Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 07:29 AM EDT

PDB ID	:	4HMY
Title	:	Structural basis for recruitment and activation of the AP-1 clathrin adaptor complex by Arf1
Authors	:	Ren, X.; Farias, G.G.; Canagarajah, B.J.; Bonifacino, J.S.; Hurley, J.H.
Deposited on	:	2012-10-18
Resolution	:	7.00 Å(reported)

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

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

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

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

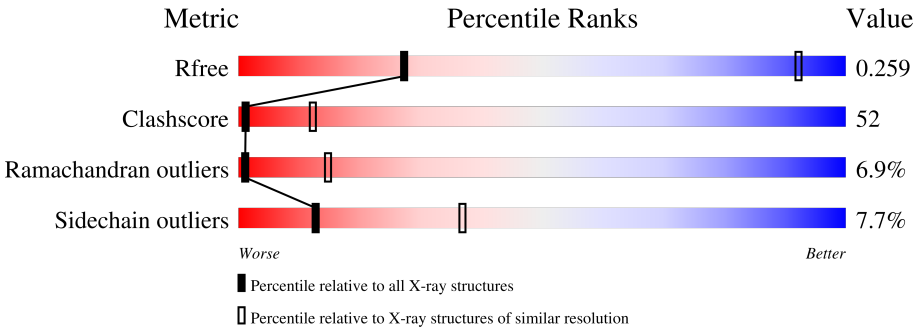
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 7.00 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))
R_{free}	130704	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)

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%

Mol	Chain	Length	Quality of chain
1	A	601	34% 56% 6% ·
2	B	586	25% 58% 11% · ·
3	M	423	25% 52% 12% · 9%
4	S	154	30% 60% 5% 6%
5	C	172	38% 52% 6% ·

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14743 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 AP-1 complex subunit gamma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	579	4583	2882	806	857	38	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	596	GLU	-	expression tag	UNP P22892
A	597	ASN	-	expression tag	UNP P22892
A	598	LEU	-	expression tag	UNP P22892
A	599	TYR	-	expression tag	UNP P22892
A	600	PHE	-	expression tag	UNP P22892
A	601	GLN	-	expression tag	UNP P22892

- Molecule 2 is a protein called AP-1 complex subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	563	4458	2847	732	852	27	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP Q10567
B	0	SER	-	expression tag	UNP Q10567
B	359	ARG	LYS	variant	UNP Q10567
B	476	LYS	GLU	variant	UNP Q10567
B	488	PHE	ILE	engineered mutation	UNP Q10567

- Molecule 3 is a protein called AP-1 complex subunit mu-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	383	Total	C	N	O	S	0	0	0
			3119	2013	523	569	14			

- Molecule 4 is a protein called AP-1 complex subunit sigma-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	S	145	Total	C	N	O	S	0	0	0
			1219	795	200	219	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	148	CYS	SER	variant	UNP Q96PC3

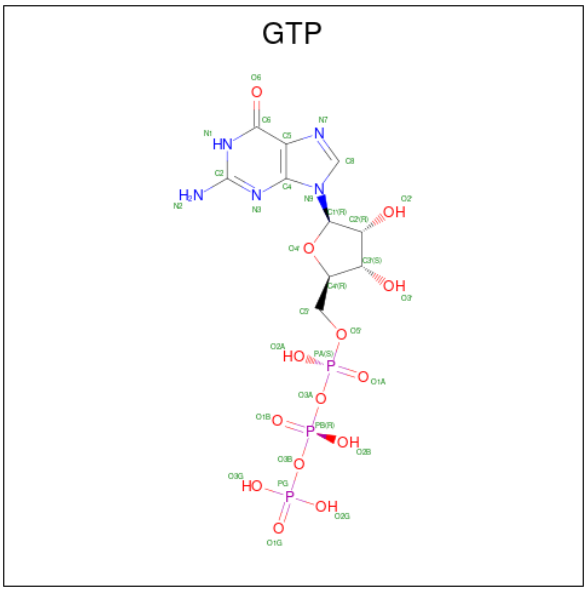
- Molecule 5 is a protein called ADP-ribosylation factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	165	Total	C	N	O	S	0	0	0
			1331	842	233	250	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	10	MET	-	expression tag	UNP P84077
C	11	HIS	-	expression tag	UNP P84077
C	12	HIS	-	expression tag	UNP P84077
C	13	HIS	-	expression tag	UNP P84077
C	14	HIS	-	expression tag	UNP P84077
C	15	HIS	-	expression tag	UNP P84077
C	16	HIS	-	expression tag	UNP P84077
C	71	LEU	GLN	engineered mutation	UNP P84077

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

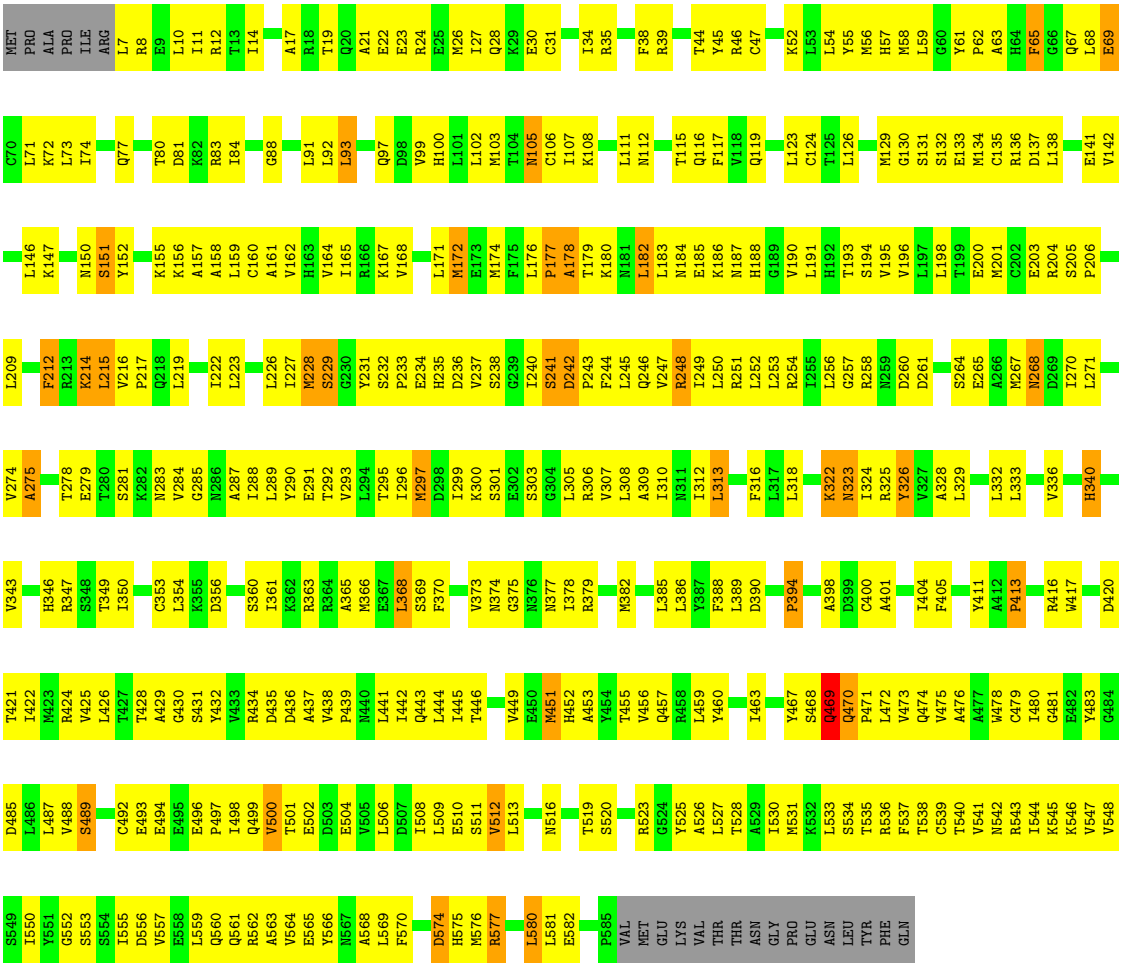
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Mg	0	0
			1	1		

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.

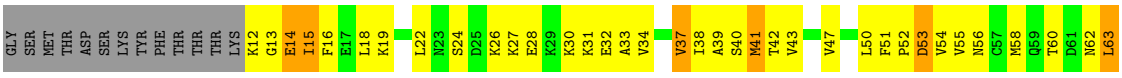
• Molecule 1: AP-1 complex subunit gamma-1

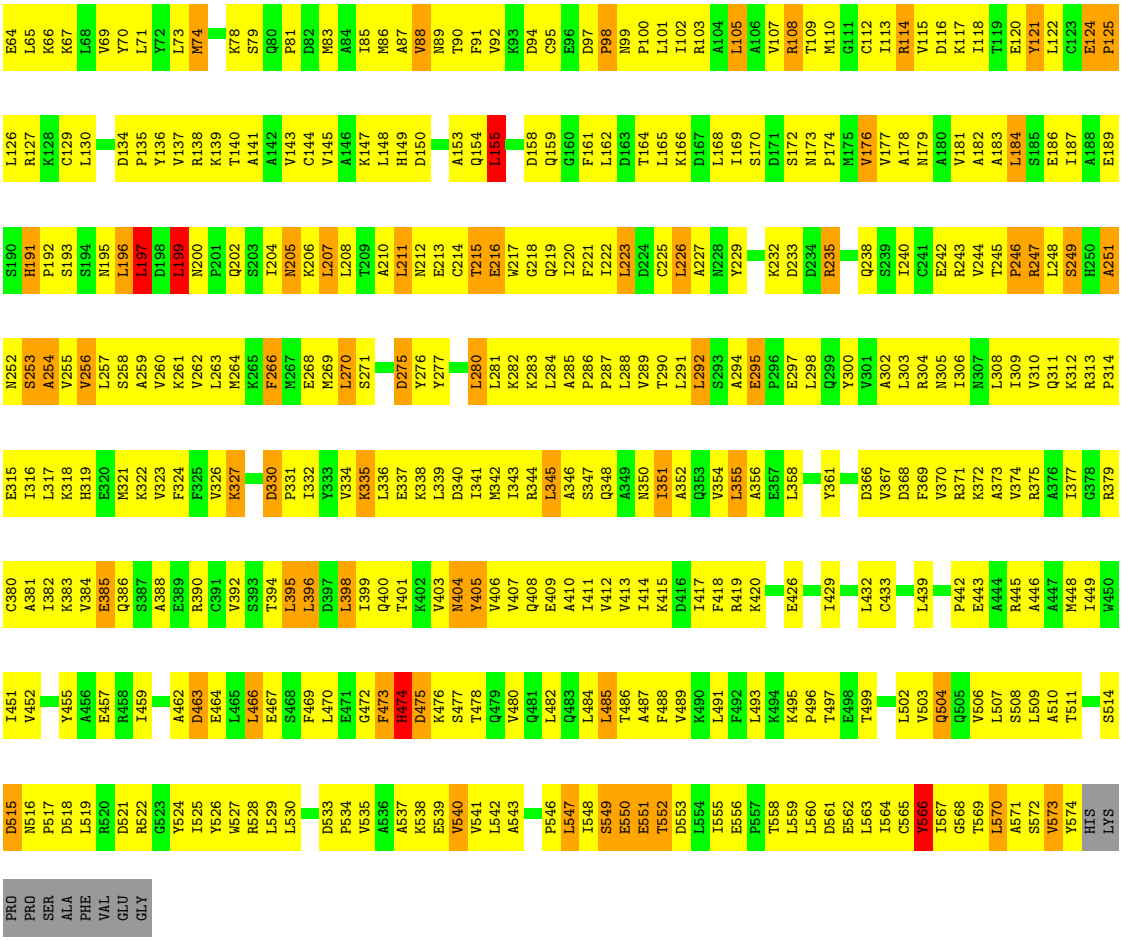
Chain A:



• Molecule 2: AP-1 complex subunit beta-1

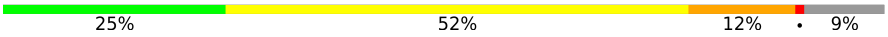
Chain B:

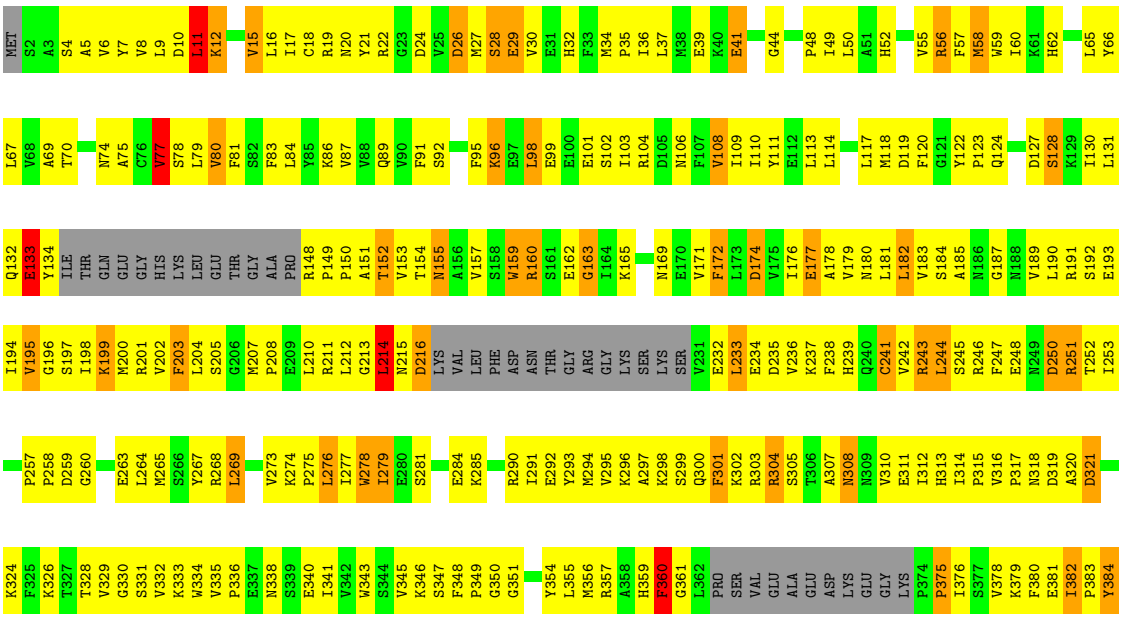




• Molecule 3: AP-1 complex subunit mu-1

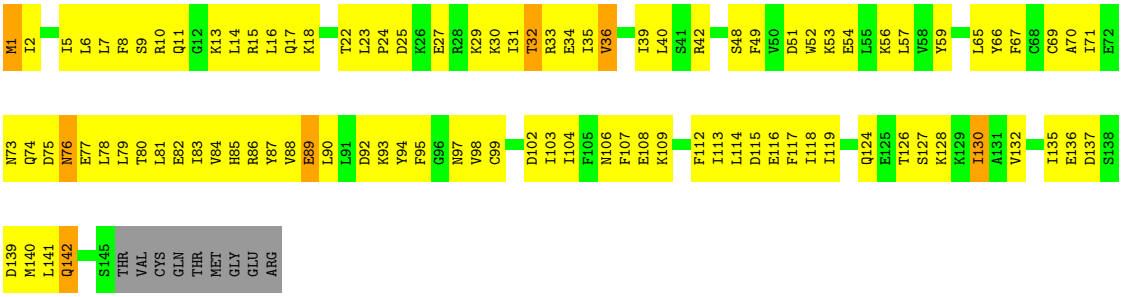
Chain M:





• Molecule 4: AP-1 complex subunit sigma-3

Chain S:



• Molecule 5: ADP-ribosylation factor 1

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α, β, γ	267.50Å 267.50Å 191.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 7.00 49.55 – 6.98	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-7.00) 93.6 (49.55-6.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 6.68Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.250 0.215 , 0.259	Depositor DCC
R_{free} test set	624 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	357.1	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 421.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.046 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	14743	wwPDB-VP
Average B, all atoms (Å^2)	321.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.23	0/4646	0.50	0/6270
2	B	0.24	0/4525	0.54	0/6134
3	M	0.26	0/3191	0.53	0/4312
4	S	0.26	0/1242	0.47	0/1669
5	C	0.24	0/1354	0.47	0/1831
All	All	0.24	0/14958	0.51	0/20216

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4583	0	4700	439	0
2	B	4458	0	4593	589	0
3	M	3119	0	3129	382	0
4	S	1219	0	1249	133	0
5	C	1331	0	1328	109	0
6	C	32	0	12	3	0
7	C	1	0	0	0	0
All	All	14743	0	15011	1548	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 52.

