HA	1.58	0.46
2:C:100:LEU:HD23	2:C:372:LEU:CD1	2.45	0.46
2:C:437:ARG:HG3	2:C:437:ARG:O	2.14	0.46
2:C:461:VAL:O	2:C:481:GLU:HG2	2.16	0.46
2:C:672:VAL:HG22	2:C:868:ASP:CG	2.36	0.46
2:C:727:PRO:O	2:C:729:LEU:N	2.48	0.46
2:C:1108:PRO:O	2:C:1109:VAL:O	2.33	0.46
3:D:552:ASN:O	3:D:556:LYS:N	2.49	0.46
3:D:660:LYS:O	3:D:664:LYS:N	2.42	0.46
3:D:695:ILE:HG23	3:D:718:PRO:HD2	1.96	0.46
3:D:701:LEU:CD1	3:D:715:ALA:HB2	2.44	0.46
3:D:709:HIS:HA	3:D:1227:GLU:CD	2.36	0.46
3:D:773:ALA:O	3:D:774:SER:CB	2.64	0.46
3:D:855:HIS:CD2	3:D:855:HIS:N	2.66	0.46
3:D:1273:VAL:O	3:D:1322:GLY:HA3	2.15	0.46
3:D:1290:LEU:O	3:D:1291:SER:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:15:SER:O	4:E:17:TYR:N	2.49	0.46
4:E:78:ASN:O	4:E:79:LEU:HB2	2.15	0.46
1:A:30:ARG:HH11	1:A:192:LEU:HD23	1.80	0.46
1:B:211:LEU:C	1:B:215:VAL:HG23	2.33	0.46
2:C:186:VAL:HG11	2:C:258:PHE:HD2	1.79	0.46
2:C:258:PHE:CD1	2:C:258:PHE:N	2.83	0.46
2:C:460:ARG:CA	2:C:468:ARG:O	2.63	0.46
2:C:494:TYR:O	2:C:495:THR:CB	2.62	0.46
2:C:549:PHE:HA	2:C:551:GLU:OE1	2.15	0.46
2:C:641:PRO:HA	2:C:656:ALA:HA	1.96	0.46
2:C:684:PHE:O	2:C:686:ASP:N	2.49	0.46
3:D:99:ALA:HB3	3:D:458:ALA:CB	2.45	0.46
3:D:654:LYS:O	3:D:655:PRO:C	2.51	0.46
3:D:772:PRO:CB	3:D:778:LEU:HD23	2.46	0.46
3:D:1089:ALA:C	3:D:1091:SER:H	2.19	0.46
3:D:1114:THR:CB	3:D:1189:ARG:HH11	2.27	0.46
3:D:1156:LEU:HB3	3:D:1173:PHE:CE1	2.50	0.46
1:A:105:GLY:HA2	1:A:136:GLY:N	2.30	0.46
1:B:101:LEU:HD23	1:B:140:MET:CE	2.45	0.46
1:B:144:VAL:HG12	1:B:145:ASP:N	2.30	0.46
2:C:122:THR:HG22	2:C:123:GLU:N	2.30	0.46
2:C:351:LEU:HA	2:C:377:PRO:HG3	1.98	0.46
2:C:358:ARG:HB2	2:C:372:LEU:CD2	2.45	0.46
2:C:395:LYS:CG	2:C:397:GLU:HG3	2.44	0.46
2:C:1639:GLN:HG2	2:C:658:GLY:HA2	1.97	0.46
2:C:756:VAL:O	2:C:790:LEU:N	2.48	0.46
2:C:805:ARG:NE	2:C:821:GLU:OE2	2.38	0.46
2:C:946:ARG:CD	2:C:984:GLU:HB2	2.45	0.46
3:D:31(U):UNK:O	3:D:32(U):UNK:CB	2.62	0.46
3:D:467:GLU:O	3:D:468:LEU:O	2.34	0.46
3:D:700:VAL:N	3:D:716:PHE:O	2.48	0.46
3:D:1109:GLU:O	3:D:1202:GLN:CB	2.64	0.46
3:D:1435:LEU:CD2	3:D:1457:ASP:OD2	2.64	0.46
3:D:1472:ILE:O	3:D:1477:GLY:HA3	2.15	0.46
4:E:48:MET:HE2	4:E:57:ASP:HB3	1.98	0.46
1:A:30:ARG:NH1	1:A:192:LEU:CD2	2.79	0.46
1:A:194:LYS:O	1:A:194:LYS:HG2	2.16	0.46
1:A:198:ARG:NH2	2:C:932:GLU:OE1	2.32	0.46
1:B:22:GLU:O	1:B:23:PHE:HD2	1.98	0.46
2:C:66:LEU:N	2:C:100:LEU:HA	2.30	0.46
2:C:143:SER:O	2:C:147:TYR:OH	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:340:MET:O	2:C:340:MET:SD	2.73	0.46
2:C:525:ALA:O	2:C:527:GLU:N	2.48	0.46
2:C:682:TYR:CE1	2:C:851:LYS:HD2	2.51	0.46
2:C:813:VAL:HG12	2:C:815:LEU:CG	2.46	0.46
2:C:816:LYS:O	2:C:819:VAL:HB	2.15	0.46
2:C:912:PRO:O	2:C:915:LYS:HB2	2.16	0.46
2:C:969:LEU:HD11	3:D:952:ASP:N	2.22	0.46
2:C:1014:SER:O	2:C:1018:GLN:OE1	2.34	0.46
2:C:1038:TRP:CH2	3:D:1096:ARG:HA	2.50	0.46
2:C:1055:ILE:HG22	2:C:1055:ILE:O	2.16	0.46
2:C:1059:ASP:HA	2:C:1083:GLU:CG	2.46	0.46
3:D:28:LYS:O	3:D:30:GLU:N	2.49	0.46
3:D:98:PRO:CB	3:D:574:LEU:HD23	2.46	0.46
3:D:23(U):UNK:CB	3:D:43(U):UNK:N	2.79	0.46
3:D:548:ILE:O	3:D:552:ASN:ND2	2.49	0.46
3:D:760:ARG:NH2	4:E:3:GLU:OE2	2.38	0.46
3:D:794:GLN:OE1	3:D:906:GLN:NE2	2.49	0.46
3:D:937:TYR:N	3:D:937:TYR:HD1	2.14	0.46
3:D:1166:LEU:HB2	3:D:1170:ASP:HB2	1.96	0.46
3:D:1377:LYS:HE2	3:D:1378:TYR:CZ	2.51	0.46
1:A:74:ASP:OD1	1:A:76:VAL:HG23	2.16	0.46
1:A:184:THR:O	1:A:184:THR:HG23	2.15	0.46
1:B:30:ARG:NH2	2:C:854:PRO:HB3	2.31	0.46
2:C:12:VAL:CG1	2:C:13:ILE:H	1.96	0.46
2:C:252:LYS:HE3	2:C:298:PHE:CE1	2.51	0.46
2:C:462:ASP:O	2:C:464:LEU:N	2.48	0.46
2:C:672:VAL:HG13	2:C:673:LEU:N	2.31	0.46
2:C:787:ASP:O	2:C:789:SER:N	2.49	0.46
3:D:75:ARG:O	3:D:77:ALA:N	2.49	0.46
3:D:6(U):UNK:CB	3:D:36(U):UNK:HA	2.46	0.46
3:D:538:SER:O	3:D:539:ASP:C	2.55	0.46
3:D:968:ASP:HA	3:D:971:LEU:HD12	1.96	0.46
3:D:1057:VAL:HG12	3:D:1067:VAL:HG21	1.98	0.46
3:D:1084:THR:C	3:D:1086:LEU:N	2.69	0.46
3:D:1277:ILE:O	3:D:1317:ASP:O	2.33	0.46
3:D:1441:GLN:O	3:D:1442:ASN:HB3	2.16	0.46
3:D:1449:GLU:O	3:D:1452:ILE:N	2.49	0.46
3:D:1489:GLN:CB	4:E:72:ARG:HD2	2.46	0.46
4:E:26:ARG:NH2	4:E:30:LEU:HD12	2.30	0.46
4:E:26:ARG:HH22	4:E:37:ASN:CB	2.29	0.46
1:A:125:PRO:O	1:A:126:ASP:C	2.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ALA:O	1:A:165:ILE:HG12	2.15	0.46
1:B:26:GLU:CG	1:B:27:PRO:HD3	2.45	0.46
1:B:64:GLU:O	1:B:75:VAL:HG21	2.16	0.46
1:B:99:LEU:HD13	1:B:114:PHE:CD2	2.51	0.46
2:C:197:LEU:HD22	2:C:202:TYR:CD1	2.43	0.46
3:D:520:LEU:HB3	3:D:521:PRO:HD2	1.97	0.46
3:D:642:CYS:SG	3:D:702:LEU:CD2	3.04	0.46
3:D:836:VAL:HB	3:D:858:LEU:HD21	1.98	0.46
3:D:1454:GLY:O	3:D:1455:LYS:HB2	2.15	0.46
3:D:1485:GLN:HA	4:E:75:PHE:HA	1.98	0.46
4:E:26:ARG:HH21	4:E:30:LEU:CD1	2.29	0.46
1:B:101:LEU:HD11	1:B:113:ASP:HB2	1.98	0.46
2:C:94:LEU:HD21	2:C:344:PHE:HZ	1.81	0.46
2:C:162:ILE:HD12	2:C:162:ILE:N	2.31	0.46
2:C:203:ASP:O	2:C:204:GLN:C	2.55	0.46
2:C:474:VAL:O	2:C:474:VAL:HG12	2.16	0.46
2:C:570:PRO:CG	2:C:635:THR:HG23	2.46	0.46
2:C:599:GLU:O	2:C:600:ASP:O	2.33	0.46
2:C:640:ARG:O	2:C:657:ASP:N	2.49	0.46
2:C:679:PHE:HE2	2:C:978:ARG:NH2	2.14	0.46
2:C:684:PHE:O	2:C:685:GLU:HB2	2.16	0.46
2:C:737:LEU:O	2:C:738:ASP:C	2.53	0.46
3:D:75:ARG:C	3:D:77:ALA:H	2.19	0.46
3:D:690:ALA:O	3:D:693:GLU:N	2.43	0.46
3:D:709:HIS:CE1	3:D:1231:GLU:HG3	2.51	0.46
3:D:859:ASP:C	3:D:861:GLN:H	2.19	0.46
3:D:901:GLN:O	3:D:905:PRO:HD3	2.16	0.46
3:D:957:PRO:CG	3:D:1007:VAL:HB	2.45	0.46
3:D:989:TYR:C	3:D:991:GLN:H	2.18	0.46
3:D:1278:ASP:CA	3:D:1317:ASP:O	2.64	0.46
3:D:1347:TYR:CE1	3:D:1351:GLU:HB2	2.51	0.46
3:D:1485:GLN:CB	4:E:75:PHE:HB3	2.46	0.46
1:A:126:ASP:O	1:A:127:LEU:C	2.54	0.45
1:A:175:ARG:HB2	1:A:201:THR:CB	2.46	0.45
1:B:43:ILE:HD12	1:B:218:LEU:HB2	1.97	0.45
1:B:57:TYR:CD2	1:B:57:TYR:C	2.88	0.45
1:B:213:GLN:O	1:B:216:ALA:HB3	2.16	0.45
2:C:157:ARG:NH1	2:C:321:GLU:HG2	2.31	0.45
2:C:172:ILE:CG2	2:C:173:ASP:N	2.79	0.45
2:C:306:THR:O	2:C:310:LEU:N	2.49	0.45
2:C:589:ARG:NH1	2:C:596:TYR:CB	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:692:GLU:O	2:C:693:GLU:C	2.53	0.45
2:C:1099:VAL:O	2:C:1099:VAL:HG12	2.16	0.45
3:D:508:ARG:HB2	3:D:510:GLU:OE2	2.15	0.45
3:D:700:VAL:CG2	3:D:718:PRO:HG3	2.46	0.45
3:D:791:TYR:CE1	3:D:1023:MET:HG3	2.51	0.45
3:D:836:VAL:HG11	3:D:858:LEU:HD11	1.98	0.45
3:D:937:TYR:N	3:D:937:TYR:CD1	2.84	0.45
3:D:1007:VAL:HG13	3:D:1008:PHE:H	1.81	0.45
3:D:1165:TYR:CE2	3:D:1214:PRO:HB3	2.51	0.45
3:D:1346:ARG:NH1	3:D:1369:GLU:OE2	2.50	0.45
3:D:1475:GLY:HA2	4:E:17:TYR:CE2	2.51	0.45
1:A:24:VAL:HG22	1:A:196:THR:HB	1.98	0.45
2:C:6:PHE:CD2	2:C:909:ALA:HA	2.52	0.45
2:C:8:ARG:C	2:C:494:TYR:OH	2.55	0.45
2:C:289:THR:HG23	2:C:302:VAL:O	2.16	0.45
2:C:321:GLU:O	2:C:322:VAL:C	2.54	0.45
2:C:540:PHE:CE1	2:C:906:PHE:HE1	2.34	0.45
2:C:574:ALA:O	2:C:575:GLN:O	2.34	0.45
2:C:880:MET:O	2:C:881:ASN:O	2.33	0.45
2:C:937:ASP:O	2:C:939:ARG:N	2.48	0.45
2:C:1004:LYS:O	2:C:1005:MET:HB3	2.15	0.45
2:C:1108:PRO:O	2:C:1109:VAL:C	2.55	0.45
3:D:638:LYS:CB	3:D:729:HIS:CE1	2.99	0.45
3:D:678:GLU:C	3:D:680:GLN:N	2.69	0.45
3:D:762:GLN:HE21	4:E:20:THR:CB	2.28	0.45
3:D:1148:VAL:HG22	3:D:1163:GLY:O	2.17	0.45
3:D:1333:HIS:HE1	3:D:1421:LEU:HB3	1.80	0.45
2:C:137:VAL:HG11	2:C:411:SER:HB2	1.97	0.45
2:C:218:VAL:O	2:C:219:GLN:C	2.54	0.45
2:C:257:LEU:HA	2:C:261:LEU:CD2	2.45	0.45
2:C:351:LEU:HG	2:C:352:ALA:N	2.31	0.45
2:C:380:ALA:O	2:C:384:GLU:CB	2.64	0.45
2:C:654:LEU:HG	2:C:655:LEU:N	2.32	0.45
2:C:733:ALA:O	2:C:734:LEU:C	2.55	0.45
2:C:959:PRO:O	2:C:962:GLN:N	2.50	0.45
3:D:78:VAL:N	3:D:81:THR:O	2.43	0.45
3:D:632:VAL:HG12	3:D:633:VAL:N	2.30	0.45
3:D:729:HIS:ND1	3:D:730:PRO:HD2	2.30	0.45
3:D:772:PRO:HG3	3:D:778:LEU:HD23	1.99	0.45
3:D:1170:ASP:C	3:D:1172:HIS:N	2.70	0.45
3:D:1462:LEU:CD2	3:D:1473:PRO:HG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLY:O	1:A:18:ASP:HB2	2.16	0.45
1:A:50:GLY:HA3	1:A:171:PHE:O	2.15	0.45
1:A:121:GLU:C	1:A:123:MET:N	2.70	0.45
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.98	0.45
2:C:152:PRO:O	2:C:153:ALA:O	2.35	0.45
2:C:215:GLY:O	2:C:216:ASP:C	2.54	0.45
2:C:224:GLU:C	2:C:226:VAL:N	2.70	0.45
2:C:520:GLU:N	2:C:521:PRO:CD	2.80	0.45
2:C:574:ALA:HB1	2:C:667:ALA:O	2.17	0.45
2:C:681:GLY:CA	3:D:939:PHE:CE2	2.99	0.45
2:C:762:LYS:HD2	2:C:786:LYS:CD	2.38	0.45
2:C:881:ASN:HB2	3:D:1061:PHE:CE2	2.52	0.45
2:C:926:PHE:HE1	2:C:929:ARG:NH1	2.14	0.45
3:D:153:LEU:C	3:D:155:ASP:H	2.19	0.45
3:D:653:PHE:O	3:D:654:LYS:C	2.55	0.45
3:D:678:GLU:O	3:D:680:GLN:N	2.45	0.45
3:D:770:LEU:CD1	3:D:770:LEU:N	2.77	0.45
3:D:845:ASN:O	3:D:847:ASP:N	2.42	0.45
3:D:963:TYR:HE2	3:D:1002:LYS:HB3	1.81	0.45
3:D:1044:LEU:HD12	3:D:1044:LEU:HA	1.73	0.45
3:D:1065:LEU:HD12	3:D:1067:VAL:HG23	1.98	0.45
3:D:1075:HIS:CD2	3:D:1075:HIS:N	2.85	0.45
3:D:1237:THR:HG22	3:D:1239:ARG:H	1.81	0.45
4:E:63:TRP:O	4:E:67:GLU:N	2.41	0.45
1:A:74:ASP:HB2	2:C:627:ARG:NH2	2.31	0.45
1:B:15:THR:C	1:B:17:GLY:H	2.18	0.45
1:B:173:PRO:HA	1:B:203:GLY:HA3	1.99	0.45
2:C:64:LEU:HA	2:C:101:ILE:O	2.16	0.45
2:C:553:ASP:HA	2:C:882:LEU:HA	1.98	0.45
2:C:588:VAL:CG2	2:C:666:LEU:HD13	2.46	0.45
2:C:848:VAL:HG12	3:D:740:PHE:O	2.16	0.45
3:D:92:HIS:O	3:D:94:GLU:N	2.50	0.45
3:D:601:ARG:HD2	3:D:605:ASP:OD2	2.16	0.45
3:D:631:ILE:HD11	3:D:743:ASP:HB2	1.97	0.45
3:D:764:LEU:HG	3:D:766:ALA:N	2.29	0.45
3:D:1051:GLU:O	3:D:1052:THR:O	2.35	0.45
3:D:1069:GLU:C	3:D:1071:PHE:N	2.70	0.45
3:D:1086:LEU:HD13	3:D:1238:MET:CB	2.38	0.45
3:D:1118:ILE:HD11	3:D:1193:THR:CG2	2.46	0.45
3:D:1130:ARG:HG2	3:D:1130:ARG:NH1	2.32	0.45
3:D:1140:ILE:O	3:D:1144:LEU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1271:LYS:O	3:D:1273:VAL:N	2.49	0.45
3:D:1283:ILE:CD1	3:D:1312:LEU:HA	2.47	0.45
1:A:30:ARG:NH1	1:A:192:LEU:HD23	2.32	0.45
1:A:42:ARG:NH2	1:B:34:VAL:HB	2.26	0.45
1:A:126:ASP:OD1	1:A:126:ASP:N	2.49	0.45
1:B:12:THR:O	1:B:24:VAL:N	2.50	0.45
2:C:32:ALA:HB2	2:C:73:ILE:HD13	1.99	0.45
2:C:78:PHE:N	2:C:78:PHE:CD1	2.83	0.45
2:C:304:LEU:H	2:C:305:PRO:HD3	1.82	0.45
2:C:374:ASN:O	2:C:376:ARG:HG2	2.17	0.45
2:C:406:HIS:ND1	2:C:406:HIS:O	2.50	0.45
2:C:630:ARG:HA	2:C:705:ILE:CD1	2.45	0.45
2:C:935:GLY:O	2:C:936:VAL:O	2.33	0.45
3:D:91:ALA:CB	3:D:518:PRO:CG	2.95	0.45
3:D:666:PHE:CZ	3:D:676:MET:SD	3.10	0.45
3:D:1085:ALA:C	3:D:1087:ARG:H	2.19	0.45
3:D:1106:VAL:HG12	3:D:1107:VAL:N	2.32	0.45
3:D:1268:PRO:HB2	3:D:1269:LYS:H	1.67	0.45
4:E:77:GLU:HG3	4:E:77:GLU:O	2.17	0.45
1:A:179:PHE:O	1:A:179:PHE:CD1	2.69	0.45
1:A:189:ARG:O	1:A:191:ASP:N	2.50	0.45
1:A:198:ARG:NH1	2:C:932:GLU:HB3	2.31	0.45
1:B:36:LEU:O	1:B:40:LEU:HD23	2.17	0.45
2:C:33:ASP:O	2:C:33:ASP:CG	2.55	0.45
2:C:115:LEU:HD13	2:C:375:SER:CB	2.47	0.45
2:C:378:LEU:HD12	2:C:378:LEU:N	2.31	0.45
2:C:758:ARG:O	2:C:788:THR:O	2.35	0.45
2:C:877:PRO:HG2	3:D:949:ILE:HD12	1.98	0.45
2:C:905:VAL:O	2:C:906:PHE:HB2	2.17	0.45
2:C:940:GLU:HA	2:C:973:VAL:CG2	2.45	0.45
3:D:21:TRP:C	3:D:23:TYR:N	2.70	0.45
3:D:106:LYS:O	3:D:109:PRO:N	2.50	0.45
3:D:609:GLY:O	3:D:611:GLN:N	2.50	0.45
3:D:860:LEU:HD12	3:D:878:GLY:CA	2.47	0.45
3:D:876:SER:O	3:D:878:GLY:N	2.50	0.45
3:D:1076:GLY:HA2	3:D:1079:LYS:HG2	1.97	0.45
3:D:1192:LEU:HG	3:D:1369:GLU:HB3	1.99	0.45
3:D:1352:ILE:O	3:D:1353:GLN:C	2.55	0.45
1:A:157:GLY:O	1:A:164:ALA:HB1	2.17	0.45
1:A:157:GLY:H	1:A:166:PRO:HB3	1.80	0.45
1:A:173:PRO:O	1:A:202:ASP:CA	2.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LEU:CG	1:B:199:ILE:HD11	2.43	0.45
2:C:282:GLY:O	2:C:283:VAL:HG23	2.17	0.45
2:C:299:LYS:O	2:C:299:LYS:CG	2.64	0.45
2:C:410:ILE:HG21	2:C:468:ARG:HH22	1.81	0.45
2:C:545:ASN:C	2:C:547:ILE:H	2.20	0.45
2:C:576:ALA:HB1	2:C:577:PRO:HD2	1.99	0.45
2:C:1035:MET:HB3	3:D:707:THR:HB	1.98	0.45
3:D:695:ILE:HD13	3:D:718:PRO:HB2	1.98	0.45
3:D:705:ALA:HB3	3:D:706:PRO:HD3	1.98	0.45
3:D:957:PRO:HG3	3:D:1007:VAL:CA	2.47	0.45
3:D:1060:SER:C	3:D:1062:ARG:N	2.69	0.45
3:D:1319:VAL:O	3:D:1320:GLU:C	2.54	0.45
1:A:23:PHE:CZ	1:A:207:PRO:HB2	2.49	0.45
1:A:88:ARG:HD3	1:A:121:GLU:CD	2.37	0.45
1:A:195:LEU:HD22	1:A:197:LEU:HD22	1.99	0.45
2:C:202:TYR:CE1	2:C:304:LEU:HD13	2.52	0.45
2:C:202:TYR:C	2:C:203:ASP:CG	2.75	0.45
2:C:246:ASP:O	2:C:248:PRO:HD3	2.17	0.45
2:C:545:ASN:O	2:C:547:ILE:N	2.49	0.45
2:C:884:GLN:HG3	2:C:885:ILE:HD12	1.98	0.45
3:D:511:TRP:CD1	3:D:511:TRP:N	2.84	0.45
3:D:679:ARG:C	3:D:680:GLN:HG2	2.38	0.45
3:D:710:ARG:NH1	3:D:768:ASN:HD21	2.15	0.45
3:D:924:MET:N	4:E:7:ASP:OD2	2.50	0.45
3:D:1266:ARG:C	3:D:1268:PRO:HD3	2.37	0.45
1:A:225:PHE:CD2	1:B:11:PHE:CE1	3.05	0.45
1:B:188:GLN:HG2	3:D:688:TRP:HD1	1.77	0.45
2:C:143:SER:OG	2:C:330:ASN:HA	2.17	0.45
2:C:150:PRO:HD3	2:C:321:GLU:HB3	1.98	0.45
2:C:163:ILE:CG2	2:C:169:GLY:HA3	2.45	0.45
2:C:405:ARG:NH1	2:C:566:THR:OG1	2.48	0.45
