



Full wwPDB EM Validation Report ⓘ

Mar 10, 2024 – 09:47 AM EDT

PDB ID : 6PSQ
EMDB ID : EMD-20460
Title : Escherichia coli RNA polymerase closed complex (TRPc) with TraR and rpsT
P2 promoter
Authors : Chen, J.; Chiu, C.E.; Campbell, E.A.; Darst, S.A.
Deposited on : 2019-07-13
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

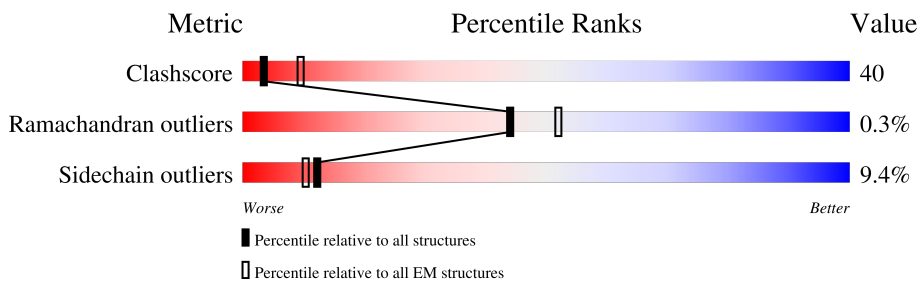
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	J	1430	
2	N	72	
3	G	329	
3	H	329	
3	M	329	
4	I	1342	
5	K	91	
6	L	616	

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Mol	Chain	Length	Quality of chain
7	O	85	 12% 47% 41%
8	P	85	 7% 52% 41%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 32933 atoms, of which 156 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 DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	J	1345	10466	6577	1867	1972	50	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	VAL	-	expression tag	UNP P0A8T7
J	1408	LEU	-	expression tag	UNP P0A8T7
J	1409	GLU	-	expression tag	UNP P0A8T7
J	1410	LEU	-	expression tag	UNP P0A8T7
J	1411	GLU	-	expression tag	UNP P0A8T7
J	1412	VAL	-	expression tag	UNP P0A8T7
J	1413	LEU	-	expression tag	UNP P0A8T7
J	1414	PHE	-	expression tag	UNP P0A8T7
J	1415	GLN	-	expression tag	UNP P0A8T7
J	1416	GLY	-	expression tag	UNP P0A8T7
J	1417	PRO	-	expression tag	UNP P0A8T7
J	1418	SER	-	expression tag	UNP P0A8T7
J	1419	SER	-	expression tag	UNP P0A8T7
J	1420	GLY	-	expression tag	UNP P0A8T7
J	1421	HIS	-	expression tag	UNP P0A8T7
J	1422	HIS	-	expression tag	UNP P0A8T7
J	1423	HIS	-	expression tag	UNP P0A8T7
J	1424	HIS	-	expression tag	UNP P0A8T7
J	1425	HIS	-	expression tag	UNP P0A8T7
J	1426	HIS	-	expression tag	UNP P0A8T7
J	1427	HIS	-	expression tag	UNP P0A8T7
J	1428	HIS	-	expression tag	UNP P0A8T7
J	1429	HIS	-	expression tag	UNP P0A8T7
J	1430	HIS	-	expression tag	UNP P0A8T7

- Molecule 2 is a protein called Protein TraR.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	72	Total	C	N	O	S	0	0
			571	353	105	108	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	230	Total	C	N	O	S	0	0
			1764	1103	314	341	6		
3	H	219	Total	C	N	O	S	0	0
			1682	1050	295	331	6		
3	M	73	Total	C	N	O	S	0	0
			572	362	100	108	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	1339	Total	C	N	O	S	0	0
			10549	6618	1840	2048	43		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	75	Total	C	N	O	S	0	0
			600	365	114	120	1		

- Molecule 6 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	551	Total	C	N	O	S	0	0
			4411	2757	774	854	26		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-2	SER	-	expression tag	UNP Q0P6L9
L	-1	GLU	-	expression tag	UNP Q0P6L9
L	0	PHE	-	expression tag	UNP Q0P6L9

- Molecule 7 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	O	50	1024	488	193	293	50	0	0

- Molecule 8 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	P	50	1026	491	178	307	50	0	0

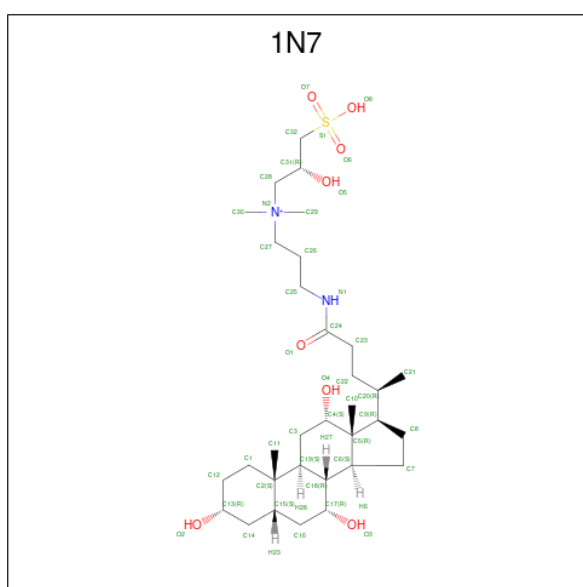
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
9	J	1	1	1	0

