



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:47 PM BST

PDB ID : 3J6P  
EMDB ID: : EMD-5931  
Title : Pseudo-atomic model of dynein microtubule binding domain-tubulin complex based on a cryoEM map  
Authors : Uchimura, S.; Fujii, T.; Takazaki, H.; Ayukawa, R.; Nishikawa, Y.; Minoura, I.; Hachikubo, Y.; Kurisu, G.; Sutoh, K.; Kon, T.; Namba, K.; Muto, E.  
Deposited on : 2014-03-20  
Resolution : 8.20 Å (reported)  
Based on PDB ID : 3VKH, 1JFF

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

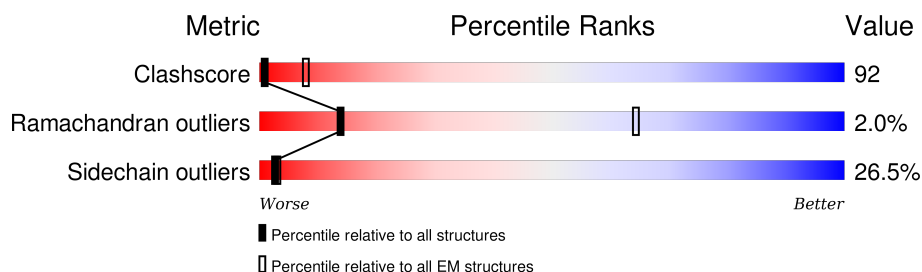
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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

Mol	Chain	Length	Quality of chain
1	D	108	<div> <div>21%</div> <div>60%</div> <div>19%</div> </div>
2	A	451	<div> <div>21%</div> <div>51%</div> <div>19%</div> <div>• 9%</div> </div>
3	B	445	<div> <div>14%</div> <div>62%</div> <div>18%</div> <div>• •</div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7563 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	108	Total	C	N	O	S	0	0
			862	557	141	157	7		

- Molecule 2 is a protein called Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLY	ALA	CONFLICT	UNP P02550

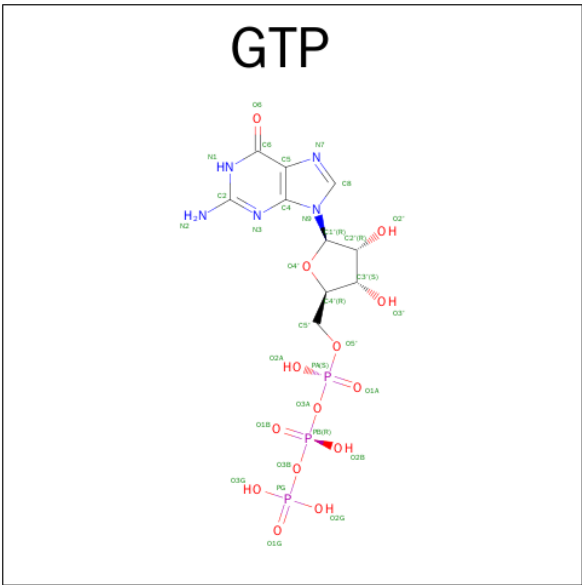
- Molecule 3 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

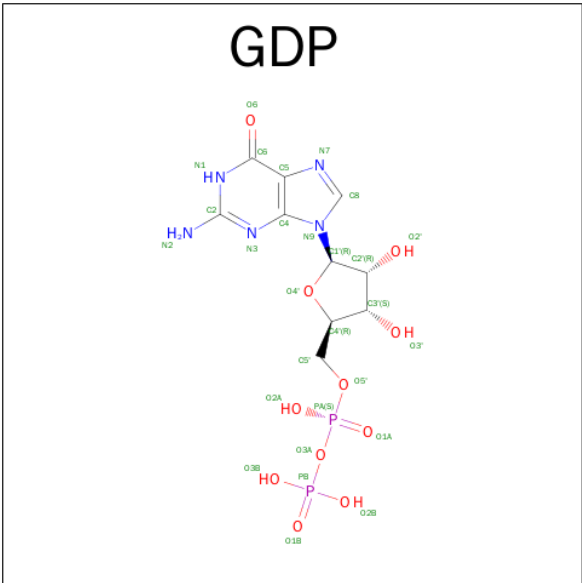
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



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

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



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

- Molecule 7 is TAXOL (three-letter code: TA1) (formula:  $C_{47}H_{51}NO_{14}$ ).

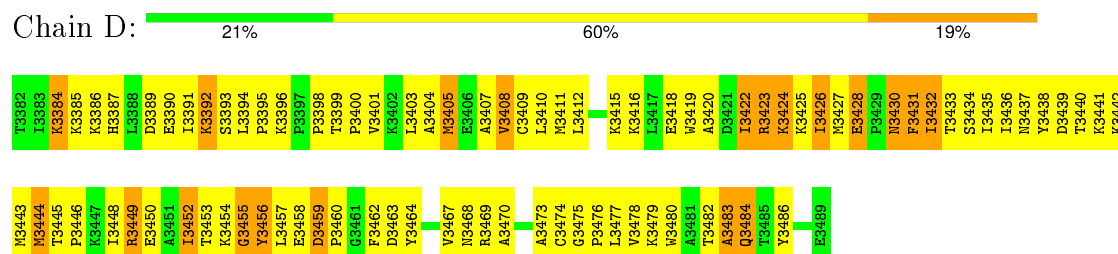


Total	C	N	O
62	47	1	14

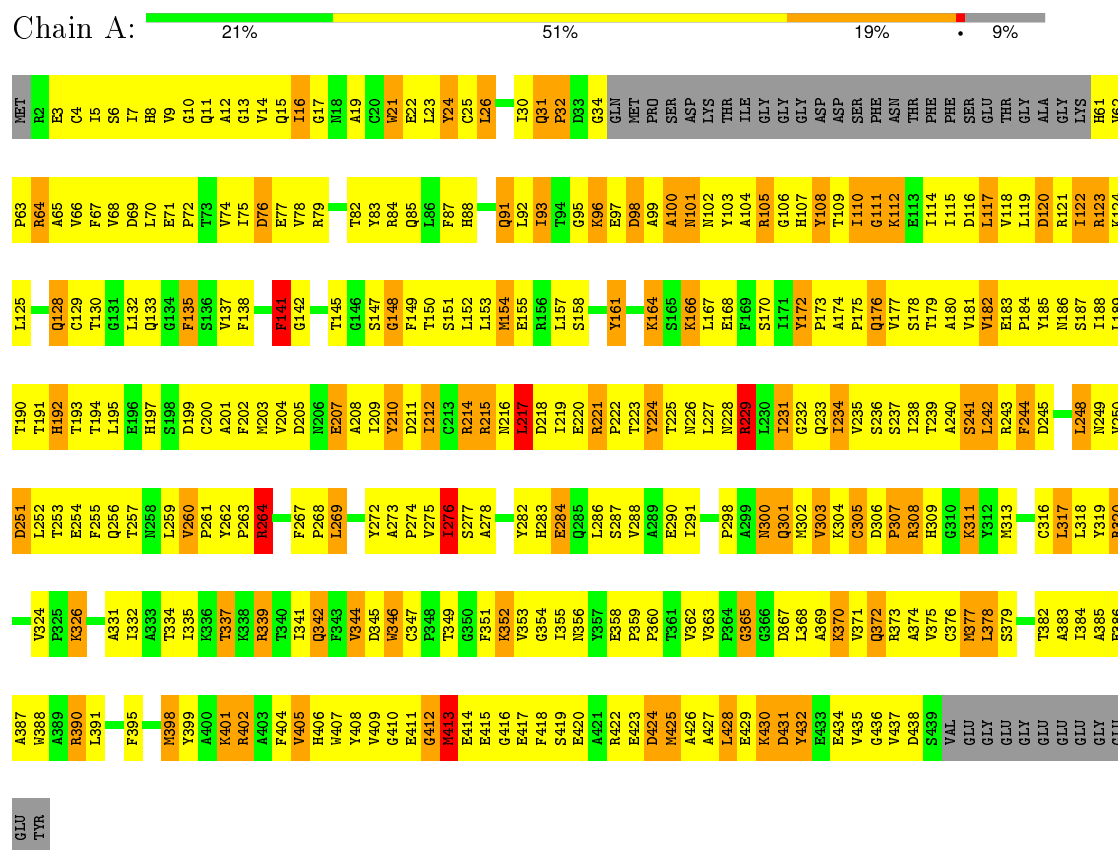
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Dynein heavy chain, cytoplasmic



- Molecule 2: Tubulin alpha-1A chain



- Molecule 3: Tubulin beta chain



## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTFFIND3 Each particle	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	60000	Depositor
Image detector	TemCam-F415MP	Depositor



## 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: GDP, GTP, MG, TA1

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	D	0.97	0/881	1.10	0/1186
2	A	0.99	1/3300 (0.0%)	1.14	5/4482 (0.1%)
3	B	0.99	0/3426	1.13	5/4642 (0.1%)
All	All	0.99	1/7607 (0.0%)	1.13	10/10310 (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	D	0	1
2	A	0	12
3	B	0	10
All	All	0	23

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	30	ILE	C-N	8.22	1.52	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	161	TYR	CA-CB-CG	-6.75	100.57	113.40
2	A	30	ILE	O-C-N	-6.64	112.07	122.70
3	B	283	TYR	CA-CB-CG	-6.38	101.28	113.40
2	A	217	LEU	N-CA-CB	5.65	121.70	110.40
3	B	404	PHE	CA-CB-CG	-5.56	100.55	113.90
2	A	365	GLY	C-N-CA	-5.55	110.64	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	229	ARG	NE-CZ-NH1	5.22	122.91	120.30
3	B	373	MET	CG-SD-CE	-5.22	91.85	100.20
3	B	52	TYR	CA-CB-CG	-5.20	103.53	113.40
3	B	28	HIS	CA-CB-CG	-5.07	104.99	113.60

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	110	ILE	Peptide
2	A	141	PHE	Peptide
2	A	176	GLN	Peptide
2	A	182	VAL	Peptide
2	A	221	ARG	Peptide
2	A	229	ARG	Sidechain
2	A	264	ARG	Peptide
2	A	283	HIS	Peptide
2	A	309	HIS	Peptide
2	A	365	GLY	Peptide
2	A	415	GLU	Peptide
2	A	64	ARG	Peptide
3	B	12	CYS	Peptide
3	B	141	LEU	Peptide
3	B	182	VAL	Peptide
3	B	277	SER	Peptide
3	B	286	LEU	Peptide
3	B	287	THR	Peptide
3	B	288	VAL	Peptide
3	B	33	THR	Peptide
3	B	379	GLY	Peptide
3	B	83	PHE	Peptide
1	D	3455	GLY	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	862	0	902	206	0
2	A	3227	0	3143	596	0
3	B	3351	0	3229	648	0
4	A	1	0	0	0	0
5	A	32	0	12	3	0
6	B	28	0	12	1	0
7	B	62	0	51	8	0
All	All	7563	0	7349	1375	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 92.

