



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 12, 2017 – 01:47 PM EST

PDB ID : 5X6O
EMDB ID: : EMD-6708
Title : Intact ATR/Mec1-ATRIP/Ddc2 complex
Authors : Wang, X.; Ran, T.; Cai, G.
Deposited on : unknown
Resolution : 3.90 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

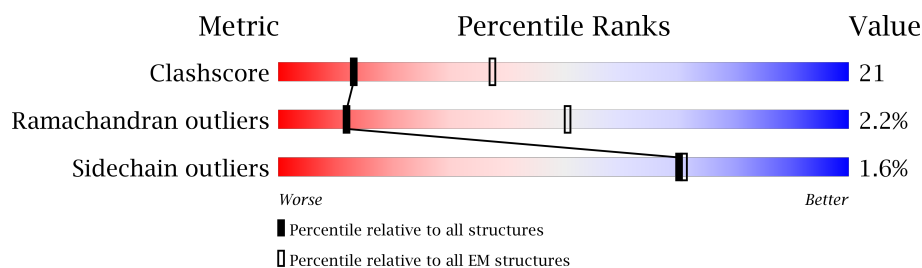
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	C	2368	
2	G	747	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 19309 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.

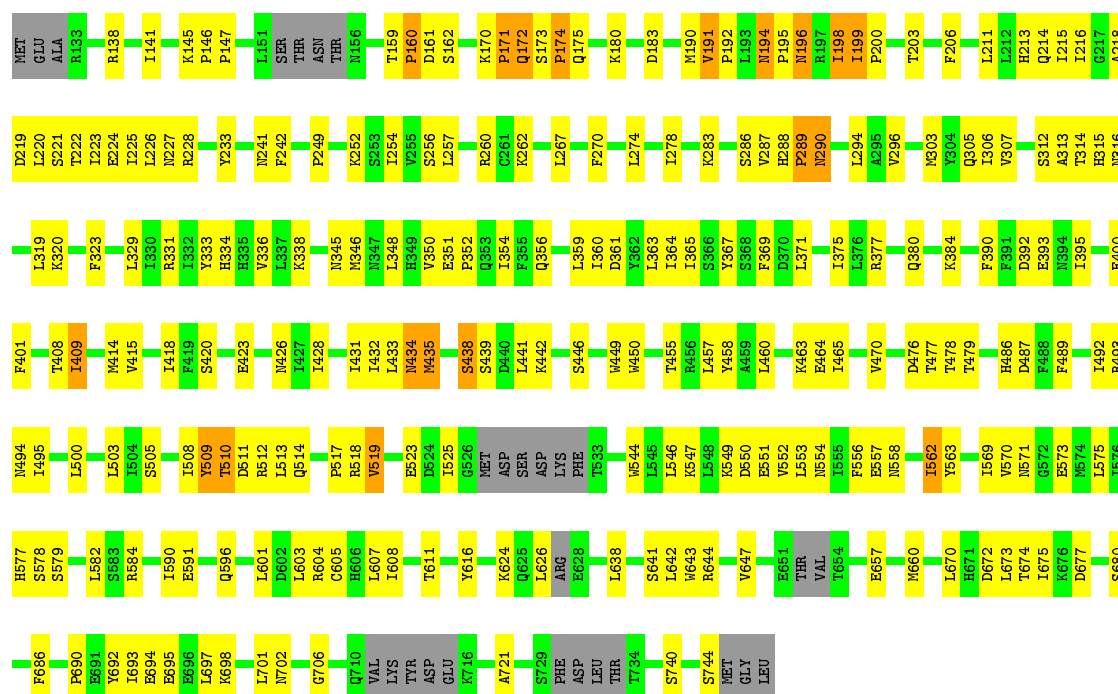
- Molecule 1 is a protein called Serine/threonine-protein kinase MEC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	1997	Total	C	N	O	S	0	0
			14240	8995	2502	2692	51		

- Molecule 2 is a protein called DNA damage checkpoint protein LCD1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	704	Total	C	N	O	S	0	0
			5069	3234	875	941	19		





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	63132	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	C	0.36	0/14428	0.55	20/19608 (0.1%)
2	G	0.41	0/5140	0.58	6/6985 (0.1%)
All	All	0.37	0/19568	0.56	26/26593 (0.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2018	PRO	N-CA-CB	6.85	111.52	103.30
2	G	160	PRO	N-CA-CB	6.70	111.34	103.30
1	C	356	PRO	N-CA-CB	6.57	111.18	103.30
2	G	171	PRO	N-CA-CB	6.24	110.79	103.30
1	C	1849	PRO	N-CA-CB	6.14	110.67	103.30
2	G	146	PRO	N-CA-CB	6.13	110.66	103.30
2	G	192	PRO	N-CA-CB	6.10	110.62	103.30
1	C	2039	PRO	N-CA-CB	6.03	110.53	103.30
1	C	1931	PRO	N-CA-CB	5.98	110.47	103.30
1	C	1893	PRO	N-CA-CB	5.95	110.44	103.30
1	C	1311	PRO	N-CA-CB	5.95	110.44	103.30
1	C	375	PRO	N-CA-CB	5.89	110.37	103.30
1	C	1207	PRO	N-CA-CB	5.74	110.19	103.30
1	C	2012	PRO	N-CA-CB	5.74	110.19	103.30
1	C	1246	PRO	N-CA-CB	5.72	110.17	103.30
1	C	1967	PRO	N-CA-CB	5.70	110.14	103.30
1	C	2042	PRO	N-CA-CB	5.69	110.12	103.30
2	G	147	PRO	N-CA-CB	5.66	110.09	103.30
1	C	2062	PRO	N-CA-CB	5.62	110.04	103.30
1	C	2028	PRO	N-CA-CB	5.61	110.03	103.30
1	C	1275	PRO	N-CA-CB	5.60	110.02	103.30
1	C	385	PRO	N-CA-CB	5.58	110.00	103.30
1	C	1396	PRO	N-CA-CB	5.57	109.98	103.30
1	C	808	PRO	N-CA-CB	5.56	109.97	103.30
2	G	174	PRO	N-CA-CB	5.54	109.95	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	1242	PRO	N-CA-CB	5.37	109.74	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	14240	0	12588	563	0
2	G	5069	0	4486	194	0
All	All	19309	0	17074	747	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 21.

All (747) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:685:SER:HB3	1:C:686:PRO:CD	1.30	1.44
1:C:2167:VAL:CG1	1:C:2168:ASP:H	1.32	1.38
2:G:191:VAL:CB	2:G:195:PRO:HD2	1.54	1.37
1:C:2265:THR:HB	1:C:2266:PRO:CD	1.57	1.29
1:C:1124:GLY:O	1:C:1125:VAL:HG22	1.35	1.24
1:C:1124:GLY:O	1:C:1125:VAL:CG2	1.86	1.24
1:C:2265:THR:CB	1:C:2266:PRO:HD2	1.64	1.23
1:C:2167:VAL:HG13	1:C:2168:ASP:N	1.42	1.21
1:C:685:SER:CB	1:C:686:PRO:CD	2.18	1.18
1:C:685:SER:CB	1:C:686:PRO:HD2	1.74	1.17
2:G:191:VAL:CB	2:G:195:PRO:CD	2.32	1.08
1:C:685:SER:HB3	1:C:686:PRO:HD3	1.38	1.03
1:C:648:LEU:HA	1:C:687:ILE:CD1	1.91	1.01
1:C:648:LEU:CA	1:C:687:ILE:HD11	1.90	0.99
2:G:233:TYR:HD2	2:G:290:ASN:O	1.49	0.94
2:G:233:TYR:CD2	2:G:290:ASN:O	2.20	0.94
2:G:198:ILE:CG2	2:G:199:ILE:N	2.31	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1852:ILE:O	1:C:1856:LEU:CB	2.16	0.93
1:C:518:ILE:HD13	1:C:518:ILE:H	1.34	0.91
1:C:1876:LYS:O	1:C:1880:ASP:N	2.03	0.91
1:C:1125:VAL:HG21	1:C:1656:ILE:HG22	1.53	0.90
1:C:1124:GLY:C	1:C:1125:VAL:HG22	1.89	0.90
1:C:2252:LYS:HD3	1:C:2360:MET:HG2	1.56	0.88
2:G:198:ILE:HG22	2:G:199:ILE:H	1.39	0.88
1:C:586:LEU:HD13	2:G:590:ILE:HD11	1.54	0.87
1:C:2167:VAL:CG1	1:C:2168:ASP:N	2.03	0.87
1:C:1570:LEU:O	1:C:1574:ASN:ND2	2.08	0.87
1:C:558:LYS:HB3	1:C:601:HIS:CD2	2.10	0.87
2:G:233:TYR:CD2	2:G:290:ASN:HB3	2.10	0.86
1:C:1124:GLY:O	1:C:1125:VAL:HG23	1.74	0.84
1:C:318:HIS:O	1:C:320:PRO:HD3	1.78	0.84
1:C:648:LEU:CA	1:C:687:ILE:CD1	2.54	0.84
1:C:585:ARG:HB3	1:C:626:ASN:HD21	1.44	0.83
1:C:2145:LYS:HB3	1:C:2184:ILE:HD13	1.61	0.82
1:C:2185:LEU:O	1:C:2185:LEU:HD23	1.78	0.82
1:C:686:PRO:O	1:C:689:PRO:HD2	1.79	0.82
1:C:846:THR:O	1:C:850:LYS:CB	2.27	0.82
1:C:2112:LEU:HD22	1:C:2212:VAL:HG11	1.62	0.82
2:G:400:GLU:HB2	2:G:449:TRP:HE1	1.44	0.82
1:C:685:SER:HB3	1:C:686:PRO:HD2	0.84	0.82
1:C:2252:LYS:CD	1:C:2360:MET:HG2	2.09	0.81
1:C:2263:ARG:HH11	1:C:2263:ARG:HG2	1.46	0.80
1:C:557:PRO:HG2	1:C:566:ILE:CG2	2.12	0.80
1:C:2196:PRO:HA	1:C:2199:TRP:HB3	1.63	0.80
1:C:558:LYS:CB	1:C:601:HIS:CD2	2.65	0.79
2:G:198:ILE:CG2	2:G:199:ILE:H	1.93	0.79
1:C:2171:LEU:HD23	1:C:2359:LYS:HB2	1.61	0.79
1:C:845:ILE:HG12	1:C:875:LYS:HZ2	1.46	0.79