All (1548) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:233:LEU:HD21	3:M:268:ARG:H	1.16	1.10
3:M:315:PRO:HA	3:M:340:GLU:HA	1.35	1.06
3:M:60:ILE:HD11	3:M:67:LEU:HD23	1.41	1.03
1:A:439:PRO:HG3	2:B:517:PRO:HD3	1.41	1.02
1:A:553:SER:HB3	2:B:546:PRO:HB2	1.48	0.95
3:M:277:ILE:HA	3:M:299:SER:HA	1.49	0.95
2:B:395:LEU:HA	2:B:398:LEU:HD23	1.48	0.94
3:M:118:MET:HA	3:M:124:GLN:H	1.32	0.94
5:C:91:VAL:HG22	5:C:124:PHE:HB2	1.51	0.92
2:B:220:ILE:HG21	2:B:254:ALA:HB1	1.50	0.91
1:A:322:LYS:HA	1:A:325:ARG:HE	1.33	0.91
1:A:492:CYS:HB3	1:A:497:PRO:HG3	1.52	0.91
3:M:92:SER:HB3	3:M:98:LEU:HD21	1.53	0.90
3:M:212:LEU:HB3	3:M:253:ILE:HD11	1.52	0.90
1:A:83:ARG:HD2	4:S:142:GLN:HG3	1.50	0.90
3:M:324:LYS:HD2	3:M:359:HIS:HB2	1.53	0.89
2:B:162:LEU:HG	2:B:166:LYS:HE3	1.53	0.89
1:A:93:LEU:HD21	1:A:99:VAL:HG21	1.56	0.88
2:B:336:LEU:HD21	2:B:369:PHE:HA	1.55	0.88
1:A:71:LEU:HA	1:A:74:ILE:HD13	1.53	0.88
1:A:93:LEU:HD13	1:A:129:MET:HE1	1.55	0.88
3:M:198:ILE:HG23	3:M:264:LEU:HB3	1.56	0.87
1:A:226:LEU:HD21	1:A:245:LEU:HD23	1.57	0.87
2:B:499:THR:HA	2:B:502:LEU:HD23	1.57	0.87
2:B:414:ILE:HA	2:B:417:ILE:HD12	1.57	0.86
3:M:202:VAL:HG23	3:M:204:LEU:HD23	1.57	0.86
2:B:564:ILE:HG23	2:B:567:ILE:HD11	1.56	0.86
2:B:260:VAL:HG22	2:B:284:LEU:HD22	1.57	0.86
3:M:314:ILE:HG23	3:M:341:ILE:HB	1.55	0.86
3:M:114:LEU:HA	3:M:117:LEU:HD12	1.56	0.86
3:M:302:LYS:HB3	3:M:304:ARG:HH22	1.39	0.86
1:A:136:ARG:HH21	1:A:168:VAL:HG22	1.38	0.85
1:A:534:SER:HB2	1:A:577:ARG:HH21	1.42	0.85
1:A:536:ARG:HH12	1:A:581:LEU:HB3	1.42	0.84
2:B:408:GLN:O	2:B:411:ILE:HG12	1.77	0.84
1:A:136:ARG:HG3	1:A:171:LEU:HD11	1.60	0.83
2:B:215:THR:HG23	2:B:218:GLY:HA3	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LEU:HD23	1:A:52:LYS:HA	1.60	0.83
2:B:533:ASP:HB2	2:B:535:VAL:HG12	1.58	0.83
4:S:86:ARG:HH22	4:S:89:GLU:HG2	1.43	0.83
1:A:46:ARG:HG3	1:A:69:GLU:HG3	1.59	0.83
2:B:452:VAL:HA	2:B:459:ILE:HD13	1.61	0.83
2:B:149:HIS:HA	2:B:153:ALA:HB3	1.61	0.83
2:B:177:VAL:HG11	2:B:210:ALA:HB1	1.61	0.82
1:A:247:VAL:HG21	4:S:79:LEU:HD13	1.62	0.82
2:B:115:VAL:HB	2:B:118:ILE:HG23	1.61	0.82
1:A:27:ILE:HD11	1:A:59:LEU:HD23	1.60	0.81
1:A:509:LEU:HD13	1:A:530:ILE:HG12	1.62	0.81
2:B:303:LEU:HD13	2:B:337:GLU:HB3	1.59	0.81
1:A:54:LEU:HD21	1:A:88:GLY:HA2	1.62	0.81
2:B:22:LEU:HD23	2:B:33:ALA:HB1	1.62	0.81
2:B:284:LEU:O	2:B:288:LEU:HG	1.79	0.81
2:B:255:VAL:HG13	2:B:256:VAL:H	1.46	0.81
2:B:374:VAL:HA	2:B:377:ILE:HD13	1.63	0.81
2:B:227:ALA:HA	2:B:262:VAL:HG13	1.62	0.80
2:B:470:LEU:HD21	2:B:484:LEU:HD22	1.62	0.80
1:A:438:VAL:HB	1:A:439:PRO:HD3	1.62	0.80
1:A:547:VAL:HA	1:A:550:ILE:HD12	1.63	0.80
3:M:118:MET:HB2	3:M:123:PRO:HA	1.63	0.80
1:A:227:ILE:HG22	1:A:228:MET:H	1.47	0.80
2:B:126:LEU:HD21	2:B:145:VAL:HG22	1.64	0.80
2:B:379:ARG:HB3	2:B:552:THR:HG22	1.63	0.80
5:C:34:LEU:HD13	5:C:65:VAL:HG11	1.64	0.80
3:M:29:GLU:HG2	3:M:55:VAL:HG21	1.65	0.79
3:M:195:VAL:HG22	3:M:196:GLY:H	1.46	0.79
1:A:459:LEU:HD13	1:A:476:ALA:HA	1.62	0.79
1:A:301:SER:HB2	1:A:305:LEU:HD23	1.63	0.78
3:M:314:ILE:HD13	3:M:376:ILE:HD11	1.65	0.78
2:B:34:VAL:HB	2:B:65:LEU:HD11	1.66	0.78
2:B:223:LEU:HA	2:B:226:LEU:HD22	1.66	0.78
4:S:23:LEU:HD23	4:S:24:PRO:HD2	1.66	0.78
3:M:118:MET:CB	3:M:123:PRO:HA	2.14	0.78
1:A:159:LEU:HD13	4:S:119:ILE:HG23	1.64	0.77
2:B:211:LEU:HG	2:B:222:ILE:HD13	1.66	0.77
3:M:397:ILE:HG21	3:M:405:ALA:HB2	1.66	0.77
3:M:383:PRO:HA	3:M:412:ILE:HG22	1.66	0.77
2:B:297:GLU:HG3	3:M:48:PRO:HB3	1.67	0.76
1:A:389:LEU:HD22	1:A:404:ILE:HD12	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:ALA:HB2	2:B:262:VAL:HG22	1.67	0.76
2:B:26:LYS:HG3	2:B:27:LYS:H	1.49	0.76
1:A:287:ALA:HB2	4:S:78:LEU:HD22	1.68	0.76
1:A:493:GLU:HG2	1:A:494:GLU:H	1.51	0.76
3:M:62:HIS:NE2	3:M:98:LEU:HD23	2.01	0.76
3:M:307:ALA:HB3	3:M:348:PHE:HB3	1.68	0.76
1:A:513:LEU:HD12	1:A:513:LEU:H	1.50	0.75
2:B:303:LEU:HA	2:B:306:ILE:HD12	1.69	0.75
3:M:108:VAL:HG23	3:M:109:ILE:H	1.51	0.75
1:A:498:ILE:HG22	1:A:499:GLN:H	1.50	0.75
2:B:184:LEU:HA	2:B:187:ILE:HD12	1.69	0.75
1:A:385:LEU:HD22	1:A:404:ILE:HG12	1.68	0.75
2:B:19:LYS:HA	2:B:22:LEU:HD12	1.69	0.75
3:M:278:TRP:HB3	3:M:298:LYS:HB3	1.67	0.75
2:B:351:ILE:HD12	2:B:352:ALA:H	1.52	0.74
2:B:336:LEU:HD22	2:B:372:LYS:HB2	1.69	0.74
2:B:398:LEU:HD11	2:B:410:ALA:HB2	1.68	0.74
3:M:238:PHE:HB3	3:M:242:VAL:HG11	1.69	0.74
1:A:246:GLN:O	1:A:250:LEU:HG	1.88	0.74
2:B:81:PRO:HB3	2:B:115:VAL:HG13	1.68	0.74
2:B:347:SER:H	2:B:350:ASN:HD21	1.33	0.74
3:M:185:ALA:HA	3:M:422:THR:HA	1.68	0.74
1:A:580:LEU:HB3	2:B:528:ARG:HB3	1.70	0.73
2:B:89:ASN:ND2	5:C:48:THR:HA	2.01	0.73
4:S:36:VAL:HA	4:S:39:ILE:HD12	1.70	0.73
1:A:247:VAL:HG11	4:S:79:LEU:HD22	1.70	0.73
2:B:211:LEU:HD21	2:B:222:ILE:HB	1.70	0.73
2:B:211:LEU:HD11	2:B:222:ILE:HG21	1.68	0.73
1:A:290:TYR:HE2	4:S:76:ASN:HA	1.52	0.73
2:B:281:LEU:HD22	2:B:316:ILE:HD11	1.69	0.72
3:M:98:LEU:HD22	3:M:98:LEU:H	1.54	0.72
5:C:70:GLY:HA2	5:C:78:TRP:HZ2	1.54	0.72
2:B:169:ILE:HG13	2:B:170:SER:H	1.53	0.72
2:B:411:ILE:HA	2:B:414:ILE:HD12	1.70	0.72
1:A:459:LEU:HD22	1:A:476:ALA:HB2	1.71	0.72
5:C:51:PHE:HA	5:C:67:ASP:O	1.90	0.72
3:M:169:ASN:HA	3:M:203:PHE:O	1.89	0.72
1:A:209:LEU:HA	1:A:212:PHE:HB2	1.71	0.71
3:M:355:LEU:HD13	3:M:356:MET:N	2.04	0.71
2:B:89:ASN:HB2	5:C:50:GLY:H	1.55	0.71
3:M:83:PHE:O	3:M:87:VAL:HG23	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:O	1:A:274:VAL:HG23	1.90	0.71
1:A:232:SER:HB3	1:A:233:PRO:HD3	1.71	0.71
1:A:542:ASN:HA	1:A:545:LYS:HE3	1.73	0.71
2:B:292:LEU:HD13	2:B:323:VAL:HG12	1.73	0.70
2:B:103:ARG:O	2:B:107:VAL:HG23	1.90	0.70
2:B:538:LYS:HD2	2:B:542:LEU:HB2	1.74	0.70
5:C:90:PHE:HB2	5:C:121:LEU:HD11	1.71	0.70
2:B:429:ILE:O	2:B:432:LEU:HG	1.91	0.70
4:S:112:PHE:O	4:S:116:GLU:HB2	1.92	0.70
1:A:244:PHE:HE2	4:S:86:ARG:HD2	1.57	0.70
1:A:487:LEU:HG	1:A:500:VAL:HG21	1.73	0.70
2:B:18:LEU:O	2:B:22:LEU:HG	1.92	0.69
2:B:54:VAL:HG12	2:B:69:VAL:HG13	1.74	0.69
1:A:288:ILE:O	1:A:292:THR:HG23	1.92	0.69
2:B:311:GLN:HB3	2:B:560:LEU:HD11	1.73	0.69
2:B:285:ALA:HB3	2:B:286:PRO:HD3	1.74	0.69
3:M:376:ILE:O	3:M:419:GLN:HA	1.92	0.69
5:C:174:SER:O	5:C:178:ARG:HG2	1.92	0.69
2:B:122:LEU:HD22	2:B:125:PRO:HB2	1.74	0.69
2:B:261:LYS:HE2	2:B:567:ILE:N	2.07	0.69
3:M:233:LEU:HD21	3:M:268:ARG:N	1.99	0.69
1:A:470:GLN:HB2	1:A:471:PRO:HD3	1.74	0.69
2:B:485:LEU:O	2:B:489:VAL:HG13	1.93	0.69
3:M:194:ILE:HD11	3:M:273:VAL:HG23	1.74	0.69
3:M:312:ILE:HG22	3:M:343:TRP:HB3	1.73	0.69
1:A:14:ILE:HD12	1:A:55:TYR:HE1	1.58	0.69
1:A:555:ILE:HD12	1:A:555:ILE:H	1.58	0.69
4:S:83:ILE:O	4:S:86:ARG:HB3	1.93	0.69
2:B:469:PHE:HZ	2:B:476:LYS:HG2	1.58	0.68
1:A:508:ILE:O	1:A:512:VAL:HG23	1.94	0.68
2:B:347:SER:H	2:B:350:ASN:ND2	1.90	0.68
1:A:244:PHE:HE1	4:S:83:ILE:HG12	1.57	0.68
1:A:340:HIS:O	1:A:343:VAL:HG22	1.92	0.68
2:B:178:ALA:HB2	2:B:214:CYS:SG	2.33	0.68
3:M:17:ILE:HD11	3:M:111:TYR:CE2	2.28	0.68
3:M:19:ARG:HD3	3:M:20:ASN:N	2.08	0.68
2:B:97:ASP:HB2	2:B:98:PRO:HD2	1.75	0.68
2:B:290:THR:HG21	3:M:237:LYS:HE2	1.74	0.68
3:M:192:SER:O	3:M:273:VAL:HG11	1.94	0.68
2:B:379:ARG:HD2	2:B:552:THR:HA	1.76	0.68
2:B:410:ALA:O	2:B:413:VAL:HG22	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:TYR:OH	1:A:504:GLU:HB3	1.94	0.67
2:B:469:PHE:CE2	2:B:484:LEU:HD11	2.29	0.67
2:B:486:THR:O	2:B:489:VAL:HG22	1.93	0.67
1:A:54:LEU:HD23	1:A:92:LEU:HG	1.76	0.67
1:A:556:ASP:HB3	1:A:559:LEU:HB2	1.77	0.67
2:B:240:ILE:O	2:B:244:VAL:HG23	1.95	0.67
4:S:76:ASN:ND2	4:S:79:LEU:H	1.93	0.67
1:A:35:ARG:HB2	1:A:65:PHE:HE2	1.59	0.67
1:A:456:VAL:HG12	1:A:487:LEU:HD13	1.77	0.67
2:B:375:ARG:HG2	2:B:379:ARG:HH22	1.58	0.67
3:M:234:GLU:HB2	3:M:268:ARG:HG3	1.77	0.67
1:A:557:VAL:HA	2:B:419:ARG:HH21	1.60	0.67
2:B:153:ALA:HB1	2:B:158:ASP:OD2	1.95	0.67
2:B:253:SER:HB2	3:M:78:SER:HB2	1.77	0.67
2:B:276:TYR:O	2:B:280:LEU:HB2	1.94	0.67
2:B:107:VAL:HG12	2:B:144:CYS:SG	2.34	0.67
2:B:166:LYS:HE2	2:B:197:LEU:HD21	1.76	0.67
1:A:322:LYS:HG3	1:A:325:ARG:HH21	1.59	0.66
2:B:478:THR:O	2:B:482:LEU:HG	1.95	0.66
4:S:95:PHE:HB2	4:S:98:VAL:HB	1.77	0.66
1:A:126:LEU:HD22	1:A:160:CYS:SG	2.35	0.66
2:B:217:TRP:HA	2:B:220:ILE:HD12	1.76	0.66
3:M:12:LYS:HE2	4:S:40:LEU:HD23	1.77	0.66
1:A:27:ILE:HG23	1:A:56:MET:SD	2.35	0.66
1:A:46:ARG:HG2	1:A:73:LEU:HG	1.78	0.66
1:A:240:ILE:HD12	1:A:284:VAL:HG12	1.76	0.66
2:B:242:GLU:HA	2:B:276:TYR:OH	1.94	0.66
1:A:441:LEU:HD23	1:A:475:VAL:HG11	1.78	0.66
1:A:449:VAL:HA	1:A:452:HIS:NE2	2.09	0.66
3:M:183:VAL:HG13	3:M:420:LEU:HB2	1.77	0.66
2:B:26:LYS:CG	2:B:27:LYS:H	2.08	0.66
2:B:372:LYS:HD2	2:B:375:ARG:HH21	1.59	0.66
1:A:115:THR:HG22	1:A:116:GLN:H	1.61	0.66
2:B:18:LEU:HD22	2:B:18:LEU:H	1.59	0.66
2:B:303:LEU:HD11	2:B:334:VAL:HG13	1.76	0.66
2:B:304:ARG:O	2:B:308:LEU:HG	1.96	0.66
2:B:310:VAL:HG22	2:B:317:LEU:HD23	1.78	0.66
2:B:89:ASN:HB2	5:C:50:GLY:N	2.11	0.66
2:B:383:LYS:HA	2:B:550:GLU:HG3	1.77	0.65
2:B:420:LYS:HD2	2:B:547:LEU:HB3	1.77	0.65
2:B:38:ILE:HA	2:B:41:MET:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:5:ALA:HB3	3:M:70:THR:HB	1.77	0.65
1:A:251:ARG:HH22	4:S:76:ASN:N	1.94	0.65
2:B:165:LEU:HD22	2:B:187:ILE:HD11	1.76	0.65
2:B:477:SER:O	2:B:480:VAL:HG12	1.96	0.65
4:S:87:TYR:O	4:S:90:LEU:HB2	1.96	0.65
5:C:34:LEU:HD11	5:C:54:GLU:HB2	1.78	0.65
1:A:250:LEU:HD22	1:A:292:THR:HG22	1.79	0.65
2:B:407:VAL:O	2:B:411:ILE:HG23	1.96	0.65
2:B:110:MET:SD	2:B:122:LEU:HD23	2.36	0.65
2:B:326:VAL:HG11	2:B:335:LYS:HG2	1.78	0.65
2:B:470:LEU:HD11	2:B:484:LEU:HD13	1.78	0.65
3:M:285:LYS:HG3	3:M:291:ILE:HD12	1.78	0.65
1:A:227:ILE:C	1:A:229:SER:H	2.01	0.65
2:B:165:LEU:HA	2:B:168:LEU:HD12	1.77	0.65
3:M:312:ILE:HD12	3:M:378:VAL:HB	1.79	0.65
4:S:113:ILE:HG12	4:S:135:ILE:HG12	1.77	0.65
1:A:249:ILE:O	1:A:253:LEU:HG	1.97	0.65
2:B:208:LEU:HA	2:B:211:LEU:HB2	1.79	0.65
2:B:469:PHE:CZ	2:B:476:LYS:HG2	2.31	0.65
3:M:397:ILE:HD12	3:M:403:TYR:HD2	1.59	0.65
1:A:228:MET:O	1:A:229:SER:HB2	1.97	0.64
2:B:396:LEU:O	2:B:400:GLN:HG2	1.97	0.64
1:A:293:VAL:HG13	1:A:309:ALA:HB1	1.79	0.64
2:B:303:LEU:HD21	2:B:338:LYS:HG2	1.79	0.64
3:M:329:VAL:HG21	3:M:354:TYR:HB3	1.76	0.64
4:S:136:GLU:O	4:S:140:MET:HB2	1.98	0.64
5:C:38:LYS:HD3	5:C:56:VAL:HG22	1.79	0.64
3:M:111:TYR:HA	3:M:114:LEU:HD12	1.79	0.64
3:M:180:ASN:ND2	3:M:195:VAL:H	1.95	0.64
1:A:8:ARG:NH2	4:S:106:ASN:HD21	1.96	0.64
1:A:73:LEU:HD22	1:A:81:ASP:HB3	1.80	0.64
2:B:205:ASN:HA	2:B:208:LEU:HG	1.80	0.64
5:C:17:GLU:HG2	5:C:62:SER:HB2	1.79	0.64
1:A:237:VAL:HG21	1:A:242:ASP:H	1.63	0.64
1:A:469:GLN:HG2	1:A:472:LEU:HD23	1.79	0.64
3:M:11:LEU:HD12	3:M:12:LYS:H	1.62	0.64
2:B:339:LEU:O	2:B:343:ILE:HG12	1.97	0.64
1:A:46:ARG:HE	1:A:69:GLU:HG3	1.63	0.64
1:A:115:THR:HG21	4:S:141:LEU:HD21	1.80	0.64
1:A:223:LEU:HB2	1:A:249:ILE:HG21	1.80	0.64
1:A:267:MET:O	1:A:271:LEU:HD23	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:LYS:O	1:A:550:ILE:HG13	1.98	0.64
2:B:67:LYS:O	2:B:71:LEU:HG	1.99	0.63
1:A:97:GLN:HA	1:A:100:HIS:HB3	1.79	0.63
2:B:394:THR:O	2:B:398:LEU:HB3	1.99	0.63
3:M:148:ARG:N	3:M:149:PRO:HD2	2.14	0.63
1:A:103:MET:O	1:A:107:ILE:HG12	1.98	0.63
3:M:183:VAL:HG22	3:M:420:LEU:HD13	1.79	0.63
3:M:301:PHE:N	3:M:301:PHE:CD1	2.67	0.63
1:A:108:LYS:HB2	1:A:138:LEU:HD11	1.79	0.63
2:B:327:LYS:HE3	2:B:338:LYS:NZ	2.13	0.63
3:M:113:LEU:HD22	3:M:131:LEU:HD21	1.79	0.63
5:C:47:PRO:HA	6:C:1001:GTP:O2G	1.99	0.63
2:B:261:LYS:NZ	2:B:566:TYR:HA	2.13	0.63
1:A:562:ARG:HE	2:B:522:ARG:HD2	1.63	0.63
1:A:216:VAL:HB	1:A:217:PRO:HD3	1.81	0.63
4:S:79:LEU:O	4:S:83:ILE:HG13	1.98	0.63
1:A:487:LEU:O	1:A:500:VAL:HG11	1.99	0.62
2:B:90:THR:HG1	2:B:91:PHE:HD1	1.47	0.62
3:M:243:ARG:HA	3:M:243:ARG:HH11	1.64	0.62
1:A:19:THR:HG22	1:A:21:ALA:H	1.64	0.62
3:M:304:ARG:HH21	3:M:305:SER:HB2	1.64	0.62
5:C:140:THR:HG23	5:C:145:LEU:HB2	1.81	0.62
1:A:548:VAL:HG21	1:A:570:PHE:HE2	1.64	0.62
3:M:202:VAL:HG13	3:M:260:GLY:H	1.64	0.62
1:A:438:VAL:HA	1:A:475:VAL:HG22	1.82	0.62
2:B:551:GLU:CD	2:B:551:GLU:H	2.03	0.62
5:C:89:ILE:HG12	5:C:122:LEU:HB3	1.81	0.62
1:A:172:MET:CE	1:A:204:ARG:HD2	2.29	0.62
2:B:60:THR:O	2:B:66:LYS:HE2	2.00	0.62
2:B:164:THR:O	2:B:168:LEU:HG	2.00	0.62
2:B:556:GLU:HB3	2:B:559:LEU:HB3	1.80	0.62
2:B:50:LEU:O	2:B:54:VAL:HG23	2.00	0.62
4:S:87:TYR:HA	4:S:90:LEU:HD13	1.80	0.62
3:M:7:TYR:HA	3:M:18:CYS:HB3	1.80	0.62
3:M:238:PHE:HA	3:M:265:MET:HB3	1.80	0.62
2:B:466:LEU:CD1	2:B:491:LEU:HD12	2.30	0.61
3:M:181:LEU:HD21	3:M:183:VAL:HG12	1.80	0.61
1:A:416:ARG:O	1:A:420:ASP:HB2	2.00	0.61
2:B:12:LYS:HE2	4:S:97:ASN:ND2	2.15	0.61
2:B:249:SER:OG	2:B:256:VAL:HG13	2.00	0.61
3:M:58:MET:HG2	3:M:80:VAL:HG11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:MET:HE3	4:S:16:LEU:HA	1.82	0.61
1:A:250:LEU:HA	1:A:253:LEU:HD12	1.82	0.61
1:A:293:VAL:HG11	1:A:313:LEU:HD21	1.80	0.61
3:M:101:GLU:O	3:M:104:ARG:HB3	2.01	0.61
3:M:160:ARG:HD2	3:M:258:PRO:HB3	1.81	0.61
1:A:227:ILE:HD12	1:A:274:VAL:HG22	1.81	0.61
2:B:248:LEU:O	3:M:237:LYS:HG3	2.01	0.61
2:B:469:PHE:HE2	2:B:484:LEU:HD11	1.65	0.61
1:A:195:VAL:HG11	1:A:248:ARG:HB3	1.83	0.61
1:A:557:VAL:HG13	2:B:419:ARG:HE	1.64	0.61
2:B:58:MET:HB2	2:B:69:VAL:HG11	1.83	0.61
2:B:173:ASN:HB2	2:B:176:VAL:HG22	1.81	0.61
4:S:23:LEU:HD22	4:S:27:GLU:HB2	1.81	0.61
1:A:457:GLN:HE22	1:A:497:PRO:HB3	1.65	0.61
2:B:181:VAL:HG21	2:B:222:ILE:HG12	1.81	0.61
1:A:108:LYS:HG3	1:A:141:GLU:HG3	1.83	0.61
1:A:172:MET:HE3	1:A:172:MET:H	1.64	0.61
1:A:254:ARG:HA	1:A:295:THR:HG23	1.83	0.61
1:A:436:ASP:O	1:A:439:PRO:HD2	2.00	0.61
3:M:56:ARG:HD2	3:M:56:ARG:N	2.15	0.61
1:A:159:LEU:HD13	4:S:119:ILE:CG2	2.30	0.61
2:B:145:VAL:HG21	2:B:165:LEU:HD11	1.81	0.61
2:B:310:VAL:HG13	2:B:314:PRO:HA	1.82	0.61
3:M:180:ASN:HD22	3:M:193:GLU:HG2	1.66	0.61
1:A:566:TYR:HA	1:A:569:LEU:CD1	2.30	0.61
2:B:126:LEU:O	2:B:130:LEU:HG	2.01	0.61
2:B:569:THR:HB	3:M:74:ASN:OD1	1.99	0.61
1:A:422:ILE:HG21	1:A:441:LEU:HD13	1.83	0.60
2:B:155:LEU:HD12	2:B:158:ASP:HB2	1.82	0.60
2:B:312:LYS:HG3	2:B:313:ARG:HG2	1.83	0.60
2:B:351:ILE:HD12	2:B:352:ALA:N	2.14	0.60
3:M:160:ARG:HD2	3:M:258:PRO:CB	2.31	0.60
3:M:193:GLU:HG3	3:M:269:LEU:C	2.22	0.60
1:A:14:ILE:HA	1:A:26:MET:SD	2.42	0.60
2:B:220:ILE:CG2	2:B:254:ALA:HB1	2.29	0.60
2:B:247:ARG:HG2	2:B:259:ALA:HB2	1.83	0.60
1:A:226:LEU:HD13	1:A:246:GLN:HG2	1.83	0.60
3:M:277:ILE:HG22	3:M:299:SER:HB3	1.83	0.60
1:A:251:ARG:O	1:A:254:ARG:HB3	2.01	0.60
2:B:247:ARG:C	2:B:249:SER:H	2.04	0.60
2:B:261:LYS:HE2	2:B:567:ILE:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:LEU:HA	2:B:398:LEU:CD2	2.28	0.60
1:A:231:TYR:HB2	1:A:241:SER:HB3	1.83	0.60
2:B:122:LEU:C	2:B:125:PRO:HD2	2.22	0.60
2:B:169:ILE:HG13	2:B:170:SER:N	2.17	0.60
1:A:562:ARG:HH21	2:B:522:ARG:HD2	1.66	0.60
3:M:244:LEU:HD12	3:M:245:SER:H	1.65	0.60
1:A:68:LEU:HG	1:A:69:GLU:N	2.17	0.60
2:B:258:SER:O	2:B:262:VAL:HG23	2.01	0.60
3:M:91:PHE:CE1	3:M:113:LEU:HD12	2.37	0.60
3:M:233:LEU:CD2	3:M:267:TYR:HB2	2.31	0.60
1:A:83:ARG:HH12	4:S:139:ASP:HA	1.65	0.59
2:B:30:LYS:O	2:B:34:VAL:HG23	2.01	0.59
2:B:295:GLU:HB3	2:B:298:LEU:HG	1.82	0.59
1:A:136:ARG:NH2	1:A:168:VAL:HG22	2.14	0.59
2:B:262:VAL:HG12	2:B:266:PHE:CE2	2.37	0.59
1:A:523:ARG:HB2	1:A:559:LEU:HD11	1.84	0.59
3:M:58:MET:HB2	3:M:69:ALA:HB3	1.85	0.59
2:B:305:ASN:HA	2:B:308:LEU:HD12	1.84	0.59
2:B:372:LYS:HD3	2:B:375:ARG:HE	1.67	0.59
3:M:378:VAL:HG22	3:M:379:LYS:H	1.67	0.59
3:M:379:LYS:HA	3:M:415:ASN:HB2	1.84	0.59
5:C:20:ILE:HG13	5:C:173:LEU:HD21	1.84	0.59
2:B:335:LYS:HB3	2:B:369:PHE:CE1	2.36	0.59
3:M:330:GLY:HA3	3:M:345:VAL:HG23	1.84	0.59
3:M:243:ARG:HA	3:M:243:ARG:NH1	2.17	0.59
2:B:51:PHE:O	2:B:55:VAL:HG23	2.03	0.59
1:A:35:ARG:HB2	1:A:65:PHE:CE2	2.37	0.59
1:A:214:LYS:O	1:A:217:PRO:HD2	2.03	0.59
1:A:459:LEU:HB3	1:A:476:ALA:HB1	1.84	0.59
2:B:144:CYS:HA	2:B:147:LYS:HB3	1.85	0.59
2:B:174:PRO:HB2	2:B:214:CYS:HA	1.85	0.59
2:B:463:ASP:OD2	2:B:464:GLU:HG3	2.03	0.59
5:C:34:LEU:HD11	5:C:54:GLU:CB	2.33	0.59
1:A:219:LEU:HA	1:A:222:ILE:HD12	1.84	0.59
1:A:574:ASP:O	1:A:577:ARG:HG2	2.03	0.59
1:A:160:CYS:O	1:A:164:VAL:HG23	2.03	0.58
2:B:502:LEU:H	2:B:502:LEU:HD22	1.68	0.58
5:C:140:THR:HA	5:C:145:LEU:HD12	1.84	0.58
1:A:289:LEU:O	1:A:293:VAL:HG23	2.03	0.58
1:A:346:HIS:O	1:A:350:ILE:HG13	2.02	0.58
2:B:141:ALA:O	2:B:145:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:MET:HG2	2:B:309:ILE:HG23	1.85	0.58
4:S:1:MET:O	4:S:71:ILE:HA	2.03	0.58
5:C:38:LYS:CD	5:C:56:VAL:HG22	2.33	0.58
1:A:543:ARG:O	1:A:547:VAL:HG23	2.02	0.58
2:B:38:ILE:H	2:B:38:ILE:HD12	1.68	0.58
3:M:385:PHE:HD1	3:M:386:THR:H	1.50	0.58
5:C:19:ARG:HD2	5:C:84:ASN:O	2.03	0.58
1:A:124:CYS:HA	4:S:119:ILE:HD13	1.86	0.58
1:A:303:SER:O	1:A:307:VAL:HG23	2.04	0.58
3:M:11:LEU:CD1	3:M:12:LYS:H	2.17	0.58
3:M:49:ILE:HA	3:M:57:PHE:O	2.03	0.58
3:M:279:ILE:HG13	3:M:296:LYS:O	2.03	0.58
1:A:267:MET:O	1:A:270:ILE:HG22	2.04	0.58
1:A:293:VAL:HG11	1:A:313:LEU:CD2	2.33	0.58
2:B:398:LEU:HD11	2:B:410:ALA:CB	2.34	0.58
3:M:384:TYR:HD1	3:M:384:TYR:H	1.52	0.58
2:B:102:ILE:HD12	2:B:102:ILE:H	1.68	0.58
2:B:130:LEU:HD23	2:B:141:ALA:HB1	1.86	0.58
3:M:60:ILE:HG13	3:M:67:LEU:HB3	1.86	0.58
