



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:59 am BST

PDB ID : 5VSW  
Title : X-ray crystal structure of Escherichia coli RNA polymerase and DksA/ppGpp complex  
Authors : Murakami, K.S.; Molodtsov, V.  
Deposited on : 2017-05-12  
Resolution : 4.29 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

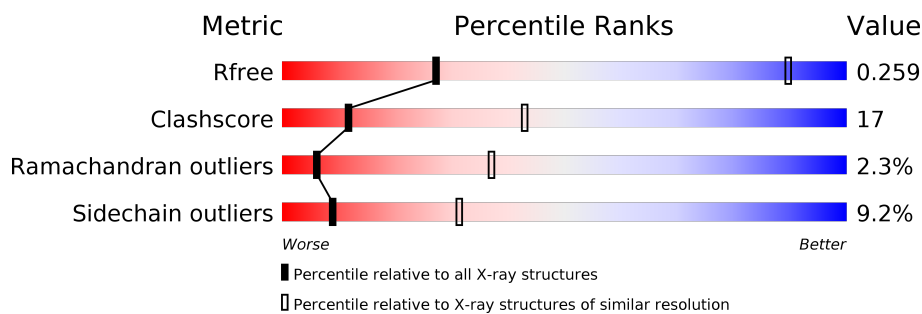
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.29 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	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	329	50% 36% 9% . .
1	B	329	43% 38% 7% . 10%
1	G	329	42% 24% . 31%
1	H	329	40% 24% . 34%
2	C	1342	60% 36% .
2	I	1342	61% 35% .
3	D	1407	49% 30% . 17%

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Mol	Chain	Length	Quality of chain
3	J	1407	
4	E	91	
4	K	91	
5	F	613	
5	L	613	
6	M	151	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 57643 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2490	1557	439	486	8			
1	B	297	Total	C	N	O	S	0	0	0
			2297	1439	403	447	8			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10570	6631	1841	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1173	Total	C	N	O	S	0	0	0
			9095	5718	1628	1703	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	46			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is a protein called RNA polymerase-binding transcription factor DksA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	140	Total	C	N	O	S	0	0	0
			1140	703	206	224	7			

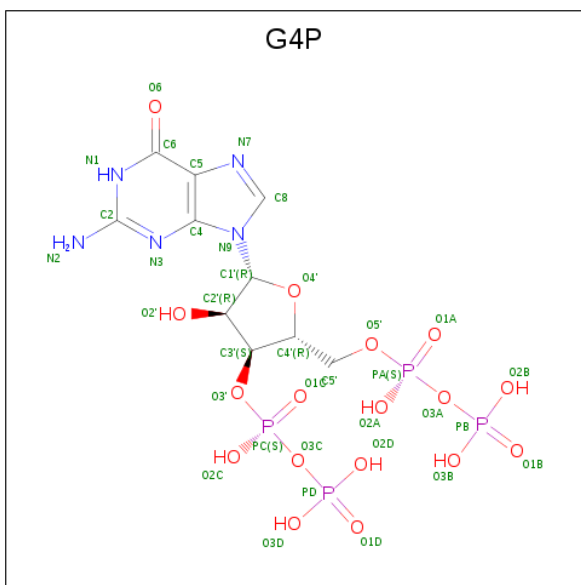
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	2	Total	Zn	0	0
			2	2		
8	D	2	Total	Zn	0	0
			2	2		
8	M	1	Total	Zn	0	0
			1	1		

- Molecule 9 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>5</sub>O<sub>17</sub>P<sub>4</sub>).



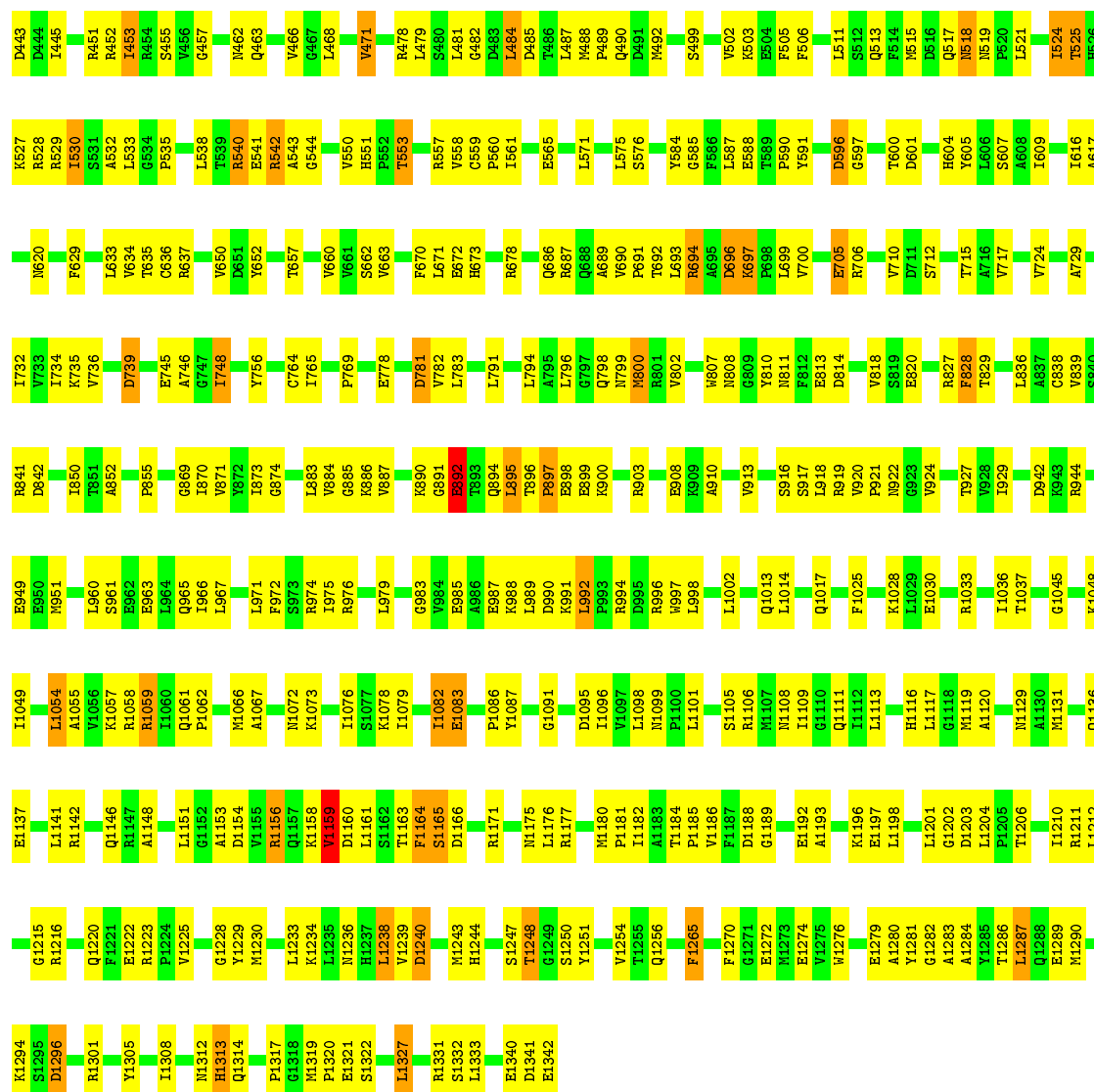
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	E	1	Total 36	C 10	N 5	O 17	P 4	0	0
9	J	1	Total 36	C 10	N 5	O 17	P 4	0	0
9	M	1	Total 36	C 10	N 5	O 17	P 4	0	0





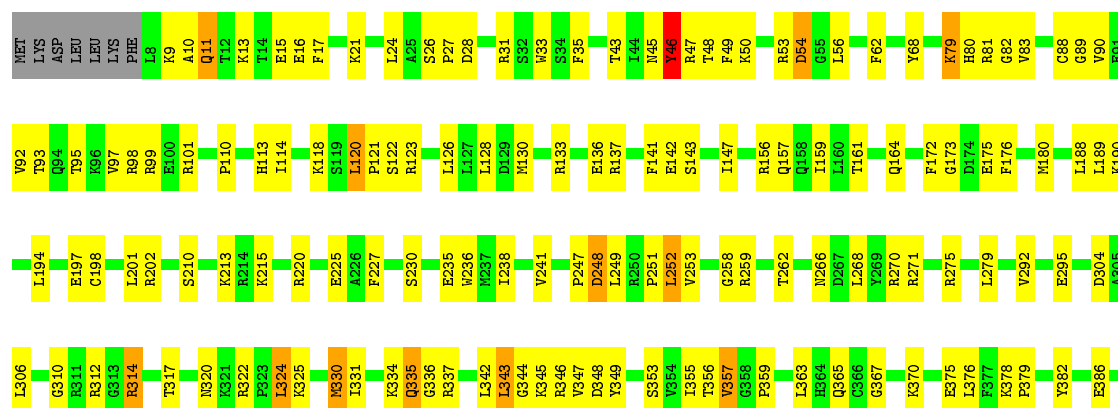






• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D: 49% 30% 17%



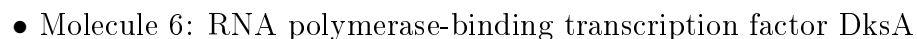


Frequency	Percentage
Daily	48%
Often	31%
Sometimes	1%
Never	18%









Response	Percentage
Yes	44%
No	46%
Don't know	7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	187.27Å 205.26Å 311.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.82 – 4.29 49.55 – 4.30	Depositor EDS
% Data completeness (in resolution range)	93.7 (46.82-4.29) 81.4 (49.55-4.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.85 (at 4.29Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.221 , 0.259 0.221 , 0.259	Depositor DCC
$R_{free}$ test set	1967 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	187.9	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 225.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	57643	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	279.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: G4P, ZN, 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	0.29	0/2524	0.62	1/3421 (0.0%)
1	B	0.31	0/2326	0.77	2/3153 (0.1%)
1	G	0.27	0/1777	0.56	0/2408
1	H	0.27	0/1681	0.61	1/2278 (0.0%)
2	C	0.29	0/10739	0.56	1/14489 (0.0%)
2	I	0.28	0/10735	0.54	1/14484 (0.0%)
3	D	0.29	0/9235	0.57	0/12472
3	J	0.28	0/9140	0.57	1/12341 (0.0%)
4	E	0.28	0/693	0.49	0/935
4	K	0.26	0/629	0.58	1/847 (0.1%)
5	F	0.26	0/3864	0.53	1/5194 (0.0%)
5	L	0.27	0/3872	0.51	0/5205
6	M	0.36	0/1155	0.65	1/1549 (0.1%)
All	All	0.29	0/58370	0.57	10/78776 (0.0%)