All (1375) 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:B:191:VAL:HA	3:B:194:LEU:HD12	1.21	1.17
3:B:250:ALA:HA	3:B:254:LYS:HE2	1.21	1.16
2:A:11:GLN:HG3	2:A:74:VAL:HG11	1.26	1.13
2:A:259:LEU:HD11	2:A:378:LEU:HD13	1.27	1.12
2:A:151:SER:HB3	2:A:193:THR:HG21	1.32	1.11
3:B:234:THR:HG21	3:B:270:PRO:HB3	1.21	1.10
2:A:316:CYS:HB2	2:A:378:LEU:HD11	1.27	1.08
2:A:71:GLU:HG3	3:B:2:ARG:HH21	1.15	1.08
2:A:303:VAL:HG13	2:A:305:CYS:H	1.18	1.08
1:D:3416:LYS:HG3	1:D:3418:GLU:H	1.14	1.08
3:B:57:ALA:HB2	3:B:60:LYS:HD2	1.30	1.08
1:D:3424:LYS:HB2	3:B:159:GLU:HB2	1.34	1.07
2:A:311:LYS:HG2	2:A:344:VAL:HG13	1.23	1.07
3:B:324:SER:HB3	3:B:327:GLU:HG2	1.08	1.06
2:A:119:LEU:HA	2:A:122:ILE:HD11	1.37	1.04
3:B:102:ASN:HB3	3:B:105:LYS:H	1.22	1.02
3:B:133:GLN:HE21	3:B:252:LEU:HB2	1.20	1.02
2:A:7:ILE:HG12	2:A:137:VAL:HG22	1.35	1.02
2:A:115:ILE:HD11	2:A:153:LEU:HD13	1.40	1.02
2:A:66:VAL:HG12	2:A:91:GLN:HG3	1.41	1.02
1:D:3387:HIS:HD2	1:D:3473:ALA:HB2	1.24	1.02
2:A:269:LEU:HD22	2:A:384:ILE:HD11	1.42	1.01
3:B:251:ASP:H	3:B:254:LYS:HG3	1.27	1.00
3:B:209:LEU:HB3	3:B:227:LEU:HD22	1.40	0.99
3:B:210:TYR:CE1	3:B:227:LEU:HD11	1.97	0.99
3:B:21:TRP:HA	3:B:24:ILE:HG22	1.42	0.98
2:A:286:LEU:HG	2:A:290:GLU:HB2	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:133:GLN:HG2	3:B:252:LEU:HD12	1.46	0.98
3:B:275:LEU:HD23	3:B:300:ASN:HD21	1.29	0.97
2:A:362:VAL:HG13	2:A:368:LEU:HB2	1.45	0.97
1:D:3390:GLU:HG3	2:A:402:ARG:HH22	1.29	0.97
2:A:102:ASN:HB2	2:A:408:TYR:CE1	2.00	0.96
2:A:219:ILE:HB	2:A:222:PRO:HG3	1.46	0.96
1:D:3424:LYS:HZ2	3:B:159:GLU:HB3	1.27	0.96
1:D:3464:TYR:CE1	1:D:3478:VAL:HG11	2.00	0.96
1:D:3416:LYS:HE2	1:D:3418:GLU:HB2	1.45	0.95
3:B:147:SER:HB3	3:B:190:SER:HB3	1.48	0.94
3:B:241:CYS:HB2	3:B:320:ARG:HE	1.31	0.94
1:D:3455:GLY:HA2	1:D:3458:GLU:H	1.32	0.94
2:A:69:ASP:HB2	2:A:75:ILE:HD11	1.50	0.94
3:B:319:PHE:CD2	3:B:375:ALA:HB2	2.03	0.94
2:A:26:LEU:HD21	2:A:363:VAL:HG13	1.49	0.93
1:D:3423:ARG:HH12	3:B:158:ARG:HD2	1.30	0.93
3:B:264:ARG:HB2	3:B:266:HIS:CD2	2.03	0.93
3:B:269:MET:SD	3:B:303:ALA:HB3	2.09	0.93
3:B:48:ARG:HG2	3:B:243:ARG:HB3	1.48	0.92
2:A:210:TYR:HE1	2:A:227:LEU:HD21	1.32	0.92
3:B:57:ALA:HB3	3:B:60:LYS:H	1.32	0.92
3:B:273:ALA:HB3	3:B:274:PRO:HD3	1.49	0.92
2:A:181:VAL:CG2	3:B:258:ASN:HB3	2.00	0.91
3:B:133:GLN:CG	3:B:252:LEU:HD12	1.99	0.91
2:A:316:CYS:HB2	2:A:378:LEU:CD1	2.00	0.91
3:B:140:SER:HB2	3:B:142:GLY:CA	2.00	0.91
3:B:27:GLU:OE1	7:B:502:TA1:H411	1.68	0.91
3:B:6:HIS:HB3	3:B:65:ALA:HB2	1.53	0.90
1:D:3387:HIS:CD2	1:D:3473:ALA:HB2	2.07	0.90
2:A:273:ALA:HB3	2:A:274:PRO:HD3	1.51	0.90
2:A:167:LEU:HD23	2:A:202:PHE:CE2	2.07	0.90
2:A:104:ALA:HB1	2:A:411:GLU:HB2	1.54	0.90
2:A:276:ILE:HG23	2:A:369:ALA:CB	2.01	0.90
1:D:3424:LYS:HE2	3:B:156:LYS:HD2	1.52	0.90
3:B:140:SER:HB2	3:B:142:GLY:HA3	1.53	0.90
2:A:31:GLN:HB3	2:A:32:PRO:HD2	1.51	0.90
2:A:179:THR:HG21	3:B:248:LEU:CD2	2.02	0.89
1:D:3431:PHE:CE1	1:D:3435:ILE:HD11	2.06	0.89
2:A:311:LYS:CG	2:A:344:VAL:HG13	2.03	0.89
1:D:3384:LYS:HD3	1:D:3386:LYS:HB2	1.54	0.89
1:D:3416:LYS:HG3	1:D:3418:GLU:N	1.88	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:132:LEU:HB3	3:B:164:ARG:HD3	1.54	0.89
3:B:241:CYS:HB2	3:B:320:ARG:NE	1.88	0.88
2:A:154:MET:HA	2:A:157:LEU:HD12	1.53	0.88
3:B:264:ARG:HB2	3:B:266:HIS:HD2	1.36	0.88
1:D:3457:LEU:HA	1:D:3462:PHE:HD2	1.39	0.88
1:D:3445:THR:HB	1:D:3446:PRO:HD3	1.54	0.88
1:D:3464:TYR:HB2	1:D:3478:VAL:HG21	1.54	0.88
2:A:110:ILE:HG23	2:A:111:GLY:H	1.39	0.87
2:A:422:ARG:HH12	2:A:426:ALA:HB2	1.39	0.87
3:B:75:MET:HE1	3:B:94:PHE:HB3	1.54	0.87
2:A:132:LEU:CD2	2:A:164:LYS:HE3	2.04	0.86
3:B:269:MET:HB2	3:B:301:MET:HE3	1.57	0.86
2:A:181:VAL:HG23	3:B:258:ASN:HB3	1.56	0.86
2:A:155:GLU:HG2	2:A:197:HIS:CE1	2.10	0.86
2:A:174:ALA:HB3	2:A:177:VAL:HB	1.55	0.86
2:A:362:VAL:CG1	2:A:368:LEU:HB2	2.06	0.86
1:D:3394:LEU:HB3	2:A:410:GLY:HA2	1.58	0.85
3:B:315:VAL:HG13	3:B:377:PHE:CE1	2.11	0.85
2:A:66:VAL:CG1	2:A:91:GLN:HG3	2.05	0.85
3:B:323:MET:HE3	3:B:373:MET:SD	2.16	0.85
1:D:3394:LEU:CB	2:A:410:GLY:HA2	2.07	0.85
2:A:119:LEU:O	2:A:122:ILE:HG12	1.76	0.85
2:A:229:ARG:HG2	2:A:229:ARG:HH11	1.40	0.85
2:A:115:ILE:HD13	2:A:152:LEU:HD11	1.58	0.85
3:B:301:MET:HE1	3:B:377:PHE:HE2	1.41	0.85
3:B:285:ALA:HB1	3:B:290:GLU:HG2	1.59	0.84
1:D:3464:TYR:CB	1:D:3478:VAL:HG21	2.07	0.84
3:B:105:LYS:HG3	3:B:110:GLU:HG2	1.58	0.84
1:D:3475:GLY:O	1:D:3478:VAL:HG12	1.76	0.84
3:B:256:ALA:O	3:B:260:VAL:HG22	1.76	0.84
2:A:317:LEU:HG	2:A:377:MET:HB2	1.58	0.84
3:B:319:PHE:HA	3:B:375:ALA:HA	1.57	0.84
3:B:189:LEU:HD23	3:B:421:ALA:CB	2.08	0.84
3:B:8:GLN:OE1	3:B:67:LEU:HD22	1.78	0.83
3:B:6:HIS:HB3	3:B:65:ALA:CB	2.08	0.83
2:A:274:PRO:HG2	2:A:374:ALA:CB	2.06	0.83
3:B:332:MET:HE3	3:B:351:VAL:HG11	1.57	0.83
1:D:3424:LYS:NZ	3:B:156:LYS:HA	1.93	0.83
2:A:112:LYS:O	2:A:115:ILE:HG22	1.78	0.83
2:A:174:ALA:HB1	2:A:207:GLU:HG2	1.60	0.83
3:B:105:LYS:CG	3:B:110:GLU:HG2	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:168:THR:HB	3:B:201:THR:HG23	1.60	0.83
2:A:311:LYS:HG2	2:A:344:VAL:CG1	2.08	0.83
2:A:151:SER:HB3	2:A:193:THR:CG2	2.08	0.83
2:A:71:GLU:HG3	3:B:2:ARG:NH2	1.93	0.83
3:B:243:ARG:HH22	3:B:252:LEU:HG	1.43	0.83
2:A:276:ILE:O	2:A:369:ALA:HB2	1.79	0.83
2:A:68:VAL:HG13	2:A:93:ILE:CG2	2.09	0.83
3:B:30:ILE:HD12	3:B:53:TYR:CE2	2.14	0.83
2:A:223:THR:HG22	2:A:224:TYR:H	1.44	0.82
3:B:133:GLN:NE2	3:B:252:LEU:HB2	1.94	0.82
3:B:75:MET:CE	3:B:94:PHE:HB3	2.09	0.82
2:A:305:CYS:SG	2:A:384:ILE:HD13	2.18	0.82
2:A:115:ILE:CD1	2:A:153:LEU:HD13	2.08	0.82
2:A:242:LEU:HG	2:A:250:VAL:O	1.78	0.82
3:B:275:LEU:HD23	3:B:300:ASN:ND2	1.93	0.82
3:B:188:THR:HG23	3:B:425:MET:HE2	1.60	0.82
1:D:3464:TYR:CG	1:D:3478:VAL:HG21	2.15	0.81
3:B:274:PRO:O	3:B:275:LEU:HD13	1.80	0.81
3:B:172:VAL:HG11	3:B:387:LEU:CD2	2.09	0.81
2:A:225:THR:O	2:A:229:ARG:HG3	1.80	0.81
2:A:276:ILE:HG23	2:A:369:ALA:HB2	1.61	0.81
1:D:3482:THR:HG23	1:D:3486:TYR:CD2	2.16	0.81
2:A:301:GLN:HE22	2:A:307:PRO:HD3	1.43	0.81
3:B:189:LEU:HD23	3:B:421:ALA:HB3	1.62	0.81
3:B:103:TRP:HD1	3:B:147:SER:HB2	1.43	0.81
2:A:22:GLU:HG2	2:A:83:TYR:CE1	2.15	0.81
3:B:155:SER:HA	3:B:197:ASN:HD21	1.46	0.81
2:A:107:HIS:HB2	2:A:148:GLY:HA2	1.62	0.80
2:A:362:VAL:HG21	2:A:370:LYS:N	1.97	0.80
3:B:70:LEU:H	3:B:145:THR:HG21	1.46	0.80
1:D:3464:TYR:CD1	1:D:3478:VAL:HG11	2.15	0.80
2:A:119:LEU:HA	2:A:122:ILE:CD1	2.11	0.80
1:D:3432:ILE:HD13	1:D:3433:THR:H	1.46	0.80
2:A:66:VAL:HA	2:A:91:GLN:HG2	1.62	0.80
3:B:234:THR:CG2	3:B:270:PRO:HB3	2.10	0.80
3:B:149:MET:O	3:B:153:LEU:HD22	1.83	0.79
2:A:223:THR:HB	2:A:225:THR:HG22	1.63	0.79
2:A:286:LEU:HG	2:A:290:GLU:CB	2.12	0.79
1:D:3455:GLY:HA2	1:D:3457:LEU:HG	1.64	0.79
1:D:3433:THR:O	1:D:3436:ILE:HG12	1.83	0.79
2:A:132:LEU:HD21	2:A:164:LYS:HE3	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4:ILE:HD11	3:B:252:LEU:CD1	2.11	0.79
2:A:301:GLN:HB2	2:A:303:VAL:H	1.48	0.79
1:D:3464:TYR:CD1	1:D:3478:VAL:HG21	2.18	0.79
1:D:3394:LEU:HD22	2:A:410:GLY:CA	2.13	0.78
2:A:431:ASP:O	2:A:435:VAL:HG23	1.82	0.78
1:D:3428:GLU:HG2	1:D:3431:PHE:H	1.47	0.78
3:B:148:GLY:O	3:B:151:THR:HG22	1.83	0.78
1:D:3424:LYS:HZ1	3:B:156:LYS:HA	1.48	0.78
3:B:31:ASP:O	3:B:34:GLY:HA3	1.83	0.78
2:A:188:ILE:HG23	2:A:425:MET:SD	2.23	0.78
1:D:3457:LEU:HA	1:D:3462:PHE:CD2	2.17	0.78
2:A:211:ASP:O	2:A:215:ARG:HG2	1.84	0.78
3:B:210:TYR:HE1	3:B:227:LEU:HD11	1.45	0.77
2:A:151:SER:CB	2:A:193:THR:HG21	2.11	0.77
2:A:103:TYR:HD2	2:A:413:MET:HE2	1.50	0.77
3:B:150:GLY:HA2	3:B:153:LEU:CD2	2.15	0.77
3:B:250:ALA:HB1	3:B:254:LYS:HB2	1.67	0.77
3:B:324:SER:HB3	3:B:327:GLU:CG	2.03	0.77
3:B:286:LEU:HD22	3:B:291:LEU:HD11	1.65	0.77
3:B:189:LEU:O	3:B:192:HIS:HB3	1.85	0.77
3:B:115:VAL:HG13	3:B:153:LEU:CD1	2.15	0.77
3:B:184:PRO:HG3	3:B:394:GLN:CB	2.14	0.77
2:A:303:VAL:HG13	2:A:305:CYS:N	1.97	0.76
3:B:250:ALA:CA	3:B:254:LYS:HE2	2.11	0.76
2:A:72:PRO:HG3	2:A:96:LYS:HA	1.67	0.76
2:A:104:ALA:CB	2:A:411:GLU:HB2	2.15	0.76
3:B:30:ILE:HG22	3:B:31:ASP:O	1.86	0.76
2:A:205:ASP:HB3	2:A:208:ALA:CB	2.15	0.76
2:A:199:ASP:HB3	2:A:256:GLN:NE2	2.01	0.76
3:B:242:LEU:HD22	3:B:250:ALA:O	1.86	0.75
2:A:74:VAL:O	2:A:77:GLU:HB2	1.86	0.75
3:B:323:MET:HG3	3:B:328:VAL:CG2	2.17	0.75
2:A:183:GLU:HB3	2:A:184:PRO:HD3	1.68	0.75
2:A:362:VAL:HG21	2:A:370:LYS:H	1.52	0.75
3:B:204:ILE:HG21	3:B:209:LEU:HD21	1.69	0.75
2:A:199:ASP:HB3	2:A:256:GLN:HE21	1.51	0.75
3:B:21:TRP:HA	3:B:24:ILE:CG2	2.17	0.75
3:B:243:ARG:NH2	3:B:252:LEU:HG	2.00	0.75
2:A:422:ARG:NH1	2:A:426:ALA:HB2	2.01	0.75
3:B:151:THR:O	3:B:154:ILE:HG13	1.86	0.75
3:B:286:LEU:HD13	3:B:373:MET:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:323:MET:HG3	3:B:328:VAL:HG21	1.68	0.75
2:A:69:ASP:HB3	2:A:75:ILE:CG1	2.17	0.75
3:B:237:GLY:O	3:B:241:CYS:HB3	1.87	0.74
3:B:324:SER:O	3:B:328:VAL:HG23	1.86	0.74
3:B:371:LEU:HG	3:B:372:LYS:N	2.00	0.74
3:B:57:ALA:HB2	3:B:60:LYS:CD	2.14	0.74
1:D:3455:GLY:CA	1:D:3458:GLU:H	2.00	0.74
3:B:19:LYS:O	3:B:22:GLU:HB2	1.86	0.74
3:B:172:VAL:HG11	3:B:387:LEU:HD23	1.67	0.74
3:B:201:THR:OG1	3:B:265:LEU:HD11	1.87	0.74
3:B:119:LEU:HA	3:B:122:VAL:CG1	2.16	0.74
2:A:7:ILE:CG1	2:A:137:VAL:HG22	2.15	0.74
3:B:103:TRP:CD1	3:B:147:SER:HB2	2.22	0.74
1:D:3459:ASP:HB2	1:D:3462:PHE:HB3	1.67	0.74
3:B:10:GLY:O	3:B:13:GLY:HA3	1.87	0.74
2:A:9:VAL:HG11	2:A:150:THR:OG1	1.87	0.74
2:A:177:VAL:HG21	2:A:207:GLU:HB3	1.69	0.74
2:A:210:TYR:CE1	2:A:227:LEU:HD21	2.20	0.74
3:B:318:VAL:HA	3:B:354:ALA:HB3	1.68	0.74
2:A:7:ILE:CG1	2:A:137:VAL:HG13	2.18	0.74
1:D:3405:MET:HA	1:D:3408:VAL:CG2	2.17	0.74
1:D:3404:ALA:O	1:D:3408:VAL:HG22	1.88	0.74
3:B:234:THR:HG23	3:B:376:THR:CG2	2.18	0.74
3:B:230:LEU:HD21	3:B:302:MET:CE	2.17	0.74
3:B:310:GLY:O	3:B:342:TYR:HB3	1.88	0.74
2:A:274:PRO:O	2:A:276:ILE:HG22	1.87	0.74
2:A:31:GLN:HB3	2:A:32:PRO:CD	2.18	0.74
1:D:3444:MET:HG2	1:D:3446:PRO:HD2	1.69	0.74
3:B:192:HIS:O	3:B:195:VAL:HG12	1.88	0.73
3:B:54:ASN:HD21	3:B:64:ARG:HB2	1.53	0.73
2:A:155:GLU:HA	2:A:197:HIS:ND1	2.02	0.73
2:A:252:LEU:O	2:A:255:PHE:HB2	1.88	0.73
3:B:275:LEU:HB2	3:B:294:GLN:OE1	1.88	0.73
3:B:234:THR:HG23	3:B:376:THR:HG22	1.68	0.73
1:D:3424:LYS:HE2	3:B:156:LYS:CD	2.17	0.73
3:B:259:MET:O	3:B:261:PRO:HD3	1.89	0.73
2:A:241:SER:O	2:A:244:PHE:HB3	1.88	0.73
2:A:402:ARG:HE	2:A:405:VAL:HG12	1.52	0.73
3:B:270:PRO:O	3:B:302:MET:HG3	1.88	0.73
2:A:7:ILE:HG13	2:A:137:VAL:HG13	1.71	0.73
3:B:315:VAL:HG13	3:B:377:PHE:HE1	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:184:PRO:HG3	3:B:394:GLN:HB3	1.69	0.73
3:B:154:ILE:HG22	3:B:166:MET:SD	2.28	0.73
3:B:219:LEU:HD21	3:B:226:ASP:OD2	1.89	0.73
3:B:141:LEU:HB3	3:B:187:ALA:HA	1.71	0.73
3:B:21:TRP:CZ3	3:B:63:PRO:HB3	2.23	0.73
2:A:133:GLN:HB2	2:A:243:ARG:HH12	1.52	0.72
1:D:3408:VAL:HA	1:D:3411:MET:HE2	1.71	0.72
3:B:100:GLY:HA3	3:B:105:LYS:HE2	1.70	0.72
3:B:169:PHE:CZ	3:B:235:MET:HB3	2.24	0.72
2:A:255:PHE:O	2:A:259:LEU:HB2	1.88	0.72
3:B:35:SER:HB3	3:B:59:ASN:OD1	1.88	0.72
2:A:362:VAL:HG21	2:A:370:LYS:CA	2.20	0.72
3:B:67:LEU:HD12	3:B:92:PHE:CD1	2.24	0.72
2:A:105:ARG:HG2	2:A:411:GLU:HG3	1.70	0.72
3:B:273:ALA:CB	3:B:375:ALA:H	2.02	0.72
3:B:199:ASP:O	3:B:265:LEU:HB2	1.89	0.72
3:B:286:LEU:HD11	3:B:371:LEU:HD21	1.72	0.72
3:B:396:THR:HG23	3:B:422:GLU:OE2	1.90	0.72
3:B:413:MET:HG2	3:B:418:PHE:HE1	1.55	0.72
3:B:304:ALA:HB3	3:B:387:LEU:CD1	2.20	0.72
3:B:93:VAL:HG11	3:B:118:VAL:HG22	1.70	0.72
3:B:57:ALA:CB	3:B:60:LYS:HD2	2.16	0.72
2:A:69:ASP:HB3	2:A:75:ILE:HG12	1.72	0.71
2:A:214:ARG:O	2:A:218:ASP:HA	1.89	0.71
2:A:242:LEU:HD21	2:A:250:VAL:HB	1.71	0.71
3:B:191:VAL:HA	3:B:194:LEU:CD1	2.12	0.71
3:B:286:LEU:O	3:B:291:LEU:HD13	1.90	0.71
3:B:175:PRO:HD2	3:B:207:GLU:OE2	1.90	0.71
2:A:175:PRO:HD2	2:A:207:GLU:HG2	1.73	0.71
2:A:179:THR:HG21	3:B:248:LEU:HD22	1.71	0.71
3:B:7:ILE:HB	3:B:137:LEU:CD1	2.20	0.71
1:D:3444:MET:O	1:D:3448:ILE:HB	1.90	0.71
3:B:102:ASN:ND2	3:B:408:TYR:HA	2.06	0.71
1:D:3433:THR:HA	1:D:3436:ILE:HD13	1.73	0.71
2:A:174:ALA:CB	2:A:177:VAL:HB	2.20	0.71
2:A:385:ALA:HB2	2:A:432:TYR:HB3	1.72	0.71
2:A:166:LYS:HE3	2:A:197:HIS:O	1.91	0.70
2:A:274:PRO:HG2	2:A:374:ALA:HB1	1.73	0.70
1:D:3449:ARG:O	1:D:3453:THR:HG23	1.90	0.70
2:A:133:GLN:CB	2:A:243:ARG:HH12	2.04	0.70
3:B:332:MET:HE3	3:B:351:VAL:CG1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:250:ALA:HA	3:B:254:LYS:CE	2.12	0.70
3:B:274:PRO:CG	3:B:374:SER:HB3	2.22	0.70
3:B:48:ARG:CG	3:B:243:ARG:HB3	2.21	0.70
2:A:19:ALA:HB2	2:A:228:ASN:HB3	1.73	0.70
3:B:119:LEU:HD11	3:B:156:LYS:CG	2.21	0.70
3:B:149:MET:C	3:B:153:LEU:HD22	2.12	0.70
3:B:268:PHE:HB3	3:B:379:GLY:H	1.57	0.70
2:A:7:ILE:HG12	2:A:137:VAL:CG2	2.16	0.70
2:A:119:LEU:HD23	2:A:122:ILE:HD11	1.72	0.70
2:A:14:VAL:HG21	2:A:75:ILE:CD1	2.22	0.70
2:A:303:VAL:CG1	2:A:305:CYS:HB2	2.20	0.70
3:B:23:VAL:HG13	7:B:502:TA1:H321	1.73	0.70
3:B:6:HIS:HD1	3:B:21:TRP:HE1	1.39	0.70
2:A:405:VAL:O	2:A:409:VAL:HG23	1.92	0.69
3:B:119:LEU:HA	3:B:122:VAL:HG13	1.74	0.69
1:D:3439:ASP:HB3	1:D:3442:LYS:HG2	1.74	0.69
3:B:115:VAL:HG13	3:B:153:LEU:HD12	1.74	0.69
1:D:3468:ASN:OD1	1:D:3475:GLY:HA2	1.92	0.69
2:A:207:GLU:O	2:A:210:TYR:HB2	1.91	0.69
1:D:3424:LYS:CE	3:B:156:LYS:HD2	2.20	0.69
3:B:89:PRO:HA	3:B:92:PHE:CE2	2.26	0.69
1:D:3459:ASP:HB2	1:D:3462:PHE:CB	2.22	0.69
3:B:385:GLN:HG2	3:B:386:GLU:N	2.05	0.69
3:B:251:ASP:N	3:B:254:LYS:HG3	2.05	0.69
3:B:346:TRP:O	3:B:348:PRO:HD3	1.93	0.69
2:A:184:PRO:O	2:A:188:ILE:HG12	1.92	0.69
3:B:10:GLY:HA2	3:B:145:THR:HB	1.74	0.69
3:B:150:GLY:HA2	3:B:153:LEU:HD22	1.73	0.69
2:A:84:ARG:HG2	2:A:84:ARG:HH11	1.57	0.68
2:A:205:ASP:HB3	2:A:208:ALA:HB3	1.74	0.68
3:B:108:TYR:CE1	3:B:413:MET:HE1	2.27	0.68
3:B:140:SER:HB2	3:B:142:GLY:HA2	1.74	0.68
3:B:230:LEU:HD23	3:B:231:VAL:N	2.08	0.68
2:A:5:ILE:O	2:A:135:PHE:HA	1.93	0.68
2:A:201:ALA:O	2:A:268:PRO:HD2	1.94	0.68
1:D:3392:LYS:HE3	1:D:3423:ARG:NH2	2.09	0.68
3:B:8:GLN:CD	3:B:67:LEU:HD22	2.13	0.68
3:B:207:GLU:HG2	3:B:208:ALA:N	2.08	0.68
2:A:79:ARG:O	2:A:84:ARG:HG3	1.94	0.68
3:B:69:ASP:OD1	3:B:71:GLU:HB3	1.94	0.68
1:D:3390:GLU:CG	2:A:402:ARG:HH22	2.04	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:6:HIS:HB3	3:B:21:TRP:HZ2	1.59	0.68
2:A:167:LEU:HD23	2:A:202:PHE:HE2	1.57	0.68
2:A:188:ILE:HG13	2:A:395:PHE:CD2	2.29	0.68
3:B:4:ILE:HD11	3:B:252:LEU:HD11	1.74	0.68
3:B:24:ILE:HD11	3:B:52:TYR:CE2	2.28	0.68
2:A:371:VAL:HG12	2:A:373:ARG:H	1.59	0.67
2:A:242:LEU:HD23	2:A:255:PHE:HE1	1.58	0.67
2:A:66:VAL:HG12	2:A:91:GLN:CG	2.21	0.67
3:B:173:PRO:HB3	3:B:183:GLU:CG	2.24	0.67
2:A:301:GLN:NE2	2:A:307:PRO:HD3	2.08	0.67
2:A:188:ILE:HD12	2:A:425:MET:SD	2.34	0.67
1:D:3464:TYR:HB2	1:D:3478:VAL:CG2	2.23	0.67
2:A:250:VAL:HG21	2:A:318:LEU:HD21	1.76	0.67
2:A:105:ARG:HB2	2:A:110:ILE:HG22	1.77	0.67
3:B:289:PRO:HG3	3:B:331:GLN:OE1	1.95	0.67
3:B:371:LEU:HG	3:B:372:LYS:H	1.59	0.67
1:D:3473:ALA:O	1:D:3476:PRO:HD2	1.94	0.67
2:A:251:ASP:H	2:A:254:GLU:HG3	1.60	0.67
2:A:242:LEU:HD23	2:A:255:PHE:CE1	2.30	0.67
1:D:3424:LYS:HE2	3:B:156:LYS:CE	2.25	0.67
3:B:413:MET:HG3	3:B:414:ASP:N	2.08	0.66
3:B:155:SER:HA	3:B:197:ASN:ND2	2.10	0.66
3:B:36:TYR:OH	3:B:43:GLN:HB2	1.96	0.66
2:A:103:TYR:H	2:A:408:TYR:HE1	1.43	0.66
2:A:69:ASP:CB	2:A:75:ILE:HD11	2.23	0.66
2:A:172:TYR:HE2	2:A:388:TRP:CZ3	2.12	0.66
3:B:204:ILE:CG2	3:B:209:LEU:HD21	2.25	0.66
1:D:3457:LEU:HD12	1:D:3458:GLU:N	2.11	0.66
