



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:19 PM BST

PDB ID : 5FLC
EMDB ID: : EMD-3213
Title : Architecture of human mTOR Complex 1 - 5.9 Angstrom reconstruction
Authors : Aylett, C.H.S.; Sauer, E.; Imseng, S.; Boehringer, D.; Hall, M.N.; Ban, N.; Maier, T.
Deposited on : 2015-10-23
Resolution : 5.90 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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

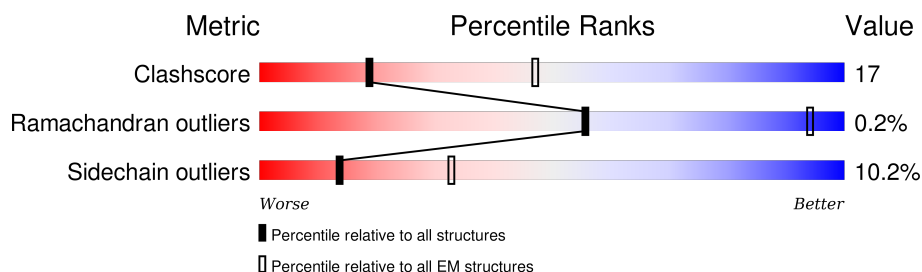
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.90 Å.

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






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

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

Mol	Chain	Length	Quality of chain
1	1	615	62% 38%
1	3	615	62% 38%
2	2	365	57% 43%
2	4	365	58% 42%
3	A	1029	76% 24%
3	E	1029	77% 23%
4	B	1168	53% 32% 5% 10%
4	F	1168	53% 32% 5% 10%
5	C	107	76% 24%

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Mol	Chain	Length	Quality of chain
5	G	107	
6	D	326	
6	H	326	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	RAP	C	999	X	-	-	-
7	RAP	G	999	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 47536 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called SERINE/THREONINE-PROTEIN KINASE MTOR.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	615	Total	C	N	O	0	0
			3690	2460	615	615		
1	3	615	Total	C	N	O	0	0
			3690	2460	615	615		

- Molecule 2 is a protein called SERINE/THREONINE-PROTEIN KINASE MTOR.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	2	365	Total	C	N	O	0	0
			2190	1460	365	365		
2	4	365	Total	C	N	O	0	0
			2190	1460	365	365		

- Molecule 3 is a protein called REGULATORY-ASSOCIATED PROTEIN OF MTOR.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	A	1029	Total	C	N	O	0	0
			6174	4116	1029	1029		
3	E	1029	Total	C	N	O	0	0
			6174	4116	1029	1029		

- Molecule 4 is a protein called SERINE/THREONINE-PROTEIN KINASE MTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	1050	Total	C	N	O	S	1	0
			8551	5439	1506	1544	62		
4	F	1050	Total	C	N	O	S	1	0
			8551	5439	1506	1544	62		

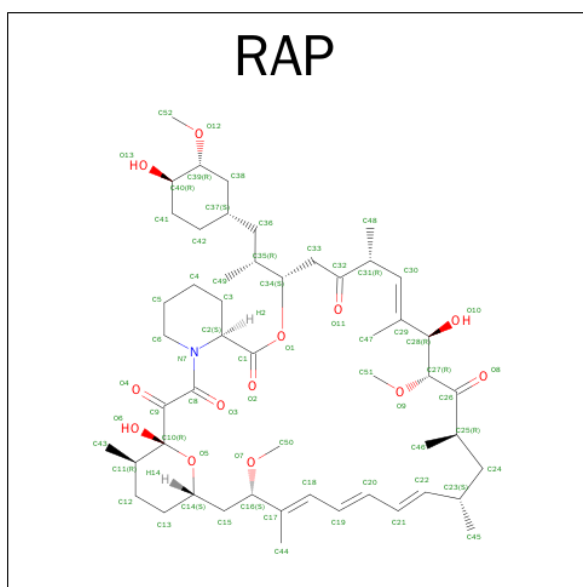
- Molecule 5 is a protein called FKBP.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	C	107	Total	C	N	O	0	0
			642	428	107	107		
5	G	107	Total	C	N	O	0	0
			642	428	107	107		

- Molecule 6 is a protein called TARGET OF RAPAMYCIN COMPLEX SUBUNIT LST8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	317	Total	C	N	O	S	0	0
			2456	1526	436	476	18		
6	H	317	Total	C	N	O	S	0	0
			2456	1526	436	476	18		

- Molecule 7 is RAPAMYCIN IMMUNOSUPPRESSANT DRUG (three-letter code: RAP) (formula: $C_{51}H_{79}NO_{13}$).

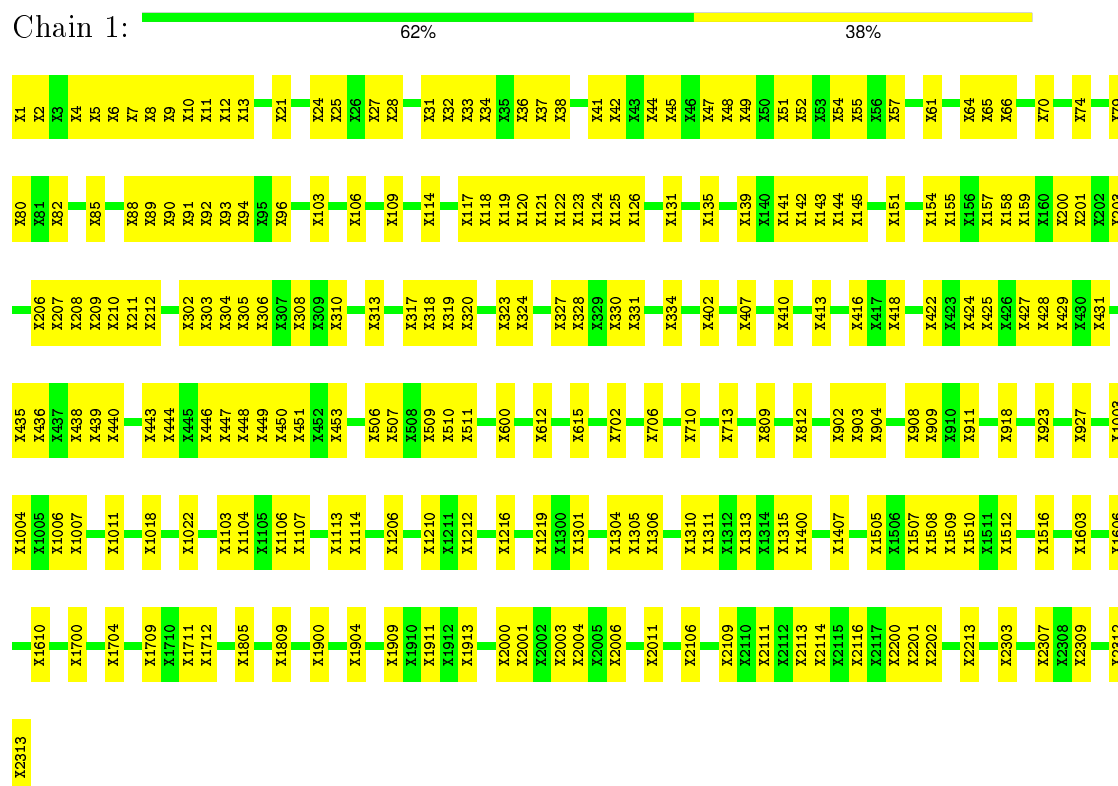


Mol	Chain	Residues	Atoms				AltConf
7	C	1	Total	C	N	O	0
			65	51	1	13	
7	G	1	Total	C	N	O	0
			65	51	1	13	

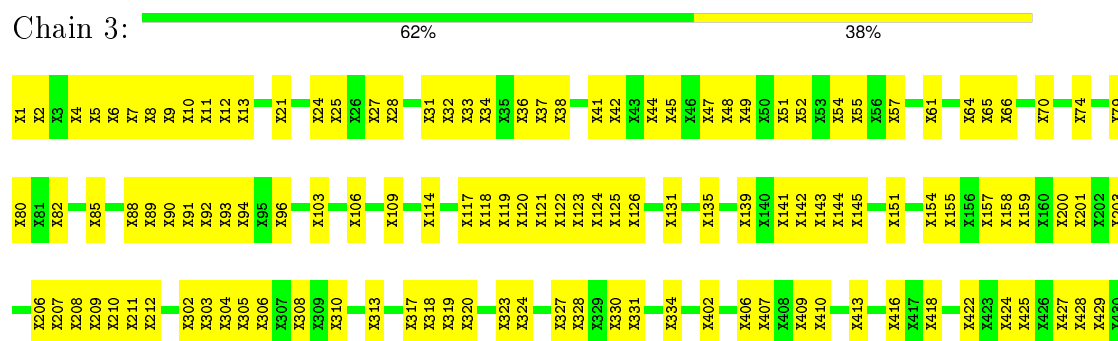
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: SERINE/THREONINE-PROTEIN KINASE MTOR



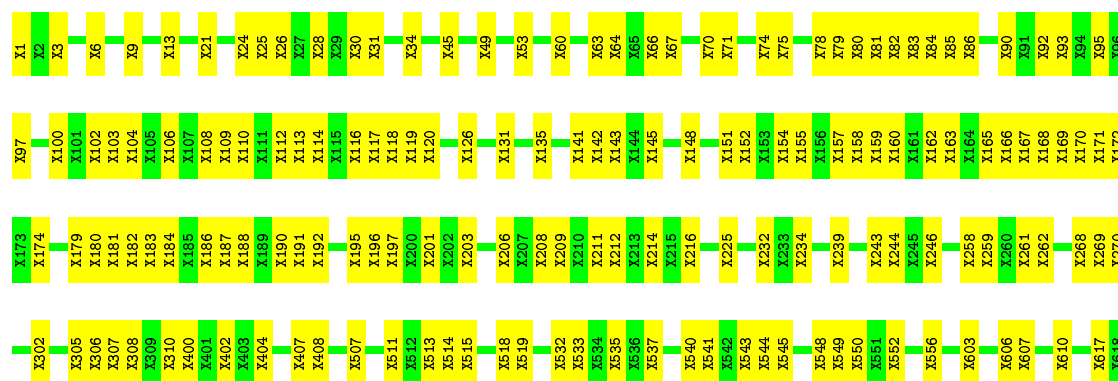
• Molecule 1: SERINE/THREONINE-PROTEIN KINASE MTOR





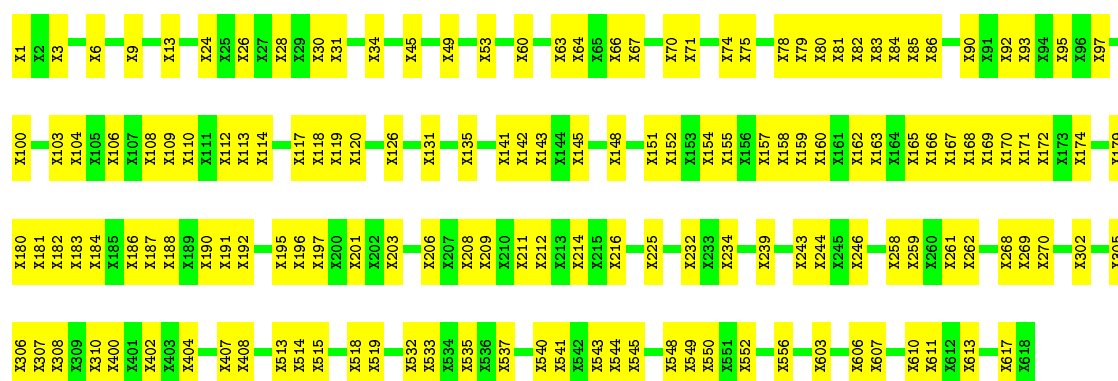
• Molecule 2: SERINE/THREONINE-PROTEIN KINASE MTOR

Chain 2: 57% 43%



• Molecule 2: SERINE/THREONINE-PROTEIN KINASE MTOR

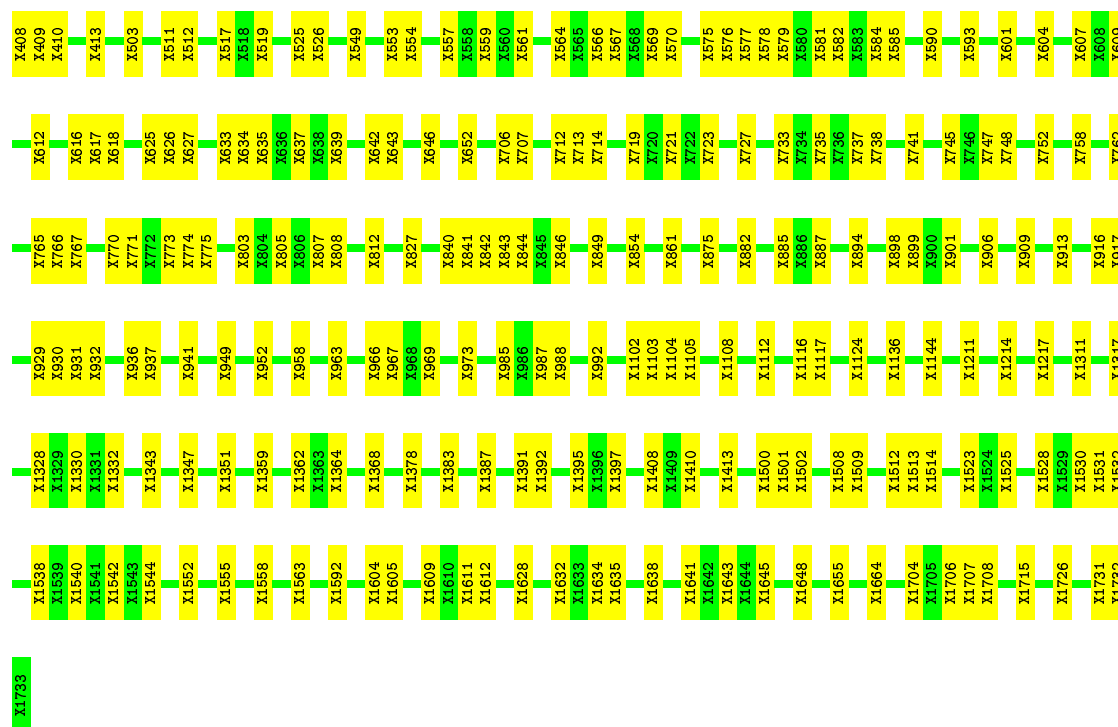
Chain 4: 58% 42%



• Molecule 3: REGULATORY-ASSOCIATED PROTEIN OF MTOR

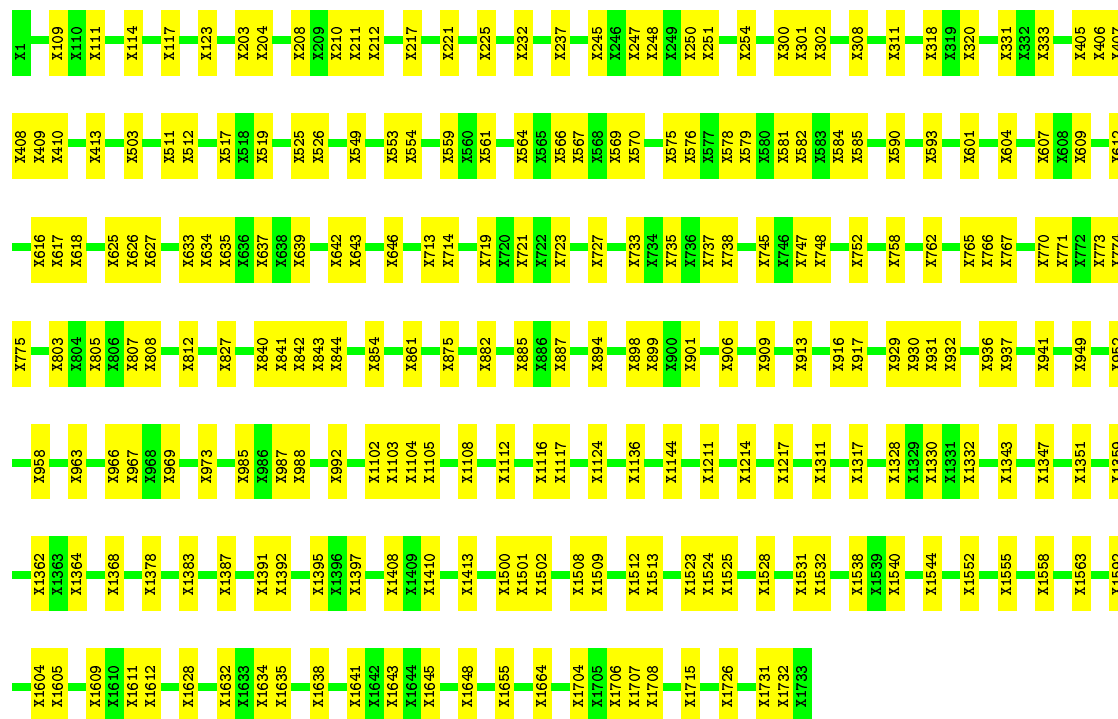
Chain A: 76% 24%





• Molecule 3: REGULATORY-ASSOCIATED PROTEIN OF MTOR

Chain E: 77% 23%

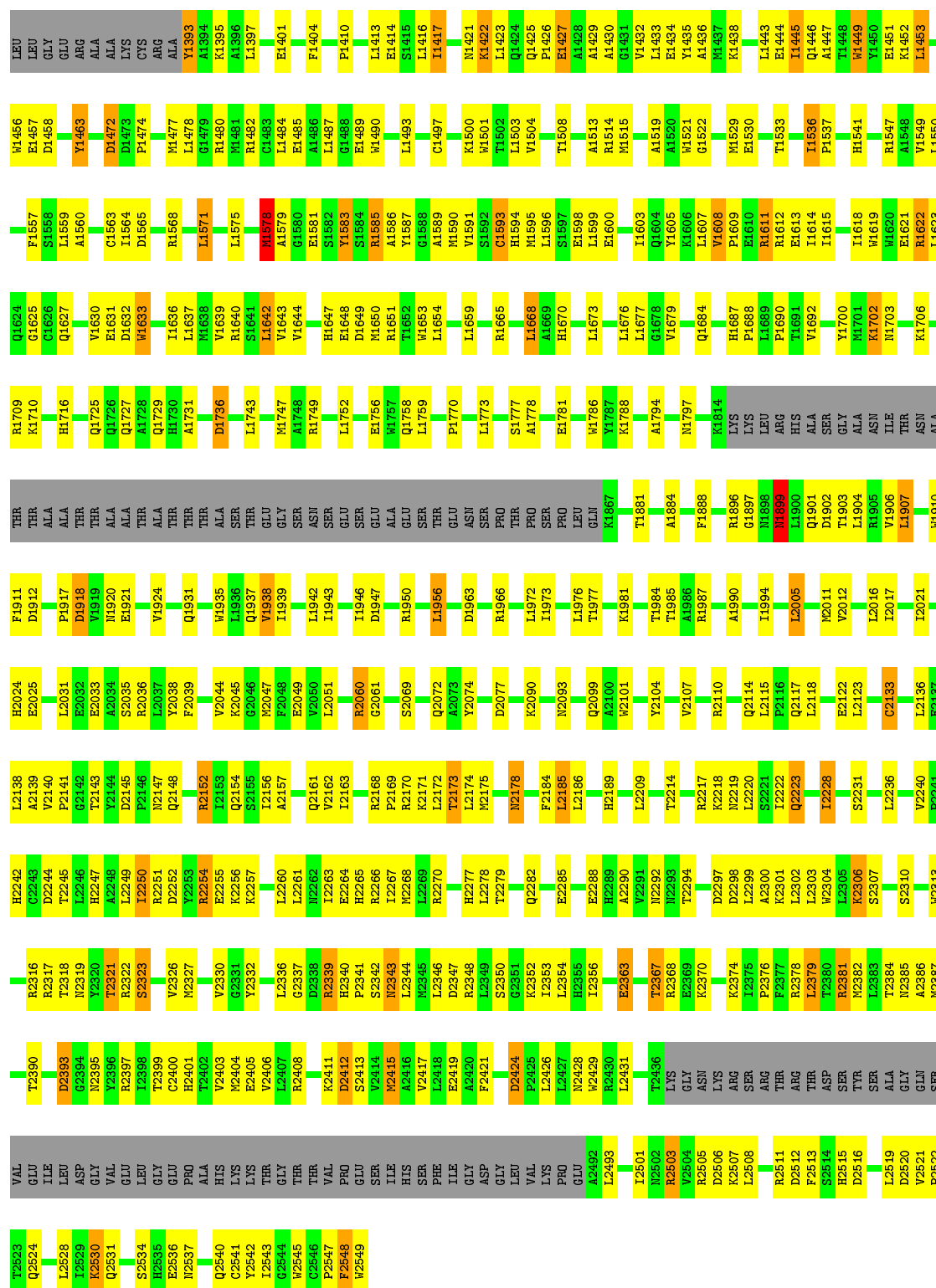


• Molecule 4: SERINE/THREONINE-PROTEIN KINASE MTOR

Chain B: 53% 32% 5% 10%



Device Type	Percentage
Smartphone	53%
Tablet	32%
Smartwatch	5%
Other	10%



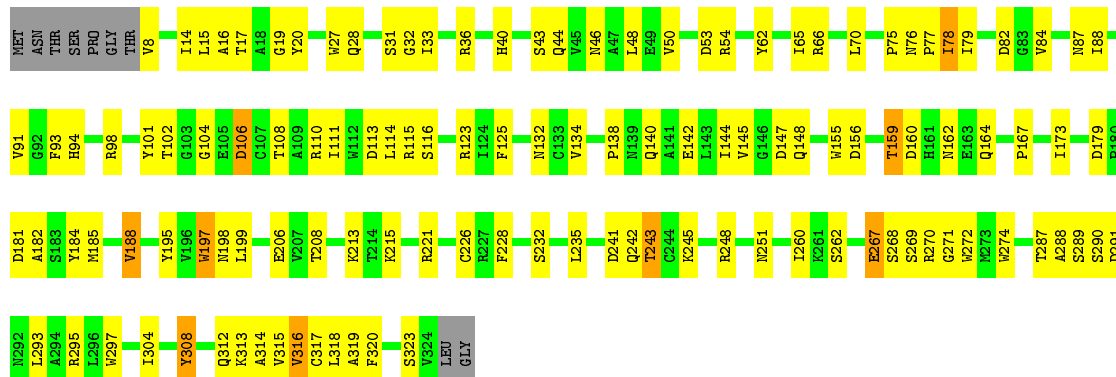
- Molecule 5: FKBP

Chain G:  74% 26%



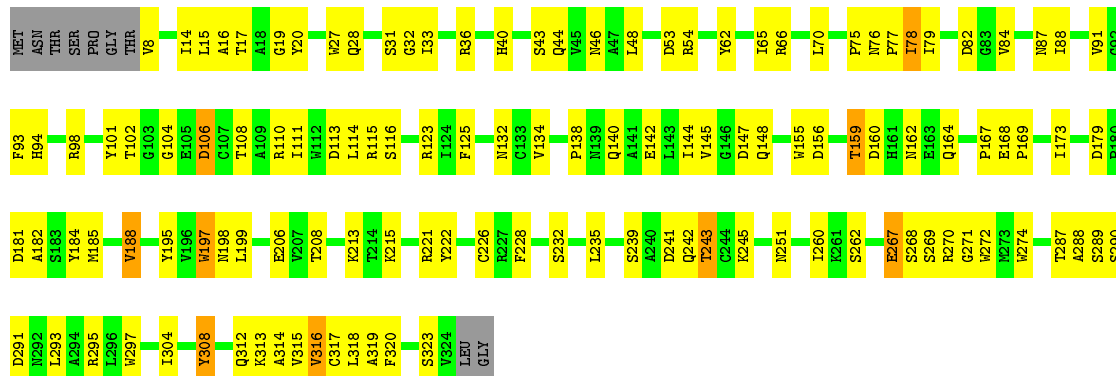
- Molecule 6: TARGET OF RAPAMYCIN COMPLEX SUBUNIT LST8

Chain D:  60% 35% . .