2:G:198:ILE:HG23	2:G:199:ILE:N	1.96	0.79
2:G:172:GLN:O	2:G:175:GLN:N	2.15	0.78
2:G:435:MET:HA	2:G:435:MET:CE	2.11	0.77
1:C:525:ASN:O	1:C:529:HIS:NE2	2.18	0.77
1:C:1290:LEU:O	1:C:1290:LEU:HD12	1.84	0.77
1:C:2285:SER:O	1:C:2288:THR:OG1	2.04	0.76
2:G:638:LEU:O	2:G:641:SER:OG	2.03	0.75
2:G:233:TYR:HD2	2:G:290:ASN:C	1.89	0.75
1:C:2295:ASN:HD21	1:C:2299:LEU:HD23	1.52	0.75
1:C:1887:GLU:O	1:C:1891:HIS:N	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2265:THR:HB	1:C:2266:PRO:HD2	0.78	0.74
1:C:440:SER:HB2	1:C:521:ILE:HD12	1.69	0.74
1:C:2167:VAL:HG13	1:C:2168:ASP:H	0.58	0.73
1:C:961:GLU:CD	1:C:962:LEU:H	1.91	0.73
1:C:493:CYS:SG	1:C:553:HIS:NE2	2.62	0.73
2:G:384:LYS:O	2:G:435:MET:CG	2.37	0.73
2:G:218:ALA:HB1	2:G:505:SER:HB2	1.70	0.73
1:C:2293:ARG:NH1	1:C:2343:GLN:OE1	2.22	0.72
1:C:648:LEU:N	1:C:687:ILE:HD11	2.03	0.72
1:C:1598:PHE:HA	1:C:1601:ILE:HG22	1.73	0.71
2:G:222:THR:HA	2:G:225:ILE:HG22	1.72	0.71
1:C:648:LEU:CB	1:C:687:ILE:HD11	2.20	0.71
2:G:463:LYS:HE2	2:G:477:THR:HA	1.73	0.71
2:G:509:TYR:HD2	2:G:511:ASP:H	1.39	0.71
1:C:1125:VAL:CG2	1:C:1656:ILE:HG22	2.20	0.71
1:C:2205:THR:O	1:C:2209:SER:HB3	1.91	0.71
1:C:465:LEU:O	1:C:469:GLU:N	2.23	0.71
1:C:2167:VAL:HG13	1:C:2168:ASP:OD1	1.90	0.70
2:G:198:ILE:HG23	2:G:199:ILE:O	1.91	0.70
1:C:506:ASN:ND2	1:C:508:ASN:O	2.24	0.70
1:C:2196:PRO:O	1:C:2200:PHE:N	2.22	0.70
2:G:348:LEU:HD13	2:G:350:VAL:HG12	1.72	0.70
1:C:1002:LEU:HD12	1:C:1006:LEU:HB2	1.74	0.69
1:C:1564:ILE:HD12	2:G:352:PRO:HD3	1.74	0.69
1:C:237:ALA:HB1	1:C:289:LEU:HD21	1.73	0.69
1:C:1958:GLU:O	1:C:1962:GLN:N	2.24	0.69
2:G:363:LEU:HD22	2:G:367:TYR:HE2	1.58	0.69
1:C:1099:LEU:HD22	1:C:1606:ILE:HD11	1.75	0.69
2:G:433:LEU:O	2:G:434:ASN:O	2.10	0.69
1:C:317:ASP:OD1	1:C:318:HIS:ND1	2.26	0.68
1:C:518:ILE:HD13	1:C:518:ILE:N	2.07	0.68
2:G:211:LEU:HD12	2:G:223:ILE:HG21	1.74	0.68
1:C:1876:LYS:O	1:C:1879:GLU:N	2.25	0.68
1:C:443:ILE:O	1:C:447:PHE:N	2.25	0.68
1:C:919:LYS:HD2	1:C:922:ILE:HD12	1.76	0.68
1:C:593:PRO:HG3	1:C:633:GLN:HB3	1.73	0.68
1:C:648:LEU:HB2	1:C:687:ILE:HD11	1.75	0.68
2:G:384:LYS:O	2:G:435:MET:HG3	1.93	0.68
1:C:579:ASN:OD1	1:C:580:SER:N	2.27	0.67
1:C:309:ASN:OD1	1:C:310:ASP:N	2.27	0.67
1:C:2265:THR:CB	1:C:2266:PRO:CD	2.35	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:518:ILE:H	1:C:518:ILE:CD1	1.99	0.67
2:G:67:GLN:O	2:G:71:ALA:N	2.26	0.67
1:C:628:VAL:HG11	1:C:664:MET:HG2	1.76	0.67
1:C:1470:LEU:HB2	1:C:1479:ALA:HB2	1.75	0.67
1:C:2110:ARG:HH22	1:C:2283:LYS:HE2	1.60	0.67
1:C:685:SER:CB	1:C:686:PRO:HD3	2.07	0.67
1:C:1127:ASP:OD1	1:C:1129:THR:OG1	2.12	0.67
1:C:1185:GLN:NE2	1:C:1220:SER:O	2.27	0.67
2:G:582:LEU:HD12	2:G:608:ILE:HD11	1.77	0.67
1:C:1185:GLN:HE21	1:C:1224:ILE:H	1.41	0.67
1:C:1021:GLY:O	1:C:1025:ARG:N	2.27	0.66
1:C:835:ASN:O	1:C:839:CYS:N	2.24	0.66
1:C:1072:LYS:O	1:C:1076:ARG:N	2.28	0.66
1:C:920:LYS:NZ	1:C:1218:SER:O	2.29	0.65
1:C:415:TYR:OH	1:C:484:MET:O	2.10	0.65
1:C:578:MET:SD	1:C:618:GLN:NE2	2.69	0.65
1:C:1897:TRP:O	1:C:1901:LEU:N	2.24	0.65
1:C:2167:VAL:CG1	1:C:2168:ASP:OD1	2.44	0.65
1:C:543:ILE:O	1:C:547:LEU:N	2.28	0.65
1:C:632:THR:O	1:C:635:THR:OG1	2.15	0.65
1:C:2265:THR:CG2	1:C:2266:PRO:HD2	2.27	0.65
2:G:241:ASN:O	2:G:260:ARG:NH2	2.30	0.65
2:G:27:ARG:O	2:G:31:ILE:N	2.21	0.65
2:G:369:PHE:O	2:G:420:SER:OG	2.10	0.65
2:G:392:ASP:H	2:G:395:ILE:HG22	1.61	0.65
1:C:2123:ARG:HB2	1:C:2126:CYS:H	1.61	0.64
1:C:2216:VAL:HA	1:C:2219:ILE:HD12	1.78	0.64
1:C:2223:GLY:HA2	1:C:2245:ASP:OD2	1.95	0.64
1:C:1102:SER:OG	1:C:1116:CYS:SG	2.51	0.64
1:C:297:LYS:O	1:C:301:ARG:N	2.29	0.64
1:C:509:ARG:HB2	1:C:510:PRO:HD2	1.78	0.64
1:C:1779:SER:HA	1:C:1782:ILE:HD12	1.79	0.64
1:C:322:ASP:HA	1:C:325:ALA:HB2	1.78	0.64
1:C:648:LEU:HA	1:C:687:ILE:HD12	1.76	0.64
1:C:1544:LEU:O	1:C:1672:SER:OG	2.16	0.64
1:C:1742:VAL:HG12	1:C:1767:PHE:HD1	1.61	0.64
1:C:440:SER:HB2	1:C:521:ILE:CD1	2.28	0.64
1:C:1594:ILE:HG21	1:C:1631:SER:HB2	1.80	0.64
2:G:28:PHE:O	2:G:32:PRO:N	2.30	0.64
1:C:1049:ASN:ND2	1:C:1061:ASN:OD1	2.29	0.63
1:C:929:ILE:O	1:C:933:LEU:N	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2139:ARG:O	1:C:2143:SER:OG	2.10	0.63
1:C:452:ILE:HG13	1:C:453:THR:HG23	1.80	0.63
1:C:1054:ASN:HB3	1:C:1057:VAL:HG12	1.80	0.63
1:C:925:ALA:O	1:C:928:GLN:N	2.32	0.63
1:C:1017:LYS:HE3	1:C:1019:GLU:HB3	1.79	0.62
1:C:845:ILE:HG12	1:C:875:LYS:NZ	2.15	0.62
1:C:2088:ASN:O	1:C:2092:GLN:N	2.25	0.62
1:C:2117:TYR:CE1	1:C:2240:LEU:HD21	2.35	0.62
1:C:517:GLU:OE2	1:C:521:ILE:CG1	2.48	0.62
1:C:895:GLU:HB3	1:C:898:THR:HG22	1.80	0.62
2:G:446:SER:O	2:G:450:TRP:N	2.29	0.62
2:G:702:ASN:O	2:G:706:GLY:N	2.31	0.62
1:C:1185:GLN:O	1:C:1189:LYS:N	2.33	0.62
1:C:2359:LYS:O	1:C:2359:LYS:HG3	2.00	0.62