3:B:11:GLN:HG3	3:B:74:THR:CG2	2.25	0.66
2:A:11:GLN:O	2:A:14:VAL:HB	1.96	0.66
2:A:227:LEU:O	2:A:231:ILE:HG12	1.95	0.66
2:A:242:LEU:HD11	2:A:250:VAL:HG23	1.76	0.66
3:B:70:LEU:O	3:B:72:PRO:HD3	1.96	0.66
3:B:100:GLY:CA	3:B:105:LYS:HE2	2.26	0.66
3:B:21:TRP:CA	3:B:24:ILE:HG22	2.20	0.66
2:A:256:GLN:O	2:A:260:VAL:HG13	1.94	0.66
3:B:390:ARG:O	3:B:394:GLN:HG3	1.95	0.66
2:A:360:PRO:HG3	2:A:374:ALA:HB3	1.78	0.66
2:A:62:VAL:HG13	2:A:63:PRO:HD2	1.78	0.65
3:B:264:ARG:O	3:B:265:LEU:HD23	1.96	0.65
2:A:98:ASP:O	2:A:110:ILE:HD13	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:68:VAL:HA	2:A:93:ILE:HG22	1.78	0.65
3:B:71:GLU:HG2	3:B:74:THR:H	1.62	0.65
3:B:31:ASP:HB2	3:B:34:GLY:HA2	1.78	0.65
2:A:217:LEU:H	2:A:217:LEU:HD23	1.60	0.65
3:B:336:GLN:HE22	3:B:350:ASN:H	1.43	0.65
2:A:101:ASN:ND2	3:B:254:LYS:HD2	2.10	0.65
3:B:173:PRO:HD2	3:B:391:ILE:HD11	1.78	0.65
3:B:339:ASN:HB3	3:B:342:TYR:CE1	2.31	0.65
3:B:140:SER:C	3:B:142:GLY:HA3	2.17	0.65
3:B:132:LEU:O	3:B:164:ARG:HG2	1.96	0.65
3:B:209:LEU:CD1	3:B:230:LEU:HD21	2.25	0.65
3:B:259:MET:HA	3:B:314:THR:HG21	1.79	0.65
1:D:3430:ASN:O	1:D:3434:SER:HB2	1.97	0.65
1:D:3399:THR:OG1	1:D:3400:PRO:HD3	1.95	0.65
2:A:242:LEU:HD21	2:A:318:LEU:HD21	1.79	0.65
3:B:272:PHE:CE2	3:B:274:PRO:HD2	2.32	0.65
3:B:119:LEU:HD11	3:B:156:LYS:HG2	1.77	0.65
2:A:132:LEU:O	2:A:132:LEU:HG	1.97	0.65
2:A:384:ILE:HG22	2:A:388:TRP:CD1	2.31	0.65
3:B:202:TYR:HE2	3:B:378:ILE:HG21	1.61	0.65
2:A:405:VAL:HG13	2:A:409:VAL:CG2	2.27	0.65
3:B:282:GLN:O	3:B:282:GLN:HG2	1.96	0.65
3:B:172:VAL:HG11	3:B:387:LEU:HD21	1.77	0.65
1:D:3392:LYS:HE2	1:D:3393:SER:HA	1.79	0.65
2:A:242:LEU:CD1	2:A:318:LEU:HD22	2.27	0.64
3:B:151:THR:HA	3:B:154:ILE:HD11	1.79	0.64
2:A:82:THR:HG22	2:A:83:TYR:CD1	2.32	0.64
3:B:241:CYS:O	3:B:244:PHE:HB2	1.96	0.64
3:B:325:MET:CE	3:B:355:VAL:HG21	2.27	0.64
3:B:6:HIS:CE1	3:B:8:GLN:HG2	2.32	0.64
2:A:176:GLN:OE1	3:B:333:LEU:HD11	1.96	0.64
2:A:104:ALA:CB	2:A:413:MET:HG2	2.28	0.64
2:A:154:MET:HE1	2:A:166:LYS:HD2	1.79	0.64
3:B:325:MET:HE3	3:B:355:VAL:HG21	1.79	0.64
1:D:3455:GLY:HA3	1:D:3458:GLU:CG	2.27	0.64
1:D:3398:PRO:HB2	1:D:3401:VAL:HG23	1.78	0.64
3:B:110:GLU:HA	3:B:110:GLU:OE1	1.98	0.64
3:B:319:PHE:CG	3:B:375:ALA:HB2	2.31	0.64
2:A:203:MET:HG3	2:A:267:PHE:HB3	1.77	0.64
2:A:185:TYR:OH	2:A:399:TYR:HA	1.98	0.64
2:A:416:GLY:O	2:A:420:GLU:HG2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3419:TRP:CE3	1:D:3422:ILE:HG12	2.33	0.64
3:B:264:ARG:HH11	3:B:264:ARG:HG3	1.62	0.64
3:B:320:ARG:HA	3:B:356:CYS:HB3	1.80	0.64
3:B:261:PRO:HB2	3:B:262:PHE:CD2	2.33	0.64
1:D:3423:ARG:NH2	3:B:162:PRO:HB3	2.12	0.64
2:A:248:LEU:HB2	2:A:355:ILE:H	1.61	0.64
2:A:386:GLU:HA	2:A:386:GLU:OE1	1.96	0.64
3:B:102:ASN:HD21	3:B:408:TYR:HA	1.62	0.64
3:B:173:PRO:HG2	3:B:391:ILE:HD13	1.78	0.64
3:B:188:THR:HG23	3:B:425:MET:CE	2.26	0.64
2:A:103:TYR:CD2	2:A:413:MET:HE2	2.33	0.64
2:A:109:THR:HG22	2:A:110:ILE:N	2.12	0.64
2:A:66:VAL:HG12	2:A:91:GLN:HA	1.79	0.64
3:B:106:GLY:O	3:B:111:GLY:HA3	1.97	0.64
2:A:311:LYS:H	2:A:382:THR:HB	1.63	0.64
2:A:362:VAL:HG21	2:A:370:LYS:HA	1.78	0.64
3:B:31:ASP:HB3	3:B:32:PRO:HD2	1.78	0.64
3:B:76:ASP:HA	3:B:79:ARG:HG3	1.80	0.64
2:A:167:LEU:HA	2:A:200:CYS:O	1.98	0.63
2:A:324:VAL:HG12	2:A:326:LYS:H	1.62	0.63
2:A:298:PRO:HA	2:A:301:GLN:OE1	1.99	0.63
3:B:7:ILE:HB	3:B:137:LEU:HD13	1.80	0.63
3:B:288:VAL:HG12	3:B:289:PRO:CD	2.28	0.63
2:A:106:GLY:O	2:A:111:GLY:HA2	1.99	0.63
2:A:238:ILE:HD12	2:A:255:PHE:CE2	2.32	0.63
1:D:3394:LEU:CG	2:A:410:GLY:HA2	2.29	0.63
1:D:3419:TRP:O	1:D:3422:ILE:HG13	1.98	0.63
2:A:278:ALA:HB2	2:A:367:ASP:O	1.99	0.63
1:D:3455:GLY:CA	1:D:3458:GLU:HG3	2.29	0.63
1:D:3455:GLY:HA3	1:D:3458:GLU:HG3	1.79	0.63
3:B:94:PHE:H	3:B:94:PHE:HD1	1.46	0.63
2:A:132:LEU:CG	2:A:164:LYS:HE3	2.28	0.63
3:B:328:VAL:O	3:B:332:MET:HG2	1.99	0.63
3:B:286:LEU:HD22	3:B:291:LEU:CD1	2.28	0.63
3:B:330:GLU:HG3	3:B:331:GLN:N	2.13	0.63
1:D:3416:LYS:CG	1:D:3418:GLU:H	2.03	0.63
3:B:89:PRO:HA	3:B:92:PHE:HE2	1.63	0.63
2:A:84:ARG:HG2	2:A:84:ARG:NH1	2.12	0.63
1:D:3469:ARG:HG3	1:D:3469:ARG:HH11	1.64	0.63
2:A:117:LEU:HD11	2:A:121:ARG:HH22	1.64	0.63
2:A:225:THR:HG23	2:A:226:ASN:HD22	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:198:THR:O	3:B:265:LEU:HD13	1.98	0.63
1:D:3436:ILE:HG13	1:D:3437:ASN:HD22	1.64	0.63
2:A:401:LYS:HE3	3:B:346:TRP:HB3	1.80	0.62
3:B:184:PRO:HG3	3:B:394:GLN:HB2	1.81	0.62
3:B:182:VAL:HB	3:B:186:ASN:HD21	1.64	0.62
7:B:502:TA1:H463	7:B:502:TA1:H261	1.80	0.62
2:A:317:LEU:HB3	2:A:319:TYR:HE1	1.64	0.62
3:B:220:THR:O	3:B:222:PRO:HD3	1.99	0.62
2:A:178:SER:HB2	2:A:183:GLU:OE2	1.98	0.62
3:B:67:LEU:HD23	3:B:67:LEU:N	2.12	0.62
2:A:179:THR:HG22	3:B:352:LYS:HE3	1.81	0.62
2:A:301:GLN:HB2	2:A:303:VAL:N	2.15	0.62
2:A:412:GLY:HA2	2:A:413:MET:O	2.00	0.62
2:A:68:VAL:HG13	2:A:93:ILE:HG22	1.81	0.62
1:D:3483:ALA:HB1	1:D:3484:GLN:NE2	2.15	0.62
2:A:303:VAL:HG11	2:A:305:CYS:HB2	1.81	0.62
2:A:320:ARG:HB2	2:A:358:GLU:O	1.99	0.62
2:A:363:VAL:H	2:A:368:LEU:HD12	1.65	0.62
2:A:179:THR:HG23	3:B:353:THR:HB	1.81	0.62
2:A:221:ARG:HG2	2:A:221:ARG:O	1.99	0.62
2:A:9:VAL:HG21	2:A:149:PHE:HD1	1.65	0.62
3:B:20:PHE:CZ	3:B:24:ILE:HD13	2.34	0.62
2:A:193:THR:HG23	2:A:194:THR:N	2.15	0.62
1:D:3424:LYS:HZ2	3:B:159:GLU:CB	2.09	0.62
2:A:275:VAL:HG11	2:A:300:ASN:HD21	1.64	0.62
1:D:3416:LYS:HE2	1:D:3418:GLU:CB	2.23	0.62
2:A:362:VAL:CG2	2:A:370:LYS:HA	2.28	0.62
3:B:55:GLU:HG2	3:B:61:TYR:CE1	2.35	0.62
2:A:118:VAL:O	2:A:122:ILE:HD13	2.00	0.61
2:A:132:LEU:HG	2:A:164:LYS:HE3	1.81	0.61
2:A:175:PRO:HG2	2:A:304:LYS:CD	2.29	0.61
3:B:157:ILE:HG21	3:B:166:MET:SD	2.39	0.61
3:B:283:TYR:O	3:B:284:ARG:HB2	2.00	0.61
3:B:150:GLY:HA2	3:B:153:LEU:HD23	1.82	0.61
3:B:288:VAL:HG12	3:B:289:PRO:N	2.15	0.61
1:D:3450:GLU:HA	1:D:3453:THR:OG1	2.01	0.61
2:A:107:HIS:HD2	2:A:108:TYR:CD1	2.17	0.61
2:A:250:VAL:CG2	2:A:318:LEU:HD21	2.31	0.61
2:A:408:TYR:CG	2:A:418:PHE:HZ	2.18	0.61
3:B:182:VAL:HG12	3:B:185:TYR:HB2	1.82	0.61
3:B:326:LYS:HE3	3:B:330:GLU:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:119:LEU:CA	3:B:122:VAL:HG13	2.31	0.61
3:B:312:TYR:HE2	3:B:377:PHE:HZ	1.49	0.61
3:B:408:TYR:CD2	3:B:418:PHE:HZ	2.18	0.61
3:B:278:ARG:HB3	3:B:279:GLY:CA	2.31	0.61
2:A:110:ILE:HG23	2:A:111:GLY:N	2.14	0.61
2:A:261:PRO:HB2	2:A:262:TYR:CD2	2.36	0.61
3:B:314:THR:H	3:B:380:ASN:HB3	1.66	0.61
3:B:388:PHE:HB2	3:B:429:VAL:HG22	1.83	0.61
3:B:172:VAL:HG23	3:B:203:CYS:HB3	1.81	0.61
3:B:372:LYS:HG3	3:B:373:MET:HB2	1.83	0.61
1:D:3384:LYS:HD3	1:D:3386:LYS:CB	2.28	0.61
2:A:68:VAL:HG13	2:A:93:ILE:HG21	1.83	0.61
1:D:3422:ILE:HG13	1:D:3423:ARG:N	2.15	0.61
3:B:209:LEU:HD11	3:B:302:MET:CE	2.31	0.61
1:D:3384:LYS:CD	1:D:3386:LYS:HB2	2.29	0.61
3:B:188:THR:HG21	3:B:422:GLU:HA	1.82	0.60
2:A:115:ILE:CD1	2:A:152:LEU:HD11	2.28	0.60
2:A:223:THR:HG22	2:A:224:TYR:N	2.14	0.60
2:A:244:PHE:HD1	2:A:245:ASP:N	1.99	0.60
2:A:269:LEU:CD2	2:A:384:ILE:HD11	2.26	0.60
3:B:172:VAL:CG1	3:B:173:PRO:HD2	2.31	0.60
2:A:419:SER:O	2:A:422:ARG:HB3	2.01	0.60
3:B:297:ASP:OD2	3:B:299:LYS:HE2	2.01	0.60
3:B:327:GLU:HA	3:B:330:GLU:HG2	1.83	0.60
2:A:205:ASP:HB3	2:A:208:ALA:HB2	1.81	0.60
2:A:316:CYS:CB	2:A:378:LEU:HD11	2.18	0.60
3:B:315:VAL:CG1	3:B:351:VAL:HG13	2.31	0.60
3:B:408:TYR:O	3:B:411:GLU:HB2	2.02	0.60
2:A:275:VAL:HG21	2:A:300:ASN:OD1	2.01	0.60
3:B:102:ASN:HB3	3:B:105:LYS:N	2.06	0.60
3:B:258:ASN:HD22	3:B:352:LYS:HG3	1.66	0.60
1:D:3418:GLU:O	1:D:3422:ILE:HG23	2.01	0.60
2:A:274:PRO:CG	2:A:374:ALA:HA	2.32	0.60
3:B:168:THR:CB	3:B:201:THR:HG23	2.30	0.60
1:D:3456:TYR:HA	1:D:3459:ASP:OD1	2.01	0.60
2:A:317:LEU:HB3	2:A:319:TYR:CE1	2.35	0.60
1:D:3436:ILE:HG13	1:D:3437:ASN:ND2	2.17	0.60
3:B:19:LYS:HG3	3:B:228:ASN:HB3	1.84	0.60
2:A:424:ASP:O	2:A:427:ALA:HB3	2.01	0.60
3:B:332:MET:CE	3:B:351:VAL:HG11	2.31	0.60
3:B:269:MET:HE3	3:B:301:MET:HG2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3384:LYS:HZ1	1:D:3386:LYS:HE3	1.67	0.60
2:A:175:PRO:HG2	2:A:304:LYS:CE	2.32	0.59
3:B:119:LEU:HD11	3:B:156:LYS:CB	2.32	0.59
2:A:119:LEU:O	2:A:123:ARG:HG2	2.03	0.59
2:A:303:VAL:HG13	2:A:305:CYS:HB2	1.84	0.59
3:B:107:HIS:CE1	3:B:152:LEU:HD13	2.37	0.59
3:B:133:GLN:HG3	3:B:252:LEU:HD12	1.81	0.59
2:A:228:ASN:HA	2:A:231:ILE:HG13	1.83	0.59
1:D:3394:LEU:HD13	2:A:409:VAL:C	2.21	0.59
3:B:314:THR:HG22	3:B:315:VAL:N	2.18	0.59
1:D:3456:TYR:O	1:D:3459:ASP:HB2	2.02	0.59
3:B:49:ILE:HG13	3:B:50:ASN:N	2.16	0.59
3:B:248:LEU:HD23	3:B:353:THR:O	2.02	0.59
1:D:3395:PRO:HD2	2:A:410:GLY:HA3	1.84	0.59
1:D:3423:ARG:CZ	3:B:162:PRO:HB3	2.32	0.59
2:A:239:THR:O	2:A:243:ARG:HG2	2.01	0.59
3:B:150:GLY:CA	3:B:153:LEU:HD22	2.33	0.59
3:B:167:ASN:HB3	3:B:202:TYR:HE1	1.67	0.59
3:B:255:LEU:O	3:B:259:MET:HG3	2.01	0.59
3:B:11:GLN:HG3	3:B:74:THR:HG21	1.84	0.59
3:B:107:HIS:HB3	3:B:108:TYR:CD1	2.36	0.59
3:B:173:PRO:HG2	3:B:391:ILE:CD1	2.32	0.59
3:B:273:ALA:CB	3:B:274:PRO:HD3	2.28	0.59
3:B:172:VAL:HB	3:B:205:ASP:OD1	2.02	0.59
3:B:209:LEU:HD11	3:B:230:LEU:HD21	1.85	0.59
3:B:198:THR:O	3:B:265:LEU:HD22	2.03	0.59
1:D:3405:MET:SD	1:D:3408:VAL:HG23	2.42	0.59
2:A:11:GLN:HG3	2:A:74:VAL:CG1	2.17	0.59
2:A:173:PRO:HG2	2:A:391:LEU:HD11	1.85	0.59
1:D:3424:LYS:CE	3:B:156:LYS:HA	2.32	0.59
1:D:3424:LYS:CB	3:B:159:GLU:HB2	2.22	0.59
3:B:139:HIS:HB2	3:B:146:GLY:O	2.03	0.59
3:B:209:LEU:HD11	3:B:302:MET:HE2	1.83	0.59
3:B:48:ARG:O	3:B:51:VAL:HG23	2.03	0.59
3:B:156:LYS:N	3:B:156:LYS:HD2	2.18	0.59
3:B:86:ILE:HG23	3:B:87:PHE:N	2.18	0.59
2:A:23:LEU:HD22	2:A:232:GLY:C	2.23	0.59
3:B:165:ILE:HG22	3:B:199:ASP:OD2	2.03	0.59
2:A:407:TRP:HE1	3:B:260:VAL:CG2	2.15	0.59
1:D:3419:TRP:CZ3	1:D:3422:ILE:HG12	2.37	0.59
2:A:231:ILE:HA	2:A:234:ILE:CG2	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:54:ASN:ND2	3:B:64:ARG:HB2	2.17	0.58
3:B:265:LEU:HG	3:B:266:HIS:N	2.15	0.58
3:B:273:ALA:HB1	3:B:291:LEU:HG	1.84	0.58
2:A:273:ALA:CB	2:A:274:PRO:HD3	2.24	0.58
2:A:120:ASP:O	2:A:124:LYS:HB2	2.03	0.58
2:A:179:THR:HG21	3:B:248:LEU:HD21	1.81	0.58
1:D:3390:GLU:CD	2:A:402:ARG:HH12	2.06	0.58
2:A:256:GLN:HG3	2:A:257:THR:N	2.18	0.58
3:B:185:TYR:OH	3:B:399:PHE:HA	2.04	0.58
3:B:266:HIS:HB3	3:B:432:TYR:OH	2.02	0.58
3:B:66:ILE:C	3:B:67:LEU:HD23	2.23	0.58
2:A:176:GLN:HB3	3:B:333:LEU:HD13	1.85	0.58
2:A:105:ARG:C	2:A:110:ILE:HG22	2.23	0.58
2:A:423:GLU:O	2:A:426:ALA:HB3	2.03	0.58
3:B:125:GLU:OE1	3:B:125:GLU:HA	2.04	0.58
2:A:9:VAL:HG22	2:A:10:GLY:N	2.19	0.58
2:A:209:ILE:HG12	2:A:302:MET:HG2	1.83	0.58
2:A:66:VAL:HA	2:A:91:GLN:CG	2.34	0.58
3:B:5:VAL:CG2	3:B:135:PHE:HD2	2.17	0.58
2:A:70:LEU:HD12	2:A:145:THR:OG1	2.03	0.58
2:A:166:LYS:HE2	2:A:199:ASP:OD1	2.03	0.58
3:B:185:TYR:HD1	3:B:395:PHE:CE1	2.22	0.58
2:A:167:LEU:HD23	2:A:202:PHE:CZ	2.38	0.58
1:D:3412:LEU:HD21	1:D:3435:ILE:CD1	2.33	0.58
2:A:413:MET:O	2:A:414:GLU:HG3	2.04	0.58
1:D:3455:GLY:HA3	1:D:3458:GLU:HB2	1.84	0.58
2:A:317:LEU:HD23	2:A:375:VAL:HG11	1.86	0.58
2:A:24:TYR:CE1	2:A:240:ALA:HB2	2.39	0.58
3:B:171:VAL:HA	3:B:204:ILE:O	2.04	0.58
2:A:274:PRO:HG2	2:A:374:ALA:CA	2.34	0.58
1:D:3469:ARG:HG3	1:D:3469:ARG:NH1	2.18	0.58
2:A:259:LEU:HD11	2:A:378:LEU:CD1	2.17	0.57
3:B:119:LEU:O	3:B:122:VAL:HG13	2.04	0.57
1:D:3464:TYR:HE1	1:D:3468:ASN:OD1	1.87	0.57
1:D:3405:MET:O	1:D:3408:VAL:HG23	2.03	0.57
2:A:231:ILE:O	2:A:234:ILE:HG23	2.04	0.57
3:B:119:LEU:C	3:B:122:VAL:HG13	2.25	0.57
1:D:3445:THR:O	1:D:3449:ARG:HB3	2.04	0.57
2:A:105:ARG:CB	2:A:110:ILE:HG22	2.34	0.57
2:A:401:LYS:HD3	3:B:346:TRP:CD2	2.39	0.57
3:B:135:PHE:HZ	3:B:161:TYR:CE1	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3392:LYS:HE3	3:B:158:ARG:HH12	1.69	0.57
1:D:3477:LEU:N	1:D:3477:LEU:HD12	2.19	0.57
3:B:273:ALA:HB2	3:B:375:ALA:H	1.68	0.57
1:D:3424:LYS:HE2	3:B:156:LYS:HE2	1.87	0.57
2:A:217:LEU:HG	2:A:219:ILE:CD1	2.34	0.57
2:A:168:GLU:HG3	2:A:201:ALA:CB	2.34	0.57
2:A:405:VAL:HG13	2:A:409:VAL:HG23	1.86	0.57
3:B:184:PRO:HD2	3:B:398:MET:HE1	1.85	0.57
3:B:359:PRO:HB2	3:B:371:LEU:O	2.05	0.57
3:B:55:GLU:HG2	3:B:61:TYR:HE1	1.70	0.57
3:B:107:HIS:HE1	3:B:152:LEU:HD13	1.68	0.57
2:A:220:GLU:OE1	2:A:220:GLU:HA	2.05	0.57
3:B:211:ASP:OD2	3:B:215:ARG:HD2	2.05	0.57
2:A:141:PHE:N	2:A:142:GLY:HA3	2.19	0.57
2:A:185:TYR:HD1	2:A:395:PHE:CE2	2.22	0.57
3:B:67:LEU:HD12	3:B:92:PHE:CE1	2.39	0.57
3:B:307:PRO:O	3:B:310:GLY:HA3	2.05	0.57
3:B:4:ILE:HD11	3:B:252:LEU:HD12	1.86	0.57
2:A:248:LEU:CB	2:A:355:ILE:H	2.18	0.57
3:B:272:PHE:HD2	3:B:274:PRO:O	1.87	0.57
1:D:3452:ILE:HG22	1:D:3453:THR:N	2.19	0.57
3:B:230:LEU:CD2	3:B:302:MET:HE1	2.35	0.56
3:B:21:TRP:CE3	3:B:24:ILE:HG21	2.40	0.56
2:A:371:VAL:HG12	2:A:372:GLN:N	2.20	0.56
2:A:331:ALA:O	2:A:335:ILE:HG12	2.04	0.56
2:A:229:ARG:HH11	2:A:229:ARG:CG	2.16	0.56
3:B:180:THR:HG22	3:B:182:VAL:H	1.69	0.56
3:B:260:VAL:HG23	3:B:260:VAL:O	2.04	0.56
1:D:3392:LYS:HE3	3:B:158:ARG:NH1	2.21	0.56
2:A:274:PRO:HG2	2:A:374:ALA:HA	1.87	0.56
3:B:299:LYS:N	3:B:299:LYS:HD3	2.20	0.56
3:B:272:PHE:CD2	3:B:274:PRO:HD2	2.39	0.56
2:A:168:GLU:HG3	2:A:201:ALA:HB1	1.88	0.56
2:A:209:ILE:O	2:A:212:ILE:HB	2.04	0.56
2:A:241:SER:HB2	2:A:356:ASN:ND2	2.20	0.56
3:B:268:PHE:HB3	3:B:379:GLY:N	2.20	0.56
2:A:67:PHE:CE2	2:A:87:PHE:CE2	2.94	0.56
3:B:230:LEU:HD21	3:B:302:MET:HE1	1.87	0.56
1:D:3416:LYS:CE	1:D:3418:GLU:HB2	2.28	0.56
1:D:3428:GLU:HG2	1:D:3431:PHE:HB2	1.88	0.56
2:A:250:VAL:HG13	2:A:254:GLU:OE1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:413:MET:CG	3:B:418:PHE:HE1	2.18	0.56
3:B:275:LEU:CD2	3:B:300:ASN:HD21	2.11	0.56
3:B:64:ARG:HD2	3:B:125:GLU:HB3	1.88	0.56
2:A:76:ASP:HA	2:A:79:ARG:HG3	1.87	0.56
2:A:362:VAL:HG13	2:A:368:LEU:CB	2.28	0.56
3:B:273:ALA:HB3	3:B:375:ALA:H	1.69	0.56
3:B:428:LEU:HD12	3:B:428:LEU:O	2.05	0.56
1:D:3407:ALA:O	1:D:3410:LEU:HB3	2.04	0.56
2:A:152:LEU:HD12	2:A:153:LEU:HA	1.86	0.56
2:A:16:ILE:HG22	2:A:17:GLY:N	2.20	0.56
2:A:237:SER:HB3	2:A:376:CYS:SG	2.46	0.56
2:A:92:LEU:N	2:A:92:LEU:HD12	2.21	0.56
3:B:180:THR:HB	3:B:183:GLU:OE1	2.06	0.56
1:D:3422:ILE:O	1:D:3425:LYS:HB2	2.05	0.56
3:B:388:PHE:CB	3:B:429:VAL:HG22	2.36	0.56
3:B:288:VAL:CB	3:B:289:PRO:HD3	2.35	0.56
2:A:219:ILE:HG22	2:A:222:PRO:HD3	1.87	0.56
3:B:132:LEU:HD23	3:B:164:ARG:HD2	1.88	0.56
3:B:36:TYR:CE2	3:B:44:LEU:HB2	2.41	0.56
2:A:229:ARG:HG2	2:A:229:ARG:NH1	2.10	0.55
1:D:3394:LEU:HD13	2:A:409:VAL:O	2.06	0.55
2:A:225:THR:HG23	2:A:226:ASN:N	2.21	0.55
2:A:189:LEU:O	2:A:193:THR:HG22	2.07	0.55
3:B:315:VAL:CG1	3:B:377:PHE:HE1	2.18	0.55
2:A:152:LEU:HD12	2:A:153:LEU:N	2.21	0.55
2:A:103:TYR:N	2:A:408:TYR:HE1	2.04	0.55
2:A:66:VAL:HG12	2:A:91:GLN:CA	2.36	0.55
3:B:122:VAL:HG22	3:B:123:ARG:N	2.21	0.55
1:D:3432:ILE:HD13	1:D:3433:THR:N	2.18	0.55
2:A:242:LEU:HD13	2:A:318:LEU:HD22	1.87	0.55
2:A:152:LEU:HD12	2:A:152:LEU:C	2.26	0.55
2:A:175:PRO:HG2	2:A:304:LYS:HE2	1.87	0.55
1:D:3392:LYS:NZ	3:B:158:ARG:HH12	2.04	0.55
1:D:3431:PHE:CZ	1:D:3435:ILE:HD11	2.42	0.55
3:B:132:LEU:HD23	3:B:164:ARG:CD	2.36	0.55
2:A:23:LEU:CD2	2:A:233:GLN:HA	2.37	0.55
2:A:21:TRP:O	2:A:24:TYR:HB2	2.06	0.55
3:B:172:VAL:CG2	3:B:203:CYS:HB3	2.36	0.55
3:B:7:ILE:HB	3:B:137:LEU:HD12	1.87	0.55
2:A:359:PRO:HB3	2:A:372:GLN:O	2.06	0.55
3:B:223:THR:HG22	3:B:224:TYR:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:185:TYR:CD1	2:A:395:PHE:CE2	2.95	0.55
3:B:173:PRO:HB3	3:B:183:GLU:HG2	1.89	0.55