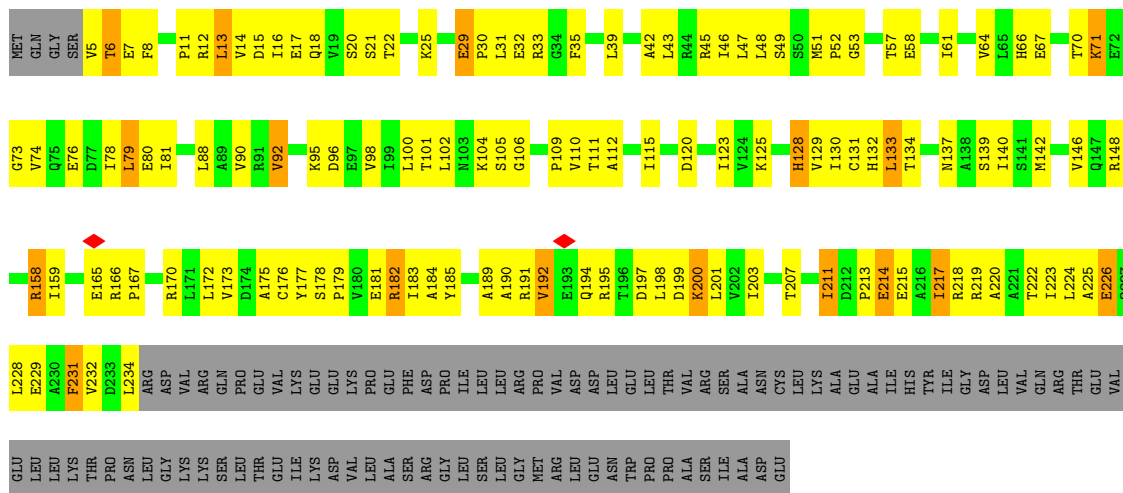
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
10	J	2	2	2	0
10	N	1	1	1	0

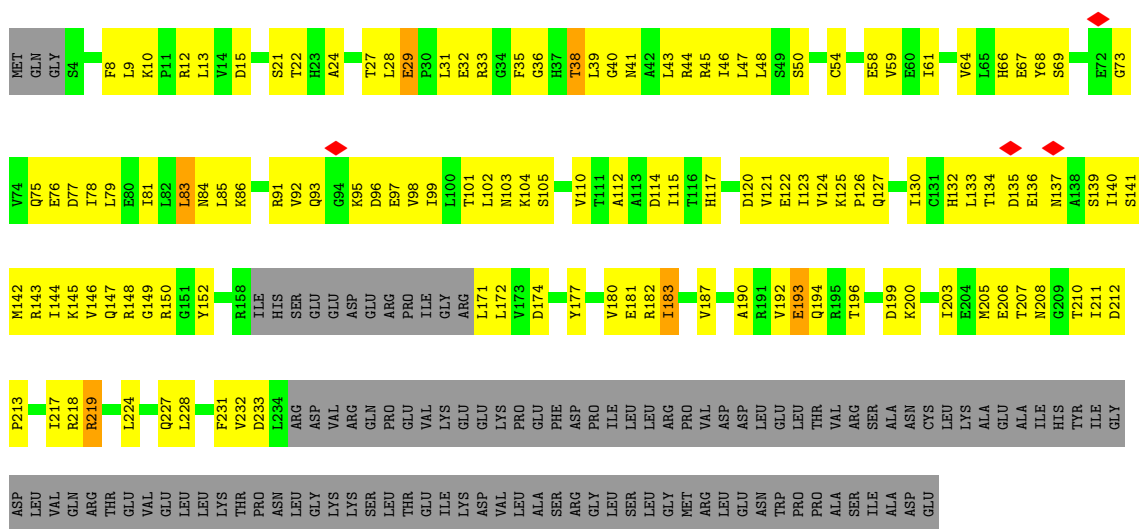
- Molecule 11 is CHAPSO (three-letter code: 1N7) (formula: C₃₂H₅₉N₂O₈S).