- Molecule 6: TARGET OF RAPAMYCIN COMPLEX SUBUNIT LST8

Chain H:  59% 35% . .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH IMAGE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1900	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4K X 4K)	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
4	B	0.36	1/8753 (0.0%)	0.55	3/11852 (0.0%)
4	F	0.36	1/8753 (0.0%)	0.54	2/11852 (0.0%)
6	D	0.26	0/2514	0.50	0/3426
6	H	0.26	0/2514	0.50	0/3426
All	All	0.34	2/22534 (0.0%)	0.54	5/30556 (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
2	2	0	1
2	4	0	1
4	B	0	5
4	F	0	4
6	D	0	1
6	H	0	1
All	All	0	13

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1583	TYR	CB-CG	5.54	1.59	1.51
4	F	1583	TYR	CB-CG	5.10	1.59	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1583	TYR	CA-CB-CG	6.74	126.21	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1583	TYR	CA-CB-CG	6.59	125.93	113.40
4	B	1445	ILE	N-CA-C	-5.12	97.18	111.00
4	F	2115	LEU	C-N-CD	5.01	138.93	128.40
4	B	2115	LEU	C-N-CD	5.01	138.93	128.40

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	216	UNK	Peptide
2	4	216	UNK	Peptide
4	B	1444	GLU	Peptide
4	B	1445	ILE	Peptide
4	B	1649	ASP	Peptide
4	B	1897	GLY	Peptide
4	B	1899	ASN	Peptide
6	D	267	GLU	Peptide
4	F	1444	GLU	Peptide
4	F	1649	ASP	Peptide
4	F	1897	GLY	Peptide
4	F	1899	ASN	Peptide
6	H	267	GLU	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	1	3690	0	3759	178	0
1	3	3690	0	3760	177	0
2	2	2190	0	2212	116	0
2	4	2190	0	2212	111	0
3	A	6174	0	6228	150	0
3	E	6174	0	6228	141	0
4	B	8551	0	8530	306	0
4	F	8551	0	8530	309	0
5	C	642	0	649	16	0
5	G	642	0	648	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	2456	0	2341	72	0
6	H	2456	0	2341	71	0
7	C	65	0	79	6	0
7	G	65	0	79	4	0
All	All	47536	0	47596	1607	0