3:B:188:THR:CG2	3:B:422:GLU:HA	2.37	0.55
3:B:202:TYR:HE2	3:B:378:ILE:CG2	2.19	0.54
2:A:114:ILE:HG22	2:A:118:VAL:CG2	2.37	0.54
2:A:9:VAL:HG21	2:A:149:PHE:CD1	2.41	0.54
3:B:283:TYR:HB3	3:B:285:ALA:H	1.72	0.54
3:B:264:ARG:HA	3:B:264:ARG:NE	2.23	0.54
1:D:3478:VAL:HG13	1:D:3479:LYS:N	2.22	0.54
2:A:104:ALA:HB1	2:A:413:MET:HG2	1.90	0.54
2:A:331:ALA:O	2:A:334:THR:HG22	2.06	0.54
3:B:299:LYS:H	3:B:299:LYS:HD3	1.71	0.54
2:A:412:GLY:N	2:A:413:MET:HB2	2.23	0.54
1:D:3409:CYS:O	1:D:3412:LEU:HB2	2.08	0.54
3:B:132:LEU:CB	3:B:164:ARG:HD3	2.35	0.54
1:D:3484:GLN:NE2	1:D:3484:GLN:H	2.05	0.54
3:B:102:ASN:HB2	3:B:105:LYS:HB2	1.89	0.54
2:A:301:GLN:O	2:A:302:MET:HB2	2.08	0.54
3:B:135:PHE:CE1	3:B:157:ILE:HG23	2.43	0.54
3:B:198:THR:HG22	3:B:265:LEU:HD13	1.89	0.54
1:D:3392:LYS:CE	3:B:158:ARG:HH12	2.21	0.54
3:B:189:LEU:HA	3:B:421:ALA:HB1	1.89	0.54
3:B:195:VAL:HG13	3:B:196:GLU:N	2.21	0.54
1:D:3455:GLY:HA3	1:D:3458:GLU:CB	2.38	0.54
1:D:3438:TYR:CZ	1:D:3443:MET:HB2	2.43	0.54
2:A:177:VAL:HG21	2:A:207:GLU:CB	2.38	0.54
2:A:301:GLN:CB	2:A:303:VAL:HG12	2.38	0.54
2:A:63:PRO:HG2	2:A:87:PHE:HA	1.89	0.54
3:B:234:THR:HG21	3:B:270:PRO:CB	2.15	0.54
2:A:210:TYR:OH	3:B:325:MET:HB3	2.07	0.54
3:B:299:LYS:CD	3:B:299:LYS:H	2.20	0.54
3:B:179:ASP:HB2	6:B:501:GDP:H3'	1.90	0.54
2:A:237:SER:HA	2:A:241:SER:OG	2.08	0.54
2:A:26:LEU:CD2	2:A:363:VAL:HG13	2.30	0.54
2:A:172:TYR:CE2	2:A:388:TRP:CZ3	2.95	0.53
2:A:172:TYR:OH	2:A:387:ALA:HB1	2.07	0.53
2:A:66:VAL:HB	2:A:91:GLN:O	2.08	0.53
3:B:264:ARG:NH1	3:B:264:ARG:HG3	2.23	0.53
3:B:288:VAL:HG12	3:B:289:PRO:HD3	1.91	0.53
3:B:318:VAL:HG23	3:B:378:ILE:HD11	1.90	0.53
3:B:18:ALA:O	3:B:22:GLU:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:6:HIS:O	3:B:65:ALA:HB1	2.07	0.53
3:B:42:LEU:HD21	3:B:245:PRO:HD2	1.89	0.53
2:A:118:VAL:HG11	2:A:153:LEU:HD22	1.90	0.53
2:A:298:PRO:O	2:A:301:GLN:HG2	2.09	0.53
2:A:402:ARG:O	2:A:402:ARG:HG3	2.08	0.53
2:A:11:GLN:CG	2:A:74:VAL:HG11	2.19	0.53
3:B:5:VAL:HG21	3:B:135:PHE:HD2	1.73	0.53
2:A:274:PRO:HB3	2:A:371:VAL:HG21	1.91	0.53
3:B:415:GLU:OE2	3:B:415:GLU:HA	2.08	0.53
3:B:337:ASN:N	3:B:337:ASN:HD22	2.05	0.53
2:A:261:PRO:HG2	2:A:313:MET:SD	2.49	0.53
2:A:269:LEU:N	2:A:269:LEU:HD23	2.24	0.53
3:B:199:ASP:C	3:B:265:LEU:HB2	2.29	0.53
1:D:3394:LEU:HD13	2:A:410:GLY:HA2	1.90	0.53
2:A:115:ILE:HG23	2:A:116:ASP:N	2.24	0.53
2:A:212:ILE:HD11	2:A:302:MET:H	1.73	0.53
3:B:182:VAL:O	3:B:182:VAL:HG12	2.09	0.53
3:B:119:LEU:HA	3:B:122:VAL:HG11	1.91	0.53
2:A:337:THR:O	2:A:339:ARG:HB2	2.08	0.53
2:A:180:ALA:HA	3:B:352:LYS:HZ1	1.73	0.53
2:A:101:ASN:O	2:A:182:VAL:HG21	2.08	0.53
2:A:68:VAL:HG22	2:A:93:ILE:CG2	2.39	0.53
3:B:168:THR:CG2	3:B:201:THR:HG23	2.38	0.53
3:B:204:ILE:HG22	3:B:205:ASP:N	2.24	0.53
3:B:360:PRO:HB2	7:B:502:TA1:H281	1.91	0.53
3:B:285:ALA:CB	3:B:290:GLU:HG2	2.36	0.53
1:D:3403:LEU:N	1:D:3403:LEU:HD23	2.24	0.53
2:A:192:HIS:HB2	2:A:424:ASP:OD2	2.09	0.53
2:A:78:VAL:HG11	2:A:92:LEU:HD21	1.91	0.53
1:D:3428:GLU:HG3	1:D:3430:ASN:OD1	2.09	0.53
2:A:155:GLU:HA	2:A:197:HIS:CE1	2.43	0.52
2:A:204:VAL:CG2	2:A:302:MET:HB3	2.39	0.52
2:A:6:SER:O	2:A:65:ALA:HB1	2.09	0.52
3:B:135:PHE:CZ	3:B:161:TYR:CE1	2.97	0.52
3:B:167:ASN:HA	3:B:200:GLU:O	2.08	0.52
3:B:201:THR:HG22	3:B:202:TYR:N	2.24	0.52
3:B:4:ILE:CD1	3:B:252:LEU:HD11	2.40	0.52
2:A:217:LEU:HG	2:A:219:ILE:HD11	1.89	0.52
3:B:172:VAL:CG1	3:B:387:LEU:HD21	2.39	0.52
2:A:304:LYS:HG3	2:A:304:LYS:O	2.10	0.52
2:A:402:ARG:O	2:A:405:VAL:HB	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3:GLU:OE2	3:B:130:ASP:HB3	2.08	0.52
3:B:52:TYR:OH	3:B:239:THR:HG21	2.09	0.52
3:B:309:HIS:N	3:B:310:GLY:HA3	2.25	0.52
3:B:57:ALA:HB3	3:B:60:LYS:N	2.12	0.52
3:B:52:TYR:HB2	3:B:53:TYR:CE1	2.45	0.52
3:B:9:ALA:O	3:B:13:GLY:HA2	2.09	0.52
2:A:332:ILE:HD13	2:A:351:PHE:CD1	2.45	0.52
2:A:250:VAL:HG21	2:A:318:LEU:CD2	2.39	0.52
3:B:229:HIS:ND1	3:B:229:HIS:C	2.62	0.52
1:D:3455:GLY:HA2	1:D:3458:GLU:N	2.13	0.52
3:B:10:GLY:HA3	3:B:146:GLY:HA2	1.91	0.52
2:A:76:ASP:HA	2:A:79:ARG:CG	2.40	0.52
2:A:251:ASP:O	2:A:255:PHE:HD1	1.93	0.52
2:A:88:HIS:O	2:A:92:LEU:HD12	2.10	0.52
2:A:288:VAL:HG23	2:A:373:ARG:HH11	1.74	0.52
2:A:388:TRP:CZ3	2:A:391:LEU:HD22	2.45	0.52
1:D:3394:LEU:HD22	2:A:410:GLY:N	2.24	0.52
2:A:185:TYR:O	2:A:189:LEU:HG	2.10	0.52
2:A:251:ASP:N	2:A:254:GLU:HG3	2.24	0.52
1:D:3426:ILE:HG22	1:D:3427:MET:N	2.25	0.52
2:A:377:MET:O	2:A:377:MET:HG3	2.08	0.52
2:A:105:ARG:NH2	2:A:110:ILE:HD12	2.24	0.52
2:A:185:TYR:HD2	2:A:408:TYR:HE2	1.59	0.52
3:B:4:ILE:N	3:B:51:VAL:HG12	2.25	0.52
2:A:217:LEU:HA	2:A:277:SER:HB3	1.92	0.52
3:B:175:PRO:HD2	3:B:207:GLU:CD	2.30	0.52
3:B:253:ARG:O	3:B:257:VAL:HG23	2.10	0.51
3:B:352:LYS:C	3:B:352:LYS:HD3	2.30	0.51
2:A:208:ALA:HB1	2:A:303:VAL:C	2.31	0.51
1:D:3395:PRO:HG2	2:A:411:GLU:OE2	2.10	0.51
3:B:44:LEU:HD12	3:B:44:LEU:O	2.09	0.51
2:A:352:LYS:HE2	2:A:353:VAL:O	2.10	0.51
3:B:313:LEU:HD23	3:B:313:LEU:N	2.25	0.51
2:A:372:GLN:HE21	2:A:372:GLN:CA	2.23	0.51
3:B:64:ARG:HG3	3:B:125:GLU:OE2	2.11	0.51
1:D:3392:LYS:HD2	1:D:3423:ARG:NE	2.26	0.51
3:B:127:GLU:OE1	3:B:127:GLU:HA	2.10	0.51
1:D:3412:LEU:HD21	1:D:3435:ILE:HD11	1.91	0.51
2:A:63:PRO:HB2	2:A:91:GLN:OE1	2.09	0.51
3:B:182:VAL:HG11	3:B:408:TYR:OH	2.10	0.51
1:D:3444:MET:CE	1:D:3448:ILE:HG12	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:248:LEU:HD12	2:A:248:LEU:O	2.11	0.51
2:A:282:TYR:CD1	2:A:284:GLU:CG	2.94	0.51
2:A:147:SER:HB2	2:A:190:THR:OG1	2.10	0.51
2:A:363:VAL:HG23	2:A:368:LEU:HD11	1.93	0.51
2:A:402:ARG:HE	2:A:405:VAL:CG1	2.22	0.51
2:A:221:ARG:N	2:A:222:PRO:HD3	2.25	0.51
2:A:408:TYR:CB	2:A:418:PHE:HZ	2.24	0.51
3:B:111:GLY:O	3:B:115:VAL:HG23	2.11	0.51
3:B:134:GLY:HA3	3:B:165:ILE:O	2.11	0.51
3:B:205:ASP:O	3:B:209:LEU:HD22	2.11	0.51
1:D:3390:GLU:O	1:D:3394:LEU:HG	2.11	0.51
2:A:429:GLU:HG3	2:A:430:LYS:N	2.26	0.51
3:B:269:MET:CE	3:B:301:MET:HE3	2.41	0.51
1:D:3392:LYS:HE2	1:D:3393:SER:CA	2.41	0.51
3:B:287:THR:HG22	3:B:288:VAL:H	1.76	0.50
3:B:4:ILE:H	3:B:51:VAL:HG12	1.76	0.50
2:A:407:TRP:HE1	3:B:260:VAL:HG23	1.75	0.50
2:A:407:TRP:NE1	3:B:257:VAL:HA	2.27	0.50
3:B:287:THR:HG22	3:B:288:VAL:N	2.26	0.50
3:B:297:ASP:CG	3:B:299:LYS:HE2	2.31	0.50
3:B:42:LEU:HD21	3:B:245:PRO:CD	2.41	0.50
2:A:102:ASN:ND2	2:A:105:ARG:H	2.09	0.50
2:A:114:ILE:HG22	2:A:118:VAL:HG23	1.93	0.50
2:A:118:VAL:O	2:A:121:ARG:HB2	2.12	0.50
3:B:230:LEU:O	3:B:233:ALA:HB3	2.11	0.50
2:A:311:LYS:HD3	2:A:342:GLN:O	2.12	0.50
2:A:152:LEU:HD12	2:A:153:LEU:CA	2.42	0.50
2:A:103:TYR:CD2	2:A:413:MET:CE	2.94	0.50
1:D:3392:LYS:HE2	1:D:3392:LYS:C	2.32	0.50
1:D:3408:VAL:HG12	1:D:3411:MET:CE	2.41	0.50
1:D:3412:LEU:CD2	1:D:3431:PHE:CE1	2.95	0.50
3:B:173:PRO:HD2	3:B:391:ILE:CD1	2.40	0.50
3:B:28:HIS:ND1	3:B:49:ILE:HG22	2.27	0.50
2:A:123:ARG:HA	2:A:161:TYR:OH	2.11	0.50
2:A:103:TYR:CD2	2:A:189:LEU:CD1	2.94	0.50
2:A:241:SER:HB2	2:A:356:ASN:HD22	1.76	0.50
3:B:123:ARG:O	3:B:127:GLU:HG2	2.12	0.50
3:B:8:GLN:HG3	3:B:66:ILE:O	2.12	0.50
2:A:287:SER:HA	2:A:373:ARG:CZ	2.42	0.50
2:A:201:ALA:O	2:A:267:PHE:HA	2.12	0.50
1:D:3394:LEU:HA	2:A:410:GLY:HA3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:224:TYR:CE1	3:B:325:MET:HG2	2.47	0.50
1:D:3408:VAL:HG12	1:D:3411:MET:HE1	1.94	0.50
1:D:3449:ARG:CG	1:D:3449:ARG:HH21	2.24	0.50
2:A:238:ILE:HD12	2:A:255:PHE:CZ	2.46	0.50
2:A:92:LEU:H	2:A:92:LEU:HD12	1.76	0.50
3:B:135:PHE:HZ	3:B:161:TYR:CD1	2.30	0.50
3:B:172:VAL:HG12	3:B:173:PRO:HD2	1.94	0.50
2:A:372:GLN:HE21	2:A:372:GLN:HA	1.75	0.50
1:D:3455:GLY:CA	1:D:3458:GLU:HB2	2.41	0.50
1:D:3428:GLU:O	1:D:3428:GLU:HG2	2.11	0.50
2:A:22:GLU:HG2	2:A:83:TYR:HE1	1.72	0.50
2:A:103:TYR:CD2	2:A:189:LEU:HD12	2.47	0.50
2:A:23:LEU:HD21	2:A:233:GLN:HA	1.93	0.50
3:B:5:VAL:CG2	3:B:135:PHE:CD2	2.95	0.50
3:B:307:PRO:HB3	3:B:312:TYR:CE1	2.47	0.50
1:D:3394:LEU:HD22	2:A:410:GLY:HA3	1.91	0.50
1:D:3438:TYR:CE2	1:D:3443:MET:HB2	2.47	0.50
2:A:407:TRP:CZ2	3:B:256:ALA:HB1	2.47	0.49
3:B:52:TYR:CB	3:B:53:TYR:CE1	2.95	0.49
2:A:105:ARG:HB2	2:A:110:ILE:CG2	2.40	0.49
2:A:276:ILE:HG12	2:A:277:SER:N	2.27	0.49
2:A:107:HIS:CD2	2:A:108:TYR:CE1	3.00	0.49
3:B:250:ALA:HB1	3:B:254:LYS:CB	2.41	0.49
2:A:288:VAL:HA	2:A:291:ILE:HD11	1.94	0.49
2:A:262:TYR:HB3	2:A:263:PRO:HD2	1.93	0.49
2:A:401:LYS:CD	3:B:346:TRP:CD2	2.94	0.49
2:A:107:HIS:CD2	2:A:108:TYR:CD1	2.99	0.49
2:A:107:HIS:HD2	2:A:108:TYR:CE1	2.31	0.49
2:A:118:VAL:HG11	2:A:153:LEU:CD2	2.42	0.49
2:A:412:GLY:H	2:A:413:MET:HB2	1.77	0.49
2:A:67:PHE:HE2	2:A:87:PHE:CE2	2.29	0.49
3:B:52:TYR:HB2	3:B:53:TYR:CD1	2.48	0.49
3:B:89:PRO:O	3:B:92:PHE:HD2	1.94	0.49
3:B:135:PHE:CE1	3:B:157:ILE:CG2	2.95	0.49
1:D:3412:LEU:CD2	1:D:3431:PHE:CZ	2.95	0.49
1:D:3449:ARG:HG2	1:D:3449:ARG:HH21	1.77	0.49
2:A:161:TYR:HB3	2:A:164:LYS:HB2	1.93	0.49
3:B:313:LEU:HB2	3:B:380:ASN:HB3	1.95	0.49
3:B:181:VAL:O	3:B:398:MET:HE1	2.13	0.49
3:B:52:TYR:CB	3:B:53:TYR:CD1	2.95	0.49
2:A:97:GLU:HB2	2:A:110:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:168:GLU:CG	2:A:201:ALA:HB2	2.43	0.49
3:B:346:TRP:CE3	3:B:347:ILE:HG12	2.46	0.49
3:B:7:ILE:HD13	3:B:66:ILE:HD11	1.94	0.49
3:B:12:CYS:HB3	3:B:140:SER:OG	2.13	0.49
2:A:108:TYR:CE1	2:A:413:MET:SD	3.06	0.49
3:B:269:MET:HE2	3:B:301:MET:HE3	1.95	0.49
2:A:268:PRO:HA	2:A:379:SER:O	2.13	0.48
3:B:24:ILE:CD1	3:B:52:TYR:CE2	2.95	0.48
2:A:426:ALA:O	2:A:429:GLU:HG2	2.13	0.48
3:B:94:PHE:N	3:B:94:PHE:CD1	2.81	0.48
2:A:324:VAL:HG12	2:A:326:LYS:N	2.26	0.48
2:A:229:ARG:NH2	2:A:363:VAL:HG11	2.28	0.48
2:A:65:ALA:O	2:A:91:GLN:HG2	2.13	0.48
3:B:274:PRO:HG2	3:B:374:SER:HB3	1.93	0.48
2:A:248:LEU:HB3	2:A:354:GLY:HA2	1.94	0.48
2:A:118:VAL:HG21	2:A:149:PHE:CZ	2.49	0.48
2:A:405:VAL:HG12	2:A:406:HIS:N	2.26	0.48
3:B:286:LEU:CD1	3:B:371:LEU:HD21	2.41	0.48
3:B:89:PRO:HA	3:B:92:PHE:CD2	2.48	0.48
2:A:275:VAL:CG1	2:A:300:ASN:HD21	2.26	0.48
2:A:244:PHE:CD1	2:A:245:ASP:N	2.80	0.48
2:A:267:PHE:CD1	2:A:267:PHE:N	2.81	0.48
3:B:67:LEU:HD21	3:B:87:PHE:CE2	2.48	0.48
2:A:317:LEU:HD23	2:A:375:VAL:CG1	2.42	0.48
2:A:210:TYR:CE1	2:A:227:LEU:CD2	2.94	0.48
3:B:318:VAL:HG13	3:B:354:ALA:HB3	1.96	0.48
3:B:408:TYR:CD2	3:B:418:PHE:CZ	2.99	0.48
2:A:274:PRO:HG3	2:A:374:ALA:HA	1.96	0.48
3:B:75:MET:HE2	3:B:94:PHE:HB3	1.95	0.48
3:B:70:LEU:HG	3:B:145:THR:HG23	1.95	0.48
2:A:308:ARG:HH11	2:A:390:ARG:HH12	1.60	0.48
2:A:132:LEU:HD21	2:A:164:LYS:CE	2.40	0.48
3:B:107:HIS:CE1	3:B:152:LEU:HB2	2.48	0.48
3:B:103:TRP:CD1	3:B:147:SER:CB	2.94	0.48
3:B:36:TYR:CZ	3:B:38:GLY:HA3	2.49	0.48
2:A:228:ASN:HA	2:A:231:ILE:CG1	2.44	0.48
2:A:62:VAL:CG1	2:A:63:PRO:HD2	2.42	0.48
3:B:241:CYS:SG	3:B:318:VAL:HG11	2.54	0.48
3:B:31:ASP:C	3:B:34:GLY:HA3	2.34	0.48
2:A:125:LEU:HD23	2:A:128:GLN:HE22	1.79	0.48
2:A:115:ILE:HD11	2:A:153:LEU:CD1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3:GLU:HA	3:B:51:VAL:HG13	1.96	0.48
3:B:42:LEU:HD12	3:B:47:GLU:OE1	2.14	0.48
2:A:9:VAL:HG22	2:A:10:GLY:H	1.78	0.48
2:A:107:HIS:CE1	2:A:152:LEU:HB3	2.48	0.48
1:D:3392:LYS:HD2	1:D:3423:ARG:CZ	2.44	0.48
2:A:341:ILE:HG23	2:A:342:GLN:N	2.29	0.48
2:A:11:GLN:HE21	2:A:74:VAL:CG1	2.26	0.48
2:A:301:GLN:HB2	2:A:303:VAL:HG12	1.96	0.48
2:A:172:TYR:CZ	2:A:391:LEU:HD13	2.48	0.48
3:B:94:PHE:O	3:B:114:LEU:HD11	2.14	0.48
2:A:22:GLU:CG	2:A:83:TYR:CE1	2.94	0.48
1:D:3398:PRO:HG2	1:D:3401:VAL:HG21	1.96	0.48
1:D:3456:TYR:HA	1:D:3456:TYR:HD1	1.57	0.47
3:B:19:LYS:HG3	3:B:228:ASN:CB	2.44	0.47
2:A:135:PHE:CD1	2:A:135:PHE:N	2.81	0.47
2:A:102:ASN:HD21	2:A:105:ARG:H	1.62	0.47
2:A:405:VAL:HA	2:A:408:TYR:HD2	1.78	0.47
3:B:255:LEU:O	3:B:259:MET:HB2	2.14	0.47
3:B:275:LEU:HD23	3:B:300:ASN:CG	2.34	0.47
2:A:346:TRP:HZ2	2:A:435:VAL:CG1	2.27	0.47
2:A:108:TYR:N	2:A:108:TYR:CD1	2.82	0.47
2:A:17:GLY:HA3	2:A:67:PHE:HE1	1.80	0.47
2:A:210:TYR:HE1	2:A:227:LEU:CD2	2.16	0.47
3:B:413:MET:HB2	3:B:413:MET:HE3	1.64	0.47
3:B:428:LEU:HG	3:B:429:VAL:N	2.29	0.47
1:D:3390:GLU:HG3	2:A:402:ARG:NH2	2.13	0.47
1:D:3392:LYS:HE2	1:D:3393:SER:N	2.29	0.47
3:B:31:ASP:HB3	3:B:32:PRO:CD	2.43	0.47
1:D:3408:VAL:O	1:D:3412:LEU:HD13	2.14	0.47
3:B:343:PHE:O	3:B:344:VAL:HB	2.14	0.47
2:A:399:TYR:O	2:A:402:ARG:HA	2.13	0.47
2:A:101:ASN:HD21	3:B:254:LYS:NZ	2.13	0.47
3:B:33:THR:HG22	3:B:34:GLY:N	2.29	0.47
3:B:53:TYR:CD1	3:B:53:TYR:N	2.83	0.47
2:A:248:LEU:HB2	2:A:355:ILE:N	2.28	0.47
3:B:427:ASP:O	3:B:430:SER:HB3	2.14	0.47
2:A:118:VAL:HG21	2:A:149:PHE:HZ	1.79	0.47
2:A:168:GLU:O	2:A:201:ALA:HA	2.15	0.47
3:B:231:VAL:HA	3:B:302:MET:HE1	1.96	0.47
3:B:259:MET:CE	3:B:268:PHE:CZ	2.97	0.47
3:B:269:MET:CG	3:B:303:ALA:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:315:VAL:HB	3:B:351:VAL:HG13	1.96	0.47
2:A:164:LYS:HD3	2:A:164:LYS:HA	1.40	0.47
3:B:272:PHE:CE1	7:B:502:TA1:H391	2.50	0.47
3:B:312:TYR:HA	3:B:381:SER:HA	1.96	0.47
2:A:372:GLN:NE2	2:A:372:GLN:HA	2.30	0.47
2:A:187:SER:O	2:A:191:THR:HG22	2.15	0.47
2:A:34:GLY:C	2:A:61:HIS:N	2.68	0.47
3:B:105:LYS:HG2	3:B:110:GLU:HG2	1.92	0.47
3:B:316:ALA:O	3:B:378:ILE:HD12	2.15	0.47
3:B:3:GLU:HA	3:B:51:VAL:HA	1.96	0.47
1:D:3428:GLU:HG2	1:D:3431:PHE:N	2.22	0.47
2:A:9:VAL:O	2:A:13:GLY:HA3	2.15	0.47
2:A:175:PRO:HD2	2:A:207:GLU:CG	2.43	0.47
2:A:288:VAL:O	2:A:291:ILE:HG12	2.15	0.47
1:D:3480:TRP:O	1:D:3483:ALA:HB3	2.15	0.47
2:A:224:TYR:CD1	3:B:325:MET:HG2	2.50	0.47
2:A:67:PHE:N	2:A:67:PHE:CD2	2.82	0.47
1:D:3422:ILE:C	1:D:3422:ILE:HD12	2.35	0.47
3:B:132:LEU:HB3	3:B:164:ARG:HH11	1.79	0.47
2:A:82:THR:HG22	2:A:83:TYR:N	2.29	0.47
2:A:388:TRP:HZ3	2:A:391:LEU:HD22	1.79	0.47
2:A:87:PHE:CD1	2:A:87:PHE:N	2.83	0.47
3:B:135:PHE:HD1	3:B:166:MET:HG2	1.79	0.47
3:B:262:PHE:HB3	3:B:263:PRO:HD2	1.97	0.47
3:B:318:VAL:HG13	3:B:354:ALA:CB	2.45	0.47
1:D:3449:ARG:HG2	1:D:3449:ARG:NH2	2.29	0.47
3:B:70:LEU:H	3:B:145:THR:CG2	2.22	0.47
3:B:267:PHE:CD1	3:B:267:PHE:N	2.82	0.47
2:A:204:VAL:HG22	2:A:302:MET:HB3	1.97	0.46
2:A:175:PRO:CG	2:A:304:LYS:HG2	2.46	0.46
3:B:301:MET:HE1	3:B:377:PHE:CE2	2.33	0.46
2:A:224:TYR:CZ	3:B:325:MET:HG2	2.50	0.46
3:B:326:LYS:HE3	3:B:330:GLU:CB	2.44	0.46
3:B:352:LYS:HD3	3:B:353:THR:N	2.30	0.46
2:A:191:THR:HG23	2:A:192:HIS:N	2.31	0.46
2:A:14:VAL:HG21	2:A:75:ILE:HD11	1.96	0.46
2:A:242:LEU:HD11	2:A:318:LEU:CD2	2.45	0.46
3:B:324:SER:OG	3:B:326:LYS:HB3	2.16	0.46
2:A:216:ASN:HA	2:A:216:ASN:HD22	1.54	0.46
2:A:100:ALA:HB3	2:A:105:ARG:HG3	1.98	0.46
2:A:153:LEU:O	2:A:157:LEU:HG	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:107:HIS:CD2	3:B:151:THR:CG2	2.98	0.46
2:A:177:VAL:HG13	3:B:329:ASP:HB3	1.96	0.46
3:B:332:MET:O	3:B:335:VAL:HB	2.16	0.46
3:B:48:ARG:HG2	3:B:243:ARG:CB	2.34	0.46
1:D:3384:LYS:HD3	1:D:3386:LYS:CG	2.45	0.46
2:A:11:GLN:HE21	2:A:74:VAL:CG2	2.29	0.46
2:A:244:PHE:HE2	2:A:358:GLU:OE1	1.98	0.46
2:A:259:LEU:O	2:A:261:PRO:HD3	2.14	0.46
3:B:135:PHE:CD1	3:B:135:PHE:N	2.84	0.46
3:B:315:VAL:HG12	3:B:351:VAL:HG13	1.97	0.46
2:A:11:GLN:O	2:A:15:GLN:HG3	2.15	0.46
2:A:8:HIS:CD2	2:A:17:GLY:HA2	2.50	0.46
2:A:24:TYR:OH	2:A:239:THR:HB	2.15	0.46
3:B:319:PHE:HA	3:B:375:ALA:CA	2.36	0.46
1:D:3442:LYS:HA	1:D:3442:LYS:HD3	1.79	0.46
3:B:108:TYR:CD1	3:B:108:TYR:N	2.82	0.46
3:B:169:PHE:CE2	3:B:235:MET:HB3	2.49	0.46
3:B:312:TYR:CD2	3:B:315:VAL:HG22	2.50	0.46
1:D:3462:PHE:O	1:D:3467:VAL:HG23	2.15	0.46
2:A:22:GLU:HG2	2:A:83:TYR:CZ	2.49	0.46
2:A:10:GLY:O	2:A:14:VAL:HG23	2.15	0.46
3:B:210:TYR:O	3:B:214:PHE:HB3	2.15	0.46
3:B:425:MET:HA	3:B:428:LEU:HD23	1.97	0.46