2:C:491:GLU:HA	2:C:531:PHE:CA	2.21	0.45
2:C:491:GLU:O	2:C:510:THR:N	2.43	0.45
2:C:531:PHE:O	2:C:532:MET:CB	2.60	0.45
2:C:537:LYS:O	2:C:540:PHE:N	2.48	0.45
2:C:674:VAL:HG21	2:C:871:LEU:HB2	1.99	0.45
2:C:778:PHE:O	2:C:780:GLU:N	2.50	0.45
2:C:840:ALA:CB	2:C:846:LYS:HA	2.47	0.45
2:C:944:LEU:O	2:C:946:ARG:N	2.50	0.45
3:D:778:LEU:HD12	3:D:778:LEU:O	2.17	0.45
3:D:907:GLU:HG3	3:D:911:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:924:MET:O	3:D:925:GLU:C	2.54	0.45
3:D:924:MET:O	3:D:927:THR:N	2.49	0.45
3:D:983:LEU:HD23	3:D:983:LEU:HA	1.73	0.45
3:D:1083:ASP:O	3:D:1086:LEU:CB	2.62	0.45
3:D:1283:ILE:HD13	3:D:1312:LEU:CD2	2.47	0.45
3:D:1311:LEU:H	3:D:1311:LEU:CD1	2.29	0.45
3:D:1435:LEU:HD21	3:D:1468:LEU:CD2	2.47	0.45
3:D:1463:LYS:HA	3:D:1466:VAL:HB	1.99	0.45
1:A:178:ALA:HB2	2:C:863:ASP:O	2.17	0.44
1:B:19:HIS:HA	1:B:207:PRO:HG3	1.98	0.44
1:B:80:LEU:HD22	3:D:839:LEU:CB	2.48	0.44
1:B:94:MET:CB	1:B:94:MET:HE3	2.47	0.44
2:C:584:GLU:C	2:C:586:ARG:H	2.19	0.44
2:C:691:SER:HB2	2:C:858:MET:HE2	1.98	0.44
2:C:874:LEU:HD12	2:C:874:LEU:HA	1.66	0.44
2:C:1008:ARG:HH22	2:C:1020:PRO:HA	1.82	0.44
3:D:149:LYS:C	3:D:151:GLN:H	2.19	0.44
3:D:638:LYS:O	3:D:639:LEU:O	2.34	0.44
3:D:663:GLU:C	3:D:665:ALA:N	2.69	0.44
3:D:905:PRO:CG	3:D:906:GLN:N	2.80	0.44
3:D:1343:ALA:O	3:D:1344:VAL:C	2.55	0.44
3:D:1478:SER:O	3:D:1481:VAL:N	2.45	0.44
4:E:9:LEU:C	4:E:11:GLY:H	2.20	0.44
1:B:99:LEU:O	1:B:141:GLU:HA	2.17	0.44
1:B:111:ALA:HA	1:B:114:PHE:CE1	2.52	0.44
2:C:30:LEU:HD13	2:C:118:LEU:HD11	1.98	0.44
2:C:378:LEU:O	2:C:382:LEU:HB2	2.17	0.44
2:C:520:GLU:O	2:C:522:VAL:N	2.49	0.44
2:C:588:VAL:HG21	2:C:666:LEU:HA	1.99	0.44
2:C:641:PRO:HA	2:C:656:ALA:CB	2.47	0.44
2:C:677:MET:H	2:C:873:PRO:HD3	1.82	0.44
2:C:897:LEU:O	2:C:899:GLN:HG3	2.17	0.44
2:C:1104:GLU:HA	3:D:6:ARG:HG3	1.99	0.44
3:D:890:VAL:HG13	3:D:926:LYS:CE	2.45	0.44
3:D:1007:VAL:HG11	3:D:1040:GLY:HA3	2.00	0.44
3:D:1094:LEU:HA	3:D:1094:LEU:HD12	1.63	0.44
3:D:1344:VAL:HG11	3:D:1421:LEU:HD11	1.99	0.44
4:E:13:VAL:HB	4:E:18:ARG:HB3	1.99	0.44
1:A:111:ALA:N	1:A:129:ILE:HG12	2.31	0.44
1:B:133:GLU:C	1:B:135:GLY:H	2.21	0.44
2:C:23:VAL:C	2:C:25:SER:H	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:182:VAL:HG12	2:C:193:LEU:CB	2.48	0.44
2:C:440:PRO:HD3	2:C:455:LEU:HA	1.96	0.44
2:C:493:ARG:NH2	3:D:1069:GLU:OE2	2.50	0.44
3:D:84:ILE:O	3:D:85:VAL:CB	2.65	0.44
3:D:691:LEU:C	3:D:693:GLU:H	2.19	0.44
3:D:792:ILE:N	3:D:792:ILE:CD1	2.79	0.44
3:D:809:PRO:C	3:D:811:GLU:H	2.19	0.44
3:D:948:THR:O	3:D:1020:LEU:CB	2.58	0.44
3:D:1400:VAL:O	3:D:1400:VAL:HG12	2.17	0.44
3:D:1467:ILE:C	3:D:1469:GLY:H	2.20	0.44
4:E:4:PRO:CG	4:E:66:LYS:HE2	2.47	0.44
1:A:26:GLU:HB3	1:A:27:PRO:HD2	1.88	0.44
1:A:74:ASP:OD2	2:C:627:ARG:NH2	2.50	0.44
1:A:160:ASP:O	1:A:161:ARG:C	2.55	0.44
1:A:185:ARG:NH2	1:A:194:LYS:CE	2.80	0.44
2:C:103:LYS:HD3	2:C:103:LYS:HA	1.85	0.44
2:C:394:PHE:HB2	5:C:1640:RFP:O8	2.18	0.44
2:C:413:LEU:HD11	2:C:448:ASN:OD1	2.17	0.44
2:C:520:GLU:C	2:C:522:VAL:N	2.69	0.44
2:C:527:GLU:O	2:C:529:VAL:N	2.50	0.44
2:C:544:THR:O	2:C:545:ASN:C	2.54	0.44
2:C:722:ILE:HD13	2:C:821:GLU:OE1	2.17	0.44
2:C:729:LEU:CB	2:C:734:LEU:HD21	2.48	0.44
2:C:754:ILE:HD13	2:C:791:ARG:NE	2.33	0.44
2:C:1070:ILE:N	2:C:1070:ILE:HD12	2.32	0.44
3:D:22:SER:C	3:D:24:GLY:H	2.21	0.44
3:D:43(U):UNK:O	3:D:44(U):UNK:CB	2.66	0.44
3:D:947:ILE:HA	3:D:1020:LEU:HD13	1.99	0.44
3:D:960:LYS:O	3:D:961:GLN:C	2.56	0.44
3:D:1133:ARG:HG3	3:D:1134:LEU:N	2.31	0.44
1:A:43:ILE:O	1:A:44:LEU:C	2.56	0.44
1:A:82:LEU:HD23	1:A:129:ILE:HD12	1.98	0.44
1:B:29:GLU:O	1:B:30:ARG:C	2.55	0.44
1:B:169:ALA:HB1	1:B:171:PHE:CE1	2.52	0.44
2:C:8:ARG:HB3	2:C:494:TYR:OH	2.18	0.44
2:C:9:ILE:O	2:C:10:ARG:HB3	2.18	0.44
2:C:15:LEU:HD21	2:C:461:VAL:HG23	1.94	0.44
2:C:73:ILE:CD1	2:C:94:LEU:HD13	2.48	0.44
2:C:79:SER:O	2:C:82:GLU:HB3	2.16	0.44
2:C:121:MET:HA	2:C:126:SER:O	2.17	0.44
2:C:202:TYR:CB	2:C:207:LEU:HD13	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:267:TYR:HD1	2:C:273:GLY:HA3	1.81	0.44
2:C:328:LEU:HB3	2:C:467:ILE:HG21	1.98	0.44
2:C:341:ALA:O	2:C:344:PHE:N	2.45	0.44
2:C:445:GLU:HG3	5:C:1640:RFP:C30	2.47	0.44
2:C:520:GLU:O	2:C:521:PRO:C	2.55	0.44
2:C:605:LYS:HA	2:C:612:ALA:N	2.30	0.44
2:C:648:ARG:HH11	2:C:648:ARG:CG	2.27	0.44
2:C:669:GLY:HA3	2:C:995:MET:HA	1.98	0.44
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.52	0.44
3:D:98:PRO:O	3:D:514:LEU:HD13	2.18	0.44
3:D:633:VAL:CG2	3:D:634:GLY:N	2.80	0.44
3:D:853:VAL:HG21	3:D:877:PRO:HB3	1.99	0.44
3:D:864:VAL:CG1	3:D:874:GLU:O	2.66	0.44
3:D:984:THR:O	3:D:988:ARG:N	2.48	0.44
3:D:1047:LYS:CA	3:D:1053:PHE:CE1	2.92	0.44
3:D:1353:GLN:O	3:D:1354:LYS:C	2.55	0.44
3:D:1461:GLY:N	3:D:1464:GLU:OE1	2.47	0.44
4:E:22:VAL:HG21	4:E:75:PHE:CD2	2.52	0.44
1:A:164:ALA:O	1:A:165:ILE:C	2.56	0.44
1:A:221:HIS:HA	1:A:224:TYR:CE2	2.52	0.44
2:C:569:VAL:HA	2:C:570:PRO:HD2	1.77	0.44
2:C:605:LYS:CG	2:C:606:VAL:H	2.30	0.44
2:C:606:VAL:O	2:C:607:ASP:HB2	2.18	0.44
2:C:713:ARG:HH12	2:C:816:LYS:CG	2.31	0.44
2:C:895:TYR:HD2	2:C:896:PHE:CE1	2.36	0.44
2:C:959:PRO:CG	2:C:960:GLU:N	2.80	0.44
3:D:629:SER:HB3	3:D:726:ILE:CD1	2.47	0.44
3:D:641:GLN:HB3	3:D:719:VAL:CG2	2.46	0.44
3:D:776:GLU:HB3	3:D:777:PRO:HD2	1.98	0.44
3:D:879:ARG:NH1	3:D:904:VAL:HG13	2.32	0.44
3:D:911:LEU:HD12	3:D:911:LEU:HA	1.85	0.44
3:D:1069:GLU:HG3	3:D:1072:ILE:CG1	2.48	0.44
3:D:1093:TYR:HE2	3:D:1097:LYS:CE	2.31	0.44
3:D:1304:LYS:N	3:D:1304:LYS:CD	2.80	0.44
4:E:63:TRP:O	4:E:64:ALA:C	2.56	0.44
1:A:18:ASP:O	1:A:19:HIS:CB	2.66	0.44
1:A:201:THR:HG22	1:A:202:ASP:N	2.31	0.44
1:A:225:PHE:HD2	1:B:11:PHE:CE1	2.36	0.44
1:B:160:ASP:O	1:B:162:ILE:N	2.50	0.44
2:C:12:VAL:CG1	2:C:13:ILE:N	2.62	0.44
2:C:141:HIS:CE1	2:C:334:ARG:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:236:VAL:CG2	2:C:250:LYS:HA	2.47	0.44
2:C:340:MET:SD	2:C:340:MET:C	2.96	0.44
2:C:399:ASN:HD21	2:C:401:LEU:CB	2.27	0.44
2:C:488:ALA:O	2:C:490:GLU:N	2.51	0.44
2:C:584:GLU:H	2:C:584:GLU:HG3	1.31	0.44
2:C:613:VAL:H	2:C:621:VAL:HA	1.83	0.44
2:C:628:TYR:HE2	2:C:703:ILE:HD13	1.81	0.44
2:C:688:ILE:CG2	2:C:869:VAL:HG23	2.48	0.44
2:C:705:ILE:HA	2:C:828:ALA:HA	2.00	0.44
2:C:714:ASP:O	2:C:715:THR:O	2.35	0.44
2:C:835:VAL:HG13	2:C:850:ALA:O	2.18	0.44
2:C:1021:LEU:O	2:C:1022:GLY:C	2.56	0.44
3:D:88:TYR:C	3:D:520:LEU:CD1	2.85	0.44
3:D:143:ASP:O	3:D:145:VAL:N	2.51	0.44
3:D:772:PRO:CG	3:D:778:LEU:HD23	2.47	0.44
3:D:791:TYR:HE1	3:D:1023:MET:HG3	1.82	0.44
3:D:906:GLN:O	3:D:907:GLU:HB2	2.18	0.44
3:D:1047:LYS:HA	3:D:1053:PHE:CZ	2.49	0.44
3:D:1114:THR:HA	3:D:1189:ARG:HH11	1.83	0.44
3:D:1125:MET:HG2	3:D:1126:ASP:H	1.81	0.44
3:D:1231:GLU:O	3:D:1233:GLY:N	2.51	0.44
4:E:32:ARG:HG3	4:E:33:HIS:N	2.32	0.44
1:A:86:VAL:HG13	1:A:123:MET:HB3	1.99	0.44
1:B:188:GLN:NE2	1:B:188:GLN:O	2.50	0.44
2:C:598:GLU:HB3	2:C:599:GLU:H	1.59	0.44
2:C:925:TYR:CE2	2:C:972:VAL:HG21	2.53	0.44
2:C:983:PHE:O	2:C:984:GLU:C	2.55	0.44
3:D:92:HIS:O	3:D:93:ILE:C	2.57	0.44
3:D:680:GLN:C	3:D:681:ARG:HG3	2.38	0.44
3:D:688:TRP:HA	3:D:688:TRP:HE3	1.82	0.44
3:D:1117:TYR:C	3:D:1118:ILE:HD12	2.38	0.44
3:D:1236:LEU:HD12	3:D:1256:LEU:CD1	2.47	0.44
2:C:11:GLU:OE1	2:C:473:ARG:CD	2.66	0.44
2:C:11:GLU:OE1	2:C:473:ARG:CG	2.66	0.44
2:C:172:ILE:HG22	2:C:173:ASP:N	2.32	0.44
2:C:278:GLU:HA	2:C:283:VAL:HA	1.99	0.44
2:C:773:LEU:O	2:C:774:LEU:C	2.56	0.44
2:C:1038:TRP:CZ2	3:D:1096:ARG:HA	2.52	0.44
2:C:1088:LEU:HD23	3:D:1468:LEU:CD2	2.48	0.44
3:D:462:GLN:O	3:D:463:GLU:C	2.56	0.44
3:D:628:ARG:O	3:D:629:SER:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:896:ALA:HA	3:D:899:LEU:HD22	2.00	0.44
3:D:1047:LYS:HB3	3:D:1048:PRO:CD	2.45	0.44
3:D:1220:ALA:O	3:D:1224:VAL:HG23	2.18	0.44
3:D:1252:ILE:HG21	3:D:1261:GLU:OE1	2.18	0.44
3:D:1274:ILE:O	3:D:1275:SER:C	2.57	0.44
4:E:3:GLU:HB3	4:E:4:PRO:HD2	1.99	0.44
1:A:100:ILE:HG22	1:A:101:LEU:H	1.82	0.43
1:B:59:GLU:OE1	1:B:60:ASP:N	2.50	0.43
1:B:95:ALA:O	1:B:96:SER:CB	2.60	0.43
2:C:64:LEU:N	2:C:101:ILE:O	2.51	0.43
2:C:100:LEU:HD11	2:C:369:PRO:CD	2.46	0.43
2:C:104:ASP:N	2:C:104:ASP:OD1	2.50	0.43
2:C:343:GLN:HG2	2:C:385:PHE:HB2	2.00	0.43
2:C:710:ILE:N	2:C:710:ILE:CD1	2.74	0.43
2:C:738:ASP:HA	2:C:743:VAL:HA	2.00	0.43
2:C:754:ILE:HG22	2:C:754:ILE:O	2.18	0.43
2:C:794:PRO:HG2	2:C:1027:PHE:CB	2.48	0.43
2:C:881:ASN:HB2	3:D:1061:PHE:HE2	1.81	0.43
3:D:564:GLU:HG3	3:D:568:ARG:NE	2.29	0.43
3:D:606:ILE:HD12	3:D:606:ILE:N	2.28	0.43
3:D:658:LEU:O	3:D:661:MET:N	2.51	0.43
3:D:1251:ASP:N	3:D:1269:LYS:HZ2	1.84	0.43
1:A:41:ARG:NH1	1:A:42:ARG:N	2.66	0.43
1:B:151:VAL:O	1:B:169:ALA:N	2.46	0.43
2:C:54:ILE:HG13	2:C:55:GLU:O	2.18	0.43
2:C:95:TYR:CD1	2:C:112:GLU:OE1	2.71	0.43
2:C:443:THR:O	2:C:444:PRO:O	2.36	0.43
2:C:626:ARG:CZ	2:C:637:PHE:CZ	3.00	0.43
2:C:760:SER:OG	2:C:762:LYS:HG3	2.18	0.43
2:C:836:GLY:C	2:C:837:ASP:OD2	2.55	0.43
2:C:1042:ALA:CB	3:D:1227:GLU:OE1	2.66	0.43
5:C:1640:RFP:N1	5:C:1640:RFP:N2	2.65	0.43
3:D:564:GLU:O	3:D:567:ILE:HG22	2.19	0.43
3:D:851:LEU:HD12	3:D:851:LEU:O	2.18	0.43
3:D:899:LEU:O	3:D:900:ILE:CG1	2.53	0.43
3:D:905:PRO:CG	3:D:906:GLN:H	2.31	0.43
3:D:931:LEU:HD13	3:D:931:LEU:HA	1.84	0.43
3:D:969:ARG:CZ	3:D:970:LYS:HE3	2.47	0.43
3:D:1011:PHE:CE2	3:D:1022:VAL:CG1	3.01	0.43
3:D:1066:THR:C	3:D:1068:LEU:N	2.71	0.43
3:D:1192:LEU:HD21	3:D:1369:GLU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:85:GLU:O	2:C:806:LEU:HD11	2.18	0.43
2:C:291:VAL:HB	2:C:299:LYS:O	2.19	0.43
2:C:380:ALA:O	2:C:384:GLU:N	2.38	0.43
2:C:605:LYS:HG2	2:C:606:VAL:N	2.33	0.43
2:C:1034:GLU:HG3	2:C:1035:MET:N	2.33	0.43
3:D:513:ILE:CG2	3:D:514:LEU:N	2.81	0.43
3:D:770:LEU:HD23	3:D:927:THR:CG2	2.49	0.43
3:D:805:ALA:O	3:D:806:PHE:CB	2.66	0.43
3:D:808:THR:O	3:D:809:PRO:O	2.36	0.43
3:D:816:TYR:HA	3:D:832:ARG:NH2	2.33	0.43
3:D:899:LEU:N	3:D:899:LEU:CD1	2.78	0.43
3:D:1071:PHE:O	3:D:1075:HIS:HD2	2.01	0.43
3:D:1253:THR:HG21	3:D:1327:ARG:HG2	2.00	0.43
3:D:1261:GLU:OE2	3:D:1268:PRO:HB3	2.18	0.43
4:E:9:LEU:C	4:E:11:GLY:N	2.72	0.43
4:E:40:LEU:HA	4:E:44:GLU:HG3	2.00	0.43
1:A:86:VAL:HG13	1:A:86:VAL:O	2.18	0.43
1:A:165:ILE:O	1:A:165:ILE:CG1	2.60	0.43
1:A:222:LEU:HD21	1:B:218:LEU:HD23	2.00	0.43
1:B:11:PHE:HZ	1:B:211:LEU:HD21	1.83	0.43
2:C:73:ILE:HD12	2:C:73:ILE:N	2.32	0.43
2:C:203:ASP:H	2:C:207:LEU:HB2	1.83	0.43
3:D:687:VAL:O	3:D:688:TRP:C	2.56	0.43
3:D:785:ILE:HD13	3:D:935:LYS:HA	2.00	0.43
3:D:1235:GLN:C	3:D:1236:LEU:HD23	2.38	0.43
3:D:1292:VAL:CG2	3:D:1305:LEU:HD23	2.49	0.43
4:E:25:LYS:HZ3	4:E:29:GLN:CD	2.21	0.43
1:A:218:LEU:O	1:A:218:LEU:HD12	2.18	0.43
1:B:214:ALA:HA	1:B:217:ILE:HG13	1.99	0.43
2:C:67:ASP:N	2:C:67:ASP:OD1	2.50	0.43
2:C:186:VAL:O	2:C:187:ASN:C	2.57	0.43
2:C:236:VAL:CG1	2:C:248:PRO:O	2.67	0.43
2:C:312:ALA:HB1	2:C:318:PRO:HG2	1.97	0.43
2:C:596:TYR:O	2:C:596:TYR:CD1	2.71	0.43
2:C:1035:MET:HB2	2:C:1036:GLU:OE2	2.17	0.43
3:D:567:ILE:CA	3:D:570:GLU:HB2	2.49	0.43
3:D:590:PRO:C	3:D:600:LEU:HD21	2.39	0.43
3:D:935:LYS:HG2	3:D:939:PHE:HD1	1.83	0.43
3:D:1011:PHE:O	3:D:1013:GLU:N	2.51	0.43
3:D:1175:ILE:O	3:D:1179:GLU:HG3	2.18	0.43
3:D:1331:ASP:C	3:D:1333:HIS:N	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:GLU:HG2	1:B:134:GLU:N	2.33	0.43
2:C:306:THR:HG22	2:C:307:LEU:N	2.34	0.43
2:C:398:THR:O	2:C:635:THR:HG21	2.19	0.43
2:C:428:ARG:O	2:C:429:ASP:HB2	2.18	0.43
2:C:491:GLU:CA	2:C:531:PHE:HA	2.21	0.43
2:C:539:VAL:HB	2:C:540:PHE:CD1	2.53	0.43
2:C:568:ALA:O	2:C:569:VAL:CG1	2.66	0.43
2:C:595:LEU:HD21	2:C:623:HIS:CB	2.47	0.43
2:C:724:ARG:C	2:C:726:ILE:HD12	2.38	0.43
3:D:669:ASN:O	3:D:672:ALA:N	2.50	0.43
3:D:700:VAL:HG13	3:D:748:HIS:O	2.18	0.43
3:D:1057:VAL:HG13	3:D:1067:VAL:HG11	2.01	0.43
3:D:1231:GLU:C	3:D:1233:GLY:H	2.21	0.43
3:D:1250:THR:HG22	3:D:1251:ASP:O	2.18	0.43
3:D:1306:PRO:O	3:D:1308:ASP:N	2.52	0.43
3:D:1323:GLN:H	3:D:1324:PRO:HD2	1.83	0.43
3:D:1443:THR:O	3:D:1444:THR:C	2.57	0.43
1:A:28:LEU:O	1:A:192:LEU:HB3	2.19	0.43
1:B:188:GLN:HG3	3:D:688:TRP:HD1	1.84	0.43
2:C:99:GLN:OE1	2:C:109:LYS:HE3	2.18	0.43
2:C:184:MET:HE2	2:C:196:LEU:HD22	1.99	0.43
2:C:399:ASN:ND2	2:C:399:ASN:O	2.44	0.43
2:C:467:ILE:HG22	2:C:484:VAL:CG2	2.48	0.43
2:C:606:VAL:HG22	2:C:606:VAL:O	2.19	0.43
2:C:944:LEU:C	2:C:946:ARG:N	2.71	0.43
3:D:764:LEU:HD23	3:D:767:HIS:CD2	2.54	0.43
3:D:806:PHE:N	3:D:827:ILE:HA	2.17	0.43
3:D:836:VAL:CB	3:D:858:LEU:HD21	2.49	0.43
3:D:853:VAL:O	3:D:854:ALA:O	2.35	0.43
3:D:885:ILE:HG12	3:D:937:TYR:CD2	2.54	0.43
3:D:1258:ARG:HG3	3:D:1258:ARG:NH1	2.33	0.43
3:D:1480:PHE:HE2	4:E:15:SER:HB2	1.82	0.43
3:D:1481:VAL:HG12	4:E:21:VAL:HG21	1.98	0.43
1:A:71:VAL:HG22	1:A:132:LEU:HB3	2.00	0.43
1:B:61:VAL:O	1:B:62:LEU:O	2.36	0.43
1:B:177:VAL:HG13	1:B:199:ILE:CD1	2.49	0.43