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	B	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	3	ARG	N-CA-C	-6.51	93.41	111.00
1	A	318	LEU	CA-CB-CG	6.18	129.50	115.30
3	J	1221	LEU	CA-CB-CG	5.99	129.08	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	236	LYS	N-CA-C	5.86	126.82	111.00
1	B	318	LEU	CA-CB-CG	5.77	128.56	115.30
1	H	65	LEU	CA-CB-CG	5.56	128.09	115.30
2	I	236	LYS	N-CA-C	5.46	125.76	111.00
5	F	608	ARG	NE-CZ-NH1	5.43	123.01	120.30
6	M	95	LEU	CA-CB-CG	5.30	127.50	115.30
1	B	82	LEU	CA-CB-CG	5.13	127.11	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	323	PRO	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	A	2490	0	2542	123	0
1	B	2297	0	2350	144	1
1	G	1755	0	1773	60	0
1	H	1662	0	1687	57	0
2	C	10570	0	10582	390	0
2	I	10566	0	10576	362	0
3	D	9095	0	9222	376	0
3	J	9001	0	9167	366	1
4	E	691	0	695	25	0
4	K	627	0	634	28	0
5	F	3813	0	3880	125	0
5	L	3821	0	3884	119	0
6	M	1140	0	1119	63	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
8	M	1	0	0	0	0
9	E	36	0	11	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	J	36	0	11	4	0
9	M	36	0	11	7	0
All	All	57643	0	58144	2018	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (2018) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:GLU:HB3	1:B:30:PRO:CD	1.26	1.46
1:B:29:GLU:CB	1:B:30:PRO:HD2	1.35	1.45
1:B:279:GLY:HA3	1:B:321:TRP:CZ2	1.55	1.41
5:F:600:HIS:O	5:F:604:SER:HB3	1.33	1.29
1:B:253:LEU:O	1:B:321:TRP:HZ2	0.98	1.26
1:B:253:LEU:O	1:B:321:TRP:CZ2	1.88	1.24
2:C:106:GLU:CB	2:C:109:ALA:HB2	1.67	1.24
1:B:29:GLU:O	1:B:31:LEU:HD22	1.36	1.20
5:F:600:HIS:O	5:F:604:SER:CB	1.93	1.16
1:B:29:GLU:CB	1:B:30:PRO:CD	2.02	1.13
5:F:600:HIS:CD2	5:F:601:PRO:HD3	1.86	1.09
2:C:106:GLU:HB3	2:C:109:ALA:CB	1.82	1.09
3:J:863:LEU:HD11	3:J:901:ARG:HG2	1.24	1.09
2:C:236:LYS:O	2:C:237:LEU:HB2	1.29	1.08
5:F:600:HIS:HD2	5:F:601:PRO:HD3	1.14	1.05
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.36	1.04
1:B:29:GLU:O	1:B:31:LEU:CD2	2.05	1.03
1:B:279:GLY:HA3	1:B:321:TRP:CH2	1.93	1.02
2:I:236:LYS:O	2:I:237:LEU:CB	2.01	1.02
3:D:1372:ARG:HA	3:J:853:THR:HG21	1.39	1.00
6:M:23:TYR:N	6:M:127:GLU:OE2	1.94	1.00
2:C:236:LYS:O	2:C:237:LEU:CB	2.10	0.97
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.47	0.96
2:C:106:GLU:HB3	2:C:109:ALA:HB2	0.96	0.95
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.48	0.94
2:I:236:LYS:O	2:I:237:LEU:HB2	1.17	0.94
1:B:279:GLY:CA	1:B:321:TRP:CZ2	2.50	0.93
1:A:316:MET:SD	5:F:600:HIS:HE1	1.92	0.92
3:D:929:GLN:NE2	6:M:66:ALA:O	2.02	0.92
1:A:316:MET:SD	5:F:600:HIS:CE1	2.63	0.92
4:K:3:ARG:O	4:K:4:VAL:HB	1.70	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:863:LEU:HD11	3:D:901:ARG:HG2	1.53	0.91
3:J:863:LEU:CD1	3:J:901:ARG:HG2	2.03	0.89
3:J:863:LEU:HD11	3:J:901:ARG:CG	2.01	0.89
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.06	0.89
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.52	0.88
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.37	0.88
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.54	0.88
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.52	0.88
3:D:1159:ILE:HG22	3:D:1177:ILE:HD12	1.56	0.87
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.54	0.86
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.40	0.86
1:B:29:GLU:CG	1:B:30:PRO:HD3	2.06	0.86
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.57	0.86
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.57	0.86
1:A:296:GLY:H	1:A:299:SER:HB2	1.38	0.85
2:I:119:GLU:HG3	2:I:489:PRO:HD2	1.59	0.85
3:J:1198:VAL:HB	3:J:1210:ILE:HG23	1.57	0.85
1:B:296:GLY:H	1:B:299:SER:HB2	1.43	0.84
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.59	0.84
3:D:905:ARG:HH21	3:D:907:HIS:HB2	1.42	0.84
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.60	0.84
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.42	0.83
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.44	0.83
2:C:235:ASN:O	2:C:236:LYS:HB2	1.78	0.83
1:B:323:PRO:HA	1:B:324:ALA:HB2	1.60	0.83
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.11	0.82
3:D:936:HIS:HA	3:D:1135:THR:HA	1.61	0.82
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.24	0.82
2:I:235:ASN:O	2:I:236:LYS:HB2	1.76	0.82
1:B:29:GLU:CG	1:B:30:PRO:CD	2.57	0.82
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.59	0.82
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.62	0.82
6:M:121:ILE:HG23	6:M:125:ARG:HH11	1.45	0.81
3:J:853:THR:HG22	3:J:854:ALA:H	1.44	0.81
1:G:45:ARG:HG2	1:H:38:THR:HB	1.62	0.81
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.62	0.81
2:C:1002:LEU:HD22	2:C:1007:LYS:HB2	1.62	0.81
2:I:942:ASP:OD2	2:I:1048:LYS:NZ	2.14	0.80
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.62	0.80
6:M:105:LYS:NZ	6:M:133:ASP:OD2	2.14	0.80
1:A:228:LEU:HD11	1:B:224:LEU:HD23	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.27	0.79
2:C:106:GLU:C	2:C:109:ALA:H	1.86	0.79
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.64	0.79
3:J:430:HIS:HD2	3:J:432:LEU:HB2	1.47	0.79
3:J:746:LEU:HD22	3:J:754:ILE:HD11	1.64	0.78
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.66	0.78
3:D:1372:ARG:HA	3:J:853:THR:CG2	2.13	0.78
2:I:268:ARG:HH21	2:I:270:THR:HG22	1.48	0.78
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.66	0.78
1:A:224:LEU:HD23	1:B:228:LEU:HD11	1.64	0.77
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.66	0.77
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.66	0.77
1:B:279:GLY:HA3	1:B:321:TRP:CE2	2.19	0.77
3:J:362:ARG:NH2	9:J:2004:G4P:O4'	2.17	0.77
1:A:150:ARG:NH1	1:B:7:GLU:O	2.17	0.77
1:B:83:LEU:HD21	3:D:526:VAL:HB	1.65	0.77
3:J:901:ARG:HB2	3:J:908:ILE:HA	1.66	0.77
3:D:430:HIS:HD2	3:D:432:LEU:HB2	1.50	0.77
4:K:40:PRO:O	4:K:52:ARG:NH2	2.18	0.77
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.65	0.77
6:M:121:ILE:HG23	6:M:125:ARG:NH1	2.00	0.77
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.65	0.76
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.50	0.76
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.67	0.76
3:J:137:ARG:HG2	3:J:142:GLU:HB2	1.66	0.76
2:I:1160:ASP:HB2	2:I:1161:LEU:HA	1.66	0.76
5:L:573:LEU:HD12	5:L:588:ARG:HE	1.49	0.76
2:C:106:GLU:H	2:C:109:ALA:HB3	1.51	0.76
2:I:6:THR:OG1	2:I:781:ASP:OD2	2.04	0.76
2:I:870:ILE:HG13	2:I:884:VAL:HG22	1.68	0.76
3:J:709:ARG:O	3:J:711:GLY:N	2.19	0.76
2:I:705:GLU:HB2	2:I:794:LEU:H	1.50	0.76
1:B:29:GLU:CB	1:B:30:PRO:HD3	2.14	0.76
9:J:2004:G4P:O3D	4:K:2:ALA:N	2.18	0.76
3:J:901:ARG:CB	3:J:908:ILE:HA	2.15	0.75
1:B:119:GLY:HA3	1:B:271:LYS:HG2	1.68	0.75
1:B:27:THR:HG23	1:B:202:VAL:HG22	1.66	0.75
3:D:1136:GLY:HA2	3:D:1140:ARG:HG2	1.69	0.75
3:J:482:ALA:HA	4:K:6:VAL:HG11	1.69	0.75
3:D:660:GLU:HG3	6:M:12:LEU:HD23	1.68	0.75
2:I:1148:ALA:HA	2:I:1201:LEU:HD21	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.69	0.74
5:L:420:GLU:OE1	5:L:423:ARG:NH2	2.19	0.74
5:L:573:LEU:H	5:L:573:LEU:HD23	1.53	0.74
2:I:30:ILE:HD12	2:I:30:ILE:H	1.50	0.74
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.52	0.74
3:D:310:GLY:HA2	3:D:314:ARG:HD2	1.70	0.74
3:J:48:THR:O	3:J:50:LYS:N	2.20	0.74
1:B:119:GLY:H	1:B:271:LYS:HE3	1.51	0.74
3:D:490:ILE:HD13	3:D:490:ILE:H	1.52	0.74
1:H:134:THR:HG23	1:H:135:ASP:H	1.53	0.74
3:J:123:ARG:HH22	3:J:1334:GLU:HG3	1.53	0.74
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.69	0.74
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.20	0.73
2:C:4:SER:HB3	2:C:7:GLU:HG3	1.70	0.73
3:D:615:LYS:NZ	9:E:101:G4P:O1C	2.20	0.73
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	1.70	0.73
2:C:557:ARG:HB3	2:C:587:LEU:HD13	1.69	0.73
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.70	0.73
3:D:709:ARG:O	3:D:711:GLY:N	2.21	0.73
6:M:91:ARG:NH1	9:M:202:G4P:O1D	2.19	0.73
5:L:481:GLU:OE1	5:L:495:ARG:NH2	2.22	0.73
2:I:811:ASN:O	2:I:1099:ASN:ND2	2.21	0.73
5:F:101:TYR:HE2	5:F:388:ILE:HD11	1.53	0.73
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.21	0.73
6:M:94:LYS:NZ	9:M:202:G4P:O1C	2.21	0.73
1:G:228:LEU:HD21	1:H:224:LEU:HB3	1.70	0.73
4:K:32:VAL:O	4:K:34:GLY:N	2.21	0.73
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.70	0.72
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.53	0.72
2:I:1119:MET:HG3	2:I:1204:LEU:HD13	1.70	0.72
1:A:191:ARG:NH1	1:A:198:LEU:O	2.21	0.72
2:C:705:GLU:HB2	2:C:794:LEU:H	1.53	0.72
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.70	0.72
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.71	0.72
1:A:252:ILE:HG21	1:A:312:LEU:HD11	1.70	0.72
2:I:1129:ASN:HB2	2:I:1177:ARG:HB2	1.70	0.72
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.72	0.72
4:K:14:GLY:O	4:K:16:ARG:N	2.22	0.72
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.54	0.72
2:C:678:ARG:NH1	2:C:1071:GLY:O	2.23	0.72
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:226:GLU:HB3	1:H:10:LYS:HE3	1.72	0.71
3:D:1298:VAL:H	3:D:1299:GLY:HA3	1.53	0.71
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.25	0.71
2:I:748:ILE:HD11	2:I:966:ILE:HG22	1.72	0.71
2:C:74:ARG:NH1	2:C:121:GLU:OE1	2.22	0.71
2:C:974:ARG:HD2	2:C:1014:LEU:HD21	1.72	0.71
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.73	0.71
3:J:853:THR:O	3:J:855:ASP:N	2.24	0.71
5:F:470:MET:HB2	5:F:478:PRO:HG3	1.73	0.71
5:F:600:HIS:O	5:F:604:SER:HB2	1.87	0.71
2:C:898:GLU:HB3	5:F:540:LEU:HD22	1.71	0.70
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.72	0.70
3:J:844:THR:OG1	3:J:860:ARG:O	2.08	0.70
1:B:279:GLY:CA	1:B:321:TRP:CH2	2.72	0.70
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.24	0.70
2:C:138:ILE:HD11	2:C:506:PHE:HB3	1.73	0.70
2:I:533:LEU:HD13	2:I:540:ARG:HE	1.57	0.70
2:I:885:GLY:HA2	2:I:917:SER:HB3	1.74	0.70
3:D:48:THR:O	3:D:50:LYS:N	2.25	0.70
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.74	0.70
2:C:106:GLU:N	2:C:109:ALA:HB3	2.07	0.70
2:I:550:VAL:HG11	3:J:776:THR:HG22	1.74	0.70
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.25	0.69
2:I:739:ASP:N	2:I:739:ASP:OD1	2.26	0.69
3:D:495:ASN:O	3:D:497:GLU:N	2.25	0.69
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.72	0.69
5:F:600:HIS:CD2	5:F:601:PRO:CD	2.71	0.69
2:C:395:TYR:HD2	2:C:419:ILE:HG22	1.57	0.69
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.75	0.69
1:G:224:LEU:HD13	1:H:228:LEU:HD11	1.75	0.69
2:I:4:SER:OG	2:I:5:TYR:N	2.26	0.69
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.75	0.69
3:D:674:THR:HG21	6:M:139:LYS:HG2	1.74	0.69
3:D:17:PHE:O	3:D:1355:ARG:NH2	2.24	0.69
3:D:418:GLU:HG3	4:E:45:LYS:H	1.57	0.69
1:B:79:LEU:HD11	3:D:526:VAL:HG11	1.74	0.69
3:D:673:VAL:HB	6:M:129:ARG:NH1	2.08	0.69
1:B:289:LEU:HD13	1:B:300:LEU:HD21	1.75	0.69
2:I:151:ARG:HH22	2:I:175:ARG:HH11	1.41	0.69
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.74	0.69
3:J:1167:LYS:NZ	3:J:1168:GLU:O	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1116:HIS:CE1	3:J:641:ILE:H	2.10	0.69
3:D:679:TYR:OH	3:D:754:ILE:O	2.09	0.68
3:J:430:HIS:CD2	3:J:432:LEU:HB2	2.28	0.68
2:C:1253:LEU:HD11	3:D:253:VAL:HG11	1.75	0.68
2:I:746:ALA:HB2	2:I:974:ARG:HE	1.57	0.68
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.74	0.68
1:A:14:VAL:HG22	1:A:15:ASP:H	1.58	0.68
1:A:7:GLU:HB3	1:B:150:ARG:HH12	1.56	0.68
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.75	0.68
3:D:1244:GLN:O	6:M:66:ALA:HB3	1.94	0.68
2:C:1160:ASP:CB	2:C:1161:LEU:HA	2.22	0.68
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.25	0.68
3:J:1365:TYR:OH	3:J:1369:ARG:NH1	2.26	0.68
1:B:77:ASP:OD1	1:B:77:ASP:N	2.26	0.68
2:C:168:GLY:O	2:C:170:VAL:N	2.22	0.68
3:D:1178:THR:HG23	3:D:1184:ASP:HB3	1.75	0.68
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.25	0.68
2:I:1073:LYS:HE3	3:J:462:ASP:HB2	1.74	0.68
3:J:853:THR:C	3:J:855:ASP:H	1.97	0.68
3:D:1233:ILE:O	3:D:1237:VAL:HG12	1.94	0.68
4:E:4:VAL:HG13	4:E:5:THR:H	1.59	0.68
1:G:102:LEU:HD23	1:G:115:ILE:HG12	1.75	0.68
2:I:560:PRO:O	3:J:780:ARG:NH2	2.26	0.68
2:I:17:LYS:NZ	2:I:1154:ASP:OD1	2.27	0.68
3:J:205:LEU:HD22	3:J:214:ARG:HB2	1.76	0.68
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.75	0.68
3:J:395:LYS:HG2	5:L:536:THR:HG21	1.76	0.68
2:C:798:GLN:OE1	2:C:827:ARG:HB2	1.94	0.67
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.76	0.67
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.75	0.67
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.76	0.67
3:J:331:ILE:HG22	3:J:1328:THR:HG21	1.76	0.67
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.76	0.67
3:J:1280:VAL:HG11	3:J:1304:ARG:NE	2.10	0.67
2:C:197:ARG:NH1	2:C:201:ARG:O	2.27	0.67
2:I:798:GLN:OE1	2:I:827:ARG:HB2	1.94	0.67
2:C:324:LYS:O	2:C:327:GLN:NE2	2.26	0.67
5:F:490:PRO:HB2	5:F:493:LYS:HG3	1.77	0.67
1:A:102:LEU:HD23	1:A:115:ILE:HG12	1.75	0.67
6:M:37:LEU:HD22	6:M:106:VAL:HG13	1.76	0.67
1:A:47:LEU:HD23	1:A:51:MET:HE2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.76	0.67
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.29	0.67
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.75	0.67
1:A:289:LEU:HD13	1:A:300:LEU:HD21	1.77	0.67
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.77	0.67
1:A:77:ASP:N	1:A:77:ASP:OD1	2.28	0.67
1:G:35:PHE:HE1	1:H:46:ILE:HG12	1.59	0.67
1:B:86:LYS:HE2	1:B:174:ASP:HB2	1.77	0.66
1:B:253:LEU:HB3	1:B:321:TRP:NE1	2.09	0.66
2:I:596:ASP:CG	2:I:597:GLY:H	1.97	0.66
5:L:561:MET:HA	5:L:567:MET:HE1	1.77	0.66
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.77	0.66
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.59	0.66
3:D:935:PHE:O	3:D:1136:GLY:N	2.29	0.66
3:J:17:PHE:O	3:J:1355:ARG:NH2	2.27	0.66
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.78	0.66
2:C:143:ARG:HH21	2:C:513:GLN:HA	1.61	0.66
2:C:97:ARG:HB3	2:C:121:GLU:HB3	1.77	0.66
3:D:690:ASN:ND2	3:D:745:GLY:HA2	2.11	0.66
5:F:465:ARG:HD2	5:F:468:ARG:HH22	1.60	0.66
2:C:1106:ARG:HG3	6:M:74:ASP:OD1	1.96	0.66
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.27	0.66
1:B:94:GLY:H	1:B:276:HIS:CD2	2.13	0.66
1:A:45:ARG:HE	2:C:1083:GLU:HB3	1.61	0.66
2:C:861:ALA:HB1	2:C:882:ILE:HD13	1.76	0.66
2:I:1160:ASP:CB	2:I:1161:LEU:HA	2.26	0.66
2:I:143:ARG:HH21	2:I:513:GLN:HA	1.61	0.66
3:J:495:ASN:O	3:J:497:GLU:N	2.29	0.65
2:C:1142:ARG:HH12	2:C:1169:VAL:HG21	1.60	0.65
2:I:1243:MET:HA	3:J:353:SER:HB3	1.79	0.65
3:J:287:ALA:HB3	3:J:292:VAL:HG12	1.78	0.65
1:B:100:LEU:HD23	1:B:115:ILE:HG21	1.79	0.65
3:D:932:MET:HA	3:D:1139:PRO:HD3	1.77	0.65
2:I:1244:HIS:HD2	2:I:1265:PHE:HB2	1.60	0.65
6:M:44:LEU:HD22	6:M:99:ILE:HG23	1.78	0.65
3:D:424:ASN:HB2	3:D:434:ILE:HG12	1.78	0.65
2:I:452:ARG:NH1	2:I:584:TYR:O	2.30	0.65
1:G:66:HIS:HB3	2:I:874:GLY:HA2	1.78	0.65
3:J:808:VAL:HG13	3:J:914:ALA:HA	1.78	0.65
3:D:664:ILE:HG22	3:D:678:ARG:HG2	1.77	0.65
2:C:106:GLU:CB	2:C:109:ALA:CB	2.57	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1234:LYS:HE2	2:C:1238:LEU:HD23	1.79	0.65
1:G:41:ASN:ND2	2:I:1216:ARG:O	2.29	0.65
1:A:59:VAL:HG22	1:A:144:ILE:HA	1.79	0.65
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.77	0.65
2:I:1248:THR:HG21	5:L:531:PRO:HG3	1.77	0.65
3:D:1289:ASN:O	3:D:1289:ASN:ND2	2.27	0.65
4:E:32:VAL:O	4:E:34:GLY:N	2.30	0.65
2:I:73:TYR:HB2	2:I:98:VAL:HG22	1.79	0.65
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.30	0.65
3:J:1291:GLU:HG2	3:J:1297:LYS:HD2	1.79	0.65
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.61	0.65
3:J:259:ARG:HD3	5:L:502:LYS:HD2	1.78	0.65
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.79	0.64
5:L:493:LYS:HG2	5:L:496:LYS:HE2	1.77	0.64
3:D:1167:LYS:NZ	3:D:1168:GLU:O	2.31	0.64
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.62	0.64
1:B:94:GLY:HA3	1:B:276:HIS:HB3	1.79	0.64
2:I:206:ALA:O	2:I:209:ILE:HG22	1.97	0.64
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.62	0.64
3:D:848:VAL:HG12	3:D:858:VAL:HG22	1.79	0.64
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.79	0.64
2:C:686:GLN:HG2	2:C:796:LEU:HD22	1.79	0.64
3:D:863:LEU:HD11	3:D:901:ARG:CG	2.25	0.64
2:I:168:GLY:O	2:I:170:VAL:N	2.30	0.64
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.79	0.64
2:I:1333:LEU:HD23	3:J:307:LEU:HD22	1.80	0.64
3:J:364:HIS:CE1	4:K:3:ARG:HH21	2.16	0.64
3:D:746:LEU:HG	3:D:758:PRO:HB3	1.80	0.64
3:D:793:SER:O	3:D:797:THR:HG23	1.98	0.64
2:I:1116:HIS:HE1	3:J:641:ILE:N	1.94	0.64
3:J:853:THR:HG22	3:J:854:ALA:N	2.12	0.64
3:D:473:THR:HG23	3:D:476:ALA:H	1.63	0.64
1:G:14:VAL:HG13	1:G:15:ASP:H	1.62	0.64
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.80	0.64
1:A:134:THR:HG21	2:C:727:VAL:O	1.98	0.64
2:I:898:GLU:HB3	5:L:540:LEU:HD22	1.78	0.64
1:B:253:LEU:CB	1:B:321:TRP:HE1	2.11	0.63
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.80	0.63
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.78	0.63
3:D:789:LYS:HD2	6:M:79:GLU:OE2	1.97	0.63
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.31	0.63
3:D:609:TYR:HE2	3:D:614:LEU:HD12	1.63	0.63
3:J:473:THR:HG23	3:J:476:ALA:H	1.63	0.63
1:B:119:GLY:N	1:B:271:LYS:HE3	2.13	0.63
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.30	0.63
3:D:658:GLU:O	3:D:661:VAL:HG22	1.97	0.63
3:D:668:PHE:HB2	3:D:678:ARG:HG3	1.80	0.63
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.80	0.63
2:C:106:GLU:O	2:C:109:ALA:N	2.31	0.63
2:C:211:ARG:NH1	2:C:357:ASN:O	2.32	0.63
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.80	0.63
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.80	0.63
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.64	0.63
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.81	0.63
2:I:125:GLY:HA3	2:I:499:SER:HB2	1.81	0.63
1:A:22:THR:O	1:A:207:THR:N	2.27	0.62
5:F:479:THR:HG23	5:F:481:GLU:H	1.63	0.62
2:I:1082:ILE:H	2:I:1082:ILE:HD12	1.64	0.62
2:I:97:ARG:HB3	2:I:121:GLU:HB3	1.80	0.62
3:J:268:LEU:HB3	3:J:306:LEU:HD23	1.81	0.62
3:D:677:GLU:HG2	6:M:129:ARG:NH1	2.14	0.62
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.81	0.62
1:A:237:VAL:HG13	1:B:13:LEU:H	1.62	0.62
1:G:118:ASP:HB3	1:G:121:VAL:HB	1.81	0.62
2:I:842:ASP:N	2:I:1045:GLY:O	2.30	0.62
3:D:1206:ARG:NH2	3:J:1295:ASN:OD1	2.32	0.62
6:M:94:LYS:O	6:M:98:LYS:HD2	1.98	0.62
1:B:253:LEU:HB3	1:B:321:TRP:HE1	1.65	0.62
1:G:161:SER:O	1:G:163:GLU:N	2.32	0.62
5:L:137:TYR:CE2	5:L:139:GLU:HB2	2.35	0.62
1:A:97:GLU:HB3	1:A:147:GLN:HG2	1.81	0.62
3:D:1198:VAL:HB	3:D:1210:ILE:HG23	1.80	0.62
3:D:133:ARG:NH1	3:D:136:GLU:OE1	2.32	0.62
2:I:149:LEU:O	2:I:532:ALA:HA	1.99	0.62
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.80	0.62
6:M:59:VAL:O	6:M:63:GLN:HG3	2.00	0.62
1:A:23:HIS:HE1	1:A:204:GLU:HG2	1.64	0.62
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.81	0.62
2:C:60:GLN:HB3	2:C:67:GLU:HG3	1.82	0.62
1:H:59:VAL:HG22	1:H:144:ILE:HG13	1.82	0.62
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:357:VAL:HG22	3:J:461:PHE:CE1	2.35	0.62
2:C:218:GLU:HG3	2:C:299:LYS:HA	1.81	0.62
2:C:724:VAL:HG11	2:C:727:VAL:HG22	1.80	0.62
1:H:118:ASP:HB2	1:H:121:VAL:HB	1.82	0.62
2:I:81:ASP:HA	2:I:92:TYR:HE1	1.63	0.62
3:J:50:LYS:HD3	3:J:71:LEU:HD21	1.81	0.62
2:C:678:ARG:NH2	2:C:1106:ARG:HG2	2.15	0.62
2:I:903:ARG:HE	2:I:910:ALA:HB2	1.64	0.62
2:C:360:LEU:HD22	2:C:378:ARG:HH21	1.65	0.61
2:I:839:VAL:HG12	2:I:1049:ILE:HG12	1.81	0.61
6:M:55:VAL:HG22	6:M:89:ARG:HG3	1.82	0.61
1:B:102:LEU:HD23	1:B:115:ILE:HG12	1.82	0.61
3:D:137:ARG:HD3	3:D:143:SER:HB2	1.83	0.61
3:D:252:LEU:HD23	3:D:262:THR:HB	1.81	0.61
3:J:479:GLU:HG3	4:K:20:VAL:HG11	1.82	0.61
3:D:678:ARG:HA	6:M:129:ARG:NH2	2.15	0.61
2:I:808:ASN:H	3:J:633:ALA:HB2	1.65	0.61
3:J:674:THR:OG1	3:J:677:GLU:HB2	2.00	0.61
2:C:1100:PRO:HB3	3:D:639:VAL:HG12	1.80	0.61
2:C:810:TYR:CE2	3:D:359:PRO:HD2	2.35	0.61
2:C:778:GLU:O	2:C:781:ASP:HB2	2.01	0.61
5:F:493:LYS:HA	5:F:496:LYS:HG3	1.82	0.61
1:A:45:ARG:HG2	1:B:38:THR:OG1	2.00	0.61
3:D:614:LEU:HD23	4:E:5:THR:HB	1.82	0.61
2:I:208:ILE:HG12	2:I:362:ALA:HB1	1.82	0.61
1:A:58:GLU:HG2	1:A:158:ARG:HH22	1.66	0.61
2:C:269:ILE:HA	2:C:273:HIS:ND1	2.16	0.61
2:C:1142:ARG:HD3	2:C:1161:LEU:HD22	1.82	0.61
2:C:1244:HIS:HD2	2:C:1265:PHE:HB2	1.66	0.61
3:D:935:PHE:HA	6:M:86:LEU:HD11	1.82	0.61
3:J:746:LEU:HG	3:J:758:PRO:HB3	1.83	0.61
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.83	0.60
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.83	0.60
2:I:1192:GLU:OE2	3:J:764:ARG:HD3	2.00	0.60
2:I:192:ASP:OD2	2:I:436:ARG:NH2	2.30	0.60
2:I:196:VAL:HG12	2:I:206:ALA:HA	1.82	0.60
3:J:418:GLU:HG3	4:K:45:LYS:H	1.65	0.60
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.35	0.60
5:L:117:ILE:HA	5:L:120:ALA:HB3	1.82	0.60
5:L:379:MET:O	5:L:383:ASN:ND2	2.34	0.60
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.82	0.60
1:A:16:ILE:HG12	1:A:26:VAL:HB	1.83	0.60
3:D:901:ARG:HB2	3:D:908:ILE:HA	1.84	0.60
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.37	0.60
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.82	0.60
3:J:853:THR:C	3:J:855:ASP:N	2.54	0.60
1:A:135:ASP:O	1:A:137:ASN:N	2.34	0.60
2:I:1294:LYS:HB3	3:J:347:VAL:HG13	1.82	0.60
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.83	0.60
2:I:1283:ALA:HB1	2:I:1286:THR:HB	1.83	0.60
2:I:37:LYS:HD2	2:I:46:GLN:HE21	1.66	0.60
1:A:211:ILE:HD12	1:A:215:GLU:HG2	1.84	0.60
1:A:316:MET:CE	5:F:600:HIS:NE2	2.65	0.60
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.82	0.60
2:C:135:THR:HG22	2:C:527:LYS:HE2	1.82	0.60
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.35	0.60
5:F:561:MET:HA	5:F:567:MET:HE1	1.84	0.60
2:I:176:ILE:HB	2:I:184:LEU:HB3	1.84	0.60
2:I:985:GLU:HG2	2:I:988:LYS:HD2	1.82	0.60
3:J:674:THR:O	3:J:678:ARG:HB3	2.02	0.60
5:L:412:LEU:HD13	5:L:435:ILE:HD11	1.84	0.60
1:B:179:PRO:HA	1:B:208:ASN:ND2	2.16	0.60
2:C:1119:MET:HE1	2:C:1210:ILE:HD11	1.84	0.60
2:C:466:VAL:HA	2:C:469:VAL:HG22	1.84	0.60
3:J:1290:ARG:HD2	3:J:1298:VAL:HG12	1.84	0.60
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.35	0.59
1:B:47:LEU:HD23	1:B:51:MET:HE2	1.84	0.59
2:C:550:VAL:HG11	3:D:776:THR:HG22	1.83	0.59
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.84	0.59
5:L:454:VAL:HA	5:L:457:ILE:HD12	1.84	0.59
2:C:408:SER:O	2:C:431:LYS:NZ	2.35	0.59
2:I:268:ARG:NH2	2:I:270:THR:HG22	2.17	0.59
3:D:325:LYS:HE2	3:D:330:MET:HG3	1.83	0.59
3:D:355:ILE:HG12	3:D:464:ASP:O	2.02	0.59
3:D:515:ARG:O	3:D:545:HIS:HB3	2.02	0.59
3:D:849:LEU:HD22	3:D:849:LEU:H	1.68	0.59
1:G:12:ARG:H	1:G:30:PRO:HD2	1.67	0.59
3:J:678:ARG:HA	3:J:681:LYS:HB3	1.84	0.59
1:B:93:GLN:HB2	1:B:276:HIS:CD2	2.38	0.59
5:F:493:LYS:HG2	5:F:496:LYS:HE2	1.83	0.59
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:106:GLU:H	2:C:109:ALA:CB	2.14	0.59
1:H:47:LEU:HD22	1:H:180:VAL:HG11	1.84	0.59
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.84	0.59
1:B:175:ALA:HB1	1:B:177:TYR:CE1	2.37	0.59
1:B:321:TRP:H	1:B:322:PRO:HD3	1.67	0.59
1:B:53:GLY:HA3	1:B:177:TYR:O	2.02	0.59
2:C:356:THR:HG21	2:C:362:ALA:HA	1.84	0.59
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.84	0.59
1:B:57:THR:HG22	1:B:58:GLU:HG3	1.84	0.59
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.02	0.59
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	1.84	0.59
1:A:45:ARG:NE	2:C:1083:GLU:HB3	2.17	0.59
3:D:1307:LEU:HD23	3:D:1312:ALA:HA	1.85	0.59
3:D:505:ASP:HB3	3:D:629:PHE:HE1	1.67	0.59
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.85	0.59
1:H:102:LEU:HG	1:H:115:ILE:HG12	1.83	0.59
3:J:140:TYR:O	3:J:297:ARG:NH1	2.36	0.59
2:I:1327:LEU:O	2:I:1331:ARG:HB2	2.02	0.59
2:C:723:VAL:O	2:C:735:LYS:N	2.33	0.59
2:I:515:MET:HG2	2:I:517:GLN:HB2	1.85	0.59
1:B:119:GLY:HA3	1:B:271:LYS:CG	2.33	0.58
2:C:814:ASP:CG	2:C:1106:ARG:HH12	2.05	0.58
3:D:137:ARG:HG2	3:D:142:GLU:HB2	1.85	0.58
2:I:557:ARG:HB3	2:I:587:LEU:HD13	1.85	0.58
3:J:128:LEU:HD23	3:J:192:MET:HE3	1.85	0.58
3:J:492:SER:HB2	3:J:499:ILE:HB	1.84	0.58
3:D:1165:PHE:HE1	3:D:1200:GLU:HB2	1.66	0.58
5:F:279:ARG:HB3	5:F:347:ILE:HD11	1.85	0.58
2:I:1234:LYS:HE2	2:I:1238:LEU:HD23	1.85	0.58
2:I:1240:ASP:N	2:I:1240:ASP:OD1	2.27	0.58
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.03	0.58
3:D:317:THR:HG22	3:D:322:ARG:O	2.03	0.58
3:D:673:VAL:HB	6:M:129:ARG:HH12	1.67	0.58
5:F:314:THR:HA	5:F:318:ALA:HB3	1.85	0.58
1:G:228:LEU:HG	1:H:221:ALA:HB1	1.85	0.58
2:I:106:GLU:HB3	2:I:109:ALA:HB2	1.83	0.58
2:I:524:ILE:HD12	2:I:712:SER:HB2	1.85	0.58
2:I:998:LEU:HD12	2:I:998:LEU:H	1.67	0.58
5:L:482:GLU:HG3	5:L:486:ARG:HH22	1.67	0.58
1:A:223:ILE:HD13	1:B:8:PHE:CE2	2.37	0.58
3:D:1221:LEU:HB2	3:D:1229:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.02	0.58
3:J:385:LEU:HD23	3:J:411:ILE:HG13	1.85	0.58
3:D:88:CYS:O	3:D:90:VAL:N	2.36	0.58
2:I:8:LYS:HE3	2:I:1171:ARG:NH2	2.17	0.58
5:L:551:LEU:HD23	5:L:597:LYS:HD2	1.84	0.58
1:A:166:ARG:O	1:A:168:ILE:N	2.37	0.58
1:A:284:ARG:HG3	1:A:288:GLU:HG3	1.85	0.58
3:J:425:ARG:HG2	3:J:426:ALA:H	1.68	0.58
1:A:57:THR:HG22	1:A:58:GLU:HG3	1.84	0.58
1:B:99:ILE:HD11	1:B:143:ARG:HB3	1.85	0.58
1:H:98:VAL:O	1:H:146:VAL:HG22	2.04	0.58
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.86	0.58
3:J:362:ARG:HE	9:J:2004:G4P:C2	2.17	0.58
2:C:488:MET:O	2:C:490:GLN:N	2.33	0.58
2:I:8:LYS:HE3	2:I:1171:ARG:HH21	1.69	0.58
3:J:708:ASN:N	3:J:708:ASN:OD1	2.37	0.58
1:B:266:SER:HB3	1:B:303:ILE:HD11	1.86	0.58
2:C:617:ALA:HA	2:C:636:CYS:SG	2.44	0.58
3:D:833:GLU:OE2	3:D:1247:LYS:NZ	2.37	0.58
2:I:324:LYS:O	2:I:327:GLN:NE2	2.37	0.58
1:B:321:TRP:H	1:B:322:PRO:CD	2.17	0.57
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.39	0.57
1:G:83:LEU:HD23	2:I:694:ARG:HE	1.69	0.57
2:I:528:ARG:NH2	2:I:576:SER:O	2.37	0.57
3:J:848:VAL:HG21	3:J:880:VAL:HG22	1.86	0.57
1:B:252:ILE:HG22	1:B:278:ILE:HD11	1.84	0.57
2:C:1247:SER:HB3	3:D:375:GLU:O	2.03	0.57
2:C:953:LEU:CD1	2:C:1033:ARG:HG3	2.34	0.57
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.87	0.57
2:I:135:THR:HG22	2:I:527:LYS:HE2	1.85	0.57
3:J:438:GLU:OE2	3:J:481:ARG:NH2	2.34	0.57
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.85	0.57
1:B:86:LYS:NZ	3:D:526:VAL:O	2.38	0.57
3:J:436:ALA:HB3	3:J:485:MET:HA	1.86	0.57
3:J:355:ILE:HD13	3:J:466:MET:HG3	1.86	0.57
2:C:470:ARG:HE	2:C:497:PRO:HB3	1.69	0.57
3:D:708:ASN:N	3:D:708:ASN:OD1	2.33	0.57
1:H:82:LEU:HD22	1:H:173:VAL:HG22	1.87	0.57
4:K:58:LEU:O	4:K:63:ILE:HG21	2.05	0.57
3:D:426:ALA:CB	3:D:427:PRO:HD3	2.34	0.57
5:F:584:ARG:HH11	5:F:584:ARG:HA	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:SER:OG	1:H:139:SER:HA	2.04	0.57
2:I:841:ARG:CZ	3:J:256:ASP:HB3	2.35	0.57
1:B:273:GLU:OE2	1:B:293:PRO:HD2	2.04	0.57
2:C:842:ASP:N	2:C:1045:GLY:O	2.37	0.57
3:D:1298:VAL:N	3:D:1299:GLY:HA3	2.18	0.57
3:D:425:ARG:HG2	3:D:426:ALA:H	1.69	0.57
2:I:106:GLU:OE1	2:I:114:VAL:HG22	2.04	0.57
2:I:1062:PRO:HA	2:I:1076:ILE:HG23	1.86	0.57
3:J:126:LEU:HD13	3:J:223:LEU:HD21	1.87	0.57
3:J:702:GLN:HA	3:J:723:TYR:CE2	2.39	0.57
1:A:137:ASN:OD1	1:A:137:ASN:N	2.38	0.57
2:C:802:VAL:HG21	2:C:1098:LEU:HD22	1.85	0.57
1:G:90:VAL:HG23	1:G:123:ILE:HD13	1.85	0.57
4:K:31:GLN:HB2	4:K:46:THR:HG21	1.87	0.57
5:L:444:ALA:HB1	5:L:457:ILE:HD13	1.87	0.57
2:C:250:THR:HA	2:C:268:ARG:HA	1.85	0.56
2:C:1271:GLY:HA3	3:D:343:LEU:HD12	1.87	0.56
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.87	0.56
5:F:245:ALA:O	5:F:249:ILE:HG13	2.04	0.56
2:I:697:LYS:HD2	2:I:1181:PRO:HG3	1.85	0.56
3:J:1257:VAL:HA	3:J:1260:MET:HG3	1.87	0.56
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.39	0.56
5:L:326:TRP:HA	5:L:329:LYS:HD2	1.86	0.56
5:L:479:THR:HG23	5:L:481:GLU:H	1.69	0.56
1:B:29:GLU:CD	1:B:30:PRO:HD3	2.24	0.56
2:C:106:GLU:O	2:C:108:GLU:HA	2.05	0.56
2:C:1116:HIS:CE1	3:D:641:ILE:H	2.17	0.56
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.86	0.56
5:L:245:ALA:O	5:L:249:ILE:HG13	2.05	0.56
2:C:708:VAL:HG11	2:C:794:LEU:HD22	1.87	0.56
5:F:388:ILE:HG22	5:F:392:LYS:HE3	1.88	0.56
3:J:422:LEU:HD13	3:J:471:PRO:HG3	1.87	0.56
1:A:13:LEU:HD12	1:A:16:ILE:HD11	1.87	0.56
3:J:609:TYR:HE2	3:J:614:LEU:HD12	1.69	0.56
4:K:15:ASN:ND2	4:K:18:ASP:OD2	2.36	0.56
5:L:573:LEU:HD11	5:L:588:ARG:HH21	1.70	0.56
2:C:1285:TYR:CD1	3:D:475:GLU:HG2	2.40	0.56
3:D:709:ARG:HD2	3:D:710:ASP:H	1.70	0.56
2:I:208:ILE:HG12	2:I:362:ALA:CB	2.36	0.56
2:I:972:PHE:HD1	2:I:994:ARG:HH21	1.54	0.56
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:102:LEU:HD23	2:C:117:ILE:HD11	1.88	0.56
2:C:93:SER:OG	2:C:126:GLU:OE1	2.17	0.56
2:I:151:ARG:HH22	2:I:175:ARG:NH1	2.04	0.56
3:J:770:LEU:HD22	3:J:770:LEU:H	1.70	0.56
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.87	0.56
3:D:194:LEU:O	3:D:198:CYS:N	2.35	0.56
3:D:62:PHE:CD1	3:D:247:PRO:HD3	2.41	0.56
2:C:808:ASN:H	3:D:633:ALA:HB2	1.71	0.56
6:M:141:LEU:O	6:M:145:ARG:HG3	2.05	0.56
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.86	0.56
1:A:300:LEU:HD13	1:A:304:LYS:HE2	1.86	0.56
3:D:1181:ASP:OD1	3:D:1182:GLY:N	2.39	0.56
3:D:903:LEU:HD22	3:D:909:ILE:HD12	1.87	0.56
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.87	0.56
3:J:824:PRO:HD3	3:J:835:LEU:HD13	1.86	0.56
5:L:312:SER:OG	5:L:313:ASP:N	2.39	0.56
1:B:275:ILE:HD11	1:B:284:ARG:HD3	1.86	0.56
3:D:842:ARG:HB3	3:D:882:VAL:HG11	1.87	0.56
4:E:8:ASP:HB2	4:E:55:GLU:OE2	2.06	0.56
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.70	0.56
3:J:749:LYS:HB3	3:J:755:ILE:HD11	1.87	0.56
3:J:644:MET:HB2	3:J:764:ARG:HG3	1.88	0.56
2:I:91:THR:HG21	2:I:503:LYS:HE3	1.87	0.56
1:A:12:ARG:H	1:A:30:PRO:HD2	1.69	0.56
2:C:582:ASN:HB3	2:C:586:PHE:H	1.71	0.56
2:C:1106:ARG:HE	3:D:731:ARG:HH21	1.53	0.56
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.88	0.56
1:B:318:LEU:O	1:B:320:ASN:N	2.32	0.55
2:C:73:TYR:HB2	2:C:98:VAL:HG22	1.89	0.55
3:D:872:LEU:HB3	3:D:877:VAL:HG11	1.88	0.55
1:A:296:GLY:N	1:A:299:SER:HB2	2.15	0.55
2:C:1158:LYS:O	2:C:1159:VAL:HG13	2.06	0.55
2:C:624:ASP:OD1	2:C:625:GLU:N	2.38	0.55
3:D:48:THR:C	3:D:50:LYS:H	2.09	0.55
2:I:462:ASN:O	2:I:466:VAL:HG23	2.06	0.55
2:I:117:ILE:HD12	2:I:488:MET:HG2	1.89	0.55
3:J:1319:PHE:HB3	3:J:1340:LYS:HD2	1.88	0.55
3:J:16:GLU:HG3	3:J:17:PHE:H	1.71	0.55
3:J:677:GLU:O	3:J:681:LYS:N	2.37	0.55
2:C:714:VAL:HB	2:C:787:PRO:HD2	1.87	0.55
2:I:93:SER:OG	2:I:126:GLU:OE1	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:156:PHE:CE1	2:I:445:ILE:HG13	2.42	0.55
5:L:562:ARG:NH2	5:L:573:LEU:HD22	2.21	0.55
1:A:66:HIS:CE1	1:A:69:SER:HB3	2.42	0.55
2:C:106:GLU:HG3	2:C:107:ARG:H	1.72	0.55
2:C:1327:LEU:HD23	2:C:1331:ARG:HH21	1.72	0.55
2:C:980:VAL:HG13	2:C:984:VAL:HB	1.88	0.55
2:I:810:TYR:CE2	3:J:359:PRO:HD2	2.42	0.55
2:C:670:PHE:CD2	2:C:1113:LEU:HB3	2.42	0.55
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.88	0.55
3:D:701:LEU:CD1	3:D:723:TYR:HB2	2.36	0.55
5:F:312:SER:OG	5:F:313:ASP:N	2.39	0.55
3:J:1289:ASN:OD1	3:J:1290:ARG:NH1	2.40	0.55
2:C:290:GLU:HG2	2:C:319:LEU:HD12	1.89	0.55
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.88	0.55
3:D:681:LYS:HZ2	6:M:12:LEU:HD22	1.72	0.55
2:I:1164:PHE:O	2:I:1166:ASP:N	2.40	0.55
2:I:670:PHE:CD1	2:I:1184:THR:HG21	2.42	0.55
1:A:44:ARG:HB2	1:A:183:ILE:HG21	1.89	0.55
1:A:98:VAL:HG22	1:A:100:LEU:HD12	1.87	0.55
1:B:48:LEU:HD22	3:D:535:ARG:HD3	1.88	0.55
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.71	0.55
2:C:1323:PHE:CE1	3:D:1353:VAL:HG23	2.41	0.55
1:H:60:GLU:OE2	1:H:143:ARG:NH1	2.40	0.55
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.42	0.55
5:L:111:LEU:HD11	5:L:119:ILE:HD12	1.88	0.55
2:C:1164:PHE:O	2:C:1166:ASP:N	2.39	0.55
3:D:901:ARG:CB	3:D:908:ILE:HA	2.36	0.55
2:I:1067:ALA:HB2	2:I:1073:LYS:HA	1.89	0.55
2:I:1131:MET:HE2	2:I:1136:GLN:HG3	1.89	0.55
3:J:1158:GLU:HA	3:J:1223:LEU:HD11	1.88	0.55
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.88	0.55