2:G:249:PRO:HG2	2:G:252:LYS:HB2	1.82	0.62
2:G:438:SER:O	2:G:441:LEU:N	2.33	0.62
2:G:287:VAL:HG12	2:G:287:VAL:O	2.00	0.62
1:C:1412:ARG:HA	1:C:2196:PRO:HG2	1.82	0.62
1:C:912:PHE:HA	1:C:915:ILE:HD12	1.82	0.62
1:C:521:ILE:O	1:C:525:ASN:ND2	2.32	0.62
1:C:1355:TYR:O	1:C:1355:TYR:HD1	1.83	0.61
1:C:1756:ASN:HB2	1:C:1759:ASP:H	1.64	0.61
1:C:775:ALA:O	1:C:779:HIS:N	2.30	0.61
1:C:2167:VAL:HG12	1:C:2168:ASP:N	2.11	0.61
1:C:2213:MET:HG2	1:C:2241:HIS:HD2	1.65	0.61
1:C:2243:ASP:OD1	1:C:2244:PHE:N	2.33	0.61
1:C:1435:LEU:HD13	1:C:1458:PHE:HD2	1.66	0.61
1:C:1778:ALA:O	1:C:1782:ILE:N	2.33	0.61
1:C:558:LYS:HB2	1:C:601:HIS:CD2	2.36	0.61
2:G:334:HIS:HB3	2:G:338:LYS:HD3	1.83	0.61
2:G:384:LYS:O	2:G:435:MET:HG2	1.99	0.61
1:C:2175:MET:CE	1:C:2358:SER:OG	2.48	0.61
2:G:345:ASN:OD1	2:G:346:MET:N	2.33	0.61
1:C:2217:GLY:O	1:C:2221:GLY:N	2.34	0.60
1:C:953:LEU:HD22	1:C:957:LEU:HD12	1.83	0.60
2:G:408:THR:O	2:G:409:ILE:HG12	2.01	0.60
1:C:1969:ASP:O	1:C:1973:SER:N	2.27	0.60
1:C:512:ALA:O	1:C:516:SER:OG	2.18	0.60
1:C:540:LEU:HD11	1:C:572:LEU:HD11	1.83	0.60
1:C:1424:ASN:HB2	1:C:1425:PRO:HD3	1.82	0.60
1:C:2365:LEU:O	1:C:2365:LEU:HD23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:516:SER:OG	1:C:519:PHE:HB3	2.02	0.60
1:C:991:ILE:O	1:C:994:THR:OG1	2.17	0.60
2:G:331:ARG:HG3	2:G:401:PHE:HE2	1.67	0.60
2:G:89:ARG:H	2:G:686:PHE:HZ	1.50	0.60
1:C:1941:LEU:O	1:C:1945:ASN:N	2.32	0.60
2:G:313:ALA:O	2:G:316:ASN:ND2	2.35	0.60
1:C:2263:ARG:HH11	1:C:2263:ARG:CG	2.15	0.59
1:C:2243:ASP:CG	1:C:2244:PHE:H	2.06	0.59
1:C:839:CYS:HA	1:C:842:ARG:HD3	1.85	0.59
1:C:880:ILE:HD12	1:C:883:ILE:HD11	1.84	0.59
1:C:926:LEU:HA	1:C:929:ILE:HG22	1.83	0.59
2:G:233:TYR:CE2	2:G:290:ASN:O	2.56	0.59
1:C:1057:VAL:O	1:C:1061:ASN:ND2	2.35	0.59
1:C:1438:LEU:HD22	1:C:1442:TYR:HE2	1.68	0.59
1:C:2252:LYS:HB3	1:C:2360:MET:HA	1.83	0.59
1:C:928:GLN:HE21	1:C:932:CYS:HB2	1.68	0.59
1:C:1960:TYR:O	1:C:1964:SER:N	2.29	0.59
1:C:386:PHE:O	1:C:389:ARG:N	2.36	0.59
1:C:741:LEU:O	1:C:745:ALA:N	2.32	0.59
1:C:266:VAL:HG23	1:C:267:CYS:H	1.66	0.59
2:G:120:LYS:O	2:G:124:GLU:N	2.27	0.59
2:G:434:ASN:O	2:G:435:MET:C	2.39	0.59
2:G:690:PRO:O	2:G:694:GLU:N	2.28	0.59
1:C:886:VAL:O	1:C:889:SER:OG	2.18	0.58
2:G:514:GLN:N	2:G:514:GLN:OE1	2.33	0.58
1:C:2145:LYS:O	1:C:2148:SER:OG	2.15	0.58
1:C:487:TRP:HZ2	1:C:490:CYS:HB2	1.68	0.58
2:G:172:GLN:O	2:G:174:PRO:N	2.36	0.58
1:C:2171:LEU:HA	1:C:2174:TYR:HE1	1.68	0.58
1:C:1568:GLU:HA	1:C:1605:PHE:HZ	1.68	0.58
1:C:919:LYS:HA	1:C:922:ILE:HD12	1.86	0.58
1:C:1982:THR:O	1:C:1986:LEU:N	2.37	0.58
1:C:290:ASP:CG	1:C:291:ASN:H	2.07	0.58
1:C:301:ARG:O	1:C:304:SER:OG	2.13	0.58
1:C:770:GLN:O	1:C:774:VAL:N	2.29	0.58
1:C:1114:GLU:HB2	1:C:1599:ARG:HG2	1.84	0.58
1:C:1356:CYS:HA	1:C:1359:TRP:HB3	1.86	0.58
1:C:512:ALA:O	1:C:519:PHE:HD2	1.87	0.58
1:C:541:SER:HA	1:C:544:LEU:HD12	1.86	0.58
1:C:585:ARG:HH21	1:C:626:ASN:ND2	2.01	0.58
1:C:1704:ASP:OD1	1:C:1704:ASP:N	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2354:GLU:OE1	1:C:2354:GLU:HA	2.03	0.57
1:C:648:LEU:HB2	1:C:687:ILE:CD1	2.34	0.57
1:C:1140:GLU:N	1:C:1140:GLU:OE1	2.37	0.57
1:C:1993:THR:O	1:C:1997:GLY:N	2.37	0.57
1:C:2086:GLN:NE2	1:C:2243:ASP:O	2.36	0.57
1:C:2092:GLN:O	1:C:2095:THR:OG1	2.13	0.57
2:G:351:GLU:HB3	2:G:352:PRO:HD2	1.86	0.57
2:G:670:LEU:O	2:G:673:LEU:N	2.38	0.57
1:C:443:ILE:HA	1:C:446:CYS:HB2	1.86	0.57
1:C:729:ILE:HG13	1:C:730:PRO:HD3	1.87	0.57
2:G:489:PHE:HB3	2:G:494:ASN:HD22	1.69	0.57
2:G:119:GLN:O	2:G:123:ASP:N	2.37	0.57
2:G:390:PHE:CZ	2:G:395:ILE:HG12	2.40	0.57
2:G:476:ASP:C	2:G:478:THR:H	2.08	0.57
1:C:609:ALA:HA	1:C:612:ILE:HD12	1.87	0.57
1:C:2185:LEU:HD23	1:C:2185:LEU:C	2.25	0.56
1:C:994:THR:O	1:C:998:GLU:N	2.35	0.56
1:C:1160:ILE:HA	1:C:1164:LEU:HD12	1.86	0.56
1:C:1322:GLU:O	1:C:1326:ILE:N	2.31	0.56
1:C:1564:ILE:HG22	1:C:1566:ASP:H	1.70	0.56
1:C:2220:LEU:HB3	1:C:2222:LEU:HD13	1.87	0.56
1:C:585:ARG:HB3	1:C:626:ASN:ND2	2.17	0.56
1:C:1064:ASP:O	1:C:1068:TYR:N	2.37	0.56
1:C:659:TYR:HA	1:C:662:ARG:HG2	1.87	0.56
1:C:2263:ARG:C	1:C:2263:ARG:HD2	2.26	0.56
2:G:380:GLN:HG3	2:G:431:ILE:HD13	1.88	0.56
1:C:317:ASP:OD1	1:C:318:HIS:N	2.38	0.56
2:G:214:GLN:NE2	2:G:218:ALA:O	2.39	0.56
1:C:590:ARG:NH2	2:G:591:GLU:O	2.38	0.56
1:C:2185:LEU:HB3	1:C:2271:ALA:HB2	1.86	0.56
1:C:868:GLN:HA	1:C:871:ALA:HB3	1.87	0.56
1:C:1412:ARG:CA	1:C:2196:PRO:HG2	2.36	0.55
1:C:2319:ALA:O	1:C:2323:LEU:HB2	2.06	0.55
1:C:1772:ASP:OD1	1:C:1782:ILE:HG12	2.07	0.55
1:C:2227:CYS:O	1:C:2230:ILE:HG22	2.07	0.55
1:C:2135:VAL:HG21	1:C:2231:LEU:HD11	1.88	0.55
1:C:2270:ASP:C	1:C:2272:LEU:H	2.08	0.55
1:C:416:ARG:O	1:C:420:LEU:N	2.40	0.55
1:C:1194:SER:O	1:C:1198:TRP:N	2.39	0.55
1:C:2302:VAL:HG13	1:C:2303:ILE:H	1.70	0.55