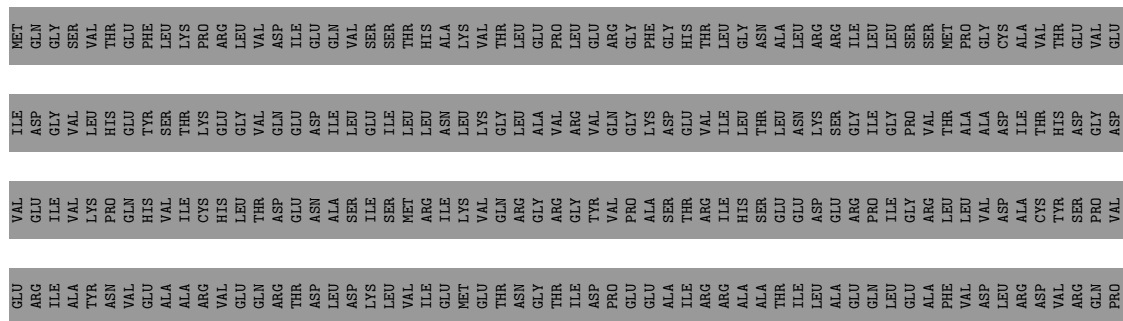
Mol	Chain	Residues	Atoms				AltConf
11	J	1	Total 66	C 24	H 39	O 3	0
11	J	1	Total 66	C 24	H 39	O 3	0
11	J	1	Total 66	C 24	H 39	O 3	0
11	I	1	Total 66	C 24	H 39	O 3	0