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

All (1607) 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)
4:B:2419:GLU:HG2	4:B:2501:ILE:HG12	1.40	1.03
4:F:2419:GLU:HG2	4:F:2501:ILE:HG12	1.39	1.02
1:1:51:UNK:O	1:1:55:UNK:N	2.06	0.89
1:3:51:UNK:O	1:3:55:UNK:N	2.06	0.88
1:3:41:UNK:HB1	1:3:79:UNK:HG1	1.58	0.86
1:1:41:UNK:HB1	1:1:79:UNK:HG1	1.58	0.83
4:F:1619:TRP:HA	4:F:1622:ARG:HH12	1.46	0.81
4:B:1595:MET:HG2	4:B:1639:VAL:HG21	1.62	0.81
1:3:201:UNK:HA	1:3:203:UNK:HG3	1.62	0.81
3:E:771:UNK:HA	3:E:775:UNK:HB2	1.62	0.81
1:1:2:UNK:H2	4:F:1622:ARG:HE	1.29	0.80
5:G:10:UNK:HB1	5:G:70:UNK:HB1	1.64	0.80
4:B:1619:TRP:HA	4:B:1622:ARG:HH12	1.45	0.80
1:1:201:UNK:HA	1:1:203:UNK:HG3	1.64	0.80
3:A:771:UNK:HA	3:A:775:UNK:HB2	1.63	0.80
1:1:47:UNK:O	1:1:51:UNK:HB1	1.82	0.80
3:A:841:UNK:HB1	3:A:844:UNK:HB2	1.64	0.79
5:C:10:UNK:HB1	5:C:70:UNK:HB1	1.64	0.79
1:3:1219:UNK:HG1	1:3:1301:UNK:HB2	1.65	0.79
1:1:52:UNK:HA	1:1:55:UNK:HG3	1.65	0.79
4:F:2168:ARG:O	4:F:2170:ARG:NH1	2.16	0.79
1:3:212:UNK:HA	1:3:303:UNK:HB2	1.65	0.79
4:F:1595:MET:HG2	4:F:1639:VAL:HG21	1.62	0.79
1:3:47:UNK:O	1:3:51:UNK:HB1	1.82	0.78
1:3:2:UNK:H2	4:B:1622:ARG:HE	1.29	0.78
4:B:2168:ARG:O	4:B:2170:ARG:NH1	2.16	0.78
3:E:841:UNK:HB1	3:E:844:UNK:HB2	1.65	0.78
2:2:244:UNK:HG1	2:2:402:UNK:HB1	1.66	0.78
1:1:212:UNK:HA	1:1:303:UNK:HB2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:52:UNK:HA	1:3:55:UNK:HG3	1.66	0.77
1:1:1219:UNK:HG1	1:1:1301:UNK:HB2	1.64	0.77
1:1:90:UNK:HA	1:1:93:UNK:HB1	1.67	0.77
1:3:2114:UNK:HG1	1:3:2313:UNK:HA	1.67	0.77
4:F:1633:TRP:HA	4:F:1636:ILE:HB	1.67	0.77
4:B:1633:TRP:HA	4:B:1636:ILE:HB	1.67	0.76
1:3:1516:UNK:HG1	1:3:1603:UNK:HB2	1.67	0.76
1:3:90:UNK:HA	1:3:93:UNK:HB1	1.67	0.76
2:4:244:UNK:HG1	2:4:402:UNK:HB1	1.67	0.76
3:A:582:UNK:HG3	3:A:635:UNK:HG1	1.68	0.76
1:1:1516:UNK:HG1	1:1:1603:UNK:HB2	1.67	0.76
1:3:118:UNK:O	1:3:120:UNK:N	2.19	0.76
3:E:584:UNK:HB1	3:E:737:UNK:HG1	1.69	0.75
1:1:320:UNK:O	1:1:324:UNK:N	2.20	0.75
3:E:582:UNK:HG3	3:E:635:UNK:HG1	1.66	0.75
1:3:320:UNK:O	1:3:324:UNK:N	2.20	0.75
1:1:118:UNK:O	1:1:120:UNK:N	2.19	0.75
1:1:2114:UNK:HG1	1:1:2313:UNK:HA	1.67	0.74
2:4:552:UNK:HG1	4:F:2304:TRP:HZ2	1.51	0.74
3:E:1413:UNK:HB1	3:E:1513:UNK:HG1	1.69	0.74
4:F:2302:LEU:O	4:F:2306:LYS:N	2.20	0.74
1:1:154:UNK:HG3	3:A:643:UNK:HB1	1.67	0.74
1:3:131:UNK:HB1	1:3:144:UNK:HG1	1.69	0.74
4:B:2302:LEU:O	4:B:2306:LYS:N	2.20	0.74
1:3:154:UNK:HG3	3:E:643:UNK:HB1	1.67	0.74
3:A:1634:UNK:HG1	3:A:1704:UNK:HA	1.70	0.74
3:A:584:UNK:HB1	3:A:737:UNK:HG1	1.69	0.73
4:F:2260:LEU:HB3	4:F:2263:ILE:HB	1.70	0.73
3:A:1413:UNK:HB1	3:A:1513:UNK:HG1	1.69	0.73
2:2:552:UNK:HG1	4:B:2304:TRP:HZ2	1.53	0.73
1:1:305:UNK:HB2	2:2:75:UNK:HG1	1.69	0.73
3:E:1634:UNK:HG1	3:E:1704:UNK:HA	1.71	0.73
1:1:131:UNK:HB1	1:1:144:UNK:HG1	1.70	0.73
2:4:53:UNK:HA	2:4:95:UNK:HG1	1.70	0.73
4:F:2163:ILE:HB	4:F:2169:PRO:HG2	1.71	0.72
2:2:53:UNK:HA	2:2:95:UNK:HG1	1.70	0.72
3:E:1112:UNK:HB1	3:E:1124:UNK:HG1	1.71	0.72
1:3:911:UNK:HG3	1:3:918:UNK:HA	1.70	0.72
3:A:1112:UNK:HB1	3:A:1124:UNK:HG1	1.71	0.72
1:3:1:UNK:HG1	4:B:1598:GLU:HG2	1.71	0.72
4:B:2260:LEU:HB3	4:B:2263:ILE:HB	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:288:ALA:HB2	6:H:318:LEU:HG	1.72	0.72
6:D:288:ALA:HB2	6:D:318:LEU:HG	1.72	0.72
2:2:603:UNK:HA	2:2:606:UNK:HB1	1.72	0.72
1:3:305:UNK:HB2	2:4:75:UNK:HG1	1.69	0.71
4:B:2404:MET:HG3	4:B:2521:VAL:HG22	1.73	0.71
4:F:2404:MET:HG3	4:F:2521:VAL:HG22	1.73	0.71
4:B:2415:MET:SD	4:B:2505:ARG:NH1	2.63	0.71
1:1:911:UNK:HG3	1:1:918:UNK:HA	1.71	0.71
4:F:2300:ALA:HB2	4:F:2386:ALA:HA	1.71	0.71
4:F:2415:MET:SD	4:F:2505:ARG:NH1	2.64	0.71
1:1:1:UNK:HG1	4:F:1598:GLU:HG2	1.71	0.71
2:2:31:UNK:HA	2:2:34:UNK:HB1	1.73	0.70
4:B:2300:ALA:HB2	4:B:2386:ALA:HA	1.71	0.70
4:F:1393:TYR:HB2	4:F:1423:LEU:HD22	1.74	0.70
4:B:1393:TYR:HB2	4:B:1423:LEU:HD22	1.74	0.70
1:1:38:UNK:HG1	4:F:1618:ILE:HG22	1.74	0.69
1:3:38:UNK:HG1	4:B:1618:ILE:HG22	1.74	0.69
4:B:2332:TYR:O	4:B:2507:LYS:NZ	2.22	0.69
2:4:603:UNK:HA	2:4:606:UNK:HB1	1.72	0.69
4:F:2332:TYR:O	4:F:2507:LYS:NZ	2.22	0.69
3:E:410:UNK:O	3:E:413:UNK:N	2.26	0.69
4:F:2222:ILE:HG12	4:F:2327:MET:HG2	1.75	0.69
4:F:1493:LEU:HD23	4:F:1519:ALA:HB2	1.75	0.69
3:E:721:UNK:HB1	3:E:733:UNK:HB1	1.74	0.69
1:3:155:UNK:O	1:3:157:UNK:N	2.26	0.69
6:D:32:GLY:HA2	6:D:308:TYR:HD2	1.58	0.69
1:3:2111:UNK:HG2	1:3:2312:UNK:HG1	1.75	0.69
1:1:158:UNK:HA	3:A:713:UNK:HG1	1.75	0.69
3:E:887:UNK:HA	3:E:930:UNK:HG1	1.76	0.68
4:F:2339:ARG:NH2	4:F:2356:ILE:O	2.26	0.68
4:B:2222:ILE:HG12	4:B:2327:MET:HG2	1.75	0.68
3:E:203:UNK:HB1	3:E:208:UNK:HG1	1.76	0.68
3:A:251:UNK:HA	3:A:254:UNK:HB1	1.75	0.68
3:A:721:UNK:HB1	3:A:733:UNK:HB1	1.74	0.68
3:A:203:UNK:HB1	3:A:208:UNK:HG1	1.75	0.68
4:B:2339:ARG:NH2	4:B:2356:ILE:O	2.26	0.68
2:4:31:UNK:HA	2:4:34:UNK:HB1	1.74	0.68
1:1:2111:UNK:HG2	1:1:2312:UNK:HG1	1.75	0.68
2:2:92:UNK:HB1	2:2:100:UNK:HG1	1.76	0.68
1:1:51:UNK:HG2	1:1:55:UNK:HB1	1.76	0.68
1:3:51:UNK:HG2	1:3:55:UNK:HB1	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:410:UNK:O	3:A:413:UNK:N	2.25	0.68
2:4:92:UNK:HB1	2:4:100:UNK:HG1	1.75	0.68
6:H:32:GLY:HA2	6:H:308:TYR:HD2	1.58	0.68
4:B:2077:ASP:OD2	4:B:2110:ARG:NH2	2.27	0.68
4:B:2163:ILE:HB	4:B:2169:PRO:HG2	1.74	0.68
1:3:1505:UNK:HA	1:3:1508:UNK:HB1	1.75	0.68
1:1:155:UNK:O	1:1:157:UNK:N	2.26	0.67
4:F:2077:ASP:OD2	4:F:2110:ARG:NH2	2.27	0.67
1:3:158:UNK:HA	3:E:713:UNK:HG1	1.75	0.67
6:D:91:VAL:HG12	6:D:102:THR:HG22	1.77	0.67
4:F:2337:GLY:O	4:F:2339:ARG:NH1	2.28	0.67
2:4:118:UNK:HG2	2:4:158:UNK:HA	1.76	0.67
3:E:406:UNK:HG1	3:E:525:UNK:HG2	1.77	0.67
3:A:887:UNK:HA	3:A:930:UNK:HG1	1.75	0.67
1:3:122:UNK:HA	1:3:125:UNK:HB1	1.76	0.67
1:1:1505:UNK:HA	1:1:1508:UNK:HB1	1.75	0.67
2:2:66:UNK:O	2:2:70:UNK:N	2.28	0.67
1:3:157:UNK:HG2	1:3:158:UNK:HG3	1.76	0.67
4:B:2395:ASN:O	4:B:2399:THR:OG1	2.10	0.67
3:A:406:UNK:HG1	3:A:525:UNK:HG2	1.77	0.66
4:B:1493:LEU:HD23	4:B:1519:ALA:HB2	1.75	0.66
1:1:157:UNK:HG2	1:1:158:UNK:HG3	1.76	0.66
4:B:2337:GLY:O	4:B:2339:ARG:NH1	2.28	0.66
6:H:91:VAL:HG12	6:H:102:THR:HG22	1.77	0.66
4:B:2247:HIS:HB2	4:B:2341:PRO:HB2	1.78	0.66
1:3:904:UNK:HG1	1:3:1003:UNK:HG3	1.78	0.66
4:F:1690:PRO:HB2	4:F:1692:VAL:HG22	1.78	0.66
3:E:251:UNK:HA	3:E:254:UNK:HB1	1.76	0.66
1:3:122:UNK:O	1:3:126:UNK:N	2.29	0.66
1:1:122:UNK:HA	1:1:125:UNK:HB1	1.76	0.66
4:F:2506:ASP:HA	4:F:2511:ARG:HB2	1.78	0.66
4:F:2247:HIS:HB2	4:F:2341:PRO:HB2	1.76	0.66
4:F:1963:ASP:OD1	4:F:1966:ARG:NH2	2.29	0.66
2:2:118:UNK:HG2	2:2:158:UNK:HA	1.77	0.66
1:1:122:UNK:O	1:1:126:UNK:N	2.29	0.65
4:B:1963:ASP:OD1	4:B:1966:ARG:NH2	2.29	0.65
4:B:2319:ASN:O	4:B:2323:SER:OG	2.14	0.65
4:B:1586:ALA:O	4:B:1590:MET:HB2	1.96	0.65
4:F:1578:MET:SD	4:F:1579:ALA:N	2.60	0.65
1:1:6:UNK:O	1:1:10:UNK:N	2.29	0.65
2:4:145:UNK:HA	2:4:148:UNK:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:29:UNK:HB1	5:G:35:UNK:HA	1.78	0.65
1:1:904:UNK:HG1	1:1:1003:UNK:HG3	1.77	0.65
4:F:1586:ALA:O	4:F:1590:MET:HB2	1.96	0.65
1:3:1106:UNK:HG1	1:3:1305:UNK:HG3	1.78	0.65
4:F:2161:GLN:O	4:F:2171:LYS:N	2.25	0.65
1:3:6:UNK:O	1:3:10:UNK:N	2.29	0.65
3:E:1211:UNK:HA	3:E:1214:UNK:HB2	1.79	0.65
4:F:2240:VAL:HG21	4:F:2354:LEU:HD22	1.77	0.65
5:C:29:UNK:HB1	5:C:35:UNK:HA	1.79	0.65
4:B:2408:ARG:NH2	4:B:2519:LEU:O	2.30	0.65
2:4:66:UNK:O	2:4:70:UNK:N	2.29	0.65
4:B:2506:ASP:HA	4:B:2511:ARG:HB2	1.79	0.65
4:F:1622:ARG:HA	4:F:1625:GLY:HA3	1.79	0.65
1:1:48:UNK:O	1:1:52:UNK:HB1	1.97	0.65
1:1:310:UNK:HA	1:1:313:UNK:HB1	1.79	0.65
1:3:48:UNK:O	1:3:52:UNK:HB1	1.96	0.65
3:E:549:UNK:HG3	3:E:553:UNK:HB1	1.79	0.65
4:F:2319:ASN:O	4:F:2323:SER:OG	2.15	0.65
4:B:2240:VAL:HG21	4:B:2354:LEU:HD22	1.77	0.64
4:B:1622:ARG:HA	4:B:1625:GLY:HA3	1.79	0.64
2:2:145:UNK:HA	2:2:148:UNK:HB2	1.77	0.64
4:B:1896:ARG:HH21	4:B:1931:GLN:HG3	1.61	0.64
1:3:1704:UNK:HG2	1:3:1904:UNK:HG1	1.79	0.64
4:B:1690:PRO:HB2	4:B:1692:VAL:HG22	1.78	0.64
1:3:310:UNK:HA	1:3:313:UNK:HB1	1.79	0.64
4:F:1896:ARG:HH21	4:F:1931:GLN:HG3	1.61	0.64
6:D:134:VAL:HG22	6:D:145:VAL:HG22	1.79	0.64
2:4:183:UNK:HA	2:4:186:UNK:HB1	1.78	0.64
1:3:702:UNK:HG1	1:3:812:UNK:HG1	1.78	0.64
1:1:331:UNK:HB1	1:1:407:UNK:HB1	1.80	0.64
3:A:549:UNK:HG3	3:A:553:UNK:HB1	1.80	0.64
1:1:1106:UNK:HG1	1:1:1305:UNK:HG3	1.78	0.64
3:E:123:UNK:HA	3:E:308:UNK:HB2	1.80	0.64
2:2:163:UNK:HA	2:2:166:UNK:HB2	1.80	0.64
4:B:1590:MET:O	4:B:1594:HIS:HB2	1.98	0.63
1:1:1704:UNK:HG2	1:1:1904:UNK:HG1	1.78	0.63
4:F:1590:MET:O	4:F:1594:HIS:HB2	1.99	0.63
3:E:901:UNK:HG3	3:E:941:UNK:HG3	1.80	0.63
4:B:2178:ASN:H	4:B:2178:ASN:HD22	1.46	0.63
4:B:2421:PHE:HA	4:B:2424:ASP:HB2	1.80	0.63
3:A:1211:UNK:HA	3:A:1214:UNK:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:702:UNK:HG1	1:1:812:UNK:HG1	1.79	0.63
4:F:2408:ARG:NH2	4:F:2519:LEU:O	2.31	0.63
3:A:901:UNK:HG3	3:A:941:UNK:HG3	1.80	0.63
3:E:1413:UNK:HG3	3:E:1523:UNK:HG1	1.80	0.63
6:D:46:ASN:ND2	6:D:87:ASN:OD1	2.31	0.63
3:A:1413:UNK:HG3	3:A:1523:UNK:HG1	1.80	0.63
4:F:2363:GLU:O	4:F:2367:THR:OG1	2.17	0.63
4:B:1749:ARG:HG2	4:B:1786:TRP:CH2	2.34	0.63
4:F:2421:PHE:HA	4:F:2424:ASP:HB2	1.81	0.63
4:F:2395:ASN:O	4:F:2399:THR:OG1	2.10	0.63
2:4:163:UNK:HA	2:4:166:UNK:HB2	1.79	0.63
1:3:331:UNK:HB1	1:3:407:UNK:HB1	1.80	0.62
3:A:123:UNK:HA	3:A:308:UNK:HB2	1.81	0.62
3:E:1391:UNK:HG3	3:E:1500:UNK:HB1	1.80	0.62
1:1:119:UNK:O	1:1:121:UNK:N	2.33	0.62
2:4:154:UNK:O	2:4:158:UNK:HB1	1.99	0.62
2:4:80:UNK:HA	2:4:120:UNK:HG1	1.81	0.62
3:A:1391:UNK:HG3	3:A:1500:UNK:HB1	1.80	0.62
4:B:2363:GLU:O	4:B:2367:THR:OG1	2.17	0.62
2:2:154:UNK:O	2:2:158:UNK:HB1	1.99	0.62
6:H:134:VAL:HG22	6:H:145:VAL:HG22	1.79	0.62
6:H:46:ASN:ND2	6:H:87:ASN:OD1	2.31	0.62
3:E:1317:UNK:HG1	3:E:1351:UNK:HA	1.81	0.62
4:F:1749:ARG:HG2	4:F:1786:TRP:CH2	2.34	0.62
3:A:311:UNK:HG2	3:A:320:UNK:HG1	1.81	0.62
6:H:181:ASP:OD2	6:H:232:SER:OG	2.18	0.62
1:3:119:UNK:O	1:3:121:UNK:N	2.33	0.62
6:D:195:TYR:OH	6:D:215:LYS:NZ	2.32	0.61
4:B:1636:ILE:HG22	4:B:1637:LEU:HD23	1.81	0.61
4:B:2161:GLN:O	4:B:2171:LYS:N	2.25	0.61
4:F:1581:GLU:CB	4:F:1585:ARG:HB2	2.30	0.61
6:D:106:ASP:OD2	6:D:108:THR:OG1	2.18	0.61
2:4:90:UNK:HG3	2:4:131:UNK:HG1	1.83	0.61
6:D:36:ARG:HH12	6:D:75:PRO:HD2	1.65	0.61
3:E:898:UNK:HG3	3:E:899:UNK:HG2	1.82	0.61
6:H:36:ARG:HH12	6:H:75:PRO:HD2	1.64	0.61
4:B:2303:LEU:HA	4:B:2306:LYS:HB2	1.83	0.61
1:3:328:UNK:HB2	1:3:431:UNK:HB2	1.82	0.61
1:1:328:UNK:HB2	1:1:431:UNK:HB2	1.81	0.61
4:B:1581:GLU:CB	4:B:1585:ARG:HB2	2.30	0.61
4:F:1549:VAL:HG13	4:F:1642:LEU:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:139:UNK:O	1:1:141:UNK:N	2.33	0.61
2:4:182:UNK:HG2	2:4:183:UNK:HG2	1.83	0.61
3:A:114:UNK:HA	3:A:300:UNK:HA	1.83	0.61
3:E:311:UNK:HG2	3:E:320:UNK:HG1	1.81	0.61
4:F:1636:ILE:HG22	4:F:1637:LEU:HD23	1.80	0.61
2:4:155:UNK:HB1	2:4:190:UNK:HG1	1.83	0.61
4:B:1786:TRP:CZ2	4:B:1788:LYS:HD3	2.36	0.61
3:A:898:UNK:HG3	3:A:899:UNK:HG2	1.82	0.61
1:3:511:UNK:HA	1:3:600:UNK:HB1	1.83	0.61
2:2:155:UNK:HB1	2:2:190:UNK:HG1	1.83	0.61
6:H:167:PRO:HG3	6:H:197:TRP:HZ2	1.66	0.61
4:F:1490:TRP:CE3	4:F:1519:ALA:HA	2.35	0.61
3:A:1317:UNK:HG1	3:A:1351:UNK:HA	1.82	0.61
4:B:1578:MET:SD	4:B:1579:ALA:N	2.60	0.61
3:E:114:UNK:HA	3:E:300:UNK:HA	1.83	0.61
2:2:80:UNK:HA	2:2:120:UNK:HG1	1.81	0.61
1:3:203:UNK:O	1:3:207:UNK:HB1	2.00	0.60
3:A:117:UNK:HA	3:A:301:UNK:HG2	1.83	0.60
3:E:117:UNK:HA	3:E:301:UNK:HG2	1.83	0.60
1:3:139:UNK:O	1:3:141:UNK:N	2.34	0.60
4:B:1549:VAL:HG13	4:B:1642:LEU:HD11	1.81	0.60
6:D:167:PRO:HG3	6:D:197:TRP:HZ2	1.66	0.60
6:H:138:PRO:HG2	6:H:182:ALA:HB2	1.83	0.60
4:F:2178:ASN:H	4:F:2178:ASN:HD22	1.47	0.60
4:B:1490:TRP:CE3	4:B:1519:ALA:HA	2.36	0.60
2:2:90:UNK:HG3	2:2:131:UNK:HG1	1.82	0.60
6:H:195:TYR:OH	6:H:215:LYS:NZ	2.32	0.60
4:F:1786:TRP:CZ2	4:F:1788:LYS:HD3	2.36	0.60
6:H:15:LEU:HD13	6:H:320:PHE:HD1	1.66	0.60
3:E:1538:UNK:HG1	3:E:1563:UNK:HG1	1.84	0.60
2:4:513:UNK:HG1	2:4:550:UNK:HB1	1.83	0.60
1:1:511:UNK:HA	1:1:600:UNK:HB1	1.83	0.60
6:D:111:ILE:HB	6:D:123:ARG:HB2	1.83	0.60
6:H:111:ILE:HB	6:H:123:ARG:HB2	1.84	0.60
1:1:203:UNK:O	1:1:207:UNK:HB1	2.01	0.60
4:F:2339:ARG:NH2	4:F:2343:ASN:OD1	2.35	0.60
4:B:2141:PRO:HB3	4:B:2228:ILE:HG21	1.84	0.60
1:3:2201:UNK:HG2	1:3:2202:UNK:HG3	1.84	0.60
6:H:106:ASP:OD2	6:H:108:THR:OG1	2.19	0.59
2:2:209:UNK:HB2	2:2:246:UNK:HB2	1.84	0.59
6:D:15:LEU:HD13	6:D:320:PHE:HD1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:2303:LEU:HA	4:F:2306:LYS:HB2	1.83	0.59
4:B:2339:ARG:NH2	4:B:2343:ASN:OD1	2.35	0.59
4:B:2347:ASP:OD1	4:B:2350:SER:N	2.35	0.59
4:B:2031:LEU:O	4:B:2035:SER:OG	2.18	0.59
2:2:182:UNK:HG2	2:2:183:UNK:HG2	1.83	0.59
4:F:2141:PRO:HB3	4:F:2228:ILE:HG21	1.83	0.59
4:B:1752:LEU:HD21	4:B:1788:LYS:HG2	1.85	0.59
3:A:408:UNK:HB1	3:A:512:UNK:HA	1.84	0.59
4:F:2347:ASP:OD1	4:F:2350:SER:N	2.36	0.59
6:D:8:VAL:HG11	6:D:36:ARG:HE	1.66	0.59
3:A:1538:UNK:HG1	3:A:1563:UNK:HG1	1.84	0.59
4:B:1673:LEU:HD22	4:B:1700:TYR:HB2	1.85	0.59
4:F:2223:GLN:HE22	4:F:2352:LYS:HB2	1.68	0.59
2:4:183:UNK:O	2:4:187:UNK:N	2.36	0.59
2:4:71:UNK:HA	2:4:74:UNK:HB2	1.85	0.58
4:F:1490:TRP:CD1	4:F:1522:GLY:HA3	2.37	0.58
6:H:8:VAL:HG11	6:H:36:ARG:HE	1.66	0.58
2:2:183:UNK:O	2:2:187:UNK:N	2.36	0.58
4:B:2244:ASP:HB2	4:B:2249:LEU:HD11	1.85	0.58
4:B:1901:GLN:HG3	4:B:2413:SER:HA	1.85	0.58
2:2:71:UNK:HA	2:2:74:UNK:HB2	1.85	0.58
4:B:1490:TRP:CD1	4:B:1522:GLY:HA3	2.38	0.58
1:3:440:UNK:HB2	1:3:444:UNK:N	2.18	0.58
1:3:1509:UNK:HG3	1:3:1606:UNK:HG3	1.85	0.58
6:D:138:PRO:HG2	6:D:182:ALA:HB2	1.83	0.58
4:F:1430:ALA:O	4:F:1434:GLU:HG2	2.03	0.58
4:B:1430:ALA:O	4:B:1434:GLU:HG2	2.03	0.58
4:F:1912:ASP:O	4:F:1950:ARG:NH1	2.37	0.58
4:F:2245:THR:HB	4:F:2342:SER:HA	1.85	0.58
6:D:93:PHE:HE1	6:D:114:LEU:HD11	1.67	0.58
5:G:62:UNK:HG1	5:G:74:UNK:HB1	1.85	0.58
4:F:1901:GLN:HG3	4:F:2413:SER:HA	1.85	0.58
3:E:1117:UNK:HB2	3:E:1410:UNK:HB2	1.86	0.58
6:H:184:TYR:OH	6:H:213:LYS:NZ	2.35	0.58
1:1:2201:UNK:HG2	1:1:2202:UNK:HG3	1.84	0.58
3:E:408:UNK:HB1	3:E:512:UNK:HA	1.84	0.58
3:A:1117:UNK:HB2	3:A:1410:UNK:HB2	1.85	0.58
4:B:1622:ARG:CZ	4:B:1622:ARG:HB3	2.33	0.58
2:2:118:UNK:HG1	2:2:159:UNK:HG2	1.86	0.58
4:F:1673:LEU:HD22	4:F:1700:TYR:HB2	1.85	0.58
1:1:1114:UNK:HB1	1:1:1315:UNK:HG1	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1752:LEU:HD21	4:F:1788:LYS:HG2	1.85	0.58
6:H:93:PHE:HE1	6:H:114:LEU:HD11	1.68	0.58
1:1:1306:UNK:HG1	1:1:1508:UNK:HA	1.86	0.58
