Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2023 – 07:13 AM EDT

PDB ID	:	1FFX
Title	:	TUBULIN:STATHMIN-LIKE DOMAIN COMPLEX
Authors	:	Gigant, B.; Martin-Barbey, C.; Knossow, M.
Deposited on	:	2000-07-26
Resolution	:	3.95 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 (i) 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 (1)) were used in the production of this report:

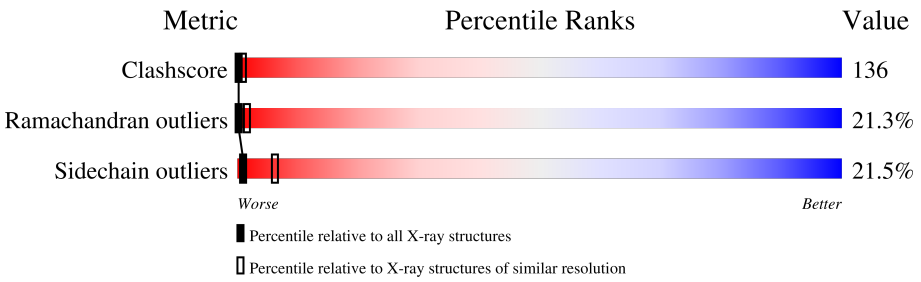
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.95 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	1085 (4.22-3.70)
Ramachandran outliers	138981	1047 (4.22-3.70)
Sidechain outliers	138945	1039 (4.22-3.70)

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	451	9% 53% 27% • 6%
1	C	451	9% 55% 25% • 6%
2	B	445	6% 57% 25% 5% 8%
2	D	445	6% 56% 24% 6% 8%
3	E	91	32% 68%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GDP	D	503	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13568 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 PROTEIN (TUBULIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	423	3295	2082	559	632	22	0	0	0
1	C	423	3295	2082	559	632	22	0	0	0

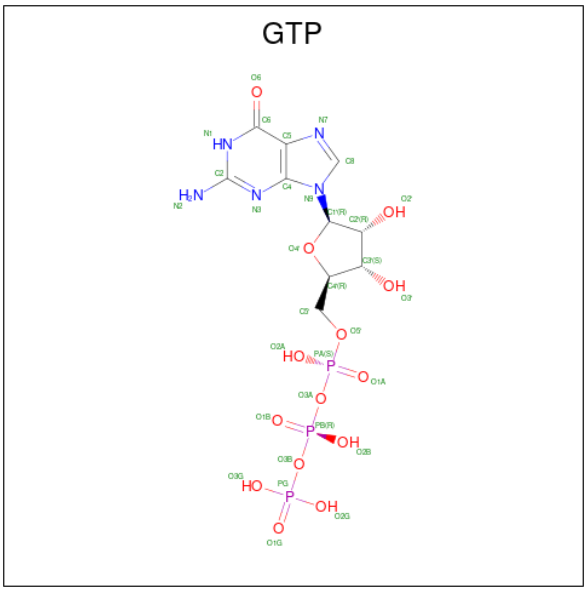
- Molecule 2 is a protein called PROTEIN (TUBULIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	410	3201	2014	550	611	26	0	0	0
2	D	410	3201	2014	550	611	26	0	0	0

- Molecule 3 is a protein called PROTEIN (STATHMIN-LIKE DOMAIN OF RB3).

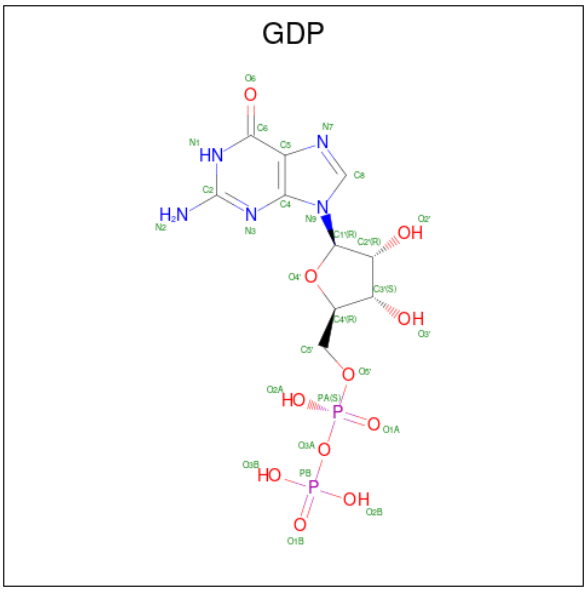
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	91	456	273	91	92	0	0	0

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	32	10	5	14	3	0	0
			Total	C	N	O	P		
4	C	1	32	10	5	14	3	0	0

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	28	10	5	11	2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	D	1	28	10	5	11	2	0	0

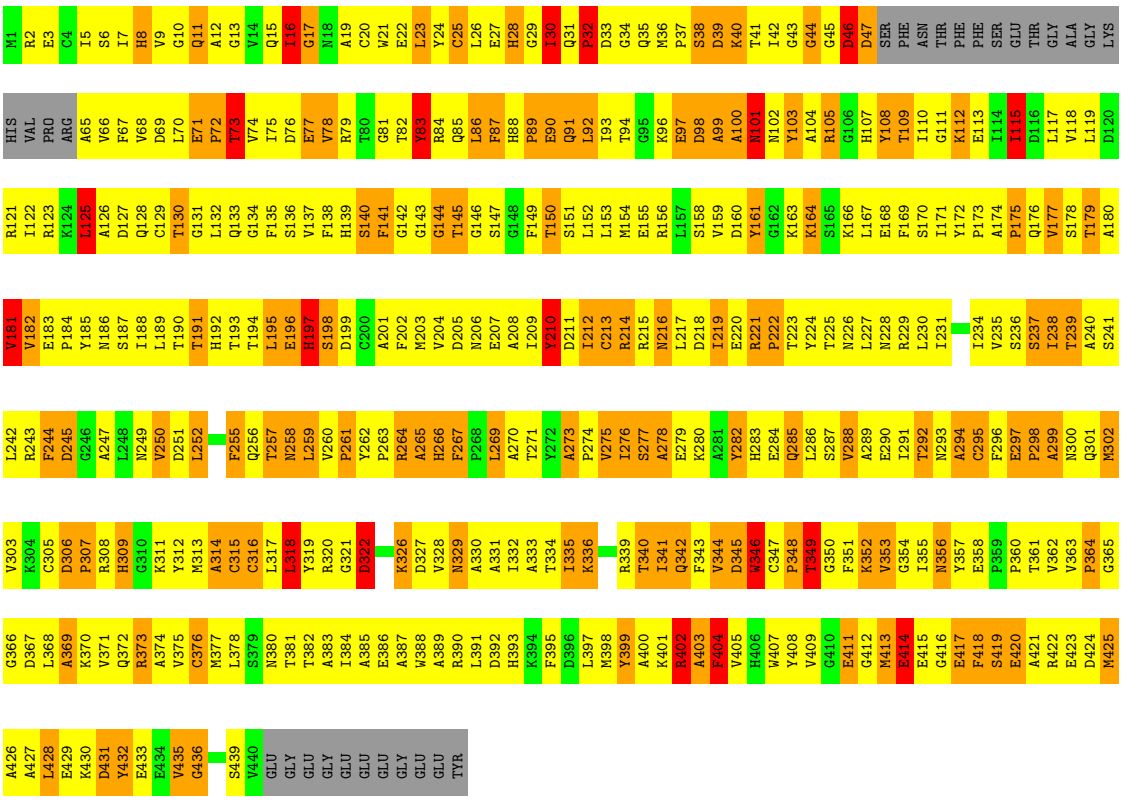
3 Residue-property plots (i)

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.

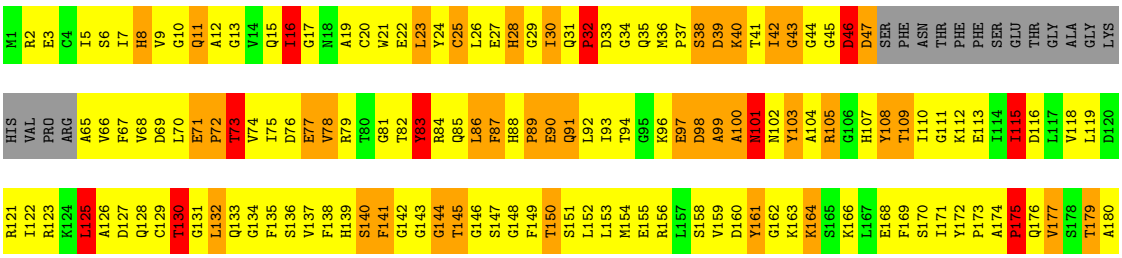
• Molecule 1: PROTEIN (TUBULIN)

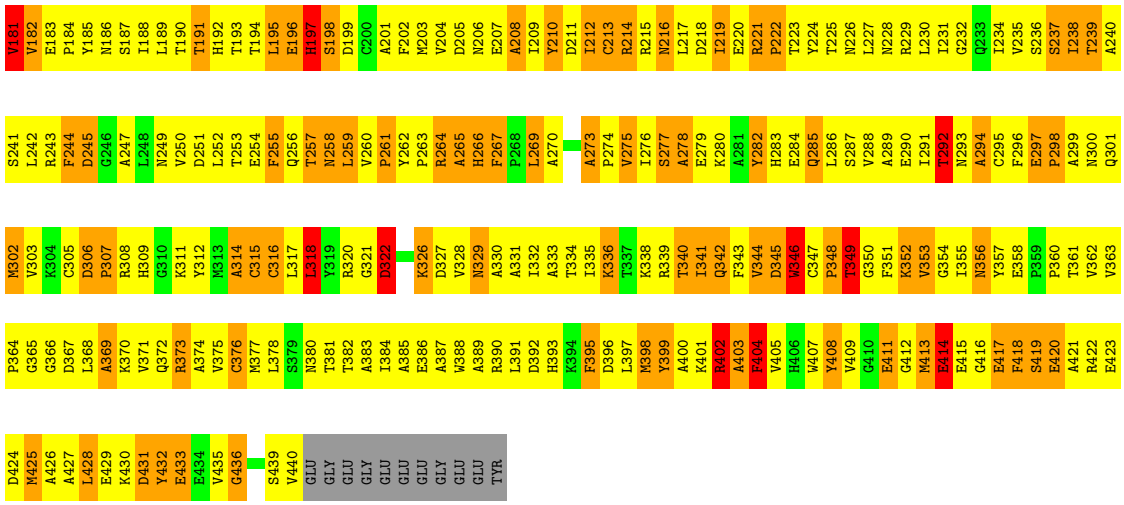
Chain A: 9% 53% 27% • 6%



• Molecule 1: PROTEIN (TUBULIN)

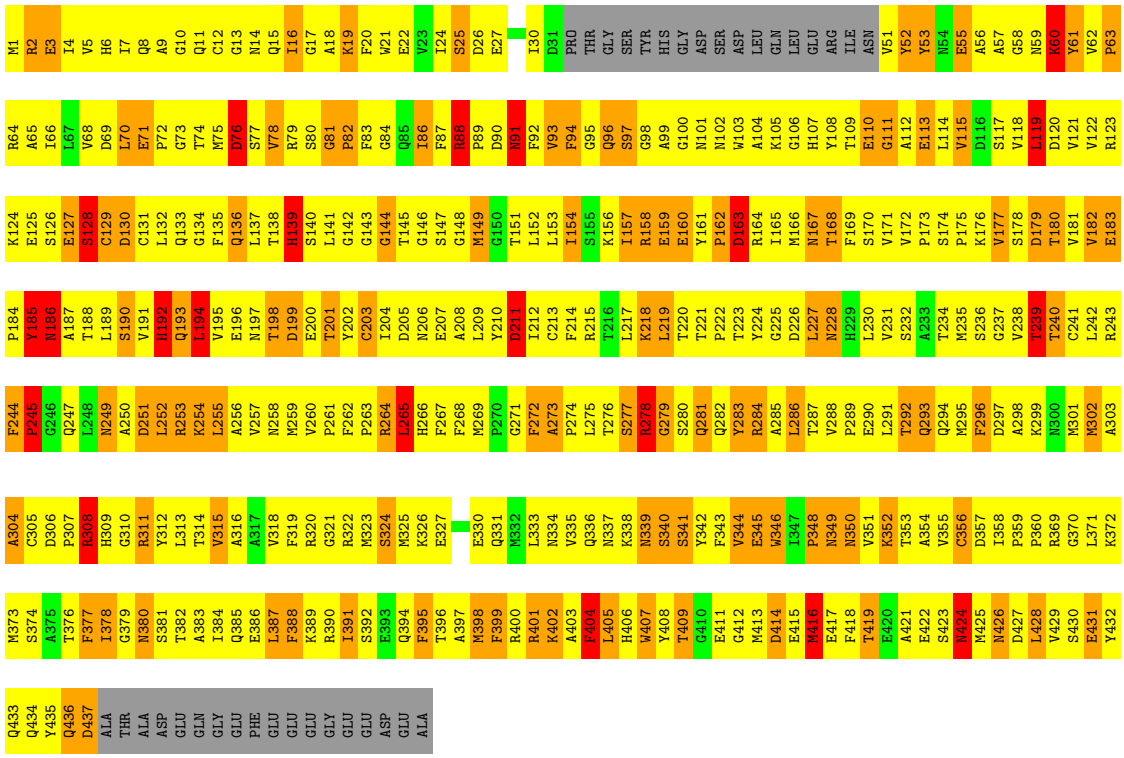
Chain C: 9% 55% 25% • 6%





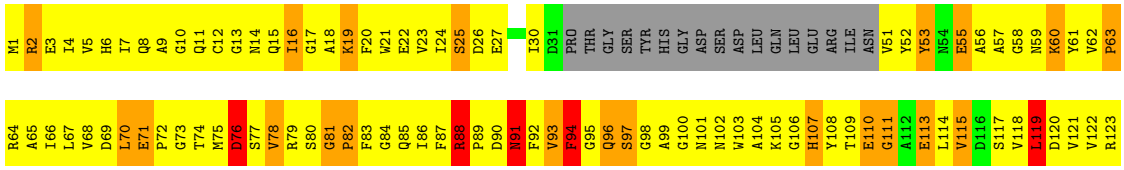
- Molecule 2: PROTEIN (TUBULIN)

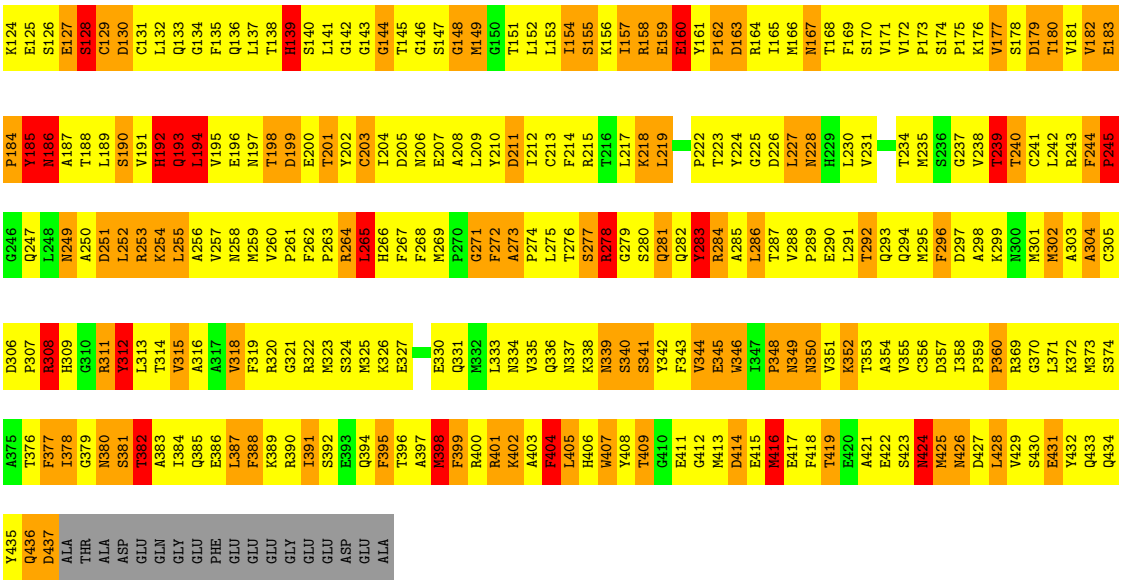
Chain B: 6% 57% 25% 5% 8%



- Molecule 2: PROTEIN (TUBULIN)

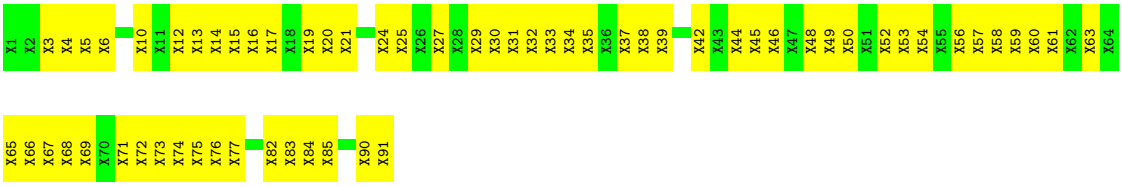
Chain D: 6% 56% 24% 6% 8%





- Molecule 3: PROTEIN (STATHMIN-LIKE DOMAIN OF RB3)

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 65	Depositor
Cell constants a, b, c, α, β, γ	328.50Å 328.50Å 54.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 3.95	Depositor
% Data completeness (in resolution range)	94.3 (7.00-3.95)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.267 , 0.367	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13568	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.59	0/3367	0.86	5/4570 (0.1%)
1	C	0.56	0/3367	0.84	5/4570 (0.1%)
2	B	0.56	0/3270	0.82	1/4428 (0.0%)
2	D	0.58	0/3270	0.84	0/4428
All	All	0.57	0/13274	0.84	11/17996 (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
1	C	0	2
2	B	0	1
2	D	0	1
All	All	0	5

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	417	GLU	N-CA-C	-5.93	94.99	111.00
1	C	318	LEU	CA-CB-CG	5.91	128.90	115.30
1	A	417	GLU	N-CA-C	-5.77	95.43	111.00
1	A	318	LEU	CA-CB-CG	5.63	128.26	115.30
1	A	294	ALA	N-CA-C	-5.38	96.46	111.00
1	C	294	ALA	N-CA-C	-5.33	96.61	111.00
2	B	356	CYS	N-CA-C	5.20	125.05	111.00
1	A	44	GLY	N-CA-C	-5.15	100.23	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	81	GLY	N-CA-C	-5.13	100.27	113.10
1	C	43	GLY	N-CA-C	-5.05	100.47	113.10
1	A	81	GLY	N-CA-C	-5.04	100.49	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	TYR	Sidechain
2	B	61	TYR	Sidechain
1	C	108	TYR	Sidechain
1	C	210	TYR	Sidechain
2	D	312	TYR	Sidechain

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	3295	0	3202	883	0
1	C	3295	0	3202	910	0
2	B	3201	0	3091	916	0
2	D	3201	0	3091	883	0
3	E	456	0	103	79	0
4	A	32	0	12	4	0
4	C	32	0	12	8	0
5	B	28	0	12	5	0
5	D	28	0	12	9	0
All	All	13568	0	12737	3585	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 136.