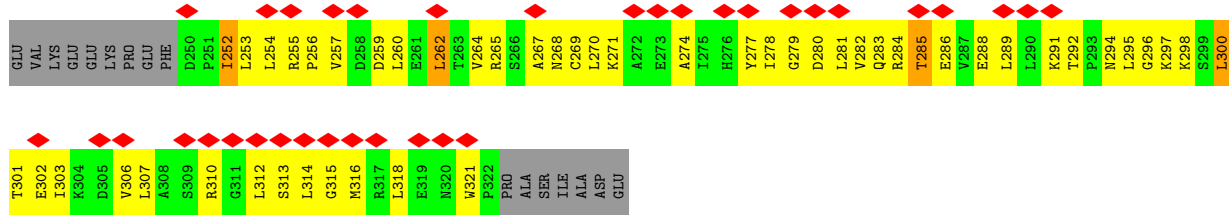


• Molecule 3: DNA-directed RNA polymerase subunit alpha

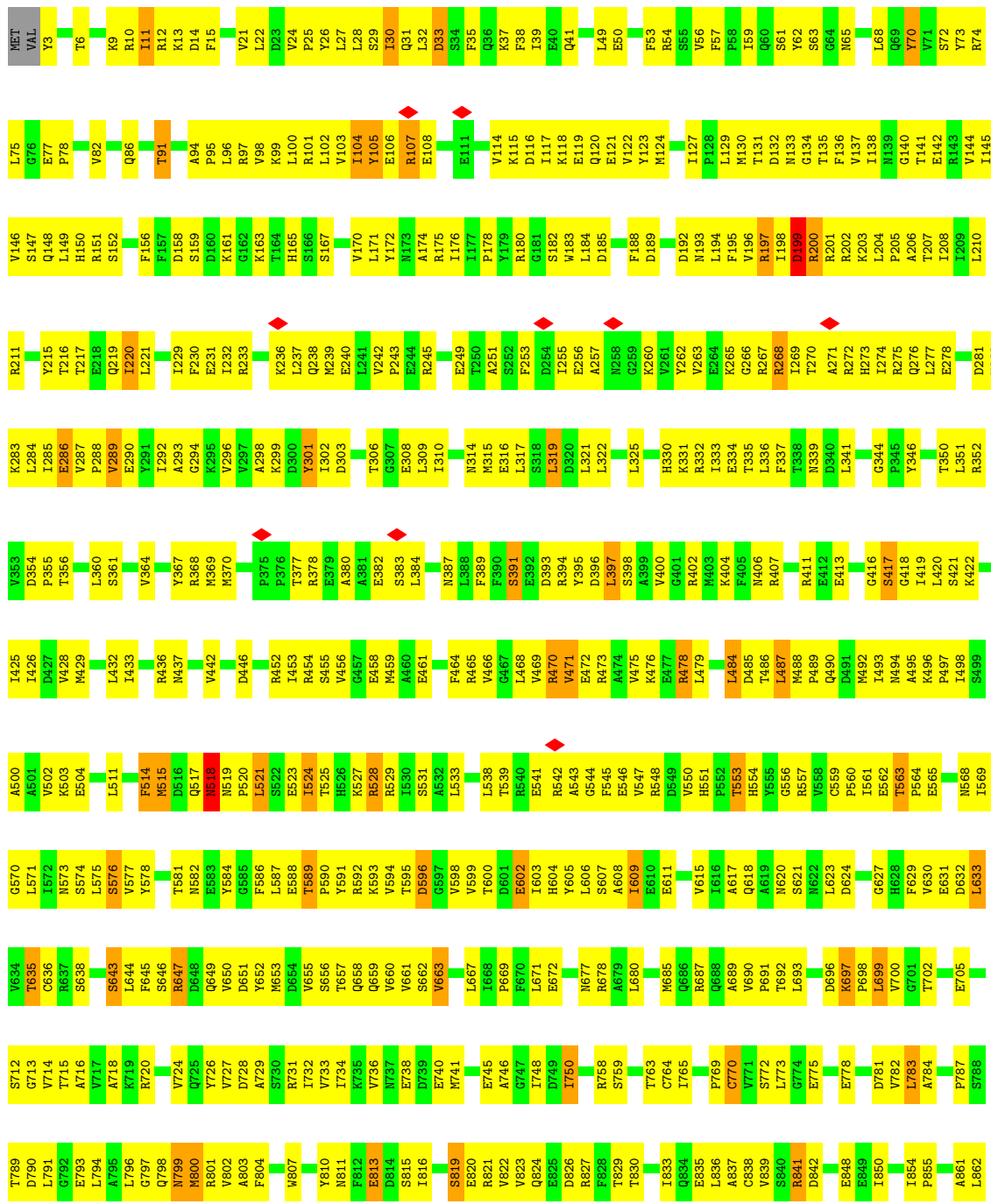


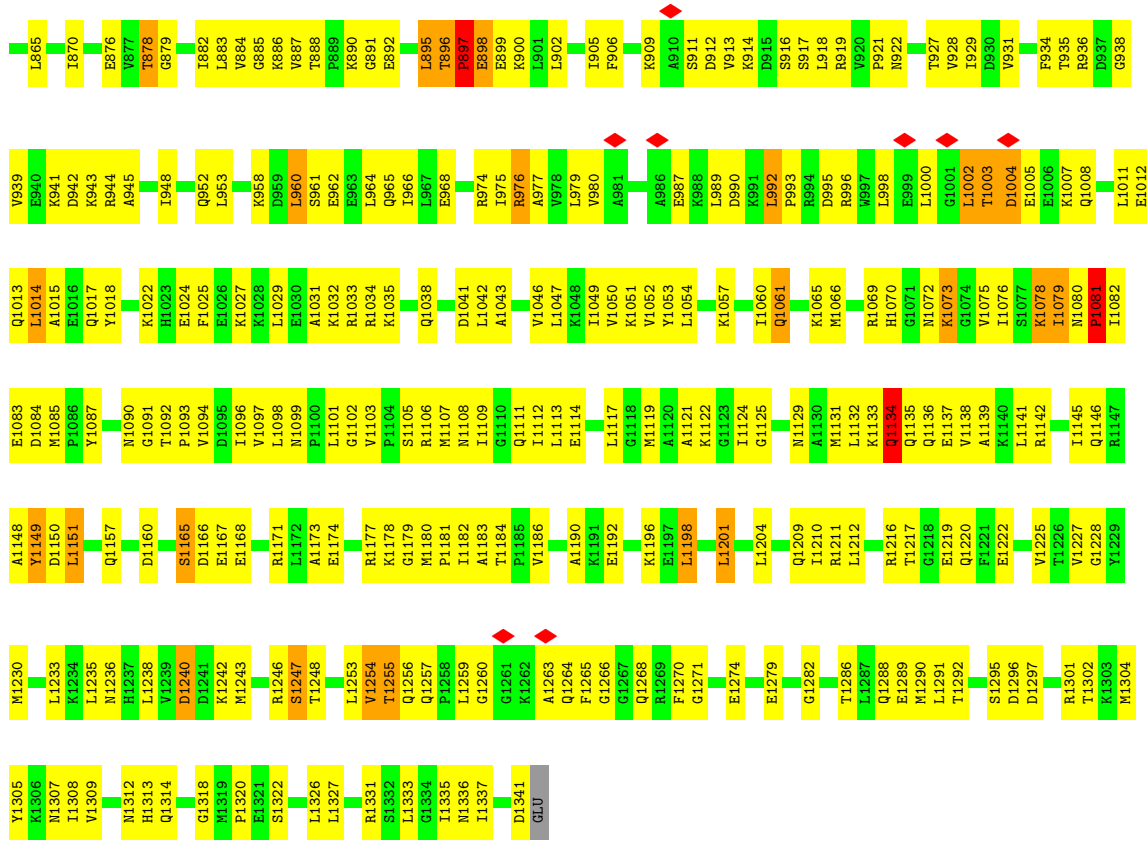
• Molecule 3: DNA-directed RNA polymerase subunit alpha



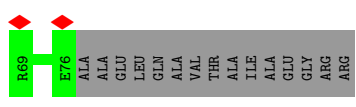
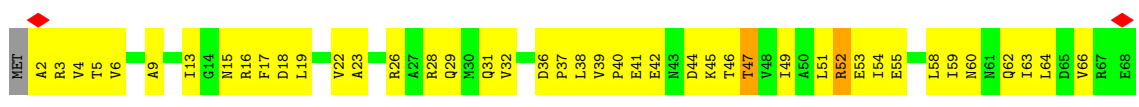