2:C:15:LEU:CD1	2:C:461:VAL:HG21	2.37	0.43
2:C:84:ARG:HE	2:C:128:ILE:HG12	1.84	0.43
2:C:89:THR:HA	2:C:130:ASN:H	1.84	0.43
2:C:163:ILE:CG2	2:C:265:LYS:HD2	2.48	0.43
2:C:413:LEU:CD2	2:C:451:LEU:HD13	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:769:PRO:HG2	2:C:770:GLU:HG3	2.00	0.43
2:C:788:THR:O	2:C:788:THR:HG23	2.19	0.43
2:C:1095:LEU:O	2:C:1096:ALA:HB3	2.18	0.43
3:D:110:SER:O	3:D:112:ILE:N	2.48	0.43
3:D:491:LYS:HE2	3:D:495:ARG:HH21	1.84	0.43
3:D:916:TYR:C	3:D:918:ALA:N	2.72	0.43
3:D:1103:HIS:O	3:D:1105:ILE:HG12	2.19	0.43
4:E:38:THR:HG23	4:E:63:TRP:CZ3	2.53	0.43
1:A:221:HIS:O	1:A:222:LEU:C	2.57	0.43
1:B:70:GLY:O	1:B:132:LEU:HB2	2.18	0.43
1:B:173:PRO:HA	1:B:203:GLY:CA	2.48	0.43
1:B:174:VAL:O	1:B:174:VAL:HG23	2.19	0.43
2:C:5:ARG:NH2	2:C:10:ARG:NH1	2.66	0.43
2:C:110:GLU:HB2	2:C:369:PRO:HB2	2.00	0.43
2:C:218:VAL:O	2:C:220:GLY:N	2.52	0.43
2:C:254:LEU:O	2:C:254:LEU:HD12	2.19	0.43
2:C:260:LEU:HD23	2:C:261:LEU:CB	2.45	0.43
2:C:397:GLU:HB2	2:C:632:ASN:HD22	1.83	0.43
2:C:648:ARG:CG	2:C:648:ARG:NH1	2.81	0.43
2:C:730:SER:CA	2:C:734:LEU:HD11	2.44	0.43
2:C:796:GLU:HA	3:D:681:ARG:NH2	2.33	0.43
2:C:967:PHE:C	2:C:969:LEU:H	2.22	0.43
2:C:974:LEU:HD23	2:C:987:ILE:HG21	2.01	0.43
3:D:15:PRO:O	3:D:19:ARG:HG3	2.19	0.43
3:D:483:HIS:N	3:D:484:PRO:CD	2.54	0.43
3:D:711:LEU:HD21	3:D:768:ASN:O	2.19	0.43
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.54	0.43
4:E:25:LYS:NZ	4:E:29:GLN:OE1	2.49	0.43
4:E:28:GLN:O	4:E:29:GLN:HB2	2.19	0.43
1:A:94:MET:HE1	1:A:119:ASP:HB2	1.95	0.43
1:B:40:LEU:O	1:B:44:LEU:HD22	2.18	0.43
1:B:41:ARG:HA	1:B:177:VAL:HG11	2.01	0.43
1:B:171:PHE:O	1:B:172:SER:OG	2.33	0.43
2:C:148:PHE:HA	2:C:159:ILE:HA	2.01	0.43
2:C:182:VAL:HG11	2:C:307:LEU:HD11	2.01	0.43
2:C:205:GLU:OE2	2:C:209:ARG:HD2	2.19	0.43
2:C:424:GLY:O	2:C:427:VAL:HG23	2.18	0.43
2:C:631:SER:C	2:C:634:GLY:H	2.23	0.43
2:C:710:ILE:HD12	2:C:710:ILE:H	1.83	0.43
3:D:472:LYS:O	3:D:473:LEU:C	2.58	0.43
3:D:759:ALA:HA	3:D:763:MET:CG	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:793:THR:CA	3:D:879:ARG:HH12	2.31	0.43
3:D:901:GLN:O	3:D:903:ASP:N	2.52	0.43
3:D:952:ASP:C	3:D:954:ALA:N	2.71	0.43
3:D:1114:THR:CB	3:D:1189:ARG:NH1	2.82	0.43
3:D:1122:LEU:CD1	3:D:1186:VAL:HG23	2.49	0.43
3:D:1154:GLU:O	3:D:1155:ALA:CB	2.63	0.43
3:D:1156:LEU:H	3:D:1182:GLU:CD	2.21	0.43
1:A:127:LEU:HG	1:A:127:LEU:O	2.19	0.42
1:A:162:ILE:CG2	1:A:163:ASN:H	2.30	0.42
2:C:63:GLY:O	2:C:64:LEU:HB2	2.19	0.42
2:C:211:LEU:HG	2:C:212:SER:N	2.33	0.42
2:C:221:LEU:O	2:C:221:LEU:HG	2.18	0.42
2:C:310:LEU:O	2:C:313:LEU:N	2.44	0.42
2:C:442:GLU:OE1	2:C:558:ALA:HB3	2.18	0.42
2:C:549:PHE:CE2	2:C:886:LEU:HB3	2.54	0.42
2:C:745:ILE:C	2:C:747:ALA:N	2.71	0.42
2:C:754:ILE:CD1	2:C:791:ARG:NE	2.80	0.42
2:C:953:VAL:HG12	2:C:954:SER:N	2.33	0.42
2:C:1112:PHE:O	2:C:1114:GLY:N	2.52	0.42
3:D:498:VAL:O	3:D:501:ALA:HB3	2.19	0.42
3:D:694:VAL:O	3:D:696:HIS:N	2.52	0.42
3:D:734:GLU:OE2	3:D:780:LYS:NZ	2.52	0.42
3:D:770:LEU:HD23	3:D:927:THR:HG21	2.00	0.42
3:D:772:PRO:CD	3:D:778:LEU:N	2.81	0.42
3:D:936:TYR:C	3:D:936:TYR:HD2	2.22	0.42
3:D:957:PRO:HD3	3:D:1007:VAL:HG23	2.01	0.42
4:E:13:VAL:HG11	4:E:19:LEU:N	2.34	0.42
1:A:36:LEU:O	1:A:40:LEU:HG	2.19	0.42
1:A:118:ALA:O	1:A:120:VAL:N	2.48	0.42
1:A:142:VAL:O	1:A:142:VAL:CG2	2.58	0.42
1:B:34:VAL:O	1:B:36:LEU:N	2.52	0.42
1:B:76:VAL:O	1:B:79:ILE:HB	2.19	0.42
2:C:79:SER:OG	2:C:82:GLU:CB	2.64	0.42
2:C:164:PRO:CG	2:C:168:ARG:HG2	2.49	0.42
2:C:254:LEU:C	2:C:254:LEU:HD12	2.39	0.42
2:C:341:ALA:CB	2:C:345:ARG:HH12	2.32	0.42
2:C:676:ILE:HD12	2:C:676:ILE:N	2.33	0.42
2:C:739:GLU:O	2:C:739:GLU:HG3	2.19	0.42
2:C:922:PHE:O	2:C:926:PHE:N	2.51	0.42
2:C:1069:ALA:O	2:C:1075:ASP:O	2.37	0.42
3:D:468:LEU:C	3:D:470:LEU:H	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:707:THR:HG23	3:D:712:GLY:HA3	2.00	0.42
3:D:752:SER:O	3:D:755:ALA:N	2.47	0.42
3:D:930:LEU:HD12	3:D:934:LEU:HG	2.01	0.42
3:D:1069:GLU:O	3:D:1070:TYR:C	2.58	0.42
3:D:1149:LEU:HD23	3:D:1188:VAL:HG23	2.00	0.42
3:D:1151:ARG:HA	3:D:1162:GLU:HG3	2.01	0.42
3:D:1252:ILE:HD12	3:D:1269:LYS:HB2	2.01	0.42
3:D:1275:SER:O	3:D:1319:VAL:HA	2.19	0.42
3:D:1303:TYR:O	3:D:1305:LEU:N	2.52	0.42
1:A:41:ARG:NE	2:C:860:HIS:CE1	2.85	0.42
1:B:183:ASP:HA	1:B:192:LEU:O	2.19	0.42
2:C:74:GLY:O	2:C:75:ASP:C	2.57	0.42
2:C:342:ASP:CA	2:C:345:ARG:HH11	2.32	0.42
2:C:348:LEU:C	2:C:350:ARG:N	2.71	0.42
2:C:349:ALA:O	2:C:350:ARG:HG3	2.20	0.42
2:C:515:ALA:CB	3:D:1069:GLU:OE2	2.67	0.42
2:C:518:ARG:C	2:C:520:GLU:N	2.70	0.42
2:C:574:ALA:O	2:C:669:GLY:O	2.37	0.42
2:C:686:ASP:CG	3:D:739:ASP:OD2	2.57	0.42
2:C:816:LYS:HA	2:C:817:PRO:HD2	1.88	0.42
2:C:1059:ASP:HA	2:C:1083:GLU:HB2	2.01	0.42
2:C:1071:ILE:HD11	3:D:655:PRO:HB3	2.00	0.42
3:D:540:LEU:HD11	3:D:603:LEU:HD13	2.00	0.42
3:D:584:ASN:HB2	3:D:602:SER:HB3	2.01	0.42
3:D:795:VAL:CA	3:D:862:ASP:CB	2.97	0.42
3:D:907:GLU:O	3:D:908:LYS:CB	2.67	0.42
3:D:1004:THR:OG1	3:D:1036:ARG:HB2	2.19	0.42
3:D:1030:GLY:O	3:D:1031:ASN:CB	2.67	0.42
3:D:1142:SER:C	3:D:1364:HIS:HD2	2.22	0.42
3:D:1194:CYS:SG	3:D:1201:CYS:CB	3.06	0.42
3:D:1326:THR:O	3:D:1327:ARG:CB	2.65	0.42
3:D:1327:ARG:HG3	3:D:1327:ARG:O	2.19	0.42
3:D:1427:SER:C	3:D:1429:LEU:N	2.72	0.42
1:A:41:ARG:HG2	1:A:177:VAL:HG12	1.99	0.42
1:A:63:HIS:HA	1:A:165:ILE:HG22	2.01	0.42
1:B:29:GLU:OE1	1:B:189:ARG:NH1	2.52	0.42
1:B:32:PHE:C	1:B:34:VAL:N	2.72	0.42
1:B:101:LEU:N	1:B:140:MET:O	2.52	0.42
1:B:109:VAL:HG23	1:B:132:LEU:HD22	2.01	0.42
2:C:11:GLU:CD	2:C:473:ARG:NE	2.73	0.42
2:C:122:THR:HG22	2:C:123:GLU:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:268:ASP:HB2	2:C:269:LEU:H	1.54	0.42
2:C:342:ASP:HA	2:C:345:ARG:HH11	1.83	0.42
2:C:517:ARG:CG	2:C:518:ARG:N	2.82	0.42
2:C:547:ILE:HD12	2:C:550:LEU:HD13	2.00	0.42
2:C:603:VAL:O	2:C:604:VAL:CG2	2.66	0.42
2:C:676:ILE:HD12	2:C:676:ILE:H	1.84	0.42
3:D:586:ARG:C	3:D:587:ARG:HD3	2.40	0.42
3:D:632:VAL:CG1	3:D:633:VAL:N	2.81	0.42
3:D:907:GLU:HB3	3:D:911:LEU:CD2	2.48	0.42
3:D:937:TYR:O	3:D:938:GLY:C	2.58	0.42
3:D:1071:PHE:O	3:D:1072:ILE:C	2.56	0.42
3:D:1114:THR:CA	3:D:1189:ARG:HH11	2.32	0.42
3:D:1471:LEU:O	3:D:1472:ILE:C	2.57	0.42
4:E:26:ARG:NH2	4:E:30:LEU:HD13	2.35	0.42
4:E:64:ALA:O	4:E:68:LEU:N	2.52	0.42
1:A:13:ALA:O	1:B:230:ALA:CB	2.68	0.42
1:A:32:PHE:O	1:A:33:GLY:C	2.57	0.42
1:A:143:ARG:NH1	1:A:145:ASP:OD1	2.52	0.42
1:B:73:GLU:HG3	1:B:77:GLU:HG2	2.01	0.42
1:B:202:ASP:O	1:B:204:SER:N	2.52	0.42
2:C:9:ILE:O	2:C:10:ARG:CB	2.68	0.42
2:C:72:ARG:NE	2:C:95:TYR:HE1	2.17	0.42
2:C:193:LEU:HD13	2:C:193:LEU:C	2.39	0.42
2:C:261:LEU:CD1	2:C:263:ASP:HB3	2.47	0.42
2:C:418:LEU:HG	2:C:418:LEU:O	2.19	0.42
2:C:534:VAL:N	2:C:538:GLN:HE22	2.17	0.42
2:C:549:PHE:CD1	2:C:886:LEU:O	2.71	0.42
2:C:923:ASN:N	2:C:924:LEU:HD23	2.35	0.42
3:D:558:LEU:HD21	3:D:567:ILE:CD1	2.49	0.42
3:D:609:GLY:HA2	3:D:615:ARG:NE	2.34	0.42
3:D:722:GLU:HB3	3:D:723:GLY:H	1.48	0.42
3:D:884:ARG:O	3:D:887:GLY:N	2.52	0.42
3:D:1258:ARG:HG3	3:D:1258:ARG:HH11	1.84	0.42
3:D:1329:ALA:O	3:D:1330:ILE:C	2.57	0.42
3:D:1336:LEU:CD1	3:D:1340:GLY:C	2.88	0.42
3:D:1378:TYR:CD1	3:D:1378:TYR:N	2.88	0.42
3:D:1476:THR:HG22	4:E:21:VAL:HG23	2.00	0.42
1:B:57:TYR:O	1:B:140:MET:HA	2.20	0.42
1:B:206:THR:OG1	1:B:209:GLU:HG3	2.20	0.42
2:C:34:VAL:O	2:C:34:VAL:HG12	2.19	0.42
2:C:266:ARG:O	2:C:266:ARG:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:395:LYS:HG2	2:C:397:GLU:CD	2.40	0.42
2:C:573:ARG:HH11	2:C:573:ARG:CG	2.29	0.42
2:C:586:ARG:O	2:C:587:VAL:C	2.58	0.42
2:C:613:VAL:CG2	2:C:619:ARG:HE	2.31	0.42
2:C:710:ILE:CG1	2:C:790:LEU:HB2	2.48	0.42
2:C:755:LEU:CD1	2:C:756:VAL:HG23	2.50	0.42
2:C:1051:GLU:OE2	3:D:751:LEU:HB3	2.19	0.42
3:D:570:GLU:HA	3:D:573:MET:HE2	2.00	0.42
3:D:713:ILE:HG22	3:D:714:GLN:N	2.35	0.42
3:D:734:GLU:O	3:D:735:ALA:C	2.57	0.42
3:D:935:LYS:HG2	3:D:939:PHE:CD1	2.54	0.42
3:D:1201:CYS:SG	3:D:1204:CYS:HB2	2.60	0.42
3:D:1466:VAL:O	3:D:1467:ILE:C	2.57	0.42
4:E:6:ILE:HG22	4:E:10:PHE:CD1	2.54	0.42
4:E:38:THR:CG2	4:E:40:LEU:H	2.24	0.42
1:A:90:LEU:HD21	1:A:121:GLU:OE2	2.20	0.42
1:A:115:THR:O	1:A:115:THR:CG2	2.67	0.42
1:B:129:ILE:O	1:B:130:ALA:CB	2.68	0.42
2:C:194:VAL:HG22	2:C:221:LEU:HD12	2.02	0.42
2:C:208:VAL:HG13	2:C:212:SER:OG	2.20	0.42
2:C:561:GLY:HA3	2:C:842:ARG:O	2.20	0.42
2:C:592:LEU:HA	2:C:592:LEU:HD23	1.80	0.42
2:C:603:VAL:HB	2:C:604:VAL:H	1.61	0.42
2:C:693:GLU:O	2:C:694:LEU:C	2.57	0.42
2:C:699:PHE:C	2:C:701:THR:H	2.22	0.42
2:C:750:LYS:HE2	2:C:753:ASP:OD2	2.18	0.42
2:C:772:ARG:HH11	2:C:776:SER:HB3	1.84	0.42
2:C:985:GLY:O	2:C:986:PRO:C	2.57	0.42
2:C:1055:ILE:HD11	2:C:1079:PRO:CG	2.49	0.42
2:C:1067:TYR:CE1	2:C:1071:ILE:HD11	2.55	0.42
2:C:1113:GLU:C	2:C:1115:LEU:N	2.69	0.42
3:D:497:GLU:CG	3:D:1389:LEU:HD21	2.50	0.42
3:D:638:LYS:O	3:D:639:LEU:C	2.55	0.42
3:D:654:LYS:HB3	3:D:655:PRO:CD	2.45	0.42
3:D:729:HIS:CE1	3:D:935:LYS:HD3	2.54	0.42
3:D:795:VAL:CG1	3:D:796:ARG:N	2.83	0.42
3:D:795:VAL:CG1	3:D:864:VAL:CG2	2.92	0.42
3:D:876:SER:O	3:D:879:ARG:N	2.53	0.42
3:D:905:PRO:CD	3:D:906:GLN:H	2.32	0.42
3:D:953:ASP:OD1	3:D:1020:LEU:CB	2.68	0.42
3:D:953:ASP:OD1	3:D:1020:LEU:CG	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:999:THR:O	3:D:1000:THR:C	2.58	0.42
4:E:26:ARG:NH2	4:E:67:GLU:OE2	2.53	0.42
4:E:80:VAL:CB	4:E:81:PRO:CD	2.97	0.42
1:A:56:VAL:CG1	1:A:167:VAL:HG21	2.50	0.42
1:B:100:ILE:HG22	1:B:101:LEU:N	2.35	0.42
2:C:32:ALA:O	2:C:34:VAL:N	2.52	0.42
2:C:257:LEU:C	2:C:259:GLY:N	2.72	0.42
2:C:342:ASP:N	2:C:345:ARG:NH1	2.68	0.42
2:C:420:ARG:HD3	2:C:420:ARG:H	1.84	0.42
2:C:892:LEU:C	2:C:894:GLY:N	2.73	0.42
3:D:106:LYS:O	3:D:110:SER:N	2.53	0.42
3:D:496:LEU:O	3:D:500:ARG:HB2	2.19	0.42
3:D:876:SER:O	3:D:879:ARG:HG3	2.20	0.42
3:D:984:THR:O	3:D:985:ASP:C	2.59	0.42
3:D:1145:TYR:CD2	3:D:1146:GLY:N	2.80	0.42
3:D:1153:VAL:O	3:D:1153:VAL:CG1	2.64	0.42
3:D:1276:GLU:HG3	3:D:1303:TYR:OH	2.20	0.42
1:A:25:LEU:HB3	1:A:26:GLU:H	1.61	0.42
1:B:21:GLY:O	1:B:23:PHE:CD2	2.73	0.42
1:B:159:LYS:O	1:B:161:ARG:N	2.40	0.42
2:C:21:ILE:HD11	2:C:455:LEU:CD2	2.50	0.42
2:C:433:THR:HG21	3:D:1075:HIS:CD2	2.55	0.42
2:C:471:TYR:O	2:C:472:ARG:HG2	2.20	0.42
2:C:597:ALA:CA	2:C:614:ARG:HH11	2.26	0.42
2:C:822:VAL:O	2:C:822:VAL:HG12	2.19	0.42
2:C:874:LEU:CD1	3:D:787:LEU:HD22	2.47	0.42
2:C:885:ILE:HD12	2:C:885:ILE:N	2.34	0.42
2:C:892:LEU:HA	2:C:895:TYR:CB	2.50	0.42
2:C:897:LEU:O	2:C:898:GLY:C	2.58	0.42
2:C:1025:ALA:HB1	2:C:1026:GLN:NE2	2.35	0.42
3:D:69:GLU:O	3:D:70:ALA:CB	2.68	0.42
3:D:151:GLN:O	3:D:154:THR:N	2.53	0.42
3:D:732:VAL:HG22	3:D:769:LEU:HD11	2.01	0.42
3:D:879:ARG:CZ	3:D:904:VAL:HG22	2.48	0.42
3:D:964:LEU:O	3:D:965:GLU:HB3	2.20	0.42
3:D:1094:LEU:O	3:D:1097:LYS:N	2.53	0.42
1:A:27:PRO:HG2	1:A:27:PRO:O	2.19	0.42
2:C:34:VAL:O	2:C:35:PRO:C	2.58	0.42
2:C:56:GLU:OE1	2:C:64:LEU:O	2.38	0.42
2:C:148:PHE:CE1	2:C:309:TYR:HD2	2.38	0.42
2:C:202:TYR:O	2:C:203:ASP:CG	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:252:LYS:HG2	2:C:256:TYR:HD1	1.83	0.42
2:C:278:GLU:O	2:C:283:VAL:HG22	2.19	0.42
2:C:332:ARG:NH1	2:C:465:GLY:O	2.53	0.42
2:C:358:ARG:HB2	2:C:372:LEU:HD23	2.00	0.42
2:C:415:PRO:O	2:C:416:GLY:C	2.58	0.42
2:C:421:GLU:O	2:C:423:ALA:N	2.53	0.42
2:C:539:VAL:HB	2:C:540:PHE:CE1	2.54	0.42
2:C:937:ASP:OD1	2:C:939:ARG:CD	2.68	0.42
3:D:638:LYS:CA	3:D:729:HIS:CD2	3.03	0.42
3:D:710:ARG:HG3	3:D:711:LEU:N	2.35	0.42
3:D:874:GLU:O	3:D:875:THR:O	2.38	0.42
3:D:920:LEU:N	3:D:920:LEU:CD2	2.83	0.42
3:D:1108:ARG:O	3:D:1109:GLU:CG	2.65	0.42
3:D:1294:VAL:O	3:D:1301:LYS:N	2.53	0.42
4:E:54:LEU:O	4:E:55:TYR:CB	2.67	0.42
1:B:15:THR:C	1:B:17:GLY:N	2.74	0.41
1:B:41:ARG:HD3	1:B:41:ARG:C	2.40	0.41
1:B:222:LEU:O	1:B:223:ASN:C	2.57	0.41
2:C:43:GLY:O	2:C:44:ILE:C	2.58	0.41
2:C:140:ILE:HD12	2:C:331:ARG:HD2	2.02	0.41
2:C:197:LEU:HD23	2:C:197:LEU:HA	1.92	0.41
2:C:200:LEU:HD21	2:C:290:LEU:HD22	2.02	0.41
2:C:552:HIS:CD2	2:C:886:LEU:HD12	2.55	0.41
2:C:605:LYS:HD2	2:C:607:ASP:CG	2.40	0.41
2:C:674:VAL:HG11	2:C:992:MET:HB2	2.02	0.41
2:C:728:HIS:C	2:C:730:SER:N	2.73	0.41
2:C:734:LEU:O	2:C:737:LEU:O	2.38	0.41
2:C:873:PRO:CG	2:C:874:LEU:N	2.78	0.41
2:C:1105:LYS:C	2:C:1108:PRO:HD3	2.40	0.41
3:D:9:ARG:HA	3:D:1456:LYS:HA	2.02	0.41
3:D:583:ASP:OD1	3:D:604:THR:OG1	2.26	0.41
3:D:974:ILE:CG2	3:D:975:GLU:N	2.83	0.41
3:D:1011:PHE:C	3:D:1013:GLU:N	2.73	0.41
3:D:1130:ARG:HG2	3:D:1130:ARG:HH11	1.85	0.41
3:D:1402:ALA:HB3	3:D:1415:VAL:HG11	2.01	0.41
1:B:51:THR:HA	1:B:145:ASP:O	2.19	0.41
1:B:109:VAL:HG23	1:B:132:LEU:CD2	2.49	0.41
2:C:137:VAL:CG2	2:C:406:HIS:HE1	2.33	0.41
2:C:167:LYS:O	2:C:168:ARG:HB2	2.19	0.41
2:C:224:GLU:O	2:C:227:LEU:N	2.46	0.41
2:C:355:VAL:CG1	2:C:356:ARG:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:521:PRO:O	2:C:522:VAL:C	2.58	0.41