3:J:658:GLU:O	3:J:661:VAL:HG22	2.06	0.55
9:M:202:G4P:O2C	9:M:202:G4P:O2'	2.23	0.55
1:B:253:LEU:HB3	1:B:321:TRP:CE2	2.42	0.55
2:C:453:ILE:HD12	2:C:587:LEU:HG	1.88	0.55
3:D:811:GLU:OE1	3:D:890:THR:OG1	2.25	0.55
2:I:710:VAL:HA	2:I:715:THR:HG21	1.88	0.55
2:I:693:LEU:HB2	2:I:829:THR:O	2.07	0.55
3:J:549:LYS:HD3	3:J:569:LEU:HD23	1.88	0.55
5:L:595:LEU:O	5:L:599:ARG:HB2	2.06	0.55
2:C:561:ILE:HD12	2:C:679:ALA:HB1	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:98:ARG:HB3	3:D:248:ASP:OD2	2.07	0.54
3:J:859:PRO:HG2	3:J:862:THR:HG21	1.88	0.54
5:L:547:VAL:HG13	5:L:598:LEU:HD22	1.89	0.54
2:C:403:MET:HG3	2:C:584:TYR:CE1	2.43	0.54
3:D:54:ASP:N	3:D:54:ASP:OD1	2.40	0.54
3:D:596:LEU:HD12	3:D:601:ILE:HG13	1.89	0.54
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.89	0.54
1:A:310:ARG:O	5:F:608:ARG:NH2	2.38	0.54
1:B:6:THR:OG1	1:B:7:GLU:N	2.40	0.54
3:D:430:HIS:ND1	3:D:925:GLU:HG3	2.22	0.54
5:F:513:ASP:C	5:F:515:GLU:H	2.11	0.54
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.89	0.54
2:I:800:MET:O	2:I:1229:TYR:HA	2.08	0.54
3:J:258:GLY:HA3	5:L:499:LYS:HE2	1.89	0.54
5:L:115:GLY:HA2	5:L:118:ASP:HB2	1.89	0.54
6:M:98:LYS:NZ	9:M:202:G4P:O4'	2.40	0.54
1:B:29:GLU:HG2	1:B:30:PRO:HD3	1.87	0.54
1:B:323:PRO:CA	1:B:324:ALA:HB2	2.35	0.54
2:C:1002:LEU:N	2:C:1008:GLN:OE1	2.39	0.54
2:C:520:PRO:HG3	2:C:714:VAL:HG21	1.88	0.54
1:G:107:ILE:HD11	1:G:136:GLU:HG2	1.90	0.54
3:J:833:GLU:OE2	3:J:1247:LYS:NZ	2.41	0.54
3:J:79:LYS:HB2	5:L:569:THR:H	1.72	0.54
1:B:277:TYR:HB2	1:B:321:TRP:HH2	1.71	0.54
5:F:489:MET:O	5:F:491:GLU:N	2.40	0.54
5:F:612:ASP:N	5:F:612:ASP:OD1	2.38	0.54
3:J:274:ASN:OD1	5:L:446:GLN:NE2	2.41	0.54
1:B:112:ALA:HB3	1:B:126:PRO:HA	1.88	0.54
3:D:1344:LEU:O	3:D:1346:GLY:N	2.39	0.54
3:D:709:ARG:HD2	3:D:710:ASP:N	2.22	0.54
5:F:309:ASN:HD21	5:F:312:SER:HB3	1.71	0.54
5:F:316:PHE:HZ	5:F:334:SER:HA	1.72	0.54
6:M:13:SER:O	6:M:17:ILE:HG13	2.08	0.54
1:B:115:ILE:HG22	1:B:116:THR:H	1.72	0.54
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.90	0.54
5:F:536:THR:O	5:F:540:LEU:N	2.38	0.54
3:J:26:SER:HB2	3:J:236:TRP:CZ2	2.43	0.54
3:J:99:ARG:HG3	3:J:249:LEU:HD21	1.90	0.54
1:A:47:LEU:O	1:A:180:VAL:HG21	2.08	0.54
1:A:11:PRO:HD2	1:B:227:GLN:HA	1.90	0.54
2:C:1075:VAL:HG21	3:D:463:GLY:HA2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:MET:CE	5:F:600:HIS:CE1	2.91	0.54
2:I:148:GLN:NE2	2:I:535:PRO:O	2.39	0.54
3:J:705:THR:HG21	3:J:719:PHE:H	1.71	0.54
5:L:515:GLU:HG2	5:L:516:ASP:N	2.23	0.54
1:B:228:LEU:O	1:B:232:VAL:HG23	2.08	0.53
1:B:268:ASN:O	1:B:271:LYS:HB3	2.07	0.53
2:C:72:SER:O	2:C:99:LYS:N	2.32	0.53
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.73	0.53
2:I:138:ILE:HD11	2:I:506:PHE:HB3	1.90	0.53
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.43	0.53
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.90	0.53
3:D:667:GLN:HG2	3:D:672:LEU:HD12	1.90	0.53
3:J:793:SER:O	3:J:797:THR:HG23	2.07	0.53
3:J:908:ILE:HG12	3:J:909:ILE:N	2.22	0.53
3:J:201:LEU:HB2	3:J:221:ILE:HD13	1.90	0.53
3:J:357:VAL:HG22	3:J:461:PHE:HE1	1.73	0.53
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.90	0.53
3:J:853:THR:CG2	3:J:854:ALA:H	2.10	0.53
2:C:130:MET:SD	2:C:134:GLY:HA2	2.48	0.53
3:D:559:ALA:HB3	3:D:562:GLU:HB3	1.89	0.53
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	1.90	0.53
2:I:138:ILE:O	2:I:139:ASN:ND2	2.41	0.53
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.90	0.53
5:F:277:MET:HG3	5:F:362:ASN:HD21	1.73	0.53
1:H:49:SER:O	1:H:151:GLY:HA2	2.09	0.53
2:I:1305:TYR:CE1	3:J:379:PRO:HG3	2.44	0.53
3:J:420:PRO:O	3:J:471:PRO:HD2	2.09	0.53
5:L:134:VAL:HG22	5:L:273:MET:HE3	1.90	0.53
3:D:576:ARG:NH1	3:D:593:ASN:O	2.41	0.53
3:D:903:LEU:HD21	3:D:913:GLU:OE1	2.09	0.53
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.91	0.53
2:C:672:GLU:HG2	2:C:1187:PHE:HD2	1.74	0.53
2:C:810:TYR:CD2	3:D:359:PRO:HD2	2.43	0.53
1:B:83:LEU:HD11	3:D:526:VAL:HG23	1.90	0.53
4:E:49:ILE:O	4:E:53:GLU:HG3	2.08	0.53
3:J:1289:ASN:O	3:J:1290:ARG:NH1	2.42	0.53
5:F:261:LEU:H	5:F:261:LEU:HD12	1.74	0.53
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.41	0.53
3:J:317:THR:HG22	3:J:322:ARG:O	2.09	0.53
3:J:591:ILE:HG23	3:J:604:MET:HE2	1.91	0.53
2:C:1288:GLN:HG2	2:C:1315:MET:HE1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1331:ARG:HG2	3:D:33:TRP:CZ3	2.43	0.53
2:C:268:ARG:HH21	2:C:270:THR:HG21	1.74	0.53
3:D:615:LYS:HB3	3:D:616:PRO:HD3	1.90	0.53
3:D:678:ARG:HA	6:M:129:ARG:HH22	1.74	0.53
5:F:391:ALA:HB3	5:F:405:ILE:HG22	1.91	0.53
1:H:27:THR:HB	1:H:202:VAL:HG22	1.91	0.53
1:A:221:ALA:HB1	1:B:228:LEU:HD23	1.90	0.53
2:C:1116:HIS:HE1	3:D:641:ILE:N	2.03	0.53
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.09	0.53
2:C:810:TYR:HE1	2:C:1078:LYS:HD2	1.74	0.53
2:I:1013:GLN:O	2:I:1017:GLN:HG2	2.08	0.53
2:I:1321:GLU:OE2	3:J:99:ARG:HD3	2.09	0.53
2:I:213:LEU:HD13	2:I:422:LYS:HG2	1.91	0.53
3:J:1326:GLN:HB3	3:J:1330:ARG:NH2	2.24	0.53
5:L:612:ASP:N	5:L:612:ASP:OD1	2.42	0.53
1:A:25:LYS:HG2	1:A:204:GLU:HG3	1.91	0.52
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.90	0.52
2:I:855:PRO:HG3	2:I:913:VAL:HG13	1.91	0.52
5:L:137:TYR:CE1	5:L:351:THR:HB	2.45	0.52
5:L:139:GLU:HG2	5:L:351:THR:HA	1.90	0.52
3:D:197:GLU:O	3:D:201:LEU:HG	2.09	0.52
3:D:262:THR:HG22	5:F:504:PRO:HB2	1.90	0.52
1:G:137:ASN:N	1:G:137:ASN:OD1	2.42	0.52
3:J:268:LEU:HD11	3:J:324:LEU:HD13	1.90	0.52
3:D:1183:SER:C	3:D:1185:PRO:HD3	2.29	0.52
3:D:932:MET:HA	3:D:1138:LEU:HB3	1.91	0.52
1:G:45:ARG:HH22	1:H:37:HIS:HB3	1.74	0.52
3:D:1372:ARG:HG3	3:J:853:THR:HB	1.91	0.52
1:A:45:ARG:HG3	1:A:46:ILE:HD13	1.90	0.52
2:C:714:VAL:HG12	2:C:765:ILE:HD12	1.91	0.52
3:D:510:LEU:HD22	3:D:601:ILE:HD11	1.92	0.52
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.45	0.52
1:A:115:ILE:HG22	1:A:116:THR:H	1.73	0.52
1:A:45:ARG:NH2	2:C:1215:GLY:O	2.43	0.52
2:C:721:GLY:N	2:C:740:GLU:OE1	2.35	0.52
2:C:998:LEU:HD12	2:C:998:LEU:H	1.74	0.52
3:D:661:VAL:HG12	3:D:685:ILE:HD11	1.92	0.52
5:F:279:ARG:NH2	5:F:350:GLU:OE2	2.36	0.52
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.92	0.52
2:I:411:ARG:NH2	2:I:424:ASP:OD1	2.38	0.52
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:891:GLY:O	2:I:892:GLU:HG3	2.10	0.52
2:C:1334:GLY:H	3:D:113:HIS:HE2	1.55	0.52
2:C:564:PRO:HG3	2:C:572:ILE:HG13	1.91	0.52
2:I:169:LYS:O	2:I:170:VAL:HG22	2.09	0.52
3:J:850:LYS:HE2	3:J:855:ASP:HB3	1.92	0.52
2:C:661:VAL:HB	2:C:665:ALA:HB3	1.92	0.52
4:E:46:THR:HA	4:E:49:ILE:HB	1.91	0.52
2:I:409:LEU:HD11	2:I:428:VAL:HG23	1.92	0.52
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.09	0.52
3:J:449:LEU:HD22	3:J:466:MET:SD	2.50	0.52
5:L:306:PHE:CZ	5:L:310:GLU:HG3	2.45	0.52
1:A:14:VAL:HG22	1:A:15:ASP:N	2.25	0.52
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.92	0.52
2:C:252:SER:H	2:C:255:ILE:HD11	1.75	0.52
5:F:380:VAL:HG13	5:F:412:LEU:HD23	1.92	0.52
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.74	0.52
2:I:175:ARG:HG3	2:I:185:ASP:OD1	2.09	0.52
2:I:38:PHE:HB2	2:I:457:GLY:HA2	1.91	0.52
3:J:1264:ALA:HB2	3:J:1280:VAL:HG22	1.91	0.52
3:J:903:LEU:HD23	3:J:905:ARG:HD3	1.92	0.52
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.33	0.52
1:A:112:ALA:O	1:A:115:ILE:HG13	2.10	0.52
3:D:128:LEU:HB3	3:D:157:GLN:HE22	1.75	0.52
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.92	0.52
1:H:102:LEU:O	1:H:141:SER:HA	2.10	0.52
2:I:356:THR:HG21	2:I:362:ALA:HA	1.92	0.52
3:J:1154:ALA:HB3	3:J:1215:GLU:HB3	1.91	0.52
3:J:218:THR:HG21	3:J:1275:LEU:HD21	1.92	0.52
3:J:668:PHE:CD1	3:J:678:ARG:HG2	2.44	0.52
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.91	0.52
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.91	0.52
3:D:156:ARG:NH1	3:D:157:GLN:HE21	2.07	0.52
3:D:425:ARG:HG2	3:D:426:ALA:N	2.24	0.52
3:D:527:LEU:HD21	3:D:536:LEU:HG	1.91	0.52
5:F:111:LEU:HD13	5:F:116:GLU:HA	1.92	0.52
1:G:75:GLN:HA	2:I:729:ALA:N	2.25	0.52
2:I:168:GLY:C	2:I:170:VAL:H	2.11	0.52
2:I:452:ARG:NH1	2:I:585:GLY:HA3	2.25	0.52
3:J:517:CYS:HB3	3:J:719:PHE:CE2	2.45	0.52
5:L:320:ILE:O	5:L:327:SER:HB3	2.10	0.52
5:L:383:ASN:HB2	5:L:412:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:106:GLU:HG3	2:C:107:ARG:N	2.25	0.51
2:C:18:ARG:NH1	2:C:622:ASN:OD1	2.38	0.51
2:I:920:VAL:HG22	2:I:1054:LEU:HD21	1.92	0.51
2:I:1142:ARG:HH11	2:I:1161:LEU:HD11	1.75	0.51
2:I:1222:GLU:OE1	3:J:512:TYR:OH	2.11	0.51
2:I:1282:GLY:O	2:I:1284:ALA:N	2.43	0.51
6:M:52:ARG:HB2	6:M:52:ARG:HH11	1.75	0.51
3:D:783:LEU:HD23	6:M:76:ALA:CB	2.40	0.51
2:C:941:LYS:HB2	2:C:946:LEU:HG	1.92	0.51
5:F:575:GLU:O	5:F:579:GLN:HG2	2.10	0.51
1:H:83:LEU:HA	1:H:86:LYS:HE2	1.92	0.51
2:I:949:GLU:HG2	2:I:1036:ILE:HG22	1.92	0.51
3:J:706:VAL:HG12	3:J:715:LYS:HB3	1.91	0.51
3:J:747:MET:HB2	3:J:774:ILE:HG22	1.92	0.51
5:L:244:THR:O	5:L:247:GLU:HG2	2.10	0.51
5:L:445:ASP:OD2	5:L:451:ARG:HD2	2.10	0.51
1:B:44:ARG:HD2	1:B:183:ILE:HD13	1.92	0.51
2:C:1106:ARG:NE	3:D:731:ARG:HH21	2.08	0.51
2:C:1142:ARG:NH1	2:C:1169:VAL:HG21	2.24	0.51
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.45	0.51
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.91	0.51
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.92	0.51
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	1.92	0.51
1:A:228:LEU:HA	1:A:231:PHE:HB2	1.93	0.51
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.75	0.51
2:C:742:TYR:HD2	2:C:743:PRO:HD2	1.76	0.51
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.92	0.51
3:D:26:SER:HB2	3:D:236:TRP:CZ2	2.45	0.51
3:D:322:ARG:HB2	3:D:322:ARG:NH1	2.26	0.51
5:F:151:VAL:HG22	5:F:156:ALA:HB3	1.92	0.51
3:J:848:VAL:HB	3:J:858:VAL:HG22	1.92	0.51
5:L:316:PHE:HZ	5:L:334:SER:HA	1.76	0.51
1:A:66:HIS:HE1	1:A:69:SER:HB3	1.75	0.51
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.91	0.51
2:C:268:ARG:NH2	2:C:270:THR:HG21	2.26	0.51
3:D:460:ASP:OD2	3:D:462:ASP:OD1	2.28	0.51
3:D:850:LYS:HD3	3:D:875:ASN:ND2	2.26	0.51
1:G:133:LEU:HD12	1:G:138:ALA:HB3	1.93	0.51
2:I:836:LEU:HD21	2:I:921:PRO:HD3	1.92	0.51
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.76	0.51
2:C:302:ILE:O	2:C:330:HIS:NE2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:21:VAL:HG13	2:C:655:VAL:HG13	1.93	0.51
3:D:268:LEU:HD11	3:D:324:LEU:HD13	1.93	0.51
5:F:399:LEU:HD22	5:F:447:ALA:HB2	1.93	0.51
5:L:476:ARG:NH1	5:L:476:ARG:HB3	2.26	0.51
2:C:106:GLU:N	2:C:109:ALA:CB	2.73	0.51
2:C:594:VAL:HG11	2:C:650:VAL:HG23	1.93	0.51
3:D:79:LYS:HG3	3:D:80:HIS:ND1	2.25	0.51
2:I:1148:ALA:HA	2:I:1201:LEU:CD2	2.38	0.51
3:J:320:ASN:OD1	3:J:322:ARG:HB3	2.11	0.51
2:I:1331:ARG:HG2	3:J:33:TRP:CZ3	2.46	0.51
3:J:504:GLN:HG3	3:J:505:ASP:H	1.76	0.51
1:B:51:MET:HE2	1:B:220:ALA:HB2	1.93	0.51
2:C:411:ARG:NH2	2:C:427:ASP:OD2	2.41	0.51
2:C:71:VAL:HB	2:C:99:LYS:HB2	1.93	0.51
2:C:80:PHE:HB3	2:C:84:GLU:HB2	1.92	0.51
2:I:972:PHE:HE2	2:I:998:LEU:HD11	1.75	0.51
3:J:291:ILE:HG23	5:L:406:GLN:HE22	1.76	0.51
1:B:186:ASN:HD22	1:B:202:VAL:HB	1.76	0.50
2:C:1327:LEU:O	2:C:1331:ARG:HB2	2.10	0.50
2:C:515:MET:HG2	2:C:517:GLN:HB2	1.93	0.50
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.20	0.50
2:I:596:ASP:CG	2:I:597:GLY:N	2.64	0.50
2:I:706:ARG:NH2	2:I:791:LEU:O	2.44	0.50
5:L:137:TYR:HE1	5:L:351:THR:HB	1.76	0.50
1:A:285:THR:OG1	1:A:286:GLU:N	2.44	0.50
3:D:1174:ARG:HG2	3:D:1189:MET:HG2	1.94	0.50
3:D:110:PRO:HB3	3:D:238:ILE:CG2	2.41	0.50
3:D:528:THR:O	3:D:551:ARG:HB3	2.12	0.50
3:D:770:LEU:H	3:D:770:LEU:HD22	1.77	0.50
1:H:46:ILE:HD11	1:H:224:LEU:HD13	1.92	0.50
2:I:1061:GLN:HG3	2:I:1239:VAL:HG11	1.93	0.50
2:I:42:ASP:O	2:I:44:GLU:N	2.43	0.50
6:M:78:GLN:HG2	6:M:82:PHE:HE2	1.77	0.50
2:C:903:ARG:HE	2:C:910:ALA:HB2	1.76	0.50
2:C:1271:GLY:HA2	3:D:344:GLY:HA3	1.92	0.50
5:F:139:GLU:HG2	5:F:351:THR:HA	1.93	0.50
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.93	0.50
2:I:921:PRO:O	2:I:924:VAL:HG22	2.11	0.50
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.92	0.50
1:A:16:ILE:HG23	1:A:26:VAL:HG12	1.94	0.50
2:C:540:ARG:HH11	2:C:540:ARG:HB2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:733:VAL:HG11	2:C:966:ILE:HG21	1.94	0.50
3:D:843:VAL:HG13	3:D:883:ARG:HD3	1.93	0.50
3:D:817:HIS:CE1	3:D:860:ARG:HH21	2.30	0.50
1:G:23:HIS:HB2	1:G:205:MET:O	2.12	0.50
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.94	0.50
2:I:620:ASN:ND2	2:I:620:ASN:O	2.44	0.50
2:C:697:LYS:HD2	2:C:1181:PRO:HG3	1.94	0.50
1:H:62:ASP:N	1:H:62:ASP:OD1	2.30	0.50
2:I:1247:SER:HB3	3:J:375:GLU:O	2.11	0.50
2:I:670:PHE:CD2	2:I:1113:LEU:HB3	2.47	0.50
3:J:1183:SER:C	3:J:1185:PRO:HD3	2.32	0.50
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.93	0.50
3:J:836:ARG:HD2	3:J:873:GLU:OE1	2.11	0.50
6:M:71:ASP:OD1	6:M:73:VAL:HG23	2.11	0.50
1:B:214:GLU:O	1:B:218:ARG:HG3	2.11	0.50
2:C:1032:LYS:O	2:C:1036:ILE:HG13	2.12	0.50
2:C:1282:GLY:O	2:C:1284:ALA:N	2.44	0.50
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.27	0.50
2:C:88:ARG:HH11	2:C:88:ARG:HB2	1.76	0.50
3:J:355:ILE:HG21	3:J:466:MET:HG3	1.93	0.50
1:B:73:GLY:O	1:B:134:THR:HG22	2.12	0.50
2:C:1283:ALA:HB1	2:C:1286:THR:HB	1.93	0.50
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.94	0.50
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.93	0.50
1:G:45:ARG:HH21	2:I:1216:ARG:HA	1.76	0.50
2:I:144:VAL:HG11	2:I:527:LYS:HA	1.93	0.50
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.94	0.50
2:I:990:ASP:HA	2:I:997:TRP:HZ2	1.76	0.50
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.12	0.50
3:J:661:VAL:HG11	3:J:686:TRP:CE2	2.47	0.50
6:M:15:LEU:HD13	6:M:22:PRO:HG3	1.93	0.50
1:B:253:LEU:HB3	1:B:321:TRP:CZ2	2.47	0.50
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.52	0.50
5:F:147:GLN:HE22	5:F:150:ARG:HH11	1.58	0.50
2:I:700:VAL:HG13	2:I:1117:LEU:HD22	1.94	0.50
2:I:1176:LEU:HD13	2:I:1180:MET:HG3	1.92	0.50
2:I:174:ALA:N	2:I:186:PHE:O	2.44	0.50
2:I:235:ASN:O	2:I:236:LYS:CB	2.52	0.50
3:J:797:THR:O	3:J:801:VAL:HG12	2.12	0.50
1:A:100:LEU:HD23	1:A:115:ILE:HG21	1.93	0.50
2:C:1255:THR:O	2:C:1257:GLN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:91:THR:HB	2:C:138:ILE:O	2.12	0.50
2:C:363:LEU:HD13	2:C:382:GLU:HG2	1.93	0.50
2:C:367:TYR:HD1	2:C:384:LEU:HD22	1.76	0.50
3:D:317:THR:HA	3:D:324:LEU:HD23	1.93	0.50
5:F:372:ALA:O	5:F:376:LYS:HG3	2.12	0.50
2:I:445:ILE:HG23	2:I:451:ARG:HE	1.76	0.50
2:I:894:GLN:HE21	3:J:78:LEU:HD21	1.77	0.50
3:J:421:VAL:HG13	3:J:439:PRO:HG3	1.92	0.50
1:B:98:VAL:HG22	1:B:100:LEU:HD12	1.92	0.49
1:B:94:GLY:H	1:B:276:HIS:HD2	1.56	0.49
1:B:29:GLU:OE1	1:B:30:PRO:HD3	2.12	0.49
2:C:1269:ARG:HG3	3:D:346:ARG:HG2	1.94	0.49
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.76	0.49
2:I:519:ASN:ND2	2:I:689:ALA:HB3	2.27	0.49
3:J:1178:THR:HA	3:J:1184:ASP:HB2	1.93	0.49
3:J:425:ARG:HG2	3:J:426:ALA:N	2.27	0.49
5:L:354:THR:O	5:L:358:VAL:HG23	2.12	0.49
3:J:253:VAL:HG21	5:L:523:ILE:HG21	1.93	0.49
2:C:13:LYS:HA	2:C:1157:GLN:OE1	2.12	0.49
2:C:478:ARG:CZ	2:C:487:LEU:HD13	2.42	0.49
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.94	0.49
2:C:730:SER:O	2:C:753:LEU:HB2	2.12	0.49
5:F:343:LYS:H	5:F:343:LYS:HD2	1.77	0.49
3:J:128:LEU:HD21	3:J:189:LEU:HD23	1.95	0.49
3:J:489:ASN:HA	3:J:904:ALA:CB	2.41	0.49
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.94	0.49
3:J:905:ARG:NH1	4:K:16:ARG:HB2	2.26	0.49
3:D:705:THR:OG1	3:D:718:SER:HA	2.12	0.49
5:F:453:PRO:O	5:F:456:MET:HB2	2.12	0.49
5:F:444:ALA:HB1	5:F:457:ILE:HD13	1.93	0.49
2:I:1211:ARG:HE	2:I:1220:GLN:NE2	2.10	0.49
3:J:1206:ARG:NH2	3:J:1223:LEU:O	2.46	0.49
3:J:657:ALA:HA	3:J:660:GLU:HB2	1.95	0.49
3:J:861:ASN:HD22	3:J:883:ARG:NH1	2.10	0.49
1:A:90:VAL:HG23	1:A:123:ILE:HD13	1.94	0.49
2:C:1106:ARG:O	2:C:1108:ASN:N	2.44	0.49
2:C:1305:TYR:OH	5:F:532:LEU:HG	2.12	0.49
2:C:359:ARG:NH1	2:C:382:GLU:OE2	2.46	0.49
3:D:1137:GLY:H	3:D:1140:ARG:HB3	1.77	0.49
2:I:1287:LEU:HD22	3:J:1357:ILE:HG13	1.94	0.49
3:J:425:ARG:NH1	3:J:459:ALA:HA	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.94	0.49
2:C:563:THR:HG22	2:C:680:LEU:HD11	1.94	0.49
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.46	0.49
5:F:233:ASP:O	5:F:236:LYS:HE2	2.13	0.49
5:F:388:ILE:O	5:F:392:LYS:HG3	2.13	0.49
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.12	0.49
2:I:924:VAL:HG12	2:I:1058:ARG:HH21	1.78	0.49
3:J:48:THR:C	3:J:50:LYS:H	2.11	0.49
3:J:56:LEU:HD12	3:J:56:LEU:H	1.77	0.49
2:C:1294:LYS:HB3	3:D:347:VAL:HG13	1.95	0.49
2:C:1340:GLU:HG3	3:D:21:LYS:HB2	1.93	0.49
3:D:1243:LEU:O	6:M:63:GLN:HG2	2.12	0.49
3:D:905:ARG:NH1	4:E:16:ARG:HB2	2.27	0.49
5:F:320:ILE:HG23	5:F:327:SER:O	2.13	0.49
5:F:449:THR:OG1	5:F:503:GLU:OE1	2.31	0.49
2:I:908:GLU:OE2	5:L:611:LEU:HD13	2.13	0.49
2:C:138:ILE:O	2:C:139:ASN:ND2	2.45	0.49
3:D:1178:THR:HG23	3:D:1184:ASP:CB	2.43	0.49
3:D:16:GLU:O	3:D:1369:ARG:NH2	2.46	0.49
3:D:436:ALA:HB3	3:D:485:MET:HA	1.94	0.49
3:D:859:PRO:HD2	3:D:862:THR:HG21	1.94	0.49
3:D:1361:THR:HG22	4:E:21:LEU:HD22	1.94	0.49
5:F:316:PHE:CZ	5:F:334:SER:HA	2.48	0.49
5:F:383:ASN:HB2	5:F:412:LEU:HD21	1.95	0.49
1:G:68:TYR:HE2	2:I:927:THR:HB	1.76	0.49
1:H:151:GLY:O	1:H:177:TYR:HB2	2.12	0.49
2:I:1120:ALA:HA	2:I:1204:LEU:HD12	1.94	0.49
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.95	0.49
2:I:1282:GLY:HA3	4:K:17:PHE:CE1	2.48	0.49
1:A:318:LEU:O	1:A:320:ASN:N	2.41	0.49
1:B:94:GLY:HA2	1:B:277:TYR:CE2	2.47	0.49
2:C:175:ARG:HG3	2:C:185:ASP:OD1	2.13	0.49
2:C:800:MET:HE1	2:C:822:VAL:HG13	1.94	0.49
3:D:504:GLN:HG3	3:D:505:ASP:H	1.76	0.49
4:E:3:ARG:HD2	9:E:101:G4P:H4'	1.95	0.49
2:I:810:TYR:CE1	2:I:1078:LYS:HD2	2.48	0.49
3:J:115:TRP:HZ2	3:J:328:ALA:HB2	1.77	0.49
1:B:79:LEU:HD21	3:D:526:VAL:HG21	1.95	0.49
2:C:1293:VAL:HG13	2:C:1301:ARG:HA	1.95	0.49
2:C:402:ARG:NE	2:C:417:SER:O	2.46	0.49
3:D:1137:GLY:O	3:D:1140:ARG:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:336:GLY:HA3	3:D:1324:SER:O	2.12	0.49
3:D:460:ASP:CG	3:D:462:ASP:OD1	2.50	0.49
5:F:484:ALA:O	5:F:491:GLU:HB2	2.12	0.49
3:D:394:ILE:HG12	5:F:536:THR:HG22	1.95	0.49
5:F:600:HIS:HB3	5:F:601:PRO:CD	2.43	0.49
1:A:251:PRO:HD2	5:F:605:GLU:HG3	1.95	0.49
1:G:231:PHE:HB3	1:H:218:ARG:HB3	1.94	0.49
1:H:76:GLU:N	1:H:76:GLU:OE1	2.46	0.49
3:J:1284:ARG:NH1	3:J:1288:ALA:HB2	2.28	0.49
5:L:463:LEU:HA	5:L:466:ILE:HD12	1.95	0.49
1:A:249:PHE:CD1	1:A:321:TRP:HZ3	2.31	0.49
1:A:257:VAL:HG13	1:A:276:HIS:O	2.13	0.49
2:C:61:SER:O	2:C:63:SER:N	2.45	0.49
2:C:796:LEU:H	2:C:796:LEU:HD12	1.78	0.49
3:D:370:LYS:HA	3:D:441:LEU:HD12	1.95	0.49
3:D:747:MET:HB2	3:D:774:ILE:HG22	1.95	0.49
9:E:101:G4P:O1C	9:E:101:G4P:O2'	2.27	0.49
2:I:1308:ILE:HD12	3:J:380:PHE:CZ	2.48	0.49
2:I:32:LEU:HD23	2:I:130:MET:SD	2.53	0.49
3:J:288:PRO:O	3:J:292:VAL:HG13	2.13	0.49
5:L:281:ARG:HG3	5:L:285:ARG:HH11	1.76	0.49
6:M:108:ASP:O	6:M:108:ASP:OD2	2.31	0.49
2:C:169:LYS:O	2:C:170:VAL:HG22	2.13	0.48
2:C:124:MET:HB3	2:C:493:ILE:HD11	1.94	0.48
3:D:1280:VAL:HG21	3:D:1304:ARG:HH21	1.76	0.48
5:F:511:ILE:HG21	5:F:522:PHE:CE2	2.48	0.48
5:F:551:LEU:HD11	5:F:598:LEU:HD11	1.94	0.48
1:A:104:LYS:HB3	1:A:110:VAL:HG13	1.95	0.48
2:C:228:VAL:HG22	2:C:245:ARG:HE	1.78	0.48
2:C:145:ILE:HA	2:C:511:LEU:O	2.13	0.48
3:D:53:ARG:HA	3:D:54:ASP:HA	1.56	0.48
4:E:4:VAL:HG13	4:E:5:THR:N	2.28	0.48
5:F:127:ILE:O	5:F:130:VAL:HG22	2.13	0.48
3:J:24:LEU:HD23	3:J:232:ASN:ND2	2.28	0.48
5:L:478:PRO:HG2	5:L:483:LEU:HD11	1.95	0.48
2:C:245:ARG:HG2	2:C:337:PHE:CE2	2.48	0.48
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.79	0.48
2:I:245:ARG:HG2	2:I:337:PHE:CE2	2.48	0.48
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.94	0.48
5:L:469:GLN:O	5:L:473:GLU:HB2	2.12	0.48
1:A:158:ARG:NH2	1:A:172:LEU:HD23	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.94	0.48
2:C:1293:VAL:HG11	2:C:1304:MET:HG2	1.95	0.48
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.44	0.48
3:D:161:THR:HG22	3:D:164:GLN:HB2	1.95	0.48
1:H:86:LYS:HD3	1:H:174:ASP:HB2	1.94	0.48
2:I:314:ASN:O	2:I:352:ARG:NH1	2.46	0.48
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.43	0.48
3:D:1227:HIS:HB2	3:J:1293:GLU:OE1	2.14	0.48
3:J:88:CYS:O	3:J:90:VAL:N	2.47	0.48
4:K:21:LEU:HD12	4:K:21:LEU:HA	1.70	0.48
1:B:195:ARG:HG3	1:B:198:LEU:HD11	1.96	0.48
2:C:670:PHE:CD1	2:C:1184:THR:HG21	2.48	0.48
1:A:250:ASP:HB2	5:F:601:PRO:HB3	1.96	0.48
1:H:59:VAL:O	1:H:171:LEU:HB2	2.13	0.48
2:I:1158:LYS:O	2:I:1159:VAL:HG13	2.13	0.48
2:I:1272:GLU:HB2	3:J:342:LEU:CB	2.44	0.48
2:I:852:ALA:HB2	2:I:869:GLY:HA2	1.95	0.48
2:I:903:ARG:HD2	2:I:908:GLU:O	2.13	0.48
3:J:123:ARG:NH2	3:J:1334:GLU:HG3	2.25	0.48
5:L:371:LYS:HA	5:L:374:ARG:NH1	2.28	0.48
1:A:224:LEU:O	1:A:228:LEU:HD12	2.14	0.48
1:A:23:HIS:HE1	1:A:204:GLU:CG	2.25	0.48
5:F:555:GLU:O	5:F:559:LEU:HB2	2.14	0.48
2:I:518:ASN:O	2:I:691:PRO:HD3	2.13	0.48
1:A:135:ASP:O	1:A:138:ALA:N	2.33	0.48
1:A:220:ALA:O	1:A:223:ILE:HG13	2.14	0.48
2:C:202:ARG:HB2	2:C:369:MET:HG2	1.94	0.48
2:C:47:TYR:OH	2:C:398:SER:HB2	2.12	0.48
2:C:519:ASN:ND2	2:C:689:ALA:HB3	2.29	0.48
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.78	0.48
3:J:131:PRO:O	3:J:135:ILE:HG13	2.13	0.48
5:L:287:ILE:HD13	5:L:315:TRP:CH2	2.48	0.48
1:B:65:LEU:O	1:B:66:HIS:ND1	2.46	0.48
2:C:395:TYR:CD2	2:C:419:ILE:HG22	2.45	0.48
2:C:994:ARG:HD2	2:C:997:TRP:CZ2	2.49	0.48
1:B:44:ARG:HE	3:D:538:ARG:HB3	1.79	0.48
1:G:13:LEU:H	1:G:13:LEU:HD23	1.78	0.48
2:I:156:PHE:CD2	2:I:175:ARG:HB3	2.48	0.48
2:I:974:ARG:HD2	2:I:1014:LEU:HD21	1.96	0.48
3:J:679:TYR:O	3:J:683:ILE:HG13	2.13	0.48
1:B:188:GLU:HG3	1:B:200:LYS:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1063:GLY:HA3	2:C:1239:VAL:HB	1.95	0.48
2:C:802:VAL:HG11	2:C:1230:MET:HB3	1.96	0.48
2:C:618:GLN:HG3	3:D:770:LEU:HD21	1.95	0.48
1:G:140:ILE:O	1:G:140:ILE:HG13	2.14	0.48
3:J:156:ARG:NH2	3:J:191:SER:OG	2.45	0.48
6:M:55:VAL:O	6:M:59:VAL:HG23	2.13	0.48
2:C:209:ILE:HD11	2:C:425:ILE:HD13	1.95	0.48
3:D:227:PHE:O	3:D:230:SER:HB3	2.13	0.48
5:F:470:MET:O	5:F:478:PRO:HD3	2.14	0.48
2:I:1086:PRO:HB3	2:I:1212:LEU:HD23	1.95	0.48
2:I:1281:TYR:OH	3:J:434:ILE:O	2.32	0.48
5:L:281:ARG:O	5:L:285:ARG:HG3	2.14	0.48
3:D:746:LEU:O	6:M:84:LEU:HD13	2.14	0.48
2:C:1124:ILE:HG21	2:C:1180:MET:HE2	1.94	0.47
2:C:131:THR:OG1	2:C:135:THR:O	2.32	0.47
2:C:227:LYS:NZ	2:C:298:ALA:HB1	2.29	0.47
2:C:27:LEU:O	2:C:528:ARG:NH1	2.46	0.47
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.96	0.47
5:F:253:SER:O	5:F:257:LYS:HG3	2.14	0.47
5:L:308:GLY:HA2	5:L:356:GLU:OE1	2.14	0.47
3:D:11:GLN:HG2	3:D:15:GLU:CD	2.34	0.47
3:D:365:GLN:O	3:D:437:PHE:HD1	1.97	0.47
1:G:76:GLU:OE2	1:G:76:GLU:N	2.47	0.47
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	1.96	0.47
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.80	0.47
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.96	0.47
3:J:848:VAL:HG12	3:J:857:LEU:CD1	2.44	0.47
3:J:915:ILE:HA	3:J:918:ILE:HG23	1.95	0.47
1:A:295:LEU:HD22	1:A:300:LEU:HD23	1.97	0.47
2:C:201:ARG:NH2	2:C:370:MET:O	2.47	0.47
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.39	0.47
5:F:608:ARG:HH11	5:F:608:ARG:HB2	1.79	0.47
1:H:73:GLY:HA3	1:H:138:ALA:HB1	1.94	0.47
2:I:678:ARG:CZ	2:I:1106:ARG:HG2	2.44	0.47
2:I:239:MET:N	2:I:285:ILE:O	2.45	0.47
2:I:1286:THR:N	3:J:479:GLU:OE2	2.42	0.47
3:J:656:GLU:OE1	3:J:692:ARG:NH2	2.41	0.47
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.96	0.47
3:D:478:LEU:HG	4:E:47:THR:HG23	1.97	0.47
3:D:452:LEU:HB3	3:D:500:ILE:HG23	1.97	0.47
3:J:1199:PHE:HB2	3:J:1202:GLU:CB	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1221:LEU:HB2	3:J:1229:VAL:HG11	1.95	0.47
6:M:144:ILE:HG23	6:M:147:LYS:HE2	1.96	0.47
3:D:27:PRO:O	3:D:31:ARG:HG3	2.13	0.47
3:D:511:TYR:OH	3:D:515:ARG:NH1	2.47	0.47
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.49	0.47
3:D:614:LEU:HD22	4:E:7:GLN:HB2	1.97	0.47
1:H:18:GLN:HA	1:H:24:ALA:HA	1.95	0.47
1:H:62:ASP:OD2	1:H:71:LYS:NZ	2.46	0.47
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.96	0.47
1:B:104:LYS:HG3	1:B:105:SER:N	2.29	0.47
1:B:270:LEU:HD22	1:B:275:ILE:HG21	1.96	0.47
1:B:29:GLU:OE1	1:B:30:PRO:CD	2.62	0.47
2:C:1111:GLN:HB2	2:C:1230:MET:CE	2.45	0.47
2:C:27:LEU:HD13	2:C:663:VAL:HG11	1.94	0.47
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.44	0.47
2:C:819:SER:HB2	2:C:1085:MET:HG3	1.97	0.47
3:D:638:SER:OG	3:D:639:VAL:N	2.47	0.47
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.97	0.47
5:F:130:VAL:HB	5:F:365:MET:HG3	1.97	0.47
1:G:44:ARG:HA	1:G:183:ILE:HG21	1.96	0.47
2:I:151:ARG:NE	2:I:445:ILE:HD11	2.30	0.47
2:I:395:TYR:HE2	2:I:397:LEU:HD12	1.79	0.47
2:I:518:ASN:N	2:I:518:ASN:OD1	2.47	0.47
2:I:601:ASP:OD1	2:I:601:ASP:N	2.46	0.47
3:J:337:ARG:NH2	3:J:1323:ALA:HB3	2.29	0.47
3:J:53:ARG:HA	3:J:54:ASP:HA	1.52	0.47
5:L:353:LEU:HD13	5:L:361:ILE:HD12	1.96	0.47
3:D:674:THR:CG2	6:M:139:LYS:HG2	2.43	0.47
1:B:112:ALA:O	1:B:115:ILE:HG13	2.15	0.47
1:B:215:GLU:HA	1:B:218:ARG:HD2	1.95	0.47
1:B:82:LEU:HD22	1:B:173:VAL:HG12	1.97	0.47
2:C:800:MET:HG3	2:C:1096:ILE:HD11	1.96	0.47
2:C:16:GLY:O	2:C:1156:ARG:HG2	2.14	0.47
2:C:616:ILE:HG13	2:C:652:TYR:HB2	1.97	0.47
3:D:405:GLU:O	3:D:408:VAL:HG22	2.15	0.47
3:D:689:ALA:O	3:D:693:VAL:HG23	2.15	0.47
4:E:2:ALA:HB2	4:E:55:GLU:OE1	2.15	0.47
1:H:215:GLU:HA	1:H:218:ARG:HG3	1.97	0.47
1:G:231:PHE:HA	1:H:218:ARG:HG2	1.97	0.47
2:I:119:GLU:HG3	2:I:489:PRO:CD	2.40	0.47
3:J:214:ARG:HA	3:J:217:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:275:ARG:HG2	3:J:278:ARG:HH12	1.80	0.47
3:J:355:ILE:HG21	3:J:466:MET:CG	2.45	0.47
3:J:850:LYS:HG2	3:J:857:LEU:CD2	2.44	0.47
5:L:114:GLU:O	5:L:117:ILE:N	2.43	0.47
5:L:395:THR:OG1	5:L:396:ASN:N	2.47	0.47
1:B:61:ILE:HG23	1:B:142:MET:HE2	1.97	0.47
2:C:1315:MET:HE2	2:C:1317:PRO:HB3	1.95	0.47
2:C:188:PHE:CE1	2:C:194:LEU:HD13	2.50	0.47
3:D:9:LYS:NZ	3:D:11:GLN:HA	2.29	0.47
1:H:100:LEU:HB3	1:H:115:ILE:CG2	2.45	0.47
3:J:337:ARG:HD2	3:J:1324:SER:HA	1.97	0.47
5:L:111:LEU:HD13	5:L:116:GLU:HA	1.96	0.47
5:L:357:GLN:HA	5:L:360:ASP:HB2	1.97	0.47
5:L:483:LEU:HD12	5:L:483:LEU:H	1.79	0.47
5:L:561:MET:HA	5:L:567:MET:CE	2.45	0.47
1:A:95:LYS:O	1:A:148:ARG:NH2	2.47	0.47
1:B:224:LEU:O	1:B:228:LEU:HD12	2.15	0.47
2:C:155:VAL:HA	2:C:175:ARG:O	2.15	0.47
2:C:325:LEU:O	2:C:330:HIS:HB2	2.15	0.47
3:D:83:VAL:HG13	3:D:92:VAL:HG13	1.96	0.47
3:D:99:ARG:HG3	3:D:249:LEU:HD21	1.97	0.47
2:I:1296:ASP:CG	2:I:1322:SER:HB3	2.35	0.47
2:I:384:LEU:O	2:I:388:LEU:HG	2.14	0.47
3:J:1262:ARG:O	3:J:1280:VAL:HG23	2.14	0.47
3:J:368:LEU:HD22	3:J:373:ALA:HB2	1.97	0.47
3:J:68:TYR:CA	3:J:92:VAL:HG23	2.44	0.47
5:L:489:MET:O	5:L:491:GLU:N	2.47	0.47
2:C:344:GLY:HA3	2:C:346:TYR:CE2	2.50	0.47
2:C:620:ASN:ND2	2:C:620:ASN:O	2.47	0.47
3:D:1163:VAL:HG23	3:D:1177:ILE:HG23	1.96	0.47
3:D:43:THR:OG1	5:F:449:THR:O	2.20	0.47
1:G:64:VAL:HG11	1:G:78:ILE:HG21	1.96	0.47
1:H:91:ARG:HD2	1:H:210:THR:HB	1.97	0.47
2:I:963:GLU:O	2:I:967:LEU:HB2	2.14	0.47
2:I:1251:TYR:OH	3:J:348:ASP:OD2	2.20	0.47
3:J:678:ARG:O	3:J:682:VAL:HG23	2.15	0.47
3:J:705:THR:OG1	3:J:718:SER:HA	2.14	0.47
5:L:515:GLU:HG2	5:L:516:ASP:H	1.79	0.47
6:M:44:LEU:CD2	6:M:99:ILE:HG23	2.43	0.47
3:D:1239:ASP:O	3:D:1243:LEU:HB2	2.14	0.47
3:D:1309:ILE:HG13	3:D:1310:THR:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:598:LYS:O	3:D:601:ILE:HG22	2.14	0.47
2:I:800:MET:SD	2:I:1096:ILE:HD11	2.55	0.47
3:J:268:LEU:CB	3:J:306:LEU:HD23	2.44	0.47
3:J:46:TYR:HD1	5:L:500:ILE:HG21	1.80	0.47
1:A:18:GLN:HE22	1:A:213:PRO:HD2	1.79	0.46
2:C:119:GLU:HG3	2:C:489:PRO:HD2	1.96	0.46
2:C:26:TYR:HE2	2:C:32:LEU:HD12	1.80	0.46
2:C:338:THR:HG22	2:C:345:PRO:HB3	1.97	0.46
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.97	0.46
3:D:491:LEU:HD22	3:D:496:GLY:O	2.15	0.46
2:I:690:VAL:HB	2:I:1236:ASN:HB3	1.97	0.46
2:I:1313:HIS:HB2	3:J:474:LEU:HD13	1.97	0.46
3:J:694:SER:O	3:J:698:MET:HB2	2.15	0.46
5:L:343:LYS:O	5:L:347:ILE:HG13	2.15	0.46
2:C:106:GLU:HB2	2:C:109:ALA:HB2	1.82	0.46
2:C:739:ASP:OD1	2:C:739:ASP:N	2.48	0.46
2:C:929:ILE:HD13	2:C:1055:ALA:HB2	1.97	0.46
3:D:556:GLU:O	3:D:564:VAL:HB	2.15	0.46
3:D:850:LYS:HG2	3:D:857:LEU:HD11	1.95	0.46
5:F:292:VAL:HG11	5:F:299:LYS:HE3	1.97	0.46
2:I:503:LYS:HD2	2:I:503:LYS:HA	1.73	0.46
3:J:809:VAL:HA	3:J:894:VAL:O	2.14	0.46
4:K:26:ARG:NH2	4:K:38:LEU:HD13	2.30	0.46
5:L:584:ARG:HA	5:L:584:ARG:HD2	1.71	0.46
1:B:250:ASP:OD1	1:B:252:ILE:HB	2.16	0.46
1:B:281:LEU:HD11	1:B:303:ILE:HG21	1.97	0.46
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.67	0.46
2:C:518:ASN:OD1	2:C:518:ASN:N	2.48	0.46
3:D:680:ASN:HB2	9:M:202:G4P:C2	2.45	0.46
5:F:138:PRO:HD2	5:F:353:LEU:HD11	1.97	0.46
5:F:600:HIS:CB	5:F:601:PRO:CD	2.93	0.46
2:I:386:GLU:HA	2:I:390:PHE:HD2	1.80	0.46
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.97	0.46
2:I:979:LEU:HA	2:I:1002:LEU:HD13	1.97	0.46
2:I:992:LEU:HD12	2:I:996:ARG:HB3	1.97	0.46
3:J:24:LEU:HD11	3:J:116:PHE:CZ	2.50	0.46
3:J:826:ILE:HD12	3:J:826:ILE:O	2.15	0.46
3:D:786:THR:CG2	6:M:75:ARG:HG2	2.45	0.46
1:A:60:GLU:CD	1:A:143:ARG:HH21	2.19	0.46
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.97	0.46
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:677:GLU:CG	6:M:129:ARG:NH1	2.79	0.46
4:E:26:ARG:NH2	4:E:38:LEU:HD13	2.30	0.46
5:F:584:ARG:HA	5:F:584:ARG:HD2	1.62	0.46
2:C:902:LEU:HD12	5:F:607:LEU:HD23	1.98	0.46
2:C:1296:ASP:OD2	2:C:1322:SER:HB3	2.16	0.46
2:C:468:LEU:O	2:C:471:VAL:HG12	2.16	0.46
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.45	0.46
3:D:356:THR:OG1	3:D:357:VAL:N	2.48	0.46
3:D:500:ILE:O	3:D:500:ILE:HG22	2.15	0.46
3:D:621:ALA:HA	3:D:624:ILE:HD12	1.98	0.46
1:G:167:PRO:HB2	1:G:170:ARG:HB2	1.97	0.46
2:I:671:LEU:HD23	2:I:1186:VAL:CG1	2.46	0.46
2:I:71:VAL:HB	2:I:99:LYS:HB2	1.96	0.46
3:J:495:ASN:C	3:J:497:GLU:H	2.19	0.46
3:J:657:ALA:O	3:J:661:VAL:HG13	2.15	0.46
2:C:147:SER:OG	2:C:455:SER:HB3	2.16	0.46
2:C:699:LEU:HA	2:C:699:LEU:HD23	1.60	0.46
3:D:797:THR:O	3:D:801:VAL:HG12	2.15	0.46
3:D:826:ILE:HD12	3:D:826:ILE:O	2.15	0.46
4:E:2:ALA:HB2	4:E:55:GLU:CD	2.36	0.46
3:J:1167:LYS:HG2	3:J:1168:GLU:H	1.80	0.46
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.97	0.46
3:J:748:ALA:O	3:J:777:HIS:HD2	1.97	0.46
1:A:115:ILE:HG22	1:A:116:THR:N	2.31	0.46
1:B:152:TYR:CE2	3:D:536:LEU:HD21	2.50	0.46
1:B:185:TYR:HA	1:B:202:VAL:O	2.15	0.46
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.23	0.46
1:A:135:ASP:HB2	2:C:726:TYR:HE1	1.80	0.46
2:C:928:VAL:HG22	2:C:1054:LEU:HD11	1.98	0.46
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.27	0.46
1:G:104:LYS:HG2	1:G:110:VAL:HG13	1.98	0.46
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.44	0.46
2:I:109:ALA:HB1	2:I:110:PRO:HD2	1.97	0.46
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.98	0.46
5:L:147:GLN:O	5:L:151:VAL:HG23	2.16	0.46
1:B:115:ILE:HG22	1:B:116:THR:N	2.29	0.46
1:B:94:GLY:HA2	1:B:277:TYR:HE2	1.81	0.46
3:D:899:TYR:CD1	3:D:915:ILE:HD12	2.51	0.46
1:G:44:ARG:HG3	1:G:183:ILE:HG22	1.97	0.46
3:J:255:LEU:HD13	3:J:255:LEU:HA	1.84	0.46
3:J:398:LYS:HE2	5:L:532:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:478:LEU:HG	4:K:47:THR:HG23	1.97	0.46
4:K:15:ASN:C	4:K:17:PHE:H	2.20	0.46
5:L:448:ARG:HE	5:L:448:ARG:HB3	1.46	0.46
3:D:518:VAL:CG1	3:D:707:ILE:HD13	2.46	0.46
3:J:57:PHE:CE2	3:J:252:LEU:HD12	2.51	0.46
3:J:57:PHE:HB3	3:J:98:ARG:NH2	2.31	0.46
3:J:700:ASN:O	3:J:704:GLU:HB2	2.16	0.46
3:J:901:ARG:HD2	3:J:906:GLY:O	2.15	0.46
6:M:18:ALA:C	6:M:20:VAL:H	2.19	0.46
1:A:223:ILE:HD13	1:B:8:PHE:HE2	1.81	0.46
1:B:187:VAL:HG13	1:B:200:LYS:O	2.16	0.46
2:C:882:ILE:H	2:C:882:ILE:HD12	1.82	0.46
5:F:525:ASP:CG	5:F:528:LEU:HG	2.36	0.46
2:I:818:VAL:HB	2:I:1076:ILE:HD11	1.98	0.46
2:I:151:ARG:NH1	2:I:542:ARG:HH12	2.13	0.46
2:I:673:HIS:O	2:I:1109:ILE:HG22	2.16	0.46
3:J:227:PHE:O	3:J:230:SER:HB3	2.16	0.46