2:G:334:HIS:HE1	2:G:401:PHE:CZ	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:648:LEU:CB	1:C:687:ILE:CD1	2.84	0.55
1:C:2087:ASP:O	1:C:2091:MET:N	2.31	0.55
2:G:392:ASP:OD1	2:G:393:GLU:N	2.39	0.55
2:G:438:SER:O	2:G:442:LYS:N	2.30	0.55
1:C:1560:SER:HB3	2:G:519:VAL:HG22	1.89	0.55
1:C:318:HIS:C	1:C:320:PRO:HD3	2.27	0.55
2:G:303:MET:HA	2:G:306:ILE:HD12	1.88	0.55
2:G:509:TYR:CE2	2:G:512:ARG:HG3	2.42	0.55
1:C:1804:GLY:HA2	1:C:1807:TYR:HB3	1.89	0.54
1:C:2190:LEU:HA	1:C:2199:TRP:CD1	2.42	0.54
1:C:447:PHE:HA	1:C:455:LEU:HD12	1.89	0.54
1:C:1764:LEU:HD23	1:C:1789:ILE:HG12	1.89	0.54
2:G:428:ILE:O	2:G:432:ILE:HG12	2.07	0.54
2:G:66:ASN:O	2:G:70:LYS:N	2.35	0.54
1:C:1614:LEU:HD12	1:C:1617:LYS:HD2	1.89	0.54
1:C:662:ARG:NH1	1:C:708:ASN:OD1	2.41	0.54
1:C:2175:MET:HE1	1:C:2358:SER:OG	2.07	0.54
1:C:2213:MET:HG2	1:C:2241:HIS:CD2	2.42	0.54
1:C:921:SER:HA	1:C:924:SER:HB2	1.90	0.54
2:G:578:SER:OG	2:G:579:SER:N	2.40	0.54
1:C:2320:LEU:O	1:C:2323:LEU:HB3	2.08	0.54
1:C:458:TRP:O	1:C:462:LEU:HG	2.07	0.54
1:C:558:LYS:HB3	1:C:601:HIS:NE2	2.23	0.54
1:C:1756:ASN:HD22	1:C:1759:ASP:HB2	1.71	0.54
2:G:53:LEU:O	2:G:57:GLN:N	2.41	0.54
1:C:506:ASN:O	1:C:509:ARG:NH1	2.40	0.54
1:C:880:ILE:HD11	1:C:913:LEU:HD21	1.89	0.54
1:C:557:PRO:HG2	1:C:566:ILE:HG23	1.88	0.53
1:C:2110:ARG:NH2	1:C:2283:LYS:HE2	2.22	0.53
1:C:2263:ARG:HG3	1:C:2263:ARG:O	2.08	0.53
2:G:557:GLU:N	2:G:557:GLU:OE1	2.37	0.53
1:C:1165:VAL:HB	1:C:1166:PRO:HD3	1.89	0.53
1:C:1734:GLU:HG2	1:C:1737:ARG:HD2	1.91	0.53
2:G:305:GLN:NE2	2:G:305:GLN:O	2.41	0.53
1:C:2273:GLY:O	1:C:2275:ILE:HG12	2.08	0.53
1:C:961:GLU:OE1	1:C:962:LEU:N	2.36	0.53
2:G:350:VAL:O	2:G:351:GLU:HG3	2.08	0.53
1:C:1300:LEU:HB3	1:C:1304:ILE:HD11	1.91	0.53
1:C:1810:LEU:HD22	1:C:1811:LEU:HD12	1.91	0.53
1:C:786:ILE:O	1:C:790:LEU:N	2.41	0.53
1:C:1001:ASP:OD1	1:C:1002:LEU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2247:LEU:HD22	1:C:2247:LEU:N	2.24	0.53
2:G:334:HIS:HE1	2:G:401:PHE:HZ	1.56	0.53
1:C:1804:GLY:O	1:C:1808:SER:N	2.32	0.53
1:C:290:ASP:OD1	1:C:291:ASN:N	2.40	0.53
2:G:191:VAL:CB	2:G:195:PRO:HD3	2.33	0.53
1:C:884:PHE:HA	1:C:887:PHE:HB2	1.90	0.53
1:C:1138:TYR:HD1	1:C:1138:TYR:H	1.53	0.52
1:C:1659:ASP:OD1	1:C:1660:PHE:N	2.40	0.52
1:C:803:ILE:O	1:C:807:LEU:N	2.40	0.52
2:G:203:THR:HB	2:G:267:LEU:HD13	1.91	0.52
2:G:352:PRO:HB2	2:G:354:ILE:HG23	1.90	0.52
2:G:435:MET:CE	2:G:435:MET:CA	2.86	0.52
1:C:1147:ASN:O	1:C:1152:THR:OG1	2.27	0.52
1:C:2143:SER:HA	1:C:2146:TYR:CE2	2.44	0.52
1:C:510:PRO:HG2	1:C:554:PHE:HD1	1.73	0.52
1:C:1690:PHE:O	1:C:1693:LEU:N	2.43	0.52
1:C:1988:ASP:O	1:C:1992:ILE:N	2.35	0.52
1:C:2137:THR:HG22	1:C:2138:LEU:N	2.25	0.52
1:C:842:ARG:HH12	1:C:916:TYR:HB2	1.74	0.52
2:G:312:SER:HB2	2:G:314:THR:HG23	1.92	0.52
1:C:1181:ALA:O	1:C:1185:GLN:HG2	2.10	0.52
1:C:2273:GLY:O	1:C:2274:ILE:HG22	2.09	0.52
1:C:891:ILE:HD12	1:C:932:CYS:SG	2.50	0.52
1:C:2185:LEU:HD22	1:C:2271:ALA:HB1	1.91	0.52
1:C:2234:ILE:HG22	1:C:2235:GLN:H	1.73	0.52
2:G:194:ASN:N	2:G:195:PRO:HD3	2.24	0.52
1:C:582:ARG:HE	1:C:586:LEU:HD11	1.75	0.52
1:C:663:ILE:O	1:C:666:THR:OG1	2.17	0.52
1:C:2175:MET:HE3	1:C:2358:SER:OG	2.09	0.52
1:C:2325:ASN:O	1:C:2329:GLY:N	2.42	0.52
1:C:987:ILE:O	1:C:990:SER:OG	2.18	0.52
1:C:456:THR:O	1:C:459:THR:OG1	2.22	0.51
2:G:294:LEU:HD12	2:G:517:PRO:HG3	1.92	0.51
1:C:923:ILE:HD11	1:C:958:ASN:ND2	2.26	0.51
1:C:1541:ALA:O	1:C:1544:LEU:N	2.43	0.51
1:C:2154:SER:O	1:C:2157:SER:OG	2.26	0.51
1:C:981:ASN:OD1	1:C:982:GLY:N	2.43	0.51
1:C:500:ASN:O	1:C:503:VAL:HG12	2.10	0.51
1:C:557:PRO:O	1:C:566:ILE:HG12	2.10	0.51
1:C:1149:SER:O	1:C:1153:ILE:HG12	2.10	0.51
1:C:2137:THR:HG22	1:C:2138:LEU:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:323:PHE:CD1	2:G:395:ILE:HD11	2.45	0.51
1:C:647:LEU:HD22	1:C:687:ILE:HG13	1.92	0.51
1:C:889:SER:O	1:C:893:ASP:N	2.44	0.51
2:G:371:LEU:O	2:G:375:ILE:HG12	2.11	0.51
1:C:1746:HIS:NE2	1:C:1764:LEU:HD13	2.26	0.51
1:C:455:LEU:HD21	1:C:526:PHE:HE1	1.76	0.51
1:C:517:GLU:OE2	1:C:521:ILE:HG12	2.10	0.51
1:C:2042:PRO:O	1:C:2045:SER:N	2.43	0.51
1:C:557:PRO:O	1:C:566:ILE:HG23	2.09	0.51
2:G:509:TYR:O	2:G:510:THR:OG1	2.22	0.51
2:G:503:LEU:HD11	2:G:525:ILE:HD13	1.93	0.51
2:G:569:ILE:HG13	2:G:570:VAL:N	2.26	0.51
1:C:1091:ILE:HG23	1:C:1126:LEU:HD21	1.92	0.51
1:C:1188:LEU:O	1:C:1192:GLY:N	2.44	0.51
1:C:1427:ASP:HB2	1:C:1430:GLN:HG2	1.93	0.51
1:C:2360:MET:O	1:C:2361:TYR:C	2.48	0.51
1:C:742:SER:O	1:C:746:LYS:N	2.39	0.51
1:C:829:SER:N	1:C:832:GLU:HB2	2.26	0.51
1:C:1356:CYS:O	1:C:1360:ALA:N	2.32	0.50
1:C:1802:SER:HA	1:C:1805:LEU:HB3	1.91	0.50
2:G:392:ASP:O	2:G:395:ILE:HG22	2.10	0.50
2:G:455:THR:HA	2:G:458:TYR:HD2	1.76	0.50
1:C:1301:ASP:HA	1:C:1304:ILE:HD12	1.93	0.50