• Molecule 4: DNA-directed RNA polymerase subunit beta

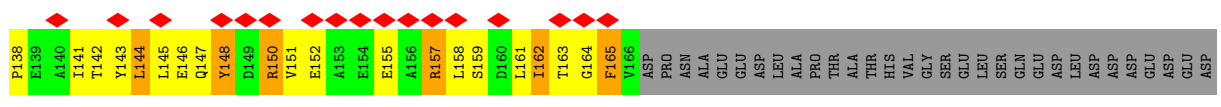
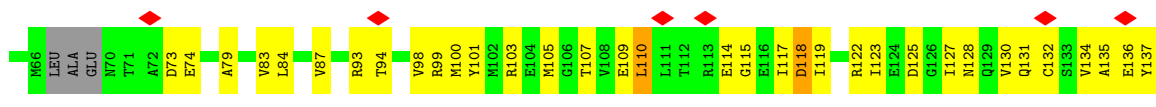
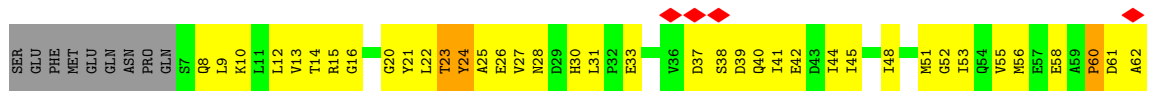