1:A:146:LEU:O	1:A:146:LEU:HD23	2.03	0.58
1:A:509:LEU:O	1:A:512:VAL:HB	2.04	0.58
2:B:205:ASN:ND2	2:B:208:LEU:HD12	2.19	0.58
3:M:103:ILE:HG23	3:M:110:ILE:HD13	1.85	0.58
3:M:152:THR:HG23	3:M:153:VAL:HG23	1.85	0.58
1:A:22:GLU:O	1:A:26:MET:HG3	2.04	0.58
1:A:278:THR:HB	1:A:289:LEU:HD11	1.86	0.58
1:A:493:GLU:HG2	1:A:494:GLU:N	2.17	0.58
3:M:34:MET:HB3	3:M:35:PRO:HD3	1.85	0.58
2:B:255:VAL:HG13	2:B:256:VAL:N	2.17	0.58
1:A:67:GLN:HE21	1:A:93:LEU:HD21	1.69	0.57
1:A:196:VAL:HG12	1:A:248:ARG:HD2	1.86	0.57
1:A:442:ILE:O	1:A:446:THR:HG22	2.04	0.57
2:B:351:ILE:HG21	2:B:384:VAL:HG21	1.86	0.57
3:M:332:VAL:HB	3:M:343:TRP:CD1	2.38	0.57
1:A:10:LEU:HD21	1:A:30:GLU:HG2	1.87	0.57
1:A:74:ILE:HG22	1:A:106:CYS:SG	2.44	0.57
1:A:566:TYR:H	1:A:566:TYR:HD1	1.52	0.57
2:B:306:ILE:HB	2:B:341:ILE:HD13	1.86	0.57
2:B:210:ALA:O	2:B:214:CYS:HB2	2.04	0.57
3:M:28:SER:O	3:M:30:VAL:N	2.36	0.57
2:B:22:LEU:CD1	2:B:50:LEU:HD13	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:GLU:O	2:B:32:GLU:HG2	2.05	0.57
2:B:97:ASP:CG	2:B:102:ILE:HB	2.23	0.57
2:B:115:VAL:HB	2:B:118:ILE:CG2	2.33	0.57
3:M:315:PRO:HG2	3:M:421:ARG:NH1	2.20	0.57
1:A:11:ILE:HG21	4:S:104:ILE:HG22	1.85	0.57
1:A:265:GLU:HA	1:A:268:ASN:HD22	1.69	0.57
2:B:154:GLN:O	2:B:158:ASP:HB3	2.04	0.57
2:B:287:PRO:HB3	3:M:237:LYS:NZ	2.19	0.57
2:B:370:VAL:HB	2:B:405:TYR:OH	2.04	0.57
1:A:219:LEU:HD23	1:A:222:ILE:HD12	1.86	0.57
2:B:40:SER:HA	2:B:43:VAL:HG22	1.87	0.57
3:M:98:LEU:HD22	3:M:98:LEU:N	2.19	0.57
3:M:355:LEU:HD22	3:M:356:MET:H	1.70	0.57
1:A:368:LEU:HD23	1:A:369:SER:N	2.20	0.57
2:B:330:ASP:O	2:B:335:LYS:HE3	2.05	0.57
2:B:495:LYS:N	2:B:496:PRO:HD3	2.20	0.57
2:B:506:VAL:HG13	2:B:507:LEU:N	2.19	0.57
3:M:195:VAL:HG22	3:M:196:GLY:N	2.16	0.57
1:A:111:LEU:HD13	1:A:141:GLU:HB3	1.86	0.57
1:A:374:ASN:O	1:A:378:ILE:HD12	2.05	0.57
1:A:439:PRO:O	1:A:443:GLN:HG3	2.04	0.57
2:B:12:LYS:HD3	2:B:14:GLU:OE1	2.05	0.57
2:B:292:LEU:HD22	3:M:191:ARG:HH12	1.69	0.57
3:M:239:HIS:O	3:M:242:VAL:HG22	2.04	0.57
2:B:47:VAL:HB	2:B:50:LEU:CD1	2.34	0.57
3:M:296:LYS:HG3	3:M:297:ALA:H	1.68	0.57
1:A:244:PHE:CE1	4:S:83:ILE:HG12	2.38	0.56
2:B:381:ALA:HB1	2:B:388:ALA:HA	1.86	0.56
2:B:413:VAL:O	2:B:417:ILE:HG13	2.05	0.56
2:B:475:ASP:O	2:B:476:LYS:HD2	2.05	0.56
3:M:194:ILE:CD1	3:M:273:VAL:HG23	2.35	0.56
4:S:35:ILE:O	4:S:39:ILE:HG13	2.04	0.56
5:C:36:LYS:HB2	5:C:42:ILE:HD13	1.86	0.56
2:B:183:ALA:O	2:B:187:ILE:HG13	2.05	0.56
2:B:323:VAL:HG13	3:M:191:ARG:NH1	2.21	0.56
2:B:388:ALA:O	2:B:392:VAL:HG23	2.04	0.56
1:A:24:ARG:HG3	1:A:61:TYR:OH	2.03	0.56
1:A:180:LYS:HE2	1:A:214:LYS:HZ2	1.70	0.56
1:A:205:SER:HB2	1:A:206:PRO:HD3	1.87	0.56
2:B:302:ALA:O	2:B:306:ILE:HG13	2.05	0.56
2:B:366:ASP:HB3	2:B:369:PHE:CB	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:GLU:O	2:B:429:ILE:HG12	2.05	0.56
3:M:10:ASP:O	3:M:12:LYS:N	2.39	0.56
3:M:10:ASP:CG	3:M:16:LEU:HD23	2.26	0.56
3:M:130:ILE:HG12	3:M:159:TRP:O	2.05	0.56
3:M:250:ASP:C	3:M:252:THR:H	2.09	0.56
5:C:25:LEU:HD11	5:C:103:ALA:HB2	1.87	0.56
3:M:295:VAL:O	3:M:355:LEU:HD22	2.05	0.56
5:C:140:THR:HA	5:C:145:LEU:CD1	2.35	0.56
2:B:395:LEU:HD22	2:B:414:ILE:HD11	1.86	0.56
1:A:249:ILE:HG22	1:A:253:LEU:HD11	1.87	0.56
2:B:223:LEU:HD13	2:B:258:SER:HB2	1.87	0.56
2:B:327:LYS:HD3	2:B:330:ASP:OD1	2.06	0.56
3:M:381:GLU:O	3:M:382:ILE:HD13	2.05	0.56
4:S:86:ARG:HH12	4:S:89:GLU:CG	2.19	0.56
1:A:46:ARG:NH2	1:A:72:LYS:HD2	2.21	0.56
1:A:178:ALA:O	1:A:182:LEU:HG	2.05	0.56
1:A:363:ARG:HA	1:A:366:MET:HE2	1.87	0.56
1:A:562:ARG:NH2	2:B:482:LEU:HD22	2.20	0.56
2:B:148:LEU:HD12	2:B:153:ALA:CB	2.36	0.56
2:B:469:PHE:CE1	2:B:476:LYS:HE3	2.40	0.56
2:B:518:ASP:HA	2:B:521:ASP:HB2	1.88	0.56
2:B:302:ALA:O	2:B:305:ASN:HB2	2.05	0.56
3:M:382:ILE:HB	3:M:384:TYR:CD1	2.40	0.56
4:S:86:ARG:NH2	4:S:89:GLU:HG2	2.16	0.56
4:S:94:TYR:HE2	4:S:109:LYS:HD3	1.71	0.56
5:C:71:LEU:O	5:C:75:ARG:HG3	2.05	0.56
1:A:61:TYR:HB3	1:A:62:PRO:HD2	1.86	0.56
2:B:286:PRO:O	2:B:289:VAL:HG22	2.05	0.56
4:S:76:ASN:C	4:S:76:ASN:HD22	2.08	0.56
2:B:78:LYS:HG3	2:B:79:SER:N	2.20	0.56
2:B:186:GLU:CD	3:M:22:ARG:HH22	2.09	0.56
2:B:375:ARG:HG2	2:B:379:ARG:NH2	2.21	0.56
3:M:182:LEU:HB3	3:M:191:ARG:HB3	1.88	0.56
4:S:93:LYS:HD3	4:S:132:VAL:HG11	1.88	0.56
5:C:167:TYR:HA	5:C:170:LEU:HD12	1.88	0.56
1:A:182:LEU:HB3	1:A:194:SER:HB3	1.88	0.55
1:A:250:LEU:HB2	1:A:291:GLU:HG3	1.88	0.55
1:A:293:VAL:HA	1:A:296:ILE:HD12	1.87	0.55
1:A:332:LEU:HG	1:A:368:LEU:HD11	1.87	0.55
2:B:408:GLN:O	2:B:412:VAL:HG23	2.06	0.55
2:B:463:ASP:CG	2:B:464:GLU:H	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:124:PHE:HE1	5:C:156:GLN:HB3	1.70	0.55
1:A:147:LYS:HE3	1:A:178:ALA:HB2	1.89	0.55
1:A:322:LYS:O	1:A:324:ILE:N	2.39	0.55
1:A:350:ILE:HA	1:A:353:CYS:SG	2.45	0.55
2:B:33:ALA:O	2:B:37:VAL:HG23	2.06	0.55
2:B:122:LEU:HD13	2:B:122:LEU:O	2.05	0.55
3:M:172:PHE:CE1	3:M:410:ARG:HG3	2.42	0.55
1:A:234:GLU:OE1	1:A:236:ASP:HB2	2.06	0.55
1:A:296:ILE:HG21	1:A:309:ALA:HB2	1.87	0.55
2:B:260:VAL:O	2:B:264:MET:N	2.32	0.55
2:B:462:ALA:O	2:B:466:LEU:HB2	2.07	0.55
2:B:521:ASP:O	2:B:525:ILE:HG12	2.07	0.55
5:C:126:ASN:HD21	5:C:160:ALA:H	1.53	0.55
2:B:31:LYS:HZ2	2:B:31:LYS:HB2	1.69	0.55
2:B:358:LEU:HB3	2:B:377:ILE:HD11	1.88	0.55
3:M:302:LYS:HB3	3:M:304:ARG:NH2	2.18	0.55
1:A:10:LEU:HD22	1:A:52:LYS:HD3	1.89	0.55
1:A:17:ALA:HA	1:A:22:GLU:OE1	2.07	0.55
1:A:24:ARG:O	1:A:28:GLN:HB2	2.07	0.55
2:B:207:LEU:HD22	2:B:222:ILE:HG21	1.88	0.55
3:M:67:LEU:HG	3:M:84:LEU:HD22	1.87	0.55
4:S:32:THR:O	4:S:36:VAL:HG23	2.07	0.55
4:S:34:GLU:HG2	4:S:52:TRP:HZ2	1.72	0.55
2:B:177:VAL:O	2:B:181:VAL:HG23	2.07	0.55
2:B:31:LYS:HG3	2:B:65:LEU:HD13	1.89	0.55
2:B:39:ALA:O	2:B:43:VAL:HG13	2.07	0.55
2:B:375:ARG:HG2	2:B:379:ARG:HH12	1.71	0.55
1:A:569:LEU:HD23	2:B:540:VAL:HG22	1.89	0.55
2:B:261:LYS:HD2	2:B:568:GLY:H	1.71	0.55
2:B:323:VAL:HG13	3:M:191:ARG:CZ	2.36	0.55
4:S:16:LEU:CD1	4:S:107:PHE:HB2	2.37	0.55
1:A:264:SER:HB3	1:A:300:LYS:O	2.07	0.55
1:A:488:VAL:HA	1:A:500:VAL:HG11	1.89	0.55
2:B:62:ASN:ND2	2:B:65:LEU:HB2	2.22	0.55
1:A:422:ILE:O	1:A:425:VAL:HG12	2.06	0.55
2:B:22:LEU:HD13	2:B:50:LEU:HD13	1.88	0.55
2:B:222:ILE:HA	2:B:225:CYS:SG	2.47	0.55
2:B:390:ARG:O	2:B:394:THR:HG23	2.07	0.55
2:B:399:ILE:HD13	2:B:407:VAL:HA	1.89	0.55
2:B:452:VAL:HA	2:B:459:ILE:CD1	2.34	0.55
2:B:466:LEU:HD22	2:B:488:PHE:CZ	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:GLU:CD	1:A:537:PHE:HB3	2.27	0.54
1:A:544:ILE:O	1:A:548:VAL:HG23	2.07	0.54
3:M:21:TYR:O	3:M:120:PHE:HA	2.08	0.54
2:B:145:VAL:O	2:B:148:LEU:HG	2.07	0.54
2:B:257:LEU:CD1	2:B:568:GLY:HA2	2.37	0.54
4:S:108:GLU:OE2	4:S:109:LYS:HG3	2.07	0.54
1:A:476:ALA:O	1:A:480:ILE:HG13	2.08	0.54
2:B:12:LYS:HE2	4:S:97:ASN:HD21	1.72	0.54
2:B:289:VAL:HG21	3:M:268:ARG:NH1	2.22	0.54
2:B:350:ASN:O	2:B:354:VAL:HG23	2.08	0.54
2:B:476:LYS:HB3	2:B:480:VAL:HG11	1.90	0.54
3:M:302:LYS:HD3	3:M:304:ARG:HH12	1.72	0.54
3:M:317:PRO:C	3:M:319:ASP:H	2.11	0.54
4:S:117:PHE:O	4:S:124:GLN:HG2	2.08	0.54
5:C:36:LYS:HA	5:C:41:GLU:O	2.07	0.54
2:B:105:LEU:HA	2:B:108:ARG:HG3	1.88	0.54
2:B:347:SER:N	2:B:350:ASN:HD21	2.02	0.54
2:B:399:ILE:HG23	2:B:407:VAL:HG13	1.89	0.54
3:M:113:LEU:O	3:M:117:LEU:HG	2.07	0.54
5:C:122:LEU:HD21	5:C:169:GLY:HA3	1.89	0.54
2:B:313:ARG:O	2:B:316:ILE:HD13	2.07	0.54
3:M:243:ARG:HB3	3:M:246:ARG:HB2	1.89	0.54
5:C:66:TRP:CE3	5:C:81:TYR:HD2	2.26	0.54
2:B:26:LYS:HG3	2:B:27:LYS:N	2.20	0.54
2:B:78:LYS:HG3	2:B:79:SER:H	1.73	0.54
2:B:410:ALA:O	2:B:414:ILE:HG13	2.08	0.54
3:M:210:LEU:HD21	3:M:395:LEU:HG	1.90	0.54
1:A:557:VAL:HG22	2:B:419:ARG:NE	2.23	0.54
2:B:126:LEU:HA	2:B:129:CYS:HB2	1.88	0.54
2:B:218:GLY:HA2	2:B:221:PHE:CD2	2.43	0.54
2:B:297:GLU:HG2	3:M:81:PHE:CE2	2.42	0.54
4:S:2:ILE:HA	4:S:70:ALA:O	2.07	0.54
5:C:94:SER:HB2	5:C:133:ALA:HB1	1.88	0.54
1:A:580:LEU:HD13	2:B:528:ARG:O	2.08	0.54
2:B:195:ASN:C	2:B:197:LEU:H	2.10	0.54
2:B:466:LEU:HD12	2:B:491:LEU:HD12	1.88	0.54
2:B:527:TRP:C	2:B:529:LEU:H	2.10	0.54
4:S:15:ARG:HB3	4:S:103:ILE:CG2	2.38	0.54
4:S:84:VAL:O	4:S:88:VAL:HG13	2.08	0.54
4:S:98:VAL:HG23	4:S:102:ASP:HB2	1.90	0.54
5:C:71:LEU:HD22	5:C:72:ASP:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:TYR:CE1	1:A:360:SER:HB3	2.43	0.54
2:B:97:ASP:OD2	2:B:102:ILE:HB	2.08	0.54
2:B:181:VAL:HG11	2:B:222:ILE:HA	1.90	0.54
2:B:445:ARG:HH12	2:B:476:LYS:NZ	2.06	0.54
3:M:77:VAL:O	3:M:80:VAL:HB	2.08	0.54
1:A:47:CYS:O	1:A:84:ILE:HG21	2.07	0.53
1:A:245:LEU:O	1:A:249:ILE:HG12	2.08	0.53
2:B:56:ASN:HA	5:C:51:PHE:HZ	1.72	0.53
2:B:134:ASP:OD2	2:B:137:VAL:HG23	2.08	0.53
2:B:366:ASP:HB3	2:B:369:PHE:HB3	1.88	0.53
3:M:174:ASP:O	3:M:198:ILE:HD12	2.09	0.53
4:S:90:LEU:HB3	4:S:113:ILE:HG21	1.91	0.53
2:B:288:LEU:HA	2:B:291:LEU:HD23	1.89	0.53
3:M:243:ARG:HD2	3:M:246:ARG:NE	2.23	0.53
1:A:431:SER:HB2	1:A:469:GLN:OE1	2.07	0.53
2:B:91:PHE:HA	2:B:94:ASP:HB2	1.89	0.53
2:B:186:GLU:OE2	2:B:189:GLU:HG3	2.08	0.53
2:B:419:ARG:HH11	2:B:419:ARG:HB3	1.74	0.53
5:C:26:ASP:HB3	5:C:70:GLY:C	2.28	0.53
1:A:283:ASN:HD22	4:S:78:LEU:HD21	1.73	0.53
1:A:329:LEU:HD13	1:A:365:ALA:HB2	1.90	0.53
2:B:24:SER:N	2:B:30:LYS:HE3	2.23	0.53
3:M:200:MET:SD	3:M:264:LEU:HD22	2.49	0.53
3:M:375:PRO:HA	3:M:421:ARG:HB3	1.91	0.53
1:A:228:MET:O	1:A:229:SER:CB	2.57	0.53
2:B:63:LEU:HG	2:B:64:GLU:H	1.74	0.53
2:B:225:CYS:SG	2:B:226:LEU:N	2.82	0.53
2:B:446:ALA:HA	2:B:449:ILE:HD12	1.90	0.53
2:B:572:SER:C	2:B:574:TYR:H	2.11	0.53
3:M:180:ASN:HD21	3:M:195:VAL:HB	1.73	0.53
1:A:354:LEU:HB3	1:A:388:PHE:CE1	2.44	0.53
2:B:13:GLY:O	2:B:15:ILE:N	2.41	0.53
2:B:304:ARG:HB2	2:B:573:VAL:HG12	1.91	0.53
2:B:355:LEU:HG	2:B:356:ALA:N	2.23	0.53
4:S:31:ILE:HG12	4:S:52:TRP:HH2	1.72	0.53
4:S:51:ASP:OD1	4:S:56:LYS:HG2	2.09	0.53
1:A:468:SER:O	1:A:469:GLN:HB2	2.07	0.53
2:B:62:ASN:ND2	2:B:65:LEU:H	2.06	0.53
2:B:229:TYR:OH	2:B:232:LYS:HE2	2.08	0.53
4:S:65:LEU:HD12	4:S:66:TYR:H	1.74	0.53
1:A:244:PHE:CD1	4:S:79:LEU:HD11	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:292:LEU:HD23	2:B:292:LEU:O	2.09	0.53
2:B:305:ASN:HA	2:B:308:LEU:CD1	2.39	0.53
5:C:126:ASN:HA	5:C:158:THR:O	2.09	0.53
1:A:150:ASN:O	1:A:152:TYR:N	2.42	0.53
3:M:165:LYS:HA	3:M:205:SER:HB3	1.89	0.53
3:M:299:SER:HB2	3:M:301:PHE:CZ	2.44	0.53
1:A:73:LEU:HB3	1:A:81:ASP:O	2.08	0.52
1:A:459:LEU:O	1:A:463:ILE:HG12	2.08	0.52
1:A:501:THR:OG1	1:A:504:GLU:HG3	2.10	0.52
2:B:27:LYS:O	2:B:31:LYS:HB2	2.09	0.52
2:B:280:LEU:O	2:B:284:LEU:HG	2.09	0.52
4:S:80:THR:HA	4:S:83:ILE:HD12	1.91	0.52
1:A:326:TYR:HE1	1:A:360:SER:HB3	1.75	0.52
1:A:513:LEU:HD11	1:A:526:ALA:HB1	1.91	0.52
2:B:122:LEU:HD21	2:B:126:LEU:HB2	1.89	0.52
2:B:358:LEU:HD13	2:B:377:ILE:HD12	1.92	0.52
1:A:519:THR:HG22	1:A:520:SER:N	2.24	0.52
2:B:56:ASN:HD21	5:C:66:TRP:HZ3	1.57	0.52
3:M:378:VAL:HG22	3:M:379:LYS:N	2.24	0.52
1:A:14:ILE:HD12	1:A:55:TYR:CE1	2.40	0.52
1:A:46:ARG:HG2	1:A:73:LEU:CG	2.39	0.52
1:A:257:GLY:O	1:A:299:ILE:HG23	2.09	0.52
1:A:313:LEU:O	1:A:316:PHE:HB2	2.10	0.52
2:B:195:ASN:O	2:B:196:LEU:HB2	2.10	0.52
1:A:442:ILE:HG12	1:A:478:TRP:HD1	1.75	0.52
1:A:463:ILE:HD12	1:A:473:VAL:HG12	1.90	0.52
1:A:489:SER:H	1:A:500:VAL:HG11	1.74	0.52
2:B:24:SER:H	2:B:30:LYS:HG3	1.74	0.52
2:B:70:TYR:HB3	2:B:109:THR:HG21	1.90	0.52
2:B:216:GLU:HG3	2:B:251:ALA:HB2	1.89	0.52
2:B:286:PRO:O	2:B:290:THR:HG23	2.09	0.52
2:B:399:ILE:HD11	2:B:410:ALA:HB3	1.91	0.52
3:M:183:VAL:HG13	3:M:419:GLN:O	2.09	0.52
1:A:562:ARG:HG2	2:B:522:ARG:NH1	2.24	0.52
3:M:275:PRO:HB2	3:M:300:GLN:HE22	1.75	0.52
3:M:329:VAL:HG21	3:M:354:TYR:CG	2.44	0.52
4:S:7:LEU:HA	4:S:66:TYR:O	2.10	0.52
1:A:67:GLN:HE21	1:A:99:VAL:HG21	1.75	0.52
2:B:429:ILE:HD12	2:B:451:ILE:HD11	1.92	0.52
3:M:7:TYR:OH	3:M:26:ASP:HA	2.10	0.52
1:A:176:LEU:N	1:A:177:PRO:CD	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:LEU:O	1:A:581:LEU:HD23	2.09	0.52
2:B:419:ARG:HB3	2:B:419:ARG:NH1	2.24	0.52
3:M:268:ARG:HG3	3:M:268:ARG:O	2.09	0.52
3:M:397:ILE:HD13	3:M:405:ALA:HB2	1.91	0.52
1:A:394:PRO:HG2	3:M:52:HIS:CE1	2.44	0.52
1:A:565:GLU:O	1:A:569:LEU:HG	2.10	0.52
2:B:122:LEU:HD22	2:B:122:LEU:O	2.09	0.52
2:B:346:ALA:N	2:B:383:LYS:HZ3	2.08	0.52
2:B:570:LEU:HG	3:M:75:ALA:O	2.10	0.52
3:M:308:ASN:HA	3:M:347:SER:HA	1.92	0.52
3:M:312:ILE:CG2	3:M:343:TRP:HB3	2.39	0.52
1:A:227:ILE:C	1:A:229:SER:N	2.62	0.52
2:B:405:TYR:HA	2:B:408:GLN:HE21	1.75	0.52
3:M:210:LEU:HD11	3:M:395:LEU:HG	1.92	0.52
1:A:275:ALA:HB1	1:A:312:ILE:HD11	1.91	0.51
1:A:347:ARG:HA	1:A:350:ILE:HD12	1.91	0.51
2:B:88:VAL:HG12	2:B:89:ASN:N	2.24	0.51
2:B:294:ALA:HB1	2:B:298:LEU:HD12	1.92	0.51
2:B:370:VAL:O	2:B:373:ALA:HB3	2.10	0.51
3:M:99:GLU:H	3:M:102:SER:HB2	1.76	0.51
1:A:38:PHE:CE2	1:A:69:GLU:HB3	2.45	0.51
2:B:145:VAL:HA	2:B:148:LEU:HD23	1.91	0.51
2:B:541:VAL:HB	2:B:542:LEU:HD12	1.93	0.51
3:M:4:SER:HB3	3:M:22:ARG:HB3	1.92	0.51
3:M:212:LEU:O	3:M:253:ILE:HG12	2.11	0.51
4:S:127:SER:O	4:S:130:ILE:HG22	2.10	0.51
5:C:124:PHE:CE1	5:C:156:GLN:HB3	2.44	0.51
1:A:71:LEU:HD21	1:A:102:LEU:O	2.10	0.51
1:A:147:LYS:HA	1:A:147:LYS:HE2	1.92	0.51
2:B:303:LEU:O	2:B:306:ILE:HB	2.10	0.51
2:B:406:VAL:HG13	2:B:407:VAL:N	2.25	0.51
3:M:17:ILE:HD11	3:M:111:TYR:CZ	2.44	0.51
4:S:49:PHE:CZ	4:S:81:LEU:HD12	2.45	0.51
1:A:35:ARG:O	1:A:39:ARG:HG2	2.09	0.51
1:A:254:ARG:CA	1:A:295:THR:HG23	2.40	0.51
1:A:481:GLY:HA2	1:A:533:LEU:HD21	1.93	0.51
2:B:117:LYS:O	2:B:120:GLU:HG2	2.10	0.51
2:B:122:LEU:HD22	2:B:126:LEU:H	1.75	0.51
2:B:529:LEU:HD21	2:B:537:ALA:HA	1.93	0.51
3:M:356:MET:HE3	3:M:357:ARG:O	2.10	0.51
5:C:63:PHE:HZ	5:C:174:SER:HB3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLU:HG3	1:A:186:LYS:N	2.26	0.51
1:A:250:LEU:CD2	1:A:292:THR:HG22	2.40	0.51
1:A:467:TYR:OH	1:A:511:SER:HB2	2.11	0.51
2:B:122:LEU:CD2	2:B:125:PRO:HB2	2.39	0.51
3:M:210:LEU:HD11	3:M:395:LEU:CG	2.40	0.51
3:M:334:TRP:HB2	3:M:341:ILE:HA	1.93	0.51
2:B:19:LYS:HA	2:B:22:LEU:CD1	2.39	0.51
2:B:442:PRO:HG2	2:B:443:GLU:OE1	2.10	0.51
2:B:448:MET:HA	2:B:451:ILE:HG22	1.91	0.51
2:B:316:ILE:N	2:B:316:ILE:HD12	2.25	0.51
2:B:502:LEU:HD22	2:B:502:LEU:N	2.26	0.51
1:A:227:ILE:CD1	1:A:274:VAL:HG22	2.40	0.51
2:B:211:LEU:CD1	2:B:222:ILE:HG21	2.39	0.51
3:M:151:ALA:HA	3:M:154:THR:HG22	1.93	0.51
3:M:301:PHE:CE1	3:M:351:GLY:N	2.79	0.51
1:A:442:ILE:CD1	1:A:475:VAL:HG13	2.41	0.51
2:B:259:ALA:O	2:B:263:LEU:HG	2.10	0.51
2:B:284:LEU:O	2:B:287:PRO:HG2	2.10	0.51
3:M:48:PRO:O	3:M:49:ILE:HD13	2.11	0.51
3:M:132:GLN:C	3:M:134:TYR:H	2.15	0.51
5:C:71:LEU:HD13	5:C:73:LYS:N	2.26	0.51
1:A:58:MET:CE	4:S:16:LEU:HA	2.40	0.51
1:A:152:TYR:O	1:A:155:LYS:HG2	2.11	0.51
1:A:52:LYS:O	1:A:56:MET:HG3	2.10	0.50
1:A:539:CYS:C	1:A:541:VAL:H	2.14	0.50
2:B:166:LYS:O	2:B:169:ILE:HG23	2.10	0.50
2:B:533:ASP:C	2:B:535:VAL:H	2.14	0.50
3:M:304:ARG:O	3:M:304:ARG:HG2	2.11	0.50
3:M:384:TYR:CE1	3:M:413:THR:HB	2.46	0.50
5:C:38:LYS:HG2	5:C:54:GLU:HG3	1.93	0.50
2:B:395:LEU:HD13	2:B:414:ILE:HG12	1.92	0.50
3:M:86:LYS:O	3:M:89:GLN:HB3	2.11	0.50
3:M:103:ILE:HG23	3:M:110:ILE:CD1	2.40	0.50
1:A:172:MET:SD	1:A:204:ARG:HD2	2.51	0.50
2:B:62:ASN:ND2	2:B:63:LEU:H	2.09	0.50
2:B:426:GLU:HA	2:B:429:ILE:HD11	1.93	0.50
3:M:60:ILE:HD13	3:M:84:LEU:HB3	1.93	0.50
3:M:148:ARG:O	3:M:152:THR:HG22	2.10	0.50
1:A:270:ILE:HG23	1:A:271:LEU:HD22	1.92	0.50
1:A:322:LYS:O	1:A:323:ASN:C	2.50	0.50
2:B:358:LEU:HA	2:B:361:TYR:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:ARG:HH22	2:B:150:ASP:HB3	1.76	0.50
2:B:245:THR:HB	2:B:246:PRO:HD3	1.92	0.50
2:B:261:LYS:HA	2:B:567:ILE:HD12	1.94	0.50
3:M:148:ARG:C	3:M:150:PRO:HD2	2.32	0.50
3:M:397:ILE:HD13	3:M:405:ALA:CB	2.41	0.50
2:B:491:LEU:HD23	2:B:491:LEU:O	2.11	0.50
2:B:522:ARG:HG2	2:B:522:ARG:HH11	1.77	0.50
3:M:244:LEU:C	3:M:246:ARG:H	2.15	0.50
2:B:181:VAL:HG11	2:B:222:ILE:CG1	2.42	0.50
2:B:264:MET:HE1	2:B:313:ARG:HG3	1.92	0.50
2:B:311:GLN:NE2	2:B:555:ILE:HG22	2.26	0.50
2:B:398:LEU:C	2:B:398:LEU:HD12	2.32	0.50
4:S:70:ALA:O	4:S:71:ILE:HD13	2.11	0.50
4:S:86:ARG:NH2	4:S:128:LYS:HG2	2.27	0.50
1:A:247:VAL:HA	1:A:250:LEU:HD12	1.92	0.50
1:A:301:SER:CB	1:A:305:LEU:HD23	2.39	0.50
3:M:157:VAL:HG12	3:M:159:TRP:CZ2	2.46	0.50
3:M:301:PHE:HE1	3:M:351:GLY:N	2.10	0.50
4:S:80:THR:HA	4:S:83:ILE:CD1	2.41	0.50
1:A:533:LEU:HB3	1:A:537:PHE:CD2	2.47	0.50
2:B:26:LYS:CG	2:B:27:LYS:N	2.74	0.50
2:B:95:CYS:HA	2:B:103:ARG:HA	1.94	0.50
2:B:449:ILE:HG21	2:B:484:LEU:HD23	1.93	0.50
2:B:459:ILE:HG22	2:B:462:ALA:N	2.26	0.50
2:B:459:ILE:HG22	2:B:462:ALA:H	1.77	0.50
3:M:20:ASN:ND2	3:M:26:ASP:HB2	2.27	0.50
3:M:383:PRO:CA	3:M:412:ILE:HG22	2.39	0.50
1:A:7:LEU:HD22	1:A:7:LEU:O	2.12	0.49
1:A:171:LEU:O	1:A:174:MET:HG2	2.12	0.49
1:A:438:VAL:HG11	1:A:525:TYR:CE2	2.47	0.49
1:A:500:VAL:HG13	1:A:500:VAL:O	2.12	0.49
2:B:124:GLU:O	2:B:127:ARG:HB3	2.12	0.49
2:B:327:LYS:HE3	2:B:338:LYS:HZ1	1.75	0.49
3:M:149:PRO:N	3:M:150:PRO:HD2	2.27	0.49
3:M:320:ALA:HA	3:M:360:PHE:CE2	2.47	0.49
1:A:54:LEU:CD2	1:A:88:GLY:HA2	2.40	0.49
1:A:332:LEU:O	1:A:336:VAL:HG23	2.11	0.49
2:B:138:ARG:HB2	2:B:176:VAL:HG12	1.93	0.49
2:B:470:LEU:CD1	2:B:484:LEU:HD13	2.41	0.49
3:M:160:ARG:HB2	3:M:258:PRO:HB3	1.94	0.49