All (3585) 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)
2:B:175:PRO:HD2	2:B:207:GLU:HB2	1.23	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:158:ARG:HD3	2:D:197:ASN:ND2	1.63	1.14
1:A:214:ARG:HH21	1:A:220:GLU:HA	1.04	1.14
2:B:179:ASP:HA	1:C:352:LYS:HE2	1.20	1.12
1:C:222:PRO:HB2	1:C:227:LEU:HD11	1.31	1.12
2:D:311:ARG:HH21	2:D:437:ASP:HB2	1.03	1.13
1:C:175:PRO:HD2	1:C:207:GLU:HB2	1.16	1.12
1:C:214:ARG:HH21	1:C:220:GLU:HA	0.99	1.12
2:D:175:PRO:HD2	2:D:207:GLU:HB2	1.26	1.12
2:B:92:PHE:HE1	2:B:118:VAL:HA	0.96	1.12
1:C:419:SER:HA	1:C:422:ARG:HD3	1.22	1.12
2:D:278:ARG:HA	2:D:278:ARG:HH11	0.96	1.12
1:A:222:PRO:HB2	1:A:227:LEU:HD11	1.31	1.11
1:A:102:ASN:HB2	1:A:105:ARG:HB2	1.31	1.11
1:A:70:LEU:HD12	1:A:145:THR:HA	1.26	1.11
2:B:92:PHE:CE1	2:B:118:VAL:HA	1.85	1.10
2:D:92:PHE:HE1	2:D:118:VAL:HA	0.98	1.10
1:A:419:SER:HA	1:A:422:ARG:HD3	1.20	1.09
1:A:175:PRO:HD2	1:A:207:GLU:HB2	1.09	1.08
1:C:70:LEU:HD12	1:C:145:THR:HA	1.22	1.08
2:B:311:ARG:HH21	2:B:437:ASP:HB2	1.04	1.08
1:C:306:ASP:OD1	1:C:308:ARG:HB3	1.54	1.08
2:D:92:PHE:CE1	2:D:118:VAL:HA	1.88	1.08
1:C:102:ASN:HB2	1:C:105:ARG:HB2	1.33	1.08
2:B:206:ASN:HD22	2:B:227:LEU:HD21	1.19	1.07
2:B:213:CYS:HB3	2:B:219:LEU:HD12	1.32	1.07
2:B:2:ARG:HG3	2:B:133:GLN:NE2	1.70	1.06
1:C:316:CYS:HB2	1:C:352:LYS:HB3	1.33	1.06
2:D:192:HIS:HA	2:D:195:VAL:HG22	1.34	1.06
1:A:133:GLN:H	1:A:164:LYS:HD3	1.12	1.06
2:D:240:THR:O	2:D:243:ARG:HB2	1.56	1.06
1:A:383:ALA:O	1:A:386:GLU:HG2	1.55	1.05
2:B:190:SER:HB2	2:B:425:MET:HG3	1.35	1.05
2:B:191:VAL:HG21	2:B:421:ALA:HB1	1.38	1.05
2:D:158:ARG:HG3	2:D:159:GLU:H	1.16	1.05
2:D:213:CYS:HB3	2:D:219:LEU:HD12	1.37	1.04
1:A:306:ASP:OD1	1:A:308:ARG:HB3	1.57	1.04
1:A:7:ILE:HG22	1:A:66:VAL:HB	1.37	1.04
2:B:178:SER:O	2:B:182:VAL:HB	1.57	1.04
2:B:192:HIS:HA	2:B:195:VAL:HG22	1.36	1.04
2:B:278:ARG:HA	2:B:278:ARG:NH1	1.72	1.04
1:C:7:ILE:HG22	1:C:66:VAL:HB	1.33	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:ARG:HA	2:B:278:ARG:HH11	0.91	1.03
2:D:2:ARG:HG3	2:D:133:GLN:NE2	1.73	1.03
2:B:158:ARG:HD3	2:B:197:ASN:ND2	1.74	1.03
1:A:409:VAL:HA	1:A:414:GLU:OE1	1.57	1.02
2:D:178:SER:O	2:D:182:VAL:HB	1.56	1.02
1:A:141:PHE:HE2	1:A:172:TYR:HA	1.23	1.02
2:B:264:ARG:HH21	2:B:428:LEU:HD12	1.22	1.02
2:B:158:ARG:HG3	2:B:159:GLU:H	1.22	1.01
1:C:133:GLN:H	1:C:164:LYS:HD3	1.19	1.01
1:A:88:HIS:HB3	1:A:91:GLN:NE2	1.75	1.01
1:C:9:VAL:HG12	1:C:68:VAL:HG13	1.43	1.01
1:A:413:MET:SD	3:E:15:UNK:HA	2.01	1.00
1:A:9:VAL:HG12	1:A:68:VAL:HG13	1.44	1.00
2:B:240:THR:O	2:B:243:ARG:HB2	1.62	1.00
1:C:93:ILE:HD13	1:C:118:VAL:HG22	1.43	0.99
1:A:242:LEU:HD21	1:A:318:LEU:HD21	1.43	0.99
2:B:322:ARG:HG2	2:B:357:ASP:HA	1.45	0.99
2:D:278:ARG:HA	2:D:278:ARG:NH1	1.76	0.99
2:D:264:ARG:HH21	2:D:428:LEU:HD12	1.25	0.99
1:C:11:GLN:HG3	1:C:74:VAL:HG21	1.45	0.98
2:D:191:VAL:HG21	2:D:421:ALA:HB1	1.42	0.98
2:D:206:ASN:HD22	2:D:227:LEU:HD21	1.26	0.98
1:A:316:CYS:HB2	1:A:352:LYS:HB3	1.41	0.98
2:B:220:THR:HB	1:C:326:LYS:HD2	1.43	0.98
1:A:387:ALA:HA	1:A:390:ARG:HD3	1.45	0.98
2:D:190:SER:HB2	2:D:425:MET:HG3	1.44	0.98
2:B:196:GLU:O	2:B:198:THR:HG22	1.64	0.97
1:C:387:ALA:HA	1:C:390:ARG:HD3	1.46	0.97
2:B:77:SER:HA	2:B:80:SER:HB3	1.46	0.97
1:A:102:ASN:HB2	1:A:105:ARG:CB	1.95	0.97
1:A:115:ILE:HD11	1:A:156:ARG:HG3	1.47	0.97
1:C:141:PHE:HE2	1:C:172:TYR:HA	1.27	0.97
1:A:11:GLN:HG3	1:A:74:VAL:HG21	1.45	0.97
1:C:88:HIS:HB3	1:C:91:GLN:NE2	1.80	0.97
1:C:115:ILE:HD11	1:C:156:ARG:HG3	1.47	0.96
2:D:158:ARG:HB2	2:D:197:ASN:HB2	1.47	0.96
1:A:69:ASP:HB3	1:A:75:ILE:HG21	1.46	0.96
2:B:132:LEU:HB3	2:B:164:ARG:NH2	1.80	0.96
1:A:322:ASP:H	1:A:357:TYR:HA	1.30	0.96
1:C:166:LYS:HE3	1:C:198:SER:H	1.31	0.96
1:C:409:VAL:HA	1:C:414:GLU:OE1	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:91:ASN:HD22	2:D:91:ASN:H	1.10	0.96
1:A:237:SER:HA	1:A:241:SER:HB2	1.48	0.96
2:B:278:ARG:HH11	2:B:278:ARG:CA	1.79	0.95
1:C:214:ARG:NH2	1:C:220:GLU:HA	1.80	0.95
2:B:91:ASN:H	2:B:91:ASN:HD22	1.05	0.95
1:C:185:TYR:HA	1:C:188:ILE:HD11	1.48	0.95
2:B:223:THR:HG22	2:B:226:ASP:OD2	1.66	0.95
1:C:386:GLU:HG3	1:C:387:ALA:H	1.32	0.95
2:D:8:GLN:HG2	2:D:14:ASN:HD22	1.30	0.95
1:C:102:ASN:HB2	1:C:105:ARG:CB	1.97	0.95
1:A:214:ARG:NH2	1:A:220:GLU:HA	1.81	0.94
1:C:362:VAL:HG13	1:C:367:ASP:HB2	1.49	0.94
1:A:311:LYS:HD3	1:A:344:VAL:HG13	1.48	0.94
2:D:322:ARG:HG2	2:D:357:ASP:HA	1.45	0.94
2:D:77:SER:HA	2:D:80:SER:HB3	1.48	0.94
2:D:196:GLU:O	2:D:198:THR:HG22	1.66	0.94
1:A:93:ILE:HD13	1:A:118:VAL:HG22	1.48	0.94
2:B:407:TRP:HZ2	1:C:256:GLN:HB2	1.30	0.94
1:A:79:ARG:HD3	1:A:89:PRO:HB3	1.50	0.93
2:D:218:LYS:HZ3	2:D:278:ARG:N	1.65	0.93
1:A:175:PRO:CD	1:A:207:GLU:HB2	1.97	0.93
2:D:263:PRO:C	2:D:265:LEU:H	1.68	0.93
1:C:322:ASP:H	1:C:357:TYR:HA	1.32	0.93
1:A:409:VAL:HG22	1:A:414:GLU:HG3	1.51	0.93
1:C:102:ASN:HD21	2:D:257:VAL:HG11	1.33	0.93
1:A:398:MET:SD	2:B:348:PRO:HD2	2.09	0.93
2:B:218:LYS:HZ3	2:B:278:ARG:H	0.96	0.92
1:A:322:ASP:N	1:A:357:TYR:HA	1.84	0.92
1:C:87:PHE:HE2	1:C:92:LEU:HD21	1.34	0.92
1:C:383:ALA:O	1:C:386:GLU:HG2	1.68	0.92
1:C:322:ASP:N	1:C:357:TYR:HA	1.84	0.92
2:B:158:ARG:HB2	2:B:197:ASN:HB2	1.51	0.92
1:A:102:ASN:HD21	2:B:257:VAL:HG11	1.31	0.92
1:A:386:GLU:HG3	1:A:387:ALA:H	1.33	0.92
1:C:409:VAL:HG22	1:C:414:GLU:CG	2.00	0.92
2:D:311:ARG:NH2	2:D:437:ASP:HB2	1.83	0.92
1:C:137:VAL:HG11	1:C:154:MET:HE2	1.51	0.92
1:C:175:PRO:C	1:C:177:VAL:H	1.65	0.92
2:D:132:LEU:HB3	2:D:164:ARG:NH2	1.84	0.91
1:C:237:SER:HA	1:C:241:SER:HB2	1.49	0.91
2:D:218:LYS:HZ3	2:D:278:ARG:H	0.91	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:VAL:HG13	1:A:367:ASP:HB2	1.50	0.91
1:C:409:VAL:HG22	1:C:414:GLU:HG3	1.50	0.91
2:D:284:ARG:O	2:D:287:THR:HG23	1.71	0.91
1:A:137:VAL:HG11	1:A:154:MET:HE2	1.50	0.91
2:B:194:LEU:HD23	2:B:195:VAL:HG13	1.52	0.91
1:A:409:VAL:HG22	1:A:414:GLU:CG	2.01	0.91
2:B:8:GLN:HG2	2:B:14:ASN:HD22	1.32	0.91
1:A:398:MET:HG3	1:A:399:TYR:HD1	1.33	0.91
1:C:335:ILE:HG13	1:C:336:LYS:H	1.32	0.91
1:A:175:PRO:C	1:A:177:VAL:H	1.70	0.90
2:D:194:LEU:HD23	2:D:195:VAL:HG13	1.50	0.90
2:B:218:LYS:HZ3	2:B:278:ARG:N	1.70	0.90
2:B:263:PRO:C	2:B:265:LEU:H	1.64	0.90
1:A:166:LYS:HE3	1:A:198:SER:H	1.35	0.90
2:D:262:PHE:HB3	2:D:263:PRO:HD2	1.53	0.90
1:A:223:THR:HB	1:A:226:ASN:OD1	1.71	0.90
2:B:2:ARG:NE	2:B:243:ARG:HD2	1.86	0.90
2:D:278:ARG:N	2:D:278:ARG:HD2	1.84	0.90
1:A:402:ARG:HD2	2:B:346:TRP:CZ3	2.07	0.90
2:B:59:ASN:HB2	2:B:64:ARG:NE	1.86	0.90
2:B:286:LEU:HD12	2:B:373:MET:HB2	1.54	0.90
1:C:398:MET:SD	2:D:348:PRO:HD2	2.11	0.90
2:B:278:ARG:N	2:B:278:ARG:HD2	1.83	0.90
2:D:70:LEU:HG	2:D:99:ALA:HB3	1.53	0.89
2:D:121:VAL:HA	2:D:124:LYS:HG2	1.54	0.89
2:B:96:GLN:HE22	1:C:130:THR:HG22	1.35	0.89
2:B:311:ARG:NH2	2:B:437:ASP:HB2	1.88	0.89
1:A:335:ILE:HG13	1:A:336:LYS:H	1.36	0.89
1:A:243:ARG:HH12	1:A:250:VAL:HG13	1.38	0.88
1:C:2:ARG:NH2	1:C:133:GLN:HE22	1.70	0.88
2:B:321:GLY:HA2	2:B:359:PRO:HB3	1.53	0.88
1:A:9:VAL:HG12	1:A:68:VAL:CG1	2.03	0.88
1:A:166:LYS:NZ	1:A:197:HIS:HB2	1.88	0.88
1:C:79:ARG:HD3	1:C:89:PRO:HB3	1.55	0.88
1:A:16:ILE:HG22	1:A:17:GLY:N	1.87	0.88
1:A:418:PHE:HD2	1:A:418:PHE:N	1.72	0.88
1:C:242:LEU:HD21	1:C:318:LEU:HD21	1.52	0.88
2:D:51:VAL:HG23	2:D:53:TYR:H	1.38	0.88
1:C:31:GLN:HB3	1:C:32:PRO:HD2	1.56	0.88
1:C:69:ASP:OD1	1:C:70:LEU:N	2.05	0.88
2:B:133:GLN:NE2	2:B:252:LEU:HB3	1.87	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:PRO:HG2	1:C:380:ASN:HD21	1.39	0.88
1:A:107:HIS:HD1	1:A:151:SER:HB2	1.37	0.88
2:D:278:ARG:HH11	2:D:278:ARG:CA	1.84	0.88
1:A:287:SER:H	1:A:290:GLU:CD	1.77	0.87
2:B:284:ARG:O	2:B:287:THR:HG23	1.73	0.87
1:A:186:ASN:ND2	1:A:391:LEU:HD11	1.90	0.87
1:C:175:PRO:CD	1:C:207:GLU:HB2	2.04	0.87
2:D:339:ASN:HB3	2:D:342:TYR:HD1	1.37	0.87
1:C:186:ASN:ND2	1:C:391:LEU:HD11	1.90	0.87
1:C:206:ASN:HB3	1:C:210:TYR:CE2	2.10	0.87
1:C:398:MET:HG3	1:C:399:TYR:HD1	1.38	0.87
1:A:216:ASN:HD22	1:A:275:VAL:HG12	1.38	0.87
1:A:409:VAL:HG13	1:A:414:GLU:OE2	1.75	0.87
1:A:144:GLY:N	1:A:147:SER:HB3	1.89	0.87
1:A:261:PRO:HG2	1:A:380:ASN:HD21	1.38	0.87
1:A:320:ARG:HB3	1:A:374:ALA:HB3	1.56	0.87
2:B:176:LYS:HD2	2:B:210:TYR:CZ	2.10	0.87
1:C:27:GLU:HG3	1:C:28:HIS:H	1.40	0.86
1:C:243:ARG:HH12	1:C:250:VAL:HG13	1.39	0.86
2:B:396:THR:HG23	2:B:400:ARG:HD3	1.54	0.86
2:D:396:THR:HG23	2:D:400:ARG:HD3	1.57	0.86
2:D:88:ARG:HB2	2:D:89:PRO:HD3	1.56	0.86
2:D:223:THR:HG22	2:D:226:ASP:OD2	1.76	0.86
1:A:322:ASP:H	1:A:357:TYR:CA	1.88	0.86
2:B:88:ARG:HB2	2:B:89:PRO:HD3	1.55	0.86
2:B:311:ARG:HB2	2:B:344:VAL:H	1.40	0.86
2:B:339:ASN:HB3	2:B:342:TYR:HD1	1.40	0.86
1:A:166:LYS:HZ2	1:A:197:HIS:HB2	1.38	0.86
2:D:358:ILE:H	2:D:358:ILE:HD12	1.40	0.86
1:C:87:PHE:CE2	1:C:92:LEU:HD21	2.10	0.86
2:D:321:GLY:HA2	2:D:359:PRO:HB3	1.58	0.86
1:C:418:PHE:HD2	1:C:418:PHE:N	1.73	0.86
2:B:223:THR:HG22	2:B:226:ASP:CG	1.97	0.86
1:C:362:VAL:HG21	1:C:370:LYS:HA	1.57	0.85
2:D:142:GLY:HA2	2:D:185:TYR:HB3	1.57	0.85
1:A:31:GLN:HB3	1:A:32:PRO:HD2	1.58	0.85
1:C:409:VAL:HG13	1:C:414:GLU:OE2	1.75	0.85
1:C:223:THR:HB	1:C:226:ASN:OD1	1.76	0.85
1:C:322:ASP:H	1:C:357:TYR:CA	1.88	0.85
1:A:138:PHE:HZ	1:A:235:VAL:HG11	1.37	0.85
1:C:190:THR:HA	1:C:193:THR:HG22	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ILE:HD11	1:A:353:VAL:HG21	1.58	0.85
1:C:102:ASN:O	1:C:104:ALA:N	2.09	0.85
1:C:344:VAL:HG11	1:C:346:TRP:NE1	1.91	0.85
2:D:103:TRP:HE1	2:D:189:LEU:HD21	1.40	0.85
2:D:344:VAL:HB	2:D:346:TRP:NE1	1.91	0.85
2:D:59:ASN:HB2	2:D:64:ARG:NE	1.90	0.85
3:E:35:UNK:C	3:E:37:UNK:N	2.35	0.85
1:C:386:GLU:HG3	1:C:387:ALA:N	1.90	0.85
2:B:19:LYS:HZ1	2:B:82:PRO:HG3	1.42	0.85
2:D:158:ARG:HG3	2:D:159:GLU:N	1.91	0.85
2:B:91:ASN:HD22	2:B:91:ASN:N	1.75	0.84
2:B:141:LEU:HB3	2:B:186:ASN:HB3	1.57	0.84
2:B:132:LEU:HB3	2:B:164:ARG:HH21	1.35	0.84
1:C:214:ARG:HA	1:C:218:ASP:O	1.77	0.84
2:D:286:LEU:HD12	2:D:373:MET:HB2	1.58	0.84
1:A:362:VAL:HB	1:A:370:LYS:HG2	1.59	0.84
1:C:206:ASN:HD22	1:C:210:TYR:HE2	1.21	0.84
1:C:418:PHE:N	1:C:418:PHE:CD2	2.45	0.84
2:D:176:LYS:HD2	2:D:210:TYR:CZ	2.13	0.84
2:B:51:VAL:HG23	2:B:53:TYR:H	1.42	0.84
2:B:133:GLN:HE21	2:B:252:LEU:HB3	1.41	0.84
1:C:166:LYS:NZ	1:C:197:HIS:HB2	1.91	0.84
2:D:13:GLY:O	2:D:16:ILE:HG23	1.76	0.84
1:A:2:ARG:NH2	1:A:133:GLN:HE22	1.76	0.84
1:C:216:ASN:HD22	1:C:275:VAL:HG12	1.42	0.84
1:C:320:ARG:HB3	1:C:374:ALA:HB3	1.60	0.84
1:A:206:ASN:HB3	1:A:210:TYR:CE2	2.11	0.84
1:A:362:VAL:HG21	1:A:370:LYS:HA	1.59	0.84
1:C:138:PHE:HZ	1:C:235:VAL:HG11	1.41	0.84
2:D:12:CYS:HB3	5:D:503:GDP:C8	2.12	0.84
1:C:362:VAL:HB	1:C:370:LYS:HG2	1.58	0.84
2:D:213:CYS:HA	2:D:217:LEU:HD23	1.58	0.84
2:B:103:TRP:HE1	2:B:189:LEU:HD21	1.42	0.83
1:C:241:SER:HA	1:C:320:ARG:NH2	1.92	0.83
1:C:284:GLU:HG2	1:C:285:GLN:HE21	1.41	0.83
2:B:121:VAL:HA	2:B:124:LYS:HG2	1.57	0.83
2:D:58:GLY:C	2:D:64:ARG:HE	1.81	0.83
2:D:141:LEU:HB3	2:D:186:ASN:HB3	1.61	0.83
1:A:402:ARG:HG2	1:A:403:ALA:H	1.43	0.83
1:C:69:ASP:HB3	1:C:75:ILE:HG21	1.60	0.83
2:D:19:LYS:NZ	2:D:82:PRO:HG3	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLU:HG3	1:A:28:HIS:H	1.43	0.83
2:B:109:THR:HG21	2:B:411:GLU:HG2	1.61	0.83
2:B:264:ARG:HH21	2:B:428:LEU:CD1	1.92	0.83
2:D:2:ARG:NE	2:D:243:ARG:HD2	1.93	0.83
2:B:192:HIS:C	2:B:194:LEU:H	1.82	0.83
2:D:3:GLU:OE2	2:D:130:ASP:HB3	1.79	0.83
2:D:92:PHE:HE1	2:D:118:VAL:CA	1.88	0.83
1:A:92:LEU:N	1:A:92:LEU:HD12	1.94	0.82
1:A:100:ALA:HB1	1:A:105:ARG:O	1.78	0.82
1:A:350:GLY:C	1:A:351:PHE:HD1	1.82	0.82
2:D:132:LEU:HB3	2:D:164:ARG:HH21	1.42	0.82
2:D:311:ARG:HB2	2:D:344:VAL:H	1.43	0.82
2:D:311:ARG:HG3	2:D:344:VAL:HA	1.61	0.82
1:A:284:GLU:HG2	1:A:285:GLN:HE21	1.42	0.82
2:B:398:MET:O	2:B:400:ARG:N	2.12	0.82
1:C:9:VAL:HG12	1:C:68:VAL:CG1	2.08	0.82
3:E:42:UNK:C	3:E:44:UNK:N	2.41	0.82
1:A:88:HIS:HB3	1:A:91:GLN:HE22	1.45	0.82
1:A:339:ARG:HD2	1:A:339:ARG:C	1.98	0.82
2:B:175:PRO:HD2	2:B:207:GLU:CB	2.09	0.82
1:A:102:ASN:O	1:A:104:ALA:N	2.12	0.82
1:A:190:THR:HA	1:A:193:THR:HG22	1.60	0.82
1:A:212:ILE:HG13	1:A:213:CYS:N	1.94	0.82
1:A:373:ARG:HB3	1:A:373:ARG:HH11	1.45	0.82
2:B:189:LEU:C	2:B:191:VAL:H	1.83	0.82
1:C:208:ALA:O	1:C:211:ASP:HB2	1.80	0.82
2:D:109:THR:O	2:D:111:GLY:N	2.13	0.82
2:D:189:LEU:C	2:D:191:VAL:H	1.83	0.82
2:D:313:LEU:HA	2:D:344:VAL:HG11	1.60	0.82
1:A:206:ASN:HD22	1:A:210:TYR:HE2	1.26	0.82
2:B:58:GLY:C	2:B:64:ARG:HE	1.83	0.82
2:B:358:ILE:H	2:B:358:ILE:HD12	1.44	0.82
2:D:59:ASN:HA	2:D:64:ARG:HH21	1.45	0.82
1:C:287:SER:H	1:C:290:GLU:CD	1.82	0.81
2:D:287:THR:HB	2:D:289:PRO:HD2	1.61	0.81
1:A:418:PHE:N	1:A:418:PHE:CD2	2.45	0.81
2:B:19:LYS:NZ	2:B:82:PRO:HG3	1.96	0.81
2:B:96:GLN:HE22	1:C:130:THR:CG2	1.94	0.81
2:B:102:ASN:HD22	2:B:105:LYS:HG3	1.45	0.81
1:C:417:GLU:HB3	1:C:418:PHE:CD2	2.14	0.81
2:D:103:TRP:NE1	2:D:189:LEU:HD21	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:175:PRO:HD2	2:D:207:GLU:CB	2.10	0.81
1:C:258:ASN:HD22	1:C:258:ASN:N	1.78	0.81
2:D:143:GLY:O	2:D:145:THR:N	2.11	0.81
1:A:115:ILE:O	1:A:115:ILE:HD13	1.80	0.81
1:A:386:GLU:HG3	1:A:387:ALA:N	1.93	0.81
1:C:115:ILE:O	1:C:115:ILE:HD13	1.81	0.81
1:C:388:TRP:CH2	1:C:428:LEU:HD13	2.15	0.81
2:D:109:THR:HG21	2:D:411:GLU:HG2	1.63	0.81
1:A:107:HIS:ND1	1:A:151:SER:HB2	1.96	0.81
2:B:179:ASP:HA	1:C:352:LYS:CE	2.09	0.81
1:C:409:VAL:HG13	1:C:414:GLU:CD	2.01	0.81
2:D:218:LYS:NZ	2:D:278:ARG:H	1.77	0.81
3:E:48:UNK:O	3:E:50:UNK:N	2.13	0.81
1:C:402:ARG:HD2	2:D:346:TRP:CZ3	2.15	0.81
2:B:287:THR:HB	2:B:289:PRO:HD2	1.63	0.80
1:A:417:GLU:HB3	1:A:418:PHE:CD2	2.16	0.80
2:B:109:THR:O	2:B:111:GLY:N	2.14	0.80
2:D:184:PRO:HB2	2:D:399:PHE:CE1	2.17	0.80
2:D:311:ARG:HH21	2:D:437:ASP:CB	1.91	0.80
2:D:390:ARG:O	2:D:392:SER:N	2.13	0.80
3:E:61:UNK:O	3:E:63:UNK:N	2.14	0.80
2:B:262:PHE:HB3	2:B:263:PRO:HD2	1.61	0.80
1:C:373:ARG:HB3	1:C:373:ARG:HH11	1.46	0.80
2:D:264:ARG:HH11	2:D:264:ARG:HG3	1.47	0.80
1:A:104:ALA:HA	1:A:108:TYR:HD2	1.46	0.80
1:A:174:ALA:O	1:A:177:VAL:N	2.15	0.80
2:D:168:THR:OG1	2:D:201:THR:HB	1.82	0.80
2:D:286:LEU:HG	2:D:373:MET:HE3	1.62	0.80
2:B:401:ARG:NH1	1:C:440:VAL:HA	1.95	0.80
2:B:115:VAL:HG11	2:B:156:LYS:HZ2	1.46	0.80
2:D:335:VAL:HA	2:D:338:LYS:CB	2.12	0.80
1:A:388:TRP:CH2	1:A:428:LEU:HD13	2.16	0.80
2:B:286:LEU:HG	2:B:286:LEU:O	1.79	0.80
1:C:291:ILE:HD12	1:C:373:ARG:HG3	1.63	0.80
2:D:133:GLN:NE2	2:D:252:LEU:HB3	1.97	0.80
2:B:142:GLY:HA2	2:B:185:TYR:HB3	1.61	0.80
2:D:12:CYS:HB2	5:D:503:GDP:O2A	1.81	0.80
3:E:21:UNK:O	3:E:24:UNK:N	2.15	0.80
2:D:285:ALA:O	2:D:286:LEU:HD23	1.82	0.80
2:D:387:LEU:O	2:D:387:LEU:HD23	1.81	0.80
1:A:133:GLN:N	1:A:164:LYS:HD3	1.94	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:TRP:NE1	2:B:189:LEU:HD21	1.96	0.79
2:D:218:LYS:HZ1	2:D:278:ARG:HB2	1.46	0.79
2:D:391:ILE:H	2:D:391:ILE:HD12	1.47	0.79
2:B:335:VAL:HA	2:B:338:LYS:HB3	1.63	0.79
1:C:16:ILE:HG22	1:C:17:GLY:N	1.96	0.79
3:E:31:UNK:HA	3:E:34:UNK:CB	2.13	0.79
2:B:59:ASN:HA	2:B:64:ARG:HH21	1.47	0.79
1:A:180:ALA:C	1:A:182:VAL:H	1.86	0.79
1:C:212:ILE:HG13	1:C:213:CYS:N	1.95	0.79
1:A:419:SER:HA	1:A:422:ARG:CD	2.10	0.79
2:B:335:VAL:HA	2:B:338:LYS:CB	2.13	0.79
1:C:311:LYS:HD3	1:C:344:VAL:HG13	1.62	0.79
2:D:102:ASN:HD22	2:D:105:LYS:HG3	1.47	0.79
1:C:339:ARG:HD2	1:C:339:ARG:C	2.03	0.79
2:D:353:THR:HG22	2:D:354:ALA:N	1.96	0.79
2:B:102:ASN:ND2	2:B:105:LYS:HG3	1.98	0.79
2:D:179:ASP:HB3	2:D:181:VAL:HG12	1.63	0.79
2:B:70:LEU:HG	2:B:99:ALA:HB3	1.62	0.79
1:C:335:ILE:HG13	1:C:336:LYS:N	1.97	0.79
1:A:417:GLU:HB3	1:A:418:PHE:CE2	2.18	0.79
2:B:179:ASP:HB3	2:B:181:VAL:HG12	1.65	0.79
2:B:182:VAL:O	2:B:182:VAL:HG12	1.81	0.79
1:C:92:LEU:N	1:C:92:LEU:HD12	1.97	0.79
1:C:417:GLU:HB3	1:C:418:PHE:CE2	2.17	0.79
1:A:388:TRP:HH2	1:A:428:LEU:HD13	1.47	0.79
2:D:274:PRO:HB2	2:D:371:LEU:HD12	1.65	0.78
2:D:322:ARG:HE	2:D:357:ASP:HB3	1.46	0.78
1:A:185:TYR:HA	1:A:188:ILE:HD11	1.63	0.78
1:A:196:GLU:O	1:A:197:HIS:HB3	1.82	0.78
1:A:344:VAL:HG11	1:A:346:TRP:NE1	1.98	0.78
2:D:205:ASP:HB2	2:D:387:LEU:HD11	1.62	0.78
1:C:175:PRO:C	1:C:177:VAL:N	2.36	0.78
1:C:227:LEU:O	1:C:231:ILE:HG12	1.84	0.78
2:D:91:ASN:HD22	2:D:91:ASN:N	1.77	0.78
2:B:217:LEU:HG	2:B:218:LYS:N	1.98	0.78
1:C:107:HIS:HD1	1:C:151:SER:HB2	1.49	0.78
1:C:362:VAL:HG13	1:C:367:ASP:CB	2.13	0.78
1:C:371:VAL:HG12	1:C:373:ARG:H	1.48	0.78
2:D:2:ARG:HG3	2:D:133:GLN:HE21	1.48	0.78
3:E:31:UNK:O	3:E:34:UNK:N	2.17	0.78
1:C:144:GLY:N	1:C:147:SER:HB3	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:223:THR:HG22	2:D:226:ASP:CG	2.03	0.78
1:A:33:ASP:HA	1:A:36:MET:HB3	1.66	0.78
2:B:285:ALA:O	2:B:286:LEU:HD23	1.84	0.78
1:A:30:ILE:HG13	1:A:31:GLN:N	1.97	0.78
1:C:234:ILE:HD13	1:C:302:MET:SD	2.24	0.78
1:C:282:TYR:N	1:C:282:TYR:CD2	2.50	0.78
2:D:292:THR:HG21	2:D:331:GLN:HB3	1.66	0.78
2:B:179:ASP:HB2	2:B:182:VAL:HG23	1.63	0.78
1:C:388:TRP:HH2	1:C:428:LEU:HD13	1.49	0.78
1:C:402:ARG:HG2	1:C:403:ALA:H	1.46	0.78
2:D:102:ASN:ND2	2:D:105:LYS:HG3	1.99	0.78
2:D:244:PHE:HB2	2:D:245:PRO:HD2	1.66	0.78
2:B:87:PHE:O	2:B:87:PHE:HD1	1.67	0.77
2:B:158:ARG:HG3	2:B:159:GLU:N	1.98	0.77
1:C:104:ALA:HA	1:C:108:TYR:HD2	1.48	0.77
1:C:212:ILE:HD11	1:C:230:LEU:HD21	1.65	0.77
2:D:288:VAL:HG11	2:D:327:GLU:OE1	1.84	0.77
2:D:339:ASN:HB3	2:D:342:TYR:CD1	2.19	0.77
3:E:35:UNK:O	3:E:37:UNK:N	2.18	0.77
2:B:402:LYS:HE3	1:C:440:VAL:HB	1.65	0.77
2:B:213:CYS:HA	2:B:217:LEU:HD23	1.67	0.77
1:C:413:MET:HG3	3:E:66:UNK:CB	2.14	0.77
2:D:274:PRO:HB2	2:D:371:LEU:CD1	2.15	0.77
1:C:298:PRO:O	1:C:301:GLN:HG3	1.85	0.77
2:D:179:ASP:CB	2:D:182:VAL:H	1.98	0.77
1:A:413:MET:CE	1:A:413:MET:H	1.97	0.77
1:C:133:GLN:N	1:C:164:LYS:HD3	1.99	0.77
1:C:322:ASP:CA	1:C:357:TYR:HA	2.15	0.77
1:A:69:ASP:OD1	1:A:70:LEU:N	2.17	0.77
2:B:4:ILE:O	2:B:58:GLY:HA2	1.84	0.77
2:D:183:GLU:C	2:D:185:TYR:H	1.88	0.77
2:D:305:CYS:SG	2:D:387:LEU:HB2	2.24	0.77
3:E:73:UNK:O	3:E:75:UNK:N	2.17	0.77
1:A:102:ASN:CB	1:A:105:ARG:HB2	2.14	0.77
2:B:344:VAL:HB	2:B:346:TRP:NE1	2.00	0.77
1:A:258:ASN:HD22	1:A:258:ASN:N	1.82	0.77
2:B:172:VAL:HG13	2:B:173:PRO:HD2	1.67	0.77
2:B:313:LEU:HA	2:B:344:VAL:HG11	1.66	0.77
1:C:419:SER:HA	1:C:422:ARG:CD	2.11	0.77
2:D:230:LEU:H	2:D:230:LEU:HD12	1.48	0.77
1:C:322:ASP:HA	1:C:357:TYR:HD1	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:LYS:HZ1	2:D:82:PRO:HG3	1.48	0.77
1:C:180:ALA:C	1:C:182:VAL:H	1.84	0.76
1:A:402:ARG:CG	1:A:403:ALA:H	1.98	0.76
2:B:175:PRO:CD	2:B:207:GLU:HB2	2.12	0.76
2:B:266:HIS:ND1	2:B:432:TYR:CZ	2.53	0.76
2:B:311:ARG:HG3	2:B:344:VAL:HA	1.65	0.76
1:C:33:ASP:HA	1:C:36:MET:HB3	1.66	0.76
1:C:151:SER:HB3	1:C:192:HIS:CE1	2.20	0.76
2:B:264:ARG:NH2	2:B:428:LEU:HD12	1.99	0.76
2:D:264:ARG:HH21	2:D:428:LEU:CD1	1.98	0.76
1:A:164:LYS:HZ2	1:A:164:LYS:N	1.83	0.76
1:A:414:GLU:HG2	1:A:415:GLU:H	1.50	0.76
2:B:149:MET:HA	2:B:149:MET:HE3	1.68	0.76
2:B:184:PRO:HB2	2:B:399:PHE:CE1	2.20	0.76
2:B:262:PHE:O	2:B:265:LEU:HA	1.85	0.76
2:D:115:VAL:HG11	2:D:156:LYS:NZ	2.00	0.76
3:E:42:UNK:O	3:E:44:UNK:N	2.18	0.76
1:A:371:VAL:HG12	1:A:373:ARG:H	1.50	0.76
1:C:388:TRP:CZ3	1:C:428:LEU:HD22	2.21	0.76
2:D:19:LYS:HA	2:D:22:GLU:CD	2.06	0.76
2:D:180:THR:HB	2:D:404:PHE:CE1	2.19	0.76
2:B:407:TRP:CZ2	1:C:256:GLN:HB2	2.19	0.76
2:D:303:ALA:HB1	2:D:387:LEU:CD1	2.14	0.76
1:A:227:LEU:O	1:A:231:ILE:HG12	1.86	0.76
1:A:243:ARG:HH12	1:A:250:VAL:CG1	1.99	0.76
2:B:91:ASN:H	2:B:91:ASN:ND2	1.82	0.76
1:C:88:HIS:HB3	1:C:91:GLN:HE22	1.48	0.76
1:C:311:LYS:HD2	1:C:436:GLY:HA2	1.66	0.76
2:D:175:PRO:CD	2:D:207:GLU:HB2	2.12	0.76
2:D:194:LEU:CD2	2:D:195:VAL:HG13	2.16	0.76
2:D:202:TYR:CE1	2:D:378:ILE:HD12	2.20	0.76
1:A:98:ASP:OD1	2:B:1:MET:HB3	1.85	0.76
2:B:401:ARG:HH11	1:C:440:VAL:HA	1.48	0.76
1:C:269:LEU:HD12	1:C:270:ALA:N	2.00	0.76
2:D:94:PHE:HB2	2:D:114:LEU:HD13	1.68	0.76
1:A:398:MET:HG3	1:A:399:TYR:CD1	2.21	0.76
1:A:409:VAL:HG13	1:A:414:GLU:CD	2.06	0.76
1:C:97:GLU:O	1:C:99:ALA:N	2.17	0.76
2:D:286:LEU:HA	2:D:290:GLU:OE2	1.84	0.76
2:D:335:VAL:HA	2:D:338:LYS:HB3	1.67	0.76
1:A:398:MET:HB3	2:B:346:TRP:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:385:GLN:HE21	2:B:433:GLN:HE21	1.31	0.76
2:B:390:ARG:O	2:B:392:SER:N	2.17	0.76
1:C:89:PRO:O	1:C:90:GLU:HB2	1.85	0.76
1:C:174:ALA:O	1:C:177:VAL:N	2.19	0.76
1:C:256:GLN:HB3	1:C:260:VAL:HB	1.68	0.76
2:D:182:VAL:O	2:D:182:VAL:HG12	1.85	0.76
2:D:390:ARG:C	2:D:392:SER:H	1.88	0.76
1:A:115:ILE:HG13	1:A:152:LEU:CD2	2.16	0.75
2:D:91:ASN:H	2:D:91:ASN:ND2	1.84	0.75
2:D:344:VAL:HB	2:D:346:TRP:CE2	2.21	0.75
2:B:179:ASP:CB	2:B:182:VAL:H	1.99	0.75
2:B:244:PHE:HB2	2:B:245:PRO:HD2	1.65	0.75
2:B:273:ALA:HB2	2:B:295:MET:HB2	1.67	0.75
2:D:70:LEU:HG	2:D:99:ALA:CB	2.15	0.75
2:D:87:PHE:O	2:D:87:PHE:HD1	1.67	0.75
1:A:151:SER:HB3	1:A:192:HIS:CE1	2.22	0.75
2:B:115:VAL:HG11	2:B:156:LYS:NZ	2.01	0.75
2:B:205:ASP:HB2	2:B:387:LEU:HD11	1.69	0.75
2:B:407:TRP:CE3	2:B:407:TRP:HA	2.20	0.75
2:D:158:ARG:CG	2:D:159:GLU:H	1.98	0.75
3:E:63:UNK:C	3:E:65:UNK:H	1.94	0.75
2:B:100:GLY:HA3	1:C:254:GLU:OE1	1.86	0.75
1:C:340:THR:OG1	1:C:341:ILE:HD12	1.86	0.75
1:C:398:MET:HB3	2:D:346:TRP:O	1.87	0.75
3:E:54:UNK:C	3:E:56:UNK:N	2.48	0.75
1:A:234:ILE:HD13	1:A:302:MET:SD	2.25	0.75
2:D:21:TRP:CZ2	2:D:65:ALA:HB2	2.22	0.75
1:A:208:ALA:O	1:A:211:ASP:HB2	1.87	0.75
2:B:218:LYS:HZ1	2:B:278:ARG:HB2	1.50	0.75
2:D:174:SER:OG	2:D:176:LYS:HG3	1.87	0.75
2:D:196:GLU:HA	2:D:196:GLU:OE2	1.86	0.75
1:A:145:THR:O	1:A:149:PHE:HB3	1.87	0.75
1:A:348:PRO:O	1:A:350:GLY:N	2.19	0.75
1:A:141:PHE:CE2	1:A:172:TYR:HA	2.15	0.75
2:B:292:THR:HG21	2:B:331:GLN:HB3	1.69	0.75
1:A:322:ASP:CA	1:A:357:TYR:HA	2.17	0.74
2:B:8:GLN:HG2	2:B:14:ASN:ND2	2.02	0.74
2:B:92:PHE:HE1	2:B:118:VAL:CA	1.89	0.74
2:B:179:ASP:CA	1:C:352:LYS:HE2	2.11	0.74
1:C:276:ILE:HG12	1:C:282:TYR:CD2	2.22	0.74
1:A:39:ASP:CG	1:A:40:LYS:H	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:PRO:HG3	1:A:399:TYR:CZ	2.22	0.74
1:A:335:ILE:HG13	1:A:336:LYS:N	2.01	0.74
2:B:143:GLY:O	2:B:145:THR:N	2.18	0.74
2:B:220:THR:HB	1:C:326:LYS:CD	2.17	0.74
1:C:107:HIS:ND1	1:C:151:SER:HB2	2.01	0.74
2:B:274:PRO:HB2	2:B:371:LEU:CD1	2.16	0.74
2:B:387:LEU:O	2:B:387:LEU:HD23	1.86	0.74
2:D:241:CYS:O	2:D:243:ARG:HG2	1.87	0.74
2:D:385:GLN:HE21	2:D:433:GLN:HE21	1.35	0.74
2:B:286:LEU:HG	2:B:373:MET:HE3	1.69	0.74
1:C:172:TYR:HB3	1:C:205:ASP:CA	2.18	0.74
1:C:177:VAL:HB	2:D:349:ASN:ND2	2.02	0.74
1:C:289:ALA:HA	1:C:292:THR:CG2	2.17	0.74
1:C:350:GLY:C	1:C:351:PHE:HD1	1.90	0.74
2:D:192:HIS:C	2:D:194:LEU:H	1.89	0.74
1:A:269:LEU:HD12	1:A:270:ALA:N	2.03	0.74
1:A:282:TYR:CD2	1:A:282:TYR:N	2.51	0.74
2:B:385:GLN:HE21	2:B:433:GLN:NE2	1.85	0.74
1:A:214:ARG:HA	1:A:218:ASP:O	1.86	0.74
2:B:179:ASP:C	2:B:181:VAL:H	1.88	0.74
1:C:166:LYS:HZ2	1:C:197:HIS:HB2	1.51	0.74
1:A:77:GLU:HB3	1:A:83:TYR:CD2	2.23	0.74
1:C:10:GLY:O	1:C:13:GLY:N	2.19	0.74
1:C:196:GLU:O	1:C:197:HIS:HB3	1.84	0.74
1:C:209:ILE:HG23	1:C:213:CYS:HB2	1.70	0.74
2:B:163:ASP:OD2	2:B:164:ARG:HD3	1.87	0.74
2:B:176:LYS:HD2	2:B:210:TYR:CE2	2.22	0.74
2:B:322:ARG:HE	2:B:357:ASP:HB3	1.53	0.74
2:B:407:TRP:HZ2	1:C:256:GLN:CB	2.01	0.74
2:D:70:LEU:HD11	2:D:110:GLU:O	1.88	0.74
1:A:291:ILE:HG21	1:A:375:VAL:CG2	2.18	0.74
1:C:101:ASN:OD1	2:D:254:LYS:HD3	1.86	0.74
2:D:179:ASP:C	2:D:181:VAL:H	1.90	0.74
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.70	0.74
1:C:183:GLU:N	1:C:184:PRO:HD2	2.03	0.74
2:D:80:SER:C	2:D:82:PRO:HD2	2.07	0.74
2:B:94:PHE:HB2	2:B:114:LEU:HD13	1.69	0.73
1:A:209:ILE:C	1:A:211:ASP:H	1.90	0.73
2:D:371:LEU:HB3	2:D:373:MET:O	1.86	0.73
2:B:145:THR:HB	5:B:501:GDP:O2B	1.88	0.73
2:B:385:GLN:NE2	2:B:433:GLN:HG2	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:179:ASP:HB2	2:D:182:VAL:H	1.53	0.73
2:B:13:GLY:O	2:B:16:ILE:HG23	1.88	0.73
2:B:123:ARG:NH2	2:B:160:GLU:HG3	2.03	0.73
2:B:166:MET:HE3	2:B:197:ASN:HB3	1.69	0.73
1:C:115:ILE:HG13	1:C:152:LEU:CD2	2.18	0.73
2:D:1:MET:O	2:D:3:GLU:N	2.19	0.73
1:A:190:THR:O	1:A:192:HIS:N	2.22	0.73
1:A:175:PRO:C	1:A:177:VAL:N	2.39	0.73
1:A:238:ILE:HG22	1:A:239:THR:N	2.03	0.73
1:A:385:ALA:HB2	1:A:432:TYR:HD2	1.53	0.73
2:B:77:SER:HA	2:B:80:SER:CB	2.18	0.73
2:B:339:ASN:HB3	2:B:342:TYR:CD1	2.23	0.73
1:C:262:TYR:HB3	1:C:263:PRO:HD2	1.70	0.73
2:D:142:GLY:CA	2:D:185:TYR:HB3	2.18	0.73
2:D:343:PHE:O	2:D:345:GLU:N	2.21	0.73
2:D:394:GLN:O	2:D:398:MET:HB3	1.87	0.73
2:B:168:THR:OG1	2:B:201:THR:HB	1.88	0.73
1:C:132:LEU:HB3	1:C:164:LYS:HD3	1.71	0.73
2:D:407:TRP:HA	2:D:407:TRP:CE3	2.22	0.73
2:B:390:ARG:C	2:B:392:SER:H	1.92	0.73
2:D:191:VAL:O	2:D:191:VAL:HG12	1.87	0.73
1:A:27:GLU:HG3	1:A:28:HIS:ND1	2.04	0.73
1:A:298:PRO:O	1:A:301:GLN:HG3	1.89	0.73
1:A:414:GLU:HB2	1:A:417:GLU:HB2	1.71	0.73
2:B:206:ASN:HD22	2:B:227:LEU:CD2	2.01	0.73
2:B:288:VAL:HG11	2:B:327:GLU:OE1	1.88	0.73
2:D:77:SER:HA	2:D:80:SER:CB	2.19	0.73
2:D:179:ASP:HB2	2:D:182:VAL:HG23	1.71	0.73
1:A:267:PHE:N	1:A:267:PHE:CD1	2.57	0.73
1:A:322:ASP:HA	1:A:357:TYR:HD1	1.54	0.73
2:B:402:LYS:HG3	1:C:440:VAL:HG12	1.70	0.73
2:D:77:SER:CA	2:D:80:SER:HB3	2.19	0.73
2:D:385:GLN:NE2	2:D:433:GLN:HG2	2.04	0.73
1:A:115:ILE:HG13	1:A:152:LEU:HD21	1.70	0.72
1:A:194:THR:O	1:A:197:HIS:O	2.06	0.72
2:B:407:TRP:HA	2:B:407:TRP:HE3	1.54	0.72
1:C:194:THR:O	1:C:197:HIS:O	2.07	0.72
1:C:322:ASP:HA	1:C:357:TYR:HA	1.71	0.72
2:D:18:ALA:C	2:D:20:PHE:H	1.92	0.72
2:D:115:VAL:HG11	2:D:156:LYS:HZ2	1.52	0.72
2:B:190:SER:CB	2:B:425:MET:HG3	2.16	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:ASP:H	1:C:357:TYR:C	1.92	0.72
2:D:263:PRO:C	2:D:265:LEU:N	2.42	0.72
2:D:286:LEU:HG	2:D:286:LEU:O	1.89	0.72
3:E:25:UNK:C	3:E:27:UNK:N	2.49	0.72
2:B:266:HIS:HA	2:B:432:TYR:OH	1.89	0.72
1:C:70:LEU:HD12	1:C:145:THR:CA	2.12	0.72
1:C:100:ALA:HB1	1:C:105:ARG:HD2	1.70	0.72
1:A:215:ARG:HH22	1:A:300:ASN:ND2	1.87	0.72
2:B:16:ILE:HB	2:B:228:ASN:HD21	1.53	0.72
1:C:267:PHE:N	1:C:267:PHE:CD1	2.55	0.72
1:A:202:PHE:HE1	1:A:378:LEU:HD22	1.55	0.72
2:B:2:ARG:HH11	2:B:251:ASP:HA	1.54	0.72
2:B:4:ILE:O	2:B:64:ARG:HD2	1.89	0.72
2:B:158:ARG:CG	2:B:159:GLU:H	1.99	0.72
2:D:18:ALA:O	2:D:20:PHE:N	2.21	0.72
1:A:345:ASP:O	1:A:347:CYS:N	2.23	0.72
2:B:77:SER:CA	2:B:80:SER:HB3	2.20	0.72
2:B:133:GLN:NE2	2:B:252:LEU:H	1.87	0.72
2:B:274:PRO:HB2	2:B:371:LEU:HD12	1.70	0.72
2:D:176:LYS:HD2	2:D:210:TYR:CE2	2.25	0.72
2:D:308:ARG:NH2	2:D:342:TYR:CD1	2.56	0.72
2:B:353:THR:HG22	2:B:354:ALA:N	2.04	0.72
1:C:263:PRO:O	1:C:265:ALA:N	2.22	0.72
2:D:132:LEU:HD22	2:D:164:ARG:HG3	1.72	0.72
2:D:331:GLN:O	2:D:334:ASN:HB3	1.89	0.72
2:B:158:ARG:O	2:B:160:GLU:N	2.22	0.72
1:C:44:GLY:C	1:C:46:ASP:H	1.92	0.72
1:C:285:GLN:OE1	1:C:372:GLN:HG2	1.90	0.72
2:D:158:ARG:CA	2:D:197:ASN:HD22	2.02	0.72
1:A:97:GLU:O	1:A:99:ALA:N	2.22	0.72
1:A:289:ALA:HA	1:A:292:THR:CG2	2.20	0.72
2:B:394:GLN:O	2:B:398:MET:HB3	1.89	0.72
2:D:194:LEU:HD11	2:D:428:LEU:HD11	1.72	0.72
2:D:273:ALA:HB2	2:D:295:MET:HB2	1.70	0.72
2:D:353:THR:CG2	2:D:354:ALA:N	2.52	0.72
2:B:138:THR:O	2:B:139:HIS:HB3	1.90	0.72
2:B:194:LEU:CD2	2:B:195:VAL:HG13	2.19	0.72
2:B:286:LEU:HA	2:B:290:GLU:OE2	1.89	0.72
1:C:39:ASP:CG	1:C:40:LYS:H	1.91	0.72
2:B:92:PHE:CE1	2:B:118:VAL:CA	2.70	0.71
2:D:16:ILE:HB	2:D:228:ASN:HD21	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:THR:O	1:C:197:HIS:N	2.22	0.71
1:C:348:PRO:O	1:C:350:GLY:N	2.23	0.71
2:D:396:THR:HG23	2:D:400:ARG:CD	2.19	0.71
1:A:256:GLN:HB3	1:A:260:VAL:HB	1.71	0.71
2:B:422:GLU:O	2:B:426:ASN:HB2	1.90	0.71
1:A:291:ILE:HG21	1:A:375:VAL:HG21	1.73	0.71
2:B:263:PRO:C	2:B:265:LEU:N	2.39	0.71
1:C:139:HIS:HB3	1:C:170:SER:HA	1.72	0.71
1:C:402:ARG:CG	1:C:403:ALA:H	2.03	0.71
3:E:58:UNK:O	3:E:61:UNK:N	2.24	0.71
1:A:109:THR:HG21	1:A:411:GLU:OE2	1.90	0.71
1:A:362:VAL:HG13	1:A:367:ASP:CB	2.19	0.71
1:A:194:THR:O	1:A:197:HIS:N	2.22	0.71
1:A:414:GLU:HG2	1:A:415:GLU:N	2.04	0.71
2:B:196:GLU:HA	2:B:196:GLU:OE2	1.91	0.71
2:B:398:MET:C	2:B:400:ARG:H	1.94	0.71
1:C:109:THR:HG21	1:C:411:GLU:OE2	1.90	0.71
2:D:322:ARG:NE	2:D:357:ASP:HB3	2.05	0.71
1:C:70:LEU:CD1	1:C:145:THR:HA	2.13	0.71
1:C:427:ALA:O	1:C:430:LYS:HB3	1.90	0.71
2:D:158:ARG:CB	2:D:197:ASN:HD22	2.02	0.71
2:D:158:ARG:HA	2:D:197:ASN:HD22	1.54	0.71
1:A:31:GLN:O	1:A:33:ASP:N	2.23	0.71
1:A:243:ARG:CZ	1:A:243:ARG:HA	2.21	0.71
2:B:142:GLY:CA	2:B:185:TYR:HB3	2.20	0.71
2:B:343:PHE:O	2:B:345:GLU:N	2.24	0.71
2:D:22:GLU:OE1	2:D:82:PRO:HB2	1.91	0.71
2:D:266:HIS:HA	2:D:432:TYR:OH	1.91	0.71
1:A:78:VAL:HG11	1:A:87:PHE:HE2	1.54	0.71
2:D:4:ILE:O	2:D:58:GLY:HA2	1.91	0.71
2:D:427:ASP:O	2:D:429:VAL:N	2.24	0.71
1:A:215:ARG:HH22	1:A:300:ASN:HD21	1.39	0.70
1:A:414:GLU:CB	1:A:417:GLU:HB2	2.21	0.70
2:B:430:SER:O	2:B:434:GLN:HG3	1.90	0.70
1:C:175:PRO:O	1:C:177:VAL:HG23	1.91	0.70
2:D:163:ASP:OD2	2:D:164:ARG:HD3	1.91	0.70
1:A:26:LEU:HG	1:A:361:THR:CB	2.21	0.70
1:A:322:ASP:HA	1:A:357:TYR:HA	1.73	0.70
2:B:87:PHE:O	2:B:90:ASP:OD1	2.08	0.70
1:C:264:ARG:O	1:C:266:HIS:N	2.24	0.70
1:C:284:GLU:HG2	1:C:285:GLN:NE2	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:HIS:CD2	1:A:17:GLY:HA3	2.27	0.70
1:C:153:LEU:O	1:C:156:ARG:HB2	1.90	0.70
1:C:171:ILE:HD12	1:C:171:ILE:N	2.06	0.70
1:C:418:PHE:O	1:C:420:GLU:N	2.23	0.70
1:A:332:ILE:CD1	1:A:353:VAL:HG21	2.21	0.70
2:B:191:VAL:O	2:B:191:VAL:HG12	1.90	0.70
2:B:206:ASN:ND2	2:B:227:LEU:HD21	2.01	0.70
2:B:405:LEU:HD13	2:B:406:HIS:N	2.06	0.70
1:C:398:MET:HG3	1:C:399:TYR:CD1	2.25	0.70
2:D:255:LEU:CD2	2:D:259:MET:HG3	2.21	0.70
1:A:340:THR:OG1	1:A:341:ILE:HD12	1.90	0.70
1:A:399:TYR:HH	1:A:408:TYR:HE2	1.37	0.70
1:C:98:ASP:OD1	2:D:1:MET:HB3	1.91	0.70
3:E:19:UNK:O	3:E:21:UNK:N	2.24	0.70
1:A:16:ILE:HD12	1:A:171:ILE:HD11	1.73	0.70
2:B:22:GLU:OE1	2:B:82:PRO:HB2	1.90	0.70
2:B:230:LEU:H	2:B:230:LEU:HD12	1.55	0.70
1:C:7:ILE:HD12	1:C:153:LEU:HD21	1.74	0.70
1:A:209:ILE:HG23	1:A:213:CYS:HB2	1.73	0.70
1:A:350:GLY:O	1:A:351:PHE:HD1	1.74	0.70
1:C:5:ILE:HD12	1:C:125:LEU:HD22	1.74	0.70
1:C:102:ASN:CB	1:C:105:ARG:HB2	2.16	0.70
1:C:115:ILE:HG13	1:C:152:LEU:HD21	1.73	0.70
1:C:362:VAL:HG21	1:C:369:ALA:O	1.92	0.70
2:D:51:VAL:HG23	2:D:53:TYR:N	2.07	0.70
1:A:418:PHE:O	1:A:420:GLU:N	2.25	0.70
2:B:391:ILE:HD12	2:B:391:ILE:N	2.07	0.70
2:D:71:GLU:HB2	2:D:72:PRO:HD2	1.74	0.70
2:D:133:GLN:HE21	2:D:252:LEU:HB3	1.54	0.70
1:A:7:ILE:HG21	1:A:122:ILE:HD11	1.73	0.70
1:A:134:GLY:H	1:A:164:LYS:CG	2.04	0.70
2:B:55:GLU:HB2	2:B:244:PHE:HA	1.73	0.70
2:B:158:ARG:HA	2:B:197:ASN:HD22	1.54	0.70
2:B:241:CYS:O	2:B:243:ARG:HG2	1.92	0.70
3:E:19:UNK:C	3:E:21:UNK:N	2.54	0.70
1:A:177:VAL:HB	2:B:349:ASN:ND2	2.06	0.70
1:C:78:VAL:C	1:C:82:THR:HA	2.13	0.70
1:C:195:LEU:HB3	1:C:196:GLU:OE2	1.90	0.70
2:D:385:GLN:HE21	2:D:433:GLN:NE2	1.90	0.70
1:A:322:ASP:H	1:A:357:TYR:C	1.94	0.69
1:C:7:ILE:HG21	1:C:122:ILE:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:GLU:HB3	1:C:83:TYR:CD2	2.26	0.69
1:C:184:PRO:HG3	1:C:399:TYR:CZ	2.28	0.69
1:C:190:THR:O	1:C:192:HIS:N	2.25	0.69
1:C:220:GLU:OE2	2:D:326:LYS:HD3	1.92	0.69
2:D:264:ARG:NH2	2:D:428:LEU:HD12	2.03	0.69
2:D:391:ILE:HD12	2:D:391:ILE:N	2.07	0.69
1:A:89:PRO:O	1:A:90:GLU:HB2	1.90	0.69
1:A:280:LYS:O	1:A:282:TYR:CE2	2.45	0.69
1:A:284:GLU:HG2	1:A:285:GLN:NE2	2.07	0.69
1:C:291:ILE:HG21	1:C:375:VAL:CG2	2.22	0.69
1:A:11:GLN:HB3	4:A:500:GTP:O2A	1.91	0.69
1:A:205:ASP:OD2	1:A:207:GLU:HB3	1.92	0.69
2:B:133:GLN:HE21	2:B:252:LEU:CB	2.05	0.69
2:D:59:ASN:HB2	2:D:64:ARG:CZ	2.22	0.69
2:D:183:GLU:O	2:D:185:TYR:N	2.24	0.69
2:D:218:LYS:NZ	2:D:278:ARG:HB2	2.07	0.69
1:A:78:VAL:O	1:A:82:THR:HG23	1.92	0.69
1:C:414:GLU:HG2	1:C:415:GLU:H	1.58	0.69
2:D:218:LYS:NZ	2:D:278:ARG:N	2.39	0.69
2:D:262:PHE:O	2:D:265:LEU:HA	1.93	0.69
2:D:138:THR:O	2:D:139:HIS:HB3	1.91	0.69
2:B:345:GLU:O	2:B:345:GLU:HG2	1.92	0.69
1:C:31:GLN:CB	1:C:32:PRO:HD2	2.23	0.69
2:D:396:THR:CG2	2:D:400:ARG:HD3	2.23	0.69
2:D:416:MET:C	2:D:418:PHE:H	1.95	0.69
1:A:78:VAL:HG11	1:A:92:LEU:HD21	1.73	0.69
1:A:86:LEU:CD2	1:A:89:PRO:HD3	2.23	0.69
1:A:154:MET:SD	1:A:197:HIS:CD2	2.86	0.69
1:A:276:ILE:HD12	1:A:277:SER:N	2.07	0.69
2:B:218:LYS:NZ	2:B:278:ARG:H	1.83	0.69
2:B:255:LEU:CD2	2:B:259:MET:HG3	2.22	0.69
1:C:30:ILE:HG13	1:C:31:GLN:N	2.07	0.69
1:C:78:VAL:O	1:C:82:THR:HG23	1.91	0.69
1:C:100:ALA:HB1	1:C:105:ARG:O	1.92	0.69
1:C:202:PHE:HE1	1:C:378:LEU:HD22	1.57	0.69
1:C:205:ASP:OD2	1:C:207:GLU:HB3	1.93	0.69
1:C:287:SER:N	1:C:290:GLU:HB2	2.07	0.69
2:D:59:ASN:CG	2:D:60:LYS:H	1.95	0.69
2:D:259:MET:HE1	2:D:316:ALA:N	2.08	0.69
2:B:183:GLU:C	2:B:185:TYR:H	1.95	0.69
2:B:274:PRO:HA	2:B:294:GLN:NE2	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:LEU:HD12	1:C:269:LEU:C	2.13	0.69
2:D:422:GLU:O	2:D:426:ASN:HB2	1.93	0.69
1:A:191:THR:CB	1:A:421:ALA:HB1	2.23	0.69
2:B:179:ASP:C	2:B:181:VAL:N	2.45	0.69
2:B:320:ARG:HG2	2:B:320:ARG:HH11	1.58	0.69
1:C:171:ILE:HD12	1:C:171:ILE:H	1.56	0.69
2:D:123:ARG:NH2	2:D:160:GLU:HG3	2.08	0.69
3:E:17:UNK:C	3:E:19:UNK:N	2.48	0.69
1:A:413:MET:O	1:A:414:GLU:HB3	1.92	0.68
2:B:333:LEU:HG	2:B:337:ASN:ND2	2.08	0.68
1:C:286:LEU:HA	1:C:290:GLU:OE1	1.93	0.68
2:D:105:LYS:HA	2:D:109:THR:OG1	1.93	0.68
3:E:71:UNK:O	3:E:73:UNK:N	2.27	0.68
2:B:132:LEU:HD22	2:B:164:ARG:HG3	1.75	0.68
1:C:258:ASN:N	1:C:258:ASN:ND2	2.39	0.68
2:D:92:PHE:CE1	2:D:118:VAL:CA	2.71	0.68
2:D:247:GLN:HB2	2:D:355:VAL:O	1.92	0.68
1:A:259:LEU:HD21	1:A:378:LEU:HB3	1.74	0.68
2:B:296:PHE:HA	2:B:377:PHE:HE2	1.59	0.68
2:B:344:VAL:HB	2:B:346:TRP:CE2	2.28	0.68
2:B:416:MET:C	2:B:418:PHE:H	1.96	0.68
1:A:10:GLY:O	1:A:13:GLY:N	2.26	0.68
2:B:111:GLY:C	2:B:113:GLU:H	1.94	0.68
1:C:209:ILE:C	1:C:211:ASP:H	1.95	0.68
1:C:414:GLU:CB	1:C:417:GLU:HB2	2.24	0.68
2:D:313:LEU:HA	2:D:344:VAL:CG1	2.23	0.68
2:D:407:TRP:HA	2:D:407:TRP:HE3	1.56	0.68
1:A:75:ILE:O	1:A:75:ILE:HG12	1.92	0.68
1:A:330:ALA:O	1:A:334:THR:HG23	1.93	0.68
2:B:175:PRO:O	2:B:177:VAL:HG23	1.93	0.68
2:D:430:SER:O	2:D:434:GLN:HG3	1.93	0.68
1:A:103:TYR:N	1:A:185:TYR:HE1	1.92	0.68
1:A:172:TYR:HB3	1:A:205:ASP:CA	2.24	0.68
1:A:311:LYS:HD3	1:A:344:VAL:HG22	1.75	0.68
2:B:21:TRP:CZ2	2:B:65:ALA:HB2	2.29	0.68
2:B:391:ILE:HD12	2:B:391:ILE:H	1.57	0.68
2:D:175:PRO:O	2:D:177:VAL:HG23	1.93	0.68
1:A:305:CYS:SG	1:A:306:ASP:N	2.65	0.68
2:B:109:THR:HG21	2:B:411:GLU:CG	2.24	0.68
2:B:102:ASN:HB3	2:B:105:LYS:HD2	1.74	0.68
1:C:433:GLU:HA	1:C:433:GLU:OE1	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:71:GLU:HB2	2:D:72:PRO:CD	2.24	0.68
2:D:126:SER:OG	2:D:127:GLU:N	2.26	0.68
1:A:134:GLY:H	1:A:164:LYS:HG2	1.58	0.68
1:A:153:LEU:O	1:A:156:ARG:HB2	1.93	0.68
1:A:171:ILE:HD12	1:A:171:ILE:N	2.08	0.68
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.75	0.68
1:A:258:ASN:O	1:A:259:LEU:HB2	1.93	0.68
2:B:51:VAL:HG23	2:B:53:TYR:N	2.08	0.68
1:C:145:THR:O	1:C:149:PHE:HB3	1.93	0.68
1:C:215:ARG:HH22	1:C:300:ASN:ND2	1.91	0.68
2:D:55:GLU:HB2	2:D:244:PHE:HA	1.75	0.68
1:A:321:GLY:HA2	1:A:357:TYR:O	1.94	0.68
2:B:163:ASP:CG	2:B:164:ARG:N	2.47	0.68
1:C:147:SER:O	1:C:189:LEU:HD23	1.93	0.68
2:D:179:ASP:C	2:D:181:VAL:N	2.47	0.68
1:A:104:ALA:HA	1:A:108:TYR:CD2	2.28	0.67
2:B:5:VAL:HB	2:B:135:PHE:CD2	2.29	0.67
1:C:31:GLN:O	1:C:33:ASP:N	2.28	0.67
1:C:414:GLU:HB2	1:C:417:GLU:HB2	1.76	0.67
2:D:16:ILE:HD12	2:D:231:VAL:HG11	1.76	0.67
2:D:405:LEU:HD13	2:D:406:HIS:N	2.09	0.67
3:E:50:UNK:O	3:E:52:UNK:N	2.27	0.67
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.29	0.67
1:A:412:GLY:O	1:A:414:GLU:OE1	2.12	0.67
1:A:427:ALA:O	1:A:430:LYS:HB3	1.93	0.67
2:B:398:MET:N	2:B:401:ARG:HB2	2.09	0.67
2:D:104:ALA:O	2:D:108:TYR:HB2	1.94	0.67
2:B:102:ASN:HD21	2:B:104:ALA:HB3	1.58	0.67
2:B:174:SER:OG	2:B:176:LYS:HG3	1.94	0.67
2:B:221:THR:OG1	1:C:326:LYS:HB2	1.94	0.67
1:A:311:LYS:HD2	1:A:436:GLY:HA2	1.76	0.67
1:A:413:MET:H	1:A:413:MET:HE2	1.58	0.67
2:D:8:GLN:HG2	2:D:14:ASN:ND2	2.06	0.67
2:D:353:THR:CG2	2:D:354:ALA:H	2.08	0.67
2:B:237:GLY:O	2:B:376:THR:HG21	1.95	0.67
2:B:263:PRO:O	2:B:265:LEU:N	2.27	0.67
2:B:331:GLN:O	2:B:334:ASN:HB3	1.95	0.67
1:C:287:SER:OG	1:C:290:GLU:N	2.28	0.67
2:B:179:ASP:HB2	2:B:182:VAL:H	1.58	0.67
1:C:213:CYS:SG	1:C:217:LEU:HD23	2.34	0.67
2:D:217:LEU:HG	2:D:218:LYS:N	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:GLU:OE2	2:B:130:ASP:HB3	1.93	0.67
1:C:264:ARG:O	1:C:266:HIS:ND1	2.28	0.67
1:C:280:LYS:O	1:C:282:TYR:CE2	2.47	0.67
1:C:404:PHE:H	1:C:404:PHE:HD1	1.42	0.67
1:C:414:GLU:HG2	1:C:415:GLU:N	2.09	0.67
2:D:122:VAL:O	2:D:126:SER:N	2.26	0.67
2:D:174:SER:HB2	2:D:207:GLU:N	2.10	0.67
1:A:44:GLY:C	1:A:46:ASP:H	1.97	0.67
1:A:287:SER:OG	1:A:290:GLU:HG3	1.94	0.67
1:C:177:VAL:HB	2:D:349:ASN:CG	2.15	0.67
2:D:205:ASP:OD2	2:D:207:GLU:HB3	1.95	0.67
2:D:266:HIS:HB2	2:D:380:ASN:OD1	1.95	0.67
2:D:386:GLU:C	2:D:388:PHE:H	1.98	0.67
1:A:88:HIS:CB	1:A:91:GLN:HE22	2.08	0.67
1:A:237:SER:CA	1:A:241:SER:HB2	2.23	0.67
2:B:92:PHE:CD1	2:B:118:VAL:HG22	2.30	0.67
2:B:264:ARG:HH22	2:B:431:GLU:HG3	1.60	0.67
1:C:141:PHE:CE2	1:C:172:TYR:HA	2.19	0.67
1:C:291:ILE:CD1	1:C:373:ARG:HG3	2.24	0.67
1:C:180:ALA:C	1:C:182:VAL:N	2.48	0.67
1:A:413:MET:SD	1:A:413:MET:N	2.68	0.66
1:C:210:TYR:CE2	1:C:227:LEU:HD23	2.30	0.66
2:D:87:PHE:O	2:D:87:PHE:CD1	2.48	0.66
2:D:255:LEU:HD23	2:D:259:MET:CG	2.25	0.66
1:A:70:LEU:CD1	1:A:145:THR:HA	2.17	0.66
1:A:164:LYS:HZ3	1:A:164:LYS:HB2	1.59	0.66
1:A:189:LEU:HD13	1:A:193:THR:HG21	1.77	0.66
2:B:305:CYS:SG	2:B:387:LEU:HB2	2.35	0.66
2:D:4:ILE:O	2:D:64:ARG:HD2	1.95	0.66
2:D:62:VAL:O	2:D:62:VAL:HG23	1.94	0.66
1:A:355:ILE:HD12	1:A:355:ILE:N	2.10	0.66
2:B:70:LEU:HG	2:B:99:ALA:CB	2.24	0.66
1:A:365:GLY:O	1:A:368:LEU:CD1	2.43	0.66
2:B:87:PHE:O	2:B:87:PHE:CD1	2.48	0.66
1:C:189:LEU:HD13	1:C:193:THR:HG21	1.77	0.66
1:C:386:GLU:CG	1:C:387:ALA:H	2.07	0.66
2:D:350:ASN:HD22	2:D:351:VAL:HG23	1.60	0.66
1:A:306:ASP:C	1:A:308:ARG:H	1.98	0.66
2:B:19:LYS:HA	2:B:22:GLU:CD	2.16	0.66
1:C:273:ALA:HB2	1:C:295:CYS:HB2	1.76	0.66
1:C:306:ASP:C	1:C:308:ARG:H	1.99	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:5:VAL:HB	2:D:135:PHE:CD2	2.30	0.66
1:A:242:LEU:O	1:A:243:ARG:NH1	2.28	0.66
1:A:287:SER:OG	1:A:290:GLU:N	2.28	0.66
2:B:16:ILE:HD12	2:B:231:VAL:HG11	1.77	0.66
2:B:255:LEU:HD23	2:B:259:MET:HG3	1.78	0.66
2:B:386:GLU:C	2:B:388:PHE:H	1.99	0.66
2:B:402:LYS:HE3	1:C:440:VAL:CB	2.24	0.66
1:A:8:HIS:ND1	1:A:8:HIS:N	2.43	0.66
2:B:102:ASN:O	2:B:105:LYS:HB2	1.96	0.66
2:B:353:THR:CG2	2:B:354:ALA:N	2.58	0.66
1:C:242:LEU:HB3	1:C:250:VAL:HG11	1.78	0.66
2:D:320:ARG:HG2	2:D:320:ARG:HH11	1.59	0.66
3:E:48:UNK:O	3:E:49:UNK:C	2.44	0.66
1:A:78:VAL:C	1:A:82:THR:HA	2.15	0.66
1:A:371:VAL:HG12	1:A:372:GLN:N	2.11	0.66
2:B:111:GLY:C	2:B:113:GLU:N	2.47	0.66
2:B:118:VAL:C	2:B:120:ASP:H	1.97	0.66
1:C:371:VAL:HG12	1:C:373:ARG:N	2.11	0.66
2:D:149:MET:HA	2:D:149:MET:HE3	1.78	0.66
3:E:25:UNK:O	3:E:29:UNK:N	2.29	0.66
1:A:261:PRO:CG	1:A:380:ASN:HD21	2.09	0.66
1:A:286:LEU:HA	1:A:290:GLU:OE1	1.96	0.66
2:B:126:SER:OG	2:B:127:GLU:N	2.28	0.66
1:C:7:ILE:HG22	1:C:66:VAL:CB	2.18	0.66