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.16	0.46
3:J:479:GLU:CG	4:K:20:VAL:HG11	2.46	0.46
1:A:72:GLU:OE2	2:C:958:LYS:NZ	2.40	0.45
2:C:810:TYR:HE2	3:D:359:PRO:HD2	1.81	0.45
3:J:803:VAL:HG22	3:J:1259:GLN:HB3	1.98	0.45
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.81	0.45
1:B:182:ARG:HG2	1:B:183:ILE:N	2.31	0.45
2:C:979:LEU:HD21	2:C:1000:LEU:HD13	1.98	0.45
2:C:820:GLU:N	2:C:1080:ASN:O	2.48	0.45
5:F:226:ALA:O	5:F:229:VAL:HG22	2.16	0.45
1:G:32:GLU:HA	1:G:198:LEU:HD22	1.98	0.45
2:I:1142:ARG:HD3	2:I:1161:LEU:HD13	1.97	0.45
2:I:1222:GLU:OE2	3:J:537:TYR:OH	2.28	0.45
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.81	0.45
2:I:478:ARG:NH2	2:I:487:LEU:HD13	2.31	0.45
2:I:617:ALA:HA	2:I:636:CYS:SG	2.56	0.45
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.98	0.45
2:I:807:TRP:HE1	2:I:1086:PRO:HD3	1.81	0.45
2:I:74:ARG:NH2	2:I:97:ARG:HG3	2.32	0.45
6:M:91:ARG:NH1	9:M:202:G4P:O2'	2.48	0.45
2:C:1142:ARG:HH12	2:C:1165:SER:HA	1.81	0.45
2:C:519:ASN:HB3	2:C:522:SER:HB2	1.98	0.45
3:D:81:ARG:C	3:D:83:VAL:H	2.20	0.45
4:E:56:GLU:HB2	4:E:58:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:166:VAL:O	5:F:167:ASP:HB2	2.16	0.45
2:I:802:VAL:HG11	2:I:1230:MET:HB3	1.98	0.45
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.16	0.45
3:J:1293:GLU:HB3	3:J:1294:ALA:H	1.56	0.45
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.30	0.45
3:J:366:CYS:HB3	3:J:437:PHE:CD1	2.51	0.45
3:J:678:ARG:HG3	3:J:679:TYR:N	2.31	0.45
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.99	0.45
1:B:321:TRP:CG	1:B:321:TRP:O	2.70	0.45
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.98	0.45
2:C:691:PRO:HA	2:C:788:SER:OG	2.15	0.45
1:H:67:GLU:O	1:H:78:ILE:HB	2.16	0.45
2:I:68:LEU:HD11	2:I:100:LEU:HB3	1.99	0.45
2:I:156:PHE:HD2	2:I:175:ARG:HB3	1.79	0.45
3:J:905:ARG:HH12	4:K:10:VAL:HG11	1.81	0.45
3:J:364:HIS:CG	4:K:4:VAL:HG23	2.51	0.45
3:D:695:LYS:HA	3:D:695:LYS:HD3	1.67	0.45
3:J:833:GLU:OE1	3:J:1242:ARG:HD3	2.16	0.45
3:J:322:ARG:NH1	3:J:322:ARG:HB2	2.31	0.45
3:J:649:LYS:O	3:J:653:ILE:HG13	2.15	0.45
5:L:247:GLU:O	5:L:251:LYS:HG3	2.16	0.45
5:L:253:SER:O	5:L:257:LYS:HG3	2.16	0.45
2:I:900:LYS:HB3	5:L:563:PHE:HD1	1.82	0.45
1:A:77:ASP:OD2	2:C:755:LYS:NZ	2.49	0.45
2:C:106:GLU:HB3	2:C:109:ALA:CA	2.43	0.45
3:D:1287:ILE:HG22	3:D:1300:ALA:H	1.81	0.45
3:D:342:LEU:HA	3:D:343:LEU:HA	1.72	0.45
5:F:608:ARG:HH11	5:F:608:ARG:CG	2.30	0.45
2:I:50:GLU:OE1	2:I:54:ARG:NE	2.44	0.45
2:I:836:LEU:HB3	2:I:918:LEU:HD11	1.98	0.45
3:J:801:VAL:O	3:J:805:GLN:HB2	2.17	0.45
4:K:49:ILE:O	4:K:53:GLU:HG3	2.17	0.45
5:L:166:VAL:O	5:L:167:ASP:HB2	2.15	0.45
1:A:195:ARG:HD2	1:A:196:THR:H	1.81	0.45
1:A:211:ILE:HD13	1:A:211:ILE:HA	1.71	0.45
1:B:151:GLY:HA2	1:B:178:SER:HB3	1.98	0.45
2:C:949:GLU:HG2	2:C:1036:ILE:HG22	1.99	0.45
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.60	0.45
2:C:236:LYS:HA	2:C:236:LYS:HD3	1.76	0.45
2:C:468:LEU:HA	2:C:471:VAL:HG12	1.99	0.45
3:D:1344:LEU:HA	3:D:1349:GLU:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:536:LEU:HD13	3:D:541:LEU:HB2	1.98	0.45
3:D:905:ARG:CZ	3:D:910:ASN:HD21	2.29	0.45
5:F:111:LEU:HD11	5:F:119:ILE:HD12	1.99	0.45
3:J:1171:GLY:HA2	3:J:1193:TRP:HZ3	1.81	0.45
3:J:115:TRP:HE1	3:J:308:ASP:HB2	1.82	0.45
3:J:598:LYS:O	3:J:601:ILE:HG22	2.17	0.45
5:L:511:ILE:HG21	5:L:522:PHE:CE2	2.52	0.45
1:B:321:TRP:N	1:B:322:PRO:CD	2.80	0.45
2:C:629:PHE:CE2	2:C:634:VAL:HG11	2.52	0.45
2:C:744:GLY:C	2:C:746:ALA:H	2.20	0.45
3:D:682:VAL:O	3:D:685:ILE:HG12	2.17	0.45
2:I:1270:PHE:CZ	2:I:1290:MET:HG2	2.52	0.45
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.98	0.45
1:A:61:ILE:HB	1:A:64:VAL:CG2	2.46	0.45
1:B:35:PHE:HA	1:B:38:THR:HB	1.99	0.45
2:C:587:LEU:HA	2:C:587:LEU:HD23	1.73	0.45
3:D:690:ASN:HD21	3:D:745:GLY:HA2	1.81	0.45
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.99	0.45
1:H:190:ALA:HB2	1:H:200:LYS:HB2	1.99	0.45
2:I:960:LEU:HD11	2:I:1028:LYS:HE2	1.99	0.45
2:I:39:ILE:HA	2:I:49:LEU:HD12	1.99	0.45
3:J:331:ILE:O	3:J:337:ARG:HA	2.17	0.45
5:L:611:LEU:HD23	5:L:611:LEU:HA	1.81	0.45
6:M:25:GLU:OE2	6:M:123:ILE:HB	2.17	0.45
1:A:282:VAL:O	1:A:315:GLY:N	2.50	0.45
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.99	0.45
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.51	0.45
2:C:684:ASN:HA	2:C:687:ARG:NH1	2.31	0.45
2:C:73:TYR:HA	2:C:98:VAL:HA	1.98	0.45
3:D:1283:SER:O	3:D:1286:LYS:N	2.49	0.45
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.52	0.45
5:F:324:LYS:HB3	5:F:325:PRO:HD2	1.99	0.45
5:F:452:ILE:HG13	5:F:457:ILE:HG13	1.99	0.45
1:H:219:ARG:HA	1:H:222:THR:HB	1.98	0.45
2:I:961:SER:O	2:I:965:GLN:N	2.40	0.45
3:J:161:THR:HG22	3:J:164:GLN:HB2	1.99	0.45
3:J:449:LEU:HD21	3:J:457:TYR:CD2	2.52	0.45
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.97	0.45
1:B:228:LEU:HA	1:B:231:PHE:HD2	1.82	0.44
1:B:253:LEU:HB2	1:B:321:TRP:HE1	1.81	0.44
1:B:65:LEU:HA	1:B:65:LEU:HD23	1.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1285:TYR:CE1	3:D:475:GLU:HG2	2.52	0.44
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.99	0.44
2:C:565:GLU:HG2	2:C:565:GLU:O	2.16	0.44
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.99	0.44
3:D:122:SER:O	3:D:126:LEU:HG	2.18	0.44
1:H:107:ILE:HG12	1:H:136:GLU:O	2.16	0.44
2:I:338:THR:HG22	2:I:345:PRO:HB3	1.98	0.44
2:I:697:LYS:HE2	2:I:697:LYS:HB3	1.72	0.44
2:I:895:LEU:HB2	2:I:899:GLU:HB2	1.98	0.44
3:J:599:LYS:HA	3:J:599:LYS:HD3	1.76	0.44
3:J:761:ALA:H	3:J:771:GLN:NE2	2.15	0.44
5:L:399:LEU:HA	5:L:399:LEU:HD12	1.69	0.44
2:C:514:PHE:HB3	2:C:760:ASN:HD22	1.82	0.44
2:C:593:LYS:HB3	2:C:602:GLU:HG3	1.99	0.44
3:D:159:ILE:HG13	3:D:159:ILE:O	2.16	0.44
2:I:960:LEU:HB3	2:I:1025:PHE:CE2	2.52	0.44
2:I:1082:ILE:H	2:I:1082:ILE:CD1	2.27	0.44
3:J:1181:ASP:OD1	3:J:1182:GLY:N	2.48	0.44
3:J:518:VAL:CG1	3:J:707:ILE:HD13	2.48	0.44
1:A:76:GLU:N	1:A:76:GLU:OE2	2.51	0.44
2:C:1086:PRO:O	2:C:1094:VAL:HG12	2.17	0.44
2:C:290:GLU:HG2	2:C:319:LEU:CD1	2.47	0.44
2:C:563:THR:OG1	2:C:564:PRO:HD2	2.16	0.44
2:C:5:TYR:O	2:C:8:LYS:HG2	2.17	0.44
2:C:946:LEU:HA	2:C:946:LEU:HD23	1.87	0.44
2:C:73:TYR:CB	2:C:98:VAL:HG22	2.47	0.44
3:D:1230:THR:O	3:D:1234:VAL:HG13	2.17	0.44
3:D:27:PRO:HB3	3:D:241:VAL:HG23	1.99	0.44
3:D:707:ILE:HD12	3:D:707:ILE:H	1.83	0.44
2:C:122:VAL:HG23	5:F:472:GLN:HG3	2.00	0.44
2:I:198:ILE:HD13	2:I:388:LEU:HD13	1.99	0.44
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.52	0.44
2:I:710:VAL:HG13	2:I:717:VAL:HG21	2.00	0.44
3:J:1167:LYS:HE3	3:J:1174:ARG:HD2	1.98	0.44
5:L:148:TYR:OH	5:L:218:ARG:HA	2.18	0.44
5:L:314:THR:O	5:L:318:ALA:HB3	2.18	0.44
1:B:212:ASP:O	1:B:215:GLU:N	2.50	0.44
2:C:541:GLU:N	2:C:541:GLU:OE1	2.49	0.44
3:D:1143:ASP:HA	3:D:1148:ARG:HH11	1.83	0.44
3:D:304:ASP:OD2	3:D:312:ARG:NH2	2.51	0.44
2:I:389:PHE:HA	2:I:395:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:588:GLU:HB3	2:I:607:SER:HA	1.99	0.44
2:I:61:SER:O	2:I:63:SER:N	2.50	0.44
3:J:1349:GLU:N	3:J:1349:GLU:OE2	2.35	0.44
5:L:99:ARG:HA	5:L:99:ARG:HD3	1.74	0.44
1:B:290:LEU:HB3	1:B:291:LYS:HE2	1.98	0.44
2:C:1083:GLU:HG3	2:C:1083:GLU:H	1.60	0.44
2:C:657:THR:HG21	2:C:1188:ASP:HB2	2.00	0.44
3:D:1252:HIS:O	3:D:1255:VAL:HG13	2.16	0.44
3:D:334:LYS:HA	3:D:335:GLN:HA	1.80	0.44
3:D:494:ALA:CB	3:D:922:SER:HB3	2.48	0.44
1:H:100:LEU:HB3	1:H:115:ILE:HG22	1.99	0.44
2:I:551:HIS:ND1	2:I:553:THR:OG1	2.50	0.44
2:I:88:ARG:HH11	2:I:88:ARG:HB2	1.83	0.44
3:J:1358:PRO:HB3	3:J:1366:HIS:CG	2.52	0.44
3:J:612:LEU:HB3	3:J:616:PRO:HG2	1.99	0.44
3:J:905:ARG:NH1	4:K:10:VAL:HG11	2.31	0.44
4:K:38:LEU:HB2	4:K:53:GLU:OE1	2.18	0.44
5:L:143:TYR:CZ	5:L:268:TYR:CE2	3.04	0.44
1:A:228:LEU:CD1	1:B:224:LEU:HD23	2.40	0.44
2:C:161:LYS:HA	2:C:170:VAL:HA	1.99	0.44
2:C:725:GLN:HE22	2:C:966:ILE:HG23	1.82	0.44
3:D:418:GLU:OE1	4:E:3:ARG:NH2	2.48	0.44
5:F:371:LYS:HA	5:F:374:ARG:NH1	2.32	0.44
2:C:490:GLN:HG3	5:F:472:GLN:CD	2.38	0.44
5:F:484:ALA:HB1	5:F:491:GLU:HG3	1.98	0.44
2:I:800:MET:HE2	2:I:1095:ASP:HB3	2.00	0.44
2:I:1332:SER:HA	3:J:243:PRO:HB2	1.99	0.44
2:I:55:SER:OG	2:I:56:VAL:N	2.50	0.44
2:I:93:SER:HA	2:I:128:PRO:HA	2.00	0.44
5:L:476:ARG:HH11	5:L:477:GLU:H	1.66	0.44
2:C:1086:PRO:HB3	2:C:1212:LEU:HD23	2.00	0.44
2:C:799:ASN:HB3	2:C:1231:TYR:HD1	1.83	0.44
2:C:238:GLN:HG2	2:C:286:GLU:HA	2.00	0.44
2:C:533:LEU:HD11	2:C:568:ASN:HD22	1.83	0.44
2:C:963:GLU:O	2:C:967:LEU:HB2	2.18	0.44
3:D:128:LEU:HD21	3:D:189:LEU:HD23	1.99	0.44
2:I:678:ARG:CG	2:I:1108:ASN:HD22	2.28	0.44
2:I:250:THR:HA	2:I:268:ARG:HA	2.00	0.44
3:J:659:ALA:O	3:J:663:GLU:HG3	2.18	0.44
3:J:825:VAL:C	3:J:826:ILE:HG13	2.38	0.44
5:L:476:ARG:HH11	5:L:476:ARG:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.98	0.44
2:C:798:GLN:HB2	2:C:828:PHE:CE1	2.53	0.44
3:D:268:LEU:HB3	3:D:306:LEU:HD23	2.00	0.44
1:H:147:GLN:HG3	1:H:148:ARG:H	1.83	0.44
2:I:478:ARG:NH1	2:I:482:GLY:HA2	2.33	0.44
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.82	0.44
5:L:470:MET:HB2	5:L:478:PRO:HG3	2.00	0.44
1:A:168:ILE:H	1:A:168:ILE:HG12	1.68	0.44
1:A:315:GLY:C	1:A:316:MET:HG3	2.38	0.44
2:C:169:LYS:HE2	2:C:190:PRO:HA	2.00	0.44
2:C:87:ILE:H	2:C:87:ILE:HG13	1.61	0.44
1:G:100:LEU:HD23	1:G:115:ILE:HG21	2.00	0.44
1:G:166:ARG:O	1:G:167:PRO:C	2.56	0.44
2:I:1142:ARG:HH12	2:I:1165:SER:HA	1.82	0.44
2:I:201:ARG:NH2	2:I:370:MET:O	2.37	0.44
2:I:541:GLU:N	2:I:541:GLU:OE1	2.48	0.44
2:I:543:ALA:HA	2:I:544:GLY:HA3	1.71	0.44
3:J:1307:LEU:HD23	3:J:1312:ALA:HA	1.99	0.44
6:M:70:PRO:HG2	6:M:78:GLN:OE1	2.18	0.44
1:A:44:ARG:HB2	1:A:183:ILE:CG2	2.47	0.43
2:C:1240:ASP:OD1	2:C:1240:ASP:N	2.45	0.43
2:C:462:ASN:O	2:C:466:VAL:HG23	2.18	0.43
2:C:716:ALA:HB3	2:C:784:ALA:HB3	2.00	0.43
3:D:1273:ASP:O	3:D:1275:LEU:N	2.47	0.43
3:D:1281:GLU:O	3:D:1285:VAL:HG13	2.18	0.43
3:D:850:LYS:HB2	3:D:852:GLY:O	2.18	0.43
5:F:320:ILE:HG21	5:F:331:HIS:CD2	2.53	0.43
1:G:35:PHE:CE1	1:H:46:ILE:HG12	2.47	0.43
2:I:1142:ARG:NH1	2:I:1161:LEU:HD11	2.33	0.43
2:I:212:ALA:HA	2:I:359:ARG:HG3	2.00	0.43
2:I:565:GLU:HG2	2:I:565:GLU:O	2.17	0.43
2:I:897:PRO:HB2	2:I:898:GLU:OE1	2.17	0.43
3:J:587:LEU:HD23	3:J:591:ILE:HG21	2.00	0.43
5:L:320:ILE:HG23	5:L:327:SER:O	2.16	0.43
1:A:266:SER:HB3	1:A:303:ILE:HD11	2.00	0.43
1:B:262:LEU:H	1:B:262:LEU:HD12	1.82	0.43
3:D:720:ASN:OD1	3:D:722:ILE:HG22	2.18	0.43
5:F:489:MET:HB2	5:F:490:PRO:HD2	1.99	0.43
1:G:67:GLU:OE1	2:I:1057:LYS:NZ	2.52	0.43
2:I:1193:ALA:O	2:I:1197:GLU:HB2	2.18	0.43
2:I:886:LYS:NZ	2:I:916:SER:HB3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:118:LYS:HE2	3:J:118:LYS:HB3	1.83	0.43
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.48	0.43
1:B:286:GLU:OE2	1:B:304:LYS:NZ	2.46	0.43
2:C:1282:GLY:H	3:D:483:LEU:HD13	1.83	0.43
5:F:101:TYR:CE2	5:F:388:ILE:HD11	2.43	0.43
1:H:71:LYS:HA	1:H:71:LYS:HD2	1.86	0.43
2:I:1308:ILE:CG2	3:J:379:PRO:HB2	2.47	0.43
2:I:850:ILE:O	2:I:850:ILE:HG22	2.18	0.43
3:J:358:GLY:N	3:J:359:PRO:HD3	2.32	0.43
5:L:573:LEU:H	5:L:573:LEU:CD2	2.25	0.43
6:M:65:GLU:HB3	6:M:82:PHE:HZ	1.82	0.43
1:A:158:ARG:HH22	1:A:172:LEU:HD23	1.82	0.43
1:B:16:ILE:HG12	1:B:26:VAL:HG13	2.00	0.43
2:C:867:GLU:H	2:C:867:GLU:HG3	1.39	0.43
3:D:331:ILE:HG22	3:D:1328:THR:HG21	1.99	0.43
3:D:347:VAL:HG12	3:D:348:ASP:O	2.18	0.43
3:D:674:THR:HG22	6:M:136:ILE:HD12	2.01	0.43
3:D:680:ASN:O	3:D:683:ILE:HG22	2.19	0.43
2:I:678:ARG:NH2	2:I:1106:ARG:HG2	2.33	0.43
2:I:18:ARG:HA	2:I:19:PRO:HD3	1.92	0.43
3:J:128:LEU:HB3	3:J:157:GLN:HE22	1.83	0.43
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.91	0.43
3:J:311:ARG:O	3:J:312:ARG:HD3	2.18	0.43
3:J:342:LEU:HA	3:J:343:LEU:HA	1.71	0.43
3:J:385:LEU:CD2	3:J:411:ILE:HG13	2.48	0.43
3:J:804:ALA:O	3:J:806:ASP:N	2.51	0.43
6:M:78:GLN:HG2	6:M:82:PHE:CE2	2.54	0.43
2:C:338:THR:CG2	2:C:345:PRO:HB3	2.49	0.43
2:C:513:GLN:HG3	2:C:526:HIS:CE1	2.53	0.43
3:D:215:LYS:HE2	3:D:215:LYS:HB3	1.86	0.43
3:D:201:LEU:CD1	3:D:220:ARG:HG2	2.49	0.43
3:D:268:LEU:HD23	3:D:268:LEU:HA	1.78	0.43
5:F:595:LEU:HB3	5:F:599:ARG:HH21	1.83	0.43
1:G:45:ARG:HD3	2:I:1083:GLU:HB3	2.01	0.43
3:J:159:ILE:O	3:J:159:ILE:HG13	2.17	0.43
3:J:513:MET:O	3:J:575:GLY:HA3	2.18	0.43
3:J:850:LYS:HB2	3:J:852:GLY:O	2.18	0.43
2:C:13:LYS:HD3	2:C:1149:TYR:HA	2.00	0.43
2:C:323:ALA:O	2:C:327:GLN:HG3	2.18	0.43
2:C:980:VAL:HA	2:C:984:VAL:HA	2.01	0.43
3:D:505:ASP:HB3	3:D:629:PHE:CE1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:68:TYR:HA	3:D:92:VAL:HG23	2.00	0.43
4:E:19:LEU:HD13	4:E:54:ILE:HG21	1.99	0.43
5:F:320:ILE:O	5:F:327:SER:HB3	2.18	0.43
5:F:399:LEU:HA	5:F:399:LEU:HD12	1.81	0.43
1:G:219:ARG:HA	1:G:222:THR:HB	2.01	0.43
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	2.00	0.43
2:I:29:SER:O	2:I:33:ASP:HB2	2.19	0.43
2:I:9:LYS:O	2:I:1175:ASN:ND2	2.49	0.43
3:J:689:ALA:O	3:J:693:VAL:HG23	2.19	0.43
5:L:580:PHE:HD1	5:L:580:PHE:HA	1.68	0.43
1:A:49:SER:O	1:A:51:MET:N	2.47	0.43
1:B:155:ALA:H	1:B:174:ASP:HA	1.84	0.43
1:B:151:GLY:O	1:B:177:TYR:N	2.51	0.43
2:C:1243:MET:HA	3:D:353:SER:HB3	2.01	0.43
1:A:261:GLU:CD	2:C:859:GLU:HB2	2.39	0.43
3:D:1165:PHE:CE1	3:D:1200:GLU:HB2	2.52	0.43
3:D:56:LEU:H	3:D:56:LEU:HD12	1.83	0.43
3:D:258:GLY:HA3	5:F:499:LYS:HE2	2.00	0.43
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.99	0.43
2:I:1066:MET:CE	2:I:1076:ILE:HB	2.49	0.43
2:I:478:ARG:CZ	2:I:487:LEU:HD13	2.49	0.43
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.43	0.43
3:J:364:HIS:CE1	4:K:3:ARG:NH2	2.84	0.43
3:J:609:TYR:HA	3:J:617:THR:OG1	2.18	0.43
3:J:263:SER:HA	5:L:507:MET:HB2	2.01	0.43
3:D:681:LYS:NZ	6:M:14:ILE:HD12	2.33	0.43
1:A:195:ARG:HD2	1:A:196:THR:N	2.34	0.43
2:C:1101:LEU:HD21	3:D:508:LEU:HD22	2.00	0.43
5:F:141:ILE:HG21	5:F:228:TYR:CD1	2.53	0.43
5:F:354:THR:O	5:F:358:VAL:HG23	2.19	0.43
2:I:1340:GLU:CG	3:J:21:LYS:HB2	2.49	0.43
2:I:974:ARG:HB3	2:I:1014:LEU:HD21	2.01	0.43
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.99	0.43
3:J:28:ASP:OD1	3:J:31:ARG:NH1	2.52	0.43
6:M:93:ARG:O	6:M:97:LYS:HG2	2.19	0.43
1:A:44:ARG:HE	1:A:183:ILE:HG22	1.83	0.43
1:A:231:PHE:HE2	1:B:39:LEU:HB3	1.83	0.43
1:A:232:VAL:O	1:B:218:ARG:HG2	2.18	0.43
2:C:1002:LEU:HD22	2:C:1007:LYS:CB	2.43	0.43
2:C:88:ARG:NH1	2:C:88:ARG:HB2	2.34	0.43
3:D:823:THR:HA	3:D:835:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:281:ARG:HD3	5:F:285:ARG:NH1	2.33	0.43
5:F:484:ALA:HB1	5:F:491:GLU:CG	2.49	0.43
1:G:197:ASP:O	1:G:198:LEU:HD23	2.19	0.43
1:H:56:VAL:HG11	1:H:144:ILE:HD11	2.01	0.43
2:I:1305:TYR:OH	5:L:532:LEU:HG	2.19	0.43
2:I:553:THR:H	2:I:553:THR:HG1	1.46	0.43
3:J:414:GLU:O	4:K:45:LYS:NZ	2.37	0.43
1:B:192:VAL:O	1:B:193:GLU:C	2.58	0.43
1:B:275:ILE:CD1	1:B:284:ARG:HD3	2.49	0.43
2:C:263:VAL:HG13	2:C:267:ARG:HB3	2.01	0.43
2:C:88:ARG:HA	2:C:934:PHE:CZ	2.54	0.43
3:D:114:ILE:HB	3:D:304:ASP:OD1	2.19	0.43
5:F:394:TYR:O	5:F:404:LEU:HD11	2.19	0.43
2:I:699:LEU:HA	2:I:699:LEU:HD23	1.88	0.43
1:A:178:SER:HA	1:A:179:PRO:HD3	1.84	0.42
1:A:310:ARG:O	5:F:608:ARG:NE	2.52	0.42
1:B:285:THR:OG1	1:B:286:GLU:N	2.52	0.42
2:C:237:LEU:HG	2:C:289:VAL:HA	2.01	0.42
3:D:529:GLY:HA2	3:D:551:ARG:O	2.19	0.42
3:D:903:LEU:HD23	3:D:905:ARG:HD3	2.00	0.42
1:G:219:ARG:HB2	1:G:219:ARG:HE	1.54	0.42
2:I:1319:MET:HA	2:I:1320:PRO:HD3	1.92	0.42
2:I:629:PHE:CD2	2:I:634:VAL:HG11	2.54	0.42
2:I:778:GLU:O	2:I:781:ASP:HB2	2.19	0.42
3:J:1166:GLY:O	3:J:1174:ARG:HB2	2.19	0.42
3:J:179:LYS:HB2	3:J:184:ALA:HB2	2.02	0.42
1:B:14:VAL:HG23	1:B:27:THR:O	2.19	0.42
2:C:1151:LEU:HD21	2:C:1198:LEU:HB2	2.01	0.42
2:C:697:LYS:HB3	2:C:697:LYS:HE2	1.78	0.42
2:C:710:VAL:HG13	2:C:717:VAL:HG21	2.01	0.42
2:C:725:GLN:NE2	2:C:966:ILE:HG23	2.34	0.42
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	2.01	0.42
3:D:416:ILE:HA	3:D:416:ILE:HD13	1.75	0.42
3:D:733:SER:O	3:D:737:ILE:HG12	2.19	0.42
3:D:860:ARG:HA	3:D:860:ARG:HD2	1.82	0.42
2:I:692:THR:OG1	2:I:827:ARG:O	2.37	0.42
3:J:1356:LEU:HA	3:J:1356:LEU:HD23	1.89	0.42
3:J:594:GLN:HB2	3:J:595:ALA:H	1.60	0.42
5:L:287:ILE:HD13	5:L:315:TRP:HH2	1.84	0.42
1:B:53:GLY:C	1:B:177:TYR:HB3	2.39	0.42
2:C:1111:GLN:HB2	2:C:1230:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.34	0.42
1:G:110:VAL:CG2	1:G:133:LEU:HD23	2.50	0.42
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.54	0.42
3:J:1266:ILE:HD12	3:J:1273:ASP:O	2.19	0.42
3:J:24:LEU:HB2	3:J:232:ASN:OD1	2.19	0.42
3:J:45:ASN:HB3	3:J:48:THR:O	2.19	0.42
3:J:596:LEU:HD11	3:J:604:MET:CE	2.49	0.42
3:J:650:LYS:O	3:J:654:ILE:HG13	2.19	0.42
5:L:316:PHE:CZ	5:L:334:SER:HA	2.53	0.42
1:A:166:ARG:N	1:A:167:PRO:HD2	2.35	0.42
1:B:183:ILE:HD12	1:B:183:ILE:H	1.83	0.42
2:C:1065:LYS:HE2	3:D:462:ASP:O	2.18	0.42
2:C:1193:ALA:O	2:C:1197:GLU:HB2	2.19	0.42
3:D:118:LYS:HE2	3:D:118:LYS:HB3	1.89	0.42
3:D:1192:LYS:HE3	3:D:1192:LYS:HB2	1.90	0.42
3:D:262:THR:HG1	3:D:266:ASN:ND2	2.15	0.42
3:D:518:VAL:HG22	3:D:709:ARG:HB2	2.01	0.42
3:D:81:ARG:HG3	3:D:82:GLY:H	1.85	0.42
5:F:584:ARG:O	5:F:588:ARG:HG3	2.20	0.42
2:I:12:ARG:NH1	2:I:1182:ILE:O	2.50	0.42
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.67	0.42
2:I:402:ARG:HG2	2:I:416:GLY:H	1.83	0.42
3:J:902:ASP:HB2	3:J:1251:LYS:HE3	2.01	0.42
1:A:175:ALA:HB1	1:A:177:TYR:CE1	2.53	0.42
1:A:18:GLN:HE22	1:A:213:PRO:CD	2.33	0.42
1:B:317:ARG:O	1:B:318:LEU:HD13	2.19	0.42
2:C:16:GLY:HA2	2:C:1188:ASP:O	2.20	0.42
2:C:696:ASP:HB3	2:C:697:LYS:H	1.61	0.42
3:D:1160:SER:OG	3:D:1203:ARG:NH1	2.53	0.42
1:G:89:ALA:HB1	1:G:210:THR:CG2	2.50	0.42
1:G:17:GLU:N	1:G:25:LYS:O	2.43	0.42
1:G:86:LYS:HB2	1:G:86:LYS:HE3	1.73	0.42
2:I:1156:ARG:HB2	2:I:1156:ARG:HH11	1.84	0.42
2:I:148:GLN:HG3	2:I:511:LEU:HD11	2.01	0.42
2:I:79:VAL:HG23	2:I:80:PHE:H	1.85	0.42
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.54	0.42
5:L:343:LYS:HD2	5:L:343:LYS:H	1.84	0.42
9:M:202:G4P:HO2'	9:M:202:G4P:PC	2.41	0.42
2:C:1156:ARG:HB2	2:C:1156:ARG:HH11	1.84	0.42
2:C:528:ARG:NH2	2:C:576:SER:O	2.52	0.42
2:C:920:VAL:HA	2:C:921:PRO:HD3	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	2.49	0.42
3:D:1174:ARG:NE	3:D:1187:GLU:OE2	2.52	0.42
3:D:126:LEU:H	3:D:126:LEU:HG	1.65	0.42
3:D:1298:VAL:N	3:D:1299:GLY:CA	2.81	0.42
3:D:842:ARG:HB3	3:D:882:VAL:CG1	2.48	0.42
5:F:277:MET:HG3	5:F:362:ASN:ND2	2.35	0.42
5:F:559:LEU:HA	5:F:559:LEU:HD12	1.89	0.42
1:H:158:ARG:HB3	1:H:172:LEU:HD23	2.00	0.42
3:J:649:LYS:HA	3:J:649:LYS:HD3	1.77	0.42
5:L:476:ARG:HD2	5:L:477:GLU:HG2	2.01	0.42
1:A:195:ARG:HE	1:A:198:LEU:HD21	1.85	0.42
1:A:321:TRP:HA	1:A:322:PRO:HA	1.78	0.42
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.83	0.42
3:D:337:ARG:HH12	3:D:1320:ILE:HG23	1.85	0.42
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.50	0.42
4:E:58:LEU:H	4:E:58:LEU:HD12	1.84	0.42
5:F:125:ASP:O	5:F:129:GLN:HG3	2.19	0.42
5:F:552:THR:OG1	5:F:554:ARG:HG2	2.20	0.42
2:I:735:LYS:HA	2:I:748:ILE:HG22	2.02	0.42
1:A:104:LYS:HG3	1:A:105:SER:N	2.35	0.42
1:B:185:TYR:HB2	1:B:201:LEU:HD11	2.02	0.42
1:B:265:ARG:O	1:B:269:CYS:HB2	2.20	0.42
1:B:48:LEU:HA	1:B:180:VAL:HG21	2.01	0.42
2:C:253:PHE:O	2:C:255:ILE:HG13	2.20	0.42
3:D:271:ARG:HD3	3:D:275:ARG:NH2	2.35	0.42
3:D:349:TYR:CD1	3:D:472:LEU:HD21	2.55	0.42
3:D:494:ALA:HB2	3:D:922:SER:HB3	2.02	0.42
5:F:379:MET:O	5:F:383:ASN:ND2	2.52	0.42
3:J:126:LEU:H	3:J:126:LEU:HG	1.67	0.42
3:J:405:GLU:O	3:J:408:VAL:HG22	2.20	0.42
3:J:902:ASP:OD1	3:J:903:LEU:N	2.53	0.42
5:L:161:LEU:C	5:L:262:VAL:HG23	2.39	0.42
1:A:249:PHE:CE2	1:A:254:LEU:HG	2.55	0.42
1:A:286:GLU:HA	1:A:289:LEU:HD12	2.01	0.42
1:A:31:LEU:HA	1:A:31:LEU:HD23	1.78	0.42
2:C:109:ALA:HA	2:C:110:PRO:HD3	1.91	0.42
2:C:297:VAL:HG23	2:C:333:ILE:HG23	2.02	0.42
2:C:198:ILE:HD13	2:C:388:LEU:HD13	2.02	0.42
2:C:466:VAL:O	2:C:470:ARG:HG2	2.19	0.42
2:C:602:GLU:O	2:C:602:GLU:HG3	2.20	0.42
3:D:133:ARG:HA	3:D:133:ARG:HD2	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:355:ILE:HG22	3:D:447:ILE:HB	2.01	0.42
3:D:363:LEU:HA	3:D:450:HIS:CD2	2.54	0.42
3:D:572:THR:OG1	3:D:576:ARG:HB2	2.20	0.42
3:D:683:ILE:HD11	3:D:754:ILE:HG23	2.01	0.42
2:I:745:GLU:N	2:I:1017:GLN:HG3	2.34	0.42
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.83	0.42
3:J:308:ASP:CG	3:J:311:ARG:HE	2.22	0.42
2:I:1274:GLU:HA	3:J:428:THR:HG21	2.02	0.42
3:J:515:ARG:NH2	3:J:717:VAL:O	2.52	0.42
3:J:596:LEU:HD11	3:J:604:MET:HE3	2.02	0.42
3:J:883:ARG:HB3	3:J:898:CYS:SG	2.59	0.42
5:L:513:ASP:C	5:L:515:GLU:H	2.22	0.42
6:M:47:TRP:O	6:M:51:LEU:HG	2.20	0.42
2:C:1131:MET:HE1	2:C:1141:LEU:HD12	2.01	0.42
2:C:117:ILE:H	2:C:117:ILE:HG12	1.62	0.42
2:C:1066:MET:HG2	2:C:1234:LYS:HA	2.01	0.42
3:D:266:ASN:O	3:D:270:ARG:HB2	2.20	0.42
3:D:422:LEU:HD13	3:D:471:PRO:HG3	2.02	0.42
3:D:487:THR:HB	3:D:618:VAL:HG21	2.01	0.42
3:D:827:GLU:O	3:D:829:GLY:N	2.50	0.42
1:G:75:GLN:HA	2:I:729:ALA:H	1.83	0.42
3:J:37:GLU:HB2	3:J:104:HIS:CE1	2.55	0.42
3:J:647:PRO:HG3	3:J:697:MET:CA	2.50	0.42
5:L:233:ASP:O	5:L:236:LYS:HE2	2.20	0.42
1:A:192:VAL:HG12	1:A:195:ARG:HB2	2.02	0.41
1:A:315:GLY:O	1:A:316:MET:HG3	2.20	0.41
2:C:593:LYS:HG3	2:C:595:THR:HG23	2.00	0.41
3:D:1299:GLY:HA2	3:D:1300:ALA:HA	1.86	0.41
3:D:123:ARG:HH12	3:D:1334:GLU:HG3	1.85	0.41
5:F:137:TYR:CE2	5:F:139:GLU:HB2	2.55	0.41
2:I:896:THR:HB	2:I:897:PRO:HD2	2.02	0.41
2:I:975:ILE:O	2:I:979:LEU:HB2	2.20	0.41
3:J:362:ARG:HH21	9:J:2004:G4P:C1'	2.33	0.41
2:C:117:ILE:HD12	2:C:488:MET:HG2	2.02	0.41
2:C:1331:ARG:HG2	3:D:33:TRP:CH2	2.55	0.41
2:C:162:GLY:O	2:C:164:THR:N	2.52	0.41
2:C:421:SER:H	2:C:424:ASP:HB2	1.85	0.41
2:C:487:LEU:HD23	2:C:487:LEU:H	1.85	0.41
2:C:463:GLN:NE2	2:C:501:ALA:O	2.53	0.41
2:C:830:THR:HG23	2:C:832:HIS:NE2	2.35	0.41
3:D:130:MET:HB2	3:D:157:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:45:ASN:O	3:D:46:TYR:HD2	2.02	0.41
3:D:835:LEU:O	3:D:839:VAL:HG23	2.20	0.41
5:F:471:LEU:HD23	5:F:476:ARG:O	2.21	0.41
1:G:192:VAL:O	1:G:194:GLN:N	2.54	0.41
1:H:67:GLU:HA	1:H:78:ILE:HG21	2.02	0.41
3:J:57:PHE:CZ	3:J:252:LEU:HB2	2.54	0.41
5:L:470:MET:O	5:L:478:PRO:HD3	2.21	0.41
3:D:786:THR:HG21	6:M:75:ARG:HG2	2.00	0.41
1:A:237:VAL:O	1:B:13:LEU:HA	2.20	0.41
2:C:42:ASP:C	2:C:44:GLU:H	2.24	0.41
3:D:661:VAL:HG12	3:D:682:VAL:HG13	2.02	0.41
3:D:749:LYS:HB2	3:D:750:PRO:HD2	2.01	0.41
5:F:515:GLU:HG2	5:F:516:ASP:N	2.35	0.41
2:I:802:VAL:HG21	2:I:1098:LEU:HD22	2.01	0.41
3:J:154:LEU:HD22	3:J:160:LEU:HD11	2.02	0.41
3:J:460:ASP:OD1	3:J:462:ASP:OD1	2.39	0.41
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.50	0.41
5:L:152:GLU:OE2	5:L:218:ARG:HG3	2.19	0.41
5:L:603:ARG:HD3	5:L:603:ARG:HA	1.84	0.41
6:M:57:ARG:O	6:M:60:THR:N	2.47	0.41
6:M:59:VAL:HA	6:M:62:MET:HB2	2.03	0.41
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	2.01	0.41
3:D:24:LEU:HD13	3:D:24:LEU:HA	1.90	0.41
3:D:425:ARG:HD2	3:D:459:ALA:HB2	2.02	0.41
5:F:483:LEU:H	5:F:483:LEU:HD12	1.85	0.41
5:F:530:LEU:HD12	5:F:533:ASP:H	1.84	0.41
1:G:51:MET:HA	1:G:52:PRO:HD3	1.93	0.41
1:H:44:ARG:CG	1:H:183:ILE:HD13	2.51	0.41
1:H:217:ILE:HA	1:H:220:ALA:HB3	2.02	0.41
2:I:194:LEU:HA	2:I:194:LEU:HD12	1.88	0.41
2:I:871:VAL:HG12	2:I:883:LEU:O	2.20	0.41
3:J:430:HIS:NE2	3:J:456:ALA:O	2.49	0.41
3:J:460:ASP:CG	3:J:462:ASP:OD1	2.59	0.41
1:B:134:THR:OG1	1:B:135:ASP:N	2.52	0.41
1:B:269:CYS:SG	1:B:295:LEU:HG	2.60	0.41
2:C:1230:MET:HG2	2:C:1232:MET:HG3	2.03	0.41
2:C:800:MET:HB3	2:C:800:MET:HE3	1.81	0.41
3:D:1221:LEU:HD13	3:D:1222:ARG:N	2.35	0.41
3:D:279:LEU:HD12	3:D:295:GLU:HG3	2.01	0.41
3:D:317:THR:HB	3:D:324:LEU:HB3	2.01	0.41
3:D:744:ARG:HG3	3:D:744:ARG:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:615:LYS:HA	4:E:5:THR:HG21	2.02	0.41
1:G:22:THR:OG1	1:G:23:HIS:N	2.54	0.41
2:I:151:ARG:CZ	2:I:445:ILE:HD11	2.51	0.41
2:I:686:GLN:HG2	2:I:796:LEU:HD22	2.03	0.41
2:I:829:THR:HA	2:I:1059:ARG:HA	2.03	0.41
3:J:147:ILE:HG13	3:J:147:ILE:O	2.20	0.41
3:J:332:LYS:HA	3:J:337:ARG:H	1.85	0.41
3:J:638:SER:OG	3:J:639:VAL:N	2.53	0.41
6:M:17:ILE:CG2	6:M:50:GLN:HG3	2.49	0.41
1:B:71:LYS:HD2	1:B:71:LYS:HA	1.81	0.41
2:C:1124:ILE:HG13	2:C:1180:MET:HE3	2.03	0.41
2:C:943:LYS:O	2:C:947:GLU:HG3	2.20	0.41
3:D:1167:LYS:HB3	3:D:1167:LYS:HE3	1.85	0.41
3:D:248:ASP:O	3:D:251:PRO:HG3	2.21	0.41
3:D:355:ILE:HG21	3:D:466:MET:HG3	2.02	0.41
5:F:139:GLU:HG3	5:F:351:THR:HG22	2.01	0.41
1:G:35:PHE:HA	1:G:35:PHE:HD1	1.78	0.41
1:H:7:GLU:HG2	1:H:8:PHE:H	1.85	0.41
2:I:1083:GLU:HG3	2:I:1083:GLU:H	1.64	0.41
2:I:1184:THR:HG23	2:I:1189:GLY:HA2	2.01	0.41
2:I:127:ILE:HG22	2:I:502:VAL:HG11	2.02	0.41
2:I:80:PHE:HB3	2:I:84:GLU:HB2	2.03	0.41
3:J:239:LEU:HD23	3:J:239:LEU:HA	1.88	0.41
3:J:686:TRP:CD1	3:J:758:PRO:HD3	2.56	0.41
5:L:316:PHE:CE1	5:L:337:VAL:HB	2.56	0.41
1:B:189:ALA:HB1	1:B:191:ARG:HH12	1.86	0.41
2:C:1054:LEU:HD12	2:C:1054:LEU:HA	1.86	0.41
2:C:1252:SER:HB3	2:C:1255:THR:O	2.21	0.41
2:C:81:ASP:HA	2:C:92:TYR:HE1	1.86	0.41
3:D:322:ARG:HB2	3:D:322:ARG:HH11	1.84	0.41
3:D:599:LYS:HA	3:D:599:LYS:HD3	1.91	0.41
3:D:735:ALA:O	3:D:738:ARG:HB3	2.21	0.41
3:D:905:ARG:NH2	3:D:907:HIS:HB2	2.22	0.41
1:G:57:THR:HG22	1:G:58:GLU:HG3	2.02	0.41
2:I:896:THR:O	2:I:897:PRO:C	2.58	0.41
3:J:761:ALA:H	3:J:771:GLN:HE22	1.67	0.41
6:M:111:PHE:CE2	6:M:126:LEU:HD13	2.56	0.41
1:A:124:VAL:HG11	1:A:210:THR:HG23	2.02	0.41
1:B:153:VAL:N	1:B:175:ALA:O	2.54	0.41
1:B:29:GLU:O	1:B:31:LEU:HD23	2.11	0.41
3:D:310:GLY:HA2	3:D:314:ARG:CD	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:591:ILE:HA	3:D:591:ILE:HD12	1.89	0.41
2:C:1321:GLU:OE2	3:D:99:ARG:HD3	2.21	0.41
4:E:15:ASN:O	4:E:16:ARG:HB3	2.21	0.41
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	2.02	0.41
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.86	0.41
2:I:1111:GLN:HB2	2:I:1230:MET:HE2	2.03	0.41
2:I:1276:TRP:HD1	2:I:1279:GLU:OE1	2.02	0.41
2:I:157:PHE:O	2:I:443:ASP:N	2.52	0.41
2:I:30:ILE:HD11	2:I:575:LEU:HD22	2.03	0.41
2:I:870:ILE:HG22	2:I:944:ARG:NH1	2.36	0.41
3:J:1179:PRO:HD2	3:J:1184:ASP:HB3	2.01	0.41
3:J:514:THR:HB	3:J:576:ARG:HG2	2.02	0.41
3:J:849:LEU:HD22	3:J:849:LEU:H	1.85	0.41
5:L:559:LEU:HA	5:L:559:LEU:HD12	1.86	0.41
1:A:97:GLU:HA	1:A:146:VAL:O	2.21	0.41
1:A:187:VAL:HG23	1:A:187:VAL:O	2.21	0.41
1:B:178:SER:HA	1:B:179:PRO:HD3	1.89	0.41
2:C:543:ALA:HA	2:C:544:GLY:HA3	1.75	0.41
3:D:1183:SER:CB	3:J:206:ASN:HD21	2.33	0.41
3:D:460:ASP:OD2	6:M:71:ASP:OD2	2.39	0.41
1:G:192:VAL:O	1:G:192:VAL:HG12	2.20	0.41
2:I:468:LEU:HA	2:I:471:VAL:HG12	2.03	0.41
3:J:426:ALA:CB	3:J:427:PRO:HD3	2.43	0.41
2:I:1281:TYR:OH	3:J:431:ARG:O	2.38	0.41
3:J:657:ALA:CB	3:J:689:ALA:HB2	2.50	0.41
3:J:647:PRO:HG3	3:J:697:MET:N	2.35	0.41
5:L:285:ARG:HA	5:L:288:MET:HB3	2.02	0.41
5:L:377:LYS:O	5:L:381:GLU:HG3	2.21	0.41
5:L:493:LYS:HA	5:L:496:LYS:HG3	2.02	0.41
6:M:140:THR:O	6:M:144:ILE:HG12	2.21	0.41
1:B:62:ASP:HB2	1:B:141:SER:O	2.21	0.41
1:B:16:ILE:HG12	1:B:26:VAL:HG22	2.03	0.41
1:B:120:ASP:OD1	1:B:276:HIS:CD2	2.74	0.41
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.42	0.41
2:C:206:ALA:O	2:C:209:ILE:HG22	2.21	0.41
2:C:42:ASP:O	2:C:44:GLU:N	2.52	0.41
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.35	0.41
3:D:1156:LEU:HD23	3:D:1219:ASP:HB3	2.02	0.41
3:D:1282:TYR:HD2	3:D:1286:LYS:HZ2	1.68	0.41
3:D:147:ILE:HG13	3:D:147:ILE:O	2.21	0.41
1:H:41:ASN:O	1:H:45:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:64:VAL:HG12	1:H:66:HIS:H	1.85	0.41
2:I:297:VAL:HB	2:I:317:LEU:HD21	2.02	0.41
2:I:734:ILE:O	2:I:748:ILE:HB	2.21	0.41
3:J:1167:LYS:HE3	3:J:1167:LYS:HB3	1.92	0.41
2:I:1294:LYS:HD2	3:J:348:ASP:O	2.21	0.41
3:J:504:GLN:OE1	3:J:731:ARG:HD2	2.21	0.41
1:A:93:GLN:HB2	1:A:120:ASP:OD2	2.20	0.41
2:C:169:LYS:HE2	2:C:190:PRO:O	2.20	0.41
3:D:17:PHE:HZ	3:D:1353:VAL:HG21	1.85	0.41
3:D:45:ASN:O	3:D:46:TYR:CD2	2.74	0.41
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.55	0.41
1:H:183:ILE:HG23	1:H:205:MET:HG3	2.03	0.41
1:H:211:ILE:HD12	1:H:211:ILE:HA	1.97	0.41
2:I:1086:PRO:CB	2:I:1212:LEU:HD23	2.51	0.41
2:I:996:ARG:HD3	2:I:996:ARG:HA	1.95	0.41
2:I:1225:VAL:HA	3:J:638:SER:CB	2.51	0.41
3:J:701:LEU:HD22	3:J:701:LEU:HA	1.95	0.41
5:L:226:ALA:O	5:L:229:VAL:HG22	2.21	0.41
2:C:1299:ASN:O	2:C:1303:LYS:HG2	2.22	0.40
3:D:13:LYS:HD3	3:D:13:LYS:HA	1.86	0.40
3:D:460:ASP:OD1	3:D:464:ASP:OD2	2.39	0.40
5:F:143:TYR:CD2	5:F:269:LEU:HD21	2.56	0.40
2:I:452:ARG:HH12	2:I:585:GLY:HA3	1.86	0.40
2:I:149:LEU:HD13	2:I:453:ILE:HG13	2.02	0.40
2:I:5:TYR:O	2:I:8:LYS:HG2	2.22	0.40
2:I:820:GLU:HA	2:I:1079:ILE:HD11	2.03	0.40
2:I:828:PHE:HD1	2:I:828:PHE:HA	1.71	0.40
3:J:1203:ARG:HH22	3:J:1205:GLU:HG2	1.86	0.40
3:J:1239:ASP:O	3:J:1243:LEU:HB2	2.21	0.40
3:J:361:LEU:HD13	3:J:366:CYS:HA	2.03	0.40
3:J:668:PHE:CE1	3:J:678:ARG:HG2	2.56	0.40
3:J:860:ARG:HB3	3:J:861:ASN:H	1.55	0.40
5:L:322:MET:HB3	5:L:324:LYS:HZ3	1.86	0.40
1:B:106:GLY:O	1:B:108:GLY:N	2.54	0.40
2:C:1082:ILE:HD12	2:C:1082:ILE:H	1.86	0.40
2:C:12:ARG:HG3	2:C:1181:PRO:HB2	2.04	0.40
2:C:145:ILE:HG22	2:C:456:VAL:HG22	2.03	0.40
2:C:221:LEU:HD12	2:C:298:ALA:O	2.21	0.40
2:C:202:ARG:HD3	2:C:369:MET:HG2	2.02	0.40
2:C:79:VAL:HG23	2:C:80:PHE:H	1.85	0.40
3:D:1243:LEU:HD12	3:D:1243:LEU:HA	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:742:GLY:O	3:D:762:ASN:HB3	2.21	0.40
5:F:320:ILE:HG21	5:F:331:HIS:NE2	2.35	0.40
5:F:492:ASP:HB2	5:F:495:ARG:NH1	2.27	0.40
2:I:540:ARG:HD2	2:I:540:ARG:H	1.86	0.40
2:I:616:ILE:HG13	2:I:652:TYR:HB2	2.03	0.40
3:J:1156:LEU:HA	3:J:1208:ASP:O	2.21	0.40
2:I:1281:TYR:CE1	3:J:484:MET:HE3	2.57	0.40
3:J:709:ARG:HD2	3:J:710:ASP:H	1.86	0.40
3:J:839:VAL:HG12	3:J:864:LEU:HD12	2.03	0.40
6:M:112:GLY:HA2	6:M:126:LEU:HD11	2.03	0.40
6:M:136:ILE:HA	6:M:136:ILE:HD12	1.89	0.40
6:M:36:GLN:O	6:M:39:HIS:HB3	2.21	0.40
1:A:110:VAL:HG21	1:A:140:ILE:HD11	2.03	0.40
2:C:1248:THR:HG22	2:C:1251:TYR:OH	2.21	0.40
2:C:1319:MET:HA	2:C:1320:PRO:HD3	1.90	0.40
3:D:1168:GLU:O	3:D:1170:LYS:N	2.54	0.40
3:D:202:ARG:NH2	3:D:225:GLU:OE1	2.54	0.40
3:D:490:ILE:N	3:D:490:ILE:HD13	2.29	0.40
5:F:281:ARG:O	5:F:285:ARG:HG3	2.20	0.40
5:F:387:VAL:HG11	5:F:409:ASN:OD1	2.21	0.40
1:H:178:SER:HA	1:H:179:PRO:HD3	1.86	0.40
1:H:74:VAL:HG11	1:H:81:ILE:HD11	2.02	0.40
2:I:521:LEU:O	2:I:525:THR:HB	2.22	0.40
3:J:416:ILE:HA	3:J:416:ILE:HD12	1.83	0.40
3:J:709:ARG:HD2	3:J:710:ASP:N	2.36	0.40
3:J:923:ILE:O	3:J:926:PRO:HD2	2.21	0.40
1:A:89:ALA:O	1:A:124:VAL:HG12	2.22	0.40
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.86	0.40
1:A:323:PRO:HB2	1:A:324:ALA:HB2	2.04	0.40
1:B:104:LYS:HD3	1:B:114:ASP:OD2	2.20	0.40
1:B:49:SER:O	1:B:51:MET:N	2.54	0.40
2:C:601:ASP:N	2:C:601:ASP:OD1	2.46	0.40
3:D:1280:VAL:HG11	3:D:1304:ARG:NH2	2.36	0.40
3:D:681:LYS:NZ	6:M:12:LEU:HD13	2.37	0.40
3:D:707:ILE:HD11	3:D:716:GLN:HG2	2.03	0.40
3:D:850:LYS:HD3	3:D:875:ASN:HD21	1.87	0.40
3:D:860:ARG:HB3	3:D:861:ASN:H	1.81	0.40
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.49	0.40
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.37	0.40
2:I:1109:ILE:HA	2:I:1109:ILE:HD12	1.91	0.40
2:I:402:ARG:HG2	2:I:416:GLY:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:195:GLU:H	3:J:195:GLU:HG3	1.61	0.40
3:J:430:HIS:ND1	3:J:925:GLU:HG3	2.37	0.40
3:J:514:THR:CB	3:J:576:ARG:HG2	2.51	0.40
3:J:664:ILE:HG21	3:J:681:LYS:HG2	2.04	0.40
6:M:90:ASP:O	6:M:94:LYS:HG3	2.22	0.40
1:A:262:LEU:HD12	1:A:262:LEU:H	1.86	0.40
2:C:149:LEU:HD12	2:C:452:ARG:O	2.21	0.40
3:D:548:VAL:HG12	3:D:550:VAL:HG13	2.03	0.40
3:D:789:LYS:HZ3	3:D:932:MET:CB	2.35	0.40
5:F:511:ILE:HG22	5:F:517:SER:O	2.22	0.40
1:G:31:LEU:HD23	1:G:31:LEU:HA	1.88	0.40
2:I:388:LEU:HD23	2:I:388:LEU:HA	1.86	0.40
2:I:74:ARG:HH12	2:I:121:GLU:CD	2.24	0.40
2:I:852:ALA:HB2	2:I:869:GLY:CA	2.51	0.40
3:J:161:THR:H	3:J:164:GLN:HB2	1.86	0.40
3:J:322:ARG:HG3	3:J:323:PRO:HD2	2.04	0.40
4:K:56:GLU:HB2	4:K:58:LEU:HD11	2.04	0.40
5:L:363:ARG:O	5:L:367:ILE:HG13	2.20	0.40
5:L:544:THR:HG22	5:L:607:LEU:HD11	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ASP:OD2	3:J:675:ALA:N[2_555]	2.03	0.17