3:M:179:VAL:HG11	3:M:418:TYR:OH	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:182:LEU:O	3:M:189:VAL:HA	2.12	0.49
5:C:74:ILE:HB	5:C:77:LEU:HD12	1.94	0.49
1:A:54:LEU:HD22	1:A:91:LEU:HD12	1.94	0.49
1:A:243:PRO:O	1:A:247:VAL:HG23	2.12	0.49
1:A:553:SER:HA	1:A:560:GLN:HG3	1.93	0.49
2:B:314:PRO:C	2:B:316:ILE:H	2.15	0.49
2:B:420:LYS:O	2:B:547:LEU:HD22	2.11	0.49
4:S:30:LYS:HE3	4:S:53:LYS:NZ	2.27	0.49
5:C:42:ILE:HD11	5:C:160:ALA:O	2.11	0.49
2:B:74:MET:SD	2:B:109:THR:HG23	2.52	0.49
2:B:184:LEU:HD22	2:B:187:ILE:HD12	1.93	0.49
2:B:248:LEU:HA	3:M:237:LYS:HZ1	1.76	0.49
2:B:257:LEU:HD13	2:B:568:GLY:HA2	1.94	0.49
2:B:287:PRO:HB3	3:M:237:LYS:HZ1	1.77	0.49
2:B:306:ILE:HD13	2:B:324:PHE:CE2	2.48	0.49
2:B:348:GLN:NE2	2:B:384:VAL:HB	2.27	0.49
3:M:208:PRO:O	3:M:257:PRO:HD2	2.12	0.49
3:M:275:PRO:HB2	3:M:300:GLN:NE2	2.28	0.49
5:C:30:LYS:HE3	5:C:68:VAL:O	2.12	0.49
2:B:474:HIS:HE1	2:B:515:ASP:H	1.60	0.49
3:M:276:LEU:HD13	3:M:418:TYR:OH	2.12	0.49
1:A:83:ARG:NH1	4:S:139:ASP:HA	2.28	0.49
1:A:561:GLN:O	1:A:565:GLU:HG3	2.12	0.49
1:A:562:ARG:O	1:A:566:TYR:HD1	1.96	0.49
2:B:211:LEU:O	2:B:219:GLN:HG2	2.12	0.49
3:M:174:ASP:O	3:M:198:ILE:HA	2.13	0.49
4:S:86:ARG:HH12	4:S:89:GLU:HG2	1.77	0.49
4:S:109:LYS:O	4:S:113:ILE:HG13	2.13	0.49
1:A:61:TYR:HB3	1:A:62:PRO:CD	2.42	0.49
1:A:172:MET:HE1	1:A:204:ARG:HD2	1.93	0.49
2:B:211:LEU:HD11	2:B:222:ILE:CG2	2.41	0.49
2:B:564:ILE:C	2:B:566:TYR:H	2.14	0.49
1:A:67:GLN:NE2	1:A:99:VAL:HG21	2.27	0.49
2:B:108:ARG:HD3	2:B:109:THR:N	2.27	0.49
2:B:227:ALA:CB	2:B:262:VAL:HG22	2.41	0.49
2:B:252:ASN:O	2:B:255:VAL:HG12	2.13	0.49
2:B:411:ILE:HA	2:B:414:ILE:CD1	2.40	0.49
3:M:198:ILE:CG2	3:M:264:LEU:HB3	2.34	0.49
3:M:277:ILE:HG13	3:M:277:ILE:O	2.12	0.49
1:A:73:LEU:HD22	1:A:81:ASP:CB	2.43	0.49
2:B:105:LEU:HD22	2:B:108:ARG:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:236:VAL:HG23	3:M:265:MET:HE2	1.94	0.49
1:A:459:LEU:HD22	1:A:476:ALA:CB	2.42	0.49
1:A:576:MET:O	1:A:580:LEU:HG	2.13	0.49
3:M:233:LEU:HD22	3:M:267:TYR:HB2	1.94	0.49
5:C:92:VAL:HG12	5:C:93:ASP:N	2.28	0.49
2:B:60:THR:HG23	2:B:62:ASN:H	1.78	0.48
2:B:199:LEU:HD13	2:B:229:TYR:CE1	2.48	0.48
4:S:17:GLN:HG3	4:S:17:GLN:O	2.12	0.48
5:C:89:ILE:HG23	5:C:122:LEU:O	2.13	0.48
3:M:19:ARG:HG3	3:M:21:TYR:CE1	2.48	0.48
3:M:238:PHE:HB2	3:M:242:VAL:HG21	1.95	0.48
2:B:165:LEU:HA	2:B:168:LEU:CD1	2.42	0.48
3:M:32:HIS:C	3:M:35:PRO:HD2	2.33	0.48
3:M:304:ARG:NH1	3:M:304:ARG:HB3	2.28	0.48
1:A:453:ALA:O	1:A:457:GLN:HG3	2.13	0.48
2:B:404:ASN:O	2:B:408:GLN:HG3	2.13	0.48
2:B:449:ILE:HG21	2:B:484:LEU:HA	1.95	0.48
3:M:316:VAL:HG12	3:M:341:ILE:HD11	1.96	0.48
4:S:27:GLU:HA	4:S:30:LYS:HB3	1.95	0.48
1:A:445:ILE:HD13	1:A:455:THR:HG21	1.95	0.48
2:B:85:ILE:HG22	5:C:49:ILE:CG2	2.44	0.48
2:B:86:MET:O	5:C:50:GLY:HA2	2.13	0.48
3:M:238:PHE:HA	3:M:265:MET:CB	2.44	0.48
1:A:107:ILE:O	1:A:111:LEU:HG	2.14	0.48
2:B:101:LEU:HD21	3:M:150:PRO:N	2.28	0.48
2:B:534:PRO:HA	2:B:537:ALA:HB2	1.94	0.48
3:M:199:LYS:HZ3	3:M:201:ARG:HG2	1.77	0.48
3:M:202:VAL:CG1	3:M:259:ASP:HA	2.44	0.48
5:C:100:VAL:CG2	5:C:142:LYS:HB3	2.44	0.48
5:C:173:LEU:O	5:C:177:LEU:HB2	2.13	0.48
1:A:329:LEU:CD1	1:A:365:ALA:HB2	2.43	0.48
1:A:333:LEU:HG	1:A:368:LEU:HB2	1.96	0.48
2:B:71:LEU:HD13	3:M:111:TYR:HB3	1.95	0.48
2:B:326:VAL:CG1	2:B:335:LYS:HG2	2.42	0.48
3:M:127:ASP:HB3	3:M:130:ILE:HG13	1.95	0.48
5:C:172:TRP:CE2	5:C:176:GLN:HG3	2.49	0.48
1:A:378:ILE:HD12	1:A:378:ILE:H	1.78	0.48
1:A:535:THR:OG1	1:A:581:LEU:HD12	2.14	0.48
2:B:121:TYR:CZ	5:C:49:ILE:HG13	2.49	0.48
2:B:139:LYS:O	2:B:143:VAL:HG23	2.13	0.48
2:B:372:LYS:CD	2:B:375:ARG:HE	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:29:GLU:HG2	3:M:55:VAL:HG11	1.96	0.48
3:M:113:LEU:HD22	3:M:131:LEU:CD2	2.44	0.48
4:S:5:ILE:C	4:S:6:LEU:HD12	2.33	0.48
3:M:277:ILE:HD11	3:M:378:VAL:HG11	1.96	0.48
5:C:20:ILE:HD12	5:C:87:GLY:HA3	1.94	0.48
2:B:18:LEU:HD22	2:B:18:LEU:N	2.26	0.48
2:B:18:LEU:H	2:B:18:LEU:CD2	2.27	0.48
4:S:2:ILE:O	4:S:2:ILE:HG13	2.13	0.48
4:S:90:LEU:HB3	4:S:113:ILE:CG2	2.43	0.48
5:C:82:PHE:CE2	5:C:113:GLU:HG3	2.49	0.48
5:C:124:PHE:CD2	5:C:158:THR:HG21	2.48	0.48
1:A:244:PHE:CE2	4:S:86:ARG:HD2	2.44	0.47
1:A:322:LYS:CG	1:A:325:ARG:HH21	2.26	0.47
2:B:395:LEU:HD21	2:B:410:ALA:HB1	1.96	0.47
2:B:418:PHE:CZ	2:B:429:ILE:HD11	2.49	0.47
2:B:426:GLU:HG3	2:B:455:TYR:CE2	2.49	0.47
5:C:38:LYS:O	5:C:39:LEU:HD23	2.14	0.47
1:A:306:ARG:O	1:A:310:ILE:HD13	2.14	0.47
2:B:88:VAL:O	2:B:92:VAL:HG23	2.15	0.47
2:B:247:ARG:O	2:B:256:VAL:HG12	2.14	0.47
2:B:346:ALA:HA	2:B:350:ASN:HD21	1.80	0.47
1:A:57:HIS:CG	1:A:92:LEU:HD23	2.48	0.47
1:A:63:ALA:HB1	1:A:92:LEU:HD22	1.95	0.47
2:B:71:LEU:HA	2:B:74:MET:SD	2.53	0.47
2:B:220:ILE:HG12	2:B:255:VAL:N	2.29	0.47
2:B:395:LEU:CD2	2:B:410:ALA:HB1	2.45	0.47
3:M:149:PRO:HG2	3:M:150:PRO:HD3	1.94	0.47
3:M:202:VAL:HG13	3:M:259:ASP:HA	1.96	0.47
3:M:393:ARG:HG2	3:M:394:TYR:CD1	2.48	0.47
4:S:13:LYS:HB2	4:S:15:ARG:CZ	2.45	0.47
1:A:68:LEU:HG	1:A:69:GLU:H	1.80	0.47
2:B:346:ALA:HA	2:B:350:ASN:ND2	2.30	0.47
4:S:130:ILE:O	4:S:130:ILE:HG13	2.15	0.47
5:C:90:PHE:HB3	5:C:123:VAL:HG22	1.96	0.47
5:C:97:ARG:O	5:C:100:VAL:HG12	2.14	0.47
1:A:112:ASN:HA	1:A:119:GLN:HE21	1.79	0.47
3:M:313:HIS:O	3:M:376:ILE:HG23	2.14	0.47
1:A:44:THR:O	1:A:45:TYR:HB2	2.15	0.47
1:A:71:LEU:HD23	1:A:71:LEU:O	2.14	0.47
1:A:176:LEU:HB3	1:A:177:PRO:HD3	1.95	0.47
1:A:237:VAL:HG12	1:A:238:SER:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:VAL:HA	2:B:148:LEU:CD2	2.45	0.47
2:B:199:LEU:HD13	2:B:229:TYR:CD1	2.50	0.47
2:B:466:LEU:HD13	2:B:491:LEU:HD12	1.95	0.47
3:M:6:VAL:O	3:M:18:CYS:HB2	2.14	0.47
3:M:310:VAL:HG12	3:M:380:PHE:CB	2.45	0.47
3:M:345:VAL:HG22	3:M:346:LYS:N	2.30	0.47
4:S:31:ILE:HG23	4:S:52:TRP:CZ3	2.50	0.47
1:A:159:LEU:HD22	4:S:119:ILE:O	2.15	0.47
1:A:284:VAL:HA	4:S:82:GLU:OE1	2.15	0.47
1:A:438:VAL:O	1:A:442:ILE:HD13	2.14	0.47
1:A:502:GLU:OE2	1:A:537:PHE:HB3	2.15	0.47
1:A:568:ALA:HB1	2:B:539:GLU:O	2.15	0.47
2:B:12:LYS:HD2	2:B:12:LYS:N	2.30	0.47
2:B:69:VAL:O	2:B:73:LEU:HD23	2.14	0.47
2:B:90:THR:HG23	5:C:50:GLY:HA3	1.96	0.47
2:B:113:ILE:HG22	2:B:115:VAL:H	1.79	0.47
2:B:246:PRO:HG3	3:M:248:GLU:HG2	1.97	0.47
2:B:319:HIS:C	2:B:321:MET:H	2.16	0.47
2:B:382:ILE:HD11	2:B:417:ILE:HA	1.97	0.47
2:B:403:VAL:O	2:B:407:VAL:HG23	2.14	0.47
2:B:474:HIS:HB3	2:B:475:ASP:H	1.53	0.47
3:M:320:ALA:HA	3:M:360:PHE:HE2	1.80	0.47
4:S:34:GLU:HG2	4:S:52:TRP:CZ2	2.49	0.47
4:S:81:LEU:HD23	4:S:81:LEU:O	2.15	0.47
4:S:94:TYR:CE2	4:S:109:LYS:HD3	2.49	0.47
2:B:85:ILE:O	5:C:49:ILE:HG22	2.15	0.47
3:M:213:GLY:C	3:M:393:ARG:HB3	2.35	0.47
5:C:26:ASP:HB3	5:C:70:GLY:O	2.13	0.47
1:A:237:VAL:HG11	1:A:243:PRO:HD3	1.96	0.47
1:A:308:LEU:O	1:A:312:ILE:HG13	2.14	0.47
2:B:38:ILE:CA	2:B:41:MET:HB3	2.45	0.47
2:B:256:VAL:O	2:B:259:ALA:HB3	2.15	0.47
2:B:326:VAL:HG22	2:B:338:LYS:HB2	1.97	0.47
3:M:10:ASP:HB3	3:M:16:LEU:HD23	1.97	0.47
1:A:142:VAL:O	1:A:146:LEU:HB2	2.14	0.47
1:A:165:ILE:HD13	1:A:172:MET:HB2	1.97	0.47
1:A:231:TYR:CD1	1:A:241:SER:HA	2.50	0.47
1:A:398:ALA:HA	1:A:432:TYR:HB3	1.96	0.47
2:B:62:ASN:CG	2:B:63:LEU:H	2.18	0.47
2:B:144:CYS:O	2:B:148:LEU:HD23	2.15	0.47
2:B:412:VAL:O	2:B:415:LYS:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:556:GLU:OE2	2:B:558:THR:HB	2.15	0.47
3:M:174:ASP:C	3:M:198:ILE:HD12	2.35	0.47
3:M:304:ARG:CZ	3:M:385:PHE:HZ	2.28	0.47
5:C:71:LEU:HD22	5:C:72:ASP:N	2.30	0.47
1:A:496:GLU:HA	1:A:497:PRO:HD3	1.75	0.46
2:B:69:VAL:HG12	2:B:73:LEU:HD23	1.96	0.46
2:B:181:VAL:HG21	2:B:207:LEU:HD21	1.97	0.46
2:B:405:TYR:CG	2:B:406:VAL:N	2.83	0.46
3:M:37:LEU:HA	3:M:50:LEU:HD21	1.96	0.46
3:M:193:GLU:HG3	3:M:269:LEU:O	2.15	0.46
5:C:66:TRP:HE3	5:C:81:TYR:HD2	1.63	0.46
1:A:135:CYS:O	1:A:164:VAL:HG13	2.15	0.46
1:A:284:VAL:O	1:A:287:ALA:HB3	2.15	0.46
2:B:13:GLY:HA3	2:B:16:PHE:CZ	2.50	0.46
2:B:191:HIS:C	2:B:193:SER:H	2.18	0.46
2:B:214:CYS:HB3	2:B:219:GLN:HG3	1.97	0.46
2:B:567:ILE:HA	2:B:572:SER:HB3	1.96	0.46
3:M:19:ARG:HB3	3:M:114:LEU:HD13	1.96	0.46
3:M:328:THR:OG1	3:M:329:VAL:HG22	2.14	0.46
1:A:528:THR:HA	1:A:566:TYR:CE2	2.49	0.46
2:B:52:PRO:HG2	2:B:53:ASP:OD1	2.15	0.46
2:B:55:VAL:HG22	2:B:73:LEU:HD21	1.96	0.46
2:B:238:GLN:O	2:B:242:GLU:HG3	2.15	0.46
2:B:253:SER:O	2:B:254:ALA:C	2.53	0.46
2:B:331:PRO:O	2:B:335:LYS:HG3	2.16	0.46
3:M:160:ARG:HB3	3:M:258:PRO:HA	1.97	0.46
3:M:214:LEU:HD22	3:M:392:VAL:HA	1.97	0.46
3:M:404:GLN:O	3:M:405:ALA:HB3	2.16	0.46
4:S:13:LYS:HB2	4:S:15:ARG:NH2	2.30	0.46
1:A:389:LEU:CD2	1:A:425:VAL:HG23	2.46	0.46
1:A:560:GLN:O	1:A:564:VAL:HG23	2.15	0.46
2:B:166:LYS:HD3	2:B:197:LEU:HD11	1.97	0.46
2:B:314:PRO:HB2	2:B:345:LEU:HD21	1.97	0.46
3:M:151:ALA:O	3:M:154:THR:HG22	2.15	0.46
3:M:233:LEU:HG	3:M:268:ARG:O	2.15	0.46
4:S:35:ILE:HG22	4:S:39:ILE:CG1	2.46	0.46
5:C:108:MET:C	5:C:110:MET:H	2.17	0.46
1:A:46:ARG:HG3	1:A:69:GLU:O	2.14	0.46
2:B:51:PHE:N	2:B:52:PRO:HD2	2.29	0.46
2:B:200:ASN:O	2:B:204:ILE:HG13	2.15	0.46
2:B:514:SER:OG	2:B:519:LEU:HD22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:180:ASN:ND2	3:M:195:VAL:N	2.62	0.46
1:A:123:LEU:HD13	1:A:157:ALA:N	2.30	0.46
1:A:400:CYS:O	1:A:404:ILE:HG13	2.15	0.46
1:A:500:VAL:O	1:A:500:VAL:HG22	2.15	0.46
2:B:42:THR:HB	3:M:111:TYR:OH	2.16	0.46
2:B:165:LEU:O	2:B:168:LEU:HB2	2.16	0.46
2:B:215:THR:H	2:B:219:GLN:HG3	1.81	0.46
2:B:252:ASN:O	2:B:253:SER:C	2.54	0.46
3:M:391:GLN:HA	3:M:411:TYR:OH	2.16	0.46
4:S:35:ILE:HD11	4:S:52:TRP:CE3	2.51	0.46
1:A:124:CYS:SG	4:S:115:ASP:HB3	2.55	0.46
1:A:227:ILE:O	1:A:229:SER:N	2.49	0.46
1:A:562:ARG:HB3	1:A:566:TYR:CE1	2.50	0.46
2:B:100:PRO:HB3	2:B:134:ASP:OD2	2.16	0.46
2:B:261:LYS:CE	2:B:566:TYR:HA	2.46	0.46
2:B:399:ILE:HB	2:B:400:GLN:NE2	2.31	0.46
3:M:281:SER:HA	3:M:294:MET:O	2.16	0.46
5:C:114:ASP:O	5:C:117:ARG:HG2	2.15	0.46
1:A:252:LEU:O	1:A:256:LEU:HG	2.16	0.46
2:B:130:LEU:HD11	2:B:161:PHE:CD1	2.51	0.46
3:M:182:LEU:O	3:M:182:LEU:HD13	2.15	0.46
5:C:24:GLY:HA3	5:C:91:VAL:O	2.16	0.46
5:C:33:ILE:HG12	5:C:160:ALA:HB2	1.96	0.46
1:A:54:LEU:HD21	1:A:88:GLY:CA	2.40	0.46
1:A:287:ALA:HA	4:S:78:LEU:HD13	1.98	0.46
1:A:438:VAL:HG11	1:A:525:TYR:CZ	2.50	0.46
1:A:452:HIS:O	1:A:456:VAL:HG23	2.15	0.46
2:B:40:SER:HA	2:B:43:VAL:CG2	2.46	0.46
2:B:342:MET:HE3	2:B:354:VAL:HG13	1.97	0.46
2:B:572:SER:O	2:B:574:TYR:N	2.49	0.46
3:M:108:VAL:HG23	3:M:109:ILE:N	2.25	0.46
5:C:160:ALA:C	5:C:162:SER:H	2.19	0.46
2:B:135:PRO:HB3	2:B:176:VAL:HG13	1.98	0.46
2:B:249:SER:HG	2:B:256:VAL:HG13	1.80	0.46
3:M:317:PRO:O	3:M:319:ASP:N	2.49	0.46
1:A:17:ALA:HB2	1:A:26:MET:SD	2.57	0.45
1:A:216:VAL:CB	1:A:217:PRO:HD3	2.46	0.45
1:A:378:ILE:CD1	1:A:411:TYR:HB3	2.47	0.45
2:B:261:LYS:CE	2:B:568:GLY:H	2.29	0.45
3:M:151:ALA:O	3:M:153:VAL:N	2.49	0.45
3:M:199:LYS:HZ3	3:M:201:ARG:CG	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:52:TRP:HB3	4:S:57:LEU:HD11	1.98	0.45
4:S:76:ASN:HD21	4:S:79:LEU:H	1.61	0.45
5:C:29:GLY:O	5:C:33:ILE:HG13	2.15	0.45
5:C:120:VAL:HG12	5:C:152:ASN:CB	2.45	0.45
1:A:267:MET:C	1:A:271:LEU:HD23	2.36	0.45
1:A:413:PRO:HD2	1:A:417:TRP:CZ3	2.52	0.45
2:B:247:ARG:HG2	2:B:259:ALA:CB	2.45	0.45
2:B:404:ASN:O	2:B:407:VAL:HB	2.16	0.45
3:M:5:ALA:HB1	3:M:7:TYR:CE1	2.51	0.45
3:M:172:PHE:CZ	3:M:408:TRP:HB3	2.51	0.45
3:M:395:LEU:O	3:M:395:LEU:HD23	2.16	0.45
3:M:397:ILE:HD12	3:M:403:TYR:CD2	2.47	0.45
5:C:18:MET:O	5:C:63:PHE:HA	2.17	0.45
5:C:86:GLN:O	5:C:119:ALA:HA	2.15	0.45
5:C:107:LEU:HG	5:C:108:MET:CE	2.47	0.45
1:A:185:GLU:HG3	1:A:186:LYS:H	1.82	0.45
1:A:401:ALA:O	1:A:405:PHE:HD1	1.98	0.45
2:B:382:ILE:HG21	2:B:551:GLU:OE1	2.15	0.45
4:S:86:ARG:O	4:S:89:GLU:HB3	2.16	0.45
1:A:46:ARG:C	1:A:73:LEU:HD11	2.37	0.45
1:A:574:ASP:O	1:A:576:MET:N	2.50	0.45
2:B:31:LYS:HB2	2:B:31:LYS:NZ	2.32	0.45
2:B:332:ILE:HD13	3:M:44:GLY:O	2.16	0.45
2:B:419:ARG:HH12	2:B:548:ILE:HG12	1.82	0.45
3:M:6:VAL:HG21	3:M:118:MET:CE	2.47	0.45
3:M:162:GLU:HG3	3:M:163:GLY:N	2.32	0.45
3:M:177:GLU:HA	3:M:196:GLY:HA3	1.97	0.45
3:M:290:ARG:HA	3:M:360:PHE:O	2.17	0.45
4:S:35:ILE:HG22	4:S:39:ILE:HG13	1.99	0.45
1:A:251:ARG:NH2	4:S:75:ASP:HA	2.32	0.45
2:B:382:ILE:HG23	2:B:420:LYS:HG2	1.97	0.45
5:C:23:VAL:HG23	5:C:90:PHE:HD1	1.81	0.45
5:C:59:LYS:O	5:C:61:ILE:HG12	2.16	0.45
1:A:35:ARG:HD3	1:A:65:PHE:CD2	2.52	0.45
1:A:46:ARG:NE	1:A:69:GLU:HG3	2.29	0.45
2:B:223:LEU:HD23	2:B:226:LEU:HD21	1.99	0.45
2:B:248:LEU:HA	3:M:237:LYS:NZ	2.32	0.45
2:B:466:LEU:HD11	2:B:487:ALA:HB1	1.99	0.45
3:M:326:LYS:CE	3:M:357:ARG:HB2	2.46	0.45
4:S:86:ARG:HG2	4:S:117:PHE:CZ	2.51	0.45
1:A:73:LEU:HD22	1:A:81:ASP:CG	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ARG:HB2	1:A:295:THR:OG1	2.17	0.45
1:A:382:MET:O	1:A:386:LEU:HG	2.17	0.45
1:A:557:VAL:HG22	2:B:419:ARG:CD	2.47	0.45
2:B:101:LEU:HD21	3:M:150:PRO:HD3	1.97	0.45
2:B:371:ARG:O	2:B:374:VAL:HG12	2.16	0.45
2:B:466:LEU:HB3	2:B:488:PHE:CE1	2.52	0.45
3:M:279:ILE:HD11	3:M:295:VAL:CG1	2.46	0.45
3:M:379:LYS:HA	3:M:415:ASN:CB	2.47	0.45
4:S:77:GLU:O	4:S:80:THR:HB	2.16	0.45
4:S:98:VAL:CG2	4:S:102:ASP:HB2	2.46	0.45
5:C:100:VAL:HG13	5:C:101:ASN:N	2.31	0.45
1:A:67:GLN:NE2	1:A:93:LEU:HD21	2.32	0.45
1:A:191:LEU:O	1:A:195:VAL:HG23	2.16	0.45
1:A:209:LEU:HA	1:A:212:PHE:CB	2.45	0.45
2:B:139:LYS:HE2	3:M:124:GLN:NE2	2.32	0.45
2:B:166:LYS:CG	2:B:184:LEU:HD21	2.45	0.45
2:B:337:GLU:O	2:B:340:ASP:HB3	2.17	0.45
2:B:375:ARG:HG2	2:B:379:ARG:NH1	2.30	0.45
2:B:539:GLU:OE1	2:B:539:GLU:HA	2.17	0.45
3:M:92:SER:N	3:M:98:LEU:HD11	2.32	0.45
3:M:214:LEU:HB3	3:M:215:ASN:H	1.61	0.45
3:M:247:PHE:O	3:M:251:ARG:N	2.43	0.45
4:S:109:LYS:HA	4:S:112:PHE:HD2	1.82	0.45
5:C:167:TYR:HA	5:C:170:LEU:CD1	2.47	0.45
1:A:7:LEU:CD2	1:A:52:LYS:HA	2.38	0.45
1:A:309:ALA:HA	1:A:312:ILE:HD12	1.99	0.45
1:A:421:THR:O	1:A:424:ARG:HB3	2.16	0.45
1:A:528:THR:HA	1:A:566:TYR:HE2	1.82	0.45
2:B:67:LYS:O	2:B:70:TYR:HB2	2.17	0.45
2:B:238:GLN:HB2	2:B:269:MET:SD	2.57	0.45
2:B:385:GLU:HG3	2:B:386:GLN:N	2.32	0.45
2:B:451:ILE:HG23	2:B:452:VAL:N	2.31	0.45
3:M:56:ARG:HD2	3:M:56:ARG:H	1.79	0.45
3:M:157:VAL:HA	3:M:159:TRP:CH2	2.51	0.45
3:M:241:CYS:SG	3:M:258:PRO:HD3	2.57	0.45
1:A:226:LEU:CD2	1:A:245:LEU:HD23	2.39	0.45
1:A:237:VAL:HG12	1:A:238:SER:N	2.32	0.45
1:A:363:ARG:HA	1:A:366:MET:CE	2.47	0.45
2:B:47:VAL:HB	2:B:50:LEU:HG	1.99	0.45
2:B:205:ASN:HD22	2:B:208:LEU:HD12	1.82	0.45
2:B:280:LEU:HD12	2:B:280:LEU:HA	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:ALA:HB2	2:B:316:ILE:CG2	2.47	0.45
2:B:316:ILE:HG22	2:B:317:LEU:HD22	1.99	0.45
2:B:448:MET:O	2:B:452:VAL:HG23	2.17	0.45
2:B:480:VAL:O	2:B:484:LEU:HG	2.16	0.45
3:M:60:ILE:CD1	3:M:84:LEU:HB3	2.47	0.45
4:S:18:LYS:HD3	4:S:114:LEU:HD22	1.99	0.45
1:A:130:GLY:HA2	1:A:134:MET:HG2	1.99	0.44
1:A:180:LYS:HE2	1:A:214:LYS:NZ	2.31	0.44
1:A:389:LEU:HD13	1:A:400:CYS:HB2	1.99	0.44
1:A:472:LEU:HG	1:A:473:VAL:N	2.32	0.44
2:B:30:LYS:O	2:B:33:ALA:HB3	2.17	0.44
2:B:108:ARG:HD3	2:B:109:THR:OG1	2.16	0.44
2:B:162:LEU:HD13	2:B:187:ILE:HG21	1.99	0.44
2:B:303:LEU:HB3	2:B:337:GLU:HG3	1.99	0.44
2:B:346:ALA:H	2:B:383:LYS:HZ3	1.65	0.44
3:M:176:ILE:HD11	3:M:197:SER:HB3	1.98	0.44
3:M:235:ASP:OD1	3:M:236:VAL:N	2.50	0.44
4:S:35:ILE:HG22	4:S:39:ILE:HD11	1.98	0.44
5:C:35:TYR:OH	5:C:52:ASN:HB3	2.16	0.44
1:A:378:ILE:HD11	1:A:411:TYR:CB	2.48	0.44
1:A:451:MET:SD	1:A:451:MET:N	2.90	0.44
1:A:556:ASP:OD1	1:A:557:VAL:N	2.50	0.44
2:B:135:PRO:HD2	3:M:154:THR:OG1	2.16	0.44
2:B:295:GLU:HB3	2:B:298:LEU:CD1	2.46	0.44
3:M:16:LEU:HD12	3:M:103:ILE:HG21	1.98	0.44
3:M:317:PRO:C	3:M:319:ASP:N	2.70	0.44
3:M:336:PRO:O	3:M:338:ASN:N	2.48	0.44
4:S:56:LYS:HE3	4:S:73:ASN:OD1	2.16	0.44
1:A:183:LEU:HD12	1:A:215:LEU:HD13	1.98	0.44
1:A:254:ARG:O	1:A:299:ILE:HD11	2.18	0.44
1:A:296:ILE:HG22	1:A:297:MET:CE	2.47	0.44
1:A:382:MET:O	1:A:385:LEU:HB2	2.17	0.44
2:B:300:TYR:HA	2:B:303:LEU:HD12	1.99	0.44
2:B:551:GLU:O	2:B:552:THR:C	2.54	0.44
3:M:77:VAL:HA	3:M:80:VAL:CG2	2.47	0.44
3:M:92:SER:CB	3:M:98:LEU:HD21	2.34	0.44
3:M:284:GLU:HB3	3:M:292:GLU:HB2	1.99	0.44
5:C:48:THR:O	5:C:69:GLY:HA3	2.17	0.44
5:C:50:GLY:O	5:C:51:PHE:C	2.56	0.44
1:A:240:ILE:O	1:A:243:PRO:HD3	2.16	0.44
1:A:318:LEU:HD21	1:A:349:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:GLY:O	1:A:378:ILE:HD12	2.17	0.44
2:B:215:THR:HG23	2:B:218:GLY:CA	2.39	0.44
2:B:489:VAL:O	2:B:493:LEU:HG	2.17	0.44
2:B:562:GLU:O	2:B:565:CYS:HB3	2.16	0.44
3:M:210:LEU:HD11	3:M:395:LEU:HD11	2.00	0.44
3:M:211:ARG:HB3	3:M:396:LYS:HB2	1.98	0.44
1:A:138:LEU:O	1:A:142:VAL:HG23	2.18	0.44
1:A:158:ALA:O	1:A:162:VAL:HG23	2.17	0.44
1:A:289:LEU:HD23	1:A:312:ILE:HG23	1.98	0.44
1:A:378:ILE:HD11	1:A:411:TYR:HB3	1.99	0.44
2:B:12:LYS:HG2	4:S:97:ASN:HD21	1.83	0.44
2:B:63:LEU:N	2:B:63:LEU:HD23	2.32	0.44
2:B:148:LEU:HD12	2:B:153:ALA:HB2	1.99	0.44
2:B:162:LEU:O	2:B:166:LYS:HG3	2.17	0.44
2:B:499:THR:O	2:B:503:VAL:HG13	2.18	0.44
2:B:506:VAL:CG1	2:B:507:LEU:N	2.79	0.44
2:B:533:ASP:CB	2:B:535:VAL:HG12	2.38	0.44
3:M:32:HIS:HD1	3:M:52:HIS:CE1	2.35	0.44
3:M:310:VAL:HG12	3:M:380:PHE:HB3	1.99	0.44
1:A:46:ARG:CZ	1:A:72:LYS:HD2	2.48	0.44