1:C:172:TYR:HB3	1:C:205:ASP:N	2.11	0.66
1:A:195:LEU:HB3	1:A:196:GLU:OE2	1.95	0.66
1:A:262:TYR:HB3	1:A:263:PRO:HD2	1.77	0.66
1:A:422:ARG:O	1:A:426:ALA:HB2	1.96	0.66
1:C:206:ASN:ND2	1:C:210:TYR:HE2	1.93	0.66
1:A:276:ILE:HG12	1:A:282:TYR:CD2	2.32	0.65
2:D:118:VAL:C	2:D:120:ASP:H	1.99	0.65
2:D:203:CYS:SG	2:D:384:ILE:HD11	2.36	0.65
1:A:144:GLY:O	1:A:146:GLY:N	2.29	0.65
2:B:1:MET:O	2:B:3:GLU:N	2.26	0.65
1:C:217:LEU:HD11	1:C:368:LEU:HD22	1.79	0.65
1:C:217:LEU:O	1:C:219:ILE:HG13	1.97	0.65
1:C:407:TRP:C	1:C:409:VAL:H	1.97	0.65
2:D:133:GLN:NE2	2:D:252:LEU:H	1.93	0.65
2:D:296:PHE:HA	2:D:377:PHE:HE2	1.61	0.65
1:A:231:ILE:O	1:A:235:VAL:HG23	1.96	0.65
1:A:363:VAL:HG13	1:A:367:ASP:OD2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:ALA:C	2:B:20:PHE:H	2.00	0.65
2:B:58:GLY:O	2:B:64:ARG:NE	2.30	0.65
1:C:134:GLY:H	1:C:164:LYS:CG	2.09	0.65
1:C:151:SER:HB3	1:C:192:HIS:NE2	2.12	0.65
1:C:422:ARG:O	1:C:426:ALA:HB2	1.97	0.65
2:D:167:ASN:HA	2:D:200:GLU:O	1.96	0.65
2:D:335:VAL:HA	2:D:338:LYS:HB2	1.79	0.65
1:A:206:ASN:HB3	1:A:210:TYR:HE2	1.58	0.65
2:B:311:ARG:HB2	2:B:344:VAL:N	2.10	0.65
1:C:413:MET:O	1:C:414:GLU:HB3	1.96	0.65
2:D:5:VAL:HA	2:D:64:ARG:CD	2.26	0.65
2:D:92:PHE:CD1	2:D:118:VAL:HG22	2.31	0.65
2:D:278:ARG:H	2:D:278:ARG:HD2	1.59	0.65
2:D:303:ALA:HB1	2:D:387:LEU:HD13	1.78	0.65
1:A:388:TRP:CZ3	1:A:428:LEU:HD22	2.31	0.65
2:B:218:LYS:NZ	2:B:278:ARG:HB2	2.11	0.65
2:B:255:LEU:HD23	2:B:259:MET:CG	2.27	0.65
1:A:174:ALA:O	1:A:176:GLN:N	2.29	0.65
1:A:186:ASN:ND2	1:A:391:LEU:HD21	2.10	0.65
1:A:286:LEU:O	1:A:373:ARG:HD2	1.97	0.65
2:B:247:GLN:HB2	2:B:355:VAL:O	1.97	0.65
2:B:264:ARG:HH11	2:B:264:ARG:HG3	1.60	0.65
1:C:330:ALA:O	1:C:334:THR:HG23	1.96	0.65
2:D:59:ASN:CG	2:D:60:LYS:N	2.50	0.65
2:D:227:LEU:O	2:D:227:LEU:HD23	1.96	0.65
1:A:247:ALA:O	1:A:249:ASN:ND2	2.30	0.65
1:A:287:SER:C	1:A:289:ALA:H	1.98	0.65
2:B:392:SER:HB2	2:B:426:ASN:ND2	2.11	0.65
1:C:12:ALA:HB3	1:C:140:SER:CB	2.27	0.65
1:C:143:GLY:O	1:C:144:GLY:O	2.13	0.65
1:C:209:ILE:N	1:C:209:ILE:HD12	2.11	0.65
2:D:274:PRO:HA	2:D:294:GLN:NE2	2.11	0.65
1:A:177:VAL:HB	2:B:349:ASN:CG	2.17	0.65
1:A:264:ARG:O	1:A:266:HIS:N	2.30	0.65
2:B:169:PHE:CD2	2:B:235:MET:SD	2.90	0.65
1:C:186:ASN:HD22	1:C:391:LEU:HD11	1.60	0.65
1:C:412:GLY:O	1:C:414:GLU:OE1	2.15	0.65
2:D:158:ARG:HB2	2:D:197:ASN:HD22	1.61	0.65
3:E:73:UNK:C	3:E:75:UNK:H	2.10	0.65
1:A:183:GLU:N	1:A:184:PRO:HD2	2.12	0.65
1:A:258:ASN:N	1:A:258:ASN:ND2	2.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:HIS:C	2:B:139:HIS:CD2	2.69	0.65
2:B:287:THR:OG1	2:B:290:GLU:HB2	1.97	0.65
2:D:163:ASP:CG	2:D:164:ARG:N	2.50	0.65
2:D:209:LEU:HB3	2:D:227:LEU:HG	1.79	0.65
2:D:398:MET:N	2:D:401:ARG:HB2	2.12	0.65
1:A:133:GLN:HA	1:A:164:LYS:HG3	1.79	0.65
2:B:122:VAL:O	2:B:126:SER:N	2.27	0.65
2:B:339:ASN:C	2:B:341:SER:H	2.00	0.65
1:C:144:GLY:O	1:C:146:GLY:N	2.30	0.65
2:D:172:VAL:HG13	2:D:173:PRO:HD2	1.78	0.65
2:D:183:GLU:C	2:D:185:TYR:N	2.47	0.65
1:A:311:LYS:HD3	1:A:344:VAL:CG1	2.23	0.64
1:A:407:TRP:C	1:A:409:VAL:H	2.00	0.64
2:B:205:ASP:OD2	2:B:207:GLU:HB3	1.96	0.64
1:C:8:HIS:ND1	1:C:8:HIS:N	2.44	0.64
1:C:133:GLN:HA	1:C:164:LYS:HG3	1.79	0.64
1:A:180:ALA:C	1:A:182:VAL:N	2.51	0.64
1:C:362:VAL:CG1	1:C:367:ASP:HB2	2.26	0.64
2:D:5:VAL:HA	2:D:64:ARG:HD2	1.79	0.64
2:D:137:LEU:HD23	2:D:154:ILE:HD11	1.80	0.64
1:A:277:SER:O	1:A:278:ALA:HB2	1.97	0.64
2:B:59:ASN:CG	2:B:60:LYS:H	1.99	0.64
2:B:96:GLN:NE2	1:C:130:THR:HG22	2.11	0.64
2:B:107:HIS:HD2	2:B:151:THR:HG23	1.62	0.64
2:B:158:ARG:CA	2:B:197:ASN:HD22	2.09	0.64
1:C:100:ALA:CB	1:C:105:ARG:HD2	2.27	0.64
1:C:360:PRO:HB3	1:C:374:ALA:HB2	1.79	0.64
1:A:78:VAL:HG11	1:A:87:PHE:CE2	2.32	0.64
1:A:183:GLU:HB2	1:A:184:PRO:CD	2.27	0.64
2:B:278:ARG:H	2:B:278:ARG:HD2	1.59	0.64
1:C:138:PHE:CZ	1:C:235:VAL:HG11	2.30	0.64
1:A:138:PHE:CZ	1:A:235:VAL:HG11	2.26	0.64
1:A:285:GLN:OE1	1:A:372:GLN:HG2	1.96	0.64
1:A:292:THR:HA	1:A:295:CYS:HB3	1.80	0.64
1:A:433:GLU:OE1	1:A:433:GLU:HA	1.97	0.64
2:B:51:VAL:C	2:B:53:TYR:H	2.00	0.64
2:B:71:GLU:HB2	2:B:72:PRO:CD	2.27	0.64
2:B:133:GLN:HE22	2:B:252:LEU:H	1.43	0.64
1:C:203:MET:SD	1:C:388:TRP:CD1	2.91	0.64
1:C:267:PHE:N	1:C:267:PHE:HD1	1.94	0.64
2:D:288:VAL:N	2:D:289:PRO:HD2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ILE:HG22	1:A:17:GLY:H	1.62	0.64
1:A:147:SER:O	1:A:189:LEU:HD23	1.97	0.64
1:A:191:THR:HB	1:A:421:ALA:HB1	1.79	0.64
2:B:2:ARG:HG3	2:B:133:GLN:HE21	1.58	0.64
2:B:192:HIS:O	2:B:194:LEU:N	2.30	0.64
1:C:191:THR:CB	1:C:421:ALA:HB1	2.27	0.64
2:D:255:LEU:HD23	2:D:259:MET:HG3	1.80	0.64
1:A:77:GLU:O	1:A:83:TYR:HB2	1.97	0.64
1:A:86:LEU:HD22	1:A:89:PRO:HD3	1.79	0.64
1:A:287:SER:N	1:A:290:GLU:HB2	2.13	0.64
1:A:350:GLY:O	1:A:351:PHE:CD1	2.50	0.64
2:B:183:GLU:HB3	2:B:184:PRO:CD	2.26	0.64
2:B:339:ASN:O	2:B:341:SER:N	2.30	0.64
2:D:386:GLU:O	2:D:388:PHE:N	2.31	0.64
1:A:87:PHE:HE2	1:A:92:LEU:HD21	1.60	0.64
1:A:111:GLY:O	1:A:113:GLU:N	2.31	0.64
1:A:276:ILE:O	1:A:369:ALA:HB3	1.98	0.64
1:C:160:ASP:O	1:C:161:TYR:CD1	2.50	0.64
2:D:92:PHE:HD1	2:D:118:VAL:HG22	1.61	0.64
2:D:184:PRO:HB2	2:D:399:PHE:CZ	2.32	0.64
2:D:311:ARG:HB2	2:D:344:VAL:N	2.12	0.64
2:D:377:PHE:O	2:D:378:ILE:HG12	1.98	0.64
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.32	0.64
1:C:331:ALA:HA	1:C:334:THR:OG1	1.98	0.64
2:D:59:ASN:ND2	2:D:60:LYS:N	2.45	0.64
2:D:111:GLY:C	2:D:113:GLU:H	1.99	0.64
2:D:129:CYS:O	2:D:130:ASP:O	2.15	0.64
2:D:391:ILE:H	2:D:391:ILE:CD1	2.10	0.64
2:B:80:SER:C	2:B:82:PRO:HD2	2.18	0.64
2:B:123:ARG:CZ	2:B:160:GLU:OE2	2.45	0.64
2:B:385:GLN:NE2	2:B:433:GLN:HE21	1.96	0.64
1:C:104:ALA:HA	1:C:108:TYR:CD2	2.31	0.64
2:D:385:GLN:HG2	2:D:433:GLN:HE21	1.62	0.64
1:A:186:ASN:HD22	1:A:391:LEU:HD11	1.63	0.63
2:B:59:ASN:HB2	2:B:64:ARG:CZ	2.28	0.63
2:B:371:LEU:HB3	2:B:373:MET:O	1.97	0.63
2:B:427:ASP:O	2:B:429:VAL:N	2.31	0.63
1:C:27:GLU:CG	1:C:28:HIS:H	2.10	0.63
2:D:140:SER:OG	2:D:171:VAL:HB	1.99	0.63
1:A:5:ILE:HD12	1:A:125:LEU:HD22	1.80	0.63
2:B:16:ILE:HG12	2:B:17:GLY:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:ARG:N	2:B:374:SER:O	2.29	0.63
1:C:287:SER:C	1:C:289:ALA:H	2.00	0.63
1:C:363:VAL:H	1:C:367:ASP:HB2	1.61	0.63
2:D:102:ASN:HD22	2:D:105:LYS:CG	2.11	0.63
2:D:345:GLU:HG2	2:D:345:GLU:O	1.96	0.63
1:A:158:SER:HB3	1:A:166:LYS:NZ	2.13	0.63
1:A:217:LEU:O	1:A:219:ILE:HG13	1.99	0.63
1:A:259:LEU:HD11	1:A:378:LEU:HD13	1.79	0.63
1:A:307:PRO:HB3	1:A:381:THR:HG21	1.80	0.63
2:B:104:ALA:O	2:B:108:TYR:HB2	1.98	0.63
2:B:140:SER:OG	2:B:171:VAL:HB	1.98	0.63
1:C:75:ILE:HG12	1:C:75:ILE:O	1.97	0.63
1:C:101:ASN:CG	2:D:254:LYS:HD3	2.17	0.63
1:C:215:ARG:HH22	1:C:300:ASN:HD21	1.45	0.63
2:D:287:THR:OG1	2:D:290:GLU:HB2	1.98	0.63
1:A:43:GLY:O	1:A:47:ASP:CG	2.37	0.63
1:A:87:PHE:CD2	1:A:87:PHE:N	2.63	0.63
1:A:217:LEU:HD11	1:A:368:LEU:HD22	1.81	0.63
1:A:241:SER:HA	1:A:320:ARG:NH2	2.13	0.63
1:A:263:PRO:O	1:A:265:ALA:N	2.28	0.63
2:B:137:LEU:HD23	2:B:154:ILE:HD11	1.80	0.63
2:B:174:SER:HB2	2:B:207:GLU:N	2.12	0.63
2:B:357:ASP:HB3	2:B:358:ILE:HD12	1.81	0.63
1:C:404:PHE:HD1	1:C:404:PHE:N	1.95	0.63
2:D:158:ARG:O	2:D:160:GLU:N	2.31	0.63
2:B:288:VAL:N	2:B:289:PRO:HD2	2.14	0.63
1:C:243:ARG:CZ	1:C:243:ARG:HA	2.28	0.63
1:C:355:ILE:N	1:C:355:ILE:HD12	2.13	0.63
1:C:404:PHE:N	1:C:404:PHE:CD1	2.67	0.63
1:A:215:ARG:NH2	1:A:216:ASN:OD1	2.32	0.63
1:A:256:GLN:HA	1:A:260:VAL:HG23	1.81	0.63
2:B:385:GLN:HG2	2:B:433:GLN:HE21	1.62	0.63
1:C:78:VAL:HG11	1:C:92:LEU:HD21	1.80	0.63
2:D:339:ASN:C	2:D:341:SER:H	2.01	0.63
2:D:5:VAL:HB	2:D:135:PHE:HD2	1.62	0.63
1:A:72:PRO:HB3	1:A:94:THR:OG1	1.98	0.63
2:B:390:ARG:C	2:B:392:SER:N	2.53	0.63
1:C:243:ARG:HH12	1:C:250:VAL:CG1	2.11	0.63
2:D:158:ARG:HD3	2:D:197:ASN:CG	2.18	0.63
1:A:291:ILE:HD12	1:A:373:ARG:HG3	1.80	0.63
1:A:311:LYS:CG	1:A:344:VAL:HG22	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:GLU:HB2	2:B:72:PRO:HD2	1.79	0.63
2:B:399:PHE:CE2	2:B:404:PHE:HB3	2.34	0.63
1:C:206:ASN:HB3	1:C:210:TYR:HE2	1.61	0.63
1:C:373:ARG:HB3	1:C:373:ARG:NH1	2.12	0.63
1:C:385:ALA:HB2	1:C:432:TYR:HD2	1.63	0.63
2:D:107:HIS:CD2	2:D:151:THR:HG23	2.33	0.63
1:A:172:TYR:HB3	1:A:205:ASP:N	2.14	0.62
1:C:93:ILE:HD13	1:C:118:VAL:CG2	2.26	0.62
2:D:215:ARG:NE	2:D:215:ARG:HA	2.13	0.62
2:D:286:LEU:HD13	2:D:371:LEU:O	1.99	0.62
2:D:391:ILE:O	2:D:425:MET:HE1	1.98	0.62
1:A:70:LEU:HD12	1:A:145:THR:CA	2.17	0.62
1:A:102:ASN:ND2	2:B:257:VAL:HG11	2.09	0.62
1:A:362:VAL:HG21	1:A:369:ALA:O	1.98	0.62
2:B:417:GLU:HG3	2:B:417:GLU:O	1.98	0.62
1:C:156:ARG:O	1:C:159:VAL:HB	2.00	0.62
2:D:107:HIS:HD2	2:D:151:THR:HG23	1.64	0.62
2:D:264:ARG:HG3	2:D:264:ARG:NH1	2.12	0.62
2:D:398:MET:O	2:D:400:ARG:N	2.32	0.62
1:A:160:ASP:O	1:A:161:TYR:CD1	2.52	0.62
1:A:171:ILE:HD12	1:A:171:ILE:H	1.62	0.62
2:B:292:THR:HG23	2:B:319:PHE:HZ	1.63	0.62
2:D:258:ASN:OD1	2:D:352:LYS:NZ	2.29	0.62
3:E:35:UNK:O	3:E:39:UNK:N	2.32	0.62
1:A:293:ASN:O	1:A:297:GLU:OE1	2.17	0.62
2:B:267:PHE:HB2	2:B:384:ILE:HD13	1.80	0.62
3:E:75:UNK:O	3:E:76:UNK:C	2.47	0.62
1:A:258:ASN:O	1:A:259:LEU:CB	2.48	0.62
1:A:280:LYS:O	1:A:282:TYR:HE2	1.82	0.62
2:B:62:VAL:HG23	2:B:62:VAL:O	1.99	0.62
2:B:165:ILE:HD13	2:B:199:ASP:OD1	1.99	0.62
2:B:192:HIS:C	2:B:194:LEU:N	2.49	0.62
2:B:241:CYS:C	2:B:243:ARG:N	2.48	0.62
2:B:292:THR:HG23	2:B:319:PHE:CZ	2.35	0.62
2:B:396:THR:CG2	2:B:400:ARG:HD3	2.28	0.62
1:C:154:MET:SD	1:C:197:HIS:CD2	2.93	0.62
1:C:307:PRO:HB3	1:C:381:THR:HG21	1.81	0.62
2:D:166:MET:HE3	2:D:197:ASN:HB3	1.82	0.62
2:D:267:PHE:HB2	2:D:384:ILE:HD13	1.81	0.62
2:D:385:GLN:HG2	2:D:433:GLN:NE2	2.13	0.62
1:A:156:ARG:O	1:A:159:VAL:HB	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:ARG:NE	2:B:160:GLU:OE2	2.32	0.62
2:B:132:LEU:O	2:B:132:LEU:HD23	2.00	0.62
2:D:191:VAL:CG1	2:D:421:ALA:HA	2.29	0.62
1:A:373:ARG:HB3	1:A:373:ARG:NH1	2.15	0.62
2:B:130:ASP:OD2	2:B:131:CYS:N	2.32	0.62
2:B:215:ARG:NE	2:B:215:ARG:HA	2.13	0.62
1:C:407:TRP:CZ2	2:D:256:ALA:O	2.53	0.62
2:D:282:GLN:HA	2:D:285:ALA:HB2	1.80	0.62
1:A:267:PHE:N	1:A:267:PHE:HD1	1.96	0.62
1:A:344:VAL:HG11	1:A:346:TRP:HE1	1.63	0.62
2:B:2:ARG:HE	2:B:243:ARG:HD2	1.64	0.62
2:B:218:LYS:O	2:B:219:LEU:HB2	2.00	0.62
1:C:27:GLU:HG3	1:C:28:HIS:ND1	2.14	0.62
1:C:291:ILE:HG21	1:C:375:VAL:HG21	1.82	0.62
1:C:311:LYS:HD3	1:C:344:VAL:HG22	1.80	0.62
1:C:331:ALA:C	1:C:333:ALA:N	2.51	0.62
1:C:344:VAL:HG12	1:C:345:ASP:N	2.15	0.62
2:D:2:ARG:O	2:D:57:ALA:HB1	1.99	0.62
2:D:24:ILE:HG22	2:D:24:ILE:O	1.98	0.62
2:D:333:LEU:HG	2:D:337:ASN:ND2	2.15	0.62
2:D:348:PRO:O	2:D:349:ASN:HB3	2.00	0.62
1:A:132:LEU:HB3	1:A:164:LYS:HD3	1.80	0.62
1:A:407:TRP:CZ2	2:B:256:ALA:O	2.53	0.62
2:B:58:GLY:C	2:B:64:ARG:NE	2.52	0.62
2:B:102:ASN:ND2	2:B:105:LYS:H	1.98	0.62
2:B:105:LYS:HA	2:B:109:THR:OG1	1.99	0.62
2:B:153:LEU:O	2:B:157:ILE:N	2.33	0.62
2:B:344:VAL:HG23	2:B:345:GLU:N	2.15	0.62
2:D:149:MET:HA	2:D:149:MET:CE	2.29	0.62
2:D:206:ASN:ND2	2:D:227:LEU:HD21	2.07	0.62
1:A:181:VAL:HG13	1:A:408:TYR:OH	2.00	0.62
1:A:365:GLY:O	1:A:368:LEU:HD11	2.00	0.62
2:B:163:ASP:CG	2:B:164:ARG:H	2.03	0.62
1:C:345:ASP:O	1:C:347:CYS:N	2.31	0.62
2:D:2:ARG:HH11	2:D:251:ASP:HA	1.64	0.62
2:D:158:ARG:HA	2:D:197:ASN:ND2	2.15	0.62
3:E:58:UNK:O	3:E:60:UNK:N	2.33	0.62
2:B:280:SER:O	2:B:282:GLN:HG2	1.99	0.61
2:B:385:GLN:HG2	2:B:433:GLN:NE2	2.14	0.61
1:C:191:THR:HB	1:C:421:ALA:HB1	1.79	0.61
1:C:242:LEU:O	1:C:243:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:PHE:HD1	1:C:267:PHE:H	1.45	0.61
1:C:344:VAL:HG11	1:C:346:TRP:HE1	1.63	0.61
2:D:358:ILE:H	2:D:358:ILE:CD1	2.13	0.61
1:A:210:TYR:CE2	1:A:227:LEU:HD23	2.34	0.61
1:A:317:LEU:HD23	1:A:377:MET:CB	2.30	0.61
2:B:22:GLU:N	2:B:22:GLU:OE2	2.33	0.61
1:C:362:VAL:CG2	1:C:370:LYS:HA	2.28	0.61
2:D:280:SER:O	2:D:282:GLN:HG2	2.00	0.61
1:A:413:MET:SD	3:E:15:UNK:CA	2.83	0.61
2:B:326:LYS:O	2:B:330:GLU:HG3	2.00	0.61
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.34	0.61
1:C:238:ILE:HG22	1:C:239:THR:N	2.15	0.61
2:D:123:ARG:NE	2:D:160:GLU:OE2	2.32	0.61
1:A:175:PRO:O	1:A:177:VAL:HG23	2.00	0.61
2:B:5:VAL:HB	2:B:135:PHE:HD2	1.65	0.61
2:B:218:LYS:NZ	2:B:278:ARG:N	2.46	0.61
2:B:241:CYS:SG	2:B:320:ARG:NH1	2.73	0.61
1:C:2:ARG:NH2	1:C:133:GLN:NE2	2.46	0.61
1:C:86:LEU:CD2	1:C:89:PRO:HD3	2.29	0.61
1:C:414:GLU:CD	1:C:414:GLU:N	2.54	0.61
2:D:237:GLY:O	2:D:376:THR:HG21	2.01	0.61
3:E:4:UNK:O	3:E:6:UNK:N	2.33	0.61
1:A:362:VAL:CG2	1:A:370:LYS:HA	2.31	0.61
2:B:353:THR:CG2	2:B:354:ALA:H	2.14	0.61
2:B:396:THR:HG23	2:B:400:ARG:CD	2.27	0.61
1:C:258:ASN:HD22	1:C:258:ASN:H	1.48	0.61
2:D:264:ARG:HH22	2:D:431:GLU:HG3	1.64	0.61
2:D:316:ALA:HB3	2:D:378:ILE:HB	1.82	0.61
1:A:88:HIS:N	1:A:91:GLN:OE1	2.33	0.61
2:B:2:ARG:NH1	2:B:251:ASP:HA	2.15	0.61
2:B:59:ASN:CG	2:B:60:LYS:N	2.54	0.61
2:B:191:VAL:HG13	2:B:421:ALA:HA	1.83	0.61
2:B:312:TYR:HA	2:B:381:SER:HA	1.81	0.61
2:D:287:THR:O	2:D:290:GLU:HB3	2.01	0.61
1:A:398:MET:O	1:A:400:ALA:N	2.34	0.61
2:B:102:ASN:HD22	2:B:105:LYS:CG	2.13	0.61
2:B:404:PHE:O	2:B:404:PHE:HD2	1.83	0.61
1:C:78:VAL:O	1:C:82:THR:HA	2.01	0.61
1:C:164:LYS:N	1:C:164:LYS:HZ1	1.98	0.61
2:D:51:VAL:C	2:D:53:TYR:H	2.03	0.61
1:A:139:HIS:NE2	1:A:150:THR:HG21	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:PHE:HD1	2:B:118:VAL:HG22	1.63	0.61
1:C:65:ALA:O	1:C:91:GLN:HB2	2.01	0.61
1:C:72:PRO:HB3	1:C:94:THR:OG1	2.01	0.61
1:C:101:ASN:OD1	2:D:254:LYS:NZ	2.30	0.61
1:C:171:ILE:CG2	1:C:206:ASN:OD1	2.48	0.61
1:C:258:ASN:ND2	1:C:258:ASN:H	1.99	0.61
2:D:94:PHE:HB2	2:D:114:LEU:CD1	2.31	0.61
1:A:27:GLU:CG	1:A:28:HIS:H	2.12	0.61
1:A:101:ASN:O	1:A:185:TYR:OH	2.19	0.61
1:A:103:TYR:CG	1:A:188:ILE:HD13	2.36	0.61
1:A:321:GLY:N	1:A:356:ASN:O	2.34	0.61
2:B:223:THR:N	2:B:226:ASP:OD2	2.30	0.61
1:C:188:ILE:HG22	1:C:417:GLU:O	2.01	0.61
1:C:259:LEU:HD21	1:C:378:LEU:HB3	1.81	0.61
1:C:393:HIS:C	1:C:395:PHE:H	2.03	0.61
2:D:60:LYS:N	2:D:60:LYS:NZ	2.49	0.61
2:D:261:PRO:HB2	2:D:262:PHE:CD1	2.36	0.61
1:A:137:VAL:CG1	1:A:154:MET:HE2	2.29	0.61
2:B:140:SER:CB	2:B:171:VAL:HB	2.31	0.61
2:B:189:LEU:C	2:B:191:VAL:N	2.55	0.61
1:C:164:LYS:HZ2	1:C:164:LYS:HB2	1.66	0.61
2:D:5:VAL:HG22	2:D:64:ARG:HD3	1.83	0.61
3:E:35:UNK:HA	3:E:38:UNK:CB	2.31	0.61
3:E:50:UNK:C	3:E:52:UNK:N	2.62	0.61
1:A:103:TYR:HB2	1:A:185:TYR:CD1	2.36	0.60
1:A:143:GLY:O	1:A:144:GLY:O	2.18	0.60
1:A:242:LEU:HB3	1:A:250:VAL:HG11	1.83	0.60
1:A:354:GLY:C	1:A:355:ILE:HD12	2.21	0.60
2:B:59:ASN:HB2	2:B:64:ARG:HE	1.63	0.60
2:B:311:ARG:HG3	2:B:311:ARG:HH11	1.65	0.60
1:C:221:ARG:CD	1:C:221:ARG:H	2.13	0.60
2:D:296:PHE:HA	2:D:377:PHE:CE2	2.35	0.60
2:D:350:ASN:ND2	2:D:351:VAL:HG23	2.16	0.60
2:D:385:GLN:HE21	2:D:433:GLN:HG2	1.65	0.60
1:A:282:TYR:N	1:A:282:TYR:HD2	1.98	0.60
1:A:283:HIS:O	1:A:284:GLU:HB3	2.00	0.60
2:B:66:ILE:O	2:B:66:ILE:HG12	2.01	0.60
2:B:75:MET:O	2:B:76:ASP:C	2.39	0.60
2:B:286:LEU:HD13	2:B:371:LEU:O	2.00	0.60
2:B:321:GLY:CA	2:B:359:PRO:HB3	2.27	0.60
2:B:380:ASN:C	2:B:380:ASN:HD22	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:109:THR:HG21	2:D:411:GLU:CG	2.30	0.60
2:D:118:VAL:O	2:D:120:ASP:N	2.32	0.60
2:D:153:LEU:O	2:D:157:ILE:N	2.34	0.60
2:D:163:ASP:CG	2:D:164:ARG:H	2.04	0.60
2:D:307:PRO:C	2:D:309:HIS:H	2.04	0.60
1:A:318:LEU:HB2	1:A:376:CYS:O	2.01	0.60
2:B:134:GLY:HA3	2:B:165:ILE:O	2.02	0.60
2:B:287:THR:O	2:B:290:GLU:HB3	2.01	0.60
2:B:308:ARG:NH2	2:B:342:TYR:CD1	2.61	0.60
2:B:348:PRO:O	2:B:349:ASN:HB3	2.01	0.60
1:C:16:ILE:HD12	1:C:171:ILE:HD11	1.83	0.60
1:C:90:GLU:O	1:C:121:ARG:NH1	2.34	0.60
1:C:126:ALA:HB1	1:C:132:LEU:HD11	1.83	0.60
1:C:183:GLU:HB2	1:C:184:PRO:CD	2.30	0.60
1:C:185:TYR:O	1:C:188:ILE:HD12	2.01	0.60
1:A:7:ILE:HG22	1:A:66:VAL:CB	2.23	0.60
2:B:118:VAL:O	2:B:120:ASP:N	2.28	0.60
2:B:149:MET:O	2:B:152:LEU:HB3	2.01	0.60
1:C:158:SER:HB3	1:C:166:LYS:NZ	2.17	0.60
2:D:265:LEU:O	2:D:266:HIS:ND1	2.34	0.60
2:D:312:TYR:HA	2:D:381:SER:HA	1.83	0.60
1:A:222:PRO:CB	1:A:227:LEU:HD11	2.19	0.60
1:A:257:THR:OG1	1:A:258:ASN:ND2	2.35	0.60
2:B:2:ARG:CG	2:B:133:GLN:NE2	2.58	0.60
1:C:276:ILE:O	1:C:369:ALA:HB3	2.01	0.60
2:D:191:VAL:HG13	2:D:421:ALA:HA	1.82	0.60
1:A:175:PRO:HD2	1:A:207:GLU:CB	2.05	0.60
1:A:269:LEU:HD21	1:A:301:GLN:NE2	2.17	0.60
2:B:11:GLN:HG3	2:B:15:GLN:NE2	2.17	0.60
2:B:107:HIS:CD2	2:B:151:THR:HG23	2.35	0.60
2:B:184:PRO:HB2	2:B:399:PHE:CZ	2.35	0.60
2:B:191:VAL:CG1	2:B:421:ALA:HA	2.30	0.60
1:C:332:ILE:HD11	1:C:353:VAL:HG21	1.84	0.60
2:D:339:ASN:O	2:D:341:SER:N	2.34	0.60
2:D:399:PHE:CE2	2:D:404:PHE:HB3	2.37	0.60
1:A:344:VAL:HG12	1:A:345:ASP:N	2.17	0.60
2:B:296:PHE:HA	2:B:377:PHE:CE2	2.36	0.60
1:C:9:VAL:HA	1:C:68:VAL:O	2.02	0.60
1:C:21:TRP:HA	1:C:24:TYR:HB2	1.82	0.60
1:C:77:GLU:O	1:C:83:TYR:HB2	2.02	0.60
1:C:139:HIS:NE2	1:C:150:THR:HG21	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:HIS:NE2	1:C:198:SER:HB3	2.17	0.60
1:C:305:CYS:SG	1:C:384:ILE:HA	2.42	0.60
1:C:371:VAL:HG12	1:C:372:GLN:N	2.17	0.60
2:D:111:GLY:C	2:D:113:GLU:N	2.53	0.60
2:D:139:HIS:C	2:D:139:HIS:CD2	2.75	0.60
1:A:23:LEU:C	1:A:25:CYS:H	2.05	0.60
1:A:220:GLU:OE2	2:B:326:LYS:HD3	2.01	0.60
1:A:291:ILE:HG22	1:A:292:THR:N	2.17	0.60
1:C:280:LYS:O	1:C:282:TYR:HE2	1.84	0.60
2:D:159:GLU:OE2	3:E:82:UNK:CB	2.50	0.60
1:A:9:VAL:HG21	1:A:150:THR:HB	1.84	0.60
1:A:31:GLN:CB	1:A:32:PRO:HD2	2.27	0.60
1:A:69:ASP:OD1	1:A:71:GLU:HG3	2.02	0.60
1:A:215:ARG:NH2	1:A:300:ASN:HD21	1.99	0.60
1:A:360:PRO:HB3	1:A:374:ALA:HB2	1.83	0.60
2:B:132:LEU:HD23	2:B:132:LEU:C	2.22	0.60
2:B:311:ARG:HH11	2:B:344:VAL:HA	1.67	0.60
1:C:26:LEU:HG	1:C:361:THR:CB	2.32	0.60
1:C:209:ILE:HD12	1:C:209:ILE:H	1.65	0.60
1:C:287:SER:OG	1:C:290:GLU:HG3	2.02	0.60
1:C:354:GLY:C	1:C:355:ILE:HD12	2.22	0.60
2:D:102:ASN:ND2	2:D:105:LYS:H	1.99	0.60
2:D:102:ASN:HB3	2:D:105:LYS:HB2	1.83	0.60
2:D:239:THR:O	2:D:241:CYS:O	2.20	0.60
2:D:398:MET:C	2:D:400:ARG:H	2.05	0.60
1:A:100:ALA:HA	1:A:105:ARG:HD2	1.83	0.60
2:B:194:LEU:HD11	2:B:428:LEU:HD11	1.84	0.60
1:C:46:ASP:OD2	1:C:46:ASP:N	2.34	0.60
1:C:332:ILE:CD1	1:C:353:VAL:HG21	2.31	0.60
3:E:83:UNK:C	3:E:85:UNK:N	2.63	0.60
1:A:69:ASP:HB3	1:A:75:ILE:CG2	2.26	0.59
2:B:60:LYS:N	2:B:60:LYS:NZ	2.50	0.59
2:B:266:HIS:HB2	2:B:380:ASN:OD1	2.02	0.59
1:C:329:ASN:HA	1:C:332:ILE:HB	1.83	0.59
2:D:58:GLY:C	2:D:64:ARG:NE	2.55	0.59
2:D:102:ASN:O	2:D:105:LYS:HB2	2.01	0.59
2:D:127:GLU:O	2:D:128:SER:C	2.40	0.59
2:D:166:MET:HG3	2:D:167:ASN:N	2.16	0.59
2:D:240:THR:C	2:D:243:ARG:HB2	2.22	0.59
2:D:263:PRO:O	2:D:265:LEU:N	2.33	0.59
2:D:380:ASN:C	2:D:380:ASN:HD22	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:ARG:HH12	2:B:252:LEU:HD12	1.67	0.59
2:B:303:ALA:HB1	2:B:387:LEU:CD1	2.32	0.59
2:B:322:ARG:NE	2:B:357:ASP:HB3	2.17	0.59
2:B:350:ASN:HD22	2:B:351:VAL:HG23	1.68	0.59
1:C:9:VAL:HG23	1:C:9:VAL:O	2.01	0.59
1:C:264:ARG:NH2	1:C:424:ASP:OD1	2.35	0.59
1:C:321:GLY:HA2	1:C:357:TYR:O	2.02	0.59
1:C:423:GLU:O	1:C:427:ALA:N	2.28	0.59
1:C:433:GLU:C	1:C:435:VAL:H	2.04	0.59
2:D:218:LYS:HZ2	2:D:277:SER:HB3	1.67	0.59
1:A:77:GLU:O	1:A:83:TYR:CB	2.50	0.59
1:A:182:VAL:CG1	1:A:183:GLU:N	2.65	0.59
1:A:209:ILE:C	1:A:211:ASP:N	2.51	0.59
2:B:259:MET:HE1	2:B:316:ALA:N	2.16	0.59
1:C:209:ILE:C	1:C:211:ASP:N	2.55	0.59
2:D:58:GLY:O	2:D:64:ARG:NE	2.34	0.59
2:D:99:ALA:HA	2:D:105:LYS:HD3	1.83	0.59
2:D:266:HIS:ND1	2:D:432:TYR:CZ	2.70	0.59
2:D:390:ARG:C	2:D:392:SER:N	2.51	0.59
1:A:44:GLY:HA3	1:A:47:ASP:HA	1.84	0.59
1:A:238:ILE:N	1:A:241:SER:HB3	2.18	0.59
1:A:395:PHE:CD1	1:A:395:PHE:C	2.75	0.59
2:B:12:CYS:HB3	5:B:501:GDP:C8	2.37	0.59
2:B:416:MET:C	2:B:418:PHE:N	2.56	0.59
1:C:86:LEU:HD22	1:C:89:PRO:HD3	1.84	0.59
1:C:237:SER:CA	1:C:241:SER:HB2	2.28	0.59
1:C:395:PHE:CD1	1:C:395:PHE:C	2.75	0.59
1:C:413:MET:H	1:C:413:MET:CE	2.15	0.59
2:D:75:MET:O	2:D:76:ASP:C	2.40	0.59
2:D:87:PHE:O	2:D:90:ASP:OD1	2.19	0.59
2:D:141:LEU:HB3	2:D:186:ASN:CB	2.32	0.59
1:A:68:VAL:HG21	1:A:118:VAL:HG21	1.83	0.59
1:A:87:PHE:CE2	1:A:92:LEU:HD21	2.38	0.59
2:B:102:ASN:HD22	2:B:105:LYS:N	2.01	0.59
2:B:247:GLN:HG2	2:B:325:MET:SD	2.42	0.59
2:B:391:ILE:H	2:B:391:ILE:CD1	2.15	0.59
1:C:196:GLU:N	1:C:196:GLU:CD	2.55	0.59
1:C:261:PRO:CG	1:C:380:ASN:HD21	2.13	0.59
2:D:66:ILE:O	2:D:66:ILE:HG12	2.02	0.59
2:B:79:ARG:HA	2:B:84:GLY:HA2	1.83	0.59
2:B:94:PHE:HB2	2:B:114:LEU:CD1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:TYR:CE1	2:B:378:ILE:HD12	2.38	0.59
1:C:413:MET:C	1:C:414:GLU:OE1	2.41	0.59
2:D:169:PHE:CD2	2:D:235:MET:SD	2.95	0.59
2:D:276:THR:HG21	2:D:281:GLN:HB3	1.84	0.59
2:D:312:TYR:CD2	2:D:381:SER:HB2	2.37	0.59
2:D:396:THR:HA	2:D:400:ARG:HB3	1.83	0.59
1:A:101:ASN:OD1	2:B:254:LYS:HD3	2.02	0.59
1:A:345:ASP:C	1:A:347:CYS:H	2.06	0.59
2:B:2:ARG:HG3	2:B:133:GLN:CD	2.21	0.59
2:B:18:ALA:O	2:B:22:GLU:OE2	2.20	0.59
2:B:239:THR:O	2:B:241:CYS:O	2.19	0.59
1:C:258:ASN:O	1:C:259:LEU:HB2	2.02	0.59
2:D:308:ARG:NH2	2:D:342:TYR:HB2	2.17	0.59
2:D:404:PHE:HD2	2:D:404:PHE:O	1.85	0.59
3:E:67:UNK:O	3:E:71:UNK:N	2.35	0.59
2:B:2:ARG:NE	2:B:243:ARG:CD	2.64	0.59
2:B:181:VAL:O	2:B:183:GLU:N	2.35	0.59
2:B:253:ARG:HG3	2:B:253:ARG:NH1	2.17	0.59
2:B:307:PRO:C	2:B:309:HIS:H	2.06	0.59
2:B:395:PHE:HB3	2:B:422:GLU:OE1	2.03	0.59
1:C:103:TYR:N	1:C:185:TYR:HE1	2.01	0.59
1:C:416:GLY:C	1:C:418:PHE:N	2.55	0.59
3:E:37:UNK:O	3:E:38:UNK:C	2.49	0.59
3:E:54:UNK:O	3:E:56:UNK:N	2.35	0.59
1:A:171:ILE:CG2	1:A:206:ASN:OD1	2.50	0.59
2:B:18:ALA:O	2:B:20:PHE:N	2.35	0.59
2:B:80:SER:OG	2:B:81:GLY:N	2.34	0.59
2:B:241:CYS:C	2:B:243:ARG:H	2.04	0.59
2:B:261:PRO:HB2	2:B:262:PHE:CD1	2.38	0.59
1:C:69:ASP:OD2	1:C:74:VAL:CG1	2.50	0.59
2:D:428:LEU:O	2:D:432:TYR:HB2	2.03	0.59
1:A:183:GLU:HB2	1:A:184:PRO:HD3	1.85	0.58
2:B:75:MET:O	2:B:76:ASP:O	2.21	0.58
2:B:385:GLN:OE1	2:B:429:VAL:HA	2.03	0.58
2:D:51:VAL:N	2:D:245:PRO:HB2	2.18	0.58
2:D:102:ASN:HB3	2:D:105:LYS:HD2	1.83	0.58
2:D:179:ASP:HB3	2:D:181:VAL:H	1.66	0.58
2:D:416:MET:C	2:D:418:PHE:N	2.56	0.58
1:A:269:LEU:HD12	1:A:269:LEU:C	2.23	0.58
1:A:389:ALA:O	1:A:392:ASP:HB3	2.03	0.58
1:C:286:LEU:O	1:C:373:ARG:HD2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:LYS:HA	2:D:22:GLU:OE2	2.02	0.58
2:D:241:CYS:C	2:D:243:ARG:N	2.49	0.58
2:D:251:ASP:CG	2:D:252:LEU:N	2.56	0.58
2:B:179:ASP:HB2	2:B:182:VAL:CG2	2.33	0.58
2:B:197:ASN:O	2:B:198:THR:HB	2.02	0.58
2:B:200:GLU:CG	2:B:268:PHE:CE2	2.86	0.58
1:C:217:LEU:HD23	1:C:219:ILE:CD1	2.33	0.58
1:C:256:GLN:O	1:C:258:ASN:N	2.36	0.58
1:A:241:SER:HB3	1:A:242:LEU:HD12	1.85	0.58
1:A:419:SER:O	1:A:422:ARG:HG2	2.02	0.58
1:A:423:GLU:O	1:A:427:ALA:N	2.29	0.58
2:B:123:ARG:C	2:B:125:GLU:H	2.06	0.58
2:B:308:ARG:NH2	2:B:342:TYR:HB2	2.19	0.58
2:D:9:ALA:HA	2:D:68:VAL:O	2.02	0.58
2:D:123:ARG:C	2:D:125:GLU:H	2.06	0.58
2:D:134:GLY:HA3	2:D:165:ILE:O	2.03	0.58
1:A:23:LEU:O	1:A:26:LEU:HD12	2.03	0.58
1:A:26:LEU:HG	1:A:361:THR:OG1	2.04	0.58
2:B:5:VAL:HA	2:B:64:ARG:CD	2.33	0.58
2:B:289:PRO:HB2	2:B:331:GLN:HE21	1.68	0.58
2:B:395:PHE:HD2	2:B:422:GLU:OE1	1.86	0.58
1:C:231:ILE:O	1:C:235:VAL:HG23	2.04	0.58
2:D:307:PRO:O	2:D:309:HIS:N	2.36	0.58
2:D:321:GLY:CA	2:D:359:PRO:HB3	2.32	0.58
3:E:66:UNK:O	3:E:69:UNK:N	2.37	0.58
1:A:186:ASN:O	1:A:189:LEU:HB3	2.03	0.58
2:B:183:GLU:C	2:B:185:TYR:N	2.54	0.58
2:B:413:MET:SD	2:B:417:GLU:HG2	2.43	0.58
2:D:12:CYS:HB2	5:D:503:GDP:PA	2.43	0.58
1:A:38:SER:O	1:A:39:ASP:HB3	2.04	0.58
2:B:158:ARG:HD3	2:B:197:ASN:CG	2.23	0.58
2:B:198:THR:O	2:B:200:GLU:N	2.37	0.58
1:C:160:ASP:O	1:C:161:TYR:CG	2.57	0.58
2:D:409:THR:HA	2:D:412:GLY:O	2.03	0.58
3:E:58:UNK:C	3:E:60:UNK:N	2.66	0.58
1:A:371:VAL:HG12	1:A:373:ARG:N	2.17	0.58
1:A:409:VAL:C	1:A:411:GLU:H	2.07	0.58
2:B:79:ARG:HA	2:B:84:GLY:CA	2.34	0.58
1:C:143:GLY:H	1:C:147:SER:CB	2.17	0.58
1:C:256:GLN:C	1:C:258:ASN:N	2.57	0.58
2:D:165:ILE:HG13	2:D:253:ARG:HG3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:183:GLU:HB3	2:D:184:PRO:CD	2.34	0.58
1:A:402:ARG:HD2	2:B:346:TRP:CE3	2.38	0.58
2:B:282:GLN:HA	2:B:285:ALA:HB2	1.86	0.58
1:C:36:MET:HA	1:C:36:MET:CE	2.34	0.58
1:C:259:LEU:HD11	1:C:378:LEU:HD13	1.85	0.58
2:D:80:SER:OG	2:D:81:GLY:N	2.36	0.58
2:D:196:GLU:O	2:D:197:ASN:C	2.39	0.58
1:A:7:ILE:HD12	1:A:153:LEU:HD21	1.85	0.58
2:B:107:HIS:HA	2:B:152:LEU:HD22	1.86	0.58
2:B:391:ILE:O	2:B:425:MET:HE1	2.03	0.58
1:C:103:TYR:HB2	1:C:185:TYR:CD1	2.38	0.58
2:D:59:ASN:OD1	2:D:60:LYS:HD2	2.04	0.58
2:D:192:HIS:C	2:D:194:LEU:N	2.56	0.58
2:D:405:LEU:HD22	2:D:405:LEU:C	2.24	0.58
1:A:132:LEU:O	1:A:133:GLN:HB2	2.04	0.57
2:B:102:ASN:ND2	2:B:105:LYS:N	2.52	0.57
2:B:251:ASP:CG	2:B:252:LEU:N	2.55	0.57
2:B:258:ASN:OD1	2:B:352:LYS:NZ	2.34	0.57
2:B:276:THR:HB	2:B:281:GLN:OE1	2.03	0.57
2:B:386:GLU:O	2:B:388:PHE:N	2.34	0.57
1:C:215:ARG:NH2	1:C:216:ASN:OD1	2.37	0.57
1:C:336:LYS:HE2	1:C:336:LYS:HA	1.85	0.57
2:D:187:ALA:HB2	2:D:391:ILE:HG22	1.85	0.57
2:D:247:GLN:HG2	2:D:325:MET:SD	2.43	0.57
3:E:17:UNK:O	3:E:19:UNK:N	2.35	0.57
1:A:88:HIS:HB3	1:A:91:GLN:CD	2.24	0.57
2:B:114:LEU:O	2:B:117:SER:N	2.36	0.57
2:B:158:ARG:HA	2:B:197:ASN:ND2	2.19	0.57
2:B:335:VAL:HA	2:B:338:LYS:HB2	1.86	0.57
1:C:317:LEU:HD23	1:C:377:MET:CB	2.34	0.57
2:D:140:SER:CB	2:D:171:VAL:HB	2.34	0.57
2:D:289:PRO:HB2	2:D:331:GLN:HE21	1.69	0.57
1:A:9:VAL:HG23	1:A:9:VAL:O	2.03	0.57
1:A:363:VAL:H	1:A:367:ASP:HB2	1.69	0.57
1:A:393:HIS:C	1:A:395:PHE:H	2.06	0.57
2:B:167:ASN:HA	2:B:200:GLU:O	2.04	0.57
2:B:313:LEU:HA	2:B:344:VAL:CG1	2.32	0.57
2:B:316:ALA:HB3	2:B:378:ILE:HB	1.86	0.57
1:C:183:GLU:HB2	1:C:184:PRO:HD3	1.85	0.57
1:C:363:VAL:HG13	1:C:367:ASP:OD2	2.05	0.57
2:D:123:ARG:CZ	2:D:160:GLU:OE2	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ASP:OD2	1:A:46:ASP:N	2.37	0.57
1:A:93:ILE:HD13	1:A:118:VAL:HA	1.86	0.57
1:A:339:ARG:HD2	1:A:340:THR:N	2.19	0.57
1:A:404:PHE:N	1:A:404:PHE:CD1	2.73	0.57
2:B:102:ASN:C	2:B:185:TYR:OH	2.43	0.57
1:C:77:GLU:O	1:C:83:TYR:CB	2.53	0.57
2:D:7:ILE:HB	2:D:137:LEU:HA	1.86	0.57
2:D:276:THR:HB	2:D:281:GLN:OE1	2.04	0.57
3:E:35:UNK:O	3:E:38:UNK:N	2.36	0.57
1:A:236:SER:O	1:A:238:ILE:N	2.31	0.57
1:A:387:ALA:HA	1:A:390:ARG:CD	2.29	0.57
2:B:59:ASN:N	2:B:64:ARG:HE	2.01	0.57
2:B:59:ASN:OD1	2:B:60:LYS:HD2	2.05	0.57
2:B:132:LEU:HB3	2:B:164:ARG:CZ	2.34	0.57
2:B:196:GLU:O	2:B:197:ASN:C	2.43	0.57
1:C:286:LEU:HB2	1:C:291:ILE:HG13	1.86	0.57
1:C:409:VAL:C	1:C:411:GLU:H	2.05	0.57
2:D:311:ARG:HG3	2:D:311:ARG:HH11	1.70	0.57
1:A:229:ARG:HH11	1:A:229:ARG:HG3	1.69	0.57
1:A:311:LYS:HB2	1:A:344:VAL:HG22	1.87	0.57
1:A:404:PHE:N	1:A:404:PHE:HD1	2.01	0.57
1:C:123:ARG:HA	1:C:161:TYR:OH	2.05	0.57
1:C:409:VAL:O	1:C:412:GLY:O	2.22	0.57
2:D:417:GLU:HG3	2:D:417:GLU:O	2.04	0.57
1:A:206:ASN:ND2	1:A:210:TYR:HE2	1.98	0.57
1:A:209:ILE:HD12	1:A:209:ILE:N	2.19	0.57
1:A:244:PHE:O	1:A:245:ASP:C	2.41	0.57
1:A:336:LYS:HE2	1:A:336:LYS:HA	1.86	0.57
2:B:409:THR:HG23	2:B:414:ASP:HA	1.86	0.57
1:C:82:THR:HG22	1:C:83:TYR:H	1.70	0.57
1:C:87:PHE:N	1:C:87:PHE:CD2	2.64	0.57
1:C:134:GLY:H	1:C:164:LYS:HG2	1.69	0.57
1:C:292:THR:HA	1:C:295:CYS:HB3	1.86	0.57
1:C:401:LYS:O	1:C:402:ARG:HB3	2.05	0.57
2:D:154:ILE:C	2:D:156:LYS:H	2.08	0.57
2:D:292:THR:HG23	2:D:319:PHE:HZ	1.70	0.57
1:A:371:VAL:HG12	1:A:372:GLN:H	1.69	0.57
2:B:223:THR:HG23	2:B:225:GLY:N	2.20	0.57
2:B:395:PHE:HE2	2:B:418:PHE:O	1.88	0.57
1:C:101:ASN:O	1:C:185:TYR:OH	2.22	0.57
1:C:102:ASN:ND2	2:D:257:VAL:HG11	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:GLY:O	1:C:182:VAL:HG23	2.04	0.57
2:D:206:ASN:HD22	2:D:227:LEU:CD2	2.09	0.57
2:D:215:ARG:HA	2:D:215:ARG:CZ	2.35	0.57
1:A:155:GLU:O	1:A:159:VAL:HG23	2.04	0.57
1:A:164:LYS:HB2	1:A:164:LYS:NZ	2.19	0.57
1:A:291:ILE:CD1	1:A:373:ARG:HG3	2.34	0.57
1:A:386:GLU:CG	1:A:387:ALA:H	2.13	0.57
1:A:401:LYS:O	1:A:402:ARG:CB	2.53	0.57
2:B:311:ARG:HH21	2:B:437:ASP:CB	1.97	0.57
1:C:35:GLN:OE1	1:C:88:HIS:NE2	2.38	0.57
1:C:78:VAL:HG11	1:C:87:PHE:HE2	1.69	0.57
1:C:111:GLY:O	1:C:113:GLU:N	2.37	0.57
1:C:220:GLU:HB3	1:C:221:ARG:NE	2.20	0.57
2:D:282:GLN:O	2:D:284:ARG:N	2.38	0.57
2:D:391:ILE:O	2:D:391:ILE:HG22	2.05	0.57
2:D:416:MET:O	2:D:417:GLU:HB3	2.04	0.57
1:A:139:HIS:HB3	1:A:170:SER:HA	1.87	0.57
1:A:196:GLU:CD	1:A:196:GLU:N	2.58	0.57
1:A:267:PHE:HD1	1:A:267:PHE:H	1.53	0.57
1:A:284:GLU:O	1:A:285:GLN:HG3	2.05	0.57
1:A:417:GLU:HB3	1:A:418:PHE:HD2	1.68	0.57
2:B:9:ALA:HA	2:B:68:VAL:O	2.04	0.57
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.39	0.57
2:B:102:ASN:HB3	2:B:105:LYS:HB2	1.86	0.57
2:B:149:MET:HA	2:B:149:MET:CE	2.34	0.57
2:B:163:ASP:OD1	2:B:164:ARG:HG2	2.05	0.57
1:C:143:GLY:H	1:C:147:SER:HB2	1.70	0.57
1:C:182:VAL:O	1:C:183:GLU:C	2.43	0.57
2:D:133:GLN:OE1	2:D:133:GLN:HA	2.05	0.57
2:D:198:THR:O	2:D:200:GLU:N	2.37	0.57
1:A:264:ARG:NH2	1:A:424:ASP:OD1	2.38	0.56
1:A:386:GLU:C	1:A:388:TRP:H	2.06	0.56
2:B:350:ASN:ND2	2:B:351:VAL:HG23	2.19	0.56
1:C:193:THR:HG23	1:C:193:THR:O	2.05	0.56
1:C:293:ASN:O	1:C:297:GLU:OE1	2.23	0.56
2:D:162:PRO:O	2:D:163:ASP:C	2.43	0.56
1:A:8:HIS:HD2	1:A:17:GLY:HA3	1.68	0.56
1:A:69:ASP:OD2	1:A:74:VAL:CG1	2.52	0.56
1:A:209:ILE:O	1:A:211:ASP:N	2.38	0.56
2:B:139:HIS:HD2	2:B:139:HIS:O	1.88	0.56
1:C:8:HIS:CD2	1:C:17:GLY:HA3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:VAL:HG21	1:C:154:MET:SD	2.45	0.56
1:C:236:SER:C	1:C:238:ILE:H	2.08	0.56
2:D:333:LEU:O	2:D:337:ASN:N	2.38	0.56
2:D:339:ASN:C	2:D:341:SER:N	2.58	0.56
1:A:7:ILE:CG1	1:A:137:VAL:HG22	2.35	0.56
1:A:401:LYS:O	1:A:402:ARG:HB3	2.05	0.56
2:B:120:ASP:O	2:B:124:LYS:HE3	2.06	0.56
2:B:200:GLU:CG	2:B:268:PHE:HE2	2.19	0.56
2:B:416:MET:O	2:B:417:GLU:HB3	2.06	0.56
1:C:23:LEU:O	1:C:26:LEU:HD12	2.06	0.56
1:C:137:VAL:CG1	1:C:154:MET:HE2	2.30	0.56
1:C:257:THR:OG1	1:C:258:ASN:ND2	2.39	0.56
1:C:399:TYR:HH	1:C:408:TYR:HE2	1.52	0.56
2:D:69:ASP:CB	2:D:74:THR:HG23	2.35	0.56
2:D:130:ASP:OD2	2:D:131:CYS:N	2.38	0.56
2:D:218:LYS:O	2:D:219:LEU:HB2	2.04	0.56
2:D:263:PRO:HG2	2:D:264:ARG:H	1.71	0.56
1:A:188:ILE:HG22	1:A:417:GLU:O	2.04	0.56
2:B:2:ARG:NH2	2:B:243:ARG:HA	2.20	0.56
2:B:103:TRP:O	2:B:105:LYS:O	2.23	0.56
1:C:331:ALA:C	1:C:333:ALA:H	2.08	0.56
2:D:194:LEU:CD1	2:D:428:LEU:HD21	2.35	0.56
2:D:223:THR:N	2:D:226:ASP:OD2	2.33	0.56
2:D:385:GLN:NE2	2:D:433:GLN:HE21	2.01	0.56
2:D:419:THR:O	2:D:423:SER:N	2.39	0.56
3:E:10:UNK:HA	3:E:13:UNK:CB	2.36	0.56
1:A:256:GLN:C	1:A:258:ASN:N	2.58	0.56
1:A:286:LEU:HB2	1:A:291:ILE:HG13	1.88	0.56
1:A:402:ARG:CG	1:A:403:ALA:N	2.68	0.56
1:A:433:GLU:C	1:A:435:VAL:H	2.07	0.56
2:B:307:PRO:O	2:B:309:HIS:N	2.38	0.56
2:B:312:TYR:CD2	2:B:381:SER:HB2	2.40	0.56
1:C:282:TYR:N	1:C:282:TYR:HD2	2.00	0.56
1:C:423:GLU:O	1:C:426:ALA:HB3	2.04	0.56
2:D:98:GLY:N	2:D:110:GLU:OE1	2.38	0.56
2:D:133:GLN:HE21	2:D:252:LEU:CB	2.18	0.56
3:E:46:UNK:C	3:E:48:UNK:N	2.62	0.56
1:A:209:ILE:HG12	1:A:231:ILE:HD11	1.88	0.56
1:A:329:ASN:HA	1:A:332:ILE:HB	1.87	0.56
2:B:141:LEU:HB3	2:B:186:ASN:CB	2.30	0.56
2:B:183:GLU:O	2:B:185:TYR:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:ALA:O	1:C:392:ASP:HB3	2.06	0.56
1:C:398:MET:O	1:C:400:ALA:N	2.38	0.56
2:D:132:LEU:HD23	2:D:132:LEU:C	2.26	0.56
2:D:151:THR:HG21	2:D:189:LEU:CD2	2.36	0.56
2:D:241:CYS:C	2:D:243:ARG:H	2.07	0.56
3:E:57:UNK:O	3:E:58:UNK:C	2.53	0.56
1:A:36:MET:HA	1:A:36:MET:CE	2.36	0.56
1:A:86:LEU:CD1	1:A:89:PRO:HD3	2.35	0.56
1:A:184:PRO:HG3	1:A:399:TYR:CE1	2.41	0.56
1:A:311:LYS:CD	1:A:344:VAL:HG22	2.36	0.56
2:B:161:TYR:O	2:B:162:PRO:C	2.42	0.56
2:B:226:ASP:C	2:B:228:ASN:H	2.08	0.56
2:B:240:THR:C	2:B:243:ARG:HB2	2.26	0.56
1:C:115:ILE:O	1:C:119:LEU:HB2	2.05	0.56
1:C:174:ALA:O	1:C:176:GLN:N	2.39	0.56
1:C:185:TYR:CE1	1:C:408:TYR:HE1	2.22	0.56
1:C:288:VAL:HA	1:C:373:ARG:HD3	1.86	0.56
1:C:399:TYR:OH	1:C:408:TYR:HE2	1.89	0.56
1:C:401:LYS:O	1:C:402:ARG:CB	2.53	0.56
2:D:158:ARG:CZ	2:D:197:ASN:HA	2.36	0.56
1:A:195:LEU:C	1:A:197:HIS:H	2.09	0.56
1:A:213:CYS:SG	1:A:217:LEU:HD23	2.46	0.56
1:A:316:CYS:O	1:A:316:CYS:SG	2.64	0.56
2:B:398:MET:C	2:B:400:ARG:N	2.57	0.56
1:C:69:ASP:HB3	1:C:75:ILE:CG2	2.35	0.56
1:C:387:ALA:HA	1:C:390:ARG:CD	2.30	0.56
2:D:133:GLN:HG3	2:D:252:LEU:HD22	1.87	0.56
2:D:372:LYS:O	2:D:373:MET:HG3	2.06	0.56
1:A:78:VAL:O	1:A:82:THR:HA	2.05	0.56
1:A:102:ASN:HD21	2:B:257:VAL:CG1	2.12	0.56
1:A:151:SER:HB3	1:A:192:HIS:NE2	2.20	0.56
1:A:189:LEU:CD1	1:A:193:THR:HG21	2.35	0.56
1:A:243:ARG:NH1	1:A:250:VAL:HG13	2.16	0.56
1:A:350:GLY:C	1:A:351:PHE:CD1	2.72	0.56
1:A:385:ALA:HB2	1:A:432:TYR:CD2	2.39	0.56
2:B:151:THR:HG21	2:B:189:LEU:CD2	2.36	0.56
1:C:102:ASN:HD21	2:D:257:VAL:CG1	2.14	0.56
1:C:182:VAL:CG1	1:C:183:GLU:N	2.68	0.56
1:C:258:ASN:O	1:C:259:LEU:CB	2.54	0.56
1:C:289:ALA:HA	1:C:292:THR:HG22	1.87	0.56
2:D:51:VAL:N	2:D:245:PRO:HG2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:88:ARG:HH11	2:D:88:ARG:HA	1.70	0.56
2:D:273:ALA:O	2:D:275:LEU:N	2.37	0.56
2:D:292:THR:HG23	2:D:319:PHE:CZ	2.41	0.56
1:A:69:ASP:OD2	1:A:74:VAL:HG12	2.05	0.56
1:A:143:GLY:H	1:A:147:SER:CB	2.19	0.56
1:A:362:VAL:CG1	1:A:367:ASP:HB2	2.29	0.56
2:D:59:ASN:CB	2:D:64:ARG:HB2	2.35	0.56
2:D:132:LEU:HD23	2:D:132:LEU:O	2.05	0.56
2:D:165:ILE:HG13	2:D:253:ARG:CG	2.36	0.56
2:D:198:THR:C	2:D:200:GLU:N	2.59	0.56
2:D:320:ARG:N	2:D:374:SER:O	2.33	0.56
1:A:16:ILE:O	1:A:19:ALA:N	2.30	0.55
1:A:26:LEU:HD12	1:A:26:LEU:H	1.71	0.55
1:A:112:LYS:NZ	3:E:12:UNK:CB	2.69	0.55
1:A:393:HIS:O	1:A:397:LEU:HB2	2.06	0.55
1:A:404:PHE:HD1	1:A:404:PHE:H	1.54	0.55
2:B:3:GLU:OE2	2:B:128:SER:O	2.24	0.55
2:B:241:CYS:O	2:B:243:ARG:N	2.39	0.55
1:C:140:SER:HB3	1:C:171:ILE:HD13	1.86	0.55
1:C:229:ARG:HH11	1:C:229:ARG:HG3	1.72	0.55
1:C:413:MET:SD	3:E:66:UNK:C	2.94	0.55
2:D:149:MET:O	2:D:152:LEU:HB3	2.06	0.55
2:D:192:HIS:CA	2:D:195:VAL:HG22	2.23	0.55
1:A:234:ILE:CD1	1:A:302:MET:SD	2.94	0.55
2:B:59:ASN:ND2	2:B:60:LYS:N	2.54	0.55
2:B:132:LEU:HD22	2:B:164:ARG:NE	2.22	0.55
1:C:166:LYS:HE3	1:C:198:SER:N	2.12	0.55
1:C:238:ILE:N	1:C:241:SER:HB3	2.21	0.55
1:C:247:ALA:O	1:C:249:ASN:ND2	2.39	0.55
1:C:287:SER:C	1:C:289:ALA:N	2.59	0.55
2:D:12:CYS:HB3	5:D:503:GDP:N7	2.21	0.55
2:D:59:ASN:HB3	2:D:64:ARG:HB2	1.87	0.55
2:D:69:ASP:HB2	2:D:74:THR:HG23	1.87	0.55
2:D:93:VAL:HG23	2:D:94:PHE:N	2.21	0.55
1:A:12:ALA:HB3	1:A:140:SER:CB	2.36	0.55
2:B:97:SER:OG	2:B:98:GLY:N	2.39	0.55
1:C:88:HIS:N	1:C:91:GLN:OE1	2.39	0.55
1:C:142:GLY:O	1:C:182:VAL:CG2	2.55	0.55
2:D:97:SER:OG	2:D:98:GLY:N	2.38	0.55
1:A:143:GLY:H	1:A:147:SER:HB2	1.71	0.55
1:A:154:MET:CE	1:A:197:HIS:NE2	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ALA:HB2	1:A:295:CYS:HA	1.89	0.55
2:B:99:ALA:HA	2:B:105:LYS:HD3	1.89	0.55
2:B:169:PHE:CG	2:B:235:MET:SD	2.99	0.55
2:B:272:PHE:HD1	2:B:275:LEU:HD23	1.71	0.55
1:C:186:ASN:O	1:C:189:LEU:HB3	2.06	0.55
1:C:284:GLU:O	1:C:285:GLN:HG3	2.06	0.55
2:D:102:ASN:HD21	2:D:104:ALA:HB3	1.71	0.55
2:D:395:PHE:HE2	2:D:418:PHE:O	1.90	0.55
3:E:31:UNK:O	3:E:32:UNK:C	2.51	0.55
1:A:75:ILE:O	1:A:75:ILE:CG1	2.54	0.55
1:C:2:ARG:HH22	1:C:133:GLN:HE22	1.54	0.55
1:C:100:ALA:CA	1:C:105:ARG:HD2	2.36	0.55
2:D:274:PRO:HG3	2:D:374:SER:CB	2.37	0.55
1:A:103:TYR:H	1:A:185:TYR:HE1	1.54	0.55
1:A:258:ASN:ND2	1:A:258:ASN:H	2.03	0.55
1:A:409:VAL:O	1:A:412:GLY:O	2.25	0.55
2:B:51:VAL:HG22	2:B:245:PRO:CG	2.36	0.55
1:C:96:LYS:O	1:C:98:ASP:N	2.39	0.55
1:C:171:ILE:H	1:C:171:ILE:CD1	2.20	0.55
1:C:386:GLU:C	1:C:388:TRP:H	2.10	0.55
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.41	0.55
2:D:338:LYS:O	2:D:340:SER:N	2.34	0.55
2:D:357:ASP:HB3	2:D:358:ILE:HD12	1.88	0.55
1:A:139:HIS:CG	1:A:140:SER:H	2.23	0.55
1:A:218:ASP:CG	1:A:219:ILE:H	2.09	0.55
1:A:236:SER:C	1:A:238:ILE:H	2.09	0.55
2:B:158:ARG:CB	2:B:197:ASN:HD22	2.19	0.55
2:B:191:VAL:HG22	2:B:421:ALA:O	2.07	0.55
1:C:222:PRO:CB	1:C:227:LEU:HD11	2.20	0.55
1:C:417:GLU:HB3	1:C:418:PHE:HD2	1.67	0.55
2:D:59:ASN:N	2:D:64:ARG:HE	2.04	0.55
2:D:189:LEU:C	2:D:191:VAL:N	2.55	0.55
2:B:320:ARG:HB2	2:B:374:SER:OG	2.07	0.55
2:B:345:GLU:O	2:B:345:GLU:CG	2.55	0.55
1:C:72:PRO:HG3	1:C:96:LYS:HA	1.89	0.55
1:C:88:HIS:HB3	1:C:91:GLN:CD	2.26	0.55
1:C:427:ALA:HA	1:C:430:LYS:HB2	1.88	0.55
2:D:120:ASP:O	2:D:124:LYS:HE3	2.06	0.55
1:A:107:HIS:CE1	1:A:151:SER:HB2	2.41	0.55
1:A:197:HIS:NE2	1:A:198:SER:HB3	2.22	0.55
2:B:10:GLY:CA	2:B:146:GLY:HA3	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:GLN:HG3	2:B:252:LEU:HD22	1.88	0.55
2:B:180:THR:HB	2:B:404:PHE:CE1	2.42	0.55
2:B:194:LEU:CD1	2:B:428:LEU:HD21	2.37	0.55
2:B:227:LEU:HD23	2:B:227:LEU:O	2.06	0.55
2:B:264:ARG:NH2	2:B:431:GLU:HG3	2.20	0.55
1:C:217:LEU:O	1:C:217:LEU:HG	2.06	0.55
1:C:286:LEU:HD12	1:C:291:ILE:HG12	1.89	0.55
2:D:230:LEU:H	2:D:230:LEU:CD1	2.19	0.55
2:D:277:SER:O	2:D:278:ARG:O	2.25	0.55
1:A:259:LEU:HD21	1:A:378:LEU:CB	2.37	0.55
1:A:331:ALA:HA	1:A:334:THR:OG1	2.07	0.55
2:B:12:CYS:HB2	5:B:501:GDP:O1A	2.07	0.55
2:B:132:LEU:HD11	2:B:135:PHE:CZ	2.42	0.55
2:B:226:ASP:O	2:B:228:ASN:N	2.37	0.55
2:B:284:ARG:O	2:B:287:THR:N	2.40	0.55
2:D:59:ASN:HA	2:D:60:LYS:HZ3	1.71	0.55
2:D:242:LEU:O	2:D:243:ARG:HD3	2.07	0.55
2:D:395:PHE:HB3	2:D:422:GLU:OE1	2.07	0.55
1:A:287:SER:C	1:A:289:ALA:N	2.60	0.54
2:B:223:THR:HG23	2:B:225:GLY:CA	2.36	0.54
2:B:263:PRO:HG2	2:B:264:ARG:H	1.72	0.54
1:C:11:GLN:NE2	4:C:502:GTP:O2A	2.40	0.54
1:C:119:LEU:HD22	1:C:156:ARG:NE	2.21	0.54
1:C:236:SER:O	1:C:238:ILE:N	2.34	0.54
1:C:318:LEU:HB2	1:C:376:CYS:O	2.07	0.54
2:D:107:HIS:HA	2:D:152:LEU:HD22	1.88	0.54
2:D:133:GLN:HE22	2:D:252:LEU:H	1.54	0.54
2:D:200:GLU:CG	2:D:268:PHE:CE2	2.90	0.54
2:D:243:ARG:HH12	2:D:252:LEU:HD12	1.72	0.54
2:D:306:ASP:HB3	2:D:309:HIS:CD2	2.42	0.54
2:D:395:PHE:HD2	2:D:422:GLU:OE1	1.89	0.54
1:A:317:LEU:HD23	1:A:377:MET:HB3	1.88	0.54
1:A:399:TYR:OH	1:A:408:TYR:HE2	1.90	0.54
2:B:218:LYS:O	2:B:219:LEU:CB	2.55	0.54
1:C:71:GLU:O	1:C:73:THR:N	2.40	0.54
1:C:100:ALA:HA	1:C:105:ARG:HD2	1.89	0.54
1:C:110:ILE:O	1:C:111:GLY:C	2.45	0.54
1:C:175:PRO:HD2	1:C:207:GLU:CB	2.11	0.54
2:D:288:VAL:N	2:D:289:PRO:CD	2.70	0.54
2:D:297:ASP:OD1	2:D:298:ALA:N	2.40	0.54
1:A:103:TYR:O	1:A:104:ALA:C	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ALA:HA	1:A:430:LYS:HB2	1.89	0.54
2:B:218:LYS:HZ2	2:B:277:SER:HB3	1.72	0.54
2:B:377:PHE:O	2:B:378:ILE:HG12	2.07	0.54
1:C:189:LEU:CD1	1:C:193:THR:HG21	2.37	0.54
1:C:316:CYS:O	1:C:316:CYS:SG	2.65	0.54
1:C:344:VAL:CG1	1:C:346:TRP:NE1	2.69	0.54
2:D:22:GLU:OE2	2:D:22:GLU:N	2.41	0.54
2:D:168:THR:OG1	2:D:201:THR:CB	2.54	0.54
2:D:428:LEU:HD12	2:D:428:LEU:H	1.73	0.54
1:A:137:VAL:O	1:A:168:GLU:HA	2.07	0.54
2:B:59:ASN:CB	2:B:64:ARG:HB2	2.37	0.54
2:B:60:LYS:N	2:B:60:LYS:HZ2	2.04	0.54
2:B:394:GLN:O	2:B:398:MET:CB	2.56	0.54
1:C:209:ILE:H	1:C:209:ILE:CD1	2.20	0.54
1:C:345:ASP:C	1:C:347:CYS:H	2.10	0.54
2:D:102:ASN:HD22	2:D:105:LYS:N	2.05	0.54
2:D:102:ASN:C	2:D:185:TYR:OH	2.46	0.54
2:D:114:LEU:O	2:D:117:SER:N	2.40	0.54
2:D:132:LEU:HD11	2:D:135:PHE:CE2	2.41	0.54
2:D:189:LEU:O	2:D:191:VAL:N	2.38	0.54
2:D:303:ALA:O	2:D:387:LEU:HD12	2.08	0.54