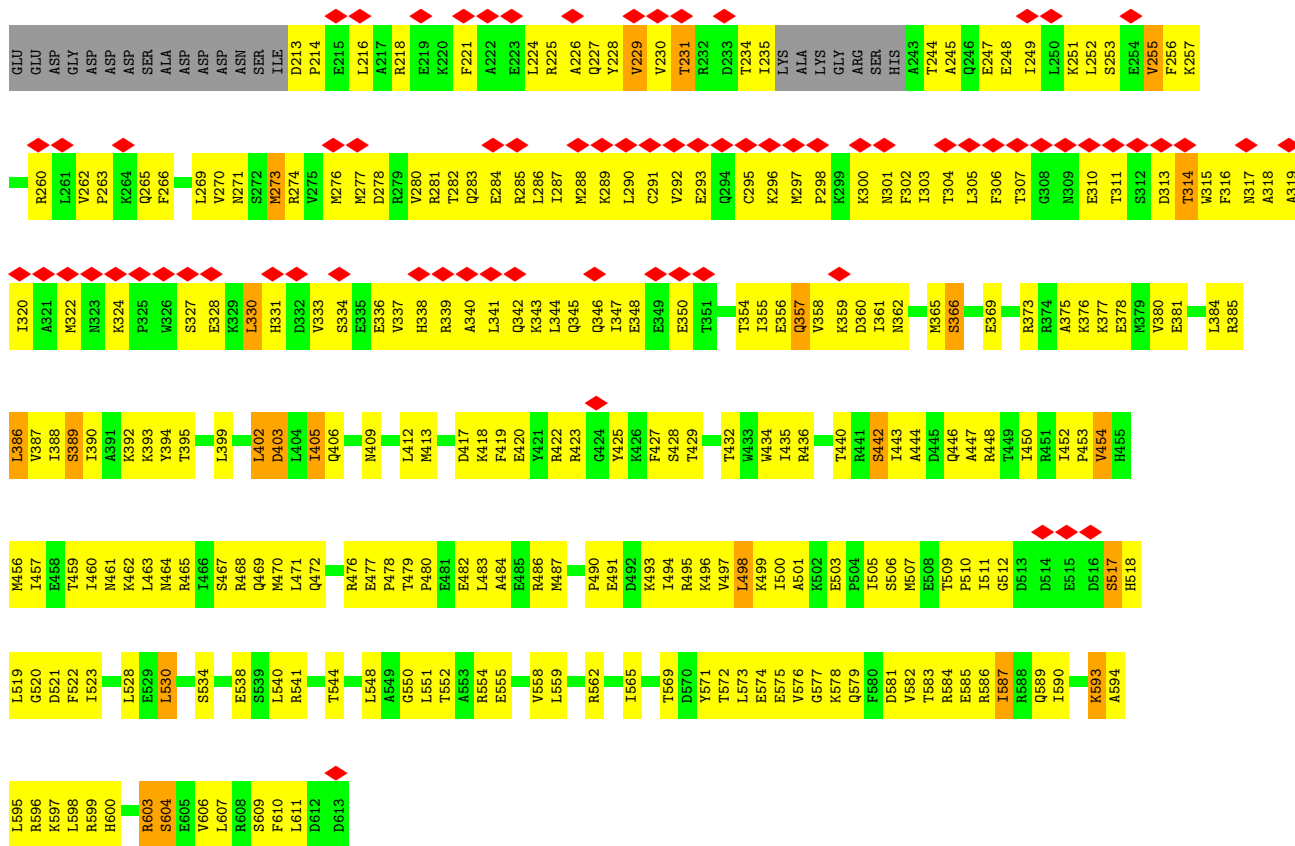


- Molecule 5: DNA-directed RNA polymerase subunit omega

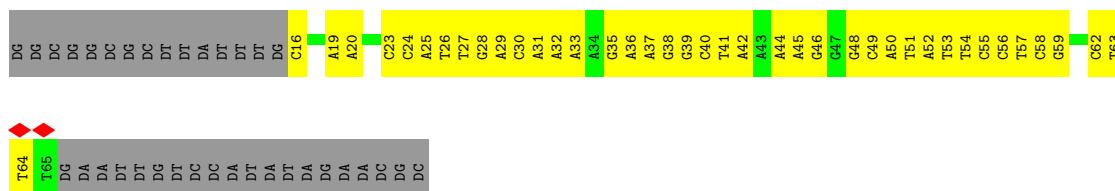


- Molecule 6: RNA polymerase sigma factor RpoD

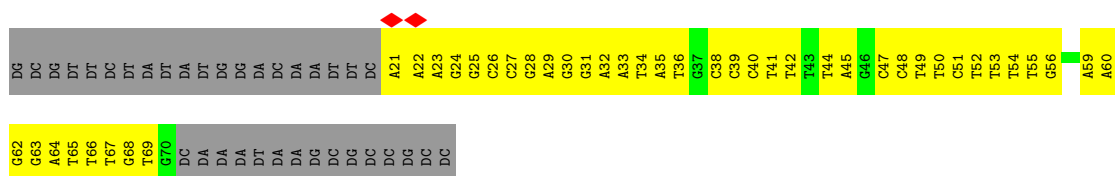




• Molecule 7: DNA (85-MER)



• Molecule 8: DNA (85-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	97182	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 ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.182	Depositor
Minimum map value	-0.094	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 1N7, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	J	0.48	0/10625	0.57	1/14345 (0.0%)
2	N	0.43	0/581	0.54	0/785
3	G	0.47	0/1786	0.56	0/2423
3	H	0.42	0/1701	0.56	0/2306
3	M	0.26	0/579	0.48	0/784
4	I	0.52	2/10717 (0.0%)	0.57	3/14461 (0.0%)
5	K	0.40	0/602	0.47	0/810
6	L	0.33	0/4466	0.49	0/6014
7	O	0.68	0/1150	1.01	0/1771
8	P	0.65	0/1148	1.00	0/1771
All	All	0.48	2/33355 (0.0%)	0.60	4/45470 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	5
4	I	0	5
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1081	PRO	N-CD	-6.69	1.38	1.47
4	I	1078	LYS	C-O	-5.61	1.12	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1081	PRO	N-CD-CG	-5.99	94.21	103.20
1	J	362	ARG	C-N-CA	-5.89	106.98	121.70
4	I	1081	PRO	N-CA-CB	-5.50	96.55	102.60
4	I	1079	ILE	N-CA-C	-5.04	97.39	111.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	I	1134	GLN	Peptide
4	I	199	ASP	Peptide
4	I	595	THR	Peptide
4	I	896	THR	Peptide
4	I	897	PRO	Peptide
1	J	1184	ASP	Peptide
1	J	416	ILE	Peptide
1	J	711	GLY	Peptide
1	J	853	THR	Peptide
1	J	934	THR	Peptide

5.2 Too-close contacts [i](#)

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	J	10466	0	10689	915	0
2	N	571	0	556	38	0
3	G	1764	0	1793	139	0
3	H	1682	0	1702	147	0
3	M	572	0	602	81	0
4	I	10549	0	10565	838	0
5	K	600	0	607	43	0
6	L	4411	0	4418	411	0
7	O	1024	0	562	68	0
8	P	1026	0	569	72	0
9	J	1	0	0	0	0
10	J	2	0	0	0	0
10	N	1	0	0	0	0
11	I	27	39	37	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	J	81	117	113	14	0
All	All	32777	156	32213	2593	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 40.