## 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	317/329 (96%)	249 (78%)	53 (17%)	15 (5%)	<b>2</b> <b>24</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	291/329 (88%)	225 (77%)	45 (16%)	21 (7%)	1	16
1	G	225/329 (68%)	200 (89%)	21 (9%)	4 (2%)	8	42
1	H	212/329 (64%)	197 (93%)	11 (5%)	4 (2%)	8	41
2	C	1338/1342 (100%)	1201 (90%)	114 (8%)	23 (2%)	9	43
2	I	1338/1342 (100%)	1196 (89%)	119 (9%)	23 (2%)	9	43
3	D	1169/1407 (83%)	1042 (89%)	99 (8%)	28 (2%)	6	36
3	J	1151/1407 (82%)	1024 (89%)	100 (9%)	27 (2%)	6	37
4	E	87/91 (96%)	81 (93%)	4 (5%)	2 (2%)	6	37
4	K	77/91 (85%)	68 (88%)	5 (6%)	4 (5%)	2	22
5	F	462/613 (75%)	425 (92%)	28 (6%)	9 (2%)	8	41
5	L	463/613 (76%)	424 (92%)	32 (7%)	7 (2%)	10	46
6	M	138/151 (91%)	128 (93%)	7 (5%)	3 (2%)	6	38
All	All	7268/8373 (87%)	6460 (89%)	638 (9%)	170 (2%)	6	37