1:C:2175:MET:SD	1:C:2176:GLU:N	2.85	0.50
1:C:247:VAL:HA	1:C:250:TYR:HB3	1.91	0.50
1:C:1042:LEU:HB3	1:C:1046:PHE:CE2	2.47	0.50
1:C:436:LEU:HD13	1:C:517:GLU:HG2	1.93	0.50
2:G:206:PHE:CE2	2:G:270:PHE:HE2	2.30	0.50
1:C:1422:ARG:NH2	1:C:1423:GLN:HE21	2.09	0.50
1:C:996:ILE:HD11	1:C:1022:ILE:HD11	1.93	0.50
2:G:553:LEU:O	2:G:556:PHE:N	2.38	0.50
2:G:180:LYS:O	2:G:183:ASP:N	2.45	0.50
2:G:605:CYS:O	2:G:608:ILE:HG22	2.11	0.50
1:C:2314:HIS:CG	1:C:2315:SER:H	2.29	0.50
1:C:585:ARG:HD2	1:C:626:ASN:HD21	1.75	0.50
1:C:1382:THR:O	1:C:1386:LEU:N	2.40	0.50
1:C:845:ILE:CG1	1:C:875:LYS:NZ	2.75	0.50
2:G:198:ILE:O	2:G:199:ILE:HG22	2.11	0.50
2:G:224:GLU:HA	2:G:227:ASN:HB2	1.94	0.50
2:G:672:ASP:HA	2:G:675:ILE:HG22	1.94	0.50
1:C:2223:GLY:HA3	1:C:2245:ASP:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:161:ASP:O	2:G:162:SER:C	2.49	0.50
1:C:2222:LEU:HD11	1:C:2246:CYS:SG	2.52	0.49
1:C:2316:ILE:HG22	1:C:2319:ALA:H	1.77	0.49
1:C:1029:PHE:O	1:C:1032:MET:N	2.39	0.49
1:C:1438:LEU:HD22	1:C:1442:TYR:CE2	2.46	0.49
1:C:1617:LYS:O	1:C:1620:LEU:N	2.40	0.49
1:C:1851:VAL:O	1:C:1855:TRP:N	2.45	0.49
1:C:2096:THR:HA	1:C:2099:PHE:HB3	1.93	0.49
1:C:1321:ILE:O	1:C:1325:SER:N	2.45	0.49
1:C:510:PRO:HG2	1:C:554:PHE:CD1	2.47	0.49
1:C:2273:GLY:C	1:C:2275:ILE:H	2.16	0.49
1:C:2234:ILE:C	1:C:2236:THR:H	2.16	0.49
1:C:2252:LYS:HD2	1:C:2360:MET:HG2	1.89	0.49
1:C:585:ARG:HD2	1:C:626:ASN:ND2	2.28	0.49
1:C:1422:ARG:HA	1:C:2274:ILE:HD12	1.94	0.49
1:C:571:LYS:O	1:C:574:GLN:HB2	2.11	0.49
2:G:296:VAL:HG12	2:G:364:ILE:HD13	1.94	0.49
1:C:1071:ARG:O	1:C:1074:THR:OG1	2.31	0.49
1:C:625:GLU:O	1:C:629:ILE:HG12	2.13	0.49
2:G:608:ILE:O	2:G:611:THR:OG1	2.23	0.49
2:G:356:GLN:HG3	2:G:517:PRO:HB2	1.94	0.49
1:C:1959:LYS:O	1:C:1963:HIS:N	2.37	0.49
1:C:2057:SER:CB	1:C:2066:ASN:H	2.26	0.49
1:C:321:ILE:O	1:C:323:GLN:N	2.45	0.49
2:G:206:PHE:HE2	2:G:270:PHE:HE2	1.61	0.49
1:C:1755:VAL:HG12	1:C:1756:ASN:H	1.78	0.48
1:C:1778:ALA:O	1:C:1781:GLN:N	2.45	0.48
1:C:2268:LEU:O	1:C:2268:LEU:HD23	2.12	0.48
2:G:9:PHE:O	2:G:13:ASP:N	2.44	0.48
1:C:937:LEU:O	1:C:943:ARG:HG2	2.12	0.48
2:G:569:ILE:HG13	2:G:570:VAL:HG23	1.95	0.48
1:C:1076:ARG:HB2	1:C:1651:TYR:CZ	2.49	0.48
1:C:868:GLN:O	1:C:871:ALA:N	2.43	0.48
1:C:1185:GLN:HE21	1:C:1224:ILE:N	2.09	0.48
1:C:1345:CYS:O	1:C:1349:ILE:HG13	2.13	0.48
1:C:1562:ARG:O	1:C:1562:ARG:HG2	2.13	0.48
1:C:2143:SER:HA	1:C:2146:TYR:CZ	2.48	0.48
1:C:964:THR:HB	1:C:1169:TRP:CZ2	2.48	0.48
1:C:582:ARG:HH12	2:G:644:ARG:HG3	1.78	0.48
1:C:1799:PRO:O	1:C:1802:SER:N	2.47	0.48
1:C:2319:ALA:HA	1:C:2322:VAL:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1513:ILE:HG13	1:C:1514:SER:N	2.28	0.48
1:C:2342:GLY:O	1:C:2345:GLU:N	2.46	0.48
1:C:343:LEU:O	1:C:346:VAL:HG12	2.13	0.48
1:C:911:SER:O	1:C:915:ILE:HG13	2.13	0.48
1:C:1042:LEU:HB3	1:C:1046:PHE:HE2	1.78	0.48
1:C:1153:ILE:O	1:C:1156:LEU:N	2.47	0.48
2:G:465:ILE:HA	2:G:479:THR:OG1	2.14	0.48
2:G:607:LEU:O	2:G:611:THR:HG23	2.13	0.48
1:C:1355:TYR:CD1	1:C:1355:TYR:C	2.86	0.48
2:G:426:ASN:ND2	2:G:551:GLU:OE2	2.47	0.48
1:C:1300:LEU:HD11	1:C:1355:TYR:CE2	2.48	0.48
1:C:1406:GLU:OE1	1:C:1413:SER:OG	2.31	0.48
1:C:2263:ARG:NH1	1:C:2263:ARG:HG2	2.22	0.48
1:C:2302:VAL:HG13	1:C:2303:ILE:N	2.29	0.48
1:C:606:GLU:O	1:C:609:ALA:N	2.43	0.48
1:C:876:LEU:O	1:C:880:ILE:N	2.47	0.48
2:G:558:ASN:O	2:G:562:ILE:HG22	2.14	0.48
1:C:1794:SER:O	1:C:1797:ASP:N	2.45	0.47
1:C:845:ILE:HD11	1:C:875:LYS:HZ3	1.79	0.47
1:C:1621:LEU:O	1:C:1625:HIS:N	2.45	0.47
2:G:400:GLU:HB2	2:G:449:TRP:NE1	2.22	0.47
2:G:509:TYR:HE2	2:G:511:ASP:HB2	1.78	0.47
1:C:570:PHE:O	1:C:574:GLN:HG2	2.14	0.47
1:C:1185:GLN:NE2	1:C:1224:ILE:H	2.11	0.47
1:C:2120:LEU:O	1:C:2128:ILE:N	2.47	0.47
1:C:2314:HIS:CD2	1:C:2315:SER:H	2.33	0.47
2:G:199:ILE:CG1	2:G:200:PRO:HD2	2.45	0.47
2:G:225:ILE:CG1	2:G:508:ILE:HG12	2.44	0.47
1:C:1781:GLN:O	1:C:1785:GLN:HG2	2.15	0.47
2:G:486:HIS:O	2:G:486:HIS:ND1	2.47	0.47
2:G:377:ARG:NH1	2:G:423:GLU:OE2	2.48	0.47
1:C:1328:THR:C	1:C:1330:ASN:H	2.18	0.47
1:C:2273:GLY:O	1:C:2275:ILE:N	2.48	0.47
1:C:2304:GLU:HG3	1:C:2323:LEU:HD11	1.96	0.47
1:C:728:ILE:HG13	1:C:729:ILE:N	2.30	0.47
1:C:949:CYS:O	1:C:952:LEU:HB2	2.15	0.47
2:G:624:LYS:HE2	2:G:626:LEU:HA	1.97	0.47
2:G:692:TYR:CE2	2:G:693:ILE:HG12	2.50	0.47
1:C:1140:GLU:H	1:C:1140:GLU:CD	2.16	0.47
1:C:1743:GLN:HA	1:C:1767:PHE:HE1	1.79	0.47
1:C:2231:LEU:HD22	1:C:2240:LEU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2268:LEU:C	1:C:2268:LEU:HD23	2.35	0.47
1:C:459:THR:O	1:C:546:SER:OG	2.24	0.47
1:C:519:PHE:CD1	1:C:519:PHE:C	2.85	0.47
1:C:545:PHE:CZ	1:C:587:LEU:HD11	2.49	0.47
1:C:596:ASN:ND2	1:C:637:THR:OG1	2.48	0.47
1:C:545:PHE:CE2	1:C:587:LEU:HD11	2.50	0.47
1:C:653:ILE:HG23	1:C:654:PHE:CD1	2.50	0.47