6:D:181:ASP:OD2	6:D:232:SER:OG	2.18	0.58
5:C:54:UNK:HG3	7:C:999:RAP:H472	1.84	0.58
4:F:1593:CYS:HA	4:F:1596:LEU:HD12	1.86	0.58
2:2:541:UNK:HG3	2:2:545:UNK:HB2	1.86	0.58
1:3:1306:UNK:HG1	1:3:1508:UNK:HA	1.86	0.58
1:3:21:UNK:O	1:3:25:UNK:HB2	2.04	0.58
3:A:917:UNK:HG3	3:A:958:UNK:HG1	1.85	0.58
1:3:410:UNK:HA	1:3:413:UNK:HB2	1.86	0.58
1:1:80:UNK:HG3	1:1:82:UNK:HB1	1.85	0.57
4:B:2245:THR:HB	4:B:2342:SER:HA	1.85	0.57
4:B:2223:GLN:HE22	4:B:2352:LYS:HB2	1.67	0.57
6:H:76:ASN:HB3	6:H:77:PRO:HD2	1.86	0.57
1:1:1509:UNK:HG3	1:1:1606:UNK:HG3	1.86	0.57
4:B:1581:GLU:HB3	4:B:1585:ARG:HB2	1.86	0.57
5:C:62:UNK:HG1	5:C:74:UNK:HB1	1.85	0.57
4:B:2264:GLU:HG3	4:B:2294:THR:HG21	1.86	0.57
5:G:54:UNK:HG3	7:G:999:RAP:H472	1.84	0.57
1:1:21:UNK:O	1:1:25:UNK:HB2	2.04	0.57
1:3:7:UNK:O	1:3:11:UNK:N	2.38	0.57
3:A:407:UNK:HG2	3:A:410:UNK:HB2	1.87	0.57
1:3:1114:UNK:HB1	1:3:1315:UNK:HG1	1.85	0.57
1:3:1809:UNK:HG1	1:3:2006:UNK:HG2	1.87	0.57
2:4:541:UNK:HG3	2:4:545:UNK:HB2	1.86	0.57
2:4:118:UNK:HG1	2:4:159:UNK:HG2	1.87	0.57
4:F:1581:GLU:HB3	4:F:1585:ARG:HB2	1.87	0.57
1:1:1809:UNK:HG1	1:1:2006:UNK:HG2	1.86	0.57
3:A:1501:UNK:HG1	3:A:1544:UNK:HA	1.86	0.57
1:1:114:UNK:O	1:1:117:UNK:HB2	2.05	0.57
3:E:917:UNK:HG3	3:E:958:UNK:HG1	1.84	0.57
3:E:1116:UNK:HG3	3:E:1392:UNK:HG3	1.87	0.57
3:E:1102:UNK:HA	3:E:1105:UNK:HB2	1.87	0.57
1:3:8:UNK:HG3	4:B:1568:ARG:HE	1.70	0.57
2:2:513:UNK:HG1	2:2:550:UNK:HB1	1.86	0.57
4:B:2101:TRP:HA	4:B:2104:TYR:HB2	1.87	0.57
1:1:440:UNK:HB2	1:1:444:UNK:N	2.18	0.57
1:3:94:UNK:O	1:3:96:UNK:N	2.38	0.57
4:B:1939:ILE:HA	4:B:1942:LEU:HD12	1.87	0.57
4:B:1912:ASP:O	4:B:1950:ARG:NH1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:76:ASN:HB3	6:D:77:PRO:HD2	1.87	0.57
4:F:2244:ASP:HB2	4:F:2249:LEU:HD11	1.87	0.57
1:3:80:UNK:HG3	1:3:82:UNK:HB1	1.86	0.56
1:3:2:UNK:H2	4:B:1622:ARG:NE	2.02	0.56
4:B:1593:CYS:HA	4:B:1596:LEU:HD12	1.86	0.56
2:4:310:UNK:C	2:4:404:UNK:HB2	2.35	0.56
4:F:2264:GLU:HG3	4:F:2294:THR:HG21	1.86	0.56
1:3:114:UNK:O	1:3:117:UNK:HB2	2.04	0.56
3:E:407:UNK:HG2	3:E:410:UNK:HB2	1.87	0.56
4:F:2321:THR:HG23	4:F:2387:MET:HG2	1.87	0.56
4:F:2412:ASP:N	4:F:2412:ASP:OD1	2.36	0.56
4:B:1899:ASN:ND2	4:B:1937:GLN:OE1	2.39	0.56
4:B:2321:THR:HG23	4:B:2387:MET:HG2	1.87	0.56
1:3:1711:UNK:HG2	1:3:1911:UNK:HG1	1.87	0.56
3:E:1501:UNK:HG1	3:E:1544:UNK:HA	1.86	0.56
1:1:94:UNK:O	1:1:96:UNK:N	2.38	0.56
4:F:1939:ILE:HA	4:F:1942:LEU:HD12	1.87	0.56
1:1:7:UNK:O	1:1:11:UNK:N	2.38	0.56
1:1:8:UNK:HG3	4:F:1568:ARG:HE	1.69	0.56
4:F:1591:VAL:O	4:F:1594:HIS:HB3	2.06	0.56
3:E:1645:UNK:HG3	3:E:1655:UNK:HG2	1.88	0.56
4:B:1513:ALA:HB1	4:B:1536:ILE:HG12	1.88	0.56
4:F:2031:LEU:O	4:F:2035:SER:OG	2.18	0.56
1:3:506:UNK:HA	1:3:509:UNK:HB2	1.88	0.56
4:B:1600:GLU:O	4:B:1603:ILE:HG22	2.05	0.56
3:E:549:UNK:HB1	3:E:554:UNK:HG2	1.88	0.56
2:4:307:UNK:HG2	2:4:407:UNK:HG1	1.87	0.56
4:F:2101:TRP:HA	4:F:2104:TYR:HB2	1.87	0.56
1:1:1711:UNK:HG2	1:1:1911:UNK:HG1	1.88	0.56
2:4:209:UNK:HB2	2:4:246:UNK:HB2	1.87	0.56
3:A:949:UNK:HA	3:A:952:UNK:HB2	1.87	0.56
4:B:2310:SER:O	4:B:2313:TRP:HB3	2.06	0.56
6:D:243:THR:HG21	6:D:245:LYS:HE3	1.88	0.56
3:A:1102:UNK:HA	3:A:1105:UNK:HB2	1.87	0.56
3:A:1116:UNK:HG3	3:A:1392:UNK:HG3	1.88	0.56
4:F:1600:GLU:O	4:F:1603:ILE:HG22	2.05	0.56
3:A:575:UNK:O	3:A:578:UNK:HB2	2.06	0.56
2:2:93:UNK:HG2	2:2:135:UNK:HB1	1.88	0.56
3:A:1645:UNK:HG3	3:A:1655:UNK:HG2	1.88	0.56
3:A:549:UNK:HB1	3:A:554:UNK:HG2	1.88	0.56
1:3:88:UNK:HG1	1:3:106:UNK:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:2534:SER:OG	4:F:2537:ASN:ND2	2.39	0.55
2:2:310:UNK:C	2:2:404:UNK:HB2	2.35	0.55
1:1:88:UNK:HG1	1:1:106:UNK:HA	1.87	0.55
4:F:2419:GLU:OE2	4:F:2505:ARG:NH1	2.38	0.55
6:D:184:TYR:OH	6:D:213:LYS:NZ	2.35	0.55
4:F:1899:ASN:ND2	4:F:1937:GLN:OE1	2.38	0.55
4:F:1410:PRO:HA	4:F:1413:LEU:HD12	1.87	0.55
4:B:2534:SER:OG	4:B:2537:ASN:ND2	2.39	0.55
4:F:1619:TRP:CH2	4:F:1640:ARG:HB3	2.42	0.55
4:F:1513:ALA:HB1	4:F:1536:ILE:HG12	1.89	0.55
3:E:949:UNK:HA	3:E:952:UNK:HB2	1.87	0.55
1:1:506:UNK:HA	1:1:509:UNK:HB2	1.88	0.55
4:B:2419:GLU:OE2	4:B:2505:ARG:NH1	2.39	0.55
1:1:2:UNK:H2	4:F:1622:ARG:NE	2.03	0.55
4:B:1943:ILE:HA	4:B:1946:ILE:HG13	1.87	0.55
4:F:2156:ILE:HG12	4:F:2174:LEU:HD22	1.89	0.55
1:1:410:UNK:HA	1:1:413:UNK:HB2	1.88	0.55
4:F:1943:ILE:HA	4:F:1946:ILE:HG13	1.87	0.55
4:B:1410:PRO:HA	4:B:1413:LEU:HD12	1.88	0.55
4:B:1591:VAL:O	4:B:1594:HIS:HB3	2.06	0.55
2:4:544:UNK:O	2:4:548:UNK:HG2	2.06	0.55
3:A:617:UNK:HG1	3:A:633:UNK:HB2	1.88	0.55
1:3:120:UNK:HB1	1:3:123:UNK:HB2	1.89	0.55
3:E:1395:UNK:O	3:E:1408:UNK:N	2.40	0.55
1:1:44:UNK:HA	1:1:47:UNK:CB	2.38	0.54
5:C:27:UNK:HG2	5:C:100:UNK:HB2	1.89	0.54
3:E:575:UNK:O	3:E:578:UNK:HB2	2.06	0.54
2:2:544:UNK:O	2:2:548:UNK:HG2	2.06	0.54
4:B:2156:ILE:HG12	4:B:2174:LEU:HD22	1.89	0.54
6:H:159:THR:OG1	6:H:206:GLU:OE1	2.25	0.54
1:3:416:UNK:O	1:3:418:UNK:N	2.26	0.54
1:3:49:UNK:O	1:3:52:UNK:HG3	2.08	0.54
4:B:1619:TRP:CH2	4:B:1640:ARG:HB3	2.42	0.54
6:D:288:ALA:HB1	6:D:315:VAL:HG12	1.89	0.54
3:E:985:UNK:HB1	3:E:988:UNK:HB2	1.89	0.54
1:1:88:UNK:HA	1:1:91:UNK:HB2	1.89	0.54
4:B:2184:PHE:HB3	4:B:2236:LEU:HD22	1.88	0.54
3:E:617:UNK:HG1	3:E:633:UNK:HB2	1.89	0.54
2:4:192:UNK:HA	2:4:195:UNK:HB2	1.89	0.54
2:2:307:UNK:HG2	2:2:407:UNK:HG1	1.87	0.54
4:F:2270:ARG:O	6:H:313:LYS:NZ	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:93:UNK:HG2	2:4:135:UNK:HB1	1.89	0.54
5:G:27:UNK:HG2	5:G:100:UNK:HB2	1.89	0.54
1:1:49:UNK:O	1:1:52:UNK:HG3	2.07	0.54
2:2:239:UNK:O	2:2:243:UNK:HB2	2.07	0.54
3:A:1395:UNK:O	3:A:1408:UNK:N	2.41	0.54
4:F:1445:ILE:HG13	4:F:1449:TRP:CZ3	2.43	0.54
6:H:243:THR:HG21	6:H:245:LYS:HE3	1.88	0.54
4:B:1653:TRP:HB2	4:B:1676:LEU:HD11	1.90	0.54
4:B:1938:VAL:HG13	4:B:1942:LEU:HG	1.89	0.54
4:F:2265:HIS:HA	4:F:2268:MET:SD	2.48	0.54
2:2:82:UNK:HA	2:2:85:UNK:HB2	1.88	0.54
1:1:1:UNK:O	1:1:5:UNK:N	2.41	0.54
4:F:1622:ARG:CZ	4:F:1622:ARG:HB3	2.34	0.54
2:4:239:UNK:O	2:4:243:UNK:HB2	2.07	0.54
2:2:192:UNK:HA	2:2:195:UNK:HB2	1.89	0.54
1:1:31:UNK:O	1:1:36:UNK:HB2	2.08	0.54
1:1:416:UNK:C	1:1:418:UNK:H	2.16	0.54
4:B:2393:ASP:OD1	4:B:2397:ARG:NH1	2.41	0.54
3:A:985:UNK:HB1	3:A:988:UNK:HB2	1.89	0.54
1:3:31:UNK:O	1:3:36:UNK:HB2	2.08	0.54
3:A:1628:UNK:HB1	3:A:1648:UNK:HG1	1.90	0.54
4:F:2304:TRP:HA	4:F:2313:TRP:CD1	2.43	0.54
4:B:2256:LYS:HZ3	4:B:2257:LYS:HE3	1.73	0.54
6:H:98:ARG:HG3	6:H:115:ARG:HD2	1.90	0.54
3:E:1311:UNK:HB2	3:E:1664:UNK:HB2	1.89	0.53
4:F:2038:TYR:HE1	4:F:2044:VAL:HG22	1.73	0.53
6:D:159:THR:OG1	6:D:206:GLU:OE1	2.25	0.53
4:B:2324:LEU:O	4:B:2328:SER:OG	2.17	0.53
1:1:44:UNK:HA	1:1:47:UNK:HB2	1.90	0.53
2:4:117:UNK:O	2:4:119:UNK:N	2.42	0.53
3:A:1311:UNK:HB2	3:A:1664:UNK:HB2	1.89	0.53
4:B:2038:TYR:HE1	4:B:2044:VAL:HG22	1.73	0.53
4:F:2310:SER:O	4:F:2313:TRP:HB3	2.07	0.53
4:B:2290:ALA:O	4:B:2294:THR:OG1	2.19	0.53
4:F:2184:PHE:HB3	4:F:2236:LEU:HD22	1.89	0.53
6:H:40:HIS:HE1	6:H:43:SER:HB3	1.74	0.53
4:B:2304:TRP:HA	4:B:2313:TRP:CD1	2.43	0.53
6:D:14:ILE:HD13	6:D:70:LEU:HD13	1.91	0.53
4:F:1598:GLU:OE2	4:F:1619:TRP:NE1	2.41	0.53
4:F:1621:GLU:O	4:F:1625:GLY:N	2.42	0.53
4:B:1598:GLU:OE2	4:B:1619:TRP:NE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:32:GLY:HA2	6:D:308:TYR:CD2	2.42	0.53
1:3:88:UNK:HA	1:3:91:UNK:HB2	1.91	0.53
1:1:334:UNK:HB2	1:1:402:UNK:HB2	1.90	0.53
3:E:517:UNK:O	3:E:519:UNK:N	2.42	0.53
4:B:2411:LYS:HB2	4:B:2508:LEU:HD13	1.90	0.53
4:F:1581:GLU:HB3	4:F:1585:ARG:H	1.74	0.53
2:2:197:UNK:O	2:2:201:UNK:N	2.42	0.53
4:F:1653:TRP:HB2	4:F:1676:LEU:HD11	1.89	0.53
1:3:334:UNK:HB2	1:3:402:UNK:HB2	1.89	0.53
1:3:44:UNK:HA	1:3:47:UNK:HB2	1.90	0.53
1:3:48:UNK:HA	1:3:51:UNK:HG3	1.91	0.53
4:B:1514:ARG:HA	4:B:1536:ILE:HD13	1.91	0.53
1:1:42:UNK:O	1:1:45:UNK:HB2	2.09	0.53
6:D:98:ARG:HG3	6:D:115:ARG:HD2	1.90	0.53
4:F:1947:ASP:HB3	4:F:1987:ARG:HG2	1.91	0.53
6:H:288:ALA:HB1	6:H:315:VAL:HG12	1.89	0.53
3:E:1628:UNK:HB1	3:E:1648:UNK:HG1	1.90	0.53
1:3:44:UNK:HA	1:3:47:UNK:CB	2.38	0.53
4:B:1590:MET:HA	4:B:1593:CYS:SG	2.48	0.53
6:H:14:ILE:HD13	6:H:70:LEU:HD13	1.91	0.53
6:D:40:HIS:HE1	6:D:43:SER:HB3	1.74	0.53
1:3:1:UNK:O	1:3:5:UNK:N	2.41	0.52
1:1:120:UNK:HB1	1:1:123:UNK:HB2	1.90	0.52
4:F:2411:LYS:HB2	4:F:2508:LEU:HD13	1.90	0.52
4:B:2265:HIS:HA	4:B:2268:MET:SD	2.48	0.52
1:1:61:UNK:O	1:1:64:UNK:HB2	2.09	0.52
2:4:259:UNK:HA	2:4:262:UNK:HG3	1.92	0.52
1:3:42:UNK:O	1:3:45:UNK:HB2	2.09	0.52
1:3:61:UNK:O	1:3:64:UNK:HB2	2.09	0.52
4:B:1644:VAL:HG13	4:B:1648:GLU:CD	2.30	0.52
3:E:1347:UNK:HG3	3:E:1359:UNK:HG2	1.91	0.52
4:F:1590:MET:HA	4:F:1593:CYS:SG	2.48	0.52
7:C:999:RAP:H432	7:C:999:RAP:O4	2.09	0.52
3:A:517:UNK:O	3:A:519:UNK:N	2.42	0.52
1:1:304:UNK:CB	2:2:71:UNK:HB1	2.39	0.52
4:F:2393:ASP:OD1	4:F:2397:ARG:NH1	2.42	0.52
3:E:320:UNK:HA	3:E:331:UNK:HA	1.92	0.52
1:3:1510:UNK:HG2	1:3:1712:UNK:HG1	1.90	0.52
4:B:2251:ARG:HA	4:B:2261:LEU:HD13	1.91	0.52
4:F:2298:ASP:HB2	4:F:2382:MET:SD	2.49	0.52
3:A:1347:UNK:HG3	3:A:1359:UNK:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:197:UNK:O	2:4:201:UNK:N	2.41	0.52
3:E:967:UNK:HB2	3:E:969:UNK:HG2	1.91	0.52
4:F:1938:VAL:HG13	4:F:1942:LEU:HG	1.90	0.52
4:F:1446:GLN:O	4:F:1449:TRP:HB2	2.09	0.52
1:1:1510:UNK:HG2	1:1:1712:UNK:HG1	1.90	0.52
4:F:2506:ASP:O	4:F:2511:ARG:N	2.37	0.52
4:B:1417:ILE:HG23	4:B:1432:VAL:HB	1.92	0.52
3:A:727:UNK:HG2	3:A:766:UNK:HG1	1.92	0.52
4:B:1621:GLU:O	4:B:1625:GLY:N	2.42	0.52
4:F:2036:ARG:HA	7:G:999:RAP:H521	1.92	0.52
4:F:1514:ARG:HA	4:F:1536:ILE:HD13	1.91	0.52
4:B:2298:ASP:HB2	4:B:2382:MET:SD	2.49	0.52
2:2:269:UNK:HG3	2:2:400:UNK:HA	1.91	0.52
1:1:446:UNK:HA	1:1:449:UNK:HB2	1.92	0.52
6:D:16:ALA:HB3	6:D:319:ALA:HB3	1.92	0.52
1:3:446:UNK:HA	1:3:449:UNK:HB2	1.91	0.52
4:B:1484:LEU:HA	4:B:1487:LEU:HB2	1.92	0.52
1:1:1700:UNK:HB1	1:1:1900:UNK:HB2	1.91	0.52
3:A:1383:UNK:HG3	3:A:1397:UNK:HA	1.92	0.52
4:B:1413:LEU:HD22	4:B:1436:ALA:HB2	1.92	0.52
2:4:82:UNK:HA	2:4:85:UNK:HB2	1.91	0.52
4:B:2346:LEU:HD23	4:B:2353:ILE:HG13	1.92	0.52
2:4:269:UNK:HG3	2:4:400:UNK:HA	1.92	0.52
4:B:1947:ASP:HB3	4:B:1987:ARG:HG2	1.91	0.52
1:3:422:UNK:C	1:3:424:UNK:H	2.22	0.52
6:D:132:ASN:HD21	6:D:148:GLN:HG2	1.74	0.52
3:E:247:UNK:HA	3:E:250:UNK:HB1	1.92	0.52
4:F:1632:ASP:O	4:F:1636:ILE:HD13	2.10	0.52
4:F:1413:LEU:HD22	4:F:1436:ALA:HB2	1.92	0.52
6:H:19:GLY:HA3	6:H:314:ALA:O	2.10	0.52
1:1:159:UNK:HB1	1:1:200:UNK:HB1	1.92	0.52
4:B:1632:ASP:O	4:B:1636:ILE:HD13	2.10	0.52
2:2:71:UNK:O	2:2:75:UNK:N	2.43	0.52
3:A:967:UNK:HB2	3:A:969:UNK:HG2	1.92	0.52
1:3:809:UNK:HG3	1:3:903:UNK:HG3	1.92	0.52
3:A:1592:UNK:HB1	3:A:1604:UNK:HA	1.92	0.52
4:F:1417:ILE:HG23	4:F:1432:VAL:HB	1.91	0.52
4:B:1446:GLN:O	4:B:1449:TRP:HB2	2.10	0.52
4:B:1918:ASP:OD1	4:B:1918:ASP:N	2.42	0.52
4:F:2264:GLU:O	4:F:2268:MET:HG3	2.10	0.51
4:B:2515:HIS:ND1	4:B:2516:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2282:GLN:HG3	6:D:274:TRP:CH2	2.45	0.51
4:F:1484:LEU:HA	4:F:1487:LEU:HB2	1.92	0.51
1:1:422:UNK:C	1:1:424:UNK:H	2.22	0.51
4:B:2024:HIS:CD2	4:B:2025:GLU:HG3	2.46	0.51
1:1:48:UNK:HA	1:1:51:UNK:HG3	1.90	0.51
6:H:195:TYR:CZ	6:H:215:LYS:HG3	2.45	0.51
7:G:999:RAP:H432	7:G:999:RAP:O4	2.09	0.51
6:D:40:HIS:CD2	6:D:66:ARG:HD2	2.45	0.51
3:E:1383:UNK:HG3	3:E:1397:UNK:HA	1.92	0.51
4:B:2412:ASP:N	4:B:2412:ASP:OD1	2.36	0.51
4:F:1918:ASP:N	4:F:1918:ASP:OD1	2.43	0.51
2:4:71:UNK:O	2:4:75:UNK:N	2.43	0.51
2:2:617:UNK:HA	4:B:1393:TYR:CE1	2.46	0.51
4:B:1749:ARG:HG2	4:B:1786:TRP:HH2	1.74	0.51
4:F:1749:ARG:HG2	4:F:1786:TRP:HH2	1.74	0.51
2:2:187:UNK:O	2:2:191:UNK:HG2	2.10	0.51
4:F:2267:ILE:HA	4:F:2270:ARG:HB3	1.92	0.51
4:F:2251:ARG:HA	4:F:2261:LEU:HD13	1.92	0.51
1:3:1700:UNK:HB1	1:3:1900:UNK:HB2	1.91	0.51
2:2:259:UNK:HA	2:2:262:UNK:HG3	1.92	0.51
1:3:1103:UNK:O	1:3:1107:UNK:HB2	2.10	0.51
3:A:1731:UNK:O	3:A:1732:UNK:HB2	2.11	0.51
4:F:2346:LEU:HD23	4:F:2353:ILE:HG13	1.92	0.51
4:B:1568:ARG:HG2	4:B:1596:LEU:HD13	1.91	0.51
2:4:617:UNK:HA	4:F:1393:TYR:CE1	2.45	0.51
3:E:405:UNK:HG1	3:E:413:UNK:HG1	1.92	0.51
1:1:1004:UNK:HG1	1:1:1104:UNK:HA	1.93	0.51
3:E:211:UNK:HB1	4:F:2118:LEU:HA	1.93	0.51
3:A:210:UNK:O	3:A:212:UNK:N	2.44	0.51
3:E:1592:UNK:HB1	3:E:1604:UNK:HA	1.92	0.51
3:E:217:UNK:O	3:E:221:UNK:HG2	2.10	0.51
3:A:217:UNK:O	3:A:221:UNK:HG2	2.10	0.51
4:F:2401:HIS:HA	4:F:2521:VAL:CG1	2.41	0.51
4:B:1581:GLU:HB3	4:B:1585:ARG:H	1.76	0.51
4:B:2267:ILE:HA	4:B:2270:ARG:HB3	1.92	0.51
4:F:2336:LEU:HG	4:F:2339:ARG:HD2	1.93	0.51
6:H:32:GLY:HA2	6:H:308:TYR:CD2	2.43	0.51
4:B:2506:ASP:O	4:B:2511:ARG:N	2.37	0.51
2:4:187:UNK:O	2:4:191:UNK:HG2	2.10	0.51
6:D:111:ILE:HD12	6:D:123:ARG:HD3	1.92	0.51
6:H:40:HIS:CD2	6:H:66:ARG:HD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:117:UNK:O	2:2:119:UNK:N	2.43	0.51
1:1:809:UNK:HG3	1:1:903:UNK:HG3	1.91	0.51
1:3:304:UNK:CB	2:4:71:UNK:HB1	2.40	0.51
3:E:1609:UNK:HG2	3:E:1632:UNK:HB1	1.92	0.51
3:E:1731:UNK:O	3:E:1732:UNK:HB2	2.11	0.51
3:A:247:UNK:HA	3:A:250:UNK:HB1	1.92	0.51
1:1:92:UNK:HA	1:1:94:UNK:HG2	1.93	0.51
4:B:2401:HIS:HA	4:B:2521:VAL:CG1	2.40	0.51
1:3:92:UNK:HA	1:3:94:UNK:HG2	1.93	0.51
1:3:416:UNK:C	1:3:418:UNK:H	2.17	0.51
6:H:16:ALA:HB3	6:H:319:ALA:HB3	1.91	0.51
2:2:126:UNK:HB1	2:2:169:UNK:HB2	1.93	0.51
1:1:435:UNK:HG1	1:1:447:UNK:HG1	1.93	0.51
4:F:2038:TYR:CE1	4:F:2044:VAL:HG22	2.46	0.51
4:B:2336:LEU:HG	4:B:2339:ARG:HD2	1.93	0.50
6:D:195:TYR:CZ	6:D:215:LYS:HG3	2.46	0.50
6:D:167:PRO:HG3	6:D:197:TRP:CZ2	2.46	0.50
4:B:2036:ARG:HA	7:C:999:RAP:H521	1.92	0.50
2:4:141:UNK:HG3	2:4:179:UNK:HG1	1.93	0.50
4:F:2282:GLN:HG3	6:H:274:TRP:CH2	2.46	0.50
1:1:1103:UNK:O	1:1:1107:UNK:HB2	2.11	0.50
1:1:327:UNK:O	1:1:330:UNK:HG2	2.11	0.50
4:F:2012:VAL:O	4:F:2016:LEU:HG	2.12	0.50
2:2:141:UNK:HG3	2:2:179:UNK:HG1	1.93	0.50
3:A:320:UNK:HA	3:A:331:UNK:HA	1.92	0.50
1:3:1004:UNK:HG1	1:3:1104:UNK:HA	1.93	0.50
4:F:1644:VAL:HG13	4:F:1648:GLU:CD	2.30	0.50
2:4:181:UNK:HA	2:4:184:UNK:HG2	1.93	0.50
3:E:894:UNK:HA	3:E:937:UNK:HG1	1.93	0.50
3:A:1609:UNK:HG2	3:A:1632:UNK:HB1	1.92	0.50
6:D:19:GLY:HA3	6:D:314:ALA:O	2.10	0.50
3:E:210:UNK:O	3:E:212:UNK:N	2.44	0.50
6:D:17:THR:HB	6:D:27:TRP:HE1	1.77	0.50
4:B:1688:PRO:HA	4:B:1716:HIS:CE1	2.47	0.50
1:3:327:UNK:O	1:3:330:UNK:HG2	2.11	0.50
2:4:180:UNK:O	2:4:183:UNK:N	2.44	0.50
4:B:2270:ARG:O	6:D:313:LYS:NZ	2.27	0.50
4:F:1907:LEU:HD13	4:F:1911:PHE:CZ	2.46	0.50
4:F:2024:HIS:CD2	4:F:2025:GLU:HG3	2.46	0.50
1:3:210:UNK:O	1:3:212:UNK:N	2.45	0.50