1:D:3438:TYR:CD1	1:D:3439:ASP:N	2.84	0.46
2:A:105:ARG:O	2:A:110:ILE:HG22	2.16	0.46
3:B:4:ILE:HD12	3:B:136:GLN:HE21	1.81	0.46
3:B:24:ILE:HD11	3:B:52:TYR:HE2	1.76	0.46
2:A:238:ILE:HD12	2:A:255:PHE:HE2	1.77	0.46
1:D:3394:LEU:CD1	2:A:410:GLY:HA2	2.46	0.46
2:A:219:ILE:HG22	2:A:221:ARG:N	2.31	0.46
1:D:3482:THR:HG23	1:D:3486:TYR:HD2	1.77	0.46
3:B:54:ASN:HD21	3:B:64:ARG:CB	2.22	0.46
1:D:3398:PRO:HB2	1:D:3401:VAL:CG2	2.44	0.46
3:B:278:ARG:HB3	3:B:279:GLY:HA3	1.97	0.46
2:A:234:ILE:HD13	2:A:235:VAL:N	2.31	0.46
2:A:26:LEU:HD23	2:A:363:VAL:HA	1.98	0.46
2:A:388:TRP:HA	2:A:388:TRP:CE3	2.51	0.46
2:A:412:GLY:CA	2:A:413:MET:HB2	2.46	0.46
3:B:161:TYR:N	3:B:161:TYR:CD1	2.82	0.46
3:B:172:VAL:HG13	3:B:173:PRO:HD2	1.98	0.46
3:B:70:LEU:HG	3:B:145:THR:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:425:MET:HB3	3:B:425:MET:HE2	1.53	0.45
3:B:236:SER:O	3:B:240:THR:HG23	2.15	0.45
2:A:251:ASP:CB	2:A:254:GLU:HG3	2.46	0.45
3:B:200:GLU:HA	3:B:265:LEU:HD12	1.98	0.45
3:B:230:LEU:HD23	3:B:231:VAL:HG23	1.99	0.45
2:A:72:PRO:HG3	2:A:95:GLY:O	2.17	0.45
2:A:99:ALA:HB1	5:A:502:GTP:O2G	2.16	0.45
3:B:187:ALA:O	3:B:191:VAL:HG12	2.16	0.45
2:A:181:VAL:HG21	3:B:258:ASN:HB3	1.93	0.45
3:B:425:MET:CG	3:B:428:LEU:HD23	2.47	0.45
1:D:3418:GLU:HG3	1:D:3420:ALA:H	1.82	0.45
1:D:3455:GLY:CA	1:D:3458:GLU:CB	2.95	0.45
1:D:3400:PRO:HA	1:D:3403:LEU:HG	1.98	0.45
3:B:358:ILE:HA	3:B:359:PRO:HD3	1.50	0.45
2:A:5:ILE:HD13	2:A:125:LEU:HB3	1.98	0.45
2:A:119:LEU:CA	2:A:122:ILE:HD11	2.27	0.45
2:A:119:LEU:CD2	2:A:153:LEU:CD1	2.95	0.45
3:B:264:ARG:O	3:B:265:LEU:HB3	2.16	0.45
2:A:100:ALA:HB1	2:A:102:ASN:OD1	2.17	0.45
3:B:273:ALA:O	3:B:294:GLN:HG2	2.16	0.45
3:B:413:MET:HG2	3:B:418:PHE:CE1	2.43	0.45
2:A:217:LEU:H	2:A:217:LEU:CD2	2.28	0.45
2:A:276:ILE:HG23	2:A:369:ALA:HB1	1.95	0.45
1:D:3399:THR:O	1:D:3403:LEU:HG	2.17	0.45
2:A:176:GLN:HB3	3:B:333:LEU:CD1	2.46	0.45
3:B:242:LEU:HD22	3:B:250:ALA:N	2.32	0.45
2:A:217:LEU:N	2:A:217:LEU:CD2	2.80	0.45
3:B:140:SER:CB	3:B:142:GLY:HA3	2.37	0.45
1:D:3444:MET:HE3	1:D:3444:MET:O	2.17	0.45
7:B:502:TA1:C26	7:B:502:TA1:H463	2.46	0.45
1:D:3459:ASP:HB2	1:D:3462:PHE:HB2	1.97	0.45
1:D:3431:PHE:HD1	1:D:3431:PHE:HA	1.43	0.45
2:A:21:TRP:HE3	2:A:21:TRP:N	2.14	0.45
2:A:182:VAL:HG11	3:B:257:VAL:CG1	2.46	0.45
3:B:288:VAL:HG12	3:B:289:PRO:CA	2.47	0.45
3:B:6:HIS:CE1	3:B:8:GLN:HE21	2.35	0.45
1:D:3464:TYR:CD1	1:D:3478:VAL:CG1	2.94	0.45
3:B:11:GLN:O	3:B:15:GLN:N	2.41	0.45
3:B:43:GLN:O	3:B:49:ILE:HG23	2.17	0.45
2:A:75:ILE:O	2:A:78:VAL:HB	2.16	0.45
2:A:93:ILE:HD12	2:A:93:ILE:HA	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:203:MET:SD	2:A:388:TRP:CZ2	3.10	0.44
2:A:272:TYR:HE1	2:A:376:CYS:HG	1.57	0.44
2:A:6:SER:OG	2:A:65:ALA:HB2	2.17	0.44
3:B:169:PHE:HD2	3:B:204:ILE:HD11	1.82	0.44
2:A:360:PRO:HG3	2:A:374:ALA:CB	2.46	0.44
2:A:12:ALA:HB2	5:A:502:GTP:C8	2.52	0.44
2:A:166:LYS:H	2:A:199:ASP:CG	2.20	0.44
2:A:302:MET:HB2	2:A:302:MET:HE3	1.88	0.44
3:B:115:VAL:O	3:B:118:VAL:HB	2.17	0.44
3:B:277:SER:N	3:B:281:GLN:HB3	2.32	0.44
2:A:98:ASP:HB3	3:B:2:ARG:HH12	1.82	0.44
3:B:431:GLU:OE1	3:B:432:TYR:HA	2.17	0.44
3:B:346:TRP:CZ2	3:B:435:TYR:CD1	3.06	0.44
2:A:432:TYR:HA	2:A:432:TYR:HD1	1.36	0.44
2:A:334:THR:HG23	2:A:335:ILE:N	2.32	0.44
2:A:107:HIS:HA	2:A:148:GLY:C	2.37	0.44
2:A:242:LEU:CD2	2:A:318:LEU:CD2	2.95	0.44
3:B:141:LEU:O	3:B:186:ASN:HB2	2.17	0.44
1:D:3395:PRO:HB3	3:B:163:ASP:OD1	2.17	0.44
3:B:262:PHE:CE2	3:B:435:TYR:CE1	3.06	0.44
3:B:229:HIS:HE2	7:B:502:TA1:H361	1.83	0.44
1:D:3418:GLU:HG3	1:D:3419:TRP:N	2.32	0.44
1:D:3384:LYS:HG2	1:D:3387:HIS:ND1	2.32	0.44
2:A:219:ILE:C	2:A:222:PRO:HD3	2.38	0.44
2:A:195:LEU:HD23	2:A:264:ARG:CZ	2.47	0.44
2:A:23:LEU:CD1	2:A:363:VAL:HG22	2.46	0.44
1:D:3394:LEU:CD2	2:A:410:GLY:CA	2.93	0.44
3:B:109:THR:HG22	3:B:110:GLU:OE2	2.17	0.44
3:B:230:LEU:HD21	3:B:302:MET:HE3	1.98	0.44
3:B:30:ILE:CD1	3:B:53:TYR:CE2	2.95	0.44
2:A:119:LEU:HD23	2:A:153:LEU:HD11	2.00	0.44
2:A:3:GLU:C	2:A:243:ARG:HH11	2.21	0.44
2:A:250:VAL:CG2	2:A:318:LEU:CD2	2.95	0.44
2:A:23:LEU:HD12	2:A:363:VAL:HG22	1.99	0.44
3:B:209:LEU:HG	3:B:230:LEU:HD22	2.00	0.44
3:B:30:ILE:HA	3:B:35:SER:O	2.18	0.44
2:A:22:GLU:CG	2:A:83:TYR:HE1	2.31	0.44
2:A:5:ILE:HG23	2:A:64:ARG:O	2.17	0.44
2:A:103:TYR:CG	2:A:189:LEU:HD12	2.53	0.44
2:A:23:LEU:HD23	2:A:236:SER:HB2	1.98	0.44
3:B:185:TYR:HD1	3:B:185:TYR:HA	1.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3438:TYR:HD1	1:D:3439:ASP:N	2.15	0.44
2:A:177:VAL:CG2	2:A:207:GLU:HB3	2.44	0.44
2:A:231:ILE:HG12	2:A:231:ILE:H	1.35	0.44
3:B:269:MET:CE	3:B:301:MET:CE	2.95	0.44
3:B:378:ILE:HG22	3:B:379:GLY:N	2.33	0.44
2:A:82:THR:CG2	2:A:83:TYR:CD1	3.00	0.44
2:A:195:LEU:HD21	2:A:428:LEU:CD2	2.48	0.44
2:A:209:ILE:HG12	2:A:302:MET:CG	2.47	0.44
2:A:269:LEU:O	2:A:378:LEU:HA	2.17	0.44
3:B:259:MET:HB3	3:B:259:MET:HE3	1.88	0.44
3:B:264:ARG:HG2	3:B:431:GLU:OE2	2.18	0.44
3:B:332:MET:HE2	3:B:353:THR:OG1	2.18	0.44
3:B:392:SER:O	3:B:395:PHE:HB3	2.17	0.44
2:A:282:TYR:HA	2:A:282:TYR:HD1	1.48	0.44
2:A:133:GLN:HB3	2:A:243:ARG:HH12	1.80	0.43
3:B:408:TYR:CD1	3:B:408:TYR:N	2.86	0.43
2:A:255:PHE:HE2	2:A:378:LEU:HD21	1.83	0.43
3:B:320:ARG:HB2	3:B:358:ILE:O	2.18	0.43
3:B:184:PRO:CB	3:B:395:PHE:HA	2.48	0.43
3:B:78:VAL:O	3:B:84:GLY:HA2	2.18	0.43
2:A:398:MET:HB2	2:A:398:MET:HE3	1.65	0.43
2:A:242:LEU:CD1	2:A:318:LEU:CD2	2.94	0.43
3:B:292:THR:HG21	3:B:331:GLN:HG2	1.98	0.43
3:B:314:THR:N	3:B:380:ASN:HB3	2.33	0.43
1:D:3405:MET:HA	1:D:3408:VAL:HG22	1.97	0.43
3:B:168:THR:HG22	3:B:169:PHE:N	2.33	0.43
3:B:191:VAL:CA	3:B:194:LEU:HD12	2.15	0.43
3:B:388:PHE:HD1	3:B:388:PHE:HA	1.59	0.43
2:A:286:LEU:O	2:A:291:ILE:HG23	2.18	0.43
3:B:36:TYR:CD2	3:B:44:LEU:HD22	2.53	0.43
3:B:382:THR:HG21	3:B:436:GLN:HA	2.00	0.43
2:A:168:GLU:CG	2:A:201:ALA:CB	2.96	0.43
2:A:6:SER:HG	2:A:21:TRP:HH2	1.66	0.43
2:A:362:VAL:HB	2:A:370:LYS:HD3	2.00	0.43
3:B:204:ILE:CG2	3:B:209:LEU:CD2	2.95	0.43
3:B:420:GLU:CG	3:B:421:ALA:N	2.82	0.43
1:D:3459:ASP:HA	1:D:3460:PRO:HD3	1.46	0.43
3:B:10:GLY:C	3:B:13:GLY:HA3	2.36	0.43
2:A:248:LEU:HD13	2:A:248:LEU:HA	1.56	0.43
2:A:264:ARG:H	2:A:264:ARG:HG2	1.62	0.43
1:D:3391:ILE:HD13	1:D:3391:ILE:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:108:TYR:O	3:B:112:ALA:HB2	2.19	0.43
3:B:276:THR:HB	3:B:281:GLN:HG3	2.00	0.43
1:D:3432:ILE:CG1	1:D:3433:THR:N	2.81	0.43
3:B:175:PRO:HD2	3:B:207:GLU:OE1	2.19	0.43
1:D:3440:THR:CG2	1:D:3441:LYS:N	2.82	0.43
3:B:346:TRP:CE3	3:B:347:ILE:CG1	3.02	0.43
3:B:359:PRO:CB	3:B:360:PRO:HD2	2.47	0.43
2:A:360:PRO:HG2	2:A:374:ALA:HB2	2.01	0.43
3:B:282:GLN:HB3	3:B:282:GLN:HE21	1.47	0.43
2:A:102:ASN:HD21	2:A:105:ARG:HG2	1.84	0.43
3:B:325:MET:HE3	3:B:355:VAL:CG2	2.47	0.43
1:D:3419:TRP:CE3	1:D:3419:TRP:HA	2.53	0.43
2:A:220:GLU:C	2:A:222:PRO:HD3	2.39	0.43
1:D:3405:MET:SD	1:D:3408:VAL:CG2	3.07	0.43
3:B:44:LEU:O	3:B:49:ILE:HG23	2.19	0.43
3:B:323:MET:HE3	3:B:373:MET:CG	2.49	0.43
3:B:137:LEU:HA	3:B:137:LEU:HD12	1.88	0.43
3:B:103:TRP:CE3	3:B:189:LEU:HD13	2.54	0.43
2:A:142:GLY:HA2	2:A:183:GLU:OE1	2.18	0.43
2:A:262:TYR:HA	2:A:263:PRO:HD3	1.81	0.43
3:B:195:VAL:CG1	3:B:196:GLU:N	2.81	0.43
2:A:185:TYR:HD2	2:A:408:TYR:CE2	2.37	0.42
3:B:198:THR:HG22	3:B:198:THR:O	2.19	0.42
3:B:425:MET:CA	3:B:428:LEU:HD23	2.49	0.42
3:B:428:LEU:HD12	3:B:428:LEU:C	2.40	0.42
2:A:7:ILE:O	2:A:7:ILE:HG13	2.18	0.42
2:A:117:LEU:HA	2:A:117:LEU:HD13	1.76	0.42
2:A:225:THR:CG2	2:A:226:ASN:N	2.82	0.42
3:B:276:THR:HB	3:B:281:GLN:CG	2.49	0.42
3:B:158:ARG:HD3	3:B:158:ARG:HA	1.75	0.42
2:A:341:ILE:CG2	2:A:342:GLN:N	2.82	0.42
3:B:7:ILE:CG2	3:B:137:LEU:CD1	2.97	0.42
1:D:3426:ILE:CG2	1:D:3427:MET:N	2.81	0.42
1:D:3455:GLY:HA2	1:D:3458:GLU:HG3	2.01	0.42
2:A:242:LEU:HD21	2:A:318:LEU:CD2	2.46	0.42
3:B:151:THR:CG2	3:B:152:LEU:N	2.82	0.42
3:B:275:LEU:HD23	3:B:300:ASN:OD1	2.19	0.42
3:B:288:VAL:CG1	3:B:289:PRO:HD3	2.48	0.42
1:D:3392:LYS:CE	1:D:3393:SER:HA	2.48	0.42
2:A:339:ARG:O	2:A:339:ARG:HG3	2.20	0.42
3:B:102:ASN:HD21	3:B:408:TYR:CA	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:259:MET:HE3	3:B:268:PHE:CE1	2.55	0.42
3:B:269:MET:HG2	3:B:303:ALA:CB	2.50	0.42
3:B:24:ILE:CG2	3:B:25:SER:N	2.82	0.42
2:A:288:VAL:HA	2:A:291:ILE:CD1	2.49	0.42
1:D:3436:ILE:CG1	1:D:3437:ASN:N	2.82	0.42
2:A:175:PRO:HD3	2:A:205:ASP:OD2	2.19	0.42
2:A:147:SER:HB3	2:A:186:ASN:HB3	2.01	0.42
2:A:237:SER:CB	2:A:376:CYS:SG	3.07	0.42
2:A:68:VAL:HG11	2:A:149:PHE:CZ	2.55	0.42
3:B:168:THR:CG2	3:B:169:PHE:N	2.83	0.42
2:A:407:TRP:NE1	3:B:260:VAL:CG2	2.82	0.42
3:B:270:PRO:HB2	3:B:302:MET:SD	2.59	0.42
3:B:311:ARG:CG	3:B:311:ARG:HH11	2.32	0.42
3:B:319:PHE:N	3:B:319:PHE:CD1	2.87	0.42
3:B:399:PHE:HE2	3:B:419:THR:HG23	1.85	0.42
3:B:4:ILE:N	3:B:51:VAL:CG1	2.82	0.42
3:B:4:ILE:CG2	3:B:5:VAL:N	2.83	0.42
3:B:86:ILE:CG2	3:B:87:PHE:N	2.83	0.42
2:A:371:VAL:CG1	2:A:372:GLN:N	2.82	0.42
1:D:3464:TYR:CD1	1:D:3478:VAL:CG2	2.96	0.42
1:D:3385:LYS:NZ	3:B:196:GLU:HG2	2.34	0.42
2:A:419:SER:O	2:A:423:GLU:HG3	2.19	0.42
3:B:133:GLN:HA	3:B:133:GLN:OE1	2.19	0.42
3:B:310:GLY:HA2	3:B:383:ALA:HB2	2.00	0.42
3:B:185:TYR:HA	3:B:395:PHE:CE1	2.54	0.42
3:B:6:HIS:CB	3:B:21:TRP:HZ2	2.28	0.42
3:B:40:SER:OG	3:B:43:GLN:HG3	2.19	0.42
3:B:241:CYS:SG	3:B:318:VAL:CG1	3.08	0.42
3:B:289:PRO:HA	3:B:292:THR:HG23	2.01	0.42
3:B:390:ARG:HA	3:B:390:ARG:HD2	1.57	0.42
2:A:15:GLN:NE2	5:A:502:GTP:N7	2.67	0.42
3:B:185:TYR:CD1	3:B:395:PHE:CE1	3.06	0.42
1:D:3478:VAL:CG1	1:D:3479:LYS:N	2.82	0.42
2:A:215:ARG:HG2	2:A:215:ARG:H	1.65	0.42
1:D:3474:CYS:O	1:D:3477:LEU:HB2	2.20	0.42
2:A:152:LEU:O	2:A:155:GLU:HB3	2.20	0.42
2:A:193:THR:CG2	2:A:194:THR:N	2.83	0.42
2:A:305:CYS:SG	2:A:383:ALA:CB	3.08	0.42
2:A:414:GLU:HB2	2:A:416:GLY:HA3	2.02	0.42
3:B:68:VAL:CG1	3:B:149:MET:SD	3.07	0.42
3:B:317:ALA:CB	3:B:319:PHE:CE1	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:156:LYS:HG3	3:B:156:LYS:HZ2	1.68	0.42
2:A:7:ILE:CD1	2:A:137:VAL:HG22	2.49	0.42
1:D:3384:LYS:NZ	1:D:3384:LYS:HB2	2.35	0.42
2:A:291:ILE:CD1	2:A:373:ARG:HG3	2.49	0.42
1:D:3467:VAL:O	1:D:3470:ALA:HB3	2.19	0.42
3:B:140:SER:O	3:B:142:GLY:HA3	2.19	0.42
1:D:3444:MET:HE2	1:D:3444:MET:HB3	1.86	0.42
1:D:3436:ILE:CG1	1:D:3437:ASN:HD22	2.33	0.42
2:A:158:SER:HB2	2:A:197:HIS:ND1	2.35	0.42
2:A:301:GLN:NE2	2:A:306:ASP:H	2.17	0.42
3:B:311:ARG:HA	3:B:342:TYR:O	2.19	0.42
2:A:117:LEU:HD12	2:A:121:ARG:NH1	2.35	0.41
2:A:9:VAL:HG12	2:A:138:PHE:O	2.19	0.41
2:A:175:PRO:HG2	2:A:304:LYS:CG	2.50	0.41
2:A:133:GLN:HG2	2:A:252:LEU:HB2	2.01	0.41
2:A:175:PRO:HG3	2:A:304:LYS:HG2	2.02	0.41
3:B:108:TYR:CE1	3:B:413:MET:CE	3.02	0.41
3:B:141:LEU:N	3:B:141:LEU:CD1	2.83	0.41
3:B:141:LEU:HD13	3:B:170:SER:HB2	2.01	0.41
3:B:24:ILE:HG23	3:B:25:SER:N	2.34	0.41
3:B:88:ARG:HA	3:B:89:PRO:HD3	1.87	0.41
3:B:28:HIS:O	3:B:36:TYR:CE1	2.73	0.41
2:A:103:TYR:CD2	2:A:189:LEU:HD13	2.55	0.41
3:B:115:VAL:HG21	3:B:152:LEU:HD23	2.02	0.41
3:B:320:ARG:CB	3:B:356:CYS:HB3	2.49	0.41
3:B:52:TYR:HB3	3:B:53:TYR:CE1	2.55	0.41
3:B:44:LEU:O	3:B:49:ILE:HG12	2.20	0.41
2:A:269:LEU:HD22	2:A:384:ILE:CD1	2.32	0.41
3:B:107:HIS:NE2	3:B:151:THR:HG23	2.35	0.41
3:B:390:ARG:HD3	3:B:390:ARG:HH11	1.75	0.41
1:D:3384:LYS:NZ	1:D:3386:LYS:HE3	2.34	0.41
3:B:86:ILE:HG23	3:B:87:PHE:CD1	2.54	0.41
2:A:430:LYS:O	2:A:434:GLU:HG3	2.20	0.41
1:D:3410:LEU:HD23	1:D:3410:LEU:C	2.41	0.41
3:B:223:THR:CG2	3:B:224:TYR:N	2.82	0.41
2:A:110:ILE:CG2	2:A:111:GLY:N	2.82	0.41
2:A:141:PHE:HB2	2:A:173:PRO:HD3	2.02	0.41
2:A:190:THR:O	2:A:193:THR:HG22	2.20	0.41
2:A:301:GLN:HE21	2:A:303:VAL:HG12	1.84	0.41
2:A:229:ARG:HH22	2:A:363:VAL:HG11	1.84	0.41
3:B:151:THR:OG1	3:B:193:GLN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:67:LEU:HD21	3:B:87:PHE:CD2	2.55	0.41
1:D:3457:LEU:O	1:D:3463:ASP:HB3	2.20	0.41
3:B:28:HIS:O	3:B:36:TYR:HE1	2.03	0.41
2:A:436:GLY:C	2:A:438:ASP:H	2.23	0.41
2:A:149:PHE:O	2:A:152:LEU:HG	2.20	0.41
1:D:3384:LYS:HZ2	1:D:3386:LYS:HG3	1.86	0.41
1:D:3427:MET:HG3	3:B:196:GLU:OE1	2.20	0.41
2:A:31:GLN:CB	2:A:32:PRO:CD	2.91	0.41
1:D:3432:ILE:CD1	1:D:3433:THR:N	2.82	0.41
2:A:104:ALA:CB	2:A:413:MET:CG	2.97	0.41
2:A:210:TYR:HA	2:A:210:TYR:HD1	1.56	0.41
2:A:238:ILE:HA	2:A:238:ILE:HD13	1.89	0.41
2:A:305:CYS:HG	2:A:384:ILE:HD13	1.80	0.41
3:B:242:LEU:HB3	3:B:250:ALA:O	2.20	0.41
2:A:217:LEU:HD23	2:A:217:LEU:N	2.32	0.41
3:B:267:PHE:HB2	3:B:384:ILE:CD1	2.51	0.41
2:A:19:ALA:CB	2:A:228:ASN:HB3	2.46	0.41
3:B:281:GLN:HA	3:B:281:GLN:OE1	2.20	0.41
1:D:3385:LYS:HZ1	3:B:196:GLU:HG2	1.86	0.41
1:D:3457:LEU:CD1	1:D:3458:GLU:N	2.83	0.41
1:D:3456:TYR:O	1:D:3462:PHE:HB3	2.20	0.41
2:A:407:TRP:HE1	3:B:260:VAL:HG22	1.86	0.41
3:B:408:TYR:CG	3:B:418:PHE:HZ	2.39	0.41
2:A:422:ARG:HH12	2:A:426:ALA:CB	2.22	0.41
1:D:3433:THR:HA	1:D:3436:ILE:CD1	2.46	0.41
2:A:119:LEU:HA	2:A:122:ILE:CG1	2.51	0.41
2:A:244:PHE:HD1	2:A:245:ASP:H	1.65	0.41
2:A:69:ASP:CB	2:A:75:ILE:CD1	2.94	0.41
3:B:133:GLN:HG2	3:B:252:LEU:CD1	2.34	0.41
3:B:314:THR:CG2	3:B:315:VAL:N	2.83	0.41
2:A:185:TYR:HA	2:A:185:TYR:HD1	1.57	0.41
2:A:63:PRO:CG	2:A:87:PHE:HA	2.51	0.41
1:D:3423:ARG:NH1	3:B:158:ARG:HD2	2.14	0.41
1:D:3424:LYS:HE3	3:B:155:SER:O	2.20	0.41
1:D:3384:LYS:HG3	1:D:3386:LYS:HB2	2.03	0.41
3:B:88:ARG:O	3:B:91:ASN:HB2	2.21	0.41
1:D:3457:LEU:HD12	1:D:3458:GLU:CA	2.51	0.41
3:B:76:ASP:HA	3:B:79:ARG:CG	2.49	0.41
2:A:172:TYR:C	2:A:172:TYR:CD1	2.94	0.41
2:A:407:TRP:NE1	3:B:260:VAL:HG23	2.36	0.41
3:B:133:GLN:HE22	3:B:253:ARG:HG3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:359:PRO:HA	2:A:360:PRO:HD3	1.92	0.41
2:A:371:VAL:HG12	2:A:373:ARG:N	2.30	0.41
3:B:64:ARG:HG2	3:B:125:GLU:HB3	2.02	0.41
3:B:223:THR:HG22	3:B:225:GLY:H	1.86	0.41
2:A:103:TYR:CE2	2:A:413:MET:HE1	2.56	0.40
2:A:404:PHE:CE2	3:B:258:ASN:O	2.74	0.40
3:B:261:PRO:HB2	3:B:262:PHE:HD2	1.80	0.40
3:B:259:MET:CE	3:B:268:PHE:CE1	3.04	0.40
3:B:325:MET:CE	3:B:355:VAL:CG2	2.98	0.40
3:B:184:PRO:HB3	3:B:394:GLN:HB2	2.03	0.40
3:B:4:ILE:CG2	3:B:136:GLN:HG2	2.51	0.40
3:B:7:ILE:CB	3:B:137:LEU:CD1	2.95	0.40
3:B:7:ILE:CD1	3:B:66:ILE:HD11	2.51	0.40
1:D:3412:LEU:HD22	1:D:3431:PHE:HZ	1.85	0.40
1:D:3477:LEU:H	1:D:3477:LEU:HD12	1.85	0.40
3:B:167:ASN:HB3	3:B:202:TYR:CE1	2.50	0.40
3:B:288:VAL:HB	3:B:289:PRO:HD3	2.03	0.40
3:B:396:THR:HA	3:B:399:PHE:HB3	2.02	0.40
2:A:276:ILE:HD13	2:A:277:SER:O	2.22	0.40
1:D:3444:MET:HG2	1:D:3445:THR:N	2.36	0.40
2:A:72:PRO:HG3	2:A:96:LYS:CA	2.44	0.40
3:B:406:HIS:CE1	3:B:407:TRP:CE2	3.09	0.40
2:A:233:GLN:HG3	2:A:272:TYR:CZ	2.56	0.40
1:D:3418:GLU:CG	1:D:3419:TRP:N	2.85	0.40
1:D:3464:TYR:CE1	1:D:3468:ASN:CG	2.95	0.40
1:D:3462:PHE:CD1	1:D:3462:PHE:O	2.74	0.40
2:A:117:LEU:CD1	2:A:121:ARG:HH22	2.31	0.40
3:B:276:THR:O	7:B:502:TA1:H192	2.21	0.40
3:B:64:ARG:HG3	3:B:125:GLU:CD	2.41	0.40
2:A:180:ALA:HB3	2:A:183:GLU:HB2	2.04	0.40
2:A:26:LEU:HD12	2:A:26:LEU:HA	1.90	0.40
2:A:402:ARG:NE	2:A:405:VAL:HG12	2.28	0.40
3:B:199:ASP:HA	3:B:265:LEU:HB2	2.04	0.40
3:B:425:MET:HA	3:B:428:LEU:HB3	2.02	0.40
2:A:219:ILE:O	2:A:222:PRO:HD3	2.22	0.40
1:D:3477:LEU:CD1	1:D:3477:LEU:N	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	106/108 (98%)	100 (94%)	5 (5%)	1 (1%)	21	67
2	A	408/451 (90%)	374 (92%)	23 (6%)	11 (3%)	6	45
3	B	424/445 (95%)	386 (91%)	31 (7%)	7 (2%)	11	55
All	All	938/1004 (93%)	860 (92%)	59 (6%)	19 (2%)	14	51