2:C:560:MET:O	2:C:564:MET:HB2	2.20	0.41
2:C:575:GLN:C	2:C:667:ALA:HB1	2.39	0.41
2:C:614:ARG:CZ	2:C:623:HIS:HE1	2.33	0.41
2:C:704:HIS:HD1	2:C:831:ARG:HD2	1.84	0.41
2:C:769:PRO:C	2:C:771:GLU:N	2.74	0.41
2:C:839:LEU:HD13	2:C:839:LEU:HA	1.76	0.41
2:C:924:LEU:HD23	2:C:924:LEU:H	1.75	0.41
2:C:1020:PRO:O	2:C:1021:LEU:CG	2.68	0.41
3:D:12:LEU:HD12	3:D:12:LEU:HA	1.79	0.41
3:D:471:GLU:O	3:D:471:GLU:HG3	2.20	0.41
3:D:496:LEU:CD1	3:D:500:ARG:HG2	2.48	0.41
3:D:566:ILE:O	3:D:570:GLU:HG3	2.20	0.41
3:D:620:GLY:O	3:D:621:LYS:HG3	2.20	0.41
3:D:645:PRO:O	3:D:646:LYS:C	2.56	0.41
3:D:887:GLY:C	3:D:889:ALA:H	2.23	0.41
3:D:962:ARG:O	3:D:966:GLU:HB2	2.19	0.41
3:D:1094:LEU:HB3	3:D:1095:THR:H	1.77	0.41
3:D:1110:ALA:O	3:D:1111:ASP:C	2.58	0.41
3:D:1436:SER:OG	3:D:1464:GLU:HG2	2.20	0.41
4:E:26:ARG:HA	4:E:26:ARG:HD2	1.79	0.41
1:A:79:ILE:HG23	1:A:167:VAL:CG2	2.50	0.41
2:C:83:CYS:HB3	2:C:88:LEU:O	2.21	0.41
2:C:334:ARG:HA	2:C:338:GLU:OE2	2.20	0.41
2:C:542:LEU:HA	2:C:545:ASN:HD22	1.85	0.41
2:C:623:HIS:HA	2:C:624:PRO:HD3	1.89	0.41
2:C:1001:VAL:O	2:C:1002:GLU:C	2.58	0.41
2:C:1023:GLY:O	2:C:1024:LYS:HG3	2.21	0.41
3:D:97:THR:O	3:D:571:LYS:CE	2.68	0.41
3:D:472:LYS:C	3:D:474:GLU:N	2.71	0.41
3:D:597:GLU:HG2	3:D:598:ARG:N	2.36	0.41
3:D:876:SER:H	3:D:879:ARG:CD	2.33	0.41
3:D:963:TYR:CE2	3:D:1002:LYS:HB3	2.55	0.41
3:D:1331:ASP:O	3:D:1334:GLN:HB2	2.20	0.41
1:A:200:TRP:O	1:A:201:THR:O	2.38	0.41
2:C:30:LEU:O	2:C:31:GLN:C	2.58	0.41
2:C:333:ILE:O	2:C:333:ILE:HG22	2.19	0.41
2:C:442:GLU:HG3	2:C:442:GLU:O	2.20	0.41
2:C:511:ASP:OD1	2:C:516:ARG:HB2	2.20	0.41
2:C:717:LEU:O	2:C:761:PHE:CB	2.68	0.41
2:C:758:ARG:HD3	2:C:788:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:947:ALA:O	2:C:950:LEU:N	2.53	0.41
2:C:1034:GLU:HG3	2:C:1035:MET:H	1.86	0.41
2:C:1112:PHE:C	2:C:1114:GLY:N	2.73	0.41
3:D:23:TYR:O	3:D:24:GLY:C	2.58	0.41
3:D:805:ALA:HB1	3:D:809:PRO:HD2	2.03	0.41
3:D:965:GLU:O	3:D:968:ASP:CB	2.67	0.41
3:D:999:THR:O	3:D:1002:LYS:N	2.53	0.41
3:D:1065:LEU:HD12	3:D:1067:VAL:CG2	2.50	0.41
3:D:1067:VAL:C	3:D:1069:GLU:N	2.74	0.41
3:D:1192:LEU:CD1	3:D:1345:GLU:HB3	2.49	0.41
3:D:1348:LEU:HD12	3:D:1348:LEU:HA	1.71	0.41
3:D:1403:LEU:CG	3:D:1415:VAL:HB	2.46	0.41
3:D:1431:THR:HG23	3:D:1432:LYS:HG2	2.03	0.41
1:A:71:VAL:HA	1:A:132:LEU:HA	2.01	0.41
1:B:110:ARG:C	1:B:112:VAL:H	2.23	0.41
1:B:122:ILE:HD12	1:B:122:ILE:N	2.35	0.41
2:C:115:LEU:HD11	2:C:378:LEU:HD22	2.01	0.41
2:C:198:ARG:HG2	2:C:228:ALA:CA	2.37	0.41
2:C:218:VAL:C	2:C:220:GLY:N	2.73	0.41
2:C:368:THR:O	2:C:371:LYS:HB2	2.21	0.41
2:C:575:GLN:HA	2:C:662:GLU:CD	2.40	0.41
2:C:588:VAL:HG21	2:C:666:LEU:HD13	2.02	0.41
2:C:657:ASP:HB3	2:C:658:GLY:H	1.46	0.41
2:C:679:PHE:C	2:C:681:GLY:N	2.73	0.41
2:C:773:LEU:O	2:C:777:ILE:HG13	2.20	0.41
2:C:806:LEU:O	2:C:821:GLU:HA	2.20	0.41
2:C:889:HIS:O	2:C:891:GLY:N	2.53	0.41
2:C:918:LEU:HD13	2:C:968:ASP:CA	2.51	0.41
2:C:1014:SER:O	2:C:1018:GLN:HA	2.20	0.41
2:C:1085:PHE:CE1	3:D:1468:LEU:HD22	2.55	0.41
3:D:99:ALA:HB1	3:D:512:MET:O	2.20	0.41
3:D:126:VAL:N	3:D:456:MET:CE	2.83	0.41
3:D:710:ARG:NH2	3:D:1219:GLU:OE2	2.51	0.41
3:D:767:HIS:O	3:D:769:LEU:N	2.49	0.41
3:D:794:GLN:O	3:D:795:VAL:CB	2.65	0.41
3:D:795:VAL:CG2	3:D:904:VAL:HG11	2.45	0.41
3:D:809:PRO:O	3:D:811:GLU:N	2.53	0.41
3:D:868:TYR:HA	3:D:871:ARG:O	2.20	0.41
3:D:891:GLY:H	3:D:926:LYS:NZ	2.17	0.41
3:D:988:ARG:O	3:D:989:TYR:C	2.59	0.41
3:D:1101:VAL:HG22	3:D:1424:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1238:MET:HE3	3:D:1257:PRO:HG3	2.02	0.41
3:D:1282:ARG:HG2	3:D:1293:PHE:CB	2.44	0.41
3:D:1394:VAL:HG11	3:D:1398:TRP:HE3	1.84	0.41
1:B:128:HIS:HE1	1:B:131:THR:N	2.18	0.41
2:C:29:ALA:O	2:C:44:ILE:HD13	2.20	0.41
2:C:498:GLN:CB	2:C:503:LEU:H	2.34	0.41
2:C:648:ARG:NH1	2:C:653:ASP:HB3	2.35	0.41
3:D:469:ASP:C	3:D:471:GLU:N	2.72	0.41
3:D:904:VAL:HG12	3:D:906:GLN:NE2	2.36	0.41
3:D:956:ILE:HD11	3:D:1062:ARG:HB3	2.01	0.41
3:D:1113:GLY:O	3:D:1114:THR:O	2.38	0.41
3:D:1456:LYS:O	3:D:1457:ASP:C	2.58	0.41
4:E:47:LYS:CD	4:E:54:LEU:HD23	2.48	0.41
1:B:174:VAL:CA	1:B:201:THR:HG22	2.48	0.41
2:C:147:TYR:O	2:C:148:PHE:CB	2.66	0.41
2:C:162:ILE:HG13	2:C:171:TRP:HZ3	1.77	0.41
2:C:202:TYR:O	2:C:203:ASP:OD2	2.39	0.41
2:C:216:ASP:O	2:C:218:VAL:N	2.54	0.41
2:C:454:SER:O	2:C:455:LEU:HB2	2.21	0.41
2:C:460:ARG:N	2:C:468:ARG:O	2.54	0.41
2:C:514:VAL:C	2:C:516:ARG:H	2.23	0.41
2:C:550:LEU:HD23	2:C:905:VAL:CG1	2.51	0.41
2:C:777:ILE:C	2:C:779:GLY:H	2.23	0.41
2:C:1051:GLU:OE2	3:D:752:SER:OG	2.34	0.41
3:D:497:GLU:O	3:D:501:ALA:HB2	2.21	0.41
3:D:521:PRO:CD	3:D:522:PRO:HD3	2.51	0.41
3:D:575:GLN:O	3:D:578:VAL:N	2.53	0.41
3:D:590:PRO:HA	3:D:600:LEU:CG	2.50	0.41
3:D:626:SER:CB	3:D:748:HIS:HA	2.50	0.41
3:D:697:GLY:O	3:D:760:ARG:NH1	2.53	0.41
3:D:850:LEU:O	3:D:853:VAL:HB	2.20	0.41
3:D:1079:LYS:C	3:D:1081:GLY:N	2.73	0.41
3:D:1486:VAL:HG21	4:E:25:LYS:CE	2.50	0.41
4:E:38:THR:HG22	4:E:39:VAL:H	1.84	0.41
1:A:14:THR:O	1:A:14:THR:HG22	2.21	0.41
1:B:205:VAL:HG13	1:B:209:GLU:OE1	2.20	0.41
2:C:80:GLN:OE1	2:C:122:THR:HG23	2.21	0.41
2:C:471:TYR:HB3	2:C:534:VAL:HG21	2.03	0.41
2:C:614:ARG:NH1	2:C:623:HIS:HE1	2.19	0.41
2:C:892:LEU:HA	2:C:895:TYR:HB2	2.03	0.41
2:C:943:VAL:O	2:C:946:ARG:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:959:PRO:HA	2:C:962:GLN:NE2	2.36	0.41
2:C:969:LEU:CD1	3:D:952:ASP:H	2.24	0.41
3:D:659:LYS:O	3:D:662:GLU:HB3	2.20	0.41
3:D:1011:PHE:CE2	3:D:1022:VAL:HG11	2.55	0.41
3:D:1141:GLU:OE1	3:D:1168:LEU:HD11	2.20	0.41
3:D:1170:ASP:C	3:D:1172:HIS:H	2.24	0.41
3:D:1321:ALA:C	3:D:1323:GLN:N	2.74	0.41
1:A:43:ILE:O	1:A:46:SER:N	2.54	0.41
1:A:212:ASN:O	1:A:213:GLN:C	2.59	0.41
1:A:220:GLU:HA	1:A:223:ASN:HD22	1.85	0.41
1:B:40:LEU:O	1:B:44:LEU:N	2.42	0.41
1:B:127:LEU:O	1:B:129:ILE:HG12	2.20	0.41
1:B:205:VAL:CG1	1:B:206:THR:N	2.84	0.41
2:C:13:ILE:HG23	2:C:14:PRO:N	2.36	0.41
2:C:34:VAL:HG13	2:C:38:LYS:HG3	2.00	0.41
2:C:137:VAL:HG23	2:C:393:GLN:HG3	2.03	0.41
2:C:149:THR:CG2	2:C:150:PRO:HD2	2.50	0.41
2:C:253:ALA:C	2:C:255:ALA:H	2.24	0.41
2:C:313:LEU:HA	2:C:319:GLY:HA2	2.03	0.41
2:C:352:ALA:C	2:C:355:VAL:HG12	2.41	0.41
2:C:361:MET:O	2:C:362:GLY:O	2.39	0.41
2:C:427:VAL:HG12	2:C:428:ARG:N	2.35	0.41
2:C:432:ARG:CZ	3:D:1048:PRO:O	2.68	0.41
2:C:445:GLU:HB3	2:C:446:GLY:H	1.67	0.41
2:C:598:GLU:HG3	2:C:614:ARG:CZ	2.51	0.41
2:C:611:ILE:HD11	2:C:641:PRO:CB	2.51	0.41
2:C:695:LEU:O	2:C:696:LYS:C	2.59	0.41
2:C:769:PRO:O	2:C:770:GLU:HB2	2.21	0.41
2:C:816:LYS:HD2	2:C:817:PRO:HG2	2.03	0.41
2:C:841:ASN:ND2	2:C:842:ARG:N	2.69	0.41
2:C:976:ASP:C	2:C:978:ARG:H	2.23	0.41
2:C:1052:MET:CE	3:D:748:HIS:HB3	2.50	0.41
3:D:631:ILE:HG21	3:D:745:MET:CE	2.47	0.41
3:D:701:LEU:HG	3:D:763:MET:CE	2.50	0.41
3:D:710:ARG:C	3:D:712:GLY:H	2.24	0.41
3:D:776:GLU:H	3:D:776:GLU:HG2	1.47	0.41
3:D:816:TYR:HA	3:D:832:ARG:HH22	1.86	0.41
3:D:879:ARG:CG	3:D:879:ARG:NH1	2.83	0.41
3:D:930:LEU:HD12	3:D:930:LEU:O	2.21	0.41
3:D:989:TYR:O	3:D:991:GLN:N	2.53	0.41
3:D:1007:VAL:C	3:D:1009:ASN:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1017:PHE:O	3:D:1018:ASN:C	2.58	0.41
3:D:1093:TYR:CE2	3:D:1097:LYS:HD2	2.56	0.41
3:D:1132:LEU:HD13	3:D:1184:ARG:NH1	2.20	0.41
3:D:1137:ARG:N	3:D:1137:ARG:HD2	2.35	0.41
3:D:1151:ARG:N	3:D:1162:GLU:HG3	2.35	0.41
3:D:1302:GLU:C	3:D:1303:TYR:CD1	2.94	0.41
3:D:1382:THR:O	3:D:1383:ASP:C	2.58	0.41
3:D:1455:LYS:O	3:D:1456:LYS:HG2	2.21	0.41
4:E:26:ARG:CZ	4:E:67:GLU:OE2	2.68	0.41
4:E:75:PHE:CD1	4:E:75:PHE:N	2.89	0.41
1:A:198:ARG:HH22	2:C:932:GLU:CD	2.17	0.41
1:B:16:GLN:CB	1:B:20:TYR:HB3	2.51	0.41
2:C:152:PRO:HD2	2:C:158:TYR:HE2	1.84	0.41
2:C:440:PRO:CD	2:C:455:LEU:N	2.80	0.41
2:C:705:ILE:CD1	2:C:705:ILE:N	2.84	0.41
2:C:750:LYS:HG2	2:C:753:ASP:OD1	2.21	0.41
3:D:558:LEU:C	3:D:560:GLN:N	2.73	0.41
3:D:782:SER:HA	3:D:786:ILE:HD11	2.03	0.41
3:D:976:GLN:C	3:D:978:TYR:N	2.71	0.41
3:D:1107:VAL:HG23	3:D:1221:VAL:HG23	2.03	0.41
3:D:1323:GLN:H	3:D:1324:PRO:CD	2.32	0.41
4:E:62:THR:O	4:E:63:TRP:C	2.58	0.41
1:A:88:ARG:O	1:A:89:PHE:HD1	2.05	0.40
1:B:32:PHE:HA	1:B:35:THR:CB	2.51	0.40
1:B:49:PRO:HB3	1:B:146:ARG:HH21	1.84	0.40
2:C:25:SER:O	2:C:28:LYS:HG2	2.20	0.40
2:C:151:ASP:N	2:C:157:ARG:HA	2.32	0.40
2:C:162:ILE:N	2:C:162:ILE:CD1	2.84	0.40
2:C:184:MET:CE	2:C:196:LEU:HD22	2.51	0.40
2:C:566:THR:O	2:C:568:ALA:N	2.53	0.40
2:C:584:GLU:C	2:C:586:ARG:N	2.74	0.40
2:C:653:ASP:O	2:C:653:ASP:CG	2.60	0.40
2:C:692:GLU:O	2:C:695:LEU:N	2.54	0.40
2:C:935:GLY:O	2:C:936:VAL:C	2.60	0.40
2:C:1049:LEU:C	2:C:1051:GLU:H	2.24	0.40
2:C:1052:MET:HE3	2:C:1056:LYS:NZ	2.35	0.40
3:D:675:ARG:CZ	3:D:675:ARG:HB2	2.50	0.40
3:D:829:VAL:O	3:D:830:ALA:CB	2.69	0.40
3:D:1102:ALA:C	3:D:1103:HIS:O	2.59	0.40
3:D:1145:TYR:HA	3:D:1171:VAL:HG21	2.02	0.40
1:A:187:GLY:HA3	1:A:192:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ASN:O	1:B:224:TYR:C	2.60	0.40
2:C:102:HIS:HB3	2:C:103:LYS:H	1.59	0.40
2:C:115:LEU:CD1	2:C:116:GLY:N	2.65	0.40
2:C:216:ASP:C	2:C:218:VAL:H	2.24	0.40
2:C:222:LEU:O	2:C:223:ASP:C	2.60	0.40
2:C:734:LEU:H	2:C:734:LEU:HG	1.68	0.40
2:C:881:ASN:ND2	3:D:1034:GLN:CG	2.85	0.40
2:C:1008:ARG:NH2	2:C:1020:PRO:CB	2.83	0.40
3:D:557:LEU:O	3:D:558:LEU:HG	2.21	0.40
3:D:655:PRO:O	3:D:656:PHE:C	2.58	0.40
3:D:709:HIS:CA	3:D:1227:GLU:HB3	2.51	0.40
3:D:1066:THR:O	3:D:1067:VAL:C	2.59	0.40
3:D:1329:ALA:O	3:D:1330:ILE:O	2.39	0.40
4:E:15:SER:O	4:E:18:ARG:N	2.30	0.40
1:A:12:THR:HG22	1:A:13:ALA:N	2.36	0.40
1:A:122:ILE:O	1:A:123:MET:C	2.60	0.40
1:A:127:LEU:O	1:A:129:ILE:HG12	2.20	0.40
1:A:185:ARG:HH21	1:A:194:LYS:CE	2.32	0.40
2:C:66:LEU:HB2	2:C:100:LEU:HB3	2.02	0.40
2:C:124:ASP:OD1	2:C:407:LYS:NZ	2.39	0.40
2:C:182:VAL:CG1	2:C:307:LEU:HD11	2.51	0.40
2:C:342:ASP:OD1	2:C:345:ARG:HD2	2.21	0.40
2:C:439:CYS:CB	2:C:468:ARG:NH1	2.84	0.40
2:C:462:ASP:O	2:C:463:ALA:C	2.59	0.40
2:C:498:GLN:CB	2:C:502:PRO:HA	2.52	0.40
2:C:840:ALA:CA	2:C:846:LYS:HA	2.52	0.40
2:C:949:LYS:C	2:C:951:GLY:N	2.74	0.40
3:D:660:LYS:NZ	4:E:58:PRO:HG2	2.36	0.40
3:D:694:VAL:C	3:D:696:HIS:N	2.73	0.40
3:D:733:CYS:O	3:D:737:ASN:N	2.47	0.40
3:D:767:HIS:C	3:D:769:LEU:H	2.24	0.40
3:D:958:GLU:C	3:D:960:LYS:H	2.23	0.40
3:D:1107:VAL:CG2	3:D:1215:VAL:HG11	2.43	0.40
4:E:57:ASP:HA	4:E:58:PRO:HD3	1.84	0.40
1:A:13:ALA:O	1:B:230:ALA:HB2	2.22	0.40
1:A:147:GLY:HA3	1:A:171:PHE:CZ	2.56	0.40
1:A:178:ALA:HB2	2:C:864:GLY:CA	2.51	0.40
1:A:191:ASP:O	1:A:192:LEU:O	2.39	0.40
1:B:65:PHE:O	1:B:65:PHE:HD1	2.05	0.40
1:B:91:ASP:HA	1:B:92:PRO:HD3	1.96	0.40
1:B:99:LEU:HB3	1:B:114:PHE:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:207:LEU:HG	2:C:208:VAL:N	2.36	0.40
2:C:336:VAL:O	2:C:338:GLU:N	2.55	0.40
2:C:533:ASP:O	2:C:535:SER:N	2.54	0.40
2:C:552:HIS:O	2:C:553:ASP:C	2.59	0.40
2:C:729:LEU:CD1	2:C:791:ARG:NH2	2.85	0.40
2:C:750:LYS:CE	2:C:753:ASP:OD2	2.70	0.40
2:C:854:PRO:C	2:C:856:GLU:N	2.74	0.40
2:C:860:HIS:HD2	2:C:977:GLY:CA	2.34	0.40
2:C:875:GLY:CA	2:C:879:ARG:HD2	2.50	0.40
2:C:895:TYR:CD1	2:C:991:GLN:NE2	2.89	0.40
2:C:916:GLU:O	2:C:919:ALA:N	2.55	0.40
2:C:969:LEU:HD13	3:D:952:ASP:OD1	2.21	0.40
3:D:776:GLU:HB3	3:D:912:LYS:HE2	2.02	0.40
3:D:948:THR:HB	3:D:949:ILE:H	1.68	0.40
3:D:1153:VAL:HG11	3:D:1174:LEU:HD21	2.03	0.40
3:D:1258:ARG:C	3:D:1260:ILE:N	2.75	0.40
3:D:1457:ASP:OD1	3:D:1459:LEU:N	2.52	0.40
3:D:1466:VAL:O	3:D:1469:GLY:CA	2.70	0.40
4:E:81:PRO:CG	4:E:84:ARG:HD2	2.49	0.40
1:A:41:ARG:HD3	1:A:177:VAL:O	2.22	0.40
1:B:175:ARG:O	1:B:176:ARG:CB	2.69	0.40
1:B:178:ALA:CB	1:B:198:ARG:HE	2.28	0.40
2:C:9:ILE:HD13	2:C:494:TYR:CE1	2.57	0.40
2:C:535:SER:HA	2:C:536:PRO:HD3	1.91	0.40
2:C:580:MET:HB2	2:C:584:GLU:OE2	2.21	0.40
2:C:611:ILE:O	2:C:611:ILE:HG22	2.21	0.40
2:C:670:GLN:OE1	2:C:699:PHE:C	2.60	0.40
2:C:1078:GLU:CD	4:E:32:ARG:HH12	2.25	0.40
2:C:1107:ASN:OD1	2:C:1107:ASN:O	2.40	0.40
3:D:77:ALA:C	3:D:79:GLU:H	2.25	0.40
3:D:121:THR:CB	3:D:461:ILE:HD11	2.51	0.40
3:D:571:LYS:O	3:D:573:MET:N	2.53	0.40
3:D:625:TYR:O	3:D:652:LEU:HD12	2.22	0.40
3:D:885:ILE:HD13	3:D:937:TYR:CD2	2.55	0.40
3:D:1192:LEU:HD21	3:D:1369:GLU:CA	2.52	0.40
3:D:1232:PRO:HB3	3:D:1361:VAL:CG1	2.51	0.40
3:D:1372:VAL:CG2	3:D:1375:MET:HE3	2.49	0.40
3:D:1425:THR:C	3:D:1427:SER:N	2.75	0.40
3:D:1431:THR:O	3:D:1432:LYS:CG	2.68	0.40
4:E:38:THR:CG2	4:E:63:TRP:HZ3	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	222/314 (71%)	111 (50%)	61 (28%)	50 (22%)	0	0
1	B	228/314 (73%)	123 (54%)	62 (27%)	43 (19%)	0	1
2	C	1111/1118 (99%)	591 (53%)	277 (25%)	243 (22%)	0	0
3	D	1126/1264 (89%)	588 (52%)	291 (26%)	247 (22%)	0	0
4	E	96/99 (97%)	50 (52%)	24 (25%)	22 (23%)	0	0
All	All	2783/3109 (90%)	1463 (53%)	715 (26%)	605 (22%)	0	0