1:1:416:UNK:O	1:1:418:UNK:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:1805:UNK:HG1	1:3:2003:UNK:HG1	1.93	0.50
4:B:1557:PHE:HD1	4:B:1603:ILE:HG13	1.77	0.50
4:B:2139:ALA:HA	4:B:2152:ARG:HA	1.94	0.50
6:H:132:ASN:HD21	6:H:148:GLN:HG2	1.74	0.50
4:B:1973:ILE:HG21	4:B:2005:LEU:HD13	1.93	0.50
4:F:1631:GLU:OE2	4:F:1665:ARG:NH2	2.45	0.50
2:4:104:UNK:O	2:4:108:UNK:HB2	2.12	0.50
4:B:1907:LEU:HD13	4:B:1911:PHE:CZ	2.46	0.50
3:E:1509:UNK:O	3:E:1525:UNK:N	2.45	0.50
4:B:1571:LEU:HD21	4:B:1589:ALA:HB1	1.94	0.50
4:B:2038:TYR:CE1	4:B:2044:VAL:HG22	2.46	0.50
4:F:1688:PRO:HA	4:F:1716:HIS:CE1	2.47	0.50
4:F:1568:ARG:HG2	4:F:1596:LEU:HD13	1.92	0.50
4:F:1571:LEU:HD21	4:F:1589:ALA:HB1	1.94	0.50
4:F:1581:GLU:HB2	4:F:1585:ARG:HB2	1.94	0.50
2:2:180:UNK:O	2:2:183:UNK:N	2.44	0.50
4:F:1591:VAL:HG13	4:F:1636:ILE:HD11	1.93	0.50
2:2:549:UNK:O	2:2:552:UNK:HG3	2.12	0.50
6:H:111:ILE:HD12	6:H:123:ARG:HD3	1.92	0.50
4:B:1910:TRP:HZ2	4:B:1956:LEU:HB3	1.77	0.50
4:F:1973:ILE:HG21	4:F:2005:LEU:HD13	1.93	0.50
6:H:242:GLN:OE1	6:H:270:ARG:N	2.45	0.50
5:C:25:UNK:HA	5:C:39:UNK:HG1	1.93	0.50
1:3:159:UNK:HB1	1:3:200:UNK:HB1	1.93	0.50
3:A:405:UNK:HG1	3:A:413:UNK:HG1	1.92	0.49
2:2:183:UNK:HA	2:2:186:UNK:HB1	1.93	0.49
3:E:1509:UNK:HB1	3:E:1525:UNK:HB2	1.93	0.49
3:A:211:UNK:HB1	4:B:2118:LEU:HA	1.94	0.49
4:B:2012:VAL:O	4:B:2016:LEU:HG	2.12	0.49
4:F:1557:PHE:HD1	4:F:1603:ILE:HG13	1.77	0.49
1:3:304:UNK:HB2	2:4:71:UNK:HB1	1.95	0.49
4:B:2264:GLU:O	4:B:2268:MET:HG3	2.11	0.49
4:F:2290:ALA:O	4:F:2294:THR:OG1	2.19	0.49
4:B:1417:ILE:HG22	4:B:1429:ALA:HB1	1.94	0.49
5:G:77:UNK:HA	5:G:96:UNK:HG3	1.93	0.49
3:E:1512:UNK:HG1	3:E:1555:UNK:HG1	1.95	0.49
5:G:25:UNK:HA	5:G:39:UNK:HG1	1.93	0.49
4:F:2408:ARG:O	4:F:2411:LYS:HG2	2.13	0.49
2:4:160:UNK:HG1	2:4:197:UNK:HB2	1.93	0.49
6:D:293:LEU:HD12	6:D:295:ARG:NH2	2.27	0.49
3:A:1512:UNK:HG1	3:A:1555:UNK:HG1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:559:UNK:HB2	3:A:566:UNK:HB2	1.93	0.49
6:H:293:LEU:HD12	6:H:295:ARG:NH2	2.27	0.49
1:1:210:UNK:O	1:1:212:UNK:N	2.45	0.49
1:3:120:UNK:O	1:3:124:UNK:N	2.46	0.49
4:B:2279:THR:N	4:B:2282:GLN:OE1	2.40	0.49
4:F:1605:TYR:O	4:F:1612:ARG:NH1	2.46	0.49
3:A:827:UNK:HG1	3:A:875:UNK:HG1	1.95	0.49
2:2:104:UNK:O	2:2:108:UNK:HB2	2.12	0.49
3:E:559:UNK:HB2	3:E:566:UNK:HB2	1.93	0.49
5:G:24:UNK:HG3	5:G:103:UNK:HA	1.95	0.49
4:B:1702:LYS:HG3	4:B:1706:LYS:HE3	1.95	0.49
4:F:2515:HIS:ND1	4:F:2516:ASP:OD1	2.43	0.49
2:4:545:UNK:HG3	4:F:1395:LYS:HZ2	1.77	0.49
4:B:1445:ILE:HG13	4:B:1449:TRP:CZ3	2.47	0.49
3:A:1509:UNK:O	3:A:1525:UNK:N	2.45	0.49
3:E:765:UNK:HG2	3:E:766:UNK:HG2	1.95	0.49
4:B:2379:LEU:O	4:B:2384:THR:OG1	2.30	0.49
4:F:2139:ALA:HA	4:F:2152:ARG:HA	1.94	0.49
4:B:2512:ASP:N	4:B:2512:ASP:OD1	2.44	0.49
4:B:1619:TRP:HA	4:B:1622:ARG:NH1	2.22	0.49
4:B:2408:ARG:O	4:B:2411:LYS:HG2	2.12	0.49
4:F:2374:LYS:HB2	4:F:2537:ASN:HB3	1.95	0.49
4:F:2254:ARG:HG3	4:F:2261:LEU:HA	1.95	0.49
3:A:1509:UNK:HB1	3:A:1525:UNK:HB2	1.94	0.49
3:E:727:UNK:HG2	3:E:766:UNK:HG1	1.93	0.49
4:F:1702:LYS:HG3	4:F:1706:LYS:HE3	1.95	0.49
4:B:1725:GLN:O	4:B:1729:GLN:HG2	2.13	0.49
1:1:1610:UNK:HG1	1:1:1709:UNK:HB1	1.95	0.49
3:A:894:UNK:HA	3:A:937:UNK:HG1	1.94	0.49
4:B:1618:ILE:HA	4:B:1621:GLU:OE1	2.13	0.49
1:1:304:UNK:HB2	2:2:71:UNK:HB1	1.95	0.49
4:F:1910:TRP:HZ2	4:F:1956:LEU:HB3	1.77	0.49
6:H:17:THR:HB	6:H:27:TRP:HE1	1.77	0.49
4:B:2074:TYR:HE2	4:B:2110:ARG:HB3	1.78	0.49
2:2:80:UNK:O	2:2:83:UNK:HG2	2.13	0.49
4:F:1425:GLN:OE1	4:F:1426:PRO:HD2	2.13	0.49
2:4:243:UNK:O	2:4:246:UNK:HG3	2.13	0.49
4:B:2374:LYS:HB2	4:B:2537:ASN:HB3	1.95	0.49
2:4:181:UNK:O	2:4:184:UNK:HB2	2.13	0.49
3:A:882:UNK:HB1	3:A:885:UNK:HB1	1.95	0.49
6:D:54:ARG:HD2	6:D:323:SER:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:827:UNK:HG1	3:E:875:UNK:HG1	1.94	0.49
5:C:77:UNK:HA	5:C:96:UNK:HG3	1.93	0.49
1:3:1206:UNK:O	1:3:1210:UNK:HB1	2.13	0.49
3:E:842:UNK:HG2	3:E:843:UNK:HG2	1.95	0.49
2:4:545:UNK:O	2:4:548:UNK:HB2	2.13	0.49
2:4:67:UNK:O	2:4:70:UNK:HB2	2.13	0.49
4:B:1581:GLU:HB2	4:B:1585:ARG:HB2	1.95	0.49
4:F:1417:ILE:HG22	4:F:1429:ALA:HB1	1.95	0.49
6:D:242:GLN:OE1	6:D:270:ARG:N	2.46	0.49
2:2:181:UNK:HA	2:2:184:UNK:HG2	1.93	0.49
4:B:1591:VAL:HG13	4:B:1636:ILE:HD11	1.93	0.48
3:A:842:UNK:HG2	3:A:843:UNK:HG2	1.95	0.48
2:4:126:UNK:HB1	2:4:169:UNK:HB2	1.94	0.48
6:H:167:PRO:HG3	6:H:197:TRP:CZ2	2.45	0.48
1:3:1103:UNK:HA	1:3:1304:UNK:HG1	1.95	0.48
2:4:232:UNK:C	2:4:234:UNK:N	2.76	0.48
4:B:2133:CYS:SG	4:B:2136:LEU:HD11	2.53	0.48
3:A:639:UNK:O	3:A:642:UNK:HB2	2.13	0.48
1:1:1113:UNK:HG1	1:1:1311:UNK:HB1	1.95	0.48
4:B:1605:TYR:O	4:B:1612:ARG:NH1	2.46	0.48
2:4:45:UNK:O	2:4:49:UNK:HG2	2.13	0.48
4:B:1631:GLU:OE2	4:B:1665:ARG:NH2	2.46	0.48
4:F:2332:TYR:CZ	4:F:2507:LYS:HE2	2.49	0.48
2:2:45:UNK:O	2:2:49:UNK:HG2	2.13	0.48
4:F:1482:ARG:HA	4:F:1485:GLU:HG2	1.94	0.48
5:C:24:UNK:HG3	5:C:103:UNK:HA	1.94	0.48
3:E:882:UNK:HB1	3:E:885:UNK:HB1	1.94	0.48
4:B:1603:ILE:O	4:B:1607:LEU:HB2	2.14	0.48
4:F:2047:MET:O	4:F:2051:LEU:HB2	2.13	0.48
1:3:1610:UNK:HG1	1:3:1709:UNK:HB1	1.94	0.48
2:4:165:UNK:O	2:4:168:UNK:HB2	2.13	0.48
1:1:1018:UNK:O	1:1:1022:UNK:HB2	2.13	0.48
3:A:916:UNK:HB1	3:A:931:UNK:HG2	1.96	0.48
4:B:2047:MET:O	4:B:2051:LEU:HB2	2.13	0.48
2:4:310:UNK:HB2	2:4:404:UNK:HB2	1.95	0.48
1:3:103:UNK:HA	1:3:106:UNK:HB1	1.95	0.48
2:2:160:UNK:HG1	2:2:197:UNK:HB2	1.94	0.48
4:F:2344:LEU:HD13	4:F:2353:ILE:HD11	1.96	0.48
4:F:1725:GLN:O	4:F:1729:GLN:HG2	2.13	0.48
2:2:232:UNK:C	2:2:234:UNK:N	2.76	0.48
1:1:1805:UNK:HG1	1:1:2003:UNK:HG1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:120:UNK:O	1:1:124:UNK:N	2.46	0.48
4:B:2322:ARG:O	4:B:2326:VAL:HG23	2.13	0.48
4:B:2547:PRO:HD2	4:B:2548:PHE:CE2	2.49	0.48
2:4:80:UNK:O	2:4:83:UNK:HG2	2.14	0.48
4:B:2344:LEU:HD13	4:B:2353:ILE:HD11	1.96	0.48
5:G:22:UNK:HB2	5:G:50:UNK:HG2	1.95	0.48
2:4:556:UNK:C	4:F:2257:LYS:HE2	2.44	0.48
3:A:109:UNK:HB2	3:A:111:UNK:HG2	1.95	0.48
4:B:2415:MET:O	4:B:2419:GLU:HG3	2.14	0.48
3:A:841:UNK:O	3:A:843:UNK:N	2.46	0.48
4:F:2547:PRO:HD2	4:F:2548:PHE:CE2	2.49	0.48
6:D:20:TYR:HB2	6:D:313:LYS:HB3	1.96	0.48
1:1:206:UNK:O	1:1:209:UNK:HG3	2.13	0.48
4:B:2060:ARG:NH2	4:B:2061:GLY:O	2.31	0.48
4:F:1529:MET:O	4:F:1533:THR:OG1	2.16	0.48
4:B:1778:ALA:HA	4:B:1781:GLU:HG2	1.96	0.48
3:E:916:UNK:HB1	3:E:931:UNK:HG2	1.96	0.48
4:F:2133:CYS:SG	4:F:2136:LEU:HD11	2.53	0.48
4:F:2415:MET:O	4:F:2419:GLU:HG3	2.14	0.48
4:F:1603:ILE:O	4:F:1607:LEU:HB2	2.13	0.48
4:F:1618:ILE:HA	4:F:1621:GLU:OE1	2.13	0.48
2:4:549:UNK:O	2:4:552:UNK:HG3	2.14	0.48
2:4:174:UNK:HG1	2:4:211:UNK:HG2	1.95	0.48
4:F:1414:GLU:HA	4:F:1417:ILE:HD11	1.96	0.48
3:E:808:UNK:O	3:E:812:UNK:N	2.47	0.48
1:1:1206:UNK:O	1:1:1210:UNK:HB1	2.13	0.48
1:3:425:UNK:O	1:3:429:UNK:N	2.47	0.48
5:C:22:UNK:HB2	5:C:50:UNK:HG2	1.96	0.48
1:1:2113:UNK:HA	1:1:2116:UNK:HG3	1.96	0.48
1:3:44:UNK:O	1:3:47:UNK:HB1	2.14	0.48
2:2:67:UNK:O	2:2:70:UNK:HB2	2.14	0.48
4:F:2172:LEU:HB3	4:F:2184:PHE:O	2.13	0.48
4:F:2256:LYS:HZ2	4:F:2257:LYS:HE3	1.77	0.48
3:A:590:UNK:HA	3:A:593:UNK:HB1	1.96	0.48
3:E:841:UNK:O	3:E:843:UNK:N	2.46	0.48
4:F:2222:ILE:HD11	4:F:2330:VAL:HG21	1.96	0.48
2:2:243:UNK:O	2:2:246:UNK:HG3	2.14	0.48
1:1:103:UNK:HA	1:1:106:UNK:HB1	1.95	0.48
4:B:2172:LEU:HB3	4:B:2184:PHE:O	2.13	0.48
1:1:1103:UNK:HA	1:1:1304:UNK:HG1	1.96	0.48
1:3:206:UNK:O	1:3:209:UNK:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:269:SER:O	6:D:271:GLY:N	2.47	0.48
1:3:1:UNK:HG2	4:B:1594:HIS:CG	2.48	0.47
4:F:2322:ARG:O	4:F:2326:VAL:HG23	2.13	0.47
4:F:2074:TYR:HE2	4:F:2110:ARG:HB3	1.77	0.47
4:B:2031:LEU:HD23	4:B:2051:LEU:HD11	1.96	0.47
4:B:1797:ASN:HB3	4:B:1884:ALA:HB2	1.95	0.47
3:E:109:UNK:HB2	3:E:111:UNK:HG2	1.95	0.47
4:B:1482:ARG:HA	4:B:1485:GLU:HG2	1.94	0.47
1:1:425:UNK:O	1:1:429:UNK:N	2.47	0.47
1:1:1:UNK:HG2	4:F:1594:HIS:CG	2.49	0.47
4:B:2332:TYR:CZ	4:B:2507:LYS:HE2	2.49	0.47
2:2:407:UNK:HG3	2:2:408:UNK:HB2	1.95	0.47
3:A:604:UNK:HA	3:A:607:UNK:HB2	1.96	0.47
2:2:165:UNK:O	2:2:168:UNK:HB2	2.13	0.47
1:3:135:UNK:HB2	1:3:139:UNK:HG1	1.95	0.47
2:2:181:UNK:O	2:2:184:UNK:HB2	2.13	0.47
4:F:2536:GLU:O	4:F:2540:GLN:NE2	2.47	0.47
6:H:54:ARG:HD2	6:H:323:SER:HB2	1.95	0.47
2:4:24:UNK:O	2:4:28:UNK:HB2	2.14	0.47
3:A:808:UNK:O	3:A:812:UNK:N	2.47	0.47
1:3:1113:UNK:HG1	1:3:1311:UNK:HB1	1.95	0.47
4:F:1778:ALA:HA	4:F:1781:GLU:HG2	1.96	0.47
3:A:581:UNK:O	3:A:585:UNK:HB2	2.14	0.47
2:4:407:UNK:HG3	2:4:408:UNK:HB2	1.97	0.47
4:B:2254:ARG:HG3	4:B:2261:LEU:HA	1.95	0.47
2:2:24:UNK:O	2:2:28:UNK:HB2	2.14	0.47
4:B:2521:VAL:HB	4:B:2522:PRO:HD3	1.96	0.47
4:B:2222:ILE:HD11	4:B:2330:VAL:HG21	1.96	0.47
2:2:556:UNK:C	4:B:2257:LYS:HE2	2.45	0.47
6:H:262:SER:HA	6:H:270:ARG:NH1	2.30	0.47
1:3:2011:UNK:HG3	1:3:2106:UNK:HG2	1.97	0.47
1:3:1018:UNK:O	1:3:1022:UNK:HB2	2.14	0.47
6:D:94:HIS:CD2	6:D:140:GLN:HE21	2.33	0.47
2:2:545:UNK:HG3	4:B:1395:LYS:HZ2	1.78	0.47
4:B:2172:LEU:HD23	4:B:2184:PHE:HB2	1.95	0.47
6:H:269:SER:O	6:H:271:GLY:N	2.47	0.47
3:A:1330:UNK:HB1	3:A:1708:UNK:HG2	1.97	0.47
4:B:1794:ALA:HB1	4:B:1888:PHE:CD2	2.50	0.47
4:F:2140:VAL:HB	4:F:2143:THR:HG21	1.95	0.47
2:4:110:UNK:O	2:4:114:UNK:HG2	2.15	0.47
4:F:1797:ASN:HB3	4:F:1884:ALA:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:1:UNK:H	1:3:5:UNK:HB2	1.80	0.47
4:F:2162:VAL:HA	4:F:2170:ARG:HA	1.97	0.47
3:E:639:UNK:O	3:E:642:UNK:HB2	2.13	0.47
2:2:545:UNK:O	2:2:548:UNK:HB2	2.13	0.47
1:1:135:UNK:HB2	1:1:139:UNK:HG1	1.95	0.47
4:F:1521:TRP:HZ2	4:F:1642:LEU:HG	1.80	0.47
2:2:310:UNK:HB2	2:2:404:UNK:HB2	1.95	0.47
4:F:2172:LEU:HD23	4:F:2184:PHE:HB2	1.95	0.47
2:4:533:UNK:O	2:4:537:UNK:HB2	2.15	0.47
4:B:2140:VAL:HB	4:B:2143:THR:HG21	1.96	0.47
4:F:2376:PRO:HD3	4:F:2531:GLN:NE2	2.30	0.47
4:F:1651:ARG:HA	4:F:1654:LEU:HD12	1.97	0.47
4:F:2521:VAL:HB	4:F:2522:PRO:HD3	1.96	0.47
5:G:27:UNK:HB1	5:G:38:UNK:HG2	1.97	0.47
6:H:94:HIS:CD2	6:H:140:GLN:HE21	2.33	0.47
4:B:2162:VAL:HA	4:B:2170:ARG:HA	1.96	0.47
4:B:2520:ASP:OD2	4:B:2522:PRO:HD2	2.15	0.47
4:F:2031:LEU:HD23	4:F:2051:LEU:HD11	1.95	0.47
6:D:262:SER:HA	6:D:270:ARG:NH1	2.30	0.47
4:B:1906:VAL:HG11	4:B:1935:TRP:HH2	1.80	0.47
4:F:2428:ASN:HB3	4:F:2493:LEU:HD13	1.97	0.47
1:1:2011:UNK:HG3	1:1:2106:UNK:HG2	1.97	0.47
1:1:44:UNK:O	1:1:47:UNK:HB1	2.14	0.47
4:F:1619:TRP:HA	4:F:1622:ARG:NH1	2.21	0.47
4:F:2520:ASP:OD2	4:F:2522:PRO:HD2	2.15	0.47
1:3:141:UNK:C	1:3:143:UNK:HG2	2.45	0.47
2:2:174:UNK:HG1	2:2:211:UNK:HG2	1.95	0.47
2:4:308:UNK:O	2:4:310:UNK:N	2.48	0.47
1:3:1507:UNK:HA	1:3:1510:UNK:HB1	1.97	0.47
4:B:2379:LEU:HA	4:B:2379:LEU:HD13	1.70	0.47
3:A:1508:UNK:HB2	3:A:1552:UNK:HB2	1.96	0.47
1:3:24:UNK:HA	1:3:27:UNK:HG2	1.97	0.47
4:F:2379:LEU:O	4:F:2384:THR:OG1	2.31	0.47
3:E:567:UNK:O	3:E:569:UNK:N	2.48	0.47
4:B:2536:GLU:O	4:B:2540:GLN:NE2	2.47	0.47
3:A:1715:UNK:HG3	3:A:1726:UNK:HG3	1.97	0.47
4:F:1794:ALA:HB1	4:F:1888:PHE:CD2	2.50	0.47
3:E:1605:UNK:HB2	3:E:1635:UNK:HG1	1.96	0.47
1:1:141:UNK:C	1:1:143:UNK:HG2	2.45	0.46
4:B:1899:ASN:HB2	4:B:1903:THR:OG1	2.15	0.46
6:H:20:TYR:HB2	6:H:313:LYS:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1414:GLU:HA	4:B:1417:ILE:HD11	1.97	0.46
3:A:765:UNK:HG2	3:A:766:UNK:HG2	1.96	0.46
2:4:142:UNK:HG3	2:4:143:UNK:HG2	1.98	0.46
6:H:222:TYR:O	6:H:239:SER:OG	2.27	0.46
1:1:2001:UNK:HG3	1:1:2200:UNK:HG3	1.98	0.46
4:F:1906:VAL:HG11	4:F:1935:TRP:HH2	1.80	0.46
3:E:604:UNK:HA	3:E:607:UNK:HB2	1.97	0.46
4:B:1425:GLN:OE1	4:B:1426:PRO:HD2	2.13	0.46
1:3:88:UNK:HA	1:3:91:UNK:CB	2.46	0.46
6:H:132:ASN:H	6:H:147:ASP:HA	1.81	0.46
6:H:297:TRP:CZ3	6:H:304:ILE:HG12	2.50	0.46
3:E:1508:UNK:HB2	3:E:1552:UNK:HB2	1.96	0.46
3:E:1104:UNK:O	3:E:1108:UNK:HB2	2.15	0.46
3:E:590:UNK:HA	3:E:593:UNK:HB1	1.96	0.46
3:A:567:UNK:O	3:A:569:UNK:N	2.48	0.46
1:1:24:UNK:HA	1:1:27:UNK:HG2	1.96	0.46
1:3:1407:UNK:HG2	1:3:1509:UNK:HG2	1.97	0.46
5:C:27:UNK:HB1	5:C:38:UNK:HG2	1.98	0.46
4:B:1605:TYR:CZ	4:B:1612:ARG:HD2	2.51	0.46
1:3:2001:UNK:HG3	1:3:2200:UNK:HG3	1.97	0.46
6:D:65:ILE:HG13	6:D:88:ILE:HD13	1.98	0.46
3:E:1330:UNK:HB1	3:E:1708:UNK:HG2	1.97	0.46
3:E:1328:UNK:HB2	3:E:1706:UNK:HG1	1.97	0.46
4:B:1651:ARG:HA	4:B:1654:LEU:HD12	1.98	0.46
1:3:7:UNK:HA	1:3:10:UNK:HB2	1.97	0.46
2:4:158:UNK:HG3	2:4:162:UNK:HB1	1.96	0.46
1:3:435:UNK:HG1	1:3:447:UNK:HG1	1.98	0.46
6:D:198:ASN:ND2	6:D:213:LYS:HB2	2.31	0.46
1:1:42:UNK:HB2	4:F:1611:ARG:NH1	2.30	0.46
6:D:88:ILE:HA	6:D:104:GLY:HA2	1.97	0.46
3:A:1104:UNK:O	3:A:1108:UNK:HB2	2.15	0.46
3:A:840:UNK:O	3:A:842:UNK:HG3	2.16	0.46
3:E:840:UNK:O	3:E:842:UNK:HG3	2.16	0.46
1:1:88:UNK:HA	1:1:91:UNK:CB	2.45	0.46
1:3:440:UNK:HB1	1:3:443:UNK:HB2	1.98	0.46
1:3:42:UNK:HB2	4:B:1611:ARG:NH1	2.30	0.46
4:F:1665:ARG:HH11	4:F:1668:LEU:HD22	1.81	0.46
1:3:612:UNK:O	1:3:615:UNK:HB1	2.15	0.46
6:H:228:PHE:CE1	6:H:235:LEU:HB2	2.51	0.46
6:D:297:TRP:CZ3	6:D:304:ILE:HG12	2.50	0.46
2:2:533:UNK:O	2:2:537:UNK:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:151:UNK:O	1:1:155:UNK:HG3	2.15	0.46
4:F:1575:LEU:HD23	4:F:1575:LEU:HA	1.77	0.46
2:4:86:UNK:O	2:4:90:UNK:HG2	2.15	0.46
2:2:86:UNK:O	2:2:90:UNK:HG2	2.15	0.46
4:F:1899:ASN:HB2	4:F:1903:THR:OG1	2.15	0.46
1:3:2113:UNK:HA	1:3:2116:UNK:HG3	1.96	0.46
1:3:142:UNK:O	1:3:145:UNK:N	2.49	0.46
1:1:82:UNK:O	1:1:85:UNK:HB2	2.16	0.46
1:3:82:UNK:O	1:3:85:UNK:HB2	2.16	0.46
1:3:151:UNK:O	1:3:155:UNK:HG3	2.16	0.46
4:B:1521:TRP:HZ2	4:B:1642:LEU:HG	1.80	0.46
4:B:2254:ARG:NH1	4:B:2298:ASP:OD2	2.49	0.46
6:D:132:ASN:H	6:D:147:ASP:HA	1.81	0.46
3:A:1328:UNK:HB2	3:A:1706:UNK:HG1	1.97	0.46
3:E:854:UNK:HG3	3:E:861:UNK:HG3	1.98	0.46
6:H:88:ILE:HA	6:H:104:GLY:HA2	1.97	0.46
4:B:2428:ASN:HB3	4:B:2493:LEU:HD13	1.97	0.46
1:1:7:UNK:HA	1:1:10:UNK:HB2	1.97	0.46
1:1:320:UNK:O	1:1:323:UNK:N	2.49	0.46
4:F:2285:GLU:HB2	6:H:272:TRP:CH2	2.51	0.46
3:A:1605:UNK:HB2	3:A:1635:UNK:HG1	1.96	0.46
1:3:1007:UNK:O	1:3:1011:UNK:HB2	2.16	0.46
3:E:576:UNK:O	3:E:579:UNK:HG2	2.16	0.46
4:B:2376:PRO:HD3	4:B:2531:GLN:NE2	2.31	0.46
1:1:612:UNK:O	1:1:615:UNK:HB1	2.15	0.46
1:3:210:UNK:C	1:3:212:UNK:N	2.79	0.46
1:1:210:UNK:C	1:1:212:UNK:N	2.79	0.46
1:3:1212:UNK:O	1:3:1216:UNK:HB2	2.16	0.46
4:F:2254:ARG:NH1	4:F:2298:ASP:OD2	2.49	0.46
3:E:1715:UNK:HG3	3:E:1726:UNK:HG3	1.97	0.46
1:3:448:UNK:HA	1:3:451:UNK:HB1	1.98	0.46
3:E:1641:UNK:O	3:E:1643:UNK:N	2.49	0.46
2:4:532:UNK:O	2:4:535:UNK:HB2	2.16	0.46
2:2:142:UNK:HG3	2:2:143:UNK:HG2	1.97	0.46