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	276	ILE
2	A	437	VAL
3	B	38	GLY
3	B	130	ASP
3	B	282	GLN
3	B	287	THR
3	B	344	VAL
2	A	100	ALA
2	A	111	GLY
2	A	249	ASN
1	D	3483	ALA
2	A	342	GLN
2	A	413	MET
2	A	148	GLY
2	A	31	GLN
2	A	307	PRO
3	B	82	PRO
2	A	412	GLY
3	B	32	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	95/95 (100%)	73 (77%)	22 (23%)	1	7
2	A	347/377 (92%)	260 (75%)	87 (25%)	1	6
3	B	367/381 (96%)	262 (71%)	105 (29%)	0	3
All	All	809/853 (95%)	595 (74%)	214 (26%)	3	5

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3384	LYS
1	D	3389	ASP
1	D	3392	LYS
1	D	3396	LYS
1	D	3405	MET
1	D	3408	VAL
1	D	3415	LYS
1	D	3422	ILE
1	D	3423	ARG
1	D	3424	LYS
1	D	3426	ILE
1	D	3428	GLU
1	D	3430	ASN
1	D	3431	PHE
1	D	3432	ILE
1	D	3444	MET
1	D	3449	ARG
1	D	3452	ILE
1	D	3454	LYS
1	D	3456	TYR
1	D	3459	ASP
1	D	3484	GLN
2	A	4	CYS
2	A	16	ILE
2	A	21	TRP
2	A	24	TYR