All (605) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	19	HIS
1	A	26	GLU
1	A	59	GLU
1	A	73	GLU
1	A	92	PRO
1	A	105	GLY
1	A	107	LYS
1	A	113	ASP
1	A	125	PRO
1	A	143	ARG
1	A	144	VAL
1	A	153	ALA
1	A	158	ILE
1	A	162	ILE
1	A	176	ARG
1	A	187	GLY
1	A	192	LEU
1	A	201	THR
1	B	4	SER
1	B	5	LYS

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Mol	Chain	Res	Type
1	B	6	LEU
1	B	26	GLU
1	B	60	ASP
1	B	62	LEU
1	B	63	HIS
1	B	75	VAL
1	B	96	SER
1	B	126	ASP
1	B	138	LEU
1	B	156	HIS
1	B	158	ILE
1	B	160	ASP
1	B	161	ARG
1	B	176	ARG
1	B	204	SER
1	B	224	TYR
2	C	31	GLN
2	C	32	ALA
2	C	33	ASP
2	C	36	PRO
2	C	44	ILE
2	C	77	PRO
2	C	153	ALA
2	C	157	ARG
2	C	204	GLN
2	C	216	ASP
2	C	258	PHE
2	C	261	LEU
2	C	268	ASP
2	C	269	LEU
2	C	276	LYS
2	C	283	VAL
2	C	287	GLY
2	C	290	LEU
2	C	295	ASP
2	C	325	ILE
2	C	360	VAL
2	C	361	MET
2	C	375	SER
2	C	388	ARG
2	C	402	SER
2	C	416	GLY