1:A:190:THR:HG21	1:A:425:MET:SD	2.47	0.54
2:B:215:ARG:HA	2:B:215:ARG:CZ	2.37	0.54
2:B:378:ILE:O	2:B:378:ILE:HG22	2.06	0.54
2:B:428:LEU:CD1	2:B:428:LEU:H	2.20	0.54
2:B:437:ASP:OD2	2:B:437:ASP:N	2.39	0.54
1:C:314:ALA:O	1:C:315:CYS:CB	2.56	0.54
1:C:419:SER:O	1:C:422:ARG:N	2.41	0.54
2:D:2:ARG:NH1	2:D:251:ASP:HA	2.23	0.54
2:D:192:HIS:O	2:D:194:LEU:N	2.36	0.54
2:D:344:VAL:HG23	2:D:345:GLU:N	2.21	0.54
1:A:389:ALA:CB	1:A:429:GLU:OE2	2.55	0.54
1:C:12:ALA:HB3	1:C:140:SER:OG	2.07	0.54
1:C:26:LEU:HD12	1:C:26:LEU:H	1.73	0.54
1:C:134:GLY:H	1:C:164:LYS:HG3	1.72	0.54
1:C:169:PHE:HE1	1:C:238:ILE:HD12	1.73	0.54
1:C:184:PRO:HG3	1:C:399:TYR:CE1	2.43	0.54
2:D:5:VAL:O	2:D:5:VAL:HG12	2.06	0.54
2:D:409:THR:HG23	2:D:414:ASP:HA	1.89	0.54
3:E:71:UNK:C	3:E:73:UNK:N	2.70	0.54
1:A:273:ALA:HB2	1:A:295:CYS:CA	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:GLY:N	2:B:110:GLU:OE1	2.40	0.54
2:B:209:LEU:HB3	2:B:227:LEU:HG	1.89	0.54
1:C:9:VAL:HG21	1:C:150:THR:CG2	2.38	0.54
1:C:244:PHE:O	1:C:245:ASP:C	2.46	0.54
2:D:132:LEU:HD11	2:D:135:PHE:CZ	2.42	0.54
2:D:148:GLY:HA2	2:D:151:THR:HG22	1.89	0.54
1:A:93:ILE:HD13	1:A:118:VAL:CG2	2.29	0.54
1:A:123:ARG:HG2	1:A:161:TYR:OH	2.08	0.54
1:A:242:LEU:HG	1:A:318:LEU:HD11	1.89	0.54
1:A:331:ALA:C	1:A:333:ALA:N	2.58	0.54
2:B:187:ALA:HB2	2:B:391:ILE:HG22	1.88	0.54
1:C:5:ILE:O	1:C:135:PHE:HA	2.07	0.54
1:C:78:VAL:HG11	1:C:87:PHE:CE2	2.42	0.54
1:C:177:VAL:HG11	2:D:349:ASN:HB3	1.90	0.54
1:C:238:ILE:O	1:C:239:THR:C	2.47	0.54
1:C:322:ASP:N	1:C:357:TYR:O	2.38	0.54
2:D:129:CYS:O	2:D:130:ASP:C	2.46	0.54
2:D:385:GLN:OE1	2:D:429:VAL:HA	2.08	0.54
1:A:103:TYR:HB2	1:A:185:TYR:HD1	1.72	0.54
1:A:322:ASP:N	1:A:357:TYR:O	2.38	0.54
2:B:60:LYS:H	2:B:60:LYS:NZ	2.06	0.54
2:B:69:ASP:HB2	2:B:74:THR:HG23	1.90	0.54
1:C:23:LEU:C	1:C:25:CYS:H	2.11	0.54
1:C:139:HIS:CG	1:C:140:SER:H	2.26	0.54
1:C:195:LEU:C	1:C:197:HIS:H	2.11	0.54
1:C:256:GLN:HA	1:C:260:VAL:HG23	1.88	0.54
2:D:2:ARG:HG3	2:D:133:GLN:CD	2.26	0.54
2:D:102:ASN:ND2	2:D:105:LYS:N	2.55	0.54
2:D:371:LEU:O	2:D:372:LYS:HB2	2.07	0.54
1:A:163:LYS:C	1:A:164:LYS:HZ2	2.10	0.54
1:A:169:PHE:HE1	1:A:238:ILE:HD12	1.73	0.54
2:B:179:ASP:HB3	2:B:181:VAL:CG1	2.37	0.54
2:B:288:VAL:N	2:B:289:PRO:CD	2.71	0.54
2:B:331:GLN:HA	2:B:331:GLN:OE1	2.08	0.54
1:C:241:SER:HB3	1:C:242:LEU:HD12	1.90	0.54
1:A:35:GLN:OE1	1:A:88:HIS:NE2	2.41	0.53
1:A:182:VAL:HG12	1:A:183:GLU:N	2.23	0.53
1:A:190:THR:CG2	1:A:425:MET:HG2	2.38	0.53
2:B:51:VAL:C	2:B:53:TYR:N	2.61	0.53
2:B:344:VAL:CG2	2:B:345:GLU:N	2.71	0.53
1:C:186:ASN:ND2	1:C:391:LEU:HD21	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:PHE:C	1:C:397:LEU:N	2.61	0.53
2:D:191:VAL:O	2:D:191:VAL:CG1	2.55	0.53
2:D:223:THR:O	2:D:226:ASP:N	2.39	0.53
1:C:86:LEU:CD1	1:C:89:PRO:HD3	2.38	0.53
1:C:92:LEU:N	1:C:92:LEU:CD1	2.71	0.53
1:C:242:LEU:HB3	1:C:250:VAL:CG1	2.38	0.53
1:C:420:GLU:C	1:C:420:GLU:OE1	2.46	0.53
2:D:398:MET:SD	2:D:399:PHE:CD2	3.01	0.53
1:A:16:ILE:CG2	1:A:17:GLY:N	2.59	0.53
1:A:87:PHE:H	1:A:87:PHE:HD2	1.54	0.53
1:A:193:THR:HG23	1:A:193:THR:O	2.07	0.53
1:A:405:VAL:O	1:A:409:VAL:HG23	2.08	0.53
2:B:130:ASP:OD2	2:B:130:ASP:C	2.46	0.53
2:B:189:LEU:O	2:B:191:VAL:N	2.39	0.53
1:C:214:ARG:CA	1:C:218:ASP:O	2.53	0.53
1:C:242:LEU:HG	1:C:318:LEU:HD11	1.89	0.53
2:D:308:ARG:NH2	2:D:342:TYR:CG	2.76	0.53
1:A:183:GLU:OE2	2:B:348:PRO:HB2	2.09	0.53
1:A:408:TYR:O	1:A:414:GLU:HG3	2.08	0.53
2:B:174:SER:OG	2:B:207:GLU:HA	2.09	0.53
2:B:204:ILE:HG21	2:B:209:LEU:HD11	1.89	0.53
2:B:371:LEU:O	2:B:372:LYS:HB2	2.08	0.53
1:C:24:TYR:HA	1:C:26:LEU:HD12	1.91	0.53
2:D:17:GLY:O	2:D:20:PHE:HB3	2.07	0.53
2:D:51:VAL:HG22	2:D:245:PRO:CG	2.38	0.53
2:D:102:ASN:HD22	2:D:105:LYS:CB	2.20	0.53
2:D:283:TYR:O	2:D:290:GLU:OE1	2.25	0.53
2:D:315:VAL:HG23	2:D:351:VAL:HG22	1.90	0.53
1:A:82:THR:O	1:A:83:TYR:HB2	2.09	0.53
1:A:220:GLU:HB3	1:A:221:ARG:NE	2.23	0.53
1:A:273:ALA:HB2	1:A:295:CYS:HB2	1.91	0.53
1:A:275:VAL:HG12	1:A:275:VAL:O	2.09	0.53
2:B:274:PRO:HA	2:B:294:GLN:CD	2.28	0.53
2:B:284:ARG:O	2:B:285:ALA:C	2.47	0.53
2:B:297:ASP:OD1	2:B:298:ALA:N	2.42	0.53
1:C:82:THR:O	1:C:83:TYR:HB2	2.07	0.53
2:D:206:ASN:HD21	5:D:503:GDP:N2	2.06	0.53
1:A:65:ALA:O	1:A:91:GLN:HB2	2.08	0.53
1:A:92:LEU:N	1:A:92:LEU:CD1	2.70	0.53
1:A:305:CYS:SG	1:A:384:ILE:HA	2.49	0.53
1:A:331:ALA:O	1:A:335:ILE:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:TYR:O	2:B:188:THR:HG22	2.08	0.53
2:B:387:LEU:O	2:B:387:LEU:CD2	2.56	0.53
1:C:217:LEU:HD23	1:C:219:ILE:HD12	1.89	0.53
1:C:238:ILE:O	1:C:242:LEU:HD12	2.09	0.53
1:C:305:CYS:SG	1:C:306:ASP:N	2.77	0.53
2:D:179:ASP:HB2	2:D:182:VAL:CG2	2.38	0.53
2:D:274:PRO:HA	2:D:294:GLN:CD	2.29	0.53
1:A:271:THR:HG23	1:A:300:ASN:O	2.08	0.53
2:B:88:ARG:CB	2:B:89:PRO:HD3	2.32	0.53
2:B:209:LEU:HD21	2:B:302:MET:HG3	1.89	0.53
2:B:223:THR:O	2:B:226:ASP:N	2.41	0.53
2:B:274:PRO:HG3	2:B:374:SER:CB	2.38	0.53
2:B:358:ILE:H	2:B:358:ILE:CD1	2.18	0.53
1:C:181:VAL:HG22	1:C:408:TYR:OH	2.09	0.53
1:C:184:PRO:HA	1:C:395:PHE:HD2	1.74	0.53
1:C:333:ALA:O	1:C:334:THR:C	2.47	0.53
2:D:223:THR:HG23	2:D:225:GLY:CA	2.39	0.53
2:D:226:ASP:C	2:D:228:ASN:H	2.12	0.53
2:D:241:CYS:O	2:D:243:ARG:N	2.42	0.53
2:B:59:ASN:HA	2:B:60:LYS:HZ3	1.73	0.53
1:C:339:ARG:HD2	1:C:340:THR:N	2.24	0.53
2:D:79:ARG:HA	2:D:84:GLY:HA2	1.90	0.53
2:D:322:ARG:HG2	2:D:357:ASP:CA	2.30	0.53
2:D:345:GLU:O	2:D:345:GLU:CG	2.57	0.53
1:A:216:ASN:HB3	1:A:275:VAL:CG1	2.39	0.53
2:B:6:HIS:O	2:B:66:ILE:HG22	2.09	0.53
1:C:206:ASN:O	1:C:210:TYR:HD2	1.92	0.53
1:C:285:GLN:C	1:C:286:LEU:HD23	2.29	0.53
2:D:190:SER:CB	2:D:425:MET:HG3	2.28	0.53
2:D:200:GLU:CG	2:D:268:PHE:HE2	2.22	0.53
2:D:282:GLN:C	2:D:285:ALA:H	2.12	0.53
2:D:392:SER:HB2	2:D:426:ASN:ND2	2.24	0.53
1:A:341:ILE:HG22	1:A:342:GLN:N	2.23	0.53
2:B:91:ASN:N	2:B:91:ASN:ND2	2.49	0.53
2:B:111:GLY:O	2:B:114:LEU:N	2.42	0.53
2:B:191:VAL:CG2	2:B:421:ALA:HB1	2.25	0.53
2:B:306:ASP:HB3	2:B:309:HIS:CD2	2.44	0.53
2:B:311:ARG:HG3	2:B:311:ARG:NH1	2.23	0.53
2:B:385:GLN:HE21	2:B:433:GLN:HG2	1.72	0.53
2:B:403:ALA:HB1	2:B:405:LEU:HD12	1.90	0.53
1:C:43:GLY:O	1:C:47:ASP:CG	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:194:LEU:HD12	2:D:428:LEU:HD21	1.91	0.53
2:D:206:ASN:ND2	5:D:503:GDP:N3	2.54	0.53
1:A:212:ILE:C	1:A:214:ARG:H	2.13	0.52
2:B:51:VAL:CG2	2:B:53:TYR:HB2	2.39	0.52
2:B:88:ARG:HH11	2:B:88:ARG:HA	1.73	0.52
2:B:223:THR:C	2:B:225:GLY:N	2.61	0.52
2:B:381:SER:C	2:B:383:ALA:H	2.11	0.52
1:C:15:GLN:HE22	1:C:224:TYR:HD1	1.56	0.52
1:C:40:LYS:HD2	1:C:41:THR:H	1.73	0.52
2:D:2:ARG:CG	2:D:133:GLN:NE2	2.61	0.52
3:E:30:UNK:O	3:E:33:UNK:N	2.42	0.52
1:A:256:GLN:O	1:A:258:ASN:N	2.43	0.52
1:C:401:LYS:O	1:C:402:ARG:CD	2.57	0.52
2:D:25:SER:HB3	2:D:369:ARG:HH22	1.74	0.52
2:D:154:ILE:O	2:D:156:LYS:N	2.42	0.52
2:D:371:LEU:C	2:D:373:MET:H	2.10	0.52
2:D:413:MET:SD	2:D:417:GLU:HG2	2.49	0.52
2:D:437:ASP:OD2	2:D:437:ASP:N	2.43	0.52
1:A:101:ASN:C	1:A:185:TYR:OH	2.46	0.52
1:A:110:ILE:O	1:A:111:GLY:C	2.46	0.52
1:A:289:ALA:HA	1:A:292:THR:HG22	1.89	0.52
1:A:333:ALA:O	1:A:334:THR:C	2.48	0.52
1:C:107:HIS:CE1	1:C:151:SER:HB2	2.43	0.52
1:C:276:ILE:CG1	1:C:282:TYR:CD2	2.92	0.52
1:C:276:ILE:HD12	1:C:277:SER:N	2.25	0.52
1:C:322:ASP:OD1	1:C:357:TYR:O	2.27	0.52
2:D:16:ILE:HG12	2:D:17:GLY:N	2.24	0.52
2:D:223:THR:C	2:D:225:GLY:N	2.60	0.52
2:D:264:ARG:NH2	2:D:431:GLU:HG3	2.24	0.52
2:D:305:CYS:O	2:D:306:ASP:C	2.47	0.52
2:D:428:LEU:CD1	2:D:428:LEU:H	2.23	0.52
3:E:73:UNK:C	3:E:75:UNK:N	2.66	0.52
1:A:213:CYS:SG	1:A:230:LEU:HD23	2.50	0.52
1:A:314:ALA:O	1:A:315:CYS:CB	2.57	0.52
1:A:416:GLY:C	1:A:418:PHE:N	2.62	0.52
2:B:306:ASP:HB3	2:B:309:HIS:NE2	2.24	0.52
1:C:101:ASN:HD22	1:C:101:ASN:C	2.13	0.52
1:C:181:VAL:HG13	1:C:408:TYR:OH	2.09	0.52
1:C:321:GLY:HA2	1:C:358:GLU:O	2.09	0.52
2:D:143:GLY:O	5:D:503:GDP:O3B	2.28	0.52
1:A:243:ARG:HA	1:A:243:ARG:NE	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:PRO:O	1:A:300:ASN:N	2.42	0.52
2:B:16:ILE:HD12	2:B:231:VAL:CG1	2.38	0.52
2:B:70:LEU:HD11	2:B:110:GLU:O	2.09	0.52
2:B:114:LEU:O	2:B:115:VAL:C	2.46	0.52
2:B:265:LEU:O	2:B:266:HIS:CG	2.63	0.52
2:B:276:THR:HG21	2:B:281:GLN:HB3	1.92	0.52
2:B:308:ARG:HH21	2:B:342:TYR:HD1	1.50	0.52
2:B:409:THR:HA	2:B:412:GLY:O	2.10	0.52
1:C:103:TYR:HB2	1:C:185:TYR:HD1	1.74	0.52
1:C:137:VAL:O	1:C:168:GLU:HA	2.10	0.52
1:C:293:ASN:C	1:C:296:PHE:H	2.13	0.52
2:D:179:ASP:HB3	2:D:181:VAL:CG1	2.37	0.52
2:D:182:VAL:O	2:D:182:VAL:CG1	2.57	0.52
1:A:7:ILE:HG13	1:A:137:VAL:HG22	1.91	0.52
1:A:252:LEU:HD22	1:A:255:PHE:HD2	1.74	0.52
2:B:183:GLU:HB3	2:B:184:PRO:HD3	1.91	0.52
2:B:322:ARG:HG2	2:B:357:ASP:CA	2.30	0.52
1:C:35:GLN:HE22	1:C:88:HIS:CD2	2.28	0.52
1:C:102:ASN:O	1:C:105:ARG:N	2.38	0.52
1:C:172:TYR:HB3	1:C:205:ASP:H	1.74	0.52
1:C:294:ALA:HA	1:C:297:GLU:OE1	2.09	0.52
1:C:311:LYS:CG	1:C:344:VAL:HG22	2.40	0.52
2:D:260:VAL:O	2:D:260:VAL:HG12	2.09	0.52
2:D:415:GLU:O	2:D:416:MET:O	2.27	0.52
1:A:30:ILE:CG1	1:A:31:GLN:N	2.70	0.52
1:A:142:GLY:O	1:A:182:VAL:CG2	2.57	0.52
2:B:129:CYS:O	2:B:130:ASP:O	2.27	0.52
2:B:287:THR:C	2:B:289:PRO:HD2	2.29	0.52
1:C:68:VAL:HG21	1:C:118:VAL:HG21	1.91	0.52
1:C:152:LEU:O	1:C:156:ARG:HG2	2.09	0.52
1:C:234:ILE:CD1	1:C:302:MET:SD	2.97	0.52
1:C:402:ARG:CG	1:C:403:ALA:N	2.69	0.52
2:D:59:ASN:ND2	2:D:60:LYS:H	2.07	0.52
2:D:127:GLU:O	2:D:128:SER:O	2.28	0.52
2:D:132:LEU:HB3	2:D:164:ARG:CZ	2.38	0.52
2:D:140:SER:HA	2:D:171:VAL:H	1.74	0.52
1:A:134:GLY:H	1:A:164:LYS:HG3	1.73	0.52
1:A:172:TYR:HB3	1:A:205:ASP:H	1.75	0.52
1:A:286:LEU:HD12	1:A:291:ILE:HG12	1.90	0.52
2:B:69:ASP:CB	2:B:74:THR:HG23	2.39	0.52
2:B:103:TRP:O	2:B:104:ALA:C	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:ASP:HB3	2:B:181:VAL:H	1.75	0.52
2:B:312:TYR:O	2:B:344:VAL:HG13	2.09	0.52
2:B:325:MET:HG2	2:B:355:VAL:HG11	1.91	0.52
1:C:71:GLU:OE2	4:C:502:GTP:O1B	2.28	0.52
1:C:307:PRO:HA	1:C:383:ALA:HB3	1.92	0.52
1:C:341:ILE:HG22	1:C:342:GLN:N	2.25	0.52
1:C:388:TRP:HZ3	1:C:428:LEU:HD22	1.71	0.52
2:D:239:THR:O	2:D:241:CYS:N	2.43	0.52
1:A:139:HIS:CG	1:A:140:SER:N	2.77	0.52
1:A:401:LYS:O	1:A:402:ARG:CD	2.58	0.52
1:A:414:GLU:CD	1:A:414:GLU:N	2.64	0.52
2:B:51:VAL:HG22	2:B:245:PRO:HG2	1.90	0.52
2:B:132:LEU:HD11	2:B:135:PHE:CE2	2.45	0.52
2:B:399:PHE:HE2	2:B:404:PHE:HB3	1.74	0.52
1:C:101:ASN:C	1:C:185:TYR:OH	2.47	0.52
1:C:139:HIS:O	1:C:140:SER:CB	2.58	0.52
1:C:190:THR:CG2	1:C:425:MET:HG2	2.40	0.52
1:C:213:CYS:O	1:C:219:ILE:HB	2.10	0.52
1:C:398:MET:C	1:C:400:ALA:H	2.13	0.52
2:D:93:VAL:HG23	2:D:95:GLY:N	2.25	0.52
2:D:142:GLY:HA2	2:D:185:TYR:CB	2.35	0.52
2:D:265:LEU:O	2:D:266:HIS:CG	2.63	0.52
1:A:2:ARG:NH2	1:A:133:GLN:NE2	2.53	0.52
1:A:212:ILE:HD11	1:A:230:LEU:HD21	1.91	0.52
1:A:414:GLU:CA	1:A:417:GLU:HB2	2.39	0.52
2:B:158:ARG:HG3	2:B:159:GLU:HG3	1.92	0.52
2:B:391:ILE:O	2:B:391:ILE:HG22	2.09	0.52
2:B:400:ARG:C	2:B:402:LYS:H	2.13	0.52
2:B:405:LEU:HD22	2:B:405:LEU:C	2.30	0.52
1:C:44:GLY:C	1:C:46:ASP:N	2.61	0.52
1:C:292:THR:O	1:C:292:THR:OG1	2.22	0.52
1:C:389:ALA:CB	1:C:429:GLU:OE2	2.58	0.52
2:D:2:ARG:HE	2:D:243:ARG:HD2	1.75	0.52
2:D:197:ASN:O	2:D:198:THR:HB	2.08	0.52
1:A:115:ILE:O	1:A:119:LEU:HB2	2.09	0.51
1:A:221:ARG:CD	1:A:221:ARG:H	2.23	0.51
1:A:387:ALA:HB1	1:A:390:ARG:CZ	2.40	0.51
2:B:58:GLY:O	2:B:64:ARG:CZ	2.59	0.51
2:B:264:ARG:HG3	2:B:264:ARG:NH1	2.25	0.51
2:B:339:ASN:C	2:B:341:SER:N	2.60	0.51
2:B:396:THR:HA	2:B:400:ARG:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:GLY:HA3	1:C:47:ASP:HA	1.91	0.51
1:C:88:HIS:CB	1:C:91:GLN:HE22	2.18	0.51
1:C:298:PRO:O	1:C:300:ASN:N	2.43	0.51
1:C:344:VAL:HG11	1:C:346:TRP:CE2	2.45	0.51
2:D:320:ARG:HB2	2:D:374:SER:OG	2.10	0.51
2:D:397:ALA:O	2:D:398:MET:HB2	2.10	0.51
1:A:20:CYS:C	1:A:22:GLU:N	2.63	0.51
1:A:264:ARG:HH22	1:A:427:ALA:HB3	1.75	0.51
1:A:285:GLN:C	1:A:286:LEU:HD23	2.31	0.51
2:B:179:ASP:CB	2:B:182:VAL:HG23	2.37	0.51
2:B:198:THR:C	2:B:200:GLU:N	2.62	0.51
2:B:249:ASN:CG	2:B:250:ALA:N	2.62	0.51
2:D:75:MET:O	2:D:76:ASP:O	2.27	0.51
2:B:104:ALA:HB1	2:B:411:GLU:HB2	1.93	0.51
2:B:247:GLN:OE1	2:B:355:VAL:O	2.28	0.51
2:B:273:ALA:O	2:B:275:LEU:N	2.40	0.51
2:B:333:LEU:O	2:B:337:ASN:N	2.43	0.51
2:B:357:ASP:CB	2:B:358:ILE:HD12	2.41	0.51
2:B:415:GLU:O	2:B:416:MET:O	2.28	0.51
1:C:322:ASP:HA	1:C:357:TYR:CD1	2.37	0.51
1:C:388:TRP:CZ3	1:C:428:LEU:HD13	2.45	0.51
2:D:18:ALA:C	2:D:20:PHE:N	2.60	0.51
2:D:223:THR:HG23	2:D:225:GLY:N	2.25	0.51
2:D:415:GLU:HG2	2:D:416:MET:H	1.75	0.51
1:A:202:PHE:CE1	1:A:378:LEU:HD22	2.42	0.51
2:B:5:VAL:HG22	2:B:64:ARG:HD3	1.92	0.51
2:B:123:ARG:NH2	2:B:160:GLU:OE2	2.44	0.51
2:B:234:THR:O	2:B:238:VAL:HG23	2.11	0.51
2:B:241:CYS:O	2:B:242:LEU:C	2.49	0.51
2:B:371:LEU:C	2:B:373:MET:H	2.14	0.51
1:C:168:GLU:HG3	1:C:201:ALA:CB	2.39	0.51
1:C:216:ASN:HB3	1:C:275:VAL:CG1	2.40	0.51
2:D:87:PHE:O	2:D:89:PRO:N	2.43	0.51
1:A:5:ILE:O	1:A:135:PHE:HA	2.10	0.51
1:A:37:PRO:HA	1:A:45:GLY:O	2.10	0.51
2:B:7:ILE:HB	2:B:137:LEU:HA	1.91	0.51
2:B:24:ILE:O	2:B:24:ILE:HG22	2.10	0.51
2:B:401:ARG:O	2:B:402:LYS:HG3	2.10	0.51
1:C:277:SER:O	1:C:278:ALA:HB2	2.10	0.51
1:C:365:GLY:O	1:C:368:LEU:CD1	2.59	0.51
2:D:51:VAL:CG2	2:D:53:TYR:HB2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:60:LYS:H	2:D:60:LYS:HD2	1.74	0.51
2:D:154:ILE:HD11	2:D:168:THR:HG21	1.92	0.51
2:D:212:ILE:C	2:D:214:PHE:H	2.13	0.51
2:D:318:VAL:HG12	2:D:318:VAL:O	2.11	0.51
1:A:41:THR:O	1:A:42:ILE:HB	2.09	0.51
1:A:160:ASP:O	1:A:161:TYR:CG	2.64	0.51
1:A:184:PRO:HA	1:A:395:PHE:HD2	1.76	0.51
1:A:288:VAL:HA	1:A:373:ARG:HD3	1.92	0.51
1:A:320:ARG:CB	1:A:374:ALA:HB3	2.37	0.51
2:B:166:MET:HG3	2:B:167:ASN:N	2.24	0.51
2:B:179:ASP:OD1	1:C:352:LYS:NZ	2.43	0.51
1:C:78:VAL:HG11	1:C:92:LEU:CD2	2.39	0.51
1:C:413:MET:H	1:C:413:MET:HE2	1.75	0.51
2:D:59:ASN:CA	2:D:64:ARG:HH21	2.19	0.51
2:D:179:ASP:HB2	2:D:182:VAL:N	2.25	0.51
2:D:400:ARG:C	2:D:402:LYS:N	2.63	0.51
1:A:15:GLN:HE22	1:A:224:TYR:HD1	1.58	0.51
1:A:72:PRO:HG3	1:A:96:LYS:HA	1.91	0.51
1:A:293:ASN:C	1:A:296:PHE:H	2.14	0.51
2:B:2:ARG:O	2:B:57:ALA:HB1	2.11	0.51
2:B:253:ARG:HG3	2:B:253:ARG:HH11	1.75	0.51
1:C:69:ASP:OD2	1:C:74:VAL:HG12	2.11	0.51
1:C:171:ILE:HA	1:C:204:VAL:HB	1.92	0.51
2:D:6:HIS:ND1	2:D:21:TRP:HZ2	2.09	0.51
2:D:11:GLN:HG3	2:D:15:GLN:NE2	2.26	0.51
2:D:51:VAL:C	2:D:53:TYR:N	2.64	0.51
2:D:103:TRP:O	2:D:105:LYS:O	2.28	0.51
2:D:253:ARG:C	2:D:255:LEU:N	2.62	0.51
2:D:297:ASP:OD1	2:D:299:LYS:N	2.32	0.51
3:E:90:UNK:O	3:E:91:UNK:O	2.29	0.51
1:A:16:ILE:O	1:A:17:GLY:C	2.49	0.51
1:A:101:ASN:C	1:A:101:ASN:HD22	2.14	0.51
2:B:212:ILE:C	2:B:214:PHE:H	2.13	0.51
2:B:372:LYS:O	2:B:373:MET:HG3	2.11	0.51
2:D:59:ASN:HB2	2:D:64:ARG:HE	1.74	0.51
2:D:242:LEU:O	2:D:243:ARG:NE	2.44	0.51
2:D:297:ASP:O	2:D:301:MET:HG2	2.11	0.51
2:D:424:ASN:O	2:D:427:ASP:N	2.44	0.51
1:A:238:ILE:O	1:A:239:THR:C	2.48	0.51
1:A:423:GLU:O	1:A:426:ALA:HB3	2.11	0.51
2:B:90:ASP:OD1	2:B:91:ASN:ND2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:PRO:O	2:B:163:ASP:C	2.47	0.51
2:B:391:ILE:N	2:B:391:ILE:CD1	2.74	0.51
1:C:38:SER:O	1:C:39:ASP:HB3	2.11	0.51
1:C:215:ARG:NH2	1:C:300:ASN:HD21	2.07	0.51
1:C:220:GLU:HB3	1:C:221:ARG:CZ	2.40	0.51
1:C:405:VAL:O	1:C:409:VAL:HG23	2.11	0.51
2:D:59:ASN:CA	2:D:60:LYS:HZ3	2.24	0.51
2:D:86:ILE:H	2:D:88:ARG:CZ	2.24	0.51
2:D:158:ARG:O	2:D:159:GLU:C	2.49	0.51
2:D:179:ASP:HB3	2:D:182:VAL:H	1.73	0.51
2:D:241:CYS:O	2:D:242:LEU:C	2.50	0.51
2:D:264:ARG:O	2:D:265:LEU:O	2.29	0.51
2:D:283:TYR:O	2:D:283:TYR:CG	2.64	0.51
1:A:21:TRP:HA	1:A:24:TYR:HB2	1.93	0.51
1:A:247:ALA:O	1:A:249:ASN:CG	2.49	0.51
2:B:79:ARG:HG3	2:B:88:ARG:HE	1.75	0.51
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.93	0.51
1:C:186:ASN:HD21	1:C:391:LEU:HD11	1.75	0.51
1:C:247:ALA:O	1:C:249:ASN:CG	2.48	0.51
2:D:159:GLU:CD	3:E:82:UNK:CB	2.80	0.51
2:D:313:LEU:HD21	2:D:435:TYR:HD2	1.76	0.51
1:A:8:HIS:HE2	1:A:21:TRP:HE1	1.59	0.50
1:A:143:GLY:O	4:A:500:GTP:O3G	2.29	0.50
1:A:177:VAL:HG11	2:B:349:ASN:HB3	1.93	0.50
1:A:180:ALA:O	1:A:182:VAL:N	2.44	0.50
2:B:203:CYS:SG	2:B:384:ILE:HD11	2.52	0.50
2:B:402:LYS:HE3	1:C:440:VAL:CG1	2.41	0.50
1:C:5:ILE:CD1	1:C:125:LEU:HD22	2.41	0.50
1:C:239:THR:OG1	1:C:240:ALA:N	2.41	0.50
1:C:273:ALA:HB2	1:C:295:CYS:CA	2.41	0.50
2:D:19:LYS:HZ2	2:D:82:PRO:HG3	1.76	0.50
2:D:186:ASN:HA	2:D:189:LEU:HD12	1.93	0.50
3:E:4:UNK:C	3:E:6:UNK:N	2.74	0.50
1:A:101:ASN:ND2	1:A:185:TYR:OH	2.44	0.50
1:A:294:ALA:HA	1:A:297:GLU:OE1	2.11	0.50
1:A:368:LEU:N	1:A:368:LEU:HD12	2.26	0.50
2:B:277:SER:O	2:B:278:ARG:O	2.29	0.50
2:B:395:PHE:CE2	2:B:418:PHE:O	2.64	0.50
1:C:75:ILE:O	1:C:75:ILE:CG1	2.58	0.50
2:D:205:ASP:HB3	2:D:303:ALA:HA	1.93	0.50
2:D:218:LYS:NZ	2:D:277:SER:HB3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:4:UNK:O	3:E:5:UNK:C	2.59	0.50
1:A:333:ALA:O	1:A:336:LYS:N	2.43	0.50
2:B:6:HIS:CE1	2:B:21:TRP:HE1	2.30	0.50
2:B:93:VAL:HG23	2:B:94:PHE:N	2.25	0.50
2:B:154:ILE:C	2:B:156:LYS:N	2.64	0.50
2:B:205:ASP:HB3	2:B:303:ALA:HA	1.93	0.50
1:C:181:VAL:HG13	1:C:181:VAL:O	2.11	0.50
1:C:208:ALA:HB2	1:C:302:MET:O	2.11	0.50
1:C:260:VAL:O	1:C:260:VAL:HG12	2.10	0.50
1:C:311:LYS:HB2	1:C:344:VAL:HG22	1.92	0.50
1:C:341:ILE:HD12	1:C:341:ILE:N	2.26	0.50
1:C:381:THR:C	1:C:383:ALA:H	2.14	0.50
1:C:414:GLU:CG	1:C:415:GLU:N	2.69	0.50
2:D:123:ARG:NH2	2:D:160:GLU:OE2	2.44	0.50
2:D:308:ARG:HH21	2:D:342:TYR:HD1	1.48	0.50
2:D:398:MET:C	2:D:400:ARG:N	2.65	0.50
1:A:38:SER:O	1:A:39:ASP:CB	2.59	0.50
1:A:82:THR:HG22	1:A:83:TYR:H	1.76	0.50
1:A:363:VAL:HG22	1:A:367:ASP:OD2	2.10	0.50
2:B:403:ALA:HB3	1:C:262:TYR:HE2	1.76	0.50
1:C:25:CYS:SG	1:C:25:CYS:O	2.69	0.50
1:C:317:LEU:HD23	1:C:377:MET:HB3	1.92	0.50
1:C:350:GLY:O	1:C:351:PHE:HD1	1.93	0.50
2:D:4:ILE:CD1	2:D:252:LEU:HD13	2.42	0.50
2:D:10:GLY:CA	2:D:146:GLY:HA3	2.41	0.50
2:D:191:VAL:HG22	2:D:421:ALA:O	2.11	0.50
2:D:289:PRO:O	2:D:292:THR:OG1	2.25	0.50
1:A:152:LEU:O	1:A:156:ARG:HG2	2.10	0.50
2:B:51:VAL:N	2:B:245:PRO:HG2	2.27	0.50
2:B:71:GLU:CB	2:B:72:PRO:CD	2.90	0.50
2:B:133:GLN:OE1	2:B:133:GLN:HA	2.11	0.50
2:B:179:ASP:HB3	2:B:182:VAL:H	1.73	0.50
2:B:228:ASN:O	2:B:231:VAL:HB	2.11	0.50
2:B:343:PHE:HB3	2:B:350:ASN:OD1	2.11	0.50
2:D:111:GLY:O	2:D:114:LEU:N	2.44	0.50
2:D:212:ILE:O	2:D:217:LEU:HB3	2.10	0.50
2:D:326:LYS:O	2:D:330:GLU:HG3	2.11	0.50
1:A:101:ASN:O	1:A:101:ASN:ND2	2.39	0.50
1:A:206:ASN:O	1:A:210:TYR:HD2	1.95	0.50
2:B:127:GLU:O	2:B:128:SER:C	2.50	0.50
2:B:140:SER:HA	2:B:171:VAL:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:ARG:CZ	2:B:197:ASN:HA	2.41	0.50
1:C:66:VAL:HG21	1:C:122:ILE:HG12	1.93	0.50
1:C:155:GLU:O	1:C:159:VAL:HG23	2.12	0.50
1:C:174:ALA:HB2	1:C:206:ASN:HB2	1.94	0.50
2:D:295:MET:O	2:D:297:ASP:N	2.43	0.50
1:A:9:VAL:HA	1:A:68:VAL:O	2.12	0.50
1:A:40:LYS:HD2	1:A:41:THR:H	1.76	0.50
1:A:74:VAL:HG13	1:A:75:ILE:N	2.27	0.50
1:A:181:VAL:HG23	1:A:404:PHE:HB2	1.93	0.50
1:A:258:ASN:HD22	1:A:258:ASN:H	1.52	0.50
1:A:332:ILE:HG23	1:A:351:PHE:CE2	2.46	0.50
1:A:344:VAL:CG1	1:A:346:TRP:NE1	2.73	0.50
1:A:413:MET:C	1:A:414:GLU:OE1	2.49	0.50
2:B:115:VAL:HG23	2:B:149:MET:HE1	1.94	0.50
2:B:211:ASP:O	2:B:215:ARG:N	2.44	0.50
2:B:266:HIS:ND1	2:B:432:TYR:CE1	2.79	0.50
2:B:311:ARG:NH1	2:B:344:VAL:HA	2.26	0.50
2:B:400:ARG:C	2:B:402:LYS:N	2.62	0.50
1:C:190:THR:CA	1:C:193:THR:HG22	2.36	0.50
1:C:203:MET:HE1	1:C:388:TRP:HD1	1.76	0.50
1:C:266:HIS:H	1:C:266:HIS:HD1	1.60	0.50
1:C:417:GLU:HB3	1:C:418:PHE:HE2	1.74	0.50
2:D:2:ARG:NE	2:D:243:ARG:CD	2.72	0.50
2:D:284:ARG:HH11	2:D:284:ARG:HG3	1.77	0.50
1:A:184:PRO:CG	1:A:399:TYR:CZ	2.93	0.50
1:A:208:ALA:O	1:A:212:ILE:HG23	2.12	0.50
1:A:244:PHE:HE1	1:A:358:GLU:OE2	1.95	0.50
1:A:401:LYS:O	1:A:402:ARG:NE	2.45	0.50
2:B:107:HIS:ND1	2:B:107:HIS:O	2.44	0.50
2:B:115:VAL:CG1	2:B:156:LYS:NZ	2.73	0.50
2:B:313:LEU:HD21	2:B:435:TYR:HD2	1.76	0.50
1:C:39:ASP:CG	1:C:40:LYS:N	2.62	0.50
1:C:77:GLU:C	1:C:83:TYR:HB2	2.32	0.50
1:C:103:TYR:O	1:C:104:ALA:C	2.47	0.50
1:C:181:VAL:O	1:C:184:PRO:HG2	2.11	0.50
1:C:183:GLU:OE2	2:D:348:PRO:HB2	2.12	0.50
1:C:184:PRO:O	1:C:188:ILE:HG13	2.11	0.50
2:D:272:PHE:HD1	2:D:275:LEU:HD23	1.77	0.50
2:D:306:ASP:HB3	2:D:309:HIS:NE2	2.26	0.50
2:D:311:ARG:HH11	2:D:344:VAL:HA	1.77	0.50
3:E:50:UNK:O	3:E:53:UNK:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:VAL:HG21	1:A:150:THR:CG2	2.42	0.50
1:A:144:GLY:CA	1:A:147:SER:HB3	2.42	0.50
1:A:171:ILE:H	1:A:171:ILE:CD1	2.25	0.50
1:A:187:SER:C	1:A:189:LEU:H	2.15	0.50
1:A:194:THR:O	1:A:195:LEU:C	2.49	0.50
1:A:194:THR:O	1:A:196:GLU:N	2.45	0.50
1:A:215:ARG:NH1	1:A:299:ALA:HB1	2.26	0.50
1:A:311:LYS:HD3	1:A:344:VAL:CG2	2.42	0.50
1:A:346:TRP:HZ2	1:A:435:VAL:HB	1.76	0.50
2:B:84:GLY:HA2	2:B:88:ARG:HH21	1.77	0.50
2:B:96:GLN:OE1	1:C:130:THR:HB	2.12	0.50
1:C:177:VAL:HG11	2:D:349:ASN:CB	2.42	0.50
1:C:194:THR:O	1:C:195:LEU:C	2.50	0.50
1:C:210:TYR:CE2	1:C:227:LEU:CD2	2.95	0.50
1:C:269:LEU:HD21	1:C:301:GLN:NE2	2.27	0.50
2:D:241:CYS:SG	2:D:320:ARG:NH1	2.85	0.50
3:E:71:UNK:O	3:E:72:UNK:C	2.60	0.50
1:A:71:GLU:O	1:A:73:THR:N	2.44	0.49
2:B:280:SER:O	2:B:282:GLN:N	2.45	0.49
2:B:315:VAL:HG23	2:B:351:VAL:HG22	1.94	0.49
1:C:242:LEU:O	1:C:243:ARG:HG2	2.12	0.49
1:C:283:HIS:O	1:C:284:GLU:HB3	2.12	0.49
2:D:6:HIS:O	2:D:66:ILE:HG22	2.12	0.49
2:D:11:GLN:C	2:D:13:GLY:H	2.15	0.49
2:D:100:GLY:C	2:D:101:ASN:HD22	2.15	0.49
2:D:218:LYS:O	2:D:219:LEU:CB	2.60	0.49
1:A:100:ALA:CA	1:A:105:ARG:HD2	2.41	0.49
1:A:102:ASN:O	1:A:105:ARG:N	2.34	0.49
1:A:174:ALA:CB	1:A:176:GLN:HG2	2.42	0.49
1:A:331:ALA:C	1:A:333:ALA:H	2.16	0.49
2:B:51:VAL:N	2:B:245:PRO:HB2	2.26	0.49
2:B:154:ILE:C	2:B:156:LYS:H	2.15	0.49
2:B:158:ARG:C	2:B:160:GLU:N	2.64	0.49
2:B:282:GLN:O	2:B:284:ARG:N	2.45	0.49
2:B:427:ASP:O	2:B:430:SER:N	2.45	0.49
1:C:41:THR:O	1:C:42:ILE:HB	2.11	0.49
1:C:393:HIS:C	1:C:395:PHE:N	2.65	0.49
1:C:402:ARG:HD2	2:D:346:TRP:CE3	2.47	0.49
2:D:87:PHE:O	2:D:89:PRO:HD2	2.12	0.49
2:D:204:ILE:HG21	2:D:209:LEU:HD11	1.93	0.49
2:D:390:ARG:HB2	2:D:391:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:MET:HE3	1:A:197:HIS:NE2	2.27	0.49
1:A:381:THR:C	1:A:383:ALA:H	2.15	0.49
1:A:386:GLU:C	1:A:388:TRP:N	2.66	0.49
2:B:4:ILE:CD1	2:B:252:LEU:HD13	2.42	0.49
2:B:59:ASN:HB3	2:B:64:ARG:HB2	1.93	0.49
2:B:344:VAL:O	2:B:345:GLU:HB3	2.13	0.49
2:B:428:LEU:HD12	2:B:428:LEU:H	1.76	0.49
1:C:213:CYS:SG	1:C:217:LEU:CD2	2.99	0.49
1:C:350:GLY:C	1:C:351:PHE:CD1	2.80	0.49
2:D:2:ARG:CG	2:D:133:GLN:HE21	2.23	0.49
2:D:107:HIS:ND1	2:D:107:HIS:O	2.46	0.49
2:D:114:LEU:O	2:D:115:VAL:C	2.49	0.49
1:A:190:THR:CA	1:A:193:THR:HG22	2.37	0.49
1:A:306:ASP:OD1	1:A:306:ASP:O	2.30	0.49
1:A:307:PRO:HA	1:A:383:ALA:CB	2.41	0.49
1:A:343:PHE:CD2	1:A:349:THR:HB	2.47	0.49
2:B:5:VAL:HA	2:B:64:ARG:HD2	1.93	0.49
2:B:271:GLY:O	2:B:272:PHE:O	2.30	0.49
2:B:398:MET:O	2:B:401:ARG:N	2.45	0.49
1:C:414:GLU:CG	1:C:415:GLU:H	2.17	0.49
2:D:79:ARG:O	2:D:79:ARG:HG2	2.13	0.49
2:D:184:PRO:CB	2:D:399:PHE:CZ	2.95	0.49
2:D:382:THR:HB	2:D:436:GLN:HG2	1.95	0.49
2:D:424:ASN:O	2:D:427:ASP:HB2	2.12	0.49
1:A:181:VAL:HG22	1:A:408:TYR:OH	2.12	0.49
2:B:295:MET:O	2:B:297:ASP:N	2.44	0.49
1:C:93:ILE:HD13	1:C:118:VAL:HA	1.95	0.49
1:C:194:THR:O	1:C:196:GLU:N	2.45	0.49
1:C:202:PHE:CE1	1:C:378:LEU:HD22	2.43	0.49
1:C:264:ARG:HH22	1:C:427:ALA:HB3	1.78	0.49
2:D:71:GLU:CB	2:D:72:PRO:CD	2.90	0.49
2:D:158:ARG:HB2	2:D:197:ASN:CB	2.31	0.49
1:A:20:CYS:C	1:A:22:GLU:H	2.16	0.49
1:A:123:ARG:O	1:A:127:ASP:HB2	2.12	0.49
1:A:142:GLY:O	1:A:182:VAL:HG23	2.13	0.49
1:A:213:CYS:SG	1:A:230:LEU:CD2	3.01	0.49
1:A:238:ILE:O	1:A:242:LEU:HD12	2.12	0.49
2:B:189:LEU:O	2:B:192:HIS:ND1	2.38	0.49
1:C:37:PRO:HA	1:C:45:GLY:O	2.13	0.49
1:C:171:ILE:N	1:C:171:ILE:CD1	2.76	0.49
2:D:242:LEU:O	2:D:243:ARG:CD	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:259:MET:CE	2:D:316:ALA:HB2	2.42	0.49
3:E:25:UNK:O	3:E:27:UNK:N	2.44	0.49
1:A:93:ILE:CD1	1:A:118:VAL:HA	2.42	0.49
1:A:217:LEU:O	1:A:217:LEU:HG	2.12	0.49
2:B:59:ASN:CB	2:B:64:ARG:HE	2.25	0.49
2:B:132:LEU:CB	2:B:164:ARG:HH21	2.15	0.49
2:B:395:PHE:CD2	2:B:422:GLU:OE1	2.66	0.49
1:C:7:ILE:HG21	1:C:122:ILE:CD1	2.42	0.49
1:C:255:PHE:CD1	1:C:259:LEU:HD12	2.48	0.49
1:C:393:HIS:O	1:C:397:LEU:HB2	2.13	0.49
2:D:2:ARG:NH2	2:D:243:ARG:HA	2.28	0.49
2:D:174:SER:C	2:D:176:LYS:N	2.66	0.49
2:D:289:PRO:CB	2:D:331:GLN:HE21	2.25	0.49
2:D:325:MET:HG2	2:D:355:VAL:HG11	1.95	0.49
1:A:2:ARG:HH22	1:A:133:GLN:HE22	1.57	0.49
1:A:68:VAL:HG13	1:A:68:VAL:O	2.13	0.49
1:A:168:GLU:HG3	1:A:201:ALA:CB	2.42	0.49
1:A:241:SER:CB	1:A:242:LEU:HD12	2.43	0.49
2:B:102:ASN:HD22	2:B:105:LYS:CB	2.26	0.49
2:B:188:THR:HA	2:B:191:VAL:HG21	1.95	0.49
2:B:381:SER:O	2:B:383:ALA:N	2.46	0.49
1:C:183:GLU:N	1:C:184:PRO:CD	2.75	0.49
1:C:283:HIS:C	1:C:285:GLN:H	2.16	0.49
1:C:420:GLU:OE1	1:C:420:GLU:O	2.30	0.49
2:D:144:GLY:HA3	2:D:185:TYR:OH	2.13	0.49
2:D:403:ALA:O	2:D:404:PHE:HB2	2.12	0.49
1:A:186:ASN:HD21	1:A:391:LEU:HD11	1.70	0.49
1:A:311:LYS:HB2	1:A:344:VAL:CG2	2.43	0.49
1:A:427:ALA:HA	1:A:430:LYS:CB	2.43	0.49
2:B:388:PHE:C	2:B:390:ARG:H	2.14	0.49
1:C:9:VAL:HG21	1:C:150:THR:HB	1.93	0.49
1:C:68:VAL:HG21	1:C:149:PHE:HE1	1.77	0.49
1:C:102:ASN:HB2	1:C:105:ARG:HB3	1.91	0.49
1:C:176:GLN:OE1	1:C:210:TYR:CE1	2.66	0.49
1:C:291:ILE:HG22	1:C:292:THR:N	2.28	0.49
2:D:6:HIS:CE1	2:D:21:TRP:HE1	2.31	0.49
3:E:58:UNK:O	3:E:59:UNK:C	2.58	0.49
1:A:26:LEU:HG	1:A:361:THR:HB	1.95	0.49
1:A:317:LEU:HD13	1:A:319:TYR:CE1	2.48	0.49
1:A:395:PHE:C	1:A:397:LEU:N	2.63	0.49
2:B:115:VAL:HG21	2:B:152:LEU:HD21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:GLN:NE2	2:B:252:LEU:CB	2.65	0.49
2:B:149:MET:CE	2:B:152:LEU:HD23	2.43	0.49
2:B:158:ARG:O	2:B:159:GLU:C	2.51	0.49
2:B:242:LEU:O	2:B:243:ARG:HD3	2.12	0.49
1:C:350:GLY:O	1:C:351:PHE:CD1	2.66	0.49
2:D:60:LYS:H	2:D:60:LYS:NZ	2.11	0.49
2:D:181:VAL:O	2:D:183:GLU:N	2.42	0.49
2:D:188:THR:HA	2:D:191:VAL:HG21	1.95	0.49
2:D:395:PHE:CE2	2:D:418:PHE:O	2.66	0.49
1:A:126:ALA:HB1	1:A:132:LEU:HD11	1.93	0.48
1:A:174:ALA:C	1:A:176:GLN:N	2.65	0.48
1:A:256:GLN:HA	1:A:260:VAL:CG2	2.43	0.48
1:A:398:MET:C	1:A:400:ALA:H	2.14	0.48
2:B:119:LEU:HD13	2:B:123:ARG:NH2	2.28	0.48
2:B:238:VAL:HG22	2:B:376:THR:HG21	1.95	0.48
1:C:185:TYR:O	1:C:186:ASN:C	2.51	0.48
2:D:8:GLN:O	2:D:67:LEU:HA	2.13	0.48
2:D:87:PHE:O	2:D:89:PRO:CD	2.61	0.48
2:D:106:GLY:O	2:D:149:MET:HA	2.13	0.48
2:D:154:ILE:C	2:D:156:LYS:N	2.65	0.48
2:D:204:ILE:HD13	2:D:231:VAL:HG13	1.94	0.48
2:D:344:VAL:CG2	2:D:345:GLU:N	2.76	0.48
1:A:102:ASN:HB2	1:A:105:ARG:HB3	1.88	0.48
1:A:294:ALA:HA	1:A:297:GLU:HB2	1.95	0.48
1:A:307:PRO:HA	1:A:383:ALA:HB3	1.95	0.48
1:A:428:LEU:C	1:A:430:LYS:N	2.66	0.48
2:B:18:ALA:C	2:B:20:PHE:N	2.66	0.48
2:B:20:PHE:HZ	2:B:239:THR:HG21	1.78	0.48
2:B:102:ASN:HB3	2:B:105:LYS:CD	2.43	0.48
2:B:262:PHE:O	2:B:265:LEU:CA	2.57	0.48
2:B:265:LEU:O	2:B:266:HIS:ND1	2.46	0.48
2:B:283:TYR:C	2:B:285:ALA:H	2.16	0.48
1:C:31:GLN:HB3	1:C:32:PRO:CD	2.37	0.48
1:C:303:VAL:HG21	1:C:384:ILE:HD11	1.94	0.48
2:D:283:TYR:C	2:D:285:ALA:H	2.15	0.48
2:D:291:LEU:H	2:D:291:LEU:CD2	2.26	0.48
2:D:313:LEU:O	2:D:314:THR:CG2	2.61	0.48
2:D:394:GLN:O	2:D:398:MET:CB	2.59	0.48
3:E:34:UNK:O	3:E:38:UNK:N	2.47	0.48
1:A:284:GLU:OE2	1:A:285:GLN:NE2	2.46	0.48
2:B:25:SER:HB3	2:B:369:ARG:HH22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:ILE:O	2:B:156:LYS:N	2.46	0.48
2:B:239:THR:O	2:B:241:CYS:N	2.46	0.48
2:B:269:MET:SD	2:B:381:SER:HB3	2.54	0.48
2:B:289:PRO:CB	2:B:331:GLN:HE21	2.26	0.48
1:C:174:ALA:CB	1:C:176:GLN:HG2	2.43	0.48
1:C:344:VAL:HG12	1:C:345:ASP:OD2	2.13	0.48
2:D:311:ARG:HG3	2:D:311:ARG:NH1	2.29	0.48
3:E:35:UNK:O	3:E:37:UNK:C	2.61	0.48
1:A:96:LYS:O	1:A:98:ASP:N	2.46	0.48
1:A:179:THR:HB	1:A:182:VAL:HB	1.94	0.48
2:B:4:ILE:HG12	2:B:133:GLN:HG2	1.95	0.48
2:B:407:TRP:HE1	1:C:257:THR:HA	1.79	0.48
1:C:77:GLU:OE2	1:C:83:TYR:CG	2.66	0.48
1:C:139:HIS:CG	1:C:140:SER:N	2.80	0.48
1:C:393:HIS:O	1:C:395:PHE:N	2.38	0.48
1:C:427:ALA:HA	1:C:430:LYS:CB	2.43	0.48
2:D:79:ARG:HA	2:D:84:GLY:CA	2.44	0.48
2:D:163:ASP:OD1	2:D:164:ARG:HG2	2.13	0.48
2:D:286:LEU:CD1	2:D:371:LEU:O	2.61	0.48
2:D:320:ARG:HB3	2:D:320:ARG:CZ	2.42	0.48
1:A:283:HIS:C	1:A:285:GLN:H	2.16	0.48
2:B:386:GLU:C	2:B:388:PHE:N	2.66	0.48
1:C:101:ASN:CB	2:D:254:LYS:HD3	2.42	0.48
1:C:181:VAL:HG23	1:C:404:PHE:HB2	1.96	0.48
1:C:244:PHE:HE1	1:C:358:GLU:OE2	1.97	0.48
1:C:274:PRO:HG3	1:C:373:ARG:O	2.13	0.48
1:C:414:GLU:CA	1:C:417:GLU:HB2	2.44	0.48
2:D:51:VAL:HG22	2:D:245:PRO:HG2	1.96	0.48
2:D:90:ASP:OD1	2:D:91:ASN:ND2	2.47	0.48
2:D:179:ASP:CB	2:D:182:VAL:HG23	2.41	0.48
2:D:279:GLY:O	2:D:281:GLN:N	2.47	0.48
1:A:408:TYR:HB2	1:A:418:PHE:HZ	1.79	0.48
2:B:137:LEU:CD2	2:B:154:ILE:HG13	2.43	0.48
2:B:181:VAL:C	2:B:184:PRO:HD2	2.34	0.48
2:B:402:LYS:CE	1:C:440:VAL:C	2.82	0.48
1:C:229:ARG:HB3	1:C:366:GLY:O	2.14	0.48
2:D:103:TRP:O	2:D:104:ALA:C	2.52	0.48
2:D:132:LEU:HD22	2:D:164:ARG:NE	2.29	0.48
2:D:132:LEU:CB	2:D:164:ARG:HH21	2.21	0.48
3:E:48:UNK:C	3:E:50:UNK:N	2.75	0.48
1:A:26:LEU:CG	1:A:361:THR:OG1	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:HIS:CD2	1:A:146:GLY:O	2.66	0.48
1:A:176:GLN:OE1	1:A:210:TYR:CE1	2.67	0.48
1:A:213:CYS:O	1:A:219:ILE:HB	2.14	0.48
2:B:62:VAL:O	2:B:63:PRO:C	2.51	0.48
2:B:93:VAL:HG23	2:B:95:GLY:N	2.28	0.48
2:B:189:LEU:HA	2:B:192:HIS:CE1	2.48	0.48
2:B:284:ARG:HB3	2:B:287:THR:OG1	2.14	0.48
2:B:397:ALA:O	2:B:398:MET:HB2	2.13	0.48
1:C:343:PHE:CD1	1:C:349:THR:HA	2.49	0.48
1:C:398:MET:HB2	1:C:403:ALA:HB2	1.96	0.48
2:D:158:ARG:HD3	2:D:197:ASN:HD22	1.67	0.48
2:D:174:SER:C	2:D:176:LYS:H	2.16	0.48
2:D:284:ARG:HB2	2:D:290:GLU:OE1	2.14	0.48
2:D:400:ARG:C	2:D:402:LYS:H	2.17	0.48
1:A:23:LEU:C	1:A:25:CYS:N	2.67	0.48
1:A:104:ALA:CA	1:A:108:TYR:HD2	2.23	0.48
1:A:209:ILE:CG2	1:A:227:LEU:HG	2.44	0.48
1:A:220:GLU:HB3	1:A:221:ARG:CZ	2.43	0.48
1:A:239:THR:OG1	1:A:240:ALA:N	2.45	0.48
1:A:286:LEU:O	1:A:287:SER:C	2.50	0.48
1:A:321:GLY:HA2	1:A:358:GLU:O	2.14	0.48
1:A:322:ASP:HA	1:A:357:TYR:CD1	2.42	0.48
2:B:102:ASN:ND2	2:B:104:ALA:HB3	2.27	0.48
2:B:139:HIS:C	2:B:139:HIS:HD2	2.17	0.48
2:B:182:VAL:O	2:B:182:VAL:CG1	2.53	0.48
2:B:212:ILE:HG21	2:B:230:LEU:HD21	1.96	0.48
1:C:103:TYR:CG	1:C:188:ILE:HD13	2.48	0.48
1:C:108:TYR:O	1:C:109:THR:C	2.52	0.48
2:D:84:GLY:HA2	2:D:88:ARG:HH21	1.78	0.48
2:D:350:ASN:HD22	2:D:350:ASN:C	2.17	0.48
2:D:383:ALA:C	2:D:385:GLN:N	2.67	0.48
1:A:174:ALA:HB2	1:A:206:ASN:HB2	1.94	0.48
1:A:417:GLU:HB3	1:A:418:PHE:HE2	1.74	0.48
1:A:426:ALA:C	1:A:428:LEU:H	2.17	0.48
2:B:59:ASN:CA	2:B:64:ARG:HH21	2.23	0.48
2:B:148:GLY:HA2	2:B:151:THR:HG22	1.95	0.48
2:B:293:GLN:C	2:B:295:MET:N	2.67	0.48
2:B:424:ASN:O	2:B:427:ASP:N	2.46	0.48
1:C:69:ASP:OD1	1:C:71:GLU:HG3	2.14	0.48
1:C:218:ASP:CG	1:C:219:ILE:H	2.16	0.48
1:C:221:ARG:H	1:C:221:ARG:NE	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:GLN:HA	1:C:260:VAL:CG2	2.44	0.48
1:C:289:ALA:HA	1:C:292:THR:HG23	1.95	0.48
2:D:62:VAL:O	2:D:62:VAL:CG2	2.62	0.48
2:D:253:ARG:HG3	2:D:253:ARG:NH1	2.27	0.48
2:D:287:THR:C	2:D:289:PRO:HD2	2.34	0.48
1:A:39:ASP:CG	1:A:40:LYS:N	2.60	0.48
1:A:77:GLU:C	1:A:83:TYR:HB2	2.35	0.48
1:A:101:ASN:CG	2:B:254:LYS:HD3	2.34	0.48
1:A:182:VAL:HG12	1:A:183:GLU:H	1.79	0.48
1:A:242:LEU:HB3	1:A:250:VAL:CG1	2.44	0.48
1:A:326:LYS:HG2	1:A:326:LYS:O	2.13	0.48
2:B:2:ARG:NH2	2:B:243:ARG:CA	2.76	0.48
2:B:22:GLU:HG3	2:B:83:PHE:CE1	2.49	0.48
2:B:106:GLY:O	2:B:149:MET:HA	2.14	0.48
2:B:297:ASP:OD1	2:B:299:LYS:N	2.36	0.48
1:C:180:ALA:O	1:C:182:VAL:N	2.47	0.48
1:C:212:ILE:C	1:C:214:ARG:H	2.17	0.48
1:C:296:PHE:HZ	1:C:317:LEU:HD21	1.79	0.48
2:D:262:PHE:HB3	2:D:263:PRO:CD	2.36	0.48
1:A:164:LYS:NZ	1:A:164:LYS:CB	2.77	0.47
1:A:311:LYS:CB	1:A:344:VAL:HG22	2.43	0.47
1:A:398:MET:CE	1:A:399:TYR:HE1	2.27	0.47
2:B:121:VAL:CG1	2:B:121:VAL:O	2.61	0.47
2:B:224:TYR:O	2:B:228:ASN:HB2	2.14	0.47
2:B:297:ASP:O	2:B:301:MET:HG2	2.13	0.47
2:B:320:ARG:HG2	2:B:320:ARG:NH1	2.29	0.47
1:C:346:TRP:HZ2	1:C:435:VAL:HB	1.79	0.47
2:D:18:ALA:O	2:D:22:GLU:OE2	2.32	0.47
2:D:381:SER:C	2:D:383:ALA:H	2.16	0.47
1:A:7:ILE:HG21	1:A:122:ILE:CD1	2.40	0.47
1:A:46:ASP:O	1:A:47:ASP:C	2.52	0.47
1:A:115:ILE:HG12	1:A:149:PHE:HE2	1.80	0.47
1:A:294:ALA:C	1:A:296:PHE:N	2.67	0.47
1:A:355:ILE:N	1:A:355:ILE:CD1	2.76	0.47
1:A:407:TRP:C	1:A:409:VAL:N	2.67	0.47
2:B:429:VAL:O	2:B:433:GLN:HG2	2.13	0.47
1:C:16:ILE:O	1:C:17:GLY:C	2.52	0.47
1:C:20:CYS:C	1:C:22:GLU:N	2.66	0.47
1:C:103:TYR:N	1:C:185:TYR:CE1	2.82	0.47
1:C:255:PHE:HD1	1:C:259:LEU:HD12	1.79	0.47
1:C:284:GLU:OE2	1:C:285:GLN:NE2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:PHE:CZ	1:C:317:LEU:HD21	2.48	0.47
1:C:417:GLU:C	1:C:418:PHE:HD2	2.15	0.47
2:D:3:GLU:O	2:D:133:GLN:N	2.38	0.47
2:D:60:LYS:N	2:D:60:LYS:HZ3	2.12	0.47
2:D:118:VAL:C	2:D:120:ASP:N	2.66	0.47
2:D:130:ASP:OD2	2:D:130:ASP:C	2.52	0.47
1:A:174:ALA:C	1:A:176:GLN:H	2.18	0.47
1:A:209:ILE:CD1	1:A:209:ILE:H	2.28	0.47
1:A:426:ALA:C	1:A:428:LEU:N	2.67	0.47
2:B:14:ASN:O	2:B:18:ALA:N	2.47	0.47
2:B:79:ARG:O	2:B:79:ARG:HG2	2.13	0.47
2:B:200:GLU:CD	2:B:268:PHE:HE2	2.17	0.47
1:C:128:GLN:OE1	1:C:128:GLN:HA	2.14	0.47
1:C:243:ARG:HA	1:C:243:ARG:NE	2.29	0.47
2:D:161:TYR:O	2:D:162:PRO:C	2.52	0.47
2:D:389:LYS:HA	2:D:392:SER:OG	2.14	0.47
1:A:217:LEU:HD23	1:A:219:ILE:CD1	2.44	0.47
2:B:427:ASP:O	2:B:428:LEU:C	2.53	0.47
1:C:307:PRO:HA	1:C:383:ALA:CB	2.45	0.47
1:C:428:LEU:C	1:C:430:LYS:N	2.68	0.47
2:D:142:GLY:HA3	2:D:186:ASN:OD1	2.15	0.47
2:D:212:ILE:HG21	2:D:230:LEU:HD21	1.95	0.47
2:D:283:TYR:HD1	2:D:284:ARG:HH21	1.62	0.47
2:D:303:ALA:HB1	2:D:387:LEU:HD12	1.95	0.47
2:D:387:LEU:O	2:D:387:LEU:CD2	2.57	0.47
2:D:405:LEU:C	2:D:407:TRP:H	2.17	0.47
1:A:343:PHE:CG	1:A:349:THR:HB	2.49	0.47
2:B:51:VAL:HG23	2:B:53:TYR:HB2	1.95	0.47
2:B:144:GLY:HA3	2:B:185:TYR:OH	2.14	0.47
2:B:154:ILE:HD11	2:B:168:THR:HG21	1.96	0.47
2:B:206:ASN:ND2	2:B:227:LEU:CD2	2.71	0.47
2:B:223:THR:HG23	2:B:225:GLY:H	1.79	0.47
2:B:235:MET:O	2:B:239:THR:OG1	2.31	0.47
2:B:242:LEU:O	2:B:243:ARG:NE	2.46	0.47
1:C:241:SER:HA	1:C:320:ARG:CZ	2.43	0.47
1:C:311:LYS:HD3	1:C:344:VAL:CG1	2.39	0.47
1:C:327:ASP:O	1:C:330:ALA:HB3	2.14	0.47
1:C:408:TYR:HB2	1:C:418:PHE:HZ	1.79	0.47
1:C:426:ALA:C	1:C:428:LEU:N	2.67	0.47
2:D:137:LEU:O	2:D:137:LEU:HG	2.15	0.47
2:D:255:LEU:HD21	2:D:259:MET:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:315:VAL:HA	2:D:379:GLY:HA2	1.97	0.47
3:E:57:UNK:O	3:E:60:UNK:N	2.48	0.47
1:A:189:LEU:HD13	1:A:193:THR:CG2	2.44	0.47
1:A:217:LEU:HD23	1:A:219:ILE:HD12	1.95	0.47
2:B:100:GLY:C	2:B:101:ASN:HD22	2.18	0.47
2:B:119:LEU:CD1	2:B:123:ARG:NH2	2.78	0.47
2:B:133:GLN:NE2	2:B:252:LEU:N	2.59	0.47
2:B:174:SER:O	2:B:176:LYS:N	2.47	0.47
2:B:178:SER:O	2:B:179:ASP:O	2.32	0.47
2:B:179:ASP:HB2	2:B:182:VAL:N	2.29	0.47
1:C:73:THR:HG23	1:C:74:VAL:H	1.79	0.47
1:C:137:VAL:HG21	1:C:154:MET:CE	2.45	0.47
1:C:286:LEU:HB3	1:C:290:GLU:HB3	1.97	0.47
1:C:295:CYS:O	1:C:295:CYS:SG	2.73	0.47
1:C:426:ALA:C	1:C:428:LEU:H	2.17	0.47
2:D:115:VAL:HG21	2:D:152:LEU:HD21	1.95	0.47
2:D:139:HIS:HD2	2:D:139:HIS:O	1.98	0.47
2:D:158:ARG:HG3	2:D:159:GLU:HG3	1.97	0.47
2:D:202:TYR:HE1	2:D:378:ILE:HD12	1.76	0.47
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.49	0.47
1:A:242:LEU:HD11	1:A:318:LEU:HG	1.97	0.47
2:B:154:ILE:HG23	2:B:197:ASN:HB3	1.97	0.47
2:B:282:GLN:C	2:B:285:ALA:H	2.17	0.47
2:B:286:LEU:CD1	2:B:371:LEU:O	2.63	0.47
1:C:35:GLN:HE22	1:C:88:HIS:CG	2.32	0.47
1:C:179:THR:HG22	1:C:180:ALA:O	2.15	0.47
1:C:190:THR:HG21	1:C:425:MET:SD	2.55	0.47
1:C:286:LEU:O	1:C:287:SER:C	2.51	0.47
1:C:294:ALA:HA	1:C:297:GLU:HB2	1.96	0.47
1:C:294:ALA:C	1:C:296:PHE:N	2.67	0.47
1:C:312:TYR:O	1:C:344:VAL:HG23	2.14	0.47
1:C:368:LEU:HD12	1:C:368:LEU:N	2.29	0.47
1:C:385:ALA:HB1	1:C:429:GLU:HG3	1.97	0.47
2:D:1:MET:C	2:D:3:GLU:N	2.68	0.47
2:D:19:LYS:HA	2:D:22:GLU:CG	2.45	0.47
2:D:81:GLY:N	2:D:82:PRO:HD2	2.29	0.47
2:D:93:VAL:CG2	2:D:94:PHE:N	2.78	0.47
2:D:124:LYS:HG3	2:D:124:LYS:O	2.15	0.47
2:D:271:GLY:O	2:D:272:PHE:O	2.33	0.47
2:D:295:MET:HG2	2:D:377:PHE:HD2	1.79	0.47
2:D:307:PRO:C	2:D:309:HIS:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:386:GLU:C	2:D:388:PHE:N	2.66	0.47
1:A:77:GLU:OE2	1:A:83:TYR:CG	2.68	0.47
1:A:86:LEU:HD13	1:A:89:PRO:HD3	1.97	0.47
1:A:152:LEU:O	1:A:153:LEU:C	2.52	0.47
1:A:184:PRO:O	1:A:188:ILE:HG13	2.14	0.47
1:A:311:LYS:CD	1:A:344:VAL:HG13	2.31	0.47
1:A:314:ALA:O	1:A:315:CYS:HB3	2.15	0.47
2:B:129:CYS:O	2:B:130:ASP:C	2.52	0.47
2:B:253:ARG:C	2:B:255:LEU:N	2.68	0.47
2:B:293:GLN:C	2:B:295:MET:H	2.17	0.47
1:C:23:LEU:O	1:C:26:LEU:CD1	2.63	0.47
1:C:401:LYS:O	1:C:402:ARG:NE	2.47	0.47
1:C:407:TRP:C	1:C:409:VAL:N	2.65	0.47
2:D:209:LEU:CB	2:D:227:LEU:HG	2.45	0.47
2:D:312:TYR:CE2	2:D:377:PHE:HZ	2.32	0.47
1:A:274:PRO:HG3	1:A:373:ARG:O	2.14	0.47
1:A:306:ASP:HB3	1:A:386:GLU:OE1	2.15	0.47
2:B:174:SER:C	2:B:176:LYS:N	2.68	0.47
2:B:218:LYS:NZ	2:B:277:SER:HB3	2.29	0.47
2:B:243:ARG:HA	2:B:243:ARG:HD3	1.47	0.47
1:C:9:VAL:HG21	1:C:150:THR:HG22	1.96	0.47
1:C:16:ILE:CG2	1:C:17:GLY:N	2.67	0.47
1:C:20:CYS:O	1:C:24:TYR:N	2.34	0.47
1:C:243:ARG:NH1	1:C:250:VAL:HG13	2.19	0.47
1:C:256:GLN:HB3	1:C:260:VAL:CB	2.41	0.47
1:C:311:LYS:CD	1:C:344:VAL:HG22	2.44	0.47
1:C:419:SER:O	1:C:422:ARG:HG2	2.14	0.47
2:D:16:ILE:HD12	2:D:231:VAL:CG1	2.42	0.47
2:D:22:GLU:HG3	2:D:83:PHE:CE1	2.50	0.47
2:D:283:TYR:C	2:D:285:ALA:N	2.67	0.47
1:A:144:GLY:H	1:A:147:SER:HB3	1.76	0.47
1:A:177:VAL:HG11	2:B:349:ASN:CB	2.45	0.47
1:A:206:ASN:O	1:A:207:GLU:C	2.53	0.47
1:A:209:ILE:HG22	1:A:227:LEU:HG	1.97	0.47
2:B:11:GLN:C	2:B:13:GLY:H	2.18	0.47
2:B:118:VAL:C	2:B:120:ASP:N	2.65	0.47
2:B:220:THR:HB	1:C:326:LYS:CE	2.45	0.47
2:B:284:ARG:HH11	2:B:284:ARG:HG3	1.79	0.47
2:B:298:ALA:HB2	2:B:307:PRO:CD	2.45	0.47
1:C:73:THR:HA	1:C:76:ASP:HB2	1.96	0.47
1:C:416:GLY:O	1:C:420:GLU:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:ILE:HG12	2:D:133:GLN:HG2	1.97	0.47
2:D:58:GLY:O	2:D:64:ARG:CZ	2.63	0.47
2:D:141:LEU:HG	2:D:170:SER:HB3	1.97	0.47
2:D:186:ASN:O	2:D:189:LEU:HB2	2.15	0.47
2:D:203:CYS:SG	2:D:384:ILE:CD1	3.02	0.47
2:D:249:ASN:CG	2:D:250:ALA:N	2.68	0.47
2:D:320:ARG:HH11	2:D:320:ARG:CG	2.25	0.47
2:D:357:ASP:CB	2:D:358:ILE:HD12	2.45	0.47
3:E:42:UNK:O	3:E:45:UNK:N	2.48	0.47
1:A:123:ARG:HA	1:A:161:TYR:OH	2.15	0.46
1:A:185:TYR:CE1	1:A:408:TYR:HE1	2.33	0.46
1:A:185:TYR:O	1:A:188:ILE:HD12	2.15	0.46
1:A:264:ARG:O	1:A:266:HIS:ND1	2.48	0.46
1:A:265:ALA:O	1:A:266:HIS:O	2.33	0.46
1:A:295:CYS:SG	1:A:377:MET:HE1	2.55	0.46
1:A:362:VAL:O	1:A:370:LYS:NZ	2.48	0.46
2:B:191:VAL:O	2:B:191:VAL:CG1	2.58	0.46
2:B:402:LYS:HE3	1:C:440:VAL:C	2.35	0.46
1:C:273:ALA:HB2	1:C:295:CYS:HA	1.97	0.46
1:C:343:PHE:CG	1:C:349:THR:HB	2.50	0.46
1:C:385:ALA:HB2	1:C:432:TYR:CD2	2.47	0.46
2:D:238:VAL:HG22	2:D:376:THR:HG21	1.96	0.46