1:A:105:ASN:HD22	1:A:105:ASN:HA	1.55	0.44
1:A:268:ASN:HB2	1:A:305:LEU:HD22	2.00	0.44
1:A:506:LEU:O	1:A:510:GLU:HG3	2.17	0.44
2:B:38:ILE:HD12	2:B:38:ILE:N	2.30	0.44
2:B:261:LYS:CD	2:B:568:GLY:H	2.30	0.44
3:M:36:ILE:CD1	3:M:52:HIS:HB2	2.47	0.44
3:M:133:GLU:CD	3:M:133:GLU:H	2.20	0.44
3:M:162:GLU:HG3	3:M:163:GLY:H	1.81	0.44
4:S:15:ARG:NH1	4:S:104:ILE:HD11	2.32	0.44
1:A:132:SER:C	1:A:134:MET:H	2.21	0.44
1:A:152:TYR:O	1:A:156:LYS:HG2	2.16	0.44
1:A:176:LEU:HA	1:A:179:THR:HG23	1.98	0.44
2:B:83:MET:HB2	2:B:86:MET:CE	2.47	0.44
2:B:312:LYS:HE3	2:B:313:ARG:HH21	1.82	0.44
2:B:549:SER:O	2:B:550:GLU:C	2.55	0.44
3:M:181:LEU:HD13	3:M:418:TYR:CE2	2.52	0.44
3:M:216:ASP:HA	3:M:232:GLU:CD	2.37	0.44
5:C:126:ASN:ND2	5:C:160:ALA:H	2.13	0.44
1:A:200:GLU:O	1:A:203:GLU:HG2	2.18	0.44
1:A:562:ARG:NE	2:B:522:ARG:HD2	2.32	0.44
2:B:139:LYS:HZ1	3:M:124:GLN:HB3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:LYS:C	2:B:284:LEU:H	2.20	0.44
2:B:286:PRO:HB2	2:B:287:PRO:CD	2.48	0.44
2:B:411:ILE:HD13	2:B:439:LEU:HD22	1.99	0.44
3:M:9:LEU:CD2	3:M:15:VAL:HA	2.48	0.44
3:M:179:VAL:HA	3:M:194:ILE:HG23	1.99	0.44
3:M:182:LEU:CD1	3:M:190:LEU:HB2	2.48	0.44
3:M:239:HIS:HB2	3:M:263:GLU:O	2.18	0.44
3:M:296:LYS:HD2	3:M:355:LEU:HB2	2.00	0.44
4:S:114:LEU:CD2	4:S:118:ILE:HD12	2.48	0.44
5:C:30:LYS:HB2	6:C:1001:GTP:O2B	2.17	0.44
1:A:287:ALA:CA	4:S:78:LEU:HD13	2.48	0.44
3:M:165:LYS:HA	3:M:205:SER:CB	2.48	0.44
3:M:189:VAL:HG13	3:M:189:VAL:O	2.18	0.44
1:A:566:TYR:HA	1:A:569:LEU:HD11	1.98	0.43
2:B:124:GLU:N	2:B:125:PRO:CD	2.81	0.43
2:B:222:ILE:O	2:B:226:LEU:HB3	2.17	0.43
2:B:401:THR:C	2:B:403:VAL:H	2.22	0.43
2:B:433:CYS:HA	2:B:448:MET:HE2	2.00	0.43
2:B:473:PHE:HB2	2:B:509:LEU:HD13	2.00	0.43
2:B:503:VAL:O	2:B:507:LEU:HB2	2.17	0.43
3:M:111:TYR:O	3:M:114:LEU:HB2	2.18	0.43
3:M:176:ILE:C	3:M:177:GLU:HG2	2.39	0.43
3:M:330:GLY:CA	3:M:345:VAL:HG23	2.48	0.43
4:S:42:ARG:HD3	4:S:59:TYR:OH	2.18	0.43
4:S:52:TRP:CH2	4:S:53:LYS:HD2	2.53	0.43
5:C:22:MET:HG3	5:C:30:LYS:HD2	2.00	0.43
1:A:253:LEU:HB3	1:A:267:MET:HE2	2.00	0.43
1:A:284:VAL:HG22	4:S:82:GLU:OE2	2.18	0.43
2:B:247:ARG:NH1	3:M:244:LEU:HD22	2.32	0.43
2:B:248:LEU:HB3	3:M:237:LYS:HZ2	1.83	0.43
2:B:287:PRO:HA	3:M:237:LYS:HE2	2.00	0.43
2:B:420:LYS:HE2	2:B:547:LEU:HD13	2.00	0.43
2:B:503:VAL:HG23	2:B:504:GLN:N	2.32	0.43
3:M:36:ILE:HD13	3:M:52:HIS:HB2	2.00	0.43
3:M:233:LEU:HD21	3:M:267:TYR:HB2	1.99	0.43
4:S:7:LEU:O	4:S:14:LEU:HD22	2.18	0.43
1:A:108:LYS:HB2	1:A:138:LEU:CD1	2.46	0.43
1:A:260:ASP:CG	1:A:261:ASP:N	2.71	0.43
1:A:438:VAL:HG11	1:A:525:TYR:OH	2.18	0.43
2:B:173:ASN:O	2:B:176:VAL:HG23	2.18	0.43
2:B:208:LEU:CA	2:B:211:LEU:HB2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:LEU:HB3	3:M:236:VAL:O	2.19	0.43
3:M:10:ASP:O	3:M:11:LEU:C	2.56	0.43
3:M:198:ILE:HG23	3:M:198:ILE:O	2.19	0.43
5:C:140:THR:HG23	5:C:145:LEU:HD12	2.01	0.43
2:B:449:ILE:HG22	2:B:487:ALA:HB2	1.99	0.43
3:M:211:ARG:HG2	3:M:212:LEU:N	2.32	0.43
3:M:257:PRO:HA	3:M:258:PRO:HD3	1.75	0.43
4:S:8:PHE:O	4:S:66:TYR:HB2	2.18	0.43
4:S:31:ILE:HG23	4:S:52:TRP:CH2	2.54	0.43
1:A:10:LEU:CD2	1:A:30:GLU:HG2	2.49	0.43
1:A:455:THR:HG22	1:A:459:LEU:HD11	2.00	0.43
1:A:536:ARG:NH1	1:A:581:LEU:HB3	2.20	0.43
1:A:557:VAL:HA	2:B:419:ARG:HE	1.84	0.43
2:B:113:ILE:HD12	2:B:113:ILE:N	2.34	0.43
2:B:244:VAL:HG11	2:B:263:LEU:HD21	2.01	0.43
2:B:261:LYS:HZ3	2:B:566:TYR:HA	1.83	0.43
2:B:311:GLN:NE2	2:B:555:ILE:H	2.16	0.43
2:B:510:ALA:HA	2:B:514:SER:OG	2.18	0.43
3:M:12:LYS:HB2	3:M:12:LYS:NZ	2.34	0.43
3:M:65:LEU:HD11	3:M:99:GLU:CA	2.48	0.43
3:M:285:LYS:HG3	3:M:291:ILE:CD1	2.47	0.43
3:M:383:PRO:HA	3:M:412:ILE:HA	1.99	0.43
4:S:86:ARG:HA	4:S:86:ARG:CZ	2.49	0.43
2:B:55:VAL:O	2:B:58:MET:HB3	2.19	0.43
2:B:244:VAL:HB	2:B:263:LEU:HD21	2.00	0.43
2:B:464:GLU:O	2:B:467:GLU:HG2	2.18	0.43
2:B:570:LEU:O	2:B:573:VAL:HG22	2.17	0.43
3:M:9:LEU:HB2	3:M:66:TYR:O	2.18	0.43
3:M:127:ASP:O	3:M:128:SER:C	2.56	0.43
3:M:176:ILE:HG13	3:M:197:SER:H	1.83	0.43
3:M:253:ILE:O	3:M:253:ILE:HG13	2.19	0.43
3:M:274:LYS:CG	3:M:275:PRO:HD2	2.48	0.43
3:M:292:GLU:HA	3:M:359:HIS:HA	2.01	0.43
3:M:345:VAL:HG22	3:M:346:LYS:H	1.83	0.43
3:M:382:ILE:HB	3:M:384:TYR:CE1	2.52	0.43
5:C:64:THR:CG2	5:C:66:TRP:HE1	2.32	0.43
5:C:108:MET:C	5:C:110:MET:N	2.72	0.43
1:A:429:ALA:O	1:A:431:SER:N	2.52	0.43
1:A:548:VAL:HG21	1:A:570:PHE:CE2	2.49	0.43
2:B:264:MET:CE	2:B:313:ARG:HG3	2.49	0.43
2:B:559:LEU:HG	2:B:563:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:332:VAL:HG23	3:M:343:TRP:HA	2.01	0.43
3:M:355:LEU:HD13	3:M:356:MET:H	1.81	0.43
5:C:91:VAL:HG13	5:C:124:PHE:O	2.19	0.43
1:A:150:ASN:O	1:A:151:SER:C	2.56	0.43
1:A:161:ALA:O	1:A:165:ILE:HG13	2.19	0.43
1:A:231:TYR:OH	1:A:237:VAL:HB	2.18	0.43
1:A:473:VAL:HG23	1:A:474:GLN:N	2.34	0.43
2:B:52:PRO:HA	2:B:86:MET:CE	2.49	0.43
2:B:165:LEU:HB3	2:B:184:LEU:HD23	2.00	0.43
2:B:502:LEU:O	2:B:506:VAL:HG12	2.18	0.43
3:M:378:VAL:HG13	3:M:415:ASN:ND2	2.33	0.43
3:M:384:TYR:O	3:M:411:TYR:HB3	2.18	0.43
5:C:21:LEU:HB3	5:C:85:THR:CG2	2.49	0.43
5:C:23:VAL:HB	5:C:110:MET:HE1	2.01	0.43
2:B:181:VAL:HG11	2:B:222:ILE:HG13	2.01	0.43
2:B:382:ILE:N	2:B:382:ILE:HD12	2.34	0.43
1:A:260:ASP:CG	1:A:261:ASP:H	2.22	0.43
2:B:108:ARG:HB3	2:B:140:THR:CG2	2.49	0.43
2:B:542:LEU:HD12	2:B:542:LEU:N	2.34	0.43
3:M:95:PHE:O	3:M:96:LYS:C	2.57	0.43
3:M:178:ALA:HB3	3:M:195:VAL:CG1	2.49	0.43
3:M:199:LYS:HE2	3:M:200:MET:N	2.34	0.43
5:C:120:VAL:HG12	5:C:152:ASN:HB2	2.00	0.43
1:A:7:LEU:HA	1:A:52:LYS:HG2	2.01	0.42
1:A:14:ILE:HG22	1:A:14:ILE:O	2.19	0.42
1:A:155:LYS:HG3	1:A:156:LYS:N	2.34	0.42
1:A:159:LEU:HD11	4:S:124:GLN:HA	2.01	0.42
1:A:577:ARG:O	1:A:581:LEU:HG	2.19	0.42
2:B:52:PRO:HA	2:B:86:MET:HE3	2.00	0.42
2:B:135:PRO:HA	2:B:138:ARG:HG3	2.01	0.42
2:B:139:LYS:HG3	2:B:179:ASN:ND2	2.34	0.42
3:M:155:ASN:C	3:M:155:ASN:HD22	2.22	0.42
3:M:193:GLU:CG	3:M:194:ILE:N	2.82	0.42
3:M:216:ASP:HA	3:M:232:GLU:OE1	2.19	0.42
4:S:108:GLU:CD	4:S:109:LYS:H	2.21	0.42
5:C:58:TYR:O	5:C:59:LYS:HB2	2.19	0.42
1:A:27:ILE:CD1	1:A:59:LEU:HD23	2.42	0.42
1:A:185:GLU:HG3	1:A:187:ASN:H	1.83	0.42
1:A:285:GLY:O	1:A:288:ILE:HB	2.19	0.42
2:B:99:ASN:HB3	2:B:102:ILE:CD1	2.49	0.42
5:C:20:ILE:HG12	5:C:63:PHE:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LYS:O	1:A:216:VAL:N	2.52	0.42
1:A:297:MET:N	1:A:297:MET:SD	2.91	0.42
2:B:233:ASP:OD2	2:B:235:ARG:HB2	2.19	0.42
2:B:261:LYS:HE2	2:B:566:TYR:HA	2.00	0.42
3:M:22:ARG:HG3	3:M:120:PHE:CE1	2.53	0.42
3:M:26:ASP:OD1	3:M:27:MET:N	2.52	0.42
3:M:106:ASN:O	3:M:109:ILE:HG13	2.20	0.42
3:M:265:MET:HE1	3:M:267:TYR:HB3	2.00	0.42
3:M:277:ILE:HG22	3:M:299:SER:CB	2.47	0.42
3:M:281:SER:OG	3:M:295:VAL:HG13	2.20	0.42
3:M:329:VAL:HG21	3:M:354:TYR:CB	2.44	0.42
1:A:513:LEU:HD11	1:A:530:ILE:HD11	2.02	0.42
1:A:577:ARG:HB2	1:A:581:LEU:CD1	2.49	0.42
2:B:382:ILE:HG13	2:B:420:LYS:HB3	2.01	0.42
2:B:478:THR:HB	2:B:516:ASN:ND2	2.35	0.42
3:M:5:ALA:N	3:M:70:THR:O	2.52	0.42
3:M:181:LEU:HG	3:M:182:LEU:N	2.34	0.42
3:M:273:VAL:O	3:M:273:VAL:HG13	2.20	0.42
4:S:13:LYS:HD2	4:S:15:ARG:HH22	1.84	0.42
1:A:23:GLU:CD	1:A:59:LEU:HD21	2.40	0.42
1:A:375:GLY:C	1:A:377:ASN:H	2.23	0.42
2:B:212:ASN:HD21	2:B:243:ARG:HD3	1.84	0.42
3:M:171:VAL:HG23	3:M:201:ARG:O	2.19	0.42
3:M:198:ILE:HG22	3:M:265:MET:SD	2.59	0.42
1:A:137:ASP:OD1	1:A:138:LEU:HD22	2.18	0.42
1:A:436:ASP:C	1:A:439:PRO:HD2	2.40	0.42
1:A:566:TYR:CD1	1:A:566:TYR:N	2.88	0.42
2:B:101:LEU:HD21	3:M:150:PRO:CD	2.49	0.42
2:B:244:VAL:CB	2:B:263:LEU:HD21	2.50	0.42
3:M:233:LEU:HD23	3:M:234:GLU:N	2.35	0.42
3:M:343:TRP:CH2	3:M:356:MET:HB2	2.54	0.42
5:C:75:ARG:N	5:C:76:PRO:CD	2.83	0.42
1:A:187:ASN:HD22	1:A:190:VAL:HG23	1.84	0.42
1:A:246:GLN:O	1:A:249:ILE:HB	2.20	0.42
1:A:533:LEU:HB3	1:A:537:PHE:HD2	1.84	0.42
1:A:562:ARG:NH2	2:B:522:ARG:HD2	2.32	0.42
2:B:105:LEU:HA	2:B:108:ARG:CG	2.49	0.42
2:B:411:ILE:HG13	2:B:412:VAL:N	2.35	0.42
2:B:522:ARG:NH1	2:B:522:ARG:HG2	2.34	0.42
2:B:556:GLU:HB3	2:B:559:LEU:CB	2.47	0.42
3:M:59:TRP:O	3:M:81:PHE:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:202:VAL:CG1	3:M:260:GLY:H	2.30	0.42
1:A:183:LEU:HD22	1:A:222:ILE:CD1	2.50	0.42
1:A:188:HIS:HB3	4:S:126:THR:OG1	2.19	0.42
1:A:313:LEU:HA	1:A:316:PHE:CD2	2.55	0.42
1:A:538:THR:HG22	1:A:539:CYS:SG	2.59	0.42
2:B:174:PRO:HA	2:B:177:VAL:HG12	2.01	0.42
2:B:223:LEU:HB3	2:B:258:SER:HB3	2.01	0.42
2:B:399:ILE:CD1	2:B:410:ALA:HB3	2.50	0.42
2:B:449:ILE:CG2	2:B:484:LEU:HD23	2.50	0.42
3:M:8:VAL:HB	3:M:17:ILE:O	2.20	0.42
3:M:36:ILE:HD11	3:M:52:HIS:CD2	2.55	0.42
3:M:210:LEU:HD23	3:M:211:ARG:O	2.20	0.42
3:M:334:TRP:HB2	3:M:341:ILE:HG12	2.02	0.42
4:S:6:LEU:HG	4:S:17:GLN:HB2	2.00	0.42
4:S:48:SER:HA	4:S:59:TYR:CE1	2.55	0.42
5:C:21:LEU:HD23	5:C:88:LEU:HD21	2.01	0.42
5:C:121:LEU:HD12	5:C:122:LEU:H	1.84	0.42
2:B:202:GLN:H	2:B:202:GLN:HG3	1.69	0.42
2:B:403:VAL:O	2:B:406:VAL:HG12	2.19	0.42
2:B:533:ASP:C	2:B:535:VAL:N	2.73	0.42
3:M:17:ILE:O	3:M:18:CYS:HB3	2.19	0.42
3:M:307:ALA:O	3:M:347:SER:HB2	2.20	0.42
3:M:316:VAL:HB	3:M:317:PRO:CD	2.50	0.42
5:C:26:ASP:OD1	5:C:75:ARG:NH2	2.53	0.42
1:A:167:LYS:NZ	4:S:22:THR:HG21	2.35	0.42
1:A:438:VAL:HG12	2:B:517:PRO:HG2	2.02	0.42
1:A:442:ILE:HD12	1:A:475:VAL:HG13	2.00	0.42
1:A:527:LEU:C	1:A:527:LEU:HD23	2.40	0.42
1:A:545:LYS:HG2	1:A:570:PHE:CD1	2.55	0.42
2:B:136:TYR:O	2:B:139:LYS:HB3	2.20	0.42
3:M:243:ARG:HH11	3:M:243:ARG:CA	2.30	0.42
4:S:29:LYS:O	4:S:33:ARG:HG2	2.20	0.42
4:S:98:VAL:HG22	4:S:99:CYS:N	2.34	0.42
1:A:198:LEU:O	1:A:201:MET:HB2	2.20	0.41
2:B:335:LYS:HB3	2:B:369:PHE:HE1	1.84	0.41
5:C:70:GLY:HA2	5:C:78:TRP:CZ2	2.44	0.41
5:C:71:LEU:O	5:C:74:ILE:HG13	2.19	0.41
5:C:124:PHE:CG	5:C:158:THR:HG21	2.55	0.41
1:A:31:CYS:SG	1:A:62:PRO:HB2	2.60	0.41
1:A:328:ALA:O	1:A:332:LEU:HB2	2.20	0.41
1:A:580:LEU:O	2:B:528:ARG:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:178:ALA:HB3	3:M:195:VAL:HG12	2.02	0.41
3:M:238:PHE:CB	3:M:242:VAL:HG11	2.45	0.41
4:S:69:CYS:SG	4:S:70:ALA:N	2.93	0.41
4:S:90:LEU:HD21	4:S:117:PHE:CG	2.55	0.41
1:A:356:ASP:OD1	1:A:361:ILE:HD12	2.21	0.41
2:B:380:CYS:HA	2:B:383:LYS:HG3	2.02	0.41
3:M:183:VAL:CG2	3:M:187:GLY:HA2	2.50	0.41
3:M:384:TYR:HE1	3:M:413:THR:HB	1.86	0.41
4:S:90:LEU:HD23	4:S:113:ILE:HG22	2.02	0.41
5:C:19:ARG:O	5:C:20:ILE:HD13	2.19	0.41
1:A:35:ARG:HD3	1:A:65:PHE:CE2	2.55	0.41
1:A:193:THR:HA	1:A:196:VAL:HG22	2.01	0.41
1:A:209:LEU:CA	1:A:212:PHE:HB2	2.43	0.41
1:A:227:ILE:HG22	1:A:228:MET:N	2.25	0.41
1:A:552:GLY:HA2	1:A:563:ALA:CB	2.50	0.41
1:A:557:VAL:HA	2:B:419:ARG:NH2	2.30	0.41
2:B:170:SER:OG	2:B:206:LYS:HD3	2.20	0.41
2:B:182:ALA:HB1	3:M:122:TYR:CD2	2.55	0.41
2:B:448:MET:HA	2:B:451:ILE:CG2	2.51	0.41
3:M:8:VAL:O	3:M:9:LEU:HD23	2.20	0.41
3:M:183:VAL:CG1	3:M:420:LEU:HB2	2.48	0.41
3:M:200:MET:SD	3:M:264:LEU:HB2	2.61	0.41
2:B:34:VAL:CB	2:B:65:LEU:HD11	2.44	0.41
2:B:85:ILE:HG22	5:C:49:ILE:HG21	2.02	0.41
2:B:162:LEU:CD1	2:B:187:ILE:HG21	2.50	0.41
2:B:269:MET:O	2:B:270:LEU:C	2.59	0.41
2:B:511:THR:HB	2:B:524:TYR:CE1	2.56	0.41
3:M:29:GLU:HG2	3:M:55:VAL:CG2	2.45	0.41
3:M:79:LEU:O	3:M:79:LEU:HD23	2.21	0.41
3:M:150:PRO:O	3:M:154:THR:HB	2.19	0.41
3:M:174:ASP:OD2	3:M:410:ARG:HD2	2.19	0.41
3:M:193:GLU:OE2	3:M:268:ARG:HB2	2.20	0.41
3:M:193:GLU:O	3:M:194:ILE:HG13	2.21	0.41
3:M:294:MET:HA	3:M:357:ARG:HD2	2.01	0.41
5:C:75:ARG:HB2	5:C:76:PRO:HD3	2.03	0.41
5:C:107:LEU:HG	5:C:108:MET:HE2	2.03	0.41
1:A:57:HIS:HB2	1:A:92:LEU:CD2	2.51	0.41
1:A:252:LEU:HD23	1:A:256:LEU:HG	2.03	0.41
2:B:98:PRO:HG2	2:B:99:ASN:H	1.85	0.41
2:B:411:ILE:O	2:B:414:ILE:HB	2.21	0.41
3:M:10:ASP:CB	3:M:16:LEU:HD23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:65:LEU:HD11	3:M:99:GLU:N	2.35	0.41
4:S:23:LEU:CD2	4:S:24:PRO:HD2	2.44	0.41
4:S:115:ASP:C	4:S:117:PHE:H	2.23	0.41
1:A:525:TYR:OH	2:B:517:PRO:HD2	2.20	0.41
2:B:102:ILE:O	2:B:103:ARG:C	2.58	0.41
2:B:143:VAL:HG11	3:M:119:ASP:OD1	2.20	0.41
2:B:173:ASN:HB3	2:B:174:PRO:HD2	2.03	0.41
2:B:429:ILE:HA	2:B:432:LEU:HG	2.02	0.41
3:M:177:GLU:O	3:M:413:THR:HG23	2.20	0.41
3:M:180:ASN:HD21	3:M:195:VAL:H	1.63	0.41
3:M:183:VAL:O	3:M:420:LEU:HD13	2.20	0.41
3:M:334:TRP:CH2	3:M:336:PRO:HA	2.56	0.41
5:C:120:VAL:HB	5:C:172:TRP:CH2	2.55	0.41
1:A:12:ARG:HD2	1:A:12:ARG:O	2.21	0.41
1:A:117:PHE:CD2	4:S:141:LEU:HD22	2.56	0.41
1:A:136:ARG:HE	1:A:168:VAL:HG21	1.84	0.41
1:A:142:VAL:HG11	1:A:161:ALA:HA	2.03	0.41
2:B:258:SER:HA	2:B:261:LYS:HB3	2.03	0.41
2:B:476:LYS:HB3	2:B:480:VAL:CG1	2.50	0.41
2:B:567:ILE:HA	2:B:572:SER:CB	2.50	0.41
3:M:10:ASP:OD1	3:M:16:LEU:HD23	2.20	0.41
3:M:301:PHE:CE1	3:M:350:GLY:HA2	2.55	0.41
4:S:18:LYS:CD	4:S:114:LEU:HD22	2.51	0.41
4:S:87:TYR:HD1	4:S:90:LEU:HD22	1.84	0.41
5:C:167:TYR:O	5:C:170:LEU:HB2	2.20	0.41
1:A:30:GLU:HG3	1:A:34:ILE:CD1	2.51	0.41
1:A:97:GLN:HA	1:A:100:HIS:CB	2.47	0.41
1:A:234:GLU:O	1:A:235:HIS:HB2	2.21	0.41
1:A:241:SER:O	1:A:242:ASP:C	2.59	0.41
1:A:378:ILE:HD11	1:A:411:TYR:CG	2.55	0.41
1:A:455:THR:HG22	1:A:459:LEU:CD1	2.51	0.41
1:A:535:THR:HB	1:A:536:ARG:HH11	1.85	0.41
2:B:166:LYS:HG2	2:B:184:LEU:HD21	2.03	0.41
2:B:247:ARG:HD3	2:B:247:ARG:HA	1.97	0.41
2:B:292:LEU:CD2	3:M:191:ARG:HH12	2.34	0.41
2:B:314:PRO:CB	2:B:345:LEU:HD21	2.50	0.41
2:B:346:ALA:H	2:B:383:LYS:NZ	2.17	0.41
2:B:351:ILE:H	2:B:351:ILE:HG13	1.74	0.41
2:B:503:VAL:HA	2:B:506:VAL:HG12	2.03	0.41
3:M:28:SER:O	3:M:30:VAL:HG12	2.21	0.41
3:M:98:LEU:H	3:M:98:LEU:CD2	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:214:LEU:CD2	3:M:392:VAL:HA	2.51	0.41
3:M:238:PHE:CD1	3:M:265:MET:HB3	2.56	0.41
3:M:248:GLU:O	3:M:248:GLU:HG3	2.21	0.41
3:M:321:ASP:HB2	3:M:361:GLY:O	2.21	0.41
4:S:7:LEU:HD22	4:S:67:PHE:HA	2.02	0.41
4:S:126:THR:O	4:S:127:SER:C	2.59	0.41
1:A:80:THR:O	1:A:84:ILE:HG12	2.21	0.41
1:A:93:LEU:CD1	1:A:129:MET:HE1	2.40	0.41
1:A:254:ARG:HA	1:A:299:ILE:HD11	2.02	0.41
2:B:34:VAL:HG21	2:B:65:LEU:HD21	2.03	0.41
2:B:65:LEU:O	2:B:69:VAL:HG23	2.20	0.41
2:B:503:VAL:O	2:B:506:VAL:HG12	2.21	0.41
3:M:301:PHE:HB2	3:M:302:LYS:H	1.55	0.41
4:S:53:LYS:O	4:S:54:GLU:HB2	2.20	0.41
4:S:87:TYR:CA	4:S:90:LEU:HD13	2.50	0.41
5:C:21:LEU:HD12	5:C:22:MET:N	2.36	0.41
5:C:22:MET:HB3	5:C:66:TRP:O	2.21	0.41
1:A:84:ILE:O	1:A:84:ILE:HG22	2.21	0.40
1:A:93:LEU:CD2	1:A:99:VAL:HG21	2.38	0.40
1:A:390:ASP:OD1	1:A:428:THR:HG21	2.20	0.40
2:B:89:ASN:CG	5:C:48:THR:HA	2.41	0.40
2:B:174:PRO:HA	2:B:177:VAL:CG1	2.51	0.40
2:B:192:PRO:O	2:B:193:SER:HB2	2.21	0.40
2:B:207:LEU:C	2:B:211:LEU:HD12	2.41	0.40
2:B:331:PRO:HG2	2:B:334:VAL:HB	2.02	0.40
2:B:409:GLU:O	2:B:412:VAL:HB	2.21	0.40
1:A:115:THR:HG22	1:A:116:GLN:N	2.34	0.40
1:A:232:SER:C	1:A:234:GLU:H	2.25	0.40
1:A:293:VAL:HG21	1:A:313:LEU:CD2	2.52	0.40
1:A:435:ASP:C	1:A:437:ALA:H	2.24	0.40
1:A:441:LEU:O	1:A:444:LEU:HB3	2.22	0.40
1:A:479:CYS:O	1:A:483:TYR:N	2.48	0.40
1:A:480:ILE:HG23	1:A:487:LEU:HD22	2.02	0.40
2:B:55:VAL:HG22	2:B:73:LEU:HD11	2.04	0.40
2:B:251:ALA:HB3	2:B:255:VAL:CG1	2.51	0.40
2:B:295:GLU:HB3	2:B:298:LEU:CG	2.49	0.40
2:B:304:ARG:HG3	2:B:573:VAL:HB	2.04	0.40
3:M:269:LEU:HD13	3:M:388:SER:OG	2.21	0.40
3:M:298:LYS:HG2	3:M:299:SER:H	1.86	0.40
4:S:85:HIS:C	4:S:88:VAL:HG22	2.42	0.40
5:C:20:ILE:CG1	5:C:63:PHE:HB3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LEU:HD11	1:A:102:LEU:HB2	2.04	0.40
1:A:438:VAL:HB	1:A:439:PRO:CD	2.41	0.40
2:B:34:VAL:O	2:B:37:VAL:HB	2.21	0.40
2:B:115:VAL:O	2:B:118:ILE:HG13	2.21	0.40
2:B:399:ILE:HD12	2:B:407:VAL:HG13	2.03	0.40
2:B:419:ARG:HH11	2:B:548:ILE:HD11	1.87	0.40
2:B:525:ILE:HA	2:B:528:ARG:HE	1.86	0.40
2:B:564:ILE:C	2:B:566:TYR:N	2.75	0.40
3:M:28:SER:O	3:M:29:GLU:C	2.59	0.40
3:M:157:VAL:HG23	3:M:157:VAL:O	2.22	0.40
3:M:299:SER:HB2	3:M:348:PHE:CE1	2.56	0.40
3:M:326:LYS:HE3	3:M:357:ARG:HB2	2.03	0.40
3:M:335:VAL:HG13	3:M:338:ASN:HB2	2.04	0.40
5:C:27:ALA:HA	6:C:1001:GTP:H5'	2.03	0.40
1:A:289:LEU:HA	1:A:292:THR:OG1	2.22	0.40
1:A:488:VAL:O	1:A:489:SER:C	2.59	0.40
2:B:58:MET:HE1	2:B:87:ALA:CB	2.51	0.40
2:B:114:ARG:NH2	2:B:150:ASP:HB3	2.36	0.40
2:B:472:GLY:O	2:B:473:PHE:C	2.59	0.40
2:B:571:ALA:HA	2:B:574:TYR:CE2	2.55	0.40
3:M:152:THR:HG23	3:M:153:VAL:N	2.36	0.40
3:M:205:SER:O	3:M:208:PRO:HD3	2.22	0.40
3:M:212:LEU:HG	3:M:394:TYR:O	2.20	0.40
4:S:9:SER:HA	4:S:65:LEU:HA	2.03	0.40
1:A:133:GLU:H	1:A:133:GLU:CD	2.24	0.40
1:A:478:TRP:HB2	1:A:525:TYR:HD2	1.86	0.40
1:A:526:ALA:O	1:A:530:ILE:HG13	2.22	0.40
3:M:39:GLU:C	3:M:41:GLU:H	2.25	0.40
3:M:180:ASN:N	3:M:193:GLU:O	2.53	0.40
3:M:182:LEU:HD12	3:M:191:ARG:N	2.36	0.40
3:M:233:LEU:CG	3:M:234:GLU:H	2.34	0.40
3:M:314:ILE:HA	3:M:376:ILE:HG12	2.04	0.40
3:M:331:SER:O	3:M:343:TRP:HD1	2.04	0.40
3:M:332:VAL:HG22	3:M:333:LYS:N	2.35	0.40
4:S:48:SER:HA	4:S:59:TYR:HE1	1.87	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	577/601 (96%)	417 (72%)	122 (21%)	38 (7%)	1 15
2	B	561/586 (96%)	392 (70%)	125 (22%)	44 (8%)	1 13
3	M	375/423 (89%)	250 (67%)	94 (25%)	31 (8%)	1 12
4	S	143/154 (93%)	115 (80%)	23 (16%)	5 (4%)	3 25
5	C	163/172 (95%)	131 (80%)	24 (15%)	8 (5%)	2 20
All	All	1819/1936 (94%)	1305 (72%)	388 (21%)	126 (7%)	1 15