All (170) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	107	ILE
1	A	136	GLU
1	A	167	PRO
1	A	242	VAL
1	A	320	ASN
1	B	20	SER
1	B	29	GLU
1	B	30	PRO
1	B	32	GLU
1	B	107	ILE
1	B	320	ASN
1	B	323	PRO
1	B	324	ALA
2	C	169	LYS
2	C	170	VAL
2	C	484	LEU
2	C	697	LYS
2	C	1137	GLU
2	C	1153	ALA
2	C	1159	VAL

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Mol	Chain	Res	Type
2	C	1165	SER
3	D	10	ALA
3	D	49	PHE
3	D	426	ALA
3	D	496	GLY
3	D	710	ASP
3	D	712	GLN
3	D	745	GLY
3	D	1169	THR
3	D	1294	ALA
4	E	33	GLY
5	F	490	PRO
5	F	566	ASP
5	F	569	THR
1	G	193	GLU
2	I	121	GLU
2	I	169	LYS
2	I	170	VAL
2	I	484	LEU
2	I	697	LYS
2	I	897	PRO
2	I	1137	GLU
2	I	1153	ALA
2	I	1159	VAL
2	I	1203	ASP
3	J	49	PHE
3	J	341	ASN
3	J	426	ALA
3	J	710	ASP
3	J	712	GLN
3	J	850	LYS
3	J	854	ALA
3	J	1294	ALA
4	K	4	VAL
4	K	15	ASN
4	K	33	GLY
5	L	584	ARG
6	M	31	TYR
1	A	50	SER
1	A	119	GLY
1	A	232	VAL
1	A	315	GLY