2:2:158:UNK:HG3	2:2:162:UNK:HB1	1.98	0.45
6:H:198:ASN:ND2	6:H:213:LYS:HB2	2.31	0.45
2:2:308:UNK:O	2:2:310:UNK:N	2.48	0.45
3:A:1136:UNK:HG3	3:A:1144:UNK:HG2	1.98	0.45
2:2:110:UNK:O	2:2:114:UNK:HG2	2.16	0.45
3:A:1332:UNK:HB2	3:A:1378:UNK:HB1	1.98	0.45
1:1:448:UNK:HA	1:1:451:UNK:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:2530:LYS:HE3	4:F:2530:LYS:HA	1.98	0.45
1:1:1212:UNK:O	1:1:1216:UNK:HB2	2.16	0.45
4:B:2039:PHE:HB3	7:C:999:RAP:H382	1.98	0.45
1:1:1407:UNK:HG2	1:1:1509:UNK:HG2	1.97	0.45
1:3:2109:UNK:O	1:3:2113:UNK:HB1	2.16	0.45
3:A:719:UNK:O	3:A:723:UNK:HB1	2.16	0.45
4:F:2147:ASN:O	4:F:2148:GLN:NE2	2.32	0.45
3:E:204:UNK:HA	3:E:526:UNK:HG2	1.99	0.45
1:1:9:UNK:O	1:1:12:UNK:HG3	2.17	0.45
4:B:2162:VAL:HG22	4:B:2170:ARG:HG3	1.98	0.45
1:3:118:UNK:C	1:3:120:UNK:N	2.79	0.45
3:E:719:UNK:O	3:E:723:UNK:HB1	2.16	0.45
4:B:2530:LYS:HE3	4:B:2530:LYS:HA	1.98	0.45
4:B:1896:ARG:NH2	4:B:1931:GLN:HG3	2.31	0.45
1:1:450:UNK:HA	1:1:453:UNK:HG3	1.99	0.45
4:B:2285:GLU:HB2	6:D:272:TRP:CH2	2.51	0.45
1:3:211:UNK:HB1	1:3:302:UNK:HB1	1.99	0.45
3:E:988:UNK:HB1	3:E:1102:UNK:HG1	1.99	0.45
4:B:2278:LEU:HB3	4:B:2282:GLN:HB2	1.97	0.45
4:F:2278:LEU:HB3	4:F:2282:GLN:HB2	1.98	0.45
4:F:2279:THR:N	4:F:2282:GLN:OE1	2.40	0.45
6:H:65:ILE:HG13	6:H:88:ILE:HD13	1.97	0.45
3:E:714:UNK:HG1	3:E:738:UNK:HG1	1.99	0.45
3:A:714:UNK:HG1	3:A:738:UNK:HG1	1.98	0.45
3:A:1641:UNK:O	3:A:1643:UNK:N	2.50	0.45
2:2:532:UNK:O	2:2:535:UNK:HB2	2.16	0.45
3:E:232:UNK:HB2	3:E:601:UNK:HG2	1.98	0.45
4:F:1433:LEU:HD12	4:F:1433:LEU:HA	1.66	0.45
1:1:1:UNK:H	1:1:5:UNK:HB2	1.81	0.45
1:3:154:UNK:HG3	3:E:643:UNK:CB	2.41	0.45
4:F:2378:ARG:NH2	4:F:2545:TRP:O	2.50	0.45
4:B:2519:LEU:HB3	4:B:2524:GLN:HB2	1.99	0.45
2:4:167:UNK:O	2:4:171:UNK:HG2	2.17	0.45
1:1:36:UNK:HG3	1:1:37:UNK:HG2	1.99	0.45
6:D:289:SER:HB2	6:D:291:ASP:OD1	2.16	0.45
1:1:2004:UNK:HG1	1:1:2200:UNK:HG1	1.99	0.45
3:A:232:UNK:HB2	3:A:601:UNK:HG2	1.97	0.45
4:B:1501:TRP:O	4:B:1504:VAL:HG22	2.17	0.45
1:1:66:UNK:O	1:1:70:UNK:N	2.50	0.45
1:1:70:UNK:O	1:1:74:UNK:HB2	2.17	0.45
1:1:118:UNK:C	1:1:120:UNK:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:552:UNK:CG	4:B:2304:TRP:HZ2	2.26	0.45
1:1:1507:UNK:HA	1:1:1510:UNK:HB1	1.97	0.45
5:C:26:UNK:O	5:C:39:UNK:N	2.50	0.45
2:4:6:UNK:O	2:4:9:UNK:HB2	2.17	0.45
4:B:1478:LEU:HD11	4:B:1508:THR:HG23	1.98	0.45
4:F:1478:LEU:HD11	4:F:1508:THR:HG23	1.99	0.45
1:1:142:UNK:O	1:1:145:UNK:N	2.50	0.45
4:F:2017:ILE:HD13	4:F:2231:SER:HB3	1.99	0.45
3:A:854:UNK:HG3	3:A:861:UNK:HG3	1.98	0.45
3:A:748:UNK:O	3:A:752:UNK:HG2	2.17	0.45
3:A:204:UNK:HA	3:A:526:UNK:HG2	1.98	0.45
4:F:2512:ASP:OD1	4:F:2512:ASP:N	2.44	0.45
3:A:639:UNK:O	3:A:643:UNK:HG3	2.17	0.45
4:B:1427:GLU:O	4:B:1430:ALA:HB3	2.17	0.45
2:4:197:UNK:C	2:4:201:UNK:HG3	2.46	0.45
4:F:1416:LEU:HD23	4:F:1432:VAL:HG13	1.98	0.45
4:B:1665:ARG:HH11	4:B:1668:LEU:HD22	1.81	0.45
3:A:225:UNK:HG3	3:A:237:UNK:HB2	1.98	0.45
3:A:503:UNK:O	3:A:626:UNK:HB2	2.17	0.45
3:E:1332:UNK:HB2	3:E:1378:UNK:HB1	1.98	0.45
2:2:302:UNK:O	2:2:306:UNK:HG2	2.17	0.45
4:B:1435:TYR:CG	4:B:2390:THR:HG21	2.51	0.45
1:1:123:UNK:O	1:1:126:UNK:HB2	2.17	0.45
4:F:2317:ARG:O	4:F:2321:THR:OG1	2.34	0.45
2:2:197:UNK:C	2:2:201:UNK:HG3	2.46	0.45
1:3:450:UNK:HA	1:3:453:UNK:HG3	1.99	0.45
4:F:1501:TRP:O	4:F:1504:VAL:HG22	2.17	0.45
3:A:805:UNK:HG3	3:A:807:UNK:HB1	1.99	0.45
4:B:1433:LEU:HA	4:B:1433:LEU:HD12	1.65	0.45
6:D:228:PHE:CE1	6:D:235:LEU:HB2	2.52	0.45
4:B:1904:LEU:HD13	4:B:2417:VAL:HA	1.99	0.45
6:H:188:VAL:HB	6:H:226:CYS:SG	2.57	0.45
1:1:706:UNK:O	1:1:710:UNK:HB1	2.17	0.45
1:3:123:UNK:O	1:3:126:UNK:HB2	2.16	0.45
1:3:36:UNK:HG3	1:3:37:UNK:HG2	1.99	0.45
4:F:1605:TYR:CZ	4:F:1612:ARG:HD2	2.51	0.45
4:F:1605:TYR:HD2	4:F:1615:ILE:HD12	1.82	0.45
3:A:735:UNK:O	3:A:738:UNK:HB1	2.16	0.45
4:F:2541:CYS:SG	4:F:2542:TYR:N	2.89	0.45
4:F:1422:LYS:HE3	4:F:1422:LYS:HB2	1.68	0.45
4:B:1890:ARG:HB2	4:B:1890:ARG:HE	1.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2411:LYS:HB2	4:B:2411:LYS:HE3	1.70	0.44
4:B:1605:TYR:HD2	4:B:1615:ILE:HD12	1.82	0.44
4:F:1777:SER:O	4:F:1781:GLU:HG2	2.17	0.44
3:E:561:UNK:HA	3:E:569:UNK:HG3	1.99	0.44
3:E:735:UNK:O	3:E:738:UNK:HB1	2.17	0.44
1:3:706:UNK:O	1:3:710:UNK:HB1	2.17	0.44
6:D:28:GLN:HE21	6:D:33:ILE:HB	1.82	0.44
6:D:188:VAL:HB	6:D:226:CYS:SG	2.57	0.44
2:4:78:UNK:HB1	3:E:634:UNK:HA	1.99	0.44
1:3:48:UNK:HA	1:3:51:UNK:CG	2.47	0.44
1:1:319:UNK:O	1:1:324:UNK:HB2	2.18	0.44
4:F:2397:ARG:HB2	4:F:2397:ARG:HH11	1.82	0.44
3:E:410:UNK:HG3	3:E:413:UNK:HB1	1.98	0.44
4:B:2545:TRP:HZ3	4:B:2547:PRO:HA	1.83	0.44
4:F:2039:PHE:HB3	7:G:999:RAP:H382	1.98	0.44
3:A:1604:UNK:HG2	3:A:1612:UNK:HG2	1.99	0.44
2:2:6:UNK:O	2:2:9:UNK:HB2	2.17	0.44
3:E:805:UNK:HG3	3:E:807:UNK:HB1	1.99	0.44
1:3:713:UNK:HG1	1:3:909:UNK:HB1	1.99	0.44
4:B:2045:LYS:NZ	4:B:2049:GLU:OE2	2.43	0.44
1:3:70:UNK:O	1:3:74:UNK:HB2	2.17	0.44
3:E:225:UNK:HG3	3:E:237:UNK:HB2	1.99	0.44
3:A:576:UNK:O	3:A:579:UNK:HG2	2.17	0.44
4:F:1568:ARG:NH2	4:F:1600:GLU:OE2	2.51	0.44
4:B:2397:ARG:HA	4:B:2400:CYS:SG	2.58	0.44
4:B:2541:CYS:SG	4:B:2542:TYR:N	2.90	0.44
2:2:167:UNK:O	2:2:171:UNK:HG2	2.17	0.44
4:F:2051:LEU:HA	4:F:2051:LEU:HD12	1.79	0.44
3:E:1604:UNK:HG2	3:E:1612:UNK:HG2	2.00	0.44
1:1:1007:UNK:O	1:1:1011:UNK:HB2	2.16	0.44
4:B:2513:PHE:HE2	4:B:2528:LEU:HG	1.82	0.44
1:1:211:UNK:HB1	1:1:302:UNK:HB1	1.99	0.44
4:F:1743:LEU:O	4:F:1747:MET:HG3	2.18	0.44
4:F:2513:PHE:HE2	4:F:2528:LEU:HG	1.82	0.44
4:B:1743:LEU:O	4:B:1747:MET:HG3	2.18	0.44
6:H:289:SER:HB2	6:H:291:ASP:OD1	2.16	0.44
3:A:410:UNK:HG3	3:A:413:UNK:HB1	1.98	0.44
4:F:1421:ASN:HD21	4:F:1452:LYS:HB3	1.83	0.44
1:3:2303:UNK:O	1:3:2307:UNK:HB2	2.18	0.44
6:H:28:GLN:HE21	6:H:33:ILE:HB	1.82	0.44
3:E:1136:UNK:HG3	3:E:1144:UNK:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1453:LEU:HA	4:F:1453:LEU:HD22	1.81	0.44
1:3:320:UNK:O	1:3:323:UNK:N	2.51	0.44
4:B:2404:MET:HB3	4:B:2521:VAL:HG13	2.00	0.44
4:F:2404:MET:HB3	4:F:2521:VAL:HG13	2.00	0.44
1:3:66:UNK:O	1:3:70:UNK:N	2.50	0.44
3:E:745:UNK:HG2	3:E:747:UNK:N	2.32	0.44
4:B:1530:GLU:HA	4:B:1550:LEU:HD11	2.00	0.44
4:B:1474:PRO:HA	4:B:1477:MET:HE2	1.99	0.44
4:F:2543:ILE:HA	4:F:2543:ILE:HD12	1.76	0.44
4:F:1515:MET:H	4:F:1515:MET:HG3	1.60	0.44
1:3:52:UNK:HG1	1:3:90:UNK:HB2	2.00	0.44
3:E:639:UNK:O	3:E:643:UNK:HG3	2.18	0.44
3:E:643:UNK:O	3:E:646:UNK:HB1	2.18	0.44
1:1:1216:UNK:HB1	1:1:1305:UNK:HG1	2.00	0.44
4:B:2317:ARG:O	4:B:2321:THR:OG1	2.35	0.44
1:1:2109:UNK:O	1:1:2113:UNK:HB1	2.17	0.44
2:4:151:UNK:O	2:4:152:UNK:C	2.65	0.44
4:B:1407:GLY:HA2	4:B:1408:PRO:HD3	1.81	0.44
1:3:32:UNK:O	1:3:34:UNK:N	2.51	0.44
4:B:1560:ALA:O	4:B:1564:ILE:HG13	2.18	0.44
4:F:1896:ARG:NH2	4:F:1931:GLN:HG3	2.31	0.44
4:F:2519:LEU:HB3	4:F:2524:GLN:HB2	1.99	0.44
3:A:1638:UNK:HG2	3:A:1707:UNK:HB1	2.00	0.44
4:B:1422:LYS:HE3	4:B:1422:LYS:HB2	1.67	0.44
1:3:8:UNK:O	1:3:12:UNK:HB1	2.18	0.44
1:3:1306:UNK:O	1:3:1310:UNK:HG2	2.18	0.44
4:F:2545:TRP:HZ3	4:F:2547:PRO:HA	1.83	0.44
4:F:1427:GLU:O	4:F:1430:ALA:HB3	2.17	0.44
2:4:9:UNK:O	2:4:13:UNK:HB2	2.18	0.44
1:1:706:UNK:HB1	1:1:902:UNK:HB1	2.00	0.44
1:3:32:UNK:O	1:3:33:UNK:C	2.66	0.44
2:4:514:UNK:O	2:4:518:UNK:HB1	2.17	0.44
4:F:1904:LEU:HD13	4:F:2417:VAL:HA	1.99	0.44
4:B:1972:LEU:HB3	4:B:1976:LEU:HD12	2.00	0.44
2:2:514:UNK:O	2:2:518:UNK:HB1	2.17	0.44
4:B:2543:ILE:HA	4:B:2543:ILE:HD12	1.77	0.44
1:3:4:UNK:O	1:3:7:UNK:HB1	2.17	0.44
4:F:2397:ARG:HG2	4:F:2401:HIS:NE2	2.33	0.44
1:1:1306:UNK:O	1:1:1310:UNK:HG2	2.18	0.44
1:3:436:UNK:HA	1:3:444:UNK:HB2	2.00	0.44
2:2:26:UNK:O	2:2:30:UNK:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:503:UNK:O	3:E:626:UNK:HB2	2.18	0.44
3:E:1362:UNK:HB1	3:E:1364:UNK:HG2	1.99	0.44
3:E:748:UNK:O	3:E:752:UNK:HG2	2.17	0.44
3:A:1362:UNK:HB1	3:A:1364:UNK:HG2	2.00	0.44
1:1:48:UNK:HA	1:1:51:UNK:CG	2.47	0.43
3:A:1538:UNK:HB1	3:A:1540:UNK:HG3	2.00	0.43
5:C:4:UNK:HG2	5:C:62:UNK:HG3	2.00	0.43
6:D:271:GLY:HA3	6:D:290:SER:HB2	2.00	0.43
4:F:1530:GLU:HA	4:F:1550:LEU:HD11	2.00	0.43
1:3:2004:UNK:HG1	1:3:2200:UNK:HG1	1.99	0.43
3:E:803:UNK:HB1	3:E:1217:UNK:HG2	2.00	0.43
1:1:54:UNK:HA	1:1:57:UNK:HB2	1.99	0.43
3:A:929:UNK:HB2	3:A:973:UNK:HB2	2.00	0.43
2:4:302:UNK:O	2:4:306:UNK:HG2	2.18	0.43
4:F:1613:GLU:H	4:F:1613:GLU:HG3	1.48	0.43
1:1:8:UNK:O	1:1:12:UNK:HB1	2.18	0.43
1:3:9:UNK:O	1:3:12:UNK:HG3	2.17	0.43
3:A:643:UNK:O	3:A:646:UNK:HB1	2.18	0.43
1:1:306:UNK:O	1:1:310:UNK:HB2	2.18	0.43
1:1:440:UNK:HB1	1:1:443:UNK:HB2	1.99	0.43
3:A:988:UNK:HB1	3:A:1102:UNK:HG1	1.99	0.43
6:D:132:ASN:ND2	6:D:148:GLN:HG2	2.33	0.43
2:4:26:UNK:O	2:4:30:UNK:HG2	2.19	0.43
1:1:1313:UNK:HG1	1:1:1400:UNK:HB1	2.00	0.43
1:1:438:UNK:HB2	1:1:439:UNK:H	1.55	0.43
4:F:2162:VAL:HG22	4:F:2170:ARG:HG3	2.00	0.43
4:F:2299:LEU:O	4:F:2302:LEU:HG	2.19	0.43
1:1:1310:UNK:CG	1:1:1512:UNK:HA	2.49	0.43
1:3:306:UNK:O	1:3:308:UNK:N	2.51	0.43
6:H:19:GLY:HA2	6:H:316:VAL:HG23	2.00	0.43
4:F:1530:GLU:O	4:F:1533:THR:HB	2.19	0.43
4:B:1777:SER:O	4:B:1781:GLU:HG2	2.17	0.43
3:A:561:UNK:HA	3:A:569:UNK:HG3	1.99	0.43
2:2:9:UNK:O	2:2:13:UNK:HB2	2.18	0.43
4:F:1972:LEU:HB3	4:F:1976:LEU:HD12	2.00	0.43
4:B:2017:ILE:HD13	4:B:2231:SER:HB3	2.00	0.43
1:1:4:UNK:O	1:1:5:UNK:C	2.67	0.43
4:F:2326:VAL:O	4:F:2330:VAL:HG23	2.19	0.43
4:B:2340:HIS:O	4:B:2343:ASN:N	2.47	0.43
4:B:2378:ARG:NH2	4:B:2545:TRP:O	2.51	0.43
3:E:1538:UNK:HB1	3:E:1540:UNK:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1426:PRO:HG2	4:F:1427:GLU:CD	2.39	0.43
4:B:1416:LEU:HD23	4:B:1432:VAL:HG13	2.00	0.43
3:E:1638:UNK:HG2	3:E:1707:UNK:HB1	2.01	0.43
4:B:1530:GLU:O	4:B:1533:THR:HB	2.19	0.43
6:H:48:LEU:HB2	6:H:317:CYS:HB3	2.00	0.43
3:A:745:UNK:HG2	3:A:747:UNK:N	2.32	0.43
4:F:1981:LYS:H	4:F:1981:LYS:HG2	1.68	0.43
3:E:929:UNK:HB2	3:E:973:UNK:HB2	2.00	0.43
4:B:1481:MET:HE2	4:B:1481:MET:HB3	1.81	0.43
4:F:1623:LEU:HD13	4:F:1640:ARG:HH12	1.83	0.43
4:B:1623:LEU:HD13	4:B:1640:ARG:HH12	1.83	0.43
4:F:2260:LEU:HD23	4:F:2263:ILE:HA	2.01	0.43
2:4:97:UNK:HG3	2:4:135:UNK:HB2	1.99	0.43
1:1:209:UNK:HB2	1:1:330:UNK:HB1	2.00	0.43
1:1:2303:UNK:O	1:1:2307:UNK:HB2	2.18	0.43
1:1:32:UNK:O	1:1:33:UNK:C	2.66	0.43
4:B:1500:LYS:HD3	4:B:1503:LEU:HD12	1.99	0.43
4:F:1474:PRO:HA	4:F:1477:MET:HE2	2.00	0.43
1:1:908:UNK:HB1	1:1:1006:UNK:HG2	2.00	0.43
4:B:1515:MET:H	4:B:1515:MET:HG3	1.59	0.43
4:F:2419:GLU:HG2	4:F:2501:ILE:CG1	2.29	0.43
4:F:2397:ARG:HA	4:F:2400:CYS:SG	2.58	0.43
1:3:1310:UNK:CG	1:3:1512:UNK:HA	2.49	0.43
4:B:1575:LEU:O	4:B:1578:MET:HG3	2.19	0.43
2:2:97:UNK:HG3	2:2:135:UNK:HB2	1.99	0.43
5:G:26:UNK:O	5:G:39:UNK:N	2.50	0.43
6:D:291:ASP:OD2	6:D:295:ARG:NH2	2.43	0.43
1:3:706:UNK:HB1	1:3:902:UNK:HB1	2.00	0.43
6:D:144:ILE:HG12	6:D:185:MET:SD	2.59	0.43
4:F:2297:ASP:O	4:F:2301:LYS:HB2	2.19	0.43
4:F:1435:TYR:CG	4:F:2390:THR:HG21	2.53	0.43
1:3:923:UNK:O	1:3:927:UNK:HB1	2.18	0.43
3:A:625:UNK:C	3:A:627:UNK:H	2.31	0.43
3:E:992:UNK:HG3	3:E:1103:UNK:HG2	2.01	0.43
3:E:932:UNK:O	3:E:936:UNK:HG2	2.19	0.43
3:E:564:UNK:HG3	3:E:570:UNK:HG2	1.99	0.43
1:3:54:UNK:HA	1:3:57:UNK:HB2	1.99	0.43
2:2:151:UNK:O	2:2:152:UNK:C	2.65	0.43
4:B:1575:LEU:HD11	4:B:1589:ALA:HB3	2.01	0.43
6:D:267:GLU:O	6:D:269:SER:N	2.52	0.43
4:F:2379:LEU:HA	4:F:2379:LEU:HD13	1.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:1913:UNK:HA	1:3:2000:UNK:HB2	1.99	0.43
4:F:1500:LYS:HD3	4:F:1503:LEU:HD12	1.99	0.43
1:3:908:UNK:HB1	1:3:1006:UNK:HG2	2.01	0.43
4:F:2209:LEU:HD23	4:F:2406:VAL:HG11	2.00	0.43
4:F:1560:ALA:O	4:F:1564:ILE:HG13	2.18	0.43
3:E:773:UNK:O	3:E:774:UNK:HB2	2.19	0.43
1:1:4:UNK:O	1:1:7:UNK:HB1	2.18	0.43
4:B:2299:LEU:O	4:B:2302:LEU:HG	2.19	0.43
1:1:328:UNK:O	1:1:331:UNK:HB2	2.19	0.43
5:G:4:UNK:HG2	5:G:62:UNK:HG3	2.00	0.43
4:F:2267:ILE:O	4:F:2270:ARG:HB3	2.19	0.43
4:B:1444:GLU:O	4:B:1445:ILE:HG12	2.19	0.43
2:2:168:UNK:O	2:2:172:UNK:HG2	2.19	0.43
6:H:78:ILE:HB	6:H:79:ILE:HG13	2.01	0.43
3:A:992:UNK:HG3	3:A:1103:UNK:HG2	2.01	0.43
4:B:2209:LEU:HD23	4:B:2406:VAL:HG11	1.99	0.43
1:3:1313:UNK:HG1	1:3:1400:UNK:HB1	2.00	0.43
2:2:607:UNK:HA	2:2:610:UNK:HG2	2.01	0.43
1:1:713:UNK:HG1	1:1:909:UNK:HB1	2.00	0.43
4:B:2214:THR:O	4:B:2217:ARG:HB3	2.18	0.43
3:E:578:UNK:O	3:E:582:UNK:HG2	2.19	0.43
4:B:1393:TYR:HD2	4:B:1423:LEU:HD13	1.83	0.43
6:D:31:SER:OG	6:D:32:GLY:N	2.51	0.43
4:B:2340:HIS:CE1	4:B:2342:SER:HB2	2.54	0.43
1:3:1216:UNK:HB1	1:3:1305:UNK:HG1	2.01	0.43
1:1:923:UNK:O	1:1:927:UNK:HB1	2.19	0.43
4:B:1951:PRO:HB2	4:B:1955:ARG:HH21	1.84	0.43
6:H:142:GLU:OE1	6:H:208:THR:HG21	2.18	0.43
2:2:109:UNK:O	2:2:113:UNK:HB1	2.19	0.43
4:B:2212:ASP:HA	4:B:2213:PRO:HD3	1.88	0.43
1:1:52:UNK:HG1	1:1:90:UNK:HB2	2.00	0.43
4:B:1568:ARG:NH2	4:B:1600:GLU:OE2	2.50	0.43
1:3:319:UNK:O	1:3:324:UNK:HB2	2.18	0.43
4:B:2307:SER:OG	4:B:2313:TRP:HB2	2.19	0.43
6:H:31:SER:OG	6:H:32:GLY:N	2.51	0.43
4:B:1611:ARG:HG2	4:B:1611:ARG:H	1.56	0.43
4:F:2254:ARG:HD2	4:F:2254:ARG:HA	1.57	0.43
4:F:2277:HIS:HB3	6:H:62:TYR:CD1	2.53	0.43
3:E:609:UNK:O	3:E:612:UNK:HB1	2.19	0.43
4:B:2397:ARG:HB2	4:B:2397:ARG:HH11	1.84	0.42
4:F:1393:TYR:HD2	4:F:1423:LEU:HD13	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:306:UNK:O	1:3:310:UNK:HB2	2.19	0.42
2:2:163:UNK:O	2:2:167:UNK:N	2.52	0.42
6:H:132:ASN:ND2	6:H:148:GLN:HG2	2.34	0.42
6:H:267:GLU:O	6:H:269:SER:N	2.52	0.42
4:B:2316:ARG:NE	4:B:2348:ARG:O	2.51	0.42
5:C:48:UNK:HG1	5:C:55:UNK:HG2	2.00	0.42
2:2:540:UNK:O	2:2:543:UNK:HG2	2.19	0.42
4:F:2157:ALA:HB3	4:F:2173:THR:HG23	2.00	0.42
4:B:1451:GLU:HG3	4:B:1456:TRP:CZ3	2.54	0.42
6:D:221:ARG:HD3	6:D:241:ASP:HA	2.01	0.42
4:B:1917:PRO:O	4:B:1921:GLU:HG3	2.19	0.42
4:B:2315:ASP:O	4:B:2318:THR:OG1	2.30	0.42
1:3:85:UNK:O	1:3:89:UNK:HB1	2.19	0.42
1:3:324:UNK:HG3	1:3:427:UNK:HB2	2.01	0.42
1:1:154:UNK:HG3	3:A:643:UNK:CB	2.41	0.42
2:4:163:UNK:O	2:4:167:UNK:N	2.52	0.42
4:B:2267:ILE:O	4:B:2270:ARG:HB3	2.19	0.42
4:B:2277:HIS:HB3	6:D:62:TYR:CD1	2.54	0.42
6:D:142:GLU:OE1	6:D:208:THR:HG21	2.19	0.42
4:F:2214:THR:O	4:F:2217:ARG:HB3	2.19	0.42
2:2:79:UNK:HB1	2:2:81:UNK:HG3	2.01	0.42
3:E:635:UNK:HG3	3:E:637:UNK:HG2	2.01	0.42
3:A:584:UNK:HB1	3:A:737:UNK:CG	2.45	0.42
2:4:617:UNK:HA	4:F:1393:TYR:CZ	2.54	0.42
4:B:2326:VAL:O	4:B:2330:VAL:HG23	2.19	0.42
1:1:510:UNK:HB1	1:1:600:UNK:HG1	2.01	0.42
4:B:1513:ALA:CB	4:B:1536:ILE:HG12	2.49	0.42
6:H:271:GLY:HA3	6:H:290:SER:HB2	2.01	0.42
4:F:2288:GLU:O	4:F:2292:ASN:ND2	2.52	0.42