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	SER
1	A	184	ASN
1	A	214	LYS
1	A	215	LEU
1	A	229	SER
1	A	281	SER
1	A	322	LYS
1	A	323	ASN
1	A	379	ARG
1	A	413	PRO
1	A	434	ARG
1	A	574	ASP
2	B	37	VAL
2	B	88	VAL
2	B	98	PRO
2	B	155	LEU
2	B	249	SER
2	B	271	SER
2	B	318	LYS
2	B	367	VAL
2	B	573	VAL

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Mol	Chain	Res	Type
3	M	11	LEU
3	M	28	SER
3	M	29	GLU
3	M	96	LYS
3	M	415	ASN
3	M	421	ARG
5	C	51	PHE
1	A	178	ALA
1	A	258	ARG
1	A	430	GLY
1	A	469	GLN
1	A	575	HIS
2	B	14	GLU
2	B	116	ASP
2	B	199	LEU
2	B	396	LEU
2	B	473	PHE
2	B	474	HIS
2	B	547	LEU
2	B	550	GLU
2	B	552	THR
3	M	26	ASP
3	M	77	VAL
3	M	80	VAL
3	M	128	SER
3	M	152	THR
3	M	184	SER
3	M	279	ILE
4	S	11	GLN
1	A	451	MET
1	A	489	SER
1	A	582	GLU
2	B	125	PRO
2	B	197	LEU
2	B	216	GLU
2	B	251	ALA
2	B	253	SER
2	B	270	LEU
2	B	275	ASP
2	B	315	GLU
2	B	322	LYS
2	B	335	LYS