3:E:61:UNK:C	3:E:63:UNK:N	2.78	0.46
1:A:102:ASN:O	1:A:103:TYR:C	2.54	0.46
2:B:320:ARG:HH11	2:B:320:ARG:CG	2.25	0.46
1:C:26:LEU:HG	1:C:361:THR:HB	1.97	0.46
1:C:172:TYR:CG	1:C:173:PRO:HD2	2.50	0.46
2:D:3:GLU:HG2	2:D:58:GLY:O	2.15	0.46
2:D:63:PRO:C	2:D:65:ALA:N	2.67	0.46
2:D:401:ARG:O	2:D:402:LYS:HG3	2.15	0.46
1:A:132:LEU:O	1:A:133:GLN:CB	2.61	0.46
1:A:317:LEU:HD23	1:A:377:MET:HB2	1.96	0.46
1:A:393:HIS:C	1:A:395:PHE:N	2.68	0.46
1:A:402:ARG:NH1	2:B:346:TRP:CD2	2.83	0.46
2:B:75:MET:SD	2:B:79:ARG:CZ	3.02	0.46
2:B:114:LEU:HD12	2:B:114:LEU:HA	1.78	0.46
2:B:142:GLY:HA2	2:B:185:TYR:CB	2.39	0.46
2:B:305:CYS:O	2:B:306:ASP:C	2.53	0.46
1:C:9:VAL:O	1:C:9:VAL:CG2	2.63	0.46
1:C:68:VAL:HG13	1:C:68:VAL:O	2.14	0.46
2:D:60:LYS:H	2:D:60:LYS:CD	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:243:ARG:HD3	2:D:243:ARG:HA	1.52	0.46
2:D:313:LEU:O	2:D:314:THR:HG23	2.15	0.46
1:A:181:VAL:O	1:A:185:TYR:CD2	2.69	0.46
1:A:243:ARG:NH1	1:A:250:VAL:CG1	2.72	0.46
1:A:275:VAL:O	1:A:275:VAL:CG1	2.63	0.46
2:B:103:TRP:N	2:B:185:TYR:OH	2.48	0.46
2:B:313:LEU:O	2:B:314:THR:CG2	2.64	0.46
2:B:389:LYS:HA	2:B:392:SER:OG	2.14	0.46
1:C:24:TYR:HA	1:C:26:LEU:CD1	2.46	0.46
1:C:101:ASN:OD1	2:D:254:LYS:CD	2.59	0.46
1:C:273:ALA:HB2	1:C:295:CYS:CB	2.42	0.46
2:D:3:GLU:OE2	2:D:128:SER:O	2.33	0.46
2:D:132:LEU:H	2:D:164:ARG:HH21	1.62	0.46
2:D:137:LEU:CD2	2:D:154:ILE:HG13	2.46	0.46
2:D:350:ASN:ND2	2:D:350:ASN:N	2.62	0.46
1:A:122:ILE:HG22	1:A:123:ARG:N	2.30	0.46
1:A:209:ILE:HD12	1:A:209:ILE:H	1.79	0.46
1:A:388:TRP:CZ3	1:A:428:LEU:HD13	2.50	0.46
2:B:124:LYS:HG3	2:B:124:LYS:O	2.15	0.46
2:B:405:LEU:C	2:B:407:TRP:H	2.18	0.46
1:C:344:VAL:CG1	1:C:345:ASP:N	2.75	0.46
1:C:386:GLU:C	1:C:388:TRP:N	2.68	0.46
1:C:398:MET:CE	1:C:399:TYR:HE1	2.29	0.46
2:D:322:ARG:NE	2:D:357:ASP:CB	2.74	0.46
2:D:350:ASN:ND2	2:D:350:ASN:H	2.13	0.46
1:A:172:TYR:CG	1:A:173:PRO:HD2	2.51	0.46
1:A:287:SER:O	1:A:289:ALA:N	2.49	0.46
2:B:60:LYS:H	2:B:60:LYS:HD2	1.79	0.46
2:B:73:GLY:O	2:B:78:VAL:HG21	2.16	0.46
2:B:320:ARG:HB3	2:B:320:ARG:CZ	2.45	0.46
1:C:122:ILE:O	1:C:125:LEU:N	2.48	0.46
1:C:265:ALA:O	1:C:266:HIS:O	2.33	0.46
1:C:344:VAL:HG12	1:C:345:ASP:CG	2.36	0.46
2:D:148:GLY:CA	2:D:151:THR:HG22	2.46	0.46
2:D:239:THR:HB	2:D:240:THR:H	1.42	0.46
1:A:23:LEU:O	1:A:26:LEU:CD1	2.63	0.46
1:A:112:LYS:HZ1	3:E:12:UNK:CB	2.29	0.46
1:A:218:ASP:CG	1:A:219:ILE:N	2.69	0.46
1:A:341:ILE:HD12	1:A:341:ILE:N	2.30	0.46
1:A:416:GLY:O	1:A:420:GLU:HB3	2.16	0.46
2:B:137:LEU:HD23	2:B:154:ILE:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:PHE:CD2	1:C:149:PHE:O	2.69	0.46
1:C:154:MET:CE	1:C:197:HIS:NE2	2.79	0.46
1:C:159:VAL:HG21	3:E:56:UNK:HA	1.98	0.46
1:C:245:ASP:O	1:C:249:ASN:OD1	2.33	0.46
2:D:18:ALA:O	2:D:21:TRP:N	2.46	0.46
2:D:378:ILE:HG22	2:D:378:ILE:O	2.16	0.46
1:A:84:ARG:C	1:A:85:GLN:HG2	2.36	0.46
1:A:398:MET:HB2	1:A:403:ALA:HB2	1.96	0.46
2:B:194:LEU:HD12	2:B:428:LEU:HD21	1.97	0.46
2:B:283:TYR:C	2:B:285:ALA:N	2.68	0.46
2:B:308:ARG:HG3	2:B:342:TYR:CZ	2.51	0.46
2:B:315:VAL:HA	2:B:379:GLY:HA2	1.98	0.46
2:B:383:ALA:C	2:B:385:GLN:N	2.68	0.46
1:C:20:CYS:C	1:C:22:GLU:H	2.19	0.46
1:C:159:VAL:CG2	3:E:56:UNK:HA	2.46	0.46
1:C:166:LYS:HD2	1:C:197:HIS:HD2	1.81	0.46
1:C:171:ILE:CG2	4:C:502:GTP:HN22	2.29	0.46
1:C:182:VAL:HG12	1:C:183:GLU:N	2.31	0.46
1:C:251:ASP:O	1:C:254:GLU:N	2.49	0.46
1:C:274:PRO:HB3	1:C:291:ILE:CD1	2.45	0.46
2:D:20:PHE:O	2:D:23:VAL:N	2.48	0.46
2:D:174:SER:O	2:D:176:LYS:N	2.49	0.46
2:D:291:LEU:HD22	2:D:291:LEU:N	2.30	0.46
2:D:331:GLN:OE1	2:D:331:GLN:HA	2.15	0.46
1:A:44:GLY:C	1:A:46:ASP:N	2.69	0.46
1:A:103:TYR:CD1	1:A:188:ILE:HD13	2.51	0.46
1:A:149:PHE:CD2	1:A:149:PHE:O	2.69	0.46
1:A:206:ASN:O	1:A:210:TYR:CD2	2.69	0.46
1:A:225:THR:HA	1:A:228:ASN:HB2	1.98	0.46
1:A:265:ALA:O	1:A:266:HIS:C	2.54	0.46
2:B:279:GLY:O	2:B:281:GLN:N	2.49	0.46
2:B:398:MET:HG3	1:C:346:TRP:O	2.16	0.46
2:B:428:LEU:HD12	2:B:428:LEU:N	2.31	0.46
2:B:430:SER:O	2:B:431:GLU:C	2.54	0.46
1:C:175:PRO:HB2	1:C:207:GLU:OE2	2.16	0.46
2:D:169:PHE:CG	2:D:235:MET:SD	3.09	0.46
2:D:215:ARG:NE	2:D:215:ARG:CA	2.78	0.46
2:D:238:VAL:HG21	2:D:378:ILE:HD11	1.98	0.46
1:A:306:ASP:OD1	1:A:309:HIS:NE2	2.49	0.46
1:A:371:VAL:CG1	1:A:372:GLN:N	2.78	0.46
1:A:371:VAL:HG11	1:A:373:ARG:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:HIS:ND1	2:B:21:TRP:HZ2	2.14	0.46
2:B:11:GLN:OE1	2:B:73:GLY:HA3	2.15	0.46
2:B:119:LEU:HD13	2:B:123:ARG:CZ	2.46	0.46
2:B:238:VAL:HG21	2:B:378:ILE:HD11	1.98	0.46
2:B:283:TYR:HD1	2:B:284:ARG:HH21	1.64	0.46
1:C:42:ILE:HD12	1:C:43:GLY:H	1.81	0.46
1:C:184:PRO:CG	1:C:399:TYR:CZ	2.98	0.46
1:C:331:ALA:O	1:C:335:ILE:HG23	2.15	0.46
2:D:122:VAL:CG1	2:D:123:ARG:N	2.78	0.46
2:D:259:MET:HE1	2:D:316:ALA:HB2	1.98	0.46
2:D:416:MET:HA	2:D:419:THR:OG1	2.16	0.46
1:A:21:TRP:CD1	1:A:21:TRP:N	2.84	0.45
1:A:36:MET:HE2	1:A:37:PRO:HD2	1.98	0.45
1:A:210:TYR:CE2	1:A:227:LEU:CD2	2.98	0.45
1:A:242:LEU:O	1:A:250:VAL:HG12	2.16	0.45
1:A:262:TYR:HE1	1:A:346:TRP:CH2	2.35	0.45
1:A:276:ILE:CG1	1:A:282:TYR:CD2	2.98	0.45
2:B:287:THR:CB	2:B:289:PRO:HD2	2.41	0.45
1:C:104:ALA:CA	1:C:108:TYR:HD2	2.23	0.45
1:C:316:CYS:HB2	1:C:352:LYS:CB	2.24	0.45
1:C:419:SER:O	1:C:420:GLU:C	2.55	0.45
2:D:20:PHE:HZ	2:D:239:THR:HG21	1.81	0.45
2:D:290:GLU:HG2	2:D:294:GLN:HB2	1.97	0.45
2:D:351:VAL:HG12	2:D:352:LYS:N	2.32	0.45
2:D:351:VAL:O	2:D:352:LYS:HG3	2.17	0.45
1:A:10:GLY:O	1:A:11:GLN:C	2.54	0.45
1:A:244:PHE:H	1:A:244:PHE:HD2	1.63	0.45
1:A:280:LYS:O	1:A:282:TYR:CD2	2.69	0.45
2:B:73:GLY:C	2:B:75:MET:H	2.20	0.45
2:B:81:GLY:N	2:B:82:PRO:HD2	2.32	0.45
2:B:158:ARG:HB2	2:B:197:ASN:HD22	1.81	0.45
2:B:174:SER:C	2:B:176:LYS:H	2.19	0.45
2:B:208:ALA:HB2	2:B:304:ALA:CB	2.47	0.45
2:B:211:ASP:O	2:B:215:ARG:HB2	2.16	0.45
2:B:247:GLN:OE1	2:B:356:CYS:HA	2.16	0.45
1:C:102:ASN:O	1:C:103:TYR:C	2.53	0.45
1:C:206:ASN:O	1:C:210:TYR:CD2	2.69	0.45
1:C:398:MET:HE3	1:C:399:TYR:HE1	1.80	0.45
2:D:58:GLY:O	2:D:64:ARG:NH2	2.49	0.45
2:D:119:LEU:HD13	2:D:123:ARG:NH2	2.30	0.45
2:D:298:ALA:HB2	2:D:307:PRO:CD	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:VAL:CG1	1:A:75:ILE:N	2.78	0.45
1:A:242:LEU:O	1:A:250:VAL:CG1	2.64	0.45
1:A:255:PHE:HD1	1:A:259:LEU:HD12	1.81	0.45
2:B:5:VAL:O	2:B:5:VAL:HG12	2.17	0.45
2:B:313:LEU:O	2:B:314:THR:HG23	2.16	0.45
1:C:139:HIS:CD2	1:C:146:GLY:O	2.69	0.45
1:C:197:HIS:CG	1:C:198:SER:N	2.83	0.45
1:C:209:ILE:O	1:C:211:ASP:N	2.49	0.45
2:D:14:ASN:O	2:D:18:ALA:N	2.46	0.45
2:D:235:MET:O	2:D:239:THR:OG1	2.35	0.45
2:D:247:GLN:OE1	2:D:356:CYS:HA	2.16	0.45
2:D:276:THR:HG21	2:D:281:GLN:CG	2.47	0.45
1:A:221:ARG:HA	1:A:222:PRO:HD2	1.71	0.45
1:A:238:ILE:O	1:A:239:THR:O	2.35	0.45
1:A:414:GLU:HA	1:A:417:GLU:HB2	1.98	0.45
1:C:5:ILE:O	1:C:136:SER:N	2.48	0.45
1:C:99:ALA:O	1:C:100:ALA:HB2	2.17	0.45
1:C:189:LEU:HD13	1:C:193:THR:CG2	2.45	0.45
2:D:276:THR:HG21	2:D:281:GLN:CB	2.47	0.45
2:D:399:PHE:HE2	2:D:404:PHE:HB3	1.80	0.45
3:E:10:UNK:C	3:E:12:UNK:N	2.71	0.45
1:A:5:ILE:HG22	1:A:6:SER:N	2.31	0.45
1:A:143:GLY:O	1:A:144:GLY:C	2.55	0.45
1:A:179:THR:HB	1:A:182:VAL:CG2	2.47	0.45
1:A:277:SER:O	1:A:278:ALA:CB	2.62	0.45
2:B:51:VAL:HG13	2:B:245:PRO:HB2	1.99	0.45
2:B:60:LYS:H	2:B:60:LYS:CD	2.29	0.45
2:B:87:PHE:O	2:B:89:PRO:N	2.49	0.45
2:B:403:ALA:O	2:B:404:PHE:HB2	2.16	0.45
2:B:424:ASN:O	2:B:427:ASP:HB2	2.17	0.45
1:C:67:PHE:O	1:C:92:LEU:HA	2.16	0.45
1:C:119:LEU:HD22	1:C:156:ARG:HE	1.81	0.45
1:C:197:HIS:CE1	1:C:198:SER:HB3	2.52	0.45
1:C:365:GLY:O	1:C:368:LEU:HD11	2.17	0.45
1:C:380:ASN:CG	1:C:380:ASN:O	2.53	0.45
2:D:2:ARG:O	2:D:2:ARG:HG2	2.17	0.45
2:D:284:ARG:O	2:D:285:ALA:C	2.54	0.45
1:A:108:TYR:O	1:A:109:THR:C	2.55	0.45
1:A:363:VAL:HG22	1:A:367:ASP:CG	2.36	0.45
1:A:364:PRO:C	1:A:366:GLY:H	2.20	0.45
1:A:398:MET:HE3	1:A:399:TYR:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:LYS:HD2	2:B:210:TYR:CE1	2.52	0.45
2:B:272:PHE:CE1	2:B:274:PRO:HG2	2.51	0.45
1:C:115:ILE:HG12	1:C:149:PHE:HE2	1.80	0.45
1:C:164:LYS:HB2	1:C:164:LYS:NZ	2.29	0.45
1:C:206:ASN:O	1:C:207:GLU:C	2.55	0.45
1:C:287:SER:O	1:C:289:ALA:N	2.50	0.45
1:C:332:ILE:HG23	1:C:351:PHE:CE2	2.52	0.45
2:D:59:ASN:HA	2:D:60:LYS:NZ	2.32	0.45
2:D:140:SER:O	2:D:147:SER:OG	2.33	0.45
2:D:211:ASP:O	2:D:215:ARG:N	2.50	0.45
2:D:234:THR:O	2:D:238:VAL:HG23	2.17	0.45
2:D:311:ARG:NE	2:D:436:GLN:O	2.50	0.45
2:D:405:LEU:HD22	2:D:405:LEU:O	2.16	0.45
1:A:327:ASP:O	1:A:330:ALA:HB3	2.16	0.45
2:B:133:GLN:CG	2:B:252:LEU:HD22	2.47	0.45
1:C:16:ILE:HG22	1:C:17:GLY:H	1.79	0.45
1:C:371:VAL:HG12	1:C:372:GLN:H	1.81	0.45
1:C:408:TYR:O	1:C:414:GLU:HG3	2.17	0.45
2:D:206:ASN:ND2	5:D:503:GDP:N2	2.64	0.45
2:D:334:ASN:O	2:D:338:LYS:N	2.50	0.45
1:A:171:ILE:HG21	4:A:500:GTP:HN22	1.81	0.45
1:A:206:ASN:CB	1:A:210:TYR:HE2	2.28	0.45
1:A:344:VAL:CG1	1:A:345:ASP:N	2.76	0.45
1:A:417:GLU:C	1:A:418:PHE:HD2	2.17	0.45
2:B:102:ASN:HB3	2:B:105:LYS:CG	2.47	0.45
1:C:172:TYR:H	1:C:205:ASP:H	1.65	0.45
1:C:344:VAL:HG12	1:C:345:ASP:H	1.81	0.45
1:C:355:ILE:N	1:C:355:ILE:CD1	2.79	0.45
2:D:209:LEU:HD21	2:D:302:MET:HG3	1.98	0.45
2:D:436:GLN:HE21	2:D:436:GLN:C	2.20	0.45
1:A:155:GLU:OE2	1:A:196:GLU:HB3	2.17	0.45
2:B:298:ALA:HA	2:B:301:MET:CG	2.47	0.45
1:C:31:GLN:CB	1:C:32:PRO:CD	2.94	0.45
1:C:171:ILE:HG21	4:C:502:GTP:N3	2.32	0.45
1:C:223:THR:O	1:C:226:ASN:N	2.50	0.45
1:C:326:LYS:O	1:C:326:LYS:HG2	2.16	0.45
1:C:343:PHE:CD2	1:C:349:THR:HB	2.52	0.45
1:C:396:ASP:O	1:C:400:ALA:HB3	2.17	0.45
2:D:85:GLN:HA	2:D:88:ARG:HG2	1.98	0.45
2:D:158:ARG:HB2	2:D:197:ASN:ND2	2.30	0.45
2:D:403:ALA:HB1	2:D:405:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:TYR:O	1:A:84:ARG:HB2	2.17	0.45
1:A:171:ILE:N	1:A:171:ILE:CD1	2.78	0.45
1:A:255:PHE:CD1	1:A:259:LEU:HD12	2.52	0.45
1:A:346:TRP:CD1	1:A:346:TRP:N	2.74	0.45
1:A:351:PHE:HB3	1:A:352:LYS:H	1.63	0.45
2:B:115:VAL:HG21	2:B:152:LEU:CD2	2.47	0.45
2:B:126:SER:O	2:B:127:GLU:C	2.54	0.45
2:B:217:LEU:CG	2:B:218:LYS:N	2.75	0.45
2:B:226:ASP:C	2:B:228:ASN:N	2.70	0.45
2:B:290:GLU:O	2:B:291:LEU:C	2.55	0.45
2:B:351:VAL:HG12	2:B:352:LYS:N	2.32	0.45
2:B:428:LEU:O	2:B:429:VAL:C	2.54	0.45
1:C:101:ASN:O	1:C:101:ASN:ND2	2.44	0.45
1:C:101:ASN:ND2	1:C:185:TYR:OH	2.50	0.45
1:C:197:HIS:CD2	1:C:198:SER:HB3	2.52	0.45
1:C:402:ARG:O	1:C:405:VAL:HG12	2.17	0.45
1:C:433:GLU:C	1:C:435:VAL:N	2.69	0.45
3:E:3:UNK:C	3:E:5:UNK:N	2.80	0.45
1:A:284:GLU:O	1:A:285:GLN:CG	2.65	0.44
2:B:59:ASN:CA	2:B:60:LYS:HZ3	2.29	0.44
2:B:115:VAL:CG1	2:B:156:LYS:HZ3	2.30	0.44
2:B:307:PRO:C	2:B:309:HIS:N	2.69	0.44
1:C:185:TYR:HA	1:C:188:ILE:CD1	2.33	0.44
1:C:256:GLN:C	1:C:258:ASN:H	2.19	0.44
2:D:115:VAL:CG1	2:D:156:LYS:HZ3	2.30	0.44
2:D:178:SER:O	2:D:179:ASP:O	2.35	0.44
1:A:88:HIS:HA	1:A:89:PRO:HD2	1.87	0.44
2:B:51:VAL:O	2:B:53:TYR:N	2.50	0.44
2:B:242:LEU:O	2:B:243:ARG:CD	2.64	0.44
1:C:86:LEU:HD13	1:C:89:PRO:HD3	1.99	0.44
1:C:163:LYS:C	1:C:164:LYS:HZ1	2.20	0.44
2:D:102:ASN:HA	2:D:408:TYR:HE1	1.82	0.44
2:D:155:SER:HB2	2:D:196:GLU:HG2	1.98	0.44
2:D:185:TYR:O	2:D:188:THR:HG22	2.16	0.44
2:D:287:THR:CB	2:D:289:PRO:HD2	2.39	0.44
1:A:9:VAL:O	1:A:9:VAL:CG2	2.66	0.44
1:A:24:TYR:HA	1:A:26:LEU:HD12	1.99	0.44
1:A:100:ALA:CB	1:A:105:ARG:HD2	2.47	0.44
1:A:137:VAL:HG21	1:A:154:MET:SD	2.57	0.44
1:A:169:PHE:HE1	1:A:238:ILE:CD1	2.30	0.44
1:A:276:ILE:HD12	1:A:277:SER:H	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:CZ	2:B:243:ARG:HD3	2.47	0.44
2:B:184:PRO:CB	2:B:399:PHE:CZ	3.00	0.44
2:B:286:LEU:HA	2:B:290:GLU:CD	2.37	0.44
1:C:331:ALA:O	1:C:333:ALA:N	2.51	0.44
2:D:25:SER:HB3	2:D:369:ARG:NH2	2.31	0.44
2:D:88:ARG:CB	2:D:89:PRO:HD3	2.34	0.44
2:D:280:SER:O	2:D:282:GLN:N	2.50	0.44
2:D:284:ARG:O	2:D:287:THR:N	2.51	0.44
1:A:164:LYS:N	1:A:164:LYS:NZ	2.60	0.44
1:A:420:GLU:C	1:A:420:GLU:OE1	2.54	0.44
2:B:138:THR:HG22	2:B:139:HIS:N	2.32	0.44
2:B:298:ALA:HB2	2:B:307:PRO:HD2	2.00	0.44
2:B:308:ARG:NH2	2:B:342:TYR:CG	2.83	0.44
1:C:11:GLN:OE1	4:C:502:GTP:O1B	2.35	0.44
1:C:16:ILE:O	1:C:19:ALA:N	2.41	0.44
1:C:273:ALA:CB	1:C:295:CYS:HB2	2.45	0.44
1:C:363:VAL:HG22	1:C:367:ASP:OD2	2.18	0.44
1:C:380:ASN:O	1:C:380:ASN:OD1	2.35	0.44
1:C:413:MET:C	1:C:414:GLU:CD	2.76	0.44
2:D:139:HIS:O	2:D:170:SER:HA	2.17	0.44
2:D:151:THR:HG21	2:D:189:LEU:HD21	1.99	0.44
1:A:139:HIS:NE2	1:A:150:THR:CG2	2.79	0.44
1:A:214:ARG:CA	1:A:218:ASP:O	2.61	0.44
1:A:256:GLN:C	1:A:258:ASN:H	2.20	0.44
1:A:344:VAL:HG12	1:A:345:ASP:OD2	2.17	0.44
2:B:4:ILE:N	2:B:58:GLY:HA2	2.33	0.44
2:B:338:LYS:O	2:B:340:SER:N	2.43	0.44
2:B:407:TRP:HE1	1:C:257:THR:CA	2.31	0.44
1:C:7:ILE:HG13	1:C:7:ILE:O	2.18	0.44
1:C:67:PHE:O	1:C:75:ILE:HD11	2.17	0.44
1:C:96:LYS:HE3	1:C:96:LYS:HB2	1.77	0.44
1:C:188:ILE:HG13	1:C:188:ILE:H	1.62	0.44
1:C:344:VAL:CG1	1:C:345:ASP:H	2.30	0.44
1:C:347:CYS:O	1:C:349:THR:N	2.50	0.44
1:C:428:LEU:C	1:C:430:LYS:H	2.21	0.44
2:D:95:GLY:O	2:D:96:GLN:HB3	2.18	0.44
2:D:97:SER:HG	2:D:110:GLU:CG	2.30	0.44
2:D:187:ALA:HB2	2:D:391:ILE:CG2	2.48	0.44
2:D:344:VAL:O	2:D:346:TRP:CD1	2.70	0.44
1:A:111:GLY:C	1:A:113:GLU:N	2.71	0.44
1:A:306:ASP:C	1:A:308:ARG:N	2.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:GLU:CG	1:A:415:GLU:H	2.13	0.44
2:B:2:ARG:CZ	2:B:243:ARG:CD	2.96	0.44
2:B:12:CYS:HB2	5:B:501:GDP:PA	2.58	0.44
2:B:58:GLY:O	2:B:64:ARG:NH2	2.50	0.44
2:B:59:ASN:ND2	2:B:60:LYS:H	2.16	0.44
2:B:271:GLY:O	2:B:377:PHE:HB2	2.18	0.44
2:B:273:ALA:HB3	2:B:274:PRO:CD	2.48	0.44
2:B:334:ASN:O	2:B:338:LYS:N	2.51	0.44
2:B:407:TRP:HE1	1:C:257:THR:N	2.15	0.44
1:C:10:GLY:O	1:C:11:GLN:C	2.56	0.44
1:C:46:ASP:O	1:C:47:ASP:C	2.56	0.44
1:C:340:THR:O	1:C:342:GLN:HG2	2.17	0.44
2:D:179:ASP:HB2	2:D:182:VAL:CB	2.47	0.44
3:E:13:UNK:C	3:E:15:UNK:N	2.77	0.44
1:A:142:GLY:HA2	1:A:185:TYR:HB2	1.98	0.44
1:A:344:VAL:HG12	1:A:345:ASP:CG	2.38	0.44
2:B:103:TRP:O	2:B:105:LYS:N	2.50	0.44
2:B:182:VAL:HG11	5:B:501:GDP:O3'	2.17	0.44
2:B:283:TYR:O	2:B:290:GLU:OE1	2.36	0.44
2:B:303:ALA:HB1	2:B:387:LEU:HD13	1.99	0.44
1:C:177:VAL:HG21	2:D:349:ASN:HB2	1.99	0.44
1:C:227:LEU:N	1:C:227:LEU:CD1	2.81	0.44
1:C:259:LEU:HD21	1:C:378:LEU:CB	2.45	0.44
1:C:312:TYR:H	1:C:312:TYR:HD1	1.65	0.44
2:D:223:THR:C	2:D:225:GLY:H	2.20	0.44
2:D:358:ILE:HD12	2:D:358:ILE:N	2.21	0.44
3:E:71:UNK:O	3:E:74:UNK:N	2.51	0.44
1:A:289:ALA:HA	1:A:292:THR:HG23	1.96	0.44
1:A:305:CYS:C	1:A:386:GLU:OE1	2.56	0.44
2:B:121:VAL:O	2:B:121:VAL:HG12	2.16	0.44
2:B:165:ILE:HG13	2:B:253:ARG:CG	2.48	0.44
2:B:274:PRO:HB2	2:B:371:LEU:HD11	1.99	0.44
2:B:320:ARG:NH1	2:B:320:ARG:CG	2.79	0.44
1:C:277:SER:O	1:C:368:LEU:HB3	2.17	0.44
1:C:288:VAL:HA	1:C:373:ARG:CD	2.47	0.44
1:C:306:ASP:C	1:C:308:ARG:N	2.69	0.44
2:D:51:VAL:HG23	2:D:53:TYR:HB2	1.99	0.44
2:D:273:ALA:H	2:D:274:PRO:HD2	1.83	0.44
2:D:430:SER:O	2:D:431:GLU:C	2.56	0.44
1:A:126:ALA:O	1:A:132:LEU:HD12	2.17	0.44
1:A:181:VAL:HG13	1:A:181:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:PRO:HB2	1:A:399:TYR:CE2	2.53	0.44
2:B:179:ASP:HB2	2:B:182:VAL:CB	2.48	0.44
2:B:223:THR:C	2:B:225:GLY:H	2.20	0.44
2:B:324:SER:HB3	2:B:327:GLU:OE1	2.18	0.44
2:B:428:LEU:O	2:B:432:TYR:HB2	2.18	0.44
1:C:152:LEU:O	1:C:153:LEU:C	2.55	0.44
1:C:206:ASN:CB	1:C:210:TYR:HE2	2.28	0.44
1:C:244:PHE:CZ	1:C:358:GLU:OE1	2.71	0.44
1:C:265:ALA:O	1:C:266:HIS:C	2.55	0.44
1:C:284:GLU:O	1:C:285:GLN:CG	2.65	0.44
1:C:349:THR:O	1:C:349:THR:OG1	2.29	0.44
1:C:402:ARG:HG2	1:C:403:ALA:N	2.24	0.44
2:D:75:MET:SD	2:D:79:ARG:CZ	3.06	0.44
2:D:106:GLY:HA2	2:D:111:GLY:HA3	1.99	0.44
2:D:381:SER:O	2:D:383:ALA:N	2.51	0.44
2:D:427:ASP:O	2:D:430:SER:N	2.51	0.44
1:A:67:PHE:O	1:A:92:LEU:HA	2.18	0.43
1:A:411:GLU:OE2	1:A:411:GLU:O	2.36	0.43
2:B:223:THR:HG23	2:B:225:GLY:C	2.38	0.43
2:B:322:ARG:NE	2:B:357:ASP:CB	2.81	0.43
1:C:320:ARG:CB	1:C:374:ALA:HB3	2.40	0.43
1:C:395:PHE:C	1:C:395:PHE:HD1	2.21	0.43
1:C:398:MET:O	1:C:401:LYS:N	2.42	0.43
2:D:185:TYR:HB3	2:D:186:ASN:H	1.56	0.43
2:D:431:GLU:HA	2:D:434:GLN:HE21	1.83	0.43
1:A:306:ASP:O	1:A:308:ARG:N	2.51	0.43
1:A:307:PRO:CB	1:A:381:THR:HG21	2.48	0.43
2:B:3:GLU:HG2	2:B:58:GLY:O	2.18	0.43
2:B:137:LEU:O	2:B:168:THR:HA	2.18	0.43
2:B:272:PHE:HD1	2:B:275:LEU:CD2	2.31	0.43
2:B:333:LEU:O	2:B:336:GLN:HB3	2.18	0.43
1:C:3:GLU:HG3	1:C:3:GLU:O	2.18	0.43
1:C:91:GLN:HG2	1:C:92:LEU:CD1	2.47	0.43
1:C:103:TYR:CD2	1:C:148:GLY:HA2	2.53	0.43
1:C:132:LEU:HB3	1:C:133:GLN:H	1.63	0.43
1:C:171:ILE:HG21	4:C:502:GTP:HN22	1.82	0.43
1:C:174:ALA:C	1:C:176:GLN:N	2.71	0.43
1:C:256:GLN:O	1:C:257:THR:C	2.57	0.43
2:D:51:VAL:N	2:D:245:PRO:CB	2.81	0.43
2:D:88:ARG:HA	2:D:91:ASN:ND2	2.33	0.43
2:D:133:GLN:NE2	2:D:252:LEU:CB	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:305:CYS:O	2:D:383:ALA:HB1	2.18	0.43
2:D:308:ARG:NH2	2:D:342:TYR:CB	2.81	0.43
2:D:383:ALA:C	2:D:385:GLN:H	2.20	0.43
2:D:427:ASP:C	2:D:429:VAL:N	2.72	0.43
1:A:303:VAL:O	1:A:305:CYS:N	2.51	0.43
1:A:402:ARG:HG2	1:A:403:ALA:N	2.22	0.43
2:B:19:LYS:HA	2:B:22:GLU:OE2	2.18	0.43
2:B:139:HIS:O	2:B:170:SER:HA	2.17	0.43
2:B:284:ARG:HB2	2:B:290:GLU:OE1	2.17	0.43
1:C:33:ASP:O	1:C:34:GLY:C	2.57	0.43
1:C:229:ARG:HD2	1:C:366:GLY:HA3	1.99	0.43
1:C:328:VAL:O	1:C:330:ALA:N	2.52	0.43
2:D:198:THR:C	2:D:200:GLU:H	2.21	0.43
2:D:320:ARG:NH1	2:D:320:ARG:CG	2.80	0.43
1:A:88:HIS:O	1:A:90:GLU:N	2.51	0.43
1:A:174:ALA:HB1	1:A:176:GLN:HG2	2.01	0.43
1:A:203:MET:HE1	1:A:388:TRP:HD1	1.83	0.43
1:A:209:ILE:N	1:A:209:ILE:CD1	2.81	0.43
1:A:371:VAL:CG1	1:A:372:GLN:H	2.32	0.43
2:B:3:GLU:O	2:B:133:GLN:N	2.40	0.43
2:B:107:HIS:HB2	2:B:148:GLY:O	2.17	0.43
2:B:154:ILE:O	2:B:157:ILE:N	2.50	0.43
2:B:159:GLU:OE2	3:E:30:UNK:HA	2.17	0.43
1:C:93:ILE:CD1	1:C:118:VAL:HA	2.48	0.43
1:C:143:GLY:O	1:C:144:GLY:C	2.56	0.43
1:C:217:LEU:HD23	1:C:219:ILE:HD11	1.99	0.43
1:C:371:VAL:HG11	1:C:373:ARG:O	2.18	0.43
2:D:137:LEU:HD23	2:D:154:ILE:CD1	2.47	0.43
2:D:174:SER:OG	2:D:207:GLU:HA	2.18	0.43
2:D:291:LEU:CD2	2:D:291:LEU:N	2.81	0.43
1:A:9:VAL:HG21	1:A:150:THR:CB	2.46	0.43
1:A:178:SER:O	1:A:179:THR:CB	2.66	0.43
1:A:205:ASP:OD2	1:A:205:ASP:C	2.56	0.43
1:A:344:VAL:HG11	1:A:346:TRP:CE2	2.52	0.43
2:B:209:LEU:CB	2:B:227:LEU:HG	2.48	0.43
2:B:327:GLU:O	2:B:331:GLN:HB2	2.19	0.43
1:C:27:GLU:CG	1:C:28:HIS:N	2.81	0.43
1:C:187:SER:C	1:C:189:LEU:H	2.21	0.43
1:C:242:LEU:HD11	1:C:318:LEU:HG	2.00	0.43
1:C:276:ILE:HG12	1:C:282:TYR:HD2	1.79	0.43
2:D:91:ASN:N	2:D:91:ASN:ND2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:158:ARG:C	2:D:160:GLU:N	2.71	0.43
2:D:238:VAL:CG2	2:D:376:THR:HG21	2.49	0.43
2:D:287:THR:O	2:D:291:LEU:HD23	2.18	0.43
1:A:15:GLN:O	1:A:16:ILE:O	2.36	0.43
1:A:36:MET:CE	1:A:37:PRO:HD2	2.48	0.43
1:A:278:ALA:HA	1:A:282:TYR:OH	2.19	0.43
1:A:368:LEU:O	1:A:369:ALA:HB3	2.19	0.43
2:B:18:ALA:O	2:B:21:TRP:N	2.51	0.43
2:B:151:THR:HG21	2:B:189:LEU:HD21	1.99	0.43
1:C:403:ALA:C	1:C:405:VAL:H	2.22	0.43
2:D:63:PRO:C	2:D:65:ALA:H	2.20	0.43
2:D:193:GLN:HE21	2:D:193:GLN:HB3	1.66	0.43
1:A:23:LEU:O	1:A:25:CYS:N	2.42	0.43
1:A:179:THR:HG22	1:A:180:ALA:O	2.18	0.43
2:B:59:ASN:CG	2:B:60:LYS:HD2	2.39	0.43
2:B:132:LEU:H	2:B:164:ARG:HH21	1.66	0.43
2:B:346:TRP:HZ2	2:B:435:TYR:HB3	1.82	0.43
1:C:71:GLU:CD	4:C:502:GTP:O3G	2.57	0.43
1:C:179:THR:HB	1:C:182:VAL:HB	2.01	0.43
1:C:333:ALA:O	1:C:336:LYS:N	2.52	0.43
2:D:51:VAL:N	2:D:245:PRO:CG	2.81	0.43
2:D:180:THR:CB	2:D:404:PHE:CE1	2.97	0.43
2:D:343:PHE:HB3	2:D:350:ASN:OD1	2.17	0.43
2:D:353:THR:HG23	2:D:354:ALA:H	1.83	0.43
1:A:43:GLY:O	1:A:47:ASP:OD2	2.37	0.43
1:A:197:HIS:CG	1:A:198:SER:N	2.85	0.43
1:A:256:GLN:HB3	1:A:260:VAL:CB	2.46	0.43
2:B:200:GLU:HG2	2:B:268:PHE:CE2	2.53	0.43
2:B:269:MET:HB3	2:B:269:MET:HE2	1.86	0.43
2:B:272:PHE:HB3	2:B:275:LEU:HD21	2.00	0.43
2:B:419:THR:O	2:B:423:SER:N	2.51	0.43
1:C:78:VAL:O	1:C:82:THR:CG2	2.63	0.43
1:C:122:ILE:HG22	1:C:123:ARG:N	2.34	0.43
2:D:208:ALA:O	2:D:212:ILE:HG13	2.19	0.43
1:A:26:LEU:HD23	1:A:361:THR:OG1	2.18	0.43
1:A:77:GLU:HB3	1:A:83:TYR:HD2	1.76	0.43
1:A:100:ALA:HA	1:A:105:ARG:CD	2.49	0.43
1:A:163:LYS:HB2	1:A:163:LYS:NZ	2.34	0.43
1:A:171:ILE:HA	1:A:204:VAL:HB	2.01	0.43
1:A:229:ARG:HG3	1:A:229:ARG:NH1	2.34	0.43
1:A:292:THR:O	1:A:292:THR:OG1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:VAL:HG11	1:A:353:VAL:HG11	2.00	0.43
1:A:395:PHE:C	1:A:397:LEU:H	2.20	0.43
1:A:409:VAL:HA	1:A:414:GLU:CD	2.32	0.43
1:A:428:LEU:C	1:A:430:LYS:H	2.22	0.43
2:B:59:ASN:CA	2:B:64:ARG:HE	2.32	0.43
2:B:276:THR:HG21	2:B:281:GLN:CG	2.49	0.43
1:C:294:ALA:C	1:C:296:PHE:H	2.22	0.43
1:C:346:TRP:CE3	1:C:347:CYS:SG	3.12	0.43
1:C:409:VAL:C	1:C:411:GLU:N	2.71	0.43
2:D:10:GLY:HA3	2:D:146:GLY:HA3	1.99	0.43
2:D:92:PHE:CZ	2:D:117:SER:O	2.71	0.43
2:D:348:PRO:O	2:D:349:ASN:CB	2.66	0.43
2:D:428:LEU:HD12	2:D:428:LEU:N	2.33	0.43
3:E:68:UNK:O	3:E:72:UNK:CB	2.66	0.43
3:E:83:UNK:O	3:E:85:UNK:N	2.51	0.43
1:A:100:ALA:HB1	1:A:105:ARG:HD2	2.00	0.43
1:A:185:TYR:O	1:A:186:ASN:C	2.56	0.43
1:A:242:LEU:CG	1:A:318:LEU:HD11	2.47	0.43
2:B:59:ASN:HA	2:B:60:LYS:NZ	2.33	0.43
2:B:132:LEU:O	2:B:164:ARG:NE	2.41	0.43
2:B:402:LYS:HE3	1:C:440:VAL:HG12	1.99	0.43
1:C:270:ALA:HB3	1:C:302:MET:HG2	2.00	0.43
2:D:60:LYS:N	2:D:60:LYS:HZ2	2.15	0.43
2:D:121:VAL:O	2:D:121:VAL:CG1	2.66	0.43
2:D:183:GLU:HB3	2:D:184:PRO:HD3	2.01	0.43
1:A:39:ASP:OD2	1:A:40:LYS:HB2	2.19	0.42
1:A:181:VAL:HG13	1:A:185:TYR:CE2	2.53	0.42
1:A:189:LEU:HD13	1:A:189:LEU:C	2.40	0.42
2:B:88:ARG:O	2:B:91:ASN:ND2	2.52	0.42
2:B:111:GLY:O	2:B:113:GLU:N	2.52	0.42
2:B:189:LEU:HA	2:B:192:HIS:HE1	1.82	0.42
2:B:211:ASP:OD1	2:B:211:ASP:N	2.52	0.42
2:B:273:ALA:HB3	2:B:274:PRO:HD3	2.01	0.42
2:B:286:LEU:CG	2:B:373:MET:HE3	2.44	0.42
1:C:217:LEU:CD2	1:C:219:ILE:HD11	2.49	0.42
2:D:86:ILE:H	2:D:88:ARG:NH2	2.17	0.42
2:D:211:ASP:O	2:D:215:ARG:HB2	2.19	0.42
2:D:273:ALA:HB3	2:D:274:PRO:HD3	2.00	0.42
2:D:283:TYR:HE2	2:D:294:GLN:NE2	2.17	0.42
2:D:311:ARG:HD3	2:D:311:ARG:H	1.84	0.42
2:D:312:TYR:CE2	2:D:377:PHE:CZ	3.06	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:389:LYS:C	2:D:392:SER:HG	2.22	0.42
3:E:14:UNK:C	3:E:16:UNK:N	2.81	0.42
1:A:46:ASP:O	1:A:47:ASP:O	2.37	0.42
1:A:306:ASP:N	1:A:307:PRO:HD3	2.33	0.42
2:B:283:TYR:O	2:B:283:TYR:CG	2.72	0.42
2:B:287:THR:OG1	2:B:290:GLU:CB	2.67	0.42
2:B:335:VAL:C	2:B:338:LYS:H	2.22	0.42
2:B:344:VAL:O	2:B:346:TRP:CD1	2.72	0.42
1:C:209:ILE:HG12	1:C:231:ILE:HD11	2.00	0.42
1:C:273:ALA:HB3	1:C:291:ILE:HG23	2.01	0.42
1:C:284:GLU:CG	1:C:285:GLN:HE21	2.22	0.42
1:C:305:CYS:C	1:C:386:GLU:OE1	2.57	0.42
1:C:306:ASP:HB3	1:C:386:GLU:OE1	2.18	0.42
1:C:312:TYR:CD1	1:C:312:TYR:N	2.87	0.42
2:D:52:TYR:CG	2:D:52:TYR:O	2.72	0.42
2:D:200:GLU:CD	2:D:268:PHE:HE2	2.21	0.42
2:D:226:ASP:O	2:D:228:ASN:N	2.44	0.42
2:D:311:ARG:NH1	2:D:344:VAL:HA	2.35	0.42
2:D:327:GLU:O	2:D:331:GLN:HB2	2.19	0.42
3:E:75:UNK:C	3:E:77:UNK:N	2.78	0.42
1:A:154:MET:C	1:A:156:ARG:N	2.70	0.42
1:A:242:LEU:CD2	1:A:318:LEU:HD21	2.33	0.42
1:A:284:GLU:CG	1:A:285:GLN:HE21	2.24	0.42
2:B:2:ARG:HH21	2:B:243:ARG:HB3	1.84	0.42
2:B:10:GLY:HA3	2:B:146:GLY:HA3	2.01	0.42
2:B:212:ILE:O	2:B:217:LEU:HB3	2.19	0.42
2:B:322:ARG:CG	2:B:357:ASP:HA	2.33	0.42
1:C:31:GLN:OE1	1:C:32:PRO:HD3	2.19	0.42
1:C:119:LEU:HD22	1:C:156:ARG:CZ	2.49	0.42
1:C:264:ARG:HD3	1:C:264:ARG:HA	1.97	0.42
2:D:176:LYS:NZ	2:D:210:TYR:CG	2.84	0.42
2:D:181:VAL:C	2:D:184:PRO:HD2	2.40	0.42
2:D:312:TYR:HE2	2:D:377:PHE:CZ	2.37	0.42
2:D:395:PHE:CD2	2:D:422:GLU:OE1	2.71	0.42
1:A:411:GLU:OE2	1:A:411:GLU:CA	2.68	0.42
2:B:22:GLU:HG3	2:B:83:PHE:CD1	2.55	0.42
2:B:93:VAL:CG2	2:B:94:PHE:N	2.82	0.42
2:B:95:GLY:O	2:B:96:GLN:O	2.37	0.42
2:B:97:SER:HG	2:B:110:GLU:CG	2.32	0.42
2:B:256:ALA:O	2:B:260:VAL:HB	2.19	0.42
2:B:312:TYR:CE2	2:B:377:PHE:HZ	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:GLU:O	2:B:331:GLN:N	2.53	0.42
1:C:20:CYS:SG	1:C:232:GLY:HA2	2.59	0.42
1:C:158:SER:HB3	1:C:166:LYS:HZ1	1.83	0.42
1:C:241:SER:CB	1:C:242:LEU:HD12	2.48	0.42
1:C:321:GLY:N	1:C:356:ASN:O	2.52	0.42
2:D:4:ILE:HD11	2:D:252:LEU:HD13	2.00	0.42
2:D:84:GLY:C	2:D:85:GLN:HG2	2.39	0.42
2:D:322:ARG:CG	2:D:357:ASP:HA	2.34	0.42
1:A:291:ILE:CG2	1:A:375:VAL:HG21	2.44	0.42
1:A:311:LYS:CE	1:A:344:VAL:HA	2.50	0.42
1:A:339:ARG:C	1:A:339:ARG:CD	2.75	0.42
1:A:340:THR:C	1:A:341:ILE:HD12	2.40	0.42
1:A:349:THR:O	1:A:349:THR:OG1	2.31	0.42
1:A:412:GLY:HA2	1:A:413:MET:HE1	2.02	0.42
2:B:3:GLU:HB3	2:B:132:LEU:HA	2.01	0.42
2:B:174:SER:HB2	2:B:206:ASN:C	2.39	0.42
2:B:383:ALA:C	2:B:385:GLN:H	2.23	0.42
1:C:5:ILE:HG22	1:C:6:SER:N	2.34	0.42
1:C:44:GLY:O	1:C:46:ASP:N	2.52	0.42
1:C:83:TYR:O	1:C:84:ARG:HB2	2.20	0.42
1:C:123:ARG:O	1:C:127:ASP:HB2	2.19	0.42
1:C:190:THR:O	1:C:193:THR:N	2.52	0.42
1:C:286:LEU:HD12	1:C:291:ILE:CG1	2.48	0.42
1:C:332:ILE:HG23	1:C:351:PHE:CZ	2.55	0.42
2:D:165:ILE:HD13	2:D:199:ASP:OD1	2.18	0.42
3:E:30:UNK:O	3:E:31:UNK:C	2.67	0.42
1:A:73:THR:O	1:A:76:ASP:N	2.48	0.42
1:A:97:GLU:CD	1:A:97:GLU:H	2.23	0.42
1:A:126:ALA:O	1:A:132:LEU:CD1	2.67	0.42
1:A:216:ASN:HB3	1:A:275:VAL:HG11	2.01	0.42
1:A:305:CYS:O	1:A:306:ASP:HB2	2.19	0.42
2:B:88:ARG:HA	2:B:91:ASN:ND2	2.35	0.42
2:B:230:LEU:H	2:B:230:LEU:CD1	2.25	0.42
1:C:21:TRP:CD1	1:C:21:TRP:N	2.87	0.42
1:C:88:HIS:O	1:C:90:GLU:N	2.52	0.42
1:C:111:GLY:C	1:C:113:GLU:N	2.73	0.42
1:C:190:THR:HA	1:C:193:THR:CG2	2.39	0.42
1:C:335:ILE:O	1:C:338:LYS:HG2	2.19	0.42
1:C:398:MET:CG	1:C:399:TYR:H	2.33	0.42
2:D:22:GLU:HG3	2:D:83:PHE:CD1	2.55	0.42
2:D:95:GLY:O	2:D:96:GLN:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:126:SER:O	2:D:127:GLU:C	2.57	0.42
2:D:346:TRP:HZ2	2:D:435:TYR:HB3	1.85	0.42
2:D:415:GLU:HG2	2:D:416:MET:SD	2.59	0.42
1:A:119:LEU:HD22	1:A:156:ARG:NE	2.34	0.42
1:A:190:THR:O	1:A:193:THR:N	2.50	0.42
1:A:286:LEU:HD12	1:A:291:ILE:CG1	2.49	0.42
2:B:350:ASN:HD22	2:B:350:ASN:C	2.21	0.42
2:B:415:GLU:HG2	2:B:416:MET:H	1.85	0.42
1:C:91:GLN:HE21	1:C:91:GLN:HB3	1.58	0.42
1:C:185:TYR:CE1	1:C:408:TYR:CE1	3.06	0.42
1:C:209:ILE:CG2	1:C:213:CYS:HB2	2.43	0.42
1:C:239:THR:O	1:C:243:ARG:HB2	2.19	0.42
2:D:311:ARG:HB3	2:D:343:PHE:N	2.35	0.42
1:A:209:ILE:CG2	1:A:213:CYS:HB2	2.47	0.42
1:A:294:ALA:C	1:A:296:PHE:H	2.23	0.42
2:B:123:ARG:C	2:B:125:GLU:N	2.72	0.42
2:B:178:SER:C	2:B:182:VAL:HB	2.35	0.42
2:B:350:ASN:ND2	2:B:350:ASN:N	2.67	0.42
1:C:320:ARG:HH21	1:C:356:ASN:ND2	2.18	0.42
1:C:405:VAL:O	1:C:405:VAL:CG2	2.68	0.42
1:C:413:MET:O	1:C:414:GLU:CB	2.66	0.42
1:C:431:ASP:C	1:C:433:GLU:H	2.23	0.42
2:D:88:ARG:HA	2:D:91:ASN:HD21	1.85	0.42
2:D:224:TYR:O	2:D:228:ASN:HB2	2.20	0.42
2:D:269:MET:HG2	2:D:384:ILE:HB	2.01	0.42
2:D:320:ARG:HG2	2:D:320:ARG:NH1	2.32	0.42
1:A:312:TYR:HD1	1:A:312:TYR:H	1.67	0.42
2:B:6:HIS:HD2	2:B:136:GLN:OE1	2.03	0.42
2:B:333:LEU:HG	2:B:337:ASN:HD21	1.82	0.42
2:B:346:TRP:CZ2	2:B:435:TYR:HB3	2.54	0.42
2:B:405:LEU:HD13	2:B:406:HIS:H	1.79	0.42
1:C:88:HIS:HA	1:C:89:PRO:HD2	1.84	0.42
1:C:192:HIS:C	1:C:194:THR:H	2.23	0.42
1:C:229:ARG:HG3	1:C:229:ARG:NH1	2.33	0.42
2:D:102:ASN:HD22	2:D:105:LYS:H	1.62	0.42
1:A:208:ALA:HB2	1:A:302:MET:O	2.20	0.42
2:B:1:MET:C	2:B:3:GLU:N	2.73	0.42
2:B:224:TYR:C	2:B:226:ASP:H	2.22	0.42
2:B:273:ALA:H	2:B:274:PRO:HD2	1.84	0.42
1:C:8:HIS:HE2	1:C:21:TRP:HE1	1.66	0.42
1:C:174:ALA:HB1	1:C:176:GLN:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ALA:O	1:C:212:ILE:HG23	2.20	0.42
1:C:269:LEU:C	1:C:269:LEU:CD1	2.84	0.42
1:C:275:VAL:HG12	1:C:275:VAL:O	2.18	0.42
1:C:277:SER:HA	1:C:368:LEU:HB3	2.02	0.42
1:C:321:GLY:CA	1:C:358:GLU:O	2.68	0.42
2:D:69:ASP:HB3	2:D:74:THR:HG23	2.02	0.42
2:D:104:ALA:HB1	2:D:411:GLU:HB2	2.02	0.42
1:A:115:ILE:HG12	1:A:149:PHE:CE2	2.54	0.41
1:A:197:HIS:CD2	1:A:198:SER:HB3	2.55	0.41
2:B:1:MET:C	2:B:3:GLU:H	2.20	0.41
2:B:122:VAL:CG1	2:B:123:ARG:N	2.82	0.41
1:C:181:VAL:HG22	1:C:399:TYR:OH	2.18	0.41
1:C:209:ILE:HA	1:C:212:ILE:HG12	2.01	0.41
2:D:60:LYS:H	2:D:60:LYS:HZ3	1.68	0.41
2:D:179:ASP:OD2	2:D:181:VAL:HG12	2.20	0.41
1:A:33:ASP:O	1:A:34:GLY:C	2.59	0.41
1:A:181:VAL:O	1:A:184:PRO:HG2	2.20	0.41
1:A:182:VAL:HA	1:A:185:TYR:HD2	1.86	0.41
1:A:245:ASP:O	1:A:249:ASN:OD1	2.37	0.41
1:A:403:ALA:C	1:A:405:VAL:H	2.23	0.41
1:A:420:GLU:OE1	1:A:420:GLU:O	2.38	0.41
2:B:86:ILE:H	2:B:88:ARG:CZ	2.33	0.41
1:C:161:TYR:O	1:C:162:GLY:C	2.59	0.41
1:C:168:GLU:HG3	1:C:168:GLU:O	2.20	0.41
1:C:215:ARG:HG2	1:C:216:ASN:N	2.36	0.41
1:C:242:LEU:CG	1:C:318:LEU:HD11	2.50	0.41
2:D:273:ALA:HB3	2:D:274:PRO:CD	2.49	0.41
3:E:16:UNK:O	3:E:20:UNK:N	2.53	0.41
1:A:5:ILE:O	1:A:136:SER:N	2.47	0.41
1:A:117:LEU:O	1:A:121:ARG:HB2	2.21	0.41
1:A:214:ARG:O	1:A:214:ARG:HG3	2.20	0.41
1:A:237:SER:C	1:A:241:SER:CB	2.88	0.41
1:A:312:TYR:HD2	1:A:315:CYS:HB2	1.84	0.41
2:B:165:ILE:HG13	2:B:253:ARG:HG2	2.02	0.41
2:B:291:LEU:CD2	2:B:291:LEU:H	2.32	0.41
1:C:38:SER:O	1:C:39:ASP:CB	2.68	0.41
1:C:42:ILE:HD12	1:C:42:ILE:HA	1.87	0.41
1:C:163:LYS:HB2	1:C:163:LYS:NZ	2.34	0.41
1:C:312:TYR:HD1	1:C:312:TYR:N	2.17	0.41
2:D:73:GLY:O	2:D:78:VAL:HG21	2.20	0.41
2:D:121:VAL:O	2:D:121:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:214:PHE:CE2	2:D:215:ARG:NE	2.88	0.41
2:D:286:LEU:HA	2:D:290:GLU:CD	2.40	0.41
1:A:3:GLU:O	1:A:3:GLU:HG3	2.19	0.41
1:A:30:ILE:HG13	1:A:31:GLN:H	1.81	0.41
1:A:35:GLN:HE22	1:A:88:HIS:CD2	2.38	0.41
1:A:229:ARG:HB3	1:A:366:GLY:O	2.20	0.41
1:A:387:ALA:CB	1:A:390:ARG:NH1	2.83	0.41
1:A:414:GLU:HB2	1:A:417:GLU:CB	2.46	0.41
2:B:103:TRP:HE1	2:B:151:THR:HG21	1.85	0.41
2:B:215:ARG:NE	2:B:215:ARG:CA	2.80	0.41
2:B:395:PHE:CE1	2:B:399:PHE:CD1	3.08	0.41
2:B:404:PHE:O	2:B:404:PHE:CD2	2.69	0.41
1:C:10:GLY:O	1:C:12:ALA:N	2.54	0.41
1:C:69:ASP:CG	1:C:71:GLU:H	2.23	0.41
1:C:253:THR:OG1	1:C:254:GLU:N	2.53	0.41
1:C:317:LEU:HD23	1:C:377:MET:HB2	2.00	0.41
1:C:363:VAL:HG22	1:C:367:ASP:CG	2.41	0.41
2:D:3:GLU:OE2	2:D:130:ASP:CB	2.60	0.41
2:D:132:LEU:HD22	2:D:164:ARG:CG	2.48	0.41
2:D:208:ALA:HB2	2:D:304:ALA:CB	2.51	0.41
2:D:218:LYS:NZ	2:D:278:ARG:CB	2.80	0.41
2:D:283:TYR:O	2:D:284:ARG:HB2	2.20	0.41
1:A:27:GLU:OE1	1:A:28:HIS:CE1	2.73	0.41
1:A:177:VAL:HG21	2:B:349:ASN:HB2	2.03	0.41
1:A:203:MET:SD	1:A:388:TRP:CD1	3.13	0.41
2:B:190:SER:O	2:B:425:MET:HB2	2.21	0.41
2:B:191:VAL:HG21	2:B:421:ALA:CB	2.28	0.41
2:B:313:LEU:C	2:B:314:THR:HG23	2.41	0.41
2:B:407:TRP:NE1	1:C:257:THR:HA	2.34	0.41
1:C:107:HIS:HB2	1:C:148:GLY:O	2.21	0.41
1:C:115:ILE:HG23	1:C:116:ASP:OD1	2.20	0.41
1:C:121:ARG:O	1:C:122:ILE:C	2.57	0.41
1:C:139:HIS:HB3	1:C:170:SER:CA	2.44	0.41
2:D:176:LYS:HD2	2:D:210:TYR:CE1	2.55	0.41
2:D:223:THR:HG23	2:D:225:GLY:C	2.41	0.41
2:D:265:LEU:HB2	2:D:266:HIS:H	1.58	0.41
2:D:335:VAL:C	2:D:338:LYS:H	2.23	0.41
1:A:105:ARG:HG3	1:A:411:GLU:HG3	2.03	0.41
1:A:167:LEU:HD13	1:A:252:LEU:HD11	2.03	0.41
1:A:180:ALA:HB3	2:B:258:ASN:ND2	2.36	0.41
1:A:238:ILE:N	1:A:241:SER:CB	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:VAL:C	1:A:411:GLU:N	2.73	0.41
1:A:419:SER:O	1:A:420:GLU:C	2.59	0.41
2:B:158:ARG:HD3	2:B:197:ASN:HD22	1.73	0.41
2:B:351:VAL:O	2:B:352:LYS:HG3	2.21	0.41
2:B:427:ASP:C	2:B:429:VAL:N	2.73	0.41
1:C:84:ARG:C	1:C:85:GLN:HG2	2.41	0.41
1:C:144:GLY:O	1:C:145:THR:C	2.59	0.41
1:C:174:ALA:HB2	1:C:206:ASN:CB	2.50	0.41
1:C:228:ASN:ND2	4:C:502:GTP:O6	2.53	0.41
1:C:395:PHE:C	1:C:397:LEU:H	2.23	0.41
1:C:416:GLY:C	1:C:418:PHE:H	2.19	0.41
2:D:97:SER:HG	2:D:110:GLU:CD	2.23	0.41
2:D:115:VAL:HG11	2:D:156:LYS:HZ3	1.80	0.41
2:D:115:VAL:HG23	2:D:149:MET:HE1	2.02	0.41
2:D:154:ILE:HG23	2:D:166:MET:HE3	2.03	0.41
2:D:320:ARG:HE	2:D:360:PRO:HG3	1.85	0.41
2:D:333:LEU:O	2:D:336:GLN:HB3	2.20	0.41
2:D:372:LYS:HE2	2:D:372:LYS:HA	2.02	0.41
1:A:24:TYR:HA	1:A:26:LEU:CD1	2.50	0.41
1:A:139:HIS:O	1:A:140:SER:CB	2.68	0.41
1:A:239:THR:O	1:A:243:ARG:HB2	2.19	0.41
1:A:242:LEU:HD21	1:A:318:LEU:CD2	2.32	0.41
1:A:251:ASP:OD2	1:A:252:LEU:N	2.54	0.41
1:A:317:LEU:HA	1:A:377:MET:HB2	2.02	0.41
1:A:409:VAL:HG22	1:A:414:GLU:CD	2.40	0.41
2:B:4:ILE:HD13	2:B:252:LEU:HD13	2.03	0.41
2:B:103:TRP:HB2	2:B:185:TYR:CE2	2.56	0.41
2:B:103:TRP:H	2:B:408:TYR:HE1	1.69	0.41
2:B:236:SER:C	2:B:238:VAL:H	2.24	0.41
2:B:262:PHE:CE1	2:B:435:TYR:CE2	3.08	0.41
2:B:304:ALA:O	2:B:305:CYS:SG	2.77	0.41
2:B:310:GLY:HA3	2:B:436:GLN:HG2	2.03	0.41
2:B:313:LEU:HD21	2:B:435:TYR:CD2	2.54	0.41
2:D:73:GLY:C	2:D:75:MET:H	2.24	0.41
2:D:102:ASN:N	2:D:185:TYR:OH	2.53	0.41
2:D:103:TRP:HE1	2:D:151:THR:HG21	1.85	0.41
2:D:289:PRO:HA	2:D:292:THR:OG1	2.21	0.41
1:A:30:ILE:C	1:A:30:ILE:HD12	2.40	0.41
1:A:197:HIS:O	1:A:198:SER:OG	2.35	0.41
1:A:335:ILE:O	1:A:336:LYS:C	2.59	0.41
1:A:335:ILE:CG1	1:A:336:LYS:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:PHE:CD1	1:A:349:THR:HA	2.55	0.41
1:A:344:VAL:HG12	1:A:345:ASP:H	1.83	0.41
2:B:95:GLY:O	2:B:96:GLN:HB3	2.21	0.41
2:B:102:ASN:HD22	2:B:105:LYS:H	1.58	0.41
2:B:271:GLY:C	2:B:272:PHE:O	2.58	0.41
1:C:142:GLY:HA2	1:C:185:TYR:HB2	2.03	0.41
1:C:255:PHE:O	1:C:259:LEU:HB2	2.21	0.41
2:D:59:ASN:CG	2:D:60:LYS:HD2	2.41	0.41
2:D:176:LYS:O	2:D:177:VAL:HB	2.21	0.41
2:D:267:PHE:CD2	2:D:267:PHE:N	2.89	0.41
1:A:115:ILE:HG13	1:A:152:LEU:CG	2.50	0.41
1:A:178:SER:O	1:A:182:VAL:HG21	2.21	0.41
1:A:184:PRO:CB	1:A:399:TYR:CE2	3.04	0.41
1:A:273:ALA:HB2	1:A:295:CYS:CB	2.51	0.41
1:A:311:LYS:HD3	1:A:344:VAL:CB	2.51	0.41
1:A:339:ARG:HD2	1:A:339:ARG:O	2.21	0.41
1:A:365:GLY:O	1:A:368:LEU:HD12	2.20	0.41
1:A:388:TRP:HZ3	1:A:428:LEU:HD22	1.82	0.41
1:A:398:MET:CG	1:A:399:TYR:H	2.34	0.41
1:A:413:MET:C	1:A:414:GLU:CD	2.80	0.41
2:B:51:VAL:HG22	2:B:245:PRO:CB	2.51	0.41
2:B:52:TYR:O	2:B:52:TYR:CG	2.74	0.41
2:B:63:PRO:C	2:B:65:ALA:N	2.74	0.41
2:B:76:ASP:HB2	2:B:77:SER:H	1.46	0.41
2:B:136:GLN:HG3	2:B:136:GLN:O	2.21	0.41
2:B:204:ILE:CG2	2:B:209:LEU:HD11	2.51	0.41
2:B:232:SER:C	2:B:234:THR:H	2.22	0.41
2:B:247:GLN:HG2	2:B:355:VAL:HB	2.03	0.41
2:B:384:ILE:O	2:B:384:ILE:HG12	2.20	0.41
2:B:404:PHE:HZ	1:C:257:THR:O	2.04	0.41
1:C:9:VAL:HG21	1:C:150:THR:CB	2.51	0.41
1:C:306:ASP:N	1:C:307:PRO:HD3	2.35	0.41
1:C:311:LYS:HB2	1:C:344:VAL:CG2	2.50	0.41
1:C:371:VAL:CG1	1:C:372:GLN:N	2.82	0.41
2:D:8:GLN:O	2:D:68:VAL:N	2.54	0.41
2:D:16:ILE:CD1	2:D:231:VAL:CG1	2.99	0.41
2:D:51:VAL:HG22	2:D:245:PRO:CB	2.51	0.41
2:D:88:ARG:O	2:D:91:ASN:ND2	2.54	0.41
2:D:103:TRP:H	2:D:408:TYR:HE1	1.68	0.41
2:D:158:ARG:NH1	2:D:197:ASN:OD1	2.54	0.41
2:D:226:ASP:C	2:D:228:ASN:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLN:HA	1:A:128:GLN:OE1	2.21	0.41
1:A:158:SER:HB3	1:A:166:LYS:HZ1	1.86	0.41
1:A:174:ALA:HB2	1:A:206:ASN:CB	2.51	0.41
1:A:204:VAL:O	1:A:205:ASP:HB3	2.21	0.41
1:A:398:MET:HE2	1:A:399:TYR:CE1	2.56	0.41
2:B:19:LYS:HA	2:B:22:GLU:CG	2.51	0.41
2:B:25:SER:HB3	2:B:369:ARG:NH2	2.34	0.41
2:B:103:TRP:C	2:B:105:LYS:N	2.74	0.41
2:B:148:GLY:CA	2:B:151:THR:HG22	2.51	0.41
2:B:179:ASP:CB	2:B:181:VAL:HG12	2.46	0.41
2:B:325:MET:CG	2:B:355:VAL:HG11	2.51	0.41
2:B:407:TRP:CZ2	1:C:256:GLN:CB	2.91	0.41
1:C:108:TYR:HB3	1:C:413:MET:HE3	2.03	0.41
1:C:238:ILE:O	1:C:239:THR:O	2.38	0.41
1:C:244:PHE:H	1:C:244:PHE:HD2	1.67	0.41
1:C:244:PHE:N	1:C:244:PHE:CD2	2.89	0.41
1:C:414:GLU:HA	1:C:417:GLU:HB2	2.02	0.41
2:D:182:VAL:O	2:D:183:GLU:HB2	2.21	0.41
1:A:183:GLU:N	1:A:184:PRO:CD	2.83	0.40
1:A:244:PHE:CE1	1:A:358:GLU:OE2	2.74	0.40
1:A:269:LEU:HD11	1:A:301:GLN:HB3	2.03	0.40
1:A:295:CYS:SG	1:A:295:CYS:O	2.78	0.40
1:A:431:ASP:C	1:A:433:GLU:H	2.22	0.40
2:B:162:PRO:HG2	2:B:163:ASP:H	1.86	0.40
2:B:269:MET:HG2	2:B:384:ILE:HB	2.03	0.40
1:C:107:HIS:HA	1:C:148:GLY:O	2.21	0.40
1:C:164:LYS:N	1:C:164:LYS:NZ	2.69	0.40
1:C:320:ARG:N	1:C:374:ALA:O	2.49	0.40
2:D:114:LEU:HD12	2:D:114:LEU:HA	1.78	0.40
2:D:115:VAL:HG21	2:D:152:LEU:CD2	2.51	0.40
2:D:253:ARG:C	2:D:255:LEU:H	2.22	0.40
2:D:350:ASN:C	2:D:351:VAL:CG2	2.89	0.40
3:E:83:UNK:O	3:E:84:UNK:C	2.67	0.40
1:A:72:PRO:HB3	1:A:94:THR:HG1	1.86	0.40
1:A:101:ASN:OD1	2:B:254:LYS:NZ	2.39	0.40
1:A:346:TRP:CZ2	1:A:435:VAL:HB	2.56	0.40
2:B:7:ILE:HG21	2:B:137:LEU:HD13	2.03	0.40
2:B:174:SER:CB	2:B:207:GLU:N	2.82	0.40
2:B:264:ARG:O	2:B:265:LEU:O	2.38	0.40
2:B:408:TYR:CD2	2:B:418:PHE:CZ	3.09	0.40
1:C:109:THR:OG1	1:C:110:ILE:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:ARG:HG3	1:C:214:ARG:NH1	2.35	0.40
1:C:362:VAL:HG12	1:C:363:VAL:N	2.36	0.40
1:C:405:VAL:O	1:C:405:VAL:HG22	2.20	0.40
2:D:123:ARG:C	2:D:125:GLU:N	2.74	0.40
2:D:154:ILE:O	2:D:157:ILE:N	2.46	0.40
2:D:180:THR:HB	2:D:404:PHE:CZ	2.55	0.40
2:D:346:TRP:CZ2	2:D:435:TYR:HB3	2.57	0.40
1:A:132:LEU:HB3	1:A:133:GLN:H	1.66	0.40
1:A:175:PRO:HB2	1:A:207:GLU:OE2	2.22	0.40
1:A:322:ASP:OD1	1:A:357:TYR:O	2.39	0.40
1:A:380:ASN:O	1:A:380:ASN:CG	2.60	0.40
1:A:409:VAL:HA	1:A:412:GLY:O	2.22	0.40
2:B:132:LEU:CD2	2:B:164:ARG:NE	2.83	0.40
2:B:172:VAL:CG1	2:B:173:PRO:HD2	2.42	0.40
1:C:139:HIS:NE2	1:C:150:THR:CG2	2.84	0.40
1:C:225:THR:HA	1:C:228:ASN:HB2	2.04	0.40
1:C:305:CYS:O	1:C:306:ASP:HB2	2.22	0.40
1:C:411:GLU:OE2	1:C:411:GLU:O	2.39	0.40
2:D:144:GLY:N	2:D:185:TYR:CZ	2.89	0.40
2:D:179:ASP:CB	2:D:181:VAL:HG12	2.42	0.40
2:D:427:ASP:O	2:D:428:LEU:C	2.59	0.40
2:D:429:VAL:O	2:D:433:GLN:HG2	2.22	0.40
1:A:79:ARG:HD3	1:A:86:LEU:HD11	2.04	0.40
1:A:142:GLY:O	1:A:182:VAL:HG22	2.20	0.40
1:A:145:THR:CB	4:A:500:GTP:PG	3.10	0.40
1:A:181:VAL:HG13	1:A:408:TYR:HH	1.86	0.40
1:A:187:SER:C	1:A:189:LEU:N	2.74	0.40
2:B:109:THR:O	2:B:112:ALA:N	2.49	0.40
2:B:147:SER:O	2:B:189:LEU:HD11	2.22	0.40
2:B:192:HIS:CA	2:B:195:VAL:HG22	2.26	0.40
2:B:267:PHE:CD2	2:B:267:PHE:N	2.89	0.40
2:B:403:ALA:HB1	2:B:405:LEU:CD1	2.51	0.40
2:B:436:GLN:HE21	2:B:436:GLN:C	2.23	0.40
1:C:107:HIS:CB	1:C:148:GLY:O	2.69	0.40
1:C:174:ALA:C	1:C:176:GLN:H	2.25	0.40
1:C:184:PRO:HB2	1:C:399:TYR:CE2	2.56	0.40
1:C:328:VAL:HG11	1:C:353:VAL:HG11	2.04	0.40
2:D:12:CYS:HB3	5:D:503:GDP:H8	1.79	0.40
2:D:62:VAL:O	2:D:63:PRO:C	2.59	0.40
2:D:223:THR:HG23	2:D:225:GLY:H	1.85	0.40
2:D:308:ARG:NH2	2:D:339:ASN:CB	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:350:ASN:O	2:D:351:VAL:HG22	2.21	0.40
3:E:21:UNK:O	3:E:24:UNK:CA	2.69	0.40
1:A:31:GLN:HB3	1:A:32:PRO:CD	2.39	0.40
1:A:221:ARG:NE	1:A:221:ARG:H	2.20	0.40
1:A:313:MET:HE2	1:A:346:TRP:HH2	1.87	0.40
1:A:317:LEU:CD2	1:A:377:MET:HB3	2.50	0.40
1:A:402:ARG:O	1:A:405:VAL:HG12	2.21	0.40
2:B:88:ARG:HA	2:B:91:ASN:HD21	1.87	0.40
2:B:117:SER:O	2:B:120:ASP:HB2	2.21	0.40
2:B:144:GLY:N	2:B:185:TYR:CZ	2.90	0.40
2:B:151:THR:HG21	2:B:189:LEU:HD22	2.03	0.40
2:B:153:LEU:O	2:B:156:LYS:HB3	2.21	0.40
2:B:168:THR:OG1	2:B:201:THR:CB	2.64	0.40
2:B:258:ASN:OD1	2:B:352:LYS:HD2	2.21	0.40
1:C:115:ILE:CD1	1:C:156:ARG:HG3	2.34	0.40
2:D:290:GLU:O	2:D:291:LEU:C	2.59	0.40
2:D:333:LEU:HA	2:D:336:GLN:HB3	2.03	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	419/451 (93%)	221 (53%)	111 (26%)	87 (21%)	0 2
1	C	419/451 (93%)	219 (52%)	114 (27%)	86 (20%)	0 2
2	B	406/445 (91%)	184 (45%)	133 (33%)	89 (22%)	0 1
2	D	406/445 (91%)	186 (46%)	130 (32%)	90 (22%)	0 1
All	All	1650/1792 (92%)	810 (49%)	488 (30%)	352 (21%)	0 1