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Mol	Chain	Res	Type
1	B	50	SER
1	B	62	ASP
1	B	119	GLY
1	B	135	ASP
1	B	315	GLY
2	C	121	GLU
2	C	237	LEU
2	C	1154	ASP
3	D	89	GLY
3	D	805	GLN
3	D	933	ARG
3	D	934	THR
5	F	584	ARG
1	G	162	GLU
1	G	167	PRO
1	H	138	ALA
2	I	237	LEU
2	I	1059	ARG
2	I	1165	SER
3	J	89	GLY
3	J	314	ARG
3	J	339	ARG
3	J	496	GLY
3	J	745	GLY
3	J	805	GLN
3	J	826	ILE
3	J	1169	THR
3	J	1297	LYS
5	L	96	ASP
5	L	490	PRO
5	L	566	ASP
5	L	569	THR
1	A	62	ASP
1	B	319	GLU
1	B	321	TRP
2	C	163	LYS
2	C	236	LYS
2	C	696	ASP
2	C	892	GLU
2	C	1317	PRO
3	D	173	GLY
3	D	314	ARG

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Mol	Chain	Res	Type
3	D	417	ARG
3	D	1274	PHE
3	D	1344	LEU
5	F	600	HIS
1	G	229	GLU
1	H	193	GLU
2	I	983	GLY
2	I	1317	PRO
3	J	332	LYS
3	J	417	ARG
6	M	58	THR
1	A	319	GLU
1	A	324	ALA
1	B	13	LEU
1	B	322	PRO
2	C	813	GLU
2	C	1059	ARG
3	D	1297	LYS
1	H	20	SER
2	I	696	ASP
2	I	813	GLU
2	I	892	GLU
3	J	344	GLY
3	J	1344	LEU
4	K	14	GLY
1	A	318	LEU
1	B	318	LEU
2	C	62	TYR
2	C	983	GLY
2	C	1158	LYS
3	D	46	TYR
3	D	345	LYS
5	F	602	SER
2	I	201	ARG
2	I	236	LYS
3	J	338	PHE
3	J	357	VAL
2	C	1256	GLN
3	D	357	VAL
3	D	828	GLY
3	D	1375	ALA
2	I	160	ASP

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Mol	Chain	Res	Type
2	I	756	TYR
3	J	333	GLY
5	L	585	GLU
6	M	27	PRO
1	A	19	VAL
1	B	19	VAL
3	D	826	ILE
5	F	96	ASP
3	J	173	GLY
3	J	336	GLY
3	D	120	LEU
3	D	831	VAL
5	F	361	ILE
5	F	601	PRO
3	J	639	VAL
1	B	217	ILE
4	E	86	ILE
2	I	1202	GLY
5	L	475	GLY
1	B	293	PRO
2	C	110	PRO
3	D	850	LYS
1	H	30	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 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	278/286 (97%)	230 (83%)	48 (17%)	2	13
1	B	256/286 (90%)	224 (88%)	32 (12%)	4	22
1	G	193/286 (68%)	169 (88%)	24 (12%)	4	22
1	H	183/286 (64%)	171 (93%)	12 (7%)	16	43
2	C	1155/1157 (100%)	1053 (91%)	102 (9%)	10	34
2	I	1154/1157 (100%)	1059 (92%)	95 (8%)	11	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	962/1168 (82%)	879 (91%)	83 (9%)	10	35
3	J	960/1168 (82%)	875 (91%)	85 (9%)	9	33
4	E	72/75 (96%)	64 (89%)	8 (11%)	6	25
4	K	67/75 (89%)	60 (90%)	7 (10%)	7	27
5	F	417/540 (77%)	387 (93%)	30 (7%)	14	41
5	L	418/540 (77%)	380 (91%)	38 (9%)	9	32
6	M	121/131 (92%)	111 (92%)	10 (8%)	11	37
All	All	6236/7155 (87%)	5662 (91%)	574 (9%)	9	31

All (574) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	8	PHE
1	A	18	GLN
1	A	26	VAL
1	A	29	GLU
1	A	44	ARG
1	A	50	SER
1	A	56	VAL
1	A	66	HIS
1	A	70	THR
1	A	71	LYS
1	A	72	GLU
1	A	74	VAL
1	A	77	ASP
1	A	83	LEU
1	A	90	VAL
1	A	98	VAL
1	A	99	ILE
1	A	105	SER
1	A	116	THR
1	A	125	LYS
1	A	133	LEU
1	A	139	SER
1	A	159	ILE
1	A	180	VAL
1	A	183	ILE
1	A	186	ASN
1	A	192	VAL

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Mol	Chain	Res	Type
1	A	195	ARG
1	A	207	THR
1	A	211	ILE
1	A	223	ILE
1	A	231	PHE
1	A	243	LYS
1	A	245	GLU
1	A	246	LYS
1	A	258	ASP
1	A	262	LEU
1	A	280	ASP
1	A	282	VAL
1	A	284	ARG
1	A	285	THR
1	A	300	LEU
1	A	302	GLU
1	A	306	VAL
1	A	316	MET
1	A	318	LEU
1	A	320	ASN
1	B	8	PHE
1	B	9	LEU
1	B	18	GLN
1	B	29	GLU
1	B	45	ARG
1	B	50	SER
1	B	54	CYS
1	B	70	THR
1	B	71	LYS
1	B	75	GLN
1	B	77	ASP
1	B	83	LEU
1	B	98	VAL
1	B	133	LEU
1	B	139	SER
1	B	159	ILE
1	B	183	ILE
1	B	186	ASN
1	B	195	ARG
1	B	223	ILE
1	B	258	ASP
1	B	262	LEU

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Mol	Chain	Res	Type
1	B	280	ASP
1	B	282	VAL
1	B	284	ARG
1	B	285	THR
1	B	300	LEU
1	B	302	GLU
1	B	306	VAL
1	B	316	MET
1	B	318	LEU
1	B	320	ASN
2	C	3	TYR
2	C	11	ILE
2	C	17	LYS
2	C	23	ASP
2	C	46	GLN
2	C	81	ASP
2	C	103	VAL
2	C	107	ARG
2	C	115	LYS
2	C	117	ILE
2	C	119	GLU
2	C	120	GLN
2	C	131	THR
2	C	135	THR
2	C	150	HIS
2	C	164	THR
2	C	201	ARG
2	C	208	ILE
2	C	236	LYS
2	C	285	ILE
2	C	306	THR
2	C	320	ASP
2	C	321	LEU
2	C	342	ASP
2	C	377	THR
2	C	384	LEU
2	C	423	ASP
2	C	455	SER
2	C	471	VAL
2	C	481	LEU
2	C	484	LEU
2	C	485	ASP

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Mol	Chain	Res	Type
2	C	490	GLN
2	C	492	MET
2	C	518	ASN
2	C	525	THR
2	C	539	THR
2	C	540	ARG
2	C	542	ARG
2	C	553	THR
2	C	561	ILE
2	C	600	THR
2	C	609	ILE
2	C	615	VAL
2	C	623	LEU
2	C	633	LEU
2	C	663	VAL
2	C	672	GLU
2	C	694	ARG
2	C	697	LYS
2	C	714	VAL
2	C	748	ILE
2	C	757	THR
2	C	764	CYS
2	C	765	ILE
2	C	778	GLU
2	C	781	ASP
2	C	791	LEU
2	C	799	ASN
2	C	800	MET
2	C	867	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	895	LEU
2	C	919	ARG
2	C	951	MET
2	C	984	VAL
2	C	992	LEU
2	C	1002	LEU
2	C	1037	THR
2	C	1054	LEU
2	C	1059	ARG
2	C	1076	ILE

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Mol	Chain	Res	Type
2	C	1082	ILE
2	C	1134	GLN
2	C	1141	LEU
2	C	1146	GLN
2	C	1151	LEU
2	C	1155	VAL
2	C	1156	ARG
2	C	1159	VAL
2	C	1163	THR
2	C	1164	PHE
2	C	1198	LEU
2	C	1206	THR
2	C	1210	ILE
2	C	1233	LEU
2	C	1237	HIS
2	C	1238	LEU
2	C	1240	ASP
2	C	1248	THR
2	C	1250	SER
2	C	1254	VAL
2	C	1255	THR
2	C	1287	LEU
2	C	1296	ASP
2	C	1310	ASP
2	C	1313	HIS
2	C	1327	LEU
2	C	1341	ASP
2	C	1342	GLU
3	D	11	GLN
3	D	46	TYR
3	D	47	ARG
3	D	54	ASP
3	D	79	LYS
3	D	93	THR
3	D	95	THR
3	D	97	VAL
3	D	172	PHE
3	D	175	GLU
3	D	176	PHE
3	D	248	ASP
3	D	252	LEU
3	D	259	ARG

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Mol	Chain	Res	Type
3	D	292	VAL
3	D	324	LEU
3	D	330	MET
3	D	335	GLN
3	D	343	LEU
3	D	376	LEU
3	D	386	GLU
3	D	392	THR
3	D	394	ILE
3	D	413	ASP
3	D	416	ILE
3	D	425	ARG
3	D	429	LEU
3	D	490	ILE
3	D	505	ASP
3	D	514	THR
3	D	536	LEU
3	D	545	HIS
3	D	560	ASN
3	D	569	LEU
3	D	571	ASP
3	D	573	THR
3	D	639	VAL
3	D	641	ILE
3	D	678	ARG
3	D	680	ASN
3	D	701	LEU
3	D	707	ILE
3	D	708	ASN
3	D	717	VAL
3	D	753	SER
3	D	754	ILE
3	D	764	ARG
3	D	772	TYR
3	D	797	THR
3	D	801	VAL
3	D	810	THR
3	D	847	ASP
3	D	849	LEU
3	D	853	THR
3	D	858	VAL
3	D	860	ARG

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Mol	Chain	Res	Type
3	D	890	THR
3	D	897	HIS
3	D	901	ARG
3	D	903	LEU
3	D	908	ILE
3	D	910	ASN
3	D	918	ILE
3	D	1155	ILE
3	D	1162	ILE
3	D	1163	VAL
3	D	1169	THR
3	D	1177	ILE
3	D	1186	TYR
3	D	1194	ARG
3	D	1199	PHE
3	D	1221	LEU
3	D	1251	LYS
3	D	1261	LEU
3	D	1266	ILE
3	D	1272	SER
3	D	1279	GLN
3	D	1289	ASN
3	D	1310	THR
3	D	1332	LEU
3	D	1333	THR
3	D	1343	GLU
3	D	1366	HIS
4	E	5	THR
4	E	13	ILE
4	E	18	ASP
4	E	21	LEU
4	E	36	ASP
4	E	39	VAL
4	E	58	LEU
4	E	62	GLN
5	F	98	VAL
5	F	114	GLU
5	F	154	GLU
5	F	163	THR
5	F	261	LEU
5	F	277	MET
5	F	305	LEU

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Mol	Chain	Res	Type
5	F	306	PHE
5	F	338	HIS
5	F	401	PHE
5	F	449	THR
5	F	471	LEU
5	F	472	GLN
5	F	482	GLU
5	F	488	LEU
5	F	491	GLU
5	F	492	ASP
5	F	516	ASP
5	F	526	THR
5	F	527	THR
5	F	547	VAL
5	F	552	THR
5	F	558	VAL
5	F	569	THR
5	F	572	THR
5	F	587	ILE
5	F	600	HIS
5	F	603	ARG
5	F	606	VAL
5	F	608	ARG
1	G	9	LEU
1	G	12	ARG
1	G	19	VAL
1	G	23	HIS
1	G	26	VAL
1	G	33	ARG
1	G	50	SER
1	G	70	THR
1	G	79	LEU
1	G	90	VAL
1	G	101	THR
1	G	121	VAL
1	G	124	VAL
1	G	133	LEU
1	G	145	LYS
1	G	156	SER
1	G	171	LEU
1	G	178	SER
1	G	187	VAL

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Mol	Chain	Res	Type
1	G	200	LYS
1	G	207	THR
1	G	211	ILE
1	G	219	ARG
1	G	231	PHE
1	H	18	GLN
1	H	27	THR
1	H	58	GLU
1	H	61	ILE
1	H	62	ASP
1	H	64	VAL
1	H	65	LEU
1	H	75	GLN
1	H	95	LYS
1	H	102	LEU
1	H	124	VAL
1	H	183	ILE
2	I	3	TYR
2	I	4	SER
2	I	46	GLN
2	I	86	GLN
2	I	107	ARG
2	I	115	LYS
2	I	117	ILE
2	I	131	THR
2	I	132	ASP
2	I	138	ILE
2	I	156	PHE
2	I	164	THR
2	I	197	ARG
2	I	201	ARG
2	I	208	ILE
2	I	236	LYS
2	I	285	ILE
2	I	320	ASP
2	I	321	LEU
2	I	342	ASP
2	I	360	LEU
2	I	423	ASP
2	I	453	ILE
2	I	455	SER
2	I	471	VAL

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Mol	Chain	Res	Type
2	I	481	LEU
2	I	484	LEU
2	I	485	ASP
2	I	490	GLN
2	I	492	MET
2	I	518	ASN
2	I	524	ILE
2	I	525	THR
2	I	530	ILE
2	I	538	LEU
2	I	540	ARG
2	I	542	ARG
2	I	553	THR
2	I	558	VAL
2	I	561	ILE
2	I	596	ASP
2	I	600	THR
2	I	604	HIS
2	I	609	ILE
2	I	633	LEU
2	I	635	THR
2	I	660	VAL
2	I	663	VAL
2	I	672	GLU
2	I	694	ARG
2	I	705	GLU
2	I	724	VAL
2	I	739	ASP
2	I	748	ILE
2	I	764	CYS
2	I	765	ILE
2	I	781	ASP
2	I	782	VAL
2	I	799	ASN
2	I	800	MET
2	I	814	ASP
2	I	828	PHE
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	919	ARG
2	I	922	ASN

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Mol	Chain	Res	Type
2	I	951	MET
2	I	992	LEU
2	I	1037	THR
2	I	1054	LEU
2	I	1082	ILE
2	I	1083	GLU
2	I	1141	LEU
2	I	1146	GLN
2	I	1151	LEU
2	I	1156	ARG
2	I	1159	VAL
2	I	1163	THR
2	I	1164	PHE
2	I	1198	LEU
2	I	1210	ILE
2	I	1233	LEU
2	I	1238	LEU
2	I	1240	ASP
2	I	1248	THR
2	I	1250	SER
2	I	1254	VAL
2	I	1265	PHE
2	I	1287	LEU
2	I	1296	ASP
2	I	1313	HIS
2	I	1327	LEU
2	I	1341	ASP
2	I	1342	GLU
3	J	20	ILE
3	J	46	TYR
3	J	47	ARG
3	J	54	ASP
3	J	79	LYS
3	J	92	VAL
3	J	93	THR
3	J	95	THR
3	J	97	VAL
3	J	98	ARG
3	J	172	PHE
3	J	175	GLU
3	J	176	PHE
3	J	206	ASN

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Mol	Chain	Res	Type
3	J	218	THR
3	J	235	GLU
3	J	244	VAL
3	J	248	ASP
3	J	252	LEU
3	J	259	ARG
3	J	292	VAL
3	J	324	LEU
3	J	343	LEU
3	J	363	LEU
3	J	374	LEU
3	J	376	LEU
3	J	386	GLU
3	J	392	THR
3	J	394	ILE
3	J	413	ASP
3	J	416	ILE
3	J	423	LEU
3	J	425	ARG
3	J	429	LEU
3	J	505	ASP
3	J	510	LEU
3	J	514	THR
3	J	536	LEU
3	J	545	HIS
3	J	560	ASN
3	J	567	THR
3	J	569	LEU
3	J	571	ASP
3	J	573	THR
3	J	641	ILE
3	J	678	ARG
3	J	701	LEU
3	J	707	ILE
3	J	708	ASN
3	J	717	VAL
3	J	754	ILE
3	J	764	ARG
3	J	772	TYR
3	J	797	THR
3	J	801	VAL
3	J	810	THR

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Mol	Chain	Res	Type
3	J	827	GLU
3	J	847	ASP
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	897	HIS
3	J	898	CYS
3	J	901	ARG
3	J	908	ILE
3	J	910	ASN
3	J	918	ILE
3	J	1155	ILE
3	J	1162	ILE
3	J	1163	VAL
3	J	1169	THR
3	J	1186	TYR
3	J	1194	ARG
3	J	1199	PHE
3	J	1221	LEU
3	J	1251	LYS
3	J	1261	LEU
3	J	1266	ILE
3	J	1273	ASP
3	J	1282	TYR
3	J	1285	VAL
3	J	1289	ASN
3	J	1292	LEU
3	J	1333	THR
3	J	1366	HIS
4	K	3	ARG
4	K	13	ILE
4	K	18	ASP
4	K	21	LEU
4	K	36	ASP
4	K	39	VAL
4	K	58	LEU
5	L	98	VAL
5	L	102	MET
5	L	114	GLU
5	L	154	GLU
5	L	261	LEU
5	L	266	PHE