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Mol	Chain	Res	Type
2	B	485	LEU
2	B	508	SER
2	B	549	SER
3	M	160	ARG
3	M	241	CYS
3	M	318	ASN
3	M	349	PRO
3	M	388	SER
4	S	32	THR
4	S	92	ASP
5	C	30	LYS
5	C	161	THR
5	C	162	SER
5	C	166	LEU
5	C	180	GLN
1	A	131	SER
1	A	182	LEU
1	A	275	ALA
1	A	485	ASP
1	A	500	VAL
1	A	516	ASN
2	B	172	SER
2	B	254	ALA
2	B	404	ASN
2	B	463	ASP
2	B	497	THR
2	B	543	ALA
3	M	12	LYS
3	M	15	VAL
3	M	133	GLU
3	M	159	TRP
3	M	163	GLY
3	M	214	LEU
3	M	303	ARG
3	M	360	PHE
5	C	47	PRO
1	A	228	MET
1	A	241	SER
1	A	268	ASN
1	A	326	TYR
1	A	340	HIS
1	A	470	GLN

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Mol	Chain	Res	Type
1	A	512	VAL
1	A	540	THR
1	A	580	LEU
2	B	235	ARG
2	B	566	TYR
3	M	251	ARG
4	S	36	VAL
2	B	266	PHE
2	B	283	LYS
3	M	108	VAL
3	M	375	PRO
4	S	130	ILE
5	C	174	SER
2	B	540	VAL
3	M	397	ILE
1	A	394	PRO
2	B	246	PRO
3	M	195	VAL
1	A	177	PRO
2	B	351	ILE
1	A	373	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	514/534 (96%)	496 (96%)	18 (4%)	36 59
2	B	503/523 (96%)	446 (89%)	57 (11%)	6 21
3	M	350/383 (91%)	312 (89%)	38 (11%)	6 23
4	S	135/143 (94%)	127 (94%)	8 (6%)	19 45
5	C	143/150 (95%)	138 (96%)	5 (4%)	36 59
All	All	1645/1733 (95%)	1519 (92%)	126 (8%)	13 37