1:C:686:PRO:O	1:C:689:PRO:CD	2.56	0.47
1:C:861:ILE:HA	1:C:863:ASN:HA	1.97	0.47
2:G:199:ILE:HG23	2:G:200:PRO:O	2.15	0.47
2:G:283:LYS:O	2:G:286:SER:OG	2.18	0.47
2:G:288:HIS:HA	2:G:289:PRO:HD3	1.73	0.47
2:G:495:ILE:HA	2:G:544:TRP:NE1	2.29	0.47
1:C:1755:VAL:HG12	1:C:1756:ASN:N	2.30	0.46
1:C:684:LEU:HD23	1:C:684:LEU:N	2.30	0.46
2:G:199:ILE:HG12	2:G:200:PRO:HD2	1.98	0.46
1:C:412:LEU:HD11	1:C:487:TRP:O	2.16	0.46
2:G:138:ARG:O	2:G:141:ILE:N	2.47	0.46
1:C:1300:LEU:O	1:C:1304:ILE:HG13	2.15	0.46
1:C:1458:PHE:O	1:C:1460:THR:HG23	2.14	0.46
1:C:2137:THR:HG21	1:C:2230:ILE:O	2.15	0.46
1:C:679:THR:O	1:C:683:LEU:N	2.48	0.46
1:C:494:ASP:OD1	2:G:596:GLN:HB2	2.16	0.46
1:C:1786:TYR:CE2	1:C:1803:ILE:HA	2.50	0.46
1:C:1968:HIS:O	1:C:1972:SER:N	2.41	0.46
1:C:2175:MET:HE3	1:C:2358:SER:CB	2.46	0.46
2:G:190:MET:O	2:G:194:ASN:HA	2.15	0.46
2:G:740:SER:O	2:G:744:SER:N	2.49	0.46
1:C:2223:GLY:CA	1:C:2245:ASP:HB3	2.46	0.46
1:C:1400:LEU:HA	1:C:1403:ARG:CB	2.45	0.46
1:C:1653:MET:O	1:C:1656:ILE:HG12	2.16	0.46
1:C:877:GLN:HG2	1:C:921:SER:HB2	1.98	0.46
1:C:1345:CYS:O	1:C:1349:ILE:N	2.35	0.46
1:C:2122:LEU:H	1:C:2127:GLY:HA2	1.81	0.46
1:C:2207:ALA:HB2	1:C:2272:LEU:HD11	1.98	0.46
1:C:2247:LEU:CD2	1:C:2247:LEU:N	2.79	0.46
1:C:321:ILE:CD1	1:C:347:TYR:HB2	2.46	0.46
1:C:455:LEU:HD21	1:C:526:PHE:CE1	2.51	0.46
2:G:457:LEU:O	2:G:460:LEU:N	2.48	0.46
2:G:692:TYR:CD2	2:G:693:ILE:HG12	2.51	0.46
1:C:918:PRO:HG2	1:C:921:SER:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:LEU:O	1:C:543:ILE:HG22	2.16	0.46
2:G:435:MET:HE1	2:G:435:MET:HA	1.93	0.46
2:G:438:SER:O	2:G:439:SER:C	2.54	0.46
1:C:1065:ILE:HA	1:C:1068:TYR:HB3	1.98	0.45
1:C:1422:ARG:HH21	1:C:1423:GLN:HE21	1.63	0.45
1:C:1796:TRP:C	1:C:1798:LYS:H	2.19	0.45
1:C:631:TRP:CD1	1:C:654:PHE:HE2	2.34	0.45
1:C:1592:LYS:NZ	2:G:523:GLU:OE2	2.41	0.45
1:C:1513:ILE:HD13	1:C:1545:GLU:HG3	1.98	0.45
1:C:1746:HIS:O	1:C:1750:GLN:HG2	2.15	0.45
1:C:2272:LEU:HD13	1:C:2281:PHE:HE2	1.80	0.45
1:C:1155:PHE:O	1:C:1159:VAL:HG23	2.15	0.45
1:C:1545:GLU:OE1	1:C:1546:GLY:N	2.48	0.45
1:C:557:PRO:HG2	1:C:566:ILE:HG21	1.94	0.45
1:C:892:HIS:NE2	1:C:935:THR:HG21	2.31	0.45
1:C:1098:LEU:HD13	1:C:1120:ILE:HG22	1.97	0.45
1:C:453:THR:HA	1:C:456:THR:HG22	1.98	0.45
2:G:348:LEU:H	2:G:348:LEU:HG	1.62	0.45
1:C:1622:MET:SD	1:C:1662:PRO:HA	2.57	0.45
1:C:983:LYS:O	1:C:986:ASN:N	2.50	0.45
1:C:1625:HIS:HE1	1:C:1652:ARG:NE	2.14	0.45
1:C:923:ILE:HD11	1:C:958:ASN:HD21	1.82	0.45
1:C:1255:LYS:O	1:C:1259:LYS:N	2.39	0.45
1:C:1362:GLU:HA	1:C:1365:GLN:HB3	1.99	0.45
1:C:606:GLU:OE1	1:C:606:GLU:N	2.48	0.45
2:G:172:GLN:C	2:G:174:PRO:N	2.70	0.45
2:G:465:ILE:O	2:G:465:ILE:HG13	2.16	0.45
2:G:546:LEU:HD23	2:G:603:LEU:HD23	1.98	0.45
1:C:1160:ILE:HA	1:C:1164:LEU:HB2	1.99	0.45
1:C:2264:LEU:CD2	1:C:2268:LEU:HD13	2.47	0.45
1:C:2107:SER:HB3	1:C:2291:LEU:HD11	1.99	0.45
2:G:203:THR:HG23	2:G:262:LYS:HE2	1.98	0.45
2:G:219:ASP:O	2:G:220:LEU:HB2	2.17	0.45
1:C:259:ALA:HB2	2:G:674:THR:HB	1.98	0.45
1:C:1017:LYS:HD2	1:C:1018:PRO:HD2	1.99	0.45
1:C:2110:ARG:HH12	1:C:2283:LYS:C	2.20	0.45
1:C:345:ILE:O	1:C:348:PHE:HB3	2.17	0.45
2:G:215:ILE:CG2	2:G:218:ALA:HB3	2.47	0.45
2:G:641:SER:OG	2:G:642:LEU:N	2.50	0.45
1:C:1410:PHE:O	1:C:1414:ALA:N	2.48	0.44
1:C:2203:ARG:O	1:C:2206:TYR:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:512:ALA:O	1:C:519:PHE:CD2	2.69	0.44
2:G:432:ILE:HG21	2:G:562:ILE:HD12	1.99	0.44
1:C:1683:ASP:O	1:C:1686:LEU:N	2.51	0.44
1:C:1756:ASN:C	1:C:1758:ARG:H	2.20	0.44
1:C:1163:ILE:HG13	1:C:1293:PHE:CZ	2.53	0.44
1:C:1411:GLU:HB3	1:C:2196:PRO:HB2	1.99	0.44
1:C:274:VAL:O	1:C:277:THR:N	2.50	0.44
2:G:196:ASN:O	2:G:196:ASN:ND2	2.50	0.44
1:C:2103:LYS:O	1:C:2107:SER:OG	2.35	0.44
1:C:517:GLU:OE1	1:C:517:GLU:HA	2.16	0.44
2:G:434:ASN:HB3	2:G:435:MET:H	1.58	0.44
2:G:508:ILE:O	2:G:508:ILE:HG13	2.17	0.44
1:C:2263:ARG:NH1	1:C:2263:ARG:CG	2.73	0.44
1:C:558:LYS:C	1:C:558:LYS:CD	2.86	0.44
1:C:729:ILE:CG1	1:C:730:PRO:HD3	2.48	0.44
1:C:1060:GLN:O	1:C:1063:ASP:N	2.49	0.44
1:C:1587:PRO:O	1:C:1591:GLN:HG2	2.18	0.44
1:C:1754:SER:H	1:C:1760:ARG:NH2	2.15	0.44
1:C:839:CYS:HA	1:C:842:ARG:CD	2.48	0.44
1:C:877:GLN:O	1:C:880:ILE:HG22	2.18	0.44
2:G:223:ILE:HD11	2:G:254:ILE:HG21	1.99	0.44
2:G:575:LEU:HA	2:G:578:SER:OG	2.18	0.44
1:C:1609:SER:OG	1:C:1610:LYS:N	2.44	0.44
1:C:2229:ASN:HD21	1:C:2243:ASP:HB3	1.82	0.44
1:C:2288:THR:O	1:C:2292:MET:HG2	2.18	0.44
2:G:359:LEU:O	2:G:363:LEU:HG	2.18	0.44
2:G:500:LEU:HB3	2:G:525:ILE:HD11	1.99	0.44
2:G:551:GLU:O	2:G:554:ASN:N	2.50	0.44
1:C:1160:ILE:HD11	1:C:1208:ASN:O	2.18	0.44
1:C:2264:LEU:HD13	1:C:2269:LEU:CD1	2.47	0.44
1:C:274:VAL:HG13	1:C:275:LEU:N	2.33	0.44
1:C:648:LEU:HD13	1:C:687:ILE:HD13	1.99	0.44