All (2593) 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)
11:J:1504:1N7:C19	11:J:1504:1N7:C3	1.83	1.57
11:J:1506:1N7:C3	11:J:1506:1N7:C19	1.82	1.57
11:I:1401:1N7:C3	11:I:1401:1N7:C19	1.82	1.56
11:J:1505:1N7:C3	11:J:1505:1N7:C19	1.82	1.56
1:J:937:ILE:CD1	1:J:1134:ILE:HG22	1.57	1.34
1:J:937:ILE:HD13	1:J:1134:ILE:HG22	1.26	1.17
6:L:231:THR:HG23	6:L:249:ILE:HG12	1.25	1.09
1:J:937:ILE:HD13	1:J:1134:ILE:CG2	1.87	1.05
3:M:262:LEU:HD21	3:M:306:VAL:HG11	1.38	1.04
1:J:937:ILE:HD11	1:J:1134:ILE:HG22	1.35	1.04
1:J:1115:ILE:HG12	1:J:1121:LEU:HD21	1.42	1.01
4:I:1165:SER:HB3	4:I:1168:GLU:HB2	1.41	1.00
1:J:193:ASP:HB3	1:J:196:GLN:HB2	1.41	0.99
4:I:322:LEU:HA	4:I:325:LEU:HD12	1.41	0.98
4:I:538:LEU:HD13	4:I:543:ALA:HB3	1.40	0.98
3:G:159:ILE:HD13	3:G:172:LEU:HD11	1.42	0.98
1:J:937:ILE:CD1	1:J:1134:ILE:CG2	2.40	0.98
6:L:213:ASP:HB3	6:L:216:LEU:HB3	1.45	0.98
1:J:1024:THR:HG23	1:J:1123:ARG:HB3	1.45	0.97
1:J:1042:ASP:HA	1:J:1046:ILE:HB	1.44	0.96
6:L:358:VAL:HA	6:L:361:ILE:HG12	1.43	0.96
1:J:1040:MET:HB3	1:J:1046:ILE:HD11	1.48	0.96
4:I:207:THR:HA	4:I:210:LEU:HD12	1.48	0.96
1:J:1089:LEU:HA	1:J:1096:PRO:HA	1.47	0.95
4:I:519:ASN:HD21	4:I:796:LEU:HD23	1.31	0.95
1:J:519:ASN:HB2	1:J:709:ARG:HB2	1.48	0.94
1:J:857:LEU:HD11	1:J:871:LEU:HD21	1.50	0.93
4:I:1103:VAL:HG11	4:I:1112:ILE:HD11	1.50	0.93
3:H:98:VAL:HG21	3:H:121:VAL:HG11	1.49	0.93
4:I:559:CYS:HG	4:I:662:SER:HG	0.94	0.93
3:H:91:ARG:HG3	3:H:122:GLU:HB3	1.51	0.93
2:N:34:VAL:HG11	2:N:56:THR:HG22	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:33:ARG:NH1	4:I:1081:PRO:HG3	1.85	0.92
3:H:33:ARG:HH11	4:I:1081:PRO:HG3	1.34	0.92
4:I:1292:THR:HG22	4:I:1320:PRO:HG3	1.52	0.92
4:I:746:ALA:HB2	4:I:974:ARG:HD2	1.49	0.91
3:G:29:GLU:HA	3:G:200:LYS:HB2	1.53	0.91
3:M:253:LEU:HD21	3:M:312:LEU:HD22	1.53	0.91
1:J:644:MET:HG2	1:J:740:LEU:HD23	1.52	0.90
4:I:563:THR:HG22	4:I:564:PRO:HD2	1.52	0.90
4:I:975:ILE:HD11	4:I:1014:LEU:HB3	1.52	0.90
1:J:1041:ILE:HB	1:J:1045:THR:HG23	1.54	0.89
6:L:141:ILE:HA	6:L:144:LEU:HD23	1.53	0.89
4:I:206:ALA:HB3	4:I:350:THR:HG21	1.55	0.89
6:L:387:VAL:HG22	6:L:435:ILE:HD13	1.54	0.89
4:I:617:ALA:HB3	4:I:653:MET:HA	1.56	0.88
4:I:1212:LEU:HD22	4:I:1225:VAL:HG21	1.54	0.88
3:M:288:GLU:HA	3:M:291:LYS:HE3	1.55	0.88
1:J:1176:VAL:HG22	1:J:1187:GLU:HA	1.53	0.88
3:G:90:VAL:HG11	3:G:146:VAL:HG21	1.56	0.88
4:I:104:ILE:HG12	4:I:116:ASP:HB2	1.57	0.87
1:J:1054:THR:HB	1:J:1056:LEU:HG	1.57	0.86
4:I:590:PRO:HB2	4:I:655:VAL:HG21	1.56	0.86
1:J:1000:GLY:HA3	1:J:1026:PRO:HG3	1.57	0.86
3:G:45:ARG:HD2	3:H:38:THR:HB	1.58	0.86
4:I:484:LEU:HD12	4:I:486:THR:HB	1.58	0.86
1:J:1178:THR:HG23	1:J:1184:ASP:HB3	1.58	0.86