All (352) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	32	PRO
1	A	46	ASP
1	A	83	TYR
1	A	90	GLU
1	A	97	GLU
1	A	98	ASP
1	A	100	ALA
1	A	103	TYR
1	A	109	THR
1	A	140	SER
1	A	177	VAL
1	A	181	VAL
1	A	191	THR
1	A	197	HIS
1	A	222	PRO
1	A	238	ILE
1	A	239	THR
1	A	265	ALA
1	A	266	HIS
1	A	278	ALA
1	A	322	ASP
1	A	346	TRP
1	A	349	THR
1	A	352	LYS
1	A	399	TYR
1	A	402	ARG
1	A	403	ALA
1	A	414	GLU
2	B	19	LYS
2	B	76	ASP
2	B	82	PRO
2	B	88	ARG
2	B	110	GLU
2	B	127	GLU
2	B	129	CYS
2	B	130	ASP
2	B	144	GLY
2	B	159	GLU
2	B	179	ASP
2	B	183	GLU
2	B	198	THR
2	B	240	THR

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Mol	Chain	Res	Type
2	B	245	PRO
2	B	265	LEU
2	B	272	PHE
2	B	278	ARG
2	B	281	GLN
2	B	296	PHE
2	B	308	ARG
2	B	324	SER
2	B	344	VAL
2	B	360	PRO
2	B	378	ILE
2	B	391	ILE
2	B	398	MET
2	B	399	PHE
2	B	402	LYS
2	B	404	PHE
2	B	416	MET
2	B	428	LEU
1	C	11	GLN
1	C	32	PRO
1	C	83	TYR
1	C	90	GLU
1	C	97	GLU
1	C	98	ASP
1	C	99	ALA
1	C	100	ALA
1	C	103	TYR
1	C	109	THR
1	C	140	SER
1	C	144	GLY
1	C	177	VAL
1	C	181	VAL
1	C	191	THR
1	C	197	HIS
1	C	222	PRO
1	C	238	ILE
1	C	259	LEU
1	C	265	ALA
1	C	266	HIS
1	C	277	SER
1	C	278	ALA
1	C	299	ALA