1:C:819:LEU:HA	1:C:838:LEU:HD21	2.00	0.44
1:C:1725:PHE:O	1:C:1728:ILE:HG13	2.18	0.43
1:C:2265:THR:HG21	1:C:2367:PHE:H	1.81	0.43
1:C:442:SER:O	1:C:445:THR:OG1	2.23	0.43
2:G:222:THR:O	2:G:226:LEU:N	2.39	0.43
2:G:464:GLU:OE2	2:G:584:ARG:NH1	2.47	0.43
1:C:1290:LEU:C	1:C:1290:LEU:HD12	2.38	0.43
1:C:257:SER:O	1:C:258:THR:OG1	2.28	0.43
1:C:512:ALA:HB2	1:C:554:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:509:TYR:HA	2:G:518:ARG:HD3	2.01	0.43
1:C:1661:VAL:CG1	1:C:1662:PRO:HD3	2.48	0.43
1:C:544:LEU:HD13	1:C:587:LEU:HD22	2.00	0.43
2:G:274:LEU:O	2:G:278:ILE:HD12	2.18	0.43
2:G:697:LEU:O	2:G:701:LEU:HD13	2.18	0.43
1:C:1170:GLN:OE1	1:C:1170:GLN:N	2.51	0.43
1:C:1117:ALA:HB2	1:C:1602:GLY:HA3	2.00	0.43
1:C:2110:ARG:HH22	1:C:2283:LYS:HB3	1.83	0.43
1:C:2212:VAL:HA	1:C:2288:THR:HG21	1.99	0.43
1:C:721:LEU:O	1:C:725:GLN:N	2.52	0.43
1:C:1457:THR:OG1	1:C:1458:PHE:N	2.52	0.43
2:G:219:ASP:OD1	2:G:219:ASP:N	2.50	0.43
2:G:643:TRP:O	2:G:647:VAL:HG23	2.18	0.43
2:G:677:ASP:O	2:G:680:SER:OG	2.30	0.43
1:C:2185:LEU:HB3	1:C:2271:ALA:CB	2.49	0.43
2:G:415:VAL:HA	2:G:418:ILE:HD12	2.01	0.43
1:C:1474:GLU:HG3	1:C:1474:GLU:O	2.19	0.43
1:C:2206:TYR:OH	1:C:2268:LEU:HD21	2.17	0.43
1:C:602:ASN:HA	1:C:605:ASP:HB2	1.99	0.43
1:C:846:THR:O	1:C:850:LYS:N	2.50	0.43
1:C:970:ILE:O	1:C:973:ILE:HG13	2.19	0.43
2:G:571:ASN:O	2:G:573:GLU:HG2	2.19	0.43
1:C:2247:LEU:HB3	1:C:2248:PHE:H	1.56	0.43
2:G:315:HIS:HB3	2:G:319:LEU:HG	2.00	0.43
1:C:620:LEU:HB2	1:C:623:VAL:HG23	2.00	0.43
1:C:1143:VAL:O	1:C:1151:GLN:NE2	2.52	0.42
1:C:2138:LEU:HA	1:C:2227:CYS:HB2	2.01	0.42
1:C:2158:LEU:HD12	1:C:2159:HIS:N	2.34	0.42
1:C:2188:TRP:O	1:C:2192:ASN:HB2	2.18	0.42
1:C:2263:ARG:C	1:C:2263:ARG:CD	2.85	0.42
1:C:710:ILE:HD12	1:C:720:ILE:HG21	2.01	0.42
2:G:254:ILE:O	2:G:257:LEU:N	2.52	0.42
1:C:1554:TRP:O	1:C:1557:GLN:N	2.50	0.42
2:G:329:LEU:HD11	2:G:333:TYR:HE2	1.84	0.42
2:G:242:PHE:CD1	2:G:257:LEU:HD22	2.54	0.42
1:C:1492:ASP:HB3	1:C:1495:THR:OG1	2.20	0.42
1:C:1806:TYR:O	1:C:1809:ARG:N	2.53	0.42
1:C:321:ILE:C	1:C:323:GLN:N	2.72	0.42
1:C:633:GLN:NE2	2:G:591:GLU:OE2	2.50	0.42
2:G:360:ILE:O	2:G:364:ILE:HG22	2.20	0.42
2:G:390:PHE:CE2	2:G:395:ILE:HG12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:549:LYS:HA	2:G:552:VAL:HG22	2.01	0.42
2:G:562:ILE:HG23	2:G:563:TYR:H	1.84	0.42
1:C:1418:GLU:O	1:C:1422:ARG:N	2.52	0.42
1:C:1646:THR:O	1:C:1650:ASP:N	2.44	0.42
1:C:512:ALA:HB1	1:C:519:PHE:CD2	2.54	0.42
1:C:1074:THR:OG1	1:C:1075:GLU:OE1	2.26	0.42
1:C:1496:THR:HB	1:C:1534:TRP:CZ2	2.55	0.42
1:C:1512:ILE:HD11	1:C:1541:ALA:HB2	2.02	0.42
1:C:1712:HIS:ND1	1:C:1712:HIS:O	2.52	0.42
1:C:2209:SER:OG	1:C:2238:LYS:HA	2.19	0.42
1:C:2270:ASP:C	1:C:2272:LEU:N	2.71	0.42
1:C:558:LYS:HB2	1:C:601:HIS:HD2	1.79	0.42
1:C:623:VAL:HG13	1:C:626:ASN:HB2	2.00	0.42
2:G:303:MET:O	2:G:307:VAL:HG23	2.19	0.42
2:G:455:THR:HA	2:G:458:TYR:CD2	2.53	0.42
2:G:657:GLU:O	2:G:660:MET:N	2.53	0.42
1:C:2179:ASP:C	1:C:2181:PHE:N	2.73	0.42
1:C:2223:GLY:CA	1:C:2245:ASP:OD2	2.64	0.42
1:C:2339:SER:O	1:C:2342:GLY:N	2.52	0.42
2:G:465:ILE:HD11	2:G:546:LEU:HD13	2.02	0.42
1:C:1573:TYR:O	1:C:1576:ALA:N	2.52	0.42
1:C:290:ASP:C	1:C:292:ASP:H	2.23	0.42
1:C:576:CYS:SG	1:C:588:SER:HB3	2.60	0.42
1:C:690:VAL:O	1:C:693:ARG:HG2	2.20	0.42
1:C:890:ASP:HA	1:C:893:ASP:OD2	2.20	0.42
1:C:842:ARG:HH12	1:C:916:TYR:CB	2.32	0.42
2:G:414:MET:O	2:G:418:ILE:HG13	2.20	0.42
2:G:458:TYR:CD1	2:G:577:HIS:CG	3.07	0.42
1:C:1991:SER:O	1:C:1995:ARG:N	2.35	0.42
1:C:2178:VAL:O	1:C:2178:VAL:HG12	2.20	0.42
1:C:2183:PRO:HB3	1:C:2267:ASN:HA	2.01	0.42
1:C:283:ASP:HA	1:C:324:TRP:HZ2	1.84	0.42
2:G:334:HIS:O	2:G:336:VAL:N	2.53	0.42
1:C:2105:ILE:HG23	1:C:2106:ALA:N	2.35	0.42
1:C:1947:SER:CB	1:C:2122:LEU:HA	2.50	0.42
1:C:321:ILE:O	1:C:322:ASP:C	2.58	0.42
2:G:476:ASP:C	2:G:478:THR:N	2.73	0.42
1:C:1125:VAL:HG21	1:C:1656:ILE:CG2	2.39	0.41
1:C:1996:SER:O	1:C:2000:LEU:N	2.47	0.41
1:C:2188:TRP:HZ2	1:C:2234:ILE:HD12	1.85	0.41
1:C:838:LEU:HD12	1:C:841:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:547:LYS:O	2:G:550:ASP:N	2.49	0.41
2:G:601:LEU:O	2:G:604:ARG:N	2.53	0.41
1:C:2135:VAL:HG23	1:C:2232:LEU:O	2.20	0.41
1:C:877:GLN:CG	1:C:921:SER:HB2	2.50	0.41
2:G:518:ARG:O	2:G:518:ARG:HG2	2.21	0.41
1:C:1396:PRO:HA	1:C:1399:LEU:CB	2.50	0.41
1:C:1562:ARG:O	1:C:1563:ASN:HB2	2.20	0.41
1:C:1128:VAL:HG23	1:C:1618:GLN:HE21	1.85	0.41
1:C:279:HIS:CE1	1:C:320:PRO:HD2	2.55	0.41
1:C:905:ARG:O	1:C:908:ASN:HB2	2.21	0.41
1:C:2081:LYS:HA	1:C:2126:CYS:O	2.21	0.41
1:C:274:VAL:HG13	1:C:275:LEU:H	1.85	0.41
1:C:528:SER:OG	1:C:529:HIS:N	2.54	0.41
1:C:605:ASP:HB3	1:C:606:GLU:OE1	2.20	0.41
1:C:688:LEU:HB2	1:C:689:PRO:HD3	2.02	0.41
1:C:833:ASN:HA	1:C:836:MET:HB2	2.02	0.41