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Mol	Chain	Res	Type
5	L	277	MET
5	L	305	LEU
5	L	306	PHE
5	L	335	GLU
5	L	338	HIS
5	L	364	ARG
5	L	395	THR
5	L	401	PHE
5	L	405	ILE
5	L	429	THR
5	L	445	ASP
5	L	469	GLN
5	L	471	LEU
5	L	476	ARG
5	L	486	ARG
5	L	491	GLU
5	L	492	ASP
5	L	526	THR
5	L	527	THR
5	L	552	THR
5	L	558	VAL
5	L	569	THR
5	L	572	THR
5	L	573	LEU
5	L	580	PHE
5	L	582	VAL
5	L	587	ILE
5	L	599	ARG
5	L	600	HIS
5	L	603	ARG
5	L	606	VAL
5	L	607	LEU
6	M	42	ARG
6	M	50	GLN
6	M	52	ARG
6	M	53	ASP
6	M	69	PHE
6	M	72	PRO
6	M	88	ASN
6	M	129	ARG
6	M	136	ILE
6	M	146	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	B	186	ASN
1	B	268	ASN
1	B	276	HIS
1	B	320	ASN
2	C	46	GLN
2	C	69	GLN
2	C	133	ASN
2	C	139	ASN
2	C	343	HIS
2	C	513	GLN
2	C	620	ASN
2	C	760	ASN
2	C	1108	ASN
2	C	1111	GLN
2	C	1116	HIS
2	C	1237	HIS
2	C	1288	GLN
3	D	157	GLN
3	D	200	GLN
3	D	320	ASN
3	D	424	ASN
3	D	680	ASN
3	D	690	ASN
3	D	777	HIS
3	D	817	HIS
3	D	910	ASN
5	F	406	GLN
5	F	446	GLN
5	F	579	GLN
5	F	600	HIS
1	G	66	HIS
2	I	46	GLN
2	I	139	ASN
2	I	357	ASN
2	I	620	ASN
2	I	808	ASN
2	I	1108	ASN
2	I	1111	GLN
2	I	1116	HIS
2	I	1146	GLN

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Mol	Chain	Res	Type
2	I	1220	GLN
2	I	1237	HIS
2	I	1244	HIS
2	I	1288	GLN
2	I	1314	GLN
3	J	200	GLN
3	J	206	ASN
3	J	364	HIS
3	J	419	HIS
3	J	424	ASN
3	J	465	GLN
3	J	716	GLN
3	J	861	ASN
5	L	301	ASN
5	L	345	GLN
5	L	362	ASN
5	L	406	GLN
5	L	446	GLN
5	L	579	GLN
6	M	36	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 7 are 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
9	G4P	E	101	-	30,38,38	1.82	7 (23%)	43,61,61	1.62	8 (18%)
9	G4P	M	202	-	30,38,38	1.95	9 (30%)	43,61,61	1.62	7 (16%)
9	G4P	J	2004	-	30,38,38	1.96	9 (30%)	43,61,61	1.53	8 (18%)

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
9	G4P	E	101	-	-	1/23/43/43	0/3/3/3
9	G4P	M	202	-	-	8/23/43/43	0/3/3/3
9	G4P	J	2004	-	-	7/23/43/43	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	2004	G4P	C2'-C1'	-5.51	1.45	1.53
9	M	202	G4P	C2'-C1'	-4.92	1.46	1.53
9	E	101	G4P	C2'-C1'	-4.82	1.46	1.53
9	M	202	G4P	C2-N2	4.50	1.42	1.33
9	J	2004	G4P	C2-N2	4.39	1.42	1.33
9	E	101	G4P	C2-N2	4.21	1.42	1.33
9	M	202	G4P	C2'-C3'	-3.45	1.45	1.52
9	M	202	G4P	C5-C4	-3.42	1.31	1.40
9	J	2004	G4P	C5-C4	-3.36	1.32	1.40
9	J	2004	G4P	C2'-C3'	-3.17	1.45	1.52
9	E	101	G4P	C5-C4	-3.12	1.32	1.40
9	E	101	G4P	C2'-C3'	-2.89	1.46	1.52
9	M	202	G4P	C3'-C4'	-2.83	1.45	1.52
9	E	101	G4P	C8-N7	2.69	1.39	1.34
9	M	202	G4P	C4-N3	2.61	1.39	1.35
9	J	2004	G4P	C8-N7	2.59	1.39	1.34
9	E	101	G4P	C4-N3	2.55	1.39	1.35
9	J	2004	G4P	C3'-C4'	-2.53	1.46	1.52
9	E	101	G4P	C3'-C4'	-2.44	1.46	1.52
9	J	2004	G4P	C4-N3	2.41	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	202	G4P	C8-N7	2.29	1.38	1.34
9	M	202	G4P	C6-C5	-2.27	1.37	1.41
9	J	2004	G4P	O4'-C1'	2.22	1.44	1.41
9	J	2004	G4P	C6-C5	-2.19	1.37	1.41
9	M	202	G4P	O4'-C1'	2.17	1.44	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	101	G4P	O3C-PC-O3'	5.63	113.83	102.48
9	M	202	G4P	O3C-PC-O3'	5.19	112.95	102.48
9	M	202	G4P	N3-C2-N1	-4.22	121.59	127.22
9	J	2004	G4P	O3C-PC-O3'	4.09	110.74	102.48
9	J	2004	G4P	PC-O3C-PD	-3.80	119.78	132.83
9	E	101	G4P	PC-O3C-PD	-3.68	120.22	132.83
9	J	2004	G4P	N3-C2-N1	-3.67	122.33	127.22
9	E	101	G4P	N3-C2-N1	-3.29	122.84	127.22
9	J	2004	G4P	C6-N1-C2	3.08	120.82	115.93
9	M	202	G4P	PA-O3A-PB	-3.04	122.39	132.83
9	J	2004	G4P	O4'-C1'-C2'	-2.95	102.61	106.93
9	M	202	G4P	C6-N1-C2	2.92	120.57	115.93
9	J	2004	G4P	C5-C6-N1	-2.91	119.45	123.43
9	E	101	G4P	C3'-C2'-C1'	2.90	106.30	99.89
9	E	101	G4P	C6-N1-C2	2.83	120.43	115.93
9	M	202	G4P	PC-O3C-PD	-2.79	123.26	132.83
9	M	202	G4P	C4-C5-N7	2.69	112.20	109.40
9	E	101	G4P	C5-C6-N1	-2.68	119.76	123.43
9	E	101	G4P	C4-C5-N7	2.60	112.11	109.40
9	J	2004	G4P	C4-C5-N7	2.49	112.00	109.40
9	J	2004	G4P	PA-O3A-PB	-2.40	124.60	132.83
9	M	202	G4P	C5-C6-N1	-2.35	120.22	123.43
9	E	101	G4P	PA-O3A-PB	-2.16	125.42	132.83

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	M	202	G4P	PA-O3A-PB-O2B
9	J	2004	G4P	C3'-O3'-PC-O1C
9	J	2004	G4P	C3'-O3'-PC-O3C
9	M	202	G4P	C4'-C5'-O5'-PA
9	M	202	G4P	PB-O3A-PA-O5'

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Mol	Chain	Res	Type	Atoms
9	J	2004	G4P	PA-O3A-PB-O1B
9	E	101	G4P	C2'-C3'-O3'-PC
9	M	202	G4P	C2'-C3'-O3'-PC
9	J	2004	G4P	C3'-O3'-PC-O2C
9	M	202	G4P	C4'-C3'-O3'-PC
9	J	2004	G4P	PB-O3A-PA-O1A
9	M	202	G4P	PA-O3A-PB-O1B
9	M	202	G4P	PC-O3C-PD-O3D
9	J	2004	G4P	PA-O3A-PB-O2B
9	J	2004	G4P	PA-O3A-PB-O3B
9	M	202	G4P	C5'-O5'-PA-O3A

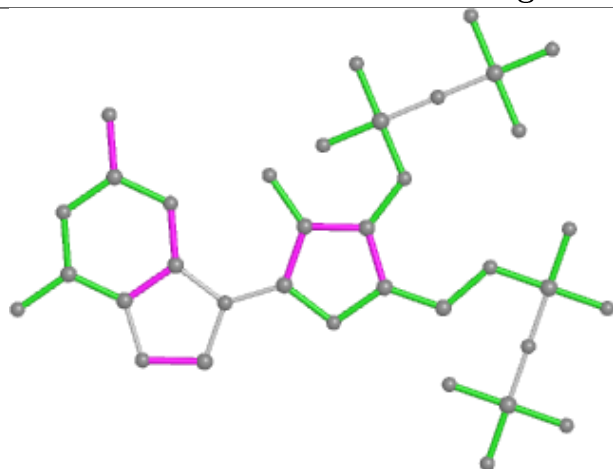
There are no ring outliers.

3 monomers are involved in 14 short contacts:

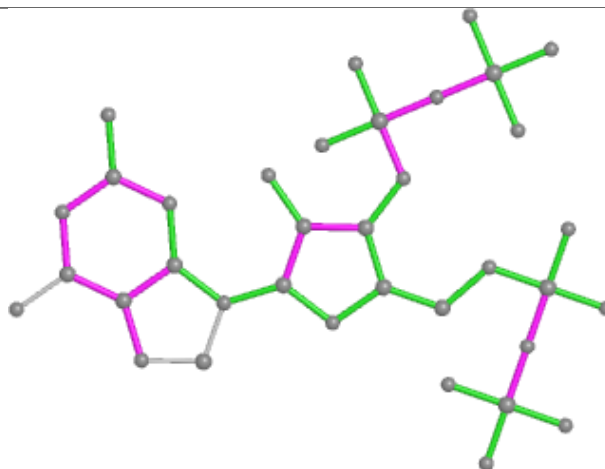
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	101	G4P	3	0
9	M	202	G4P	7	0
9	J	2004	G4P	4	0

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

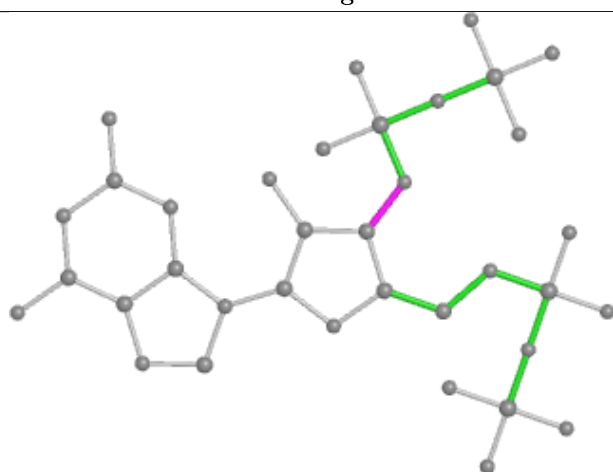
## Ligand G4P E 101



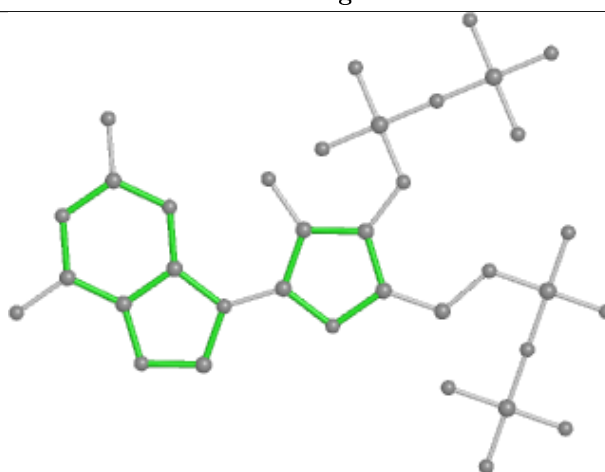
Bond lengths



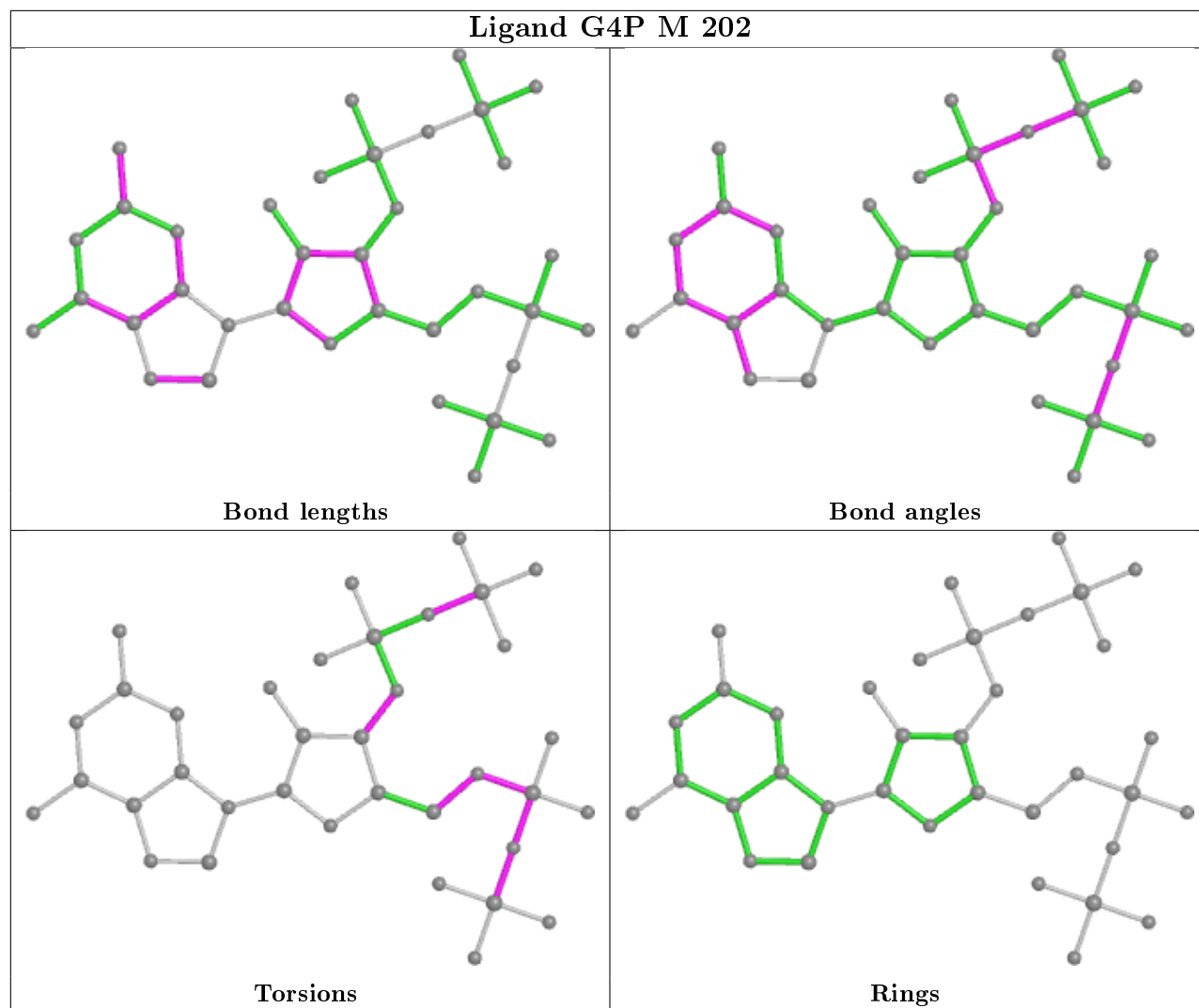
Bond angles

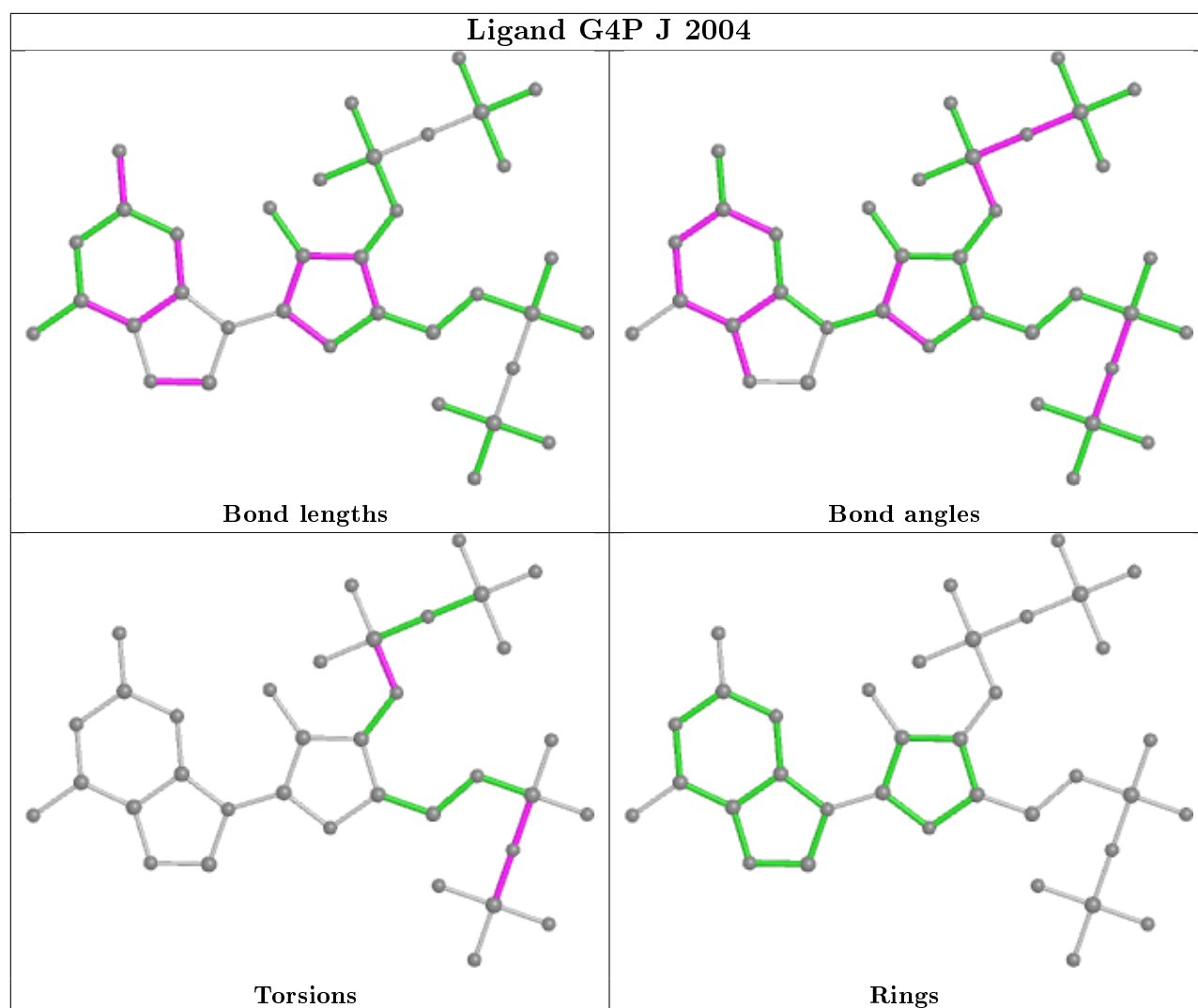


Torsions



Rings





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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.

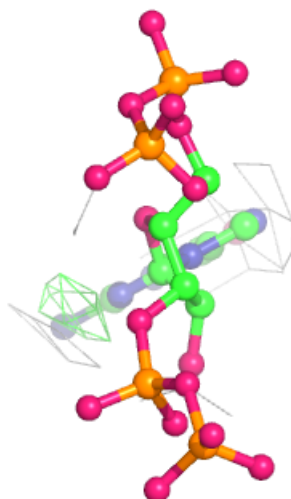
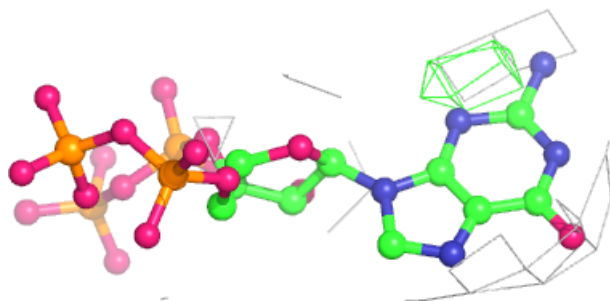
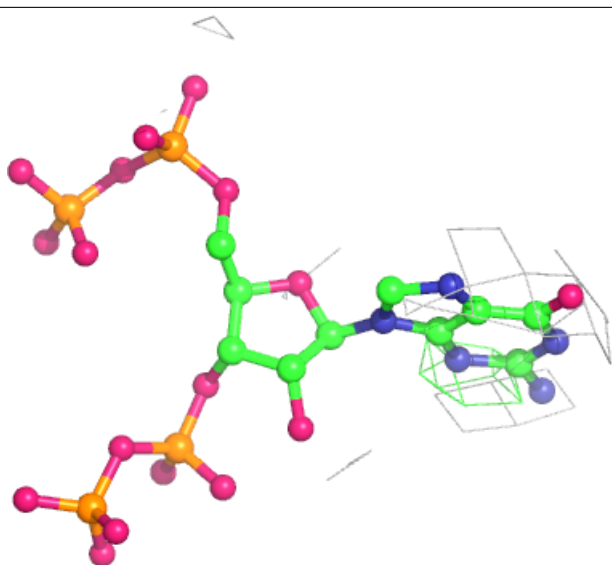
### 6.4 Ligands ⓘ

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 G4P E 101:**

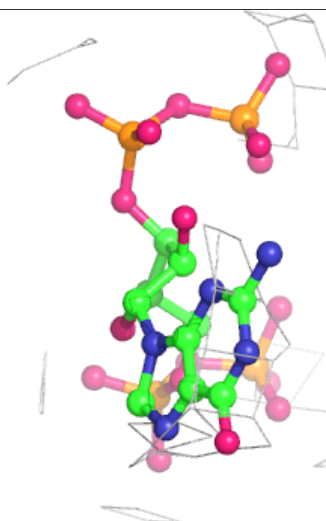
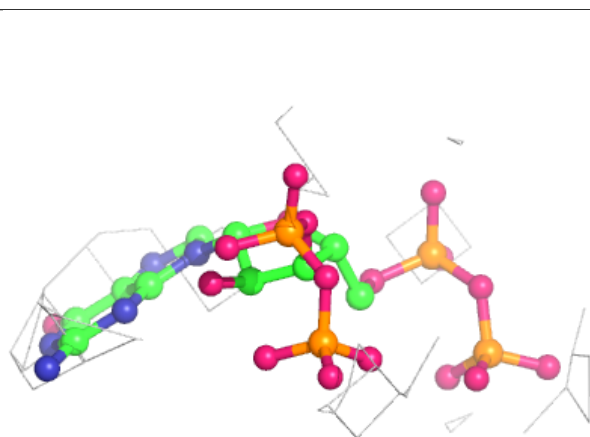
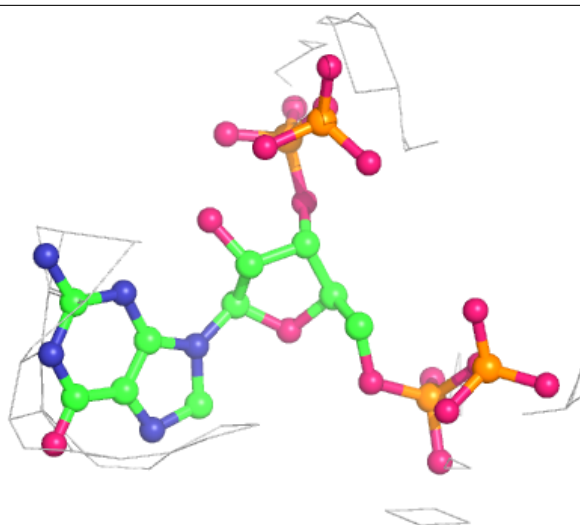
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





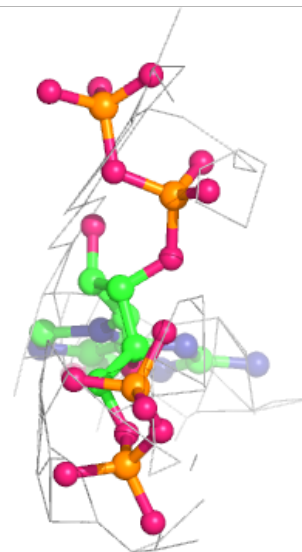
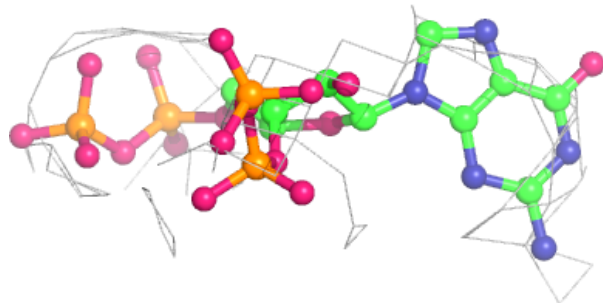
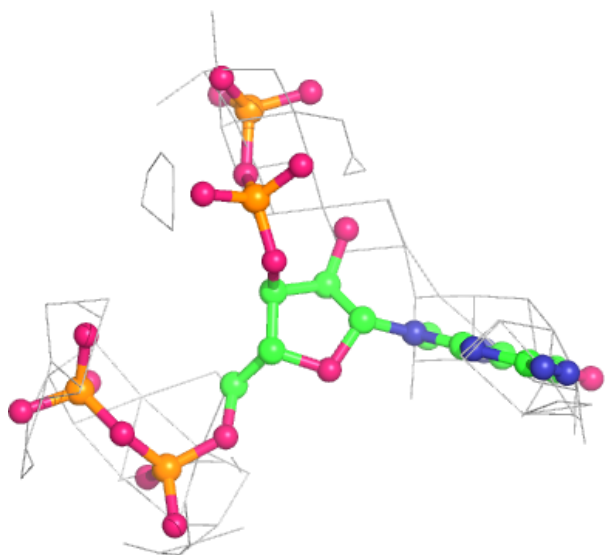
**Electron density around G4P M 202:**

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



**Electron density around G4P J 2004:**

$2mF_o-DF_c$  (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.