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	PHE
1	A	69	GLU
1	A	77	GLN
1	A	93	LEU
1	A	105	ASN
1	A	172	MET
1	A	212	PHE
1	A	242	ASP
1	A	248	ARG
1	A	279	GLU
1	A	297	MET
1	A	313	LEU
1	A	368	LEU
1	A	370	PHE
1	A	426	LEU
1	A	469	GLN
1	A	531	MET
1	A	577	ARG
2	B	15	ILE
2	B	41	MET
2	B	53	ASP
2	B	63	LEU
2	B	74	MET
2	B	105	LEU
2	B	108	ARG
2	B	112	CYS
2	B	114	ARG
2	B	121	TYR
2	B	124	GLU
2	B	155	LEU
2	B	159	GLN
2	B	176	VAL
2	B	184	LEU
2	B	191	HIS
2	B	196	LEU
2	B	197	LEU
2	B	199	LEU
2	B	205	ASN
2	B	207	LEU
2	B	211	LEU
2	B	213	GLU
2	B	215	THR
2	B	223	LEU

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Mol	Chain	Res	Type
2	B	226	LEU
2	B	247	ARG
2	B	256	VAL
2	B	268	GLU
2	B	275	ASP
2	B	277	TYR
2	B	280	LEU
2	B	292	LEU
2	B	295	GLU
2	B	327	LYS
2	B	330	ASP
2	B	344	ARG
2	B	345	LEU
2	B	355	LEU
2	B	368	ASP
2	B	385	GLU
2	B	395	LEU
2	B	398	LEU
2	B	405	TYR
2	B	457	GLU
2	B	466	LEU
2	B	474	HIS
2	B	475	ASP
2	B	504	GLN
2	B	515	ASP
2	B	526	TYR
2	B	530	LEU
2	B	551	GLU
2	B	553	ASP
2	B	561	ASP
2	B	566	TYR
2	B	570	LEU
3	M	11	LEU
3	M	24	ASP
3	M	41	GLU
3	M	56	ARG
3	M	58	MET
3	M	77	VAL
3	M	98	LEU
3	M	133	GLU
3	M	155	ASN
3	M	172	PHE

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Mol	Chain	Res	Type
3	M	174	ASP
3	M	177	GLU
3	M	182	LEU
3	M	199	LYS
3	M	203	PHE
3	M	207	MET
3	M	214	LEU
3	M	216	ASP
3	M	233	LEU
3	M	243	ARG
3	M	244	LEU
3	M	250	ASP
3	M	269	LEU
3	M	276	LEU
3	M	278	TRP
3	M	293	TYR
3	M	301	PHE
3	M	304	ARG
3	M	308	ASN
3	M	311	GLU
3	M	321	ASP
3	M	360	PHE
3	M	382	ILE
3	M	384	TYR
3	M	385	PHE
3	M	393	ARG
3	M	394	TYR
3	M	419	GLN
4	S	1	MET
4	S	10	ARG
4	S	25	ASP
4	S	74	GLN
4	S	76	ASN
4	S	89	GLU
4	S	137	ASP
4	S	142	GLN
5	C	19	ARG
5	C	94	SER
5	C	177	LEU
5	C	178	ARG
5	C	180	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	43	ASN
1	A	67	GLN
1	A	77	GLN
1	A	105	ASN
1	A	119	GLN
1	A	187	ASN
1	A	246	GLN
1	A	268	ASN
1	A	273	GLN
1	A	277	ASN
1	A	283	ASN
1	A	474	GLN
1	A	560	GLN
1	A	567	ASN
2	B	56	ASN
2	B	62	ASN
2	B	80	GLN
2	B	152	ASN
2	B	205	ASN
2	B	212	ASN
2	B	228	ASN
2	B	252	ASN
2	B	307	ASN
2	B	311	GLN
2	B	329	ASN
2	B	348	GLN
2	B	350	ASN
2	B	400	GLN
2	B	435	ASN
3	M	64	ASN
3	M	169	ASN
3	M	180	ASN
3	M	249	ASN
3	M	270	ASN
3	M	318	ASN
3	M	338	ASN
3	M	359	HIS
3	M	391	GLN
4	S	76	ASN
4	S	85	HIS
4	S	97	ASN

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Mol	Chain	Res	Type
4	S	142	GLN
5	C	83	GLN
5	C	95	ASN
5	C	128	GLN
5	C	132	ASN
5	C	156	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	GTP	C	1001	7	26,34,34	0.96	2 (7%)	32,54,54	1.20	4 (12%)

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
6	GTP	C	1001	7	-	1/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1001	GTP	C5-C6	-2.50	1.42	1.47
6	C	1001	GTP	C2-N3	2.30	1.38	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1001	GTP	C8-N7-C5	3.17	109.03	102.99
6	C	1001	GTP	C5-C6-N1	2.53	118.41	113.95
6	C	1001	GTP	O6-C6-N1	-2.12	118.15	120.65
6	C	1001	GTP	N1-C2-N3	-2.01	119.57	123.32

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1001	GTP	PA-O3A-PB-O2B

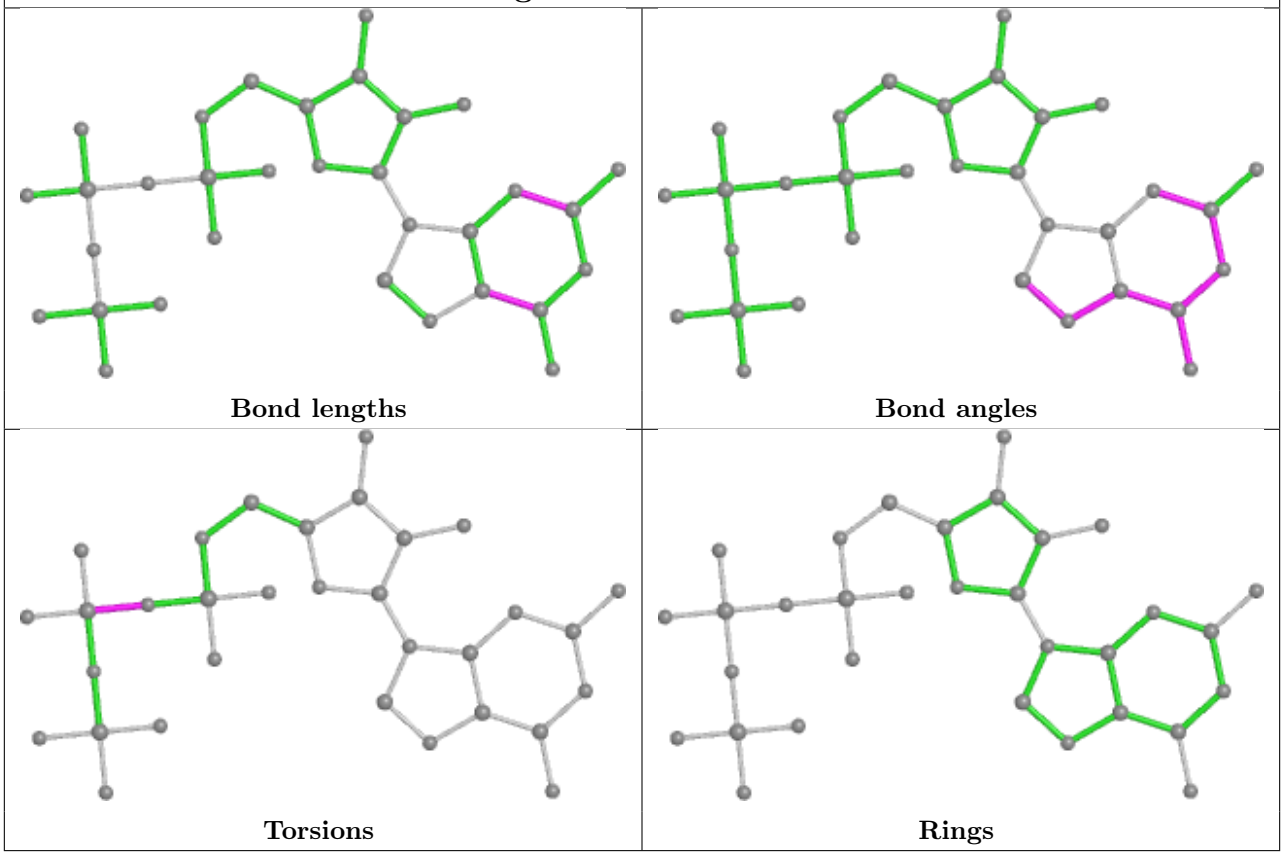
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1001	GTP	3	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 C 1001



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

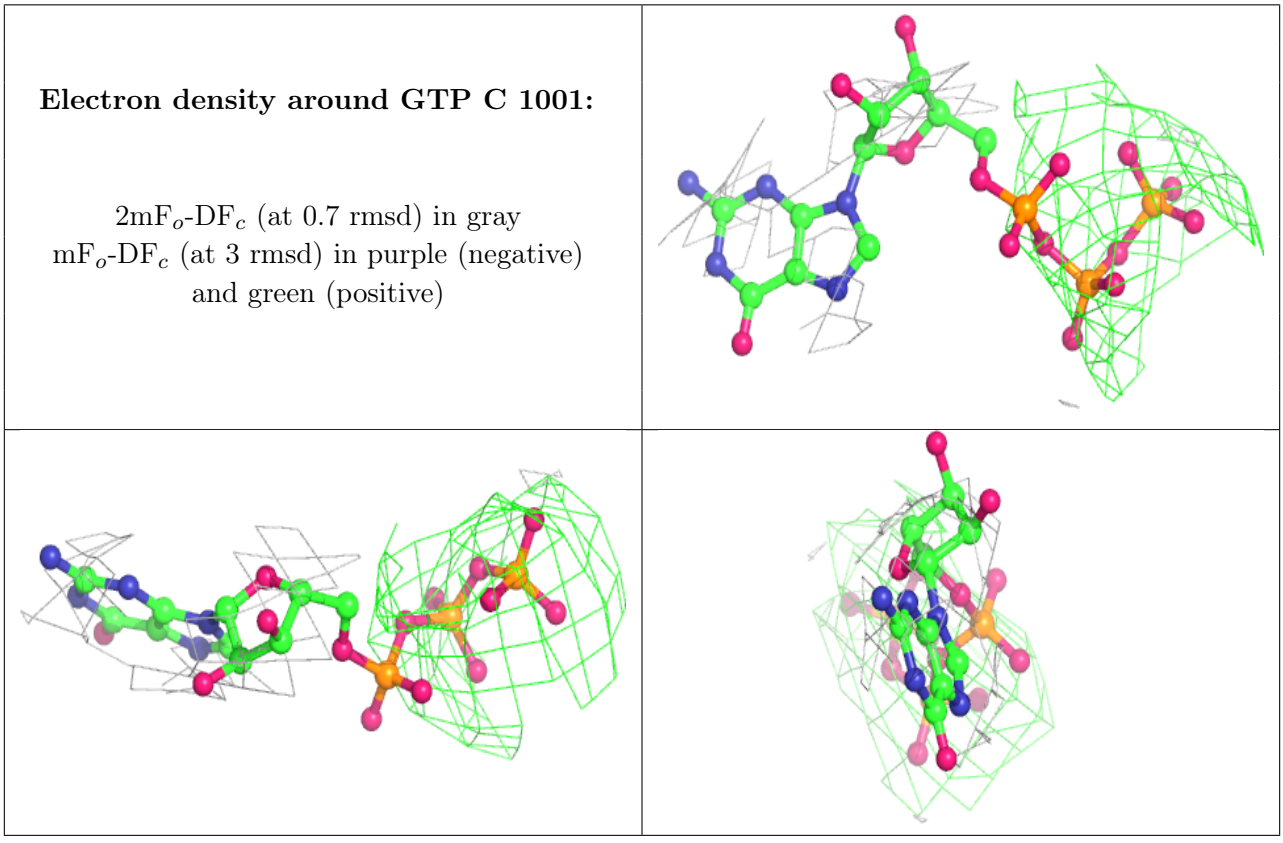
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GTP C 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.