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Mol	Chain	Res	Type
1	C	322	ASP
1	C	340	THR
1	C	346	TRP
1	C	349	THR
1	C	352	LYS
1	C	399	TYR
1	C	402	ARG
1	C	403	ALA
1	C	414	GLU
2	D	19	LYS
2	D	27	GLU
2	D	61	TYR
2	D	71	GLU
2	D	76	ASP
2	D	82	PRO
2	D	88	ARG
2	D	110	GLU
2	D	127	GLU
2	D	129	CYS
2	D	130	ASP
2	D	144	GLY
2	D	159	GLU
2	D	179	ASP
2	D	183	GLU
2	D	198	THR
2	D	240	THR
2	D	245	PRO
2	D	265	LEU
2	D	272	PHE
2	D	278	ARG
2	D	281	GLN
2	D	296	PHE
2	D	308	ARG
2	D	324	SER
2	D	344	VAL
2	D	360	PRO
2	D	378	ILE
2	D	391	ILE
2	D	398	MET
2	D	402	LYS
2	D	404	PHE
2	D	416	MET

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Mol	Chain	Res	Type
2	D	428	LEU
1	A	11	GLN
1	A	39	ASP
1	A	73	THR
1	A	99	ALA
1	A	112	LYS
1	A	144	GLY
1	A	195	LEU
1	A	237	SER
1	A	245	ASP
1	A	259	LEU
1	A	277	SER
1	A	299	ALA
1	A	340	THR
1	A	341	ILE
1	A	344	VAL
1	A	353	VAL
1	A	419	SER
2	B	26	ASP
2	B	27	GLU
2	B	56	ALA
2	B	60	LYS
2	B	61	TYR
2	B	71	GLU
2	B	96	GLN
2	B	115	VAL
2	B	119	LEU
2	B	128	SER
2	B	139	HIS
2	B	185	TYR
2	B	199	ASP
2	B	219	LEU
2	B	239	THR
2	B	264	ARG
2	B	293	GLN
2	B	304	ALA
2	B	340	SER
2	B	349	ASN
2	B	382	THR
2	B	387	LEU
1	C	16	ILE
1	C	38	SER