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Mol	Chain	Res	Type
2	C	426	ASP
2	C	427	VAL
2	C	432	ARG
2	C	449	ILE
2	C	450	GLY
2	C	460	ARG
2	C	461	VAL
2	C	462	ASP
2	C	467	ILE
2	C	468	ARG
2	C	469	THR
2	C	476	ASN
2	C	477	GLY
2	C	479	VAL
2	C	480	THR
2	C	484	VAL
2	C	488	ALA
2	C	489	SER
2	C	495	THR
2	C	496	ILE
2	C	502	PRO
2	C	517	ARG
2	C	526	PRO
2	C	528	GLU
2	C	568	ALA
2	C	569	VAL
2	C	573	ARG
2	C	575	GLN
2	C	600	ASP
2	C	602	GLU
2	C	603	VAL
2	C	604	VAL
2	C	606	VAL
2	C	613	VAL
2	C	615	TYR
2	C	629	ALA
2	C	636	ALA
2	C	654	LEU
2	C	660	ALA
2	C	677	MET
2	C	680	ASP
2	C	700	TYR

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Mol	Chain	Res	Type
2	C	715	THR
2	C	730	SER
2	C	734	LEU
2	C	762	LYS
2	C	788	THR
2	C	791	ARG
2	C	796	GLU
2	C	811	PRO
2	C	821	GLU
2	C	832	LYS
2	C	837	ASP
2	C	840	ALA
2	C	876	VAL
2	C	881	ASN
2	C	887	GLU
2	C	936	VAL
2	C	943	VAL
2	C	973	VAL
2	C	992	MET
2	C	993	PHE
2	C	1001	VAL
2	C	1018	GLN
2	C	1021	LEU
2	C	1022	GLY
2	C	1034	GLU
2	C	1055	ILE
2	C	1080	SER
2	C	1104	GLU
2	C	1109	VAL
3	D	28	LYS
3	D	83	SER
3	D	84	ILE
3	D	85	VAL
3	D	86	ARG
3	D	93	ILE
3	D	98	PRO
3	D	104	PHE
3	D	112	ILE
3	D	113	ALA
3	D	127	LEU
3	D	130	ASN
3	D	133	ILE