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Mol	Chain	Res	Type
2	A	25	CYS
2	A	26	LEU
2	A	32	PRO
2	A	76	ASP
2	A	85	GLN
2	A	91	GLN
2	A	93	ILE
2	A	96	LYS
2	A	98	ASP
2	A	101	ASN
2	A	105	ARG
2	A	108	TYR
2	A	112	LYS
2	A	117	LEU
2	A	120	ASP
2	A	122	ILE
2	A	123	ARG
2	A	128	GLN
2	A	129	CYS
2	A	130	THR
2	A	135	PHE
2	A	141	PHE
2	A	154	MET
2	A	164	LYS
2	A	166	LYS
2	A	170	SER
2	A	172	TYR
2	A	192	HIS
2	A	207	GLU
2	A	210	TYR
2	A	212	ILE
2	A	214	ARG
2	A	215	ARG
2	A	217	LEU
2	A	224	TYR
2	A	229	ARG
2	A	231	ILE
2	A	234	ILE
2	A	241	SER
2	A	242	LEU
2	A	244	PHE
2	A	248	LEU

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Mol	Chain	Res	Type
2	A	251	ASP
2	A	253	THR
2	A	260	VAL
2	A	264	ARG
2	A	269	LEU
2	A	276	ILE
2	A	284	GLU
2	A	300	ASN
2	A	301	GLN
2	A	303	VAL
2	A	305	CYS
2	A	308	ARG
2	A	311	LYS
2	A	317	LEU
2	A	320	ARG
2	A	326	LYS
2	A	337	THR
2	A	339	ARG
2	A	344	VAL
2	A	345	ASP
2	A	346	TRP
2	A	347	CYS
2	A	349	THR
2	A	352	LYS
2	A	370	LYS
2	A	372	GLN
2	A	377	MET
2	A	378	LEU
2	A	390	ARG
2	A	398	MET
2	A	401	LYS
2	A	402	ARG
2	A	405	VAL
2	A	413	MET
2	A	417	GLU
2	A	424	ASP
2	A	425	MET
2	A	428	LEU
2	A	430	LYS
2	A	431	ASP
2	A	432	TYR
3	B	7	ILE