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Mol	Chain	Res	Type
1	C	39	ASP
1	C	46	ASP
1	C	73	THR
1	C	112	LYS
1	C	195	LEU
1	C	237	SER
1	C	239	THR
1	C	245	ASP
1	C	257	THR
1	C	264	ARG
1	C	315	CYS
1	C	341	ILE
1	C	344	VAL
1	C	353	VAL
1	C	404	PHE
1	C	419	SER
2	D	2	ARG
2	D	26	ASP
2	D	56	ALA
2	D	96	GLN
2	D	115	VAL
2	D	119	LEU
2	D	128	SER
2	D	139	HIS
2	D	185	TYR
2	D	186	ASN
2	D	199	ASP
2	D	219	LEU
2	D	239	THR
2	D	293	GLN
2	D	340	SER
2	D	382	THR
2	D	387	LEU
2	D	399	PHE
1	A	28	HIS
1	A	29	GLY
1	A	38	SER
1	A	89	PRO
1	A	101	ASN
1	A	115	ILE
1	A	129	CYS
1	A	175	PRO

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Mol	Chain	Res	Type
1	A	198	SER
1	A	210	TYR
1	A	219	ILE
1	A	257	THR
1	A	261	PRO
1	A	264	ARG
1	A	306	ASP
1	A	315	CYS
1	A	404	PHE
2	B	2	ARG
2	B	91	ASN
2	B	94	PHE
2	B	97	SER
2	B	186	ASN
2	B	190	SER
2	B	192	HIS
2	B	194	LEU
2	B	211	ASP
2	B	227	LEU
2	B	273	ALA
2	B	277	SER
2	B	348	PRO
2	B	370	GLY
1	C	29	GLY
1	C	72	PRO
1	C	89	PRO
1	C	101	ASN
1	C	129	CYS
1	C	130	THR
1	C	161	TYR
1	C	198	SER
1	C	208	ALA
1	C	219	ILE
1	C	261	PRO
1	C	329	ASN
1	C	364	PRO
1	C	432	TYR
2	D	78	VAL
2	D	81	GLY
2	D	91	ASN
2	D	94	PHE
2	D	97	SER

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Mol	Chain	Res	Type
2	D	155	SER
2	D	190	SER
2	D	192	HIS
2	D	194	LEU
2	D	264	ARG
2	D	273	ALA
2	D	277	SER
2	D	283	TYR
2	D	304	ALA
2	D	339	ASN
2	D	348	PRO
2	D	370	GLY
1	A	72	PRO
1	A	125	LEU
1	A	130	THR
1	A	131	GLY
1	A	145	THR
1	A	314	ALA
1	A	326	LYS
1	A	436	GLY
2	B	30	ILE
2	B	52	TYR
2	B	63	PRO
2	B	78	VAL
2	B	177	VAL
2	B	424	ASN
1	C	28	HIS
1	C	132	LEU
1	C	145	THR
1	C	292	THR
1	C	306	ASP
1	C	314	ALA
1	C	326	LYS
1	C	348	PRO
1	C	382	THR
1	C	408	TYR
1	C	436	GLY
2	D	63	PRO
2	D	154	ILE
2	D	177	VAL
2	D	211	ASP
2	D	227	LEU

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Mol	Chain	Res	Type
2	D	318	VAL
2	D	349	ASN
2	D	424	ASN
2	D	431	GLU
1	A	161	TYR
1	A	329	ASN
1	A	342	GLN
1	A	348	PRO
1	A	364	PRO
1	A	369	ALA
1	A	382	THR
1	A	432	TYR
2	B	3	GLU
2	B	162	PRO
2	B	193	GLN
2	B	339	ASN
1	C	125	LEU
1	C	175	PRO
1	C	369	ALA
2	D	148	GLY
2	D	160	GLU
2	D	193	GLN
1	A	17	GLY
1	A	307	PRO
2	B	81	GLY
2	B	154	ILE
2	B	163	ASP
2	B	182	VAL
2	B	431	GLU
1	C	115	ILE
1	C	298	PRO
1	C	342	GLN
2	D	30	ILE
2	D	107	HIS
2	D	111	GLY
2	D	162	PRO
2	D	182	VAL
1	A	298	PRO
2	B	93	VAL
2	B	222	PRO
2	B	318	VAL
1	C	78	VAL

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Mol	Chain	Res	Type
1	C	131	GLY
2	D	93	VAL
2	D	222	PRO
1	A	288	VAL
2	B	86	ILE
1	A	30	ILE
2	B	111	GLY
1	C	307	PRO
2	D	184	PRO
1	A	78	VAL
2	B	279	GLY
1	C	273	ALA
1	A	273	ALA
1	A	435	VAL
2	D	271	GLY

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	354/377 (94%)	278 (78%)	76 (22%)	1 6
1	C	354/377 (94%)	279 (79%)	75 (21%)	1 6
2	B	347/381 (91%)	274 (79%)	73 (21%)	1 6
2	D	347/381 (91%)	270 (78%)	77 (22%)	1 6
All	All	1402/1516 (92%)	1101 (78%)	301 (22%)	1 6

All (301) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	16	ILE
1	A	23	LEU
1	A	25	CYS
1	A	30	ILE
1	A	32	PRO

Continued on next page...

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Mol	Chain	Res	Type
1	A	40	LYS
1	A	46	ASP
1	A	47	ASP
1	A	71	GLU
1	A	73	THR
1	A	77	GLU
1	A	83	TYR
1	A	86	LEU
1	A	87	PHE
1	A	91	GLN
1	A	92	LEU
1	A	101	ASN
1	A	105	ARG
1	A	115	ILE
1	A	125	LEU
1	A	130	THR
1	A	141	PHE
1	A	150	THR
1	A	164	LYS
1	A	179	THR
1	A	181	VAL
1	A	182	VAL
1	A	196	GLU
1	A	197	HIS
1	A	199	ASP
1	A	210	TYR
1	A	212	ILE
1	A	213	CYS
1	A	214	ARG
1	A	216	ASN
1	A	221	ARG
1	A	244	PHE
1	A	250	VAL
1	A	252	LEU
1	A	255	PHE
1	A	258	ASN
1	A	267	PHE
1	A	269	LEU
1	A	275	VAL
1	A	276	ILE
1	A	279	GLU
1	A	282	TYR

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Mol	Chain	Res	Type
1	A	285	GLN
1	A	292	THR
1	A	295	CYS
1	A	297	GLU
1	A	302	MET
1	A	309	HIS
1	A	316	CYS
1	A	318	LEU
1	A	322	ASP
1	A	335	ILE
1	A	336	LYS
1	A	345	ASP
1	A	346	TRP
1	A	349	THR
1	A	356	ASN
1	A	373	ARG
1	A	376	CYS
1	A	402	ARG
1	A	404	PHE
1	A	411	GLU
1	A	413	MET
1	A	414	GLU
1	A	418	PHE
1	A	420	GLU
1	A	425	MET
1	A	428	LEU
1	A	431	ASP
1	A	439	SER
2	B	16	ILE
2	B	25	SER
2	B	53	TYR
2	B	55	GLU
2	B	60	LYS
2	B	70	LEU
2	B	76	ASP
2	B	88	ARG
2	B	91	ASN
2	B	113	GLU
2	B	119	LEU
2	B	128	SER
2	B	136	GLN
2	B	139	HIS

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Mol	Chain	Res	Type
2	B	149	MET
2	B	157	ILE
2	B	158	ARG
2	B	160	GLU
2	B	163	ASP
2	B	167	ASN
2	B	168	THR
2	B	180	THR
2	B	185	TYR
2	B	186	ASN
2	B	192	HIS
2	B	193	GLN
2	B	194	LEU
2	B	201	THR
2	B	203	CYS
2	B	211	ASP
2	B	218	LYS
2	B	228	ASN
2	B	239	THR
2	B	244	PHE
2	B	245	PRO
2	B	249	ASN
2	B	251	ASP
2	B	252	LEU
2	B	253	ARG
2	B	254	LYS
2	B	255	LEU
2	B	265	LEU
2	B	278	ARG
2	B	283	TYR
2	B	284	ARG
2	B	286	LEU
2	B	292	THR
2	B	302	MET
2	B	308	ARG
2	B	311	ARG
2	B	315	VAL
2	B	323	MET
2	B	341	SER
2	B	345	GLU
2	B	346	TRP
2	B	350	ASN

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Mol	Chain	Res	Type
2	B	352	LYS
2	B	377	PHE
2	B	380	ASN
2	B	388	PHE
2	B	395	PHE
2	B	401	ARG
2	B	404	PHE
2	B	405	LEU
2	B	407	TRP
2	B	409	THR
2	B	414	ASP
2	B	416	MET
2	B	419	THR
2	B	424	ASN
2	B	426	ASN
2	B	436	GLN
2	B	437	ASP
1	C	8	HIS
1	C	16	ILE
1	C	23	LEU
1	C	25	CYS
1	C	30	ILE
1	C	32	PRO
1	C	40	LYS
1	C	42	ILE
1	C	46	ASP
1	C	47	ASP
1	C	71	GLU
1	C	73	THR
1	C	77	GLU
1	C	83	TYR
1	C	86	LEU
1	C	87	PHE
1	C	91	GLN
1	C	101	ASN
1	C	105	ARG
1	C	115	ILE
1	C	125	LEU
1	C	130	THR
1	C	141	PHE
1	C	150	THR
1	C	164	LYS

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Mol	Chain	Res	Type
1	C	175	PRO
1	C	179	THR
1	C	181	VAL
1	C	182	VAL
1	C	196	GLU
1	C	197	HIS
1	C	199	ASP
1	C	212	ILE
1	C	213	CYS
1	C	214	ARG
1	C	216	ASN
1	C	221	ARG
1	C	244	PHE
1	C	252	LEU
1	C	255	PHE
1	C	258	ASN
1	C	267	PHE
1	C	269	LEU
1	C	275	VAL
1	C	279	GLU
1	C	282	TYR
1	C	285	GLN
1	C	292	THR
1	C	297	GLU
1	C	302	MET
1	C	309	HIS
1	C	316	CYS
1	C	318	LEU
1	C	322	ASP
1	C	336	LYS
1	C	345	ASP
1	C	346	TRP
1	C	349	THR
1	C	356	ASN
1	C	373	ARG
1	C	376	CYS
1	C	395	PHE
1	C	398	MET
1	C	402	ARG
1	C	404	PHE
1	C	411	GLU
1	C	413	MET

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Mol	Chain	Res	Type
1	C	414	GLU
1	C	418	PHE
1	C	420	GLU
1	C	425	MET
1	C	428	LEU
1	C	431	ASP
1	C	433	GLU
1	C	439	SER
2	D	16	ILE
2	D	25	SER
2	D	53	TYR
2	D	55	GLU
2	D	60	LYS
2	D	70	LEU
2	D	76	ASP
2	D	88	ARG
2	D	91	ASN
2	D	94	PHE
2	D	113	GLU
2	D	119	LEU
2	D	128	SER
2	D	136	GLN
2	D	139	HIS
2	D	149	MET
2	D	157	ILE
2	D	158	ARG
2	D	160	GLU
2	D	163	ASP
2	D	167	ASN
2	D	180	THR
2	D	185	TYR
2	D	186	ASN
2	D	192	HIS
2	D	193	GLN
2	D	194	LEU
2	D	201	THR
2	D	203	CYS
2	D	218	LYS
2	D	228	ASN
2	D	239	THR
2	D	244	PHE
2	D	245	PRO

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Mol	Chain	Res	Type
2	D	249	ASN
2	D	251	ASP
2	D	252	LEU
2	D	253	ARG
2	D	254	LYS
2	D	255	LEU
2	D	265	LEU
2	D	278	ARG
2	D	283	TYR
2	D	284	ARG
2	D	286	LEU
2	D	292	THR
2	D	302	MET
2	D	308	ARG
2	D	311	ARG
2	D	312	TYR
2	D	315	VAL
2	D	323	MET
2	D	341	SER
2	D	345	GLU
2	D	346	TRP
2	D	350	ASN
2	D	352	LYS
2	D	377	PHE
2	D	380	ASN
2	D	381	SER
2	D	382	THR
2	D	388	PHE
2	D	395	PHE
2	D	398	MET
2	D	401	ARG
2	D	404	PHE
2	D	405	LEU
2	D	407	TRP
2	D	409	THR
2	D	414	ASP
2	D	416	MET
2	D	419	THR
2	D	424	ASN
2	D	425	MET
2	D	426	ASN
2	D	436	GLN

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Mol	Chain	Res	Type
2	D	437	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	102	ASN
1	A	133	GLN
1	A	176	GLN
1	A	186	ASN
1	A	258	ASN
1	A	285	GLN
1	A	300	ASN
1	A	301	GLN
1	A	356	ASN
1	A	380	ASN
2	B	6	HIS
2	B	8	GLN
2	B	14	ASN
2	B	15	GLN
2	B	85	GLN
2	B	91	ASN
2	B	101	ASN
2	B	102	ASN
2	B	133	GLN
2	B	139	HIS
2	B	193	GLN
2	B	197	ASN
2	B	206	ASN
2	B	228	ASN
2	B	282	GLN
2	B	294	GLN
2	B	337	ASN
2	B	350	ASN
2	B	380	ASN
2	B	426	ASN
2	B	433	GLN
2	B	434	GLN
1	C	15	GLN
1	C	35	GLN
1	C	102	ASN
1	C	133	GLN

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Mol	Chain	Res	Type
1	C	176	GLN
1	C	186	ASN
1	C	256	GLN
1	C	258	ASN
1	C	285	GLN
1	C	300	ASN
1	C	301	GLN
1	C	356	ASN
2	D	6	HIS
2	D	8	GLN
2	D	14	ASN
2	D	15	GLN
2	D	85	GLN
2	D	91	ASN
2	D	101	ASN
2	D	102	ASN
2	D	133	GLN
2	D	193	GLN
2	D	197	ASN
2	D	206	ASN
2	D	228	ASN
2	D	282	GLN
2	D	294	GLN
2	D	349	ASN
2	D	350	ASN
2	D	380	ASN
2	D	426	ASN
2	D	433	GLN
2	D	434	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GTP	A	500	-	26,34,34	1.36	5 (19%)	32,54,54	0.92	0
4	GTP	C	502	-	26,34,34	1.31	2 (7%)	32,54,54	1.02	2 (6%)
5	GDP	D	503	-	24,30,30	1.35	4 (16%)	30,47,47	0.96	2 (6%)
5	GDP	B	501	-	24,30,30	1.53	5 (20%)	30,47,47	0.91	0

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
4	GTP	A	500	-	-	5/18/38/38	0/3/3/3
4	GTP	C	502	-	-	3/18/38/38	0/3/3/3
5	GDP	D	503	-	-	6/12/32/32	0/3/3/3
5	GDP	B	501	-	-	4/12/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	GDP	C6-N1	3.79	1.43	1.37
5	D	503	GDP	C6-N1	3.44	1.43	1.37
4	A	500	GTP	C5-C6	-3.33	1.40	1.47
5	B	501	GDP	C2'-C1'	-3.28	1.48	1.53
4	C	502	GTP	C5-C6	-3.06	1.41	1.47
4	C	502	GTP	C6-N1	3.00	1.42	1.37
5	D	503	GDP	C2'-C1'	-2.77	1.49	1.53
5	B	501	GDP	O4'-C1'	-2.74	1.37	1.41
4	A	500	GTP	C6-N1	2.45	1.41	1.37
4	A	500	GTP	C8-N7	-2.41	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	GDP	C5-C6	-2.30	1.42	1.47
4	A	500	GTP	O5'-C5'	-2.23	1.36	1.44
5	D	503	GDP	PA-O2A	-2.10	1.45	1.55
4	A	500	GTP	PA-O2A	-2.08	1.45	1.55
5	D	503	GDP	C5-C6	-2.05	1.43	1.47
5	B	501	GDP	PA-O2A	-2.03	1.45	1.55

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	502	GTP	PA-O3A-PB	2.75	142.26	132.83
4	C	502	GTP	O2G-PG-O3B	2.65	113.51	104.64
5	D	503	GDP	O2B-PB-O3A	2.31	112.38	104.64
5	D	503	GDP	O3B-PB-O3A	2.10	111.68	104.64

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	500	GTP	C3'-C4'-C5'-O5'
5	B	501	GDP	C5'-O5'-PA-O1A
5	B	501	GDP	C5'-O5'-PA-O2A
5	B	501	GDP	C4'-C5'-O5'-PA
5	D	503	GDP	C5'-O5'-PA-O1A
5	D	503	GDP	C5'-O5'-PA-O2A
5	D	503	GDP	C4'-C5'-O5'-PA
5	D	503	GDP	C3'-C4'-C5'-O5'
5	D	503	GDP	O4'-C4'-C5'-O5'
4	A	500	GTP	O4'-C4'-C5'-O5'
4	A	500	GTP	PG-O3B-PB-O1B
4	C	502	GTP	C3'-C4'-C5'-O5'
4	A	500	GTP	PA-O3A-PB-O1B
4	C	502	GTP	O4'-C4'-C5'-O5'
5	B	501	GDP	C5'-O5'-PA-O3A
5	D	503	GDP	C5'-O5'-PA-O3A
4	A	500	GTP	C5'-O5'-PA-O1A
4	C	502	GTP	C5'-O5'-PA-O1A

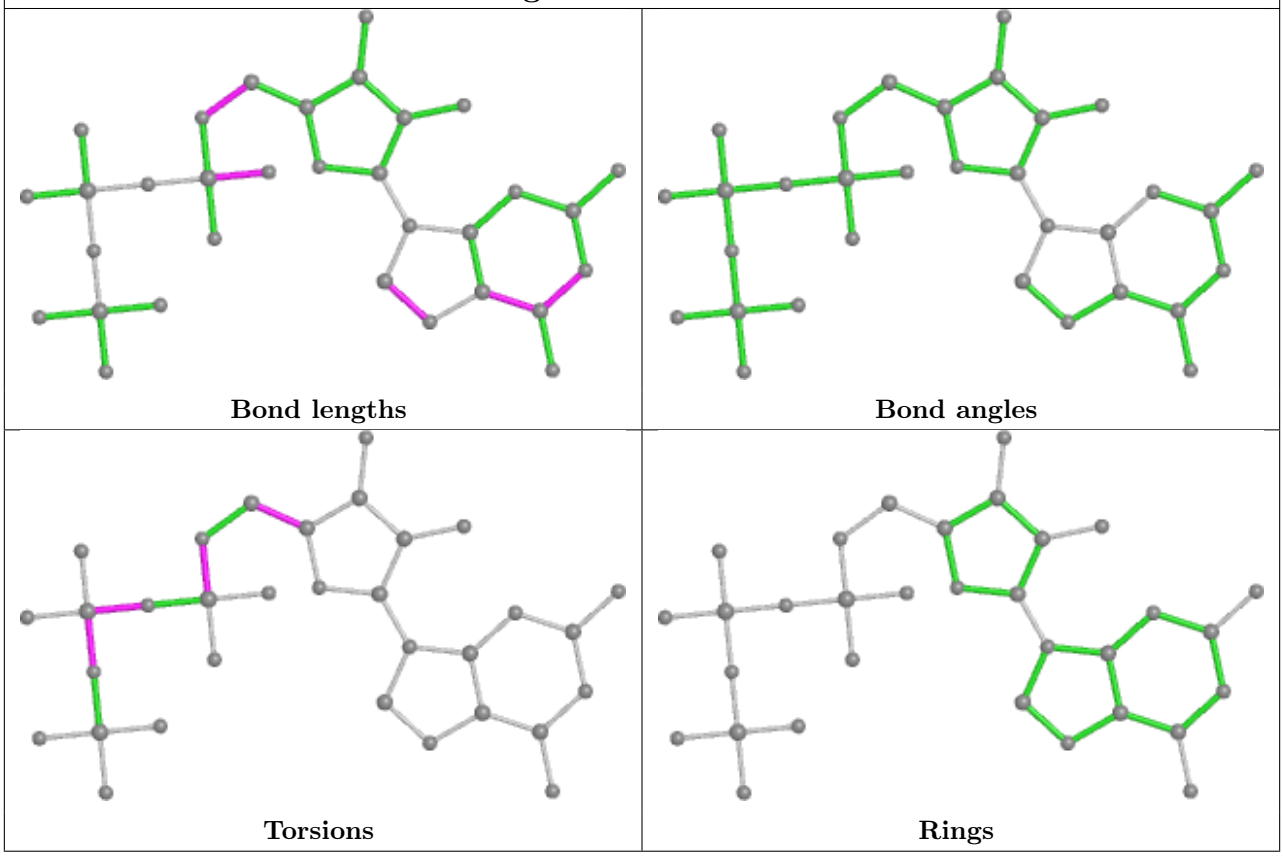
There are no ring outliers.

4 monomers are involved in 26 short contacts:

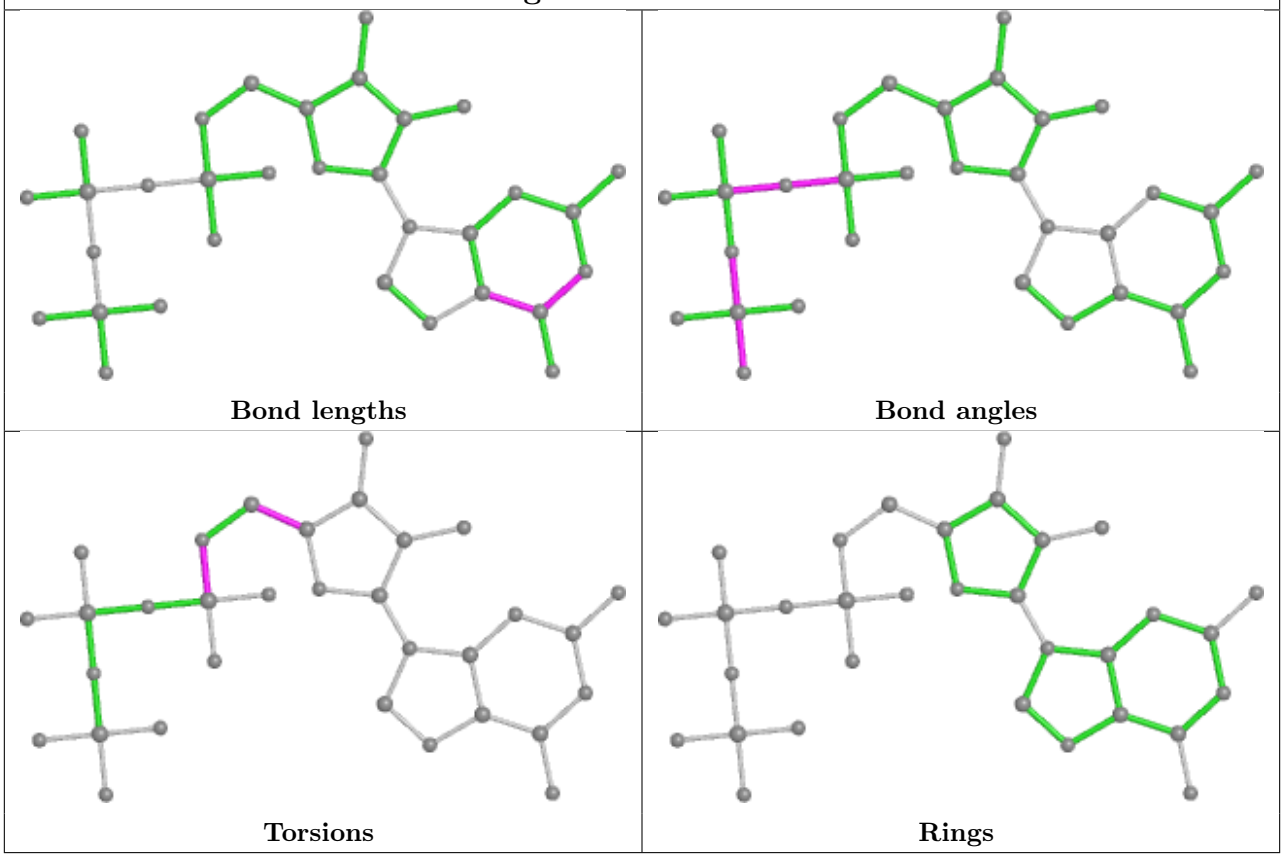
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	500	GTP	4	0
4	C	502	GTP	8	0
5	D	503	GDP	9	0
5	B	501	GDP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

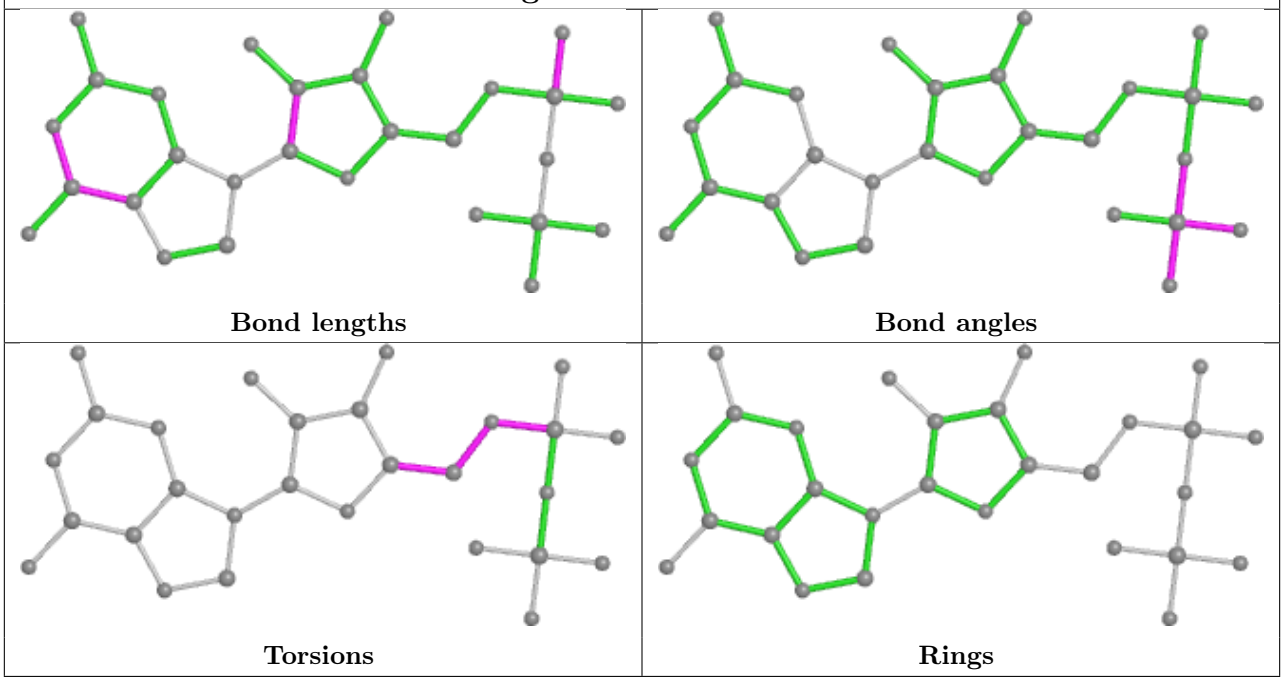
Ligand GTP A 500



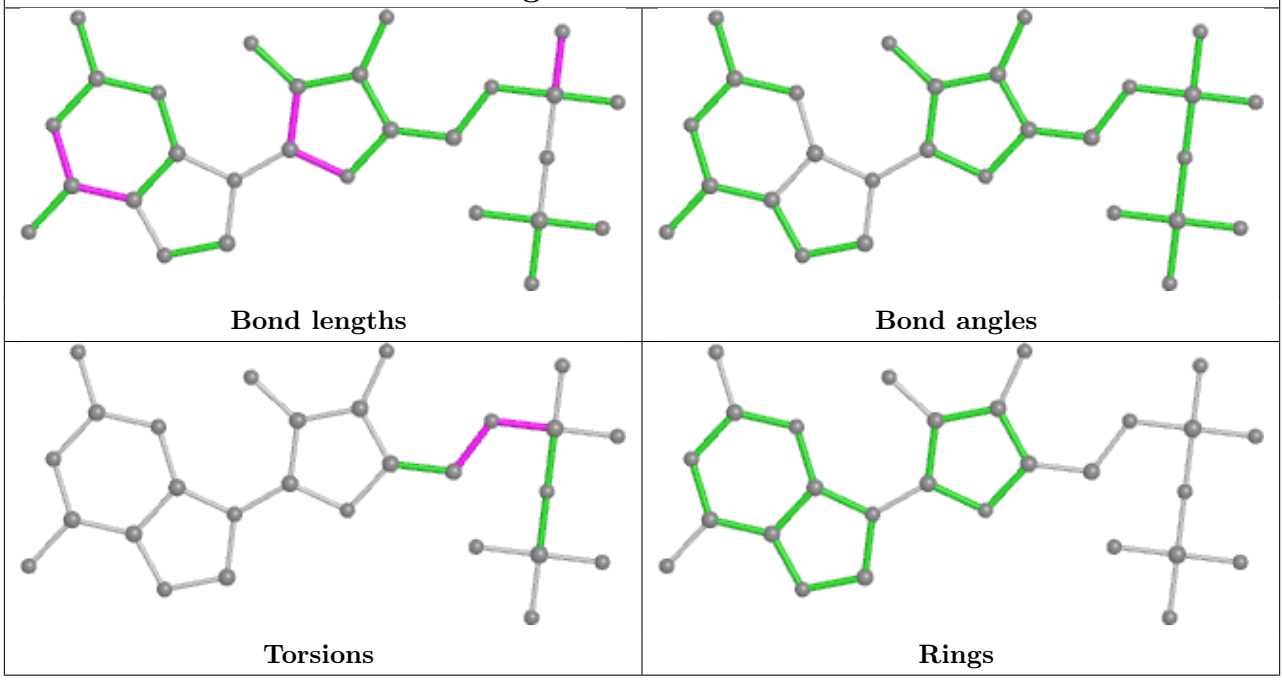
Ligand GTP C 502



Ligand GDP D 503



Ligand GDP B 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.