1:C:956:HIS:O	1:C:956:HIS:CG	2.74	0.41
2:G:616:TYR:CE1	2:G:721:ALA:HB1	2.56	0.41
2:G:695:GLU:O	2:G:698:LYS:HB2	2.21	0.41
1:C:2162:TRP:CD1	1:C:2174:TYR:CZ	3.09	0.41
1:C:963:SER:OG	1:C:964:THR:N	2.54	0.41
2:G:350:VAL:O	2:G:350:VAL:HG13	2.21	0.41
1:C:2265:THR:CG2	1:C:2266:PRO:CD	2.92	0.41
1:C:2344:THR:O	1:C:2348:ILE:HG22	2.20	0.41
1:C:548:HIS:ND1	1:C:594:LEU:HD11	2.35	0.41
1:C:962:LEU:HD12	1:C:999:LYS:NZ	2.35	0.41
1:C:1168:PHE:CB	1:C:1180:VAL:HG11	2.51	0.41
1:C:2226:HIS:CE1	1:C:2229:ASN:HB2	2.55	0.41
1:C:547:LEU:HD11	1:C:551:PHE:CZ	2.56	0.41
2:G:213:HIS:O	2:G:221:SER:HB2	2.21	0.41
1:C:1156:LEU:O	1:C:1160:ILE:HG23	2.21	0.41
1:C:1295:LEU:HB3	1:C:1296:PRO:HD3	2.02	0.41
1:C:1495:THR:OG1	1:C:1496:THR:N	2.54	0.41
1:C:241:LEU:HD23	1:C:241:LEU:O	2.20	0.41
2:G:294:LEU:O	2:G:294:LEU:HD23	2.20	0.41
2:G:579:SER:HA	2:G:582:LEU:HB3	2.03	0.41
1:C:1611:GLU:HG3	1:C:1611:GLU:O	2.21	0.41
1:C:539:LEU:O	1:C:542:GLY:N	2.54	0.41
2:G:320:LYS:HA	2:G:390:PHE:HE1	1.86	0.41
1:C:1463:LEU:HD12	1:C:1466:LYS:HB2	2.01	0.41
1:C:1789:ILE:HG23	1:C:1789:ILE:HD12	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2297:VAL:O	1:C:2301:ASN:N	2.53	0.41
1:C:557:PRO:O	1:C:566:ILE:CG2	2.69	0.41
1:C:1596:ASN:OD1	2:G:350:VAL:HB	2.21	0.41
2:G:361:ASP:O	2:G:365:ILE:HG12	2.21	0.41
1:C:1163:ILE:HG13	1:C:1293:PHE:CE1	2.56	0.40
1:C:1789:ILE:O	1:C:1789:ILE:HG22	2.21	0.40
1:C:2179:ASP:O	1:C:2181:PHE:N	2.54	0.40
1:C:2171:LEU:HB3	1:C:2359:LYS:CB	2.51	0.40
1:C:1036:ILE:O	1:C:1039:THR:OG1	2.37	0.40
1:C:1778:ALA:O	1:C:1782:ILE:HG13	2.21	0.40
1:C:2147:GLU:C	1:C:2150:LYS:H	2.24	0.40
1:C:290:ASP:O	1:C:293:PRO:HD3	2.21	0.40
1:C:1360:ALA:HA	1:C:1363:PHE:HB3	2.04	0.40
1:C:1592:LYS:O	1:C:1596:ASN:HB2	2.21	0.40
1:C:2100:LEU:HD21	1:C:2112:LEU:HB2	2.04	0.40
1:C:2243:ASP:CG	1:C:2244:PHE:N	2.73	0.40
1:C:272:LYS:HE3	1:C:314:CYS:SG	2.61	0.40
1:C:915:ILE:HG22	1:C:916:TYR:CE1	2.56	0.40
2:G:196:ASN:C	2:G:196:ASN:ND2	2.74	0.40
1:C:1539:LEU:HD13	1:C:1554:TRP:HB3	2.02	0.40
1:C:1723:LEU:HD21	1:C:1766:LYS:HE3	2.04	0.40
1:C:1764:LEU:HA	1:C:1767:PHE:HB3	2.04	0.40
1:C:908:ASN:O	1:C:911:SER:OG	2.24	0.40
2:G:228:ARG:HB2	2:G:513:LEU:HA	2.02	0.40
1:C:1661:VAL:HG13	1:C:1662:PRO:HD3	2.03	0.40
1:C:1809:ARG:HA	1:C:1812:GLU:HB3	2.03	0.40
1:C:2269:LEU:O	1:C:2276:GLY:HA2	2.22	0.40
1:C:283:ASP:HA	1:C:324:TRP:CZ2	2.55	0.40
2:G:256:SER:OG	2:G:260:ARG:NE	2.52	0.40
2:G:314:THR:OG1	2:G:315:HIS:N	2.54	0.40
2:G:487:ASP:N	2:G:487:ASP:OD1	2.53	0.40
2:G:492:ILE:HD13	2:G:493:ARG:NH2	2.36	0.40
2:G:670:LEU:HA	2:G:670:LEU:HD23	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1943/2368 (82%)	1595 (82%)	311 (16%)	37 (2%)	9	50
2	G	678/747 (91%)	556 (82%)	102 (15%)	20 (3%)	5	42
All	All	2621/3115 (84%)	2151 (82%)	413 (16%)	57 (2%)	12	47

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	356	PRO
1	C	685	SER
1	C	845	ILE
1	C	1241	VAL
1	C	1395	THR
1	C	2017	VAL
1	C	2018	PRO
1	C	2061	LYS
1	C	2062	PRO
1	C	2274	ILE
2	G	159	THR
2	G	160	PRO
2	G	170	LYS
2	G	171	PRO
2	G	289	PRO
2	G	409	ILE
2	G	434	ASN
1	C	1755	VAL
1	C	2055	VAL
2	G	510	THR
1	C	687	ILE
1	C	2114	ILE
1	C	2180	LYS
1	C	2271	ALA
2	G	172	GLN

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Mol	Chain	Res	Type
2	G	173	SER
2	G	191	VAL
2	G	290	ASN
1	C	307	ILE
1	C	322	ASP
1	C	357	VAL
1	C	2010	VAL
1	C	2167	VAL
1	C	2265	THR
2	G	199	ILE
2	G	438	SER
2	G	509	TYR
1	C	2248	PHE
1	C	2354	GLU
1	C	603	SER
1	C	623	VAL
1	C	652	ASP
1	C	2041	ARG
1	C	2195	ASP
2	G	145	LYS
1	C	489	VAL
2	G	216	ILE
2	G	470	VAL
2	G	519	VAL
1	C	780	GLY
2	G	562	ILE
1	C	1125	VAL
1	C	1224	ILE
1	C	2025	ILE
1	C	2026	ILE
1	C	529	HIS
1	C	1274	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	1257/2174 (58%)	1233 (98%)	24 (2%)	62	84
2	G	447/698 (64%)	443 (99%)	4 (1%)	82	92
All	All	1704/2872 (59%)	1676 (98%)	28 (2%)	70	86

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	518	ILE
1	C	519	PHE
1	C	558	LYS
1	C	684	LEU
1	C	685	SER
1	C	687	ILE
1	C	1126	LEU
1	C	1138	TYR
1	C	1290	LEU
1	C	1355	TYR
1	C	2167	VAL
1	C	2175	MET
1	C	2179	ASP
1	C	2209	SER
1	C	2246	CYS
1	C	2247	LEU
1	C	2263	ARG
1	C	2265	THR
1	C	2267	ASN
1	C	2269	LEU
1	C	2353	SER
1	C	2355	ASP
1	C	2357	LEU
1	C	2359	LYS
2	G	194	ASN
2	G	196	ASN
2	G	198	ILE
2	G	435	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	270	GLN
1	C	444	GLN

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Mol	Chain	Res	Type
1	C	506	ASN
1	C	596	ASN
1	C	601	HIS
1	C	626	ASN
1	C	877	GLN
1	C	879	ASN
1	C	928	GLN
1	C	1185	GLN
1	C	1423	GLN
1	C	1480	GLN
1	C	1618	GLN
1	C	1625	HIS
1	C	1756	ASN
1	C	2089	GLN
1	C	2229	ASN
1	C	2314	HIS
2	G	196	ASN
2	G	214	GLN
2	G	305	GLN
2	G	334	HIS
2	G	416	ASN
2	G	494	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.