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Mol	Chain	Res	Type
3	D	137	PRO
3	D	143	ASP
3	D	467	GLU
3	D	468	LEU
3	D	483	HIS
3	D	509	PRO
3	D	511	TRP
3	D	512	MET
3	D	513	ILE
3	D	515	GLU
3	D	539	ASP
3	D	564	GLU
3	D	583	ASP
3	D	584	ASN
3	D	587	ARG
3	D	610	LYS
3	D	638	LYS
3	D	657	LEU
3	D	658	LEU
3	D	680	GLN
3	D	682	ASP
3	D	689	ASP
3	D	705	ALA
3	D	709	HIS
3	D	722	GLU
3	D	725	SER
3	D	740	PHE
3	D	748	HIS
3	D	753	SER
3	D	774	SER
3	D	783	ARG
3	D	795	VAL
3	D	824	ASN
3	D	827	ILE
3	D	828	VAL
3	D	835	SER
3	D	838	ARG
3	D	839	LEU
3	D	854	ALA
3	D	856	GLY
3	D	869	LEU
3	D	875	THR

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Mol	Chain	Res	Type
3	D	892	ASP
3	D	902	MET
3	D	908	LYS
3	D	969	ARG
3	D	1015	TYR
3	D	1018	ASN
3	D	1028	ALA
3	D	1052	THR
3	D	1075	HIS
3	D	1076	GLY
3	D	1089	ALA
3	D	1111	ASP
3	D	1112	CYS
3	D	1114	THR
3	D	1137	ARG
3	D	1197	ARG
3	D	1203	LYS
3	D	1206	GLY
3	D	1268	PRO
3	D	1270	ALA
3	D	1271	LYS
3	D	1279	GLY
3	D	1281	VAL
3	D	1282	ARG
3	D	1307	LYS
3	D	1312	LEU
3	D	1313	VAL
3	D	1315	ASP
3	D	1317	ASP
3	D	1320	GLU
3	D	1322	GLY
3	D	1323	GLN
3	D	1325	LEU
3	D	1339	LYS
3	D	1364	HIS
3	D	1392	GLY
3	D	1403	LEU
3	D	1442	ASN
3	D	1472	ILE
3	D	1482	ARG
4	E	29	GLN
4	E	31	LEU

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Mol	Chain	Res	Type
4	E	34	ARG
4	E	35	PHE
4	E	43	GLU
4	E	51	LEU
4	E	55	TYR
4	E	80	VAL
4	E	94	PRO
1	A	14	THR
1	A	30	ARG
1	A	90	LEU
1	A	96	SER
1	A	123	MET
1	A	139	TYR
1	A	161	ARG
1	A	182	GLU
1	A	190	THR
1	A	200	TRP
1	A	224	TYR
1	B	35	THR
1	B	47	SER
1	B	105	GLY
1	B	107	LYS
1	B	116	PRO
1	B	119	ASP
1	B	120	VAL
1	B	130	ALA
1	B	152	PRO
1	B	195	LEU
1	B	196	THR
2	C	10	ARG
2	C	23	VAL
2	C	42	VAL
2	C	59	LYS
2	C	90	TYR
2	C	148	PHE
2	C	155	PRO
2	C	168	ARG
2	C	262	ALA
2	C	303	PHE
2	C	309	TYR
2	C	315	ALA
2	C	319	GLY

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Mol	Chain	Res	Type
2	C	320	HIS
2	C	322	VAL
2	C	362	GLY
2	C	435	TYR
2	C	444	PRO
2	C	474	VAL
2	C	482	GLU
2	C	524	VAL
2	C	529	VAL
2	C	534	VAL
2	C	546	LEU
2	C	567	GLN
2	C	581	THR
2	C	587	VAL
2	C	643	VAL
2	C	657	ASP
2	C	663	GLU
2	C	713	ARG
2	C	728	HIS
2	C	731	GLU
2	C	769	PRO
2	C	777	ILE
2	C	779	GLY
2	C	812	GLY
2	C	874	LEU
2	C	886	LEU
2	C	922	PHE
2	C	938	LYS
2	C	945	ALA
2	C	969	LEU
2	C	970	GLY
2	C	975	TYR
2	C	977	GLY
2	C	1002	GLU
2	C	1025	ALA
2	C	1059	ASP
2	C	1074	GLU
2	C	1110	ASP
3	D	9	ARG
3	D	22	SER
3	D	29	PRO
3	D	72	VAL

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Mol	Chain	Res	Type
3	D	76	CYS
3	D	78	VAL
3	D	87	ARG
3	D	89	ARG
3	D	95	LEU
3	D	111	LYS
3	D	126	VAL
3	D	144	ALA
3	D	150	ARG
3	D	453	ASP
3	D	561	GLY
3	D	567	ILE
3	D	590	PRO
3	D	613	ARG
3	D	617	ASN
3	D	643	GLY
3	D	668	PRO
3	D	730	PRO
3	D	733	CYS
3	D	747	VAL
3	D	773	ALA
3	D	784	ASP
3	D	799	LYS
3	D	806	PHE
3	D	822	ALA
3	D	825	ALA
3	D	855	HIS
3	D	858	LEU
3	D	917	GLN
3	D	935	LYS
3	D	946	GLY
3	D	983	LEU
3	D	995	LEU
3	D	1070	TYR
3	D	1103	HIS
3	D	1109	GLU
3	D	1130	ARG
3	D	1151	ARG
3	D	1155	ALA
3	D	1156	LEU
3	D	1200	VAL
3	D	1220	ALA

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Mol	Chain	Res	Type
3	D	1272	ALA
3	D	1291	SER
3	D	1304	LYS
3	D	1316	GLY
3	D	1324	PRO
3	D	1330	ILE
3	D	1354	LYS
3	D	1366	LYS
3	D	1367	HIS
3	D	1408	ILE
3	D	1470	ARG
4	E	16	LYS
4	E	70	THR
1	A	20	TYR
1	A	48	ILE
1	A	112	VAL
1	A	160	ASP
1	A	199	ILE
1	B	90	LEU
1	B	207	PRO
2	C	55	GLU
2	C	75	ASP
2	C	103	LYS
2	C	156	GLY
2	C	203	ASP
2	C	210	GLU
2	C	264	PRO
2	C	328	LEU
2	C	420	ARG
2	C	457	ALA
2	C	463	ALA
2	C	512	ARG
2	C	527	GLU
2	C	531	PHE
2	C	551	GLU
2	C	555	ALA
2	C	610	ARG
2	C	692	GLU
2	C	732	ALA
2	C	738	ASP
2	C	857	ASP
2	C	873	PRO

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Mol	Chain	Res	Type
2	C	875	GLY
2	C	966	LEU
2	C	986	PRO
2	C	998	TYR
2	C	1043	TYR
2	C	1061	GLU
2	C	1072	LYS
2	C	1105	LYS
2	C	1112	PHE
2	C	1113	GLU
3	D	11	ALA
3	D	125	GLN
3	D	486	ARG
3	D	507	ASN
3	D	543	LEU
3	D	652	LEU
3	D	711	LEU
3	D	714	GLN
3	D	734	GLU
3	D	768	ASN
3	D	793	THR
3	D	809	PRO
3	D	816	TYR
3	D	840	LYS
3	D	862	ASP
3	D	893	GLU
3	D	905	PRO
3	D	953	ASP
3	D	959	GLU
3	D	968	ASP
3	D	990	ASP
3	D	1090	ASP
3	D	1152	GLU
3	D	1251	ASP
3	D	1252	ILE
3	D	1283	ILE
3	D	1309	ALA
3	D	1319	VAL
3	D	1426	LYS
3	D	1452	ILE
3	D	1488	ASP
4	E	30	LEU

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Mol	Chain	Res	Type
1	A	67	THR
1	A	119	ASP
1	A	126	ASP
1	A	128	HIS
1	A	152	PRO
1	B	15	THR
1	B	202	ASP
2	C	9	ILE
2	C	51	THR
2	C	58	ASP
2	C	66	LEU
2	C	105	THR
2	C	149	THR
2	C	181	VAL
2	C	187	ASN
2	C	232	GLU
2	C	324	ASP
2	C	326	ASP
2	C	380	ALA
2	C	425	PHE
2	C	431	HIS
2	C	499	ALA
2	C	626	ARG
2	C	685	GLU
2	C	699	PHE
2	C	781	LYS
2	C	890	LEU
2	C	894	GLY
2	C	1012	PRO
2	C	1044	GLY
3	D	522	PRO
3	D	599	PRO
3	D	629	SER
3	D	639	LEU
3	D	679	ARG
3	D	685	ASP
3	D	695	ILE
3	D	737	ASN
3	D	805	ALA
3	D	823	LEU
3	D	829	VAL
3	D	830	ALA

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Mol	Chain	Res	Type
3	D	904	VAL
3	D	906	GLN
3	D	907	GLU
3	D	961	GLN
3	D	1009	ASN
3	D	1031	ASN
3	D	1036	ARG
3	D	1060	SER
3	D	1061	PHE
3	D	1138	SER
3	D	1161	GLU
3	D	1207	TYR
3	D	1327	ARG
3	D	1344	VAL
4	E	2	ALA
4	E	12	MET
4	E	49	ARG
4	E	56	ASP
4	E	95	THR
1	A	64	GLU
1	A	111	ALA
1	A	118	ALA
1	A	122	ILE
1	A	134	GLU
1	A	189	ARG
1	A	196	THR
1	B	37	GLY
1	B	159	LYS
2	C	12	VAL
2	C	15	LEU
2	C	39	ARG
2	C	46	ALA
2	C	112	GLU
2	C	182	VAL
2	C	617	ASP
2	C	656	ALA
2	C	716	LYS
2	C	793	PRO
2	C	858	MET
2	C	877	PRO
2	C	898	GLY
2	C	921	ALA