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Mol	Chain	Res	Type
3	B	8	GLN
3	B	14	ASN
3	B	24	ILE
3	B	26	ASP
3	B	33	THR
3	B	41	ASP
3	B	44	LEU
3	B	53	TYR
3	B	54	ASN
3	B	64	ARG
3	B	66	ILE
3	B	67	LEU
3	B	76	ASP
3	B	79	ARG
3	B	88	ARG
3	B	90	ASP
3	B	94	PHE
3	B	97	SER
3	B	101	ASN
3	B	116	ASP
3	B	117	SER
3	B	124	LYS
3	B	126	SER
3	B	135	PHE
3	B	138	THR
3	B	140	SER
3	B	141	LEU
3	B	145	THR
3	B	153	LEU
3	B	154	ILE
3	B	156	LYS
3	B	158	ARG
3	B	160	GLU
3	B	161	TYR
3	B	164	ARG
3	B	165	ILE
3	B	178	SER
3	B	186	ASN
3	B	193	GLN
3	B	198	THR
3	B	207	GLU
3	B	209	LEU

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Mol	Chain	Res	Type
3	B	211	ASP
3	B	213	CYS
3	B	218	LYS
3	B	219	LEU
3	B	221	THR
3	B	224	TYR
3	B	230	LEU
3	B	236	SER
3	B	240	THR
3	B	241	CYS
3	B	243	ARG
3	B	259	MET
3	B	265	LEU
3	B	275	LEU
3	B	277	SER
3	B	278	ARG
3	B	280	SER
3	B	282	GLN
3	B	283	TYR
3	B	284	ARG
3	B	288	VAL
3	B	293	GLN
3	B	294	GLN
3	B	299	LYS
3	B	306	ASP
3	B	308	ARG
3	B	309	HIS
3	B	311	ARG
3	B	320	ARG
3	B	322	ARG
3	B	323	MET
3	B	325	MET
3	B	330	GLU
3	B	337	ASN
3	B	342	TYR
3	B	343	PHE
3	B	344	VAL
3	B	346	TRP
3	B	352	LYS
3	B	369	ARG
3	B	372	LYS
3	B	376	THR

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Mol	Chain	Res	Type
3	B	378	ILE
3	B	380	ASN
3	B	384	ILE
3	B	385	GLN
3	B	390	ARG
3	B	400	ARG
3	B	401	ARG
3	B	402	LYS
3	B	405	LEU
3	B	409	THR
3	B	413	MET
3	B	419	THR
3	B	423	SER
3	B	425	MET
3	B	427	ASP
3	B	428	LEU
3	B	430	SER
3	B	431	GLU
3	B	432	TYR
3	B	437	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	3437	ASN
1	D	3484	GLN
2	A	11	GLN
2	A	15	GLN
2	A	61	HIS
2	A	101	ASN
2	A	102	ASN
2	A	107	HIS
2	A	128	GLN
2	A	133	GLN
2	A	139	HIS
2	A	216	ASN
2	A	226	ASN
2	A	256	GLN
2	A	301	GLN
2	A	372	GLN
2	A	380	ASN
3	B	8	GLN

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Mol	Chain	Res	Type
3	B	14	ASN
3	B	43	GLN
3	B	54	ASN
3	B	91	ASN
3	B	101	ASN
3	B	102	ASN
3	B	107	HIS
3	B	133	GLN
3	B	136	GLN
3	B	139	HIS
3	B	167	ASN
3	B	186	ASN
3	B	258	ASN
3	B	282	GLN
3	B	300	ASN
3	B	334	ASN
3	B	336	GLN
3	B	337	ASN
3	B	349	ASN
3	B	380	ASN
3	B	406	HIS
3	B	424	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	GTP	A	502	4	26,34,34	1.34	1 (3%)	29,54,54	2.28	4 (13%)
6	GDP	B	501	-	24,30,30	2.65	8 (33%)	26,47,47	3.29	9 (34%)
7	TA1	B	502	-	68,68,68	1.93	20 (29%)	102,105,105	1.31	8 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	502	4	-	0/18/38/38	0/3/3/3
6	GDP	B	501	-	-	0/12/32/32	0/3/3/3
7	TA1	B	502	-	-	0/41/127/127	0/5/7/7

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	502	TA1	C08-C07	-4.92	1.25	1.38
6	B	501	GDP	PB-O2B	-4.19	1.40	1.54
7	B	502	TA1	C04-C03	-2.38	1.44	1.49
7	B	502	TA1	C10-C02	2.04	1.62	1.57
7	B	502	TA1	C41-C42	2.04	1.42	1.38
6	B	501	GDP	O3'-C3'	2.06	1.47	1.43
7	B	502	TA1	C37-C29	2.11	1.54	1.51
7	B	502	TA1	C18-C20	2.12	1.62	1.56
7	B	502	TA1	C11-C10	2.16	1.61	1.55
7	B	502	TA1	C01-C45	2.17	1.66	1.56
7	B	502	TA1	C16-C15	2.19	1.56	1.52
6	B	501	GDP	C5-C4	2.37	1.45	1.40
7	B	502	TA1	C26-C25	2.43	1.56	1.51
7	B	502	TA1	C43-C26	2.47	1.58	1.52
6	B	501	GDP	PB-O3B	2.61	1.63	1.54
7	B	502	TA1	C43-C01	2.81	1.60	1.54
7	B	502	TA1	C46-C45	2.87	1.59	1.53
7	B	502	TA1	C25-C24	3.06	1.39	1.34
6	B	501	GDP	C8-N7	3.33	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	502	TA1	C45-C24	3.38	1.61	1.54
7	B	502	TA1	O02-C03	3.42	1.42	1.34
7	B	502	TA1	C36-C31	3.53	1.45	1.39
6	B	501	GDP	O6-C6	4.03	1.34	1.24
7	B	502	TA1	C18-C10	4.15	1.68	1.57
7	B	502	TA1	C05-C04	4.56	1.46	1.39
5	A	502	GTP	C6-N1	4.76	1.41	1.33
7	B	502	TA1	C06-C05	5.68	1.50	1.38
6	B	501	GDP	O4'-C1'	6.02	1.49	1.41
6	B	501	GDP	C2-N1	7.29	1.49	1.35

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	GDP	C6-C5-C4	-9.89	109.55	120.86
5	A	502	GTP	C5-C6-N1	-7.76	113.38	123.52
6	B	501	GDP	N2-C2-N1	-5.68	107.83	117.20
6	B	501	GDP	N3-C2-N1	-5.39	120.23	127.56
7	B	502	TA1	C06-C05-C04	-4.81	114.61	120.35
7	B	502	TA1	C05-C04-C03	-3.92	111.54	120.38
5	A	502	GTP	N3-C2-N1	-3.51	122.78	127.56
6	B	501	GDP	C1'-N9-C4	-2.65	123.84	126.81
7	B	502	TA1	O04-C11-C14	-2.49	101.75	108.08
5	A	502	GTP	C6-C5-C4	-2.08	118.48	120.86
6	B	501	GDP	C6-N1-C2	2.01	118.24	115.88
6	B	501	GDP	O2'-C2'-C3'	2.25	119.14	111.86
7	B	502	TA1	O01-C01-C43	2.52	113.40	106.82
7	B	502	TA1	C17-C18-C20	2.54	109.75	102.14
7	B	502	TA1	C45-C01-C02	3.06	115.17	111.64
6	B	501	GDP	C2'-C3'-C4'	3.19	109.17	102.64
7	B	502	TA1	C09-C04-C03	3.57	128.41	120.38
6	B	501	GDP	C4'-O4'-C1'	4.11	114.00	109.64
7	B	502	TA1	C07-C08-C09	5.12	127.31	120.20
5	A	502	GTP	C6-N1-C2	7.47	124.64	115.88
6	B	501	GDP	N2-C2-N3	7.57	131.93	117.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	502	GTP	3	0
6	B	501	GDP	1	0
7	B	502	TA1	8	0

## 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.