6:H:221:ARG:HD3	6:H:241:ASP:HA	2.02	0.42
3:A:803:UNK:HB1	3:A:1217:UNK:HG2	2.00	0.42
3:E:616:UNK:C	3:E:618:UNK:N	2.83	0.42
3:A:767:UNK:O	3:A:770:UNK:HB2	2.20	0.42
4:F:2185:LEU:HD12	4:F:2185:LEU:HA	1.80	0.42
4:B:1736:ASP:N	4:B:1736:ASP:OD1	2.52	0.42
4:B:2419:GLU:HG2	4:B:2501:ILE:CG1	2.30	0.42
4:B:2397:ARG:HG2	4:B:2401:HIS:NE2	2.34	0.42
4:F:1575:LEU:O	4:F:1578:MET:HG3	2.18	0.42
6:H:108:THR:OG1	6:H:110:ARG:NH1	2.52	0.42
1:1:436:UNK:HA	1:1:444:UNK:HB2	2.00	0.42
4:F:1668:LEU:HD12	4:F:1668:LEU:HA	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:32:UNK:O	1:1:34:UNK:N	2.52	0.42
6:D:48:LEU:HB2	6:D:317:CYS:HB3	2.00	0.42
4:B:2297:ASP:O	4:B:2301:LYS:HB2	2.19	0.42
4:B:2218:LYS:HE3	4:B:2220:LEU:HD11	2.01	0.42
1:1:85:UNK:O	1:1:89:UNK:HB1	2.19	0.42
4:F:2307:SER:OG	4:F:2313:TRP:HB2	2.20	0.42
3:E:721:UNK:HG1	3:E:733:UNK:HA	2.00	0.42
4:F:2340:HIS:CE1	4:F:2342:SER:HB2	2.54	0.42
4:F:2074:TYR:HD2	4:F:2107:VAL:HG12	1.84	0.42
1:3:328:UNK:O	1:3:331:UNK:HB2	2.19	0.42
1:1:1913:UNK:HA	1:1:2000:UNK:HB2	2.00	0.42
3:E:625:UNK:C	3:E:627:UNK:H	2.31	0.42
4:B:2157:ALA:HB3	4:B:2173:THR:HG23	2.00	0.42
2:2:1:UNK:H	2:2:3:UNK:HG2	1.85	0.42
4:B:1447:ALA:HB1	4:B:1463:TYR:CE2	2.55	0.42
4:F:2045:LYS:NZ	4:F:2049:GLU:OE2	2.43	0.42
2:4:109:UNK:O	2:4:113:UNK:HB1	2.19	0.42
3:A:564:UNK:HG3	3:A:570:UNK:HG2	2.02	0.42
4:F:1575:LEU:HD11	4:F:1589:ALA:HB3	2.02	0.42
6:D:108:THR:OG1	6:D:110:ARG:NH1	2.52	0.42
4:B:1426:PRO:HG2	4:B:1427:GLU:CD	2.39	0.42
2:2:81:UNK:O	2:2:84:UNK:HG2	2.20	0.42
3:E:581:UNK:O	3:E:585:UNK:HB2	2.20	0.42
5:G:48:UNK:HG1	5:G:55:UNK:HG2	2.01	0.42
4:F:2316:ARG:NE	4:F:2348:ARG:O	2.53	0.42
1:3:121:UNK:HB1	1:3:203:UNK:CB	2.50	0.42
4:F:2186:LEU:HA	4:F:2186:LEU:HD12	1.82	0.42
4:B:2260:LEU:HD23	4:B:2263:ILE:HA	2.00	0.42
1:1:306:UNK:O	1:1:308:UNK:N	2.52	0.42
4:F:2249:LEU:O	4:F:2252:ASP:HB2	2.20	0.42
4:F:1513:ALA:CB	4:F:1536:ILE:HG12	2.49	0.42
6:D:19:GLY:HA2	6:D:316:VAL:HG23	2.01	0.42
6:H:242:GLN:HG2	6:H:271:GLY:O	2.20	0.42
4:B:2381:ARG:HA	4:B:2384:THR:HB	2.02	0.42
4:F:1990:ALA:O	4:F:1994:ILE:HG13	2.20	0.42
4:B:2288:GLU:O	4:B:2292:ASN:ND2	2.52	0.42
1:1:208:UNK:C	1:1:210:UNK:N	2.82	0.42
2:2:549:UNK:HB2	4:B:1395:LYS:NZ	2.35	0.42
4:B:2341:PRO:HD3	4:B:2378:ARG:HH22	1.85	0.42
3:E:117:UNK:HG3	3:E:302:UNK:N	2.35	0.42
3:E:985:UNK:O	3:E:987:UNK:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:168:UNK:O	2:4:172:UNK:HG2	2.20	0.42
6:H:144:ILE:HG12	6:H:185:MET:SD	2.59	0.42
2:4:540:UNK:O	2:4:543:UNK:HG2	2.20	0.42
4:B:1727:GLN:O	4:B:1731:ALA:HB3	2.20	0.42
4:F:2069:SER:O	4:F:2072:GLN:HB2	2.20	0.42
4:B:1607:LEU:O	4:B:1608:VAL:HG13	2.20	0.42
4:F:2397:ARG:HB2	4:F:2397:ARG:NH1	2.35	0.42
6:H:40:HIS:CE1	6:H:43:SER:HB3	2.55	0.42
1:3:61:UNK:O	1:3:65:UNK:HG2	2.20	0.42
4:B:1417:ILE:H	4:B:1417:ILE:HG13	1.42	0.42
1:3:1913:UNK:O	1:3:2116:UNK:HG1	2.20	0.42
4:B:1472:ASP:CG	4:B:1503:LEU:HD13	2.40	0.42
4:B:1421:ASN:HD21	4:B:1452:LYS:HB3	1.85	0.42
6:D:78:ILE:HB	6:D:79:ILE:HG13	2.01	0.42
3:A:932:UNK:O	3:A:936:UNK:HG2	2.19	0.42
1:3:117:UNK:C	1:3:118:UNK:O	2.66	0.42
1:1:324:UNK:HG3	1:1:427:UNK:HB2	2.02	0.42
3:E:405:UNK:HB1	3:E:410:UNK:HG1	2.01	0.42
2:4:157:UNK:O	2:4:159:UNK:N	2.53	0.42
4:F:2341:PRO:HD3	4:F:2378:ARG:HH22	1.84	0.42
4:F:1536:ILE:HA	4:F:1537:PRO:HD3	1.94	0.42
4:F:1987:ARG:NH1	4:F:2426:LEU:HD21	2.35	0.42
4:B:2250:ILE:O	4:B:2254:ARG:HG2	2.20	0.42
3:E:1605:UNK:HG3	3:E:1611:UNK:HG3	2.01	0.42
4:B:2147:ASN:O	4:B:2148:GLN:NE2	2.31	0.42
4:F:1920:ASN:O	4:F:1924:VAL:HG23	2.20	0.42
5:C:21:UNK:HG3	5:C:49:UNK:HG3	2.01	0.42
1:3:406:UNK:HA	1:3:409:UNK:HG2	2.02	0.42
2:2:515:UNK:O	2:2:519:UNK:HG3	2.20	0.42
1:1:89:UNK:HG3	1:1:90:UNK:HG2	2.02	0.41
4:F:1607:LEU:O	4:F:1608:VAL:HG13	2.19	0.41
1:3:4:UNK:O	1:3:5:UNK:C	2.67	0.41
3:A:635:UNK:HG3	3:A:637:UNK:HG2	2.02	0.41
4:B:2397:ARG:HB2	4:B:2397:ARG:NH1	2.35	0.41
2:2:617:UNK:HA	4:B:1393:TYR:CZ	2.55	0.41
3:A:405:UNK:HB1	3:A:410:UNK:HG1	2.01	0.41
2:2:166:UNK:O	2:2:169:UNK:HB1	2.20	0.41
4:F:2399:THR:O	4:F:2403:VAL:HG23	2.20	0.41
2:4:167:UNK:O	2:4:170:UNK:HB2	2.20	0.41
1:3:444:UNK:HA	1:3:447:UNK:HB1	2.02	0.41
2:4:209:UNK:C	2:4:211:UNK:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:985:UNK:O	3:A:987:UNK:N	2.53	0.41
6:D:313:LYS:HA	6:D:313:LYS:HD3	1.91	0.41
4:F:2381:ARG:HA	4:F:2384:THR:HB	2.01	0.41
3:A:409:UNK:N	3:A:511:UNK:O	2.53	0.41
3:A:966:UNK:N	3:A:1528:UNK:O	2.53	0.41
3:A:706:UNK:HB1	3:A:707:UNK:H	1.66	0.41
4:B:2114:GLN:HG2	4:B:2117:GLN:OE1	2.20	0.41
4:F:1684:GLN:HB3	4:F:1687:HIS:HD2	1.84	0.41
4:F:1736:ASP:OD1	4:F:1736:ASP:N	2.52	0.41
2:2:258:UNK:O	2:2:261:UNK:HG2	2.20	0.41
1:3:89:UNK:HG3	1:3:90:UNK:HG2	2.01	0.41
3:A:578:UNK:O	3:A:582:UNK:HG2	2.20	0.41
2:4:155:UNK:C	2:4:157:UNK:H	2.33	0.41
3:A:549:UNK:HB1	3:A:554:UNK:CG	2.50	0.41
4:F:2411:LYS:HB2	4:F:2411:LYS:HE3	1.69	0.41
2:4:166:UNK:O	2:4:169:UNK:HB1	2.20	0.41
3:A:117:UNK:HG3	3:A:302:UNK:N	2.34	0.41
4:F:1611:ARG:H	4:F:1611:ARG:HG2	1.56	0.41
4:F:1472:ASP:CG	4:F:1503:LEU:HD13	2.41	0.41
3:A:609:UNK:O	3:A:612:UNK:HB1	2.20	0.41
4:B:2154:GLN:N	4:B:2175:MET:O	2.50	0.41
4:B:1977:THR:O	4:B:1981:LYS:HE2	2.21	0.41
2:2:63:UNK:CG	2:2:103:UNK:HG1	2.50	0.41
1:1:317:UNK:HG3	1:1:318:UNK:O	2.19	0.41
3:E:1343:UNK:HA	3:E:1368:UNK:O	2.20	0.41
4:B:2399:THR:O	4:B:2403:VAL:HG23	2.19	0.41
4:F:2503:ARG:O	4:F:2506:ASP:HB2	2.21	0.41
2:2:155:UNK:C	2:2:157:UNK:H	2.34	0.41
6:H:101:TYR:CD1	6:H:111:ILE:HG12	2.56	0.41
2:2:211:UNK:HA	2:2:214:UNK:HG3	2.02	0.41
2:4:211:UNK:O	2:4:214:UNK:N	2.53	0.41
2:4:108:UNK:O	2:4:112:UNK:HG2	2.21	0.41
6:D:242:GLN:HG2	6:D:271:GLY:O	2.20	0.41
3:E:1531:UNK:HG3	3:E:1532:UNK:HG2	2.02	0.41
4:F:1451:GLU:HG3	4:F:1456:TRP:CZ3	2.55	0.41
3:A:1531:UNK:HG3	3:A:1532:UNK:HG2	2.01	0.41
4:F:1917:PRO:O	4:F:1921:GLU:HG3	2.19	0.41
4:F:1647:HIS:O	4:F:1650:MET:HE3	2.20	0.41
3:E:409:UNK:N	3:E:511:UNK:O	2.52	0.41
3:A:773:UNK:O	3:A:774:UNK:HB2	2.20	0.41
4:F:2340:HIS:O	4:F:2343:ASN:N	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:721:UNK:HG1	3:A:733:UNK:HA	2.01	0.41
2:2:167:UNK:O	2:2:170:UNK:HB2	2.20	0.41
4:F:2250:ILE:O	4:F:2254:ARG:HG2	2.20	0.41
4:F:1417:ILE:H	4:F:1417:ILE:HG13	1.41	0.41
4:B:1684:GLN:HB3	4:B:1687:HIS:HD2	1.84	0.41
3:A:616:UNK:C	3:A:618:UNK:N	2.82	0.41
3:A:1387:UNK:HG1	3:A:1502:UNK:HB1	2.02	0.41
2:4:60:UNK:O	2:4:64:UNK:HG3	2.21	0.41
2:4:81:UNK:O	2:4:84:UNK:HG2	2.19	0.41
1:1:117:UNK:C	1:1:118:UNK:O	2.66	0.41
2:4:549:UNK:HB2	4:F:1395:LYS:NZ	2.35	0.41
1:1:444:UNK:HA	1:1:447:UNK:HB1	2.02	0.41
2:2:192:UNK:O	2:2:196:UNK:HG3	2.20	0.41
1:1:42:UNK:HB2	4:F:1611:ARG:HH12	1.84	0.41
2:2:184:UNK:O	2:2:188:UNK:N	2.53	0.41
1:3:425:UNK:HA	1:3:428:UNK:HB2	2.03	0.41
1:1:1909:UNK:O	1:1:1913:UNK:HB2	2.20	0.41
3:A:1638:UNK:HB2	3:A:1643:UNK:O	2.20	0.41
2:2:302:UNK:O	2:2:305:UNK:HB2	2.21	0.41
4:B:1670:HIS:HD2	4:B:1703:ASN:HD21	1.69	0.41
2:4:268:UNK:C	2:4:270:UNK:N	2.83	0.41
4:F:2114:GLN:HG2	4:F:2117:GLN:OE1	2.20	0.41
1:3:2213:UNK:HG1	1:3:2309:UNK:HG1	2.02	0.41
2:2:60:UNK:O	2:2:64:UNK:HG3	2.21	0.41
3:E:767:UNK:O	3:E:770:UNK:HB2	2.19	0.41
2:4:63:UNK:CG	2:4:103:UNK:HG1	2.50	0.41
3:E:966:UNK:N	3:E:1528:UNK:O	2.53	0.41
4:F:2060:ARG:NH2	4:F:2061:GLY:O	2.30	0.41
1:3:317:UNK:HG3	1:3:318:UNK:O	2.20	0.41
4:B:1920:ASN:O	4:B:1924:VAL:HG23	2.20	0.41
3:A:1523:UNK:HG3	3:A:1530:UNK:HG2	2.03	0.41
4:B:2541:CYS:HB3	4:B:2547:PRO:HG3	2.02	0.41
2:2:157:UNK:O	2:2:159:UNK:N	2.54	0.41
4:B:1434:GLU:O	4:B:1438:LYS:HD2	2.21	0.41
1:3:13:UNK:HB1	1:3:21:UNK:HG3	2.03	0.41
1:1:13:UNK:HB1	1:1:21:UNK:HG3	2.02	0.41
2:4:206:UNK:O	2:4:209:UNK:HB1	2.21	0.41
2:4:192:UNK:O	2:4:196:UNK:HG3	2.20	0.41
1:3:1909:UNK:O	1:3:1913:UNK:HB2	2.21	0.41
5:G:21:UNK:HG3	5:G:49:UNK:HG3	2.02	0.41
4:B:1541:HIS:CG	4:B:1542:ASP:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:212:UNK:HG1	2:4:225:UNK:HG1	2.01	0.41
3:E:245:UNK:HA	3:E:248:UNK:HB1	2.02	0.41
4:F:2370:LYS:HD2	4:F:2370:LYS:HA	1.86	0.41
1:1:121:UNK:HB1	1:1:203:UNK:CB	2.50	0.41
4:B:2074:TYR:HD2	4:B:2107:VAL:HG12	1.84	0.41
1:3:510:UNK:HB1	1:3:600:UNK:HG1	2.02	0.41
4:B:1571:LEU:O	4:B:1574:GLU:HB3	2.20	0.41
2:2:211:UNK:O	2:2:214:UNK:N	2.54	0.41
4:B:2249:LEU:O	4:B:2252:ASP:HB2	2.20	0.41
1:3:106:UNK:O	1:3:109:UNK:HB1	2.20	0.41
1:1:106:UNK:O	1:1:109:UNK:HB1	2.20	0.41
1:1:28:UNK:HA	1:1:31:UNK:HB2	2.01	0.41
4:B:2256:LYS:NZ	4:B:2257:LYS:HE3	2.34	0.41
2:4:117:UNK:C	2:4:119:UNK:N	2.84	0.41
1:3:42:UNK:HB2	4:B:1611:ARG:HH12	1.86	0.41
2:4:515:UNK:O	2:4:519:UNK:HG3	2.19	0.41
2:4:611:UNK:C	2:4:613:UNK:N	2.83	0.41
3:A:1514:UNK:HB1	3:A:1542:UNK:HB1	2.02	0.41
4:B:1990:ALA:O	4:B:1994:ILE:HG13	2.20	0.41
4:F:2218:LYS:HE3	4:F:2220:LEU:HD11	2.01	0.41
4:F:1401:GLU:O	4:F:1404:PHE:HB3	2.21	0.41
4:B:2423:TYR:CE2	4:B:2501:ILE:HD13	2.56	0.41
2:2:209:UNK:C	2:2:211:UNK:N	2.83	0.41
1:1:435:UNK:CG	1:1:447:UNK:HG1	2.51	0.41
4:F:2374:LYS:HD3	4:F:2374:LYS:HA	1.89	0.41
6:H:78:ILE:HG13	6:H:78:ILE:H	1.60	0.41
4:B:2069:SER:O	4:B:2072:GLN:HB2	2.20	0.41
4:B:2166:LYS:HA	4:B:2166:LYS:HD2	1.87	0.41
6:H:113:ASP:HB3	6:H:116:SER:OG	2.21	0.41
1:3:48:UNK:HA	1:3:51:UNK:CB	2.51	0.41
4:F:1623:LEU:HD12	4:F:1623:LEU:HA	1.95	0.41
4:F:1608:VAL:HA	4:F:1609:PRO:HD3	1.77	0.41
1:3:1:UNK:HA	4:B:1622:ARG:NE	2.36	0.41
4:B:2503:ARG:O	4:B:2506:ASP:HB2	2.20	0.41
1:1:507:UNK:O	1:1:511:UNK:HG2	2.21	0.41
6:D:101:TYR:CD1	6:D:111:ILE:HG12	2.55	0.41
4:F:1434:GLU:O	4:F:1438:LYS:HD2	2.20	0.41
4:F:1673:LEU:HD13	4:F:1700:TYR:HD1	1.86	0.41
2:4:203:UNK:O	2:4:206:UNK:HB1	2.20	0.41
1:1:416:UNK:C	1:1:418:UNK:N	2.84	0.41
3:A:517:UNK:C	3:A:519:UNK:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:197:UNK:O	2:4:201:UNK:HG3	2.21	0.41
4:B:1987:ARG:NH1	4:B:2426:LEU:HD21	2.35	0.41
2:2:116:UNK:HG3	2:2:119:UNK:HB1	2.02	0.41
2:4:184:UNK:O	2:4:188:UNK:N	2.54	0.41
2:2:106:UNK:O	2:2:110:UNK:HG2	2.21	0.41
1:3:33:UNK:HB2	1:3:34:UNK:H	1.55	0.41
2:2:63:UNK:HG1	2:2:103:UNK:HG1	2.02	0.41
2:4:208:UNK:O	2:4:212:UNK:HG3	2.21	0.41
3:E:906:UNK:HA	3:E:909:UNK:HB2	2.03	0.41
3:E:1387:UNK:HG1	3:E:1502:UNK:HB1	2.02	0.41
4:F:1770:PRO:HA	4:F:1773:LEU:HB2	2.02	0.41
3:E:758:UNK:O	3:E:762:UNK:HG2	2.21	0.41
3:A:577:UNK:HG2	3:A:741:UNK:HB1	2.03	0.41
2:2:507:UNK:O	2:2:511:UNK:HG2	2.21	0.41
4:B:2090:LYS:HE2	4:B:2090:LYS:HB2	1.91	0.41
4:B:2370:LYS:HA	4:B:2370:LYS:HD2	1.85	0.41
3:E:963:UNK:HG3	3:E:1112:UNK:HG1	2.03	0.41
4:F:2343:ASN:HD22	4:F:2343:ASN:HA	1.70	0.41
1:3:507:UNK:O	1:3:511:UNK:HG2	2.21	0.41
3:A:913:UNK:O	3:A:917:UNK:HG2	2.22	0.41
3:E:1544:UNK:HG3	3:E:1558:UNK:HG3	2.03	0.41
4:B:2253:TYR:CE1	4:B:2257:LYS:HG3	2.56	0.41
1:1:61:UNK:O	1:1:65:UNK:HG2	2.20	0.41
1:3:209:UNK:HB2	1:3:330:UNK:HB1	2.01	0.41
1:1:1913:UNK:O	1:1:2116:UNK:HG1	2.20	0.41
2:4:106:UNK:O	2:4:110:UNK:HG2	2.21	0.41
2:4:79:UNK:HB1	2:4:81:UNK:HG3	2.03	0.41
2:2:203:UNK:O	2:2:206:UNK:HB1	2.20	0.41
3:A:906:UNK:HA	3:A:909:UNK:HB2	2.03	0.41
3:A:1343:UNK:HA	3:A:1368:UNK:O	2.20	0.41
2:2:212:UNK:HG1	2:2:225:UNK:HG1	2.02	0.41
3:A:846:UNK:O	3:A:849:UNK:HB2	2.21	0.41
4:F:1397:LEU:HA	4:F:1397:LEU:HD12	1.81	0.41
1:3:208:UNK:C	1:3:210:UNK:N	2.83	0.40
2:2:552:UNK:HG1	4:B:2304:TRP:CZ2	2.44	0.40
4:F:2256:LYS:NZ	4:F:2257:LYS:HE3	2.34	0.40
3:A:1605:UNK:HG3	3:A:1611:UNK:HG3	2.02	0.40
4:F:1977:THR:O	4:F:1981:LYS:HE2	2.20	0.40
2:2:268:UNK:C	2:2:270:UNK:N	2.83	0.40
2:4:258:UNK:O	2:4:261:UNK:HG2	2.20	0.40
5:G:81:UNK:HG1	5:G:97:UNK:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:21:UNK:O	2:2:25:UNK:HB1	2.21	0.40
4:F:2170:ARG:HB2	4:F:2186:LEU:HB3	2.03	0.40
3:E:913:UNK:O	3:E:917:UNK:HG2	2.22	0.40
1:3:28:UNK:HA	1:3:31:UNK:HB2	2.02	0.40
2:2:197:UNK:O	2:2:201:UNK:HG3	2.21	0.40
6:D:50:VAL:HG23	6:D:319:ALA:HB1	2.03	0.40
4:B:2431:LEU:HB2	4:B:2493:LEU:HD22	2.03	0.40
4:B:1433:LEU:HD22	4:B:1453:LEU:HG	2.03	0.40
3:A:315:UNK:O	3:A:317:UNK:HG2	2.21	0.40
2:4:607:UNK:HA	2:4:610:UNK:HG2	2.03	0.40
4:F:1670:HIS:HD2	4:F:1703:ASN:HD21	1.70	0.40
5:C:60:UNK:O	5:C:64:UNK:HB2	2.22	0.40
4:F:1447:ALA:HB1	4:F:1463:TYR:CE2	2.56	0.40
3:A:557:UNK:HG2	3:A:652:UNK:HG1	2.03	0.40
2:4:1:UNK:H	2:4:3:UNK:HG2	1.86	0.40
5:G:60:UNK:O	5:G:64:UNK:HB2	2.22	0.40
2:4:552:UNK:CG	4:F:2304:TRP:HZ2	2.26	0.40
2:2:549:UNK:HB2	4:B:1395:LYS:HZ1	1.86	0.40
3:A:114:UNK:HG2	3:A:300:UNK:C	2.52	0.40
2:2:108:UNK:O	2:2:112:UNK:HG2	2.21	0.40
4:F:2515:HIS:HD1	4:F:2516:ASP:N	2.20	0.40
4:F:1881:THR:O	4:F:1884:ALA:HB3	2.22	0.40
4:F:2431:LEU:HB2	4:F:2493:LEU:HD22	2.03	0.40
3:E:1638:UNK:HB2	3:E:1643:UNK:O	2.20	0.40
3:E:1641:UNK:HG3	3:E:1643:UNK:HB2	2.03	0.40
2:2:208:UNK:O	2:2:212:UNK:HG3	2.21	0.40
1:1:2213:UNK:HG1	1:1:2309:UNK:HG1	2.02	0.40
6:D:113:ASP:HB3	6:D:116:SER:OG	2.21	0.40
4:B:1756:GLU:O	4:B:1759:LEU:HB2	2.22	0.40
2:2:78:UNK:HB1	3:A:634:UNK:HA	2.02	0.40
4:F:1756:GLU:O	4:F:1759:LEU:HB2	2.22	0.40
3:E:318:UNK:HG1	3:E:333:UNK:HB1	2.03	0.40
6:D:248:ARG:H	6:D:248:ARG:HG2	1.73	0.40
3:A:963:UNK:HG3	3:A:1112:UNK:HG1	2.04	0.40
3:E:549:UNK:HB1	3:E:554:UNK:CG	2.51	0.40
6:D:195:TYR:CE2	6:D:215:LYS:HG3	2.56	0.40
5:C:54:UNK:O	7:C:999:RAP:O10	2.40	0.40
3:A:1544:UNK:HG3	3:A:1558:UNK:HG3	2.03	0.40
1:1:425:UNK:HA	1:1:428:UNK:HB2	2.03	0.40
3:A:1641:UNK:HG3	3:A:1643:UNK:HB2	2.03	0.40
3:A:712:UNK:HG2	3:A:748:UNK:HG1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1743:LEU:HA	4:F:1743:LEU:HD12	1.96	0.40
3:A:318:UNK:HG1	3:A:333:UNK:HB1	2.03	0.40
4:F:1727:GLN:O	4:F:1731:ALA:HB3	2.20	0.40
4:F:2154:GLN:N	4:F:2175:MET:O	2.51	0.40
6:D:125:PHE:HB2	6:D:155:TRP:CZ2	2.56	0.40
4:B:2185:LEU:HD12	4:B:2185:LEU:HA	1.81	0.40
1:1:80:UNK:C	1:1:82:UNK:N	2.85	0.40
1:1:1:UNK:HA	4:F:1622:ARG:NE	2.36	0.40
4:B:2303:LEU:HA	4:B:2303:LEU:HD23	1.80	0.40
2:2:100:UNK:C	2:2:102:UNK:N	2.85	0.40
4:F:2247:HIS:HA	4:F:2549:TRP:HZ3	1.87	0.40
4:B:2051:LEU:HD12	4:B:2051:LEU:HA	1.80	0.40
4:B:2039:PHE:CZ	7:C:999:RAP:H502	2.57	0.40
2:4:302:UNK:O	2:4:305:UNK:HB2	2.21	0.40
4:F:2242:HIS:HA	4:F:2348:ARG:NH1	2.37	0.40
3:E:1524:UNK:O	3:E:1528:UNK:N	2.55	0.40
4:B:2199:MET:HE1	4:B:2225:TYR:H	1.86	0.40
6:H:125:PHE:HB2	6:H:155:TRP:CZ2	2.56	0.40
6:H:168:GLU:HA	6:H:169:PRO:HD3	1.93	0.40
3:A:758:UNK:O	3:A:762:UNK:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B	1045/1168 (90%)	996 (95%)	47 (4%)	2 (0%)	52	86
4	F	1045/1168 (90%)	997 (95%)	46 (4%)	2 (0%)	52	86
6	D	315/326 (97%)	293 (93%)	21 (7%)	1 (0%)	46	83
6	H	315/326 (97%)	293 (93%)	21 (7%)	1 (0%)	46	83
All	All	2720/2988 (91%)	2579 (95%)	135 (5%)	6 (0%)	56	86