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Mol	Chain	Res	Type
2	C	1077	PRO
3	D	94	GLU
3	D	132	TYR
3	D	134	VAL
3	D	145	VAL
3	D	540	LEU
3	D	558	LEU
3	D	572	ARG
3	D	582	ILE
3	D	644	LEU
3	D	654	LYS
3	D	673	ALA
3	D	861	GLN
3	D	894	LYS
3	D	1008	PHE
3	D	1321	ALA
3	D	1453	ALA
3	D	1476	THR
4	E	71	GLY
4	E	72	ARG
4	E	93	TYR
1	B	42	ARG
1	B	115	THR
1	B	128	HIS
1	B	134	GLU
2	C	35	PRO
2	C	376	ARG
2	C	856	GLU
2	C	1000	MET
2	C	1010	THR
2	C	1107	ASN
3	D	542	ASP
3	D	609	GLY
3	D	640	HIS
3	D	667	ALA
3	D	1332	PRO
3	D	1396	GLU
4	E	62	THR
1	A	109	VAL
1	A	203	GLY
2	C	113	VAL
2	C	164	PRO

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Mol	Chain	Res	Type
2	C	166	PRO
2	C	337	GLY
2	C	478	VAL
2	C	520	GLU
2	C	982	PRO
2	C	1011	GLY
3	D	771	SER
3	D	864	VAL
3	D	1043	GLY
3	D	1081	GLY
3	D	1381	VAL
1	B	24	VAL
1	B	125	PRO
1	B	136	GLY
2	C	54	ILE
2	C	144	PRO
2	C	819	VAL
3	D	1064	GLY
2	C	470	PRO
2	C	972	VAL
3	D	719	VAL
3	D	900	ILE
3	D	1267	ARG
2	C	535	SER
2	C	951	GLY
2	C	959	PRO
2	C	1079	PRO
3	D	136	ASP
3	D	1050	GLY
3	D	1222	GLY
4	E	41	GLU
1	A	136	GLY
1	B	71	VAL
2	C	443	THR
2	C	931	GLY
3	D	634	GLY
3	D	845	ASN
3	D	890	VAL

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	189/271 (70%)	161 (85%)	28 (15%)	3 13
1	B	190/271 (70%)	169 (89%)	21 (11%)	6 23
2	C	870/935 (93%)	770 (88%)	100 (12%)	5 22
3	D	782/1035 (76%)	671 (86%)	111 (14%)	3 15
4	E	67/88 (76%)	62 (92%)	5 (8%)	13 39
All	All	2098/2600 (81%)	1833 (87%)	265 (13%)	4 19

All (265) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	25	LEU
1	A	26	GLU
1	A	27	PRO
1	A	30	ARG
1	A	41	ARG
1	A	57	TYR
1	A	63	HIS
1	A	67	THR
1	A	74	ASP
1	A	77	GLU
1	A	91	ASP
1	A	97	THR
1	A	101	LEU
1	A	110	ARG
1	A	123	MET
1	A	126	ASP
1	A	132	LEU
1	A	142	VAL
1	A	143	ARG
1	A	144	VAL
1	A	192	LEU
1	A	195	LEU

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Mol	Chain	Res	Type
1	A	196	THR
1	A	197	LEU
1	A	200	TRP
1	A	213	GLN
1	A	222	LEU
1	B	19	HIS
1	B	20	TYR
1	B	25	LEU
1	B	38	ASN
1	B	41	ARG
1	B	44	LEU
1	B	51	THR
1	B	56	VAL
1	B	57	TYR
1	B	89	PHE
1	B	90	LEU
1	B	94	MET
1	B	123	MET
1	B	132	LEU
1	B	151	VAL
1	B	167	VAL
1	B	171	PHE
1	B	183	ASP
1	B	188	GLN
1	B	191	ASP
1	B	199	ILE
2	C	13	ILE
2	C	34	VAL
2	C	36	PRO
2	C	52	PHE
2	C	56	GLU
2	C	67	ASP
2	C	70	GLU
2	C	75	ASP
2	C	95	TYR
2	C	100	LEU
2	C	104	ASP
2	C	115	LEU
2	C	126	SER
2	C	129	ILE
2	C	135	VAL
2	C	138	SER

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Mol	Chain	Res	Type
2	C	142	ARG
2	C	147	TYR
2	C	157	ARG
2	C	158	TYR
2	C	163	ILE
2	C	176	VAL
2	C	194	VAL
2	C	198	ARG
2	C	203	ASP
2	C	214	TYR
2	C	232	GLU
2	C	251	ASP
2	C	254	LEU
2	C	258	PHE
2	C	261	LEU
2	C	263	ASP
2	C	267	TYR
2	C	285	LEU
2	C	303	PHE
2	C	304	LEU
2	C	306	THR
2	C	335	THR
2	C	344	PHE
2	C	351	LEU
2	C	356	ARG
2	C	393	GLN
2	C	399	ASN
2	C	407	LYS
2	C	425	PHE
2	C	433	THR
2	C	434	HIS
2	C	435	TYR
2	C	438	ILE
2	C	445	GLU
2	C	461	VAL
2	C	479	VAL
2	C	502	PRO
2	C	526	PRO
2	C	534	VAL
2	C	559	LEU
2	C	575	GLN
2	C	603	VAL

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Mol	Chain	Res	Type
2	C	630	ARG
2	C	633	GLN
2	C	635	THR
2	C	637	PHE
2	C	672	VAL
2	C	673	LEU
2	C	686	ASP
2	C	688	ILE
2	C	691	SER
2	C	698	ASP
2	C	699	PHE
2	C	705	ILE
2	C	710	ILE
2	C	714	ASP
2	C	723	THR
2	C	739	GLU
2	C	743	VAL
2	C	758	ARG
2	C	764	GLU
2	C	803	ARG
2	C	810	ASP
2	C	815	LEU
2	C	837	ASP
2	C	839	LEU
2	C	841	ASN
2	C	846	LYS
2	C	852	ILE
2	C	859	PRO
2	C	866	PRO
2	C	881	ASN
2	C	882	LEU
2	C	888	THR
2	C	892	LEU
2	C	924	LEU
2	C	981	GLU
2	C	1005	MET
2	C	1013	TYR
2	C	1018	GLN
2	C	1027	PHE
2	C	1031	ARG
2	C	1043	TYR
2	C	1115	LEU

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Mol	Chain	Res	Type
3	D	5	VAL
3	D	21	TRP
3	D	469	ASP
3	D	502	PHE
3	D	509	PRO
3	D	567	ILE
3	D	576	GLU
3	D	587	ARG
3	D	619	LEU
3	D	640	HIS
3	D	651	GLU
3	D	674	ARG
3	D	678	GLU
3	D	685	ASP
3	D	688	TRP
3	D	691	LEU
3	D	701	LEU
3	D	702	LEU
3	D	722	GLU
3	D	724	GLN
3	D	752	SER
3	D	754	PHE
3	D	762	GLN
3	D	769	LEU
3	D	772	PRO
3	D	776	GLU
3	D	778	LEU
3	D	791	TYR
3	D	794	GLN
3	D	796	ARG
3	D	798	GLU
3	D	834	THR
3	D	851	LEU
3	D	857	LEU
3	D	860	LEU
3	D	876	SER
3	D	879	ARG
3	D	886	VAL
3	D	899	LEU
3	D	904	VAL
3	D	906	GLN
3	D	911	LEU

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Mol	Chain	Res	Type
3	D	914	LEU
3	D	920	LEU
3	D	925	GLU
3	D	931	LEU
3	D	932	ASP
3	D	936	TYR
3	D	941	LEU
3	D	947	ILE
3	D	951	ILE
3	D	953	ASP
3	D	955	VAL
3	D	964	LEU
3	D	971	LEU
3	D	974	ILE
3	D	984	THR
3	D	989	TYR
3	D	1009	ASN
3	D	1031	ASN
3	D	1038	LEU
3	D	1041	MET
3	D	1042	ARG
3	D	1045	MET
3	D	1052	THR
3	D	1057	VAL
3	D	1061	PHE
3	D	1062	ARG
3	D	1068	LEU
3	D	1078	ARG
3	D	1093	TYR
3	D	1103	HIS
3	D	1104	GLU
3	D	1119	SER
3	D	1126	ASP
3	D	1130	ARG
3	D	1134	LEU
3	D	1137	ARG
3	D	1142	SER
3	D	1145	TYR
3	D	1154	GLU
3	D	1161	GLU
3	D	1166	LEU
3	D	1188	VAL

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Mol	Chain	Res	Type
3	D	1190	SER
3	D	1192	LEU
3	D	1194	CYS
3	D	1196	THR
3	D	1207	TYR
3	D	1210	SER
3	D	1213	ARG
3	D	1260	ILE
3	D	1273	VAL
3	D	1274	ILE
3	D	1278	ASP
3	D	1299	PHE
3	D	1304	LYS
3	D	1315	ASP
3	D	1327	ARG
3	D	1332	PRO
3	D	1348	LEU
3	D	1372	VAL
3	D	1373	ARG
3	D	1376	LEU
3	D	1390	LEU
3	D	1399	ASP
3	D	1424	VAL
3	D	1434	TRP
3	D	1447	LEU
3	D	1476	THR
3	D	1483	PHE
4	E	32	ARG
4	E	61	VAL
4	E	75	PHE
4	E	78	ASN
4	E	92	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	81	ASN
1	A	128	HIS
1	A	156	HIS
1	A	180	GLN
1	A	212	ASN

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Mol	Chain	Res	Type
1	A	223	ASN
1	A	227	ASN
1	B	38	ASN
1	B	81	ASN
1	B	156	HIS
1	B	188	GLN
1	B	213	GLN
1	B	221	HIS
1	B	223	ASN
2	C	22	GLN
2	C	102	HIS
2	C	141	HIS
2	C	320	HIS
2	C	343	GLN
2	C	393	GLN
2	C	399	ASN
2	C	538	GLN
2	C	545	ASN
2	C	565	GLN
2	C	623	HIS
2	C	632	ASN
2	C	1639	GLN
2	C	671	ASN
2	C	841	ASN
2	C	845	ASN
2	C	860	HIS
2	C	872	ASN
2	C	881	ASN
2	C	884	GLN
2	C	889	HIS
2	C	962	GLN
2	C	991	GLN
2	C	1026	GLN
2	C	1030	GLN
2	C	1107	ASN
3	D	507	ASN
3	D	549	ASN
3	D	551	ASN
3	D	552	ASN
3	D	636	GLN
3	D	640	HIS
3	D	696	HIS

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Mol	Chain	Res	Type
3	D	709	HIS
3	D	724	GLN
3	D	727	GLN
3	D	729	HIS
3	D	756	GLN
3	D	762	GLN
3	D	767	HIS
3	D	768	ASN
3	D	855	HIS
3	D	861	GLN
3	D	897	GLN
3	D	909	ASN
3	D	1018	ASN
3	D	1034	GLN
3	D	1333	HIS
3	D	1353	GLN
3	D	1364	HIS
3	D	1374	GLN
3	D	1393	GLN
3	D	1445	HIS
3	D	1465	ASN
4	E	33	HIS
4	E	59	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
5	RFP	C	1640	-	63,63,63	1.26	9 (14%)	94,94,94	0.95	4 (4%)

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
5	RFP	C	1640	-	-	13/60/85/85	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1640	RFP	O5-C29	3.47	1.48	1.39
5	C	1640	RFP	O4-C11	3.12	1.27	1.21
5	C	1640	RFP	C5-C10	2.99	1.49	1.43
5	C	1640	RFP	C39-N4	2.98	1.52	1.46
5	C	1640	RFP	C8-C9	2.77	1.51	1.43
5	C	1640	RFP	C42-N4	2.22	1.51	1.46
5	C	1640	RFP	C2-C1	2.07	1.43	1.38
5	C	1640	RFP	O6-C27	2.05	1.48	1.43
5	C	1640	RFP	O2-C8	-2.02	1.28	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1640	RFP	C34-C26-C25	-2.37	107.15	111.40
5	C	1640	RFP	C5-C10-C9	-2.33	115.41	119.66
5	C	1640	RFP	O12-C4-C10	2.16	124.19	119.00
5	C	1640	RFP	C24-C23-C22	2.12	118.97	115.43

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1640	RFP	C17-C18-C19-C20
5	C	1640	RFP	C26-C27-C28-C29
5	C	1640	RFP	O6-C27-C28-C29
5	C	1640	RFP	C32-C22-C23-C24
5	C	1640	RFP	C21-C22-C23-C24
5	C	1640	RFP	C32-C22-C23-O9
5	C	1640	RFP	C43-N2-N3-C40
5	C	1640	RFP	C21-C22-C23-O9
5	C	1640	RFP	C43-N2-N3-C41
5	C	1640	RFP	C3-C2-N1-C15
5	C	1640	RFP	C28-C29-O5-C12
5	C	1640	RFP	C33-C24-C25-C26
5	C	1640	RFP	C23-C24-C25-C26

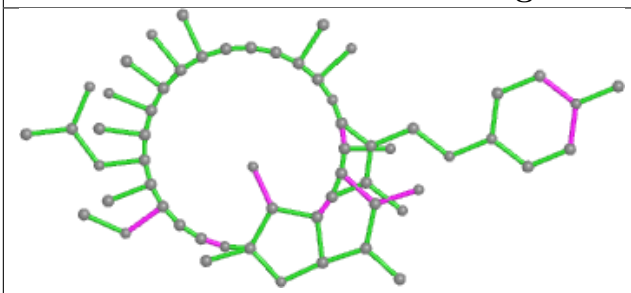
There are no ring outliers.

1 monomer is involved in 6 short contacts:

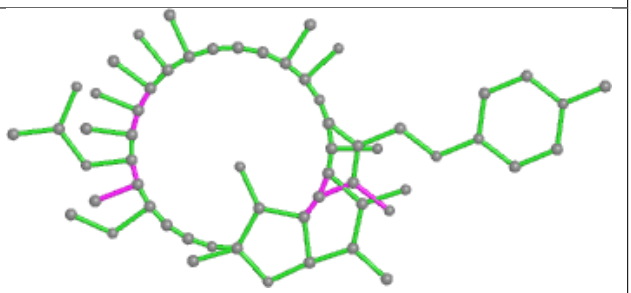
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1640	RFP	6	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

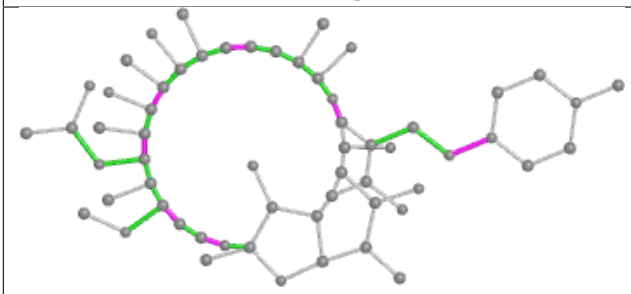
Ligand RFP C 1640



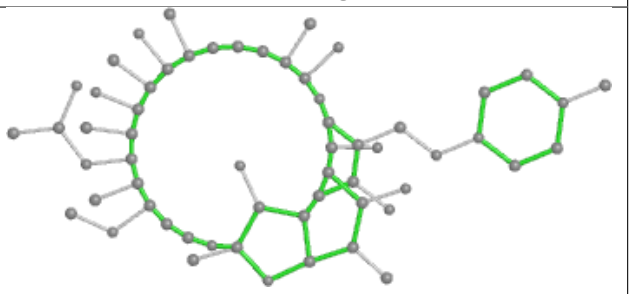
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	D	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	155:ASP	C	2(U):UNK	N	54.72
1	D	46(U):UNK	C	452:ILE	N	47.08
1	D	10(U):UNK	C	20(U):UNK	N	15.58
1	D	1270:ALA	C	1271:LYS	N	1.06

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.