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	268	SER
6	H	268	SER
4	B	1578	MET
4	F	1578	MET
4	B	1679	VAL
4	F	1679	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	927/1019 (91%)	829 (89%)	98 (11%)	8	36
4	F	927/1019 (91%)	828 (89%)	99 (11%)	8	36
6	D	269/276 (98%)	246 (91%)	23 (9%)	13	47
6	H	269/276 (98%)	246 (91%)	23 (9%)	13	47
All	All	2392/2590 (92%)	2149 (90%)	243 (10%)	14	38

All (243) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	1393	TYR
4	B	1417	ILE
4	B	1420	ASN
4	B	1422	LYS
4	B	1427	GLU
4	B	1443	LEU
4	B	1445	ILE
4	B	1449	TRP
4	B	1453	LEU
4	B	1457	GLU
4	B	1458	ASP
4	B	1463	TYR
4	B	1472	ASP
4	B	1480	ARG

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Mol	Chain	Res	Type
4	B	1489	GLU
4	B	1497	CYS
4	B	1536	ILE
4	B	1541	HIS
4	B	1547	ARG
4	B	1559	LEU
4	B	1563	CYS
4	B	1565	ASP
4	B	1571	LEU
4	B	1578	MET
4	B	1583	TYR
4	B	1585	ARG
4	B	1587	TYR
4	B	1599	LEU
4	B	1608	VAL
4	B	1611	ARG
4	B	1614	ILE
4	B	1622	ARG
4	B	1627	GLN
4	B	1630	VAL
4	B	1633	TRP
4	B	1642	LEU
4	B	1643	VAL
4	B	1659	LEU
4	B	1668	LEU
4	B	1677	LEU
4	B	1702	LYS
4	B	1709	ARG
4	B	1710	LYS
4	B	1736	ASP
4	B	1758	GLN
4	B	1899	ASN
4	B	1902	ASP
4	B	1907	LEU
4	B	1918	ASP
4	B	1938	VAL
4	B	1956	LEU
4	B	1984	THR
4	B	1985	THR
4	B	2005	LEU
4	B	2011	MET
4	B	2021	ILE

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Mol	Chain	Res	Type
4	B	2033	GLU
4	B	2060	ARG
4	B	2090	LYS
4	B	2093	ASN
4	B	2099	GLN
4	B	2122	GLU
4	B	2123	LEU
4	B	2133	CYS
4	B	2138	LEU
4	B	2145	ASP
4	B	2152	ARG
4	B	2173	THR
4	B	2178	ASN
4	B	2185	LEU
4	B	2189	HIS
4	B	2223	GLN
4	B	2228	ILE
4	B	2250	ILE
4	B	2254	ARG
4	B	2255	GLU
4	B	2266	ARG
4	B	2306	LYS
4	B	2318	THR
4	B	2321	THR
4	B	2323	SER
4	B	2339	ARG
4	B	2343	ASN
4	B	2363	GLU
4	B	2367	THR
4	B	2368	ARG
4	B	2379	LEU
4	B	2381	ARG
4	B	2385	ASN
4	B	2393	ASP
4	B	2405	GLU
4	B	2412	ASP
4	B	2415	MET
4	B	2424	ASP
4	B	2429	TRP
4	B	2503	ARG
4	B	2530	LYS
4	B	2548	PHE

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Mol	Chain	Res	Type
6	D	44	GLN
6	D	53	ASP
6	D	78	ILE
6	D	82	ASP
6	D	84	VAL
6	D	106	ASP
6	D	156	ASP
6	D	159	THR
6	D	160	ASP
6	D	162	ASN
6	D	164	GLN
6	D	173	ILE
6	D	179	ASP
6	D	188	VAL
6	D	197	TRP
6	D	199	LEU
6	D	243	THR
6	D	251	ASN
6	D	260	ILE
6	D	287	THR
6	D	308	TYR
6	D	312	GLN
6	D	316	VAL
4	F	1393	TYR
4	F	1417	ILE
4	F	1422	LYS
4	F	1427	GLU
4	F	1443	LEU
4	F	1445	ILE
4	F	1449	TRP
4	F	1453	LEU
4	F	1457	GLU
4	F	1458	ASP
4	F	1463	TYR
4	F	1472	ASP
4	F	1480	ARG
4	F	1489	GLU
4	F	1497	CYS
4	F	1536	ILE
4	F	1541	HIS
4	F	1547	ARG
4	F	1559	LEU

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Mol	Chain	Res	Type
4	F	1563	CYS
4	F	1565	ASP
4	F	1571	LEU
4	F	1578	MET
4	F	1583	TYR
4	F	1585	ARG
4	F	1587	TYR
4	F	1593	CYS
4	F	1599	LEU
4	F	1608	VAL
4	F	1611	ARG
4	F	1614	ILE
4	F	1622	ARG
4	F	1627	GLN
4	F	1630	VAL
4	F	1633	TRP
4	F	1642	LEU
4	F	1643	VAL
4	F	1659	LEU
4	F	1668	LEU
4	F	1677	LEU
4	F	1702	LYS
4	F	1709	ARG
4	F	1710	LYS
4	F	1736	ASP
4	F	1758	GLN
4	F	1899	ASN
4	F	1902	ASP
4	F	1907	LEU
4	F	1918	ASP
4	F	1938	VAL
4	F	1956	LEU
4	F	1984	THR
4	F	1985	THR
4	F	2005	LEU
4	F	2011	MET
4	F	2021	ILE
4	F	2033	GLU
4	F	2060	ARG
4	F	2090	LYS
4	F	2093	ASN
4	F	2099	GLN

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Mol	Chain	Res	Type
4	F	2122	GLU
4	F	2123	LEU
4	F	2133	CYS
4	F	2138	LEU
4	F	2145	ASP
4	F	2152	ARG
4	F	2173	THR
4	F	2178	ASN
4	F	2185	LEU
4	F	2189	HIS
4	F	2219	ASN
4	F	2223	GLN
4	F	2228	ILE
4	F	2250	ILE
4	F	2254	ARG
4	F	2255	GLU
4	F	2266	ARG
4	F	2306	LYS
4	F	2318	THR
4	F	2321	THR
4	F	2323	SER
4	F	2339	ARG
4	F	2343	ASN
4	F	2363	GLU
4	F	2367	THR
4	F	2368	ARG
4	F	2379	LEU
4	F	2381	ARG
4	F	2385	ASN
4	F	2393	ASP
4	F	2405	GLU
4	F	2412	ASP
4	F	2415	MET
4	F	2424	ASP
4	F	2429	TRP
4	F	2503	ARG
4	F	2530	LYS
4	F	2548	PHE
6	H	44	GLN
6	H	53	ASP
6	H	78	ILE
6	H	82	ASP

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Mol	Chain	Res	Type
6	H	84	VAL
6	H	106	ASP
6	H	156	ASP
6	H	159	THR
6	H	160	ASP
6	H	162	ASN
6	H	164	GLN
6	H	173	ILE
6	H	179	ASP
6	H	188	VAL
6	H	197	TRP
6	H	199	LEU
6	H	243	THR
6	H	251	ASN
6	H	260	ILE
6	H	287	THR
6	H	308	TYR
6	H	312	GLN
6	H	316	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	1627	GLN
4	B	1634	GLN
4	B	1647	HIS
4	B	1687	HIS
4	B	1693	HIS
4	B	1695	GLN
4	B	1703	ASN
4	B	1758	GLN
4	B	1760	ASN
4	B	1968	HIS
4	B	2024	HIS
4	B	2082	GLN
4	B	2124	GLN
4	B	2167	GLN
4	B	2178	ASN
4	B	2292	ASN
4	B	2410	HIS
4	B	2537	ASN
4	B	2540	GLN

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Mol	Chain	Res	Type
6	D	28	GLN
6	D	137	HIS
6	D	139	ASN
6	D	140	GLN
6	D	153	HIS
6	D	161	HIS
6	D	209	GLN
6	D	219	HIS
6	D	312	GLN
4	F	1634	GLN
4	F	1647	HIS
4	F	1687	HIS
4	F	1695	GLN
4	F	1703	ASN
4	F	1758	GLN
4	F	1760	ASN
4	F	1968	HIS
4	F	2024	HIS
4	F	2082	GLN
4	F	2124	GLN
4	F	2167	GLN
4	F	2178	ASN
4	F	2292	ASN
4	F	2395	ASN
4	F	2410	HIS
4	F	2537	ASN
4	F	2540	GLN
6	H	28	GLN
6	H	140	GLN
6	H	153	HIS
6	H	161	HIS
6	H	209	GLN
6	H	219	HIS
6	H	312	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
7	RAP	C	999	-	64,68,68	1.37	6 (9%)	63,96,96	2.91	21 (33%)
7	RAP	G	999	-	64,68,68	1.37	6 (9%)	63,96,96	2.91	21 (33%)

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
7	RAP	C	999	-	1/1/23/29	2/81/124/124	0/2/4/4
7	RAP	G	999	-	1/1/23/29	2/81/124/124	0/2/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	999	RAP	C8-C9	-5.20	1.47	1.53
7	G	999	RAP	C8-C9	-5.16	1.47	1.53
7	C	999	RAP	O1-C34	-2.03	1.42	1.46
7	G	999	RAP	O1-C34	-2.02	1.42	1.46
7	C	999	RAP	C27-C28	2.61	1.56	1.52
7	G	999	RAP	C27-C28	2.65	1.56	1.52
7	G	999	RAP	C2-N7	2.98	1.50	1.47
7	C	999	RAP	C2-N7	3.04	1.50	1.47
7	G	999	RAP	O6-C10	3.32	1.44	1.39
7	C	999	RAP	O6-C10	3.34	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	999	RAP	O1-C1	4.30	1.44	1.34
7	G	999	RAP	O1-C1	4.31	1.44	1.34

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	999	RAP	O5-C10-C11	-11.84	94.90	110.23
7	C	999	RAP	O5-C10-C11	-11.82	94.94	110.23
7	C	999	RAP	C48-C31-C30	-6.67	104.58	110.75
7	G	999	RAP	C48-C31-C30	-6.66	104.59	110.75
7	C	999	RAP	C43-C11-C12	-4.90	102.51	110.44
7	G	999	RAP	C43-C11-C12	-4.89	102.53	110.44
7	G	999	RAP	C47-C29-C30	-4.14	112.80	123.66
7	C	999	RAP	C47-C29-C30	-4.14	112.80	123.66
7	G	999	RAP	C20-C19-C18	-4.03	114.54	123.23
7	C	999	RAP	C20-C19-C18	-4.00	114.60	123.23
7	C	999	RAP	C12-C13-C14	-3.76	104.80	110.81
7	G	999	RAP	C12-C13-C14	-3.76	104.81	110.81
7	C	999	RAP	C45-C23-C22	-3.00	104.70	110.69
7	G	999	RAP	C45-C23-C22	-3.00	104.70	110.69
7	C	999	RAP	C16-C17-C18	-2.64	113.53	119.61
7	G	999	RAP	C16-C17-C18	-2.63	113.55	119.61
7	C	999	RAP	C5-C4-C3	-2.23	106.84	111.44
7	G	999	RAP	C5-C4-C3	-2.22	106.85	111.44
7	C	999	RAP	O11-C32-C33	-2.22	118.58	121.45
7	G	999	RAP	O11-C32-C33	-2.22	118.58	121.45
7	G	999	RAP	O1-C1-O2	-2.09	119.83	123.88
7	C	999	RAP	O1-C1-O2	-2.07	119.86	123.88
7	C	999	RAP	C51-O9-C27	2.24	117.24	113.92
7	G	999	RAP	C15-C16-C17	2.31	116.99	113.68
7	C	999	RAP	C36-C35-C34	2.33	116.97	111.54
7	G	999	RAP	C36-C35-C34	2.34	116.99	111.54
7	C	999	RAP	C15-C16-C17	2.34	117.03	113.68
7	G	999	RAP	C51-O9-C27	2.44	117.54	113.92
7	C	999	RAP	O1-C1-C2	2.67	116.61	110.75
7	G	999	RAP	O1-C1-C2	2.68	116.63	110.75
7	C	999	RAP	O5-C14-C15	3.49	112.07	106.00
7	G	999	RAP	O5-C14-C15	3.51	112.11	106.00
7	C	999	RAP	O5-C14-C13	3.89	115.04	109.98
7	G	999	RAP	O5-C14-C13	3.91	115.06	109.98
7	G	999	RAP	C44-C17-C16	4.23	125.36	115.22
7	C	999	RAP	C44-C17-C16	4.26	125.41	115.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	999	RAP	C47-C29-C28	4.35	126.61	116.08
7	C	999	RAP	C47-C29-C28	4.35	126.62	116.08
7	G	999	RAP	C12-C11-C10	4.52	117.03	109.93
7	C	999	RAP	C12-C11-C10	4.56	117.09	109.93
7	C	999	RAP	C43-C11-C10	9.85	121.40	111.97
7	G	999	RAP	C43-C11-C10	9.89	121.44	111.97

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	G	999	RAP	C10
7	C	999	RAP	C10

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	999	RAP	C50-O7-C16-C15
7	C	999	RAP	C50-O7-C16-C15
7	G	999	RAP	C31-C30-C29-C28
7	C	999	RAP	C31-C30-C29-C28

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	999	RAP	6	0
7	G	999	RAP	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.