6:L:558:VAL:HG21	6:L:590:ILE:HG21	1.58	0.86
6:L:593:LYS:HG3	6:L:596:ARG:HH12	1.39	0.86
7:O:19:DA:H1'	7:O:20:DA:H5'	1.55	0.86
1:J:1271:SER:HB3	1:J:1297:LYS:HD3	1.56	0.85
4:I:6:THR:HA	4:I:9:LYS:HD3	1.57	0.85
4:I:992:LEU:HD11	4:I:1000:LEU:HD11	1.58	0.85
1:J:784:ALA:HA	4:I:569:ILE:HD12	1.58	0.84
1:J:1120:THR:HB	1:J:1123:ARG:HG2	1.59	0.84
3:G:104:LYS:HG2	3:G:110:VAL:HG22	1.59	0.84
4:I:993:PRO:HG2	4:I:996:ARG:HB2	1.59	0.84
1:J:1038:THR:O	1:J:1077:ALA:HB3	1.77	0.84
1:J:1172:LYS:HB3	1:J:1189:MET:HB3	1.60	0.84
3:G:105:SER:HB3	3:G:139:SER:HB3	1.59	0.84
1:J:973:LEU:HB3	1:J:1003:LEU:HB2	1.58	0.83
4:I:271:ALA:HA	4:I:274:ILE:HD12	1.60	0.83
6:L:98:VAL:HB	6:L:402:LEU:HD11	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:986:ASP:HB3	1:J:992:LYS:HD2	1.59	0.83
1:J:287:ALA:HB1	1:J:291:ILE:HD11	1.58	0.82
3:M:257:VAL:HA	3:M:260:LEU:HG	1.59	0.82
3:G:90:VAL:HG23	3:G:123:ILE:HD13	1.61	0.82
1:J:961:SER:O	1:J:980:THR:HA	1.79	0.82
4:I:748:ILE:HD11	4:I:966:ILE:HG22	1.59	0.82
1:J:1190:ILE:HG21	1:J:1196:LEU:HD21	1.60	0.82
3:H:93:GLN:HB2	3:H:120:ASP:HB2	1.62	0.82
4:I:905:ILE:HD11	6:L:598:LEU:HD23	1.59	0.82
3:M:257:VAL:HG12	3:M:260:LEU:HD11	1.62	0.82
6:L:270:VAL:HG13	6:L:365:MET:HE3	1.60	0.81
6:L:389:SER:HA	6:L:392:LYS:HE3	1.61	0.81
1:J:338:PHE:HA	1:J:342:LEU:HD22	1.62	0.81
4:I:823:VAL:HG22	4:I:1060:ILE:HG23	1.63	0.81
3:M:269:CYS:HB3	3:M:292:THR:HG21	1.61	0.81
4:I:563:THR:HG21	4:I:570:GLY:H	1.46	0.81
3:H:133:LEU:HD11	3:H:140:ILE:HG21	1.62	0.81
4:I:545:PHE:HA	4:I:548:ARG:HB2	1.63	0.81
8:P:35:DA:H1'	8:P:36:DT:H5'	1.63	0.80
4:I:836:LEU:HD21	4:I:921:PRO:HD3	1.61	0.80
6:L:131:GLN:HB3	6:L:257:LYS:HE3	1.61	0.80
6:L:147:GLN:HA	6:L:150:ARG:HB3	1.62	0.80
1:J:147:ILE:HD11	1:J:179:LYS:HD3	1.62	0.80
4:I:292:ILE:HG22	4:I:317:LEU:HD12	1.64	0.80
4:I:301:TYR:OH	4:I:332:ARG:O	2.00	0.80
3:G:45:ARG:HH21	4:I:1216:ARG:HA	1.45	0.80
4:I:633:LEU:HB2	4:I:644:LEU:HD12	1.60	0.80
1:J:30:ILE:HD13	1:J:243:PRO:HG3	1.63	0.80
4:I:898:GLU:HG3	6:L:565:ILE:HG12	1.64	0.80
3:G:102:LEU:HD23	3:G:115:ILE:HG12	1.65	0.79
1:J:1031:VAL:HG21	1:J:1088:VAL:HG11	1.63	0.79
7:O:52:DA:H1'	7:O:53:DT:H5''	1.63	0.79
1:J:559:ALA:HB3	1:J:562:GLU:HB2	1.64	0.79
4:I:528:ARG:NH2	4:I:576:SER:O	2.14	0.79
1:J:316:ILE:HD11	1:J:324:LEU:HD11	1.65	0.79
1:J:1025:MET:HB2	1:J:1124:ILE:HB	1.63	0.79
3:H:47:LEU:HD22	3:H:180:VAL:HG21	1.64	0.79
5:K:39:VAL:HG23	5:K:52:ARG:HH21	1.46	0.79
1:J:975:ILE:HD11	1:J:1003:LEU:HD12	1.62	0.79
2:N:48:ARG:HE	2:N:55:VAL:HG21	1.48	0.79
3:H:205:MET:HE1	3:H:217:ILE:HG13	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:48:LEU:HD22	3:H:183:ILE:HD11	1.64	0.79
7:O:24:DC:O2	8:P:62:DG:N2	2.16	0.79
1:J:931:THR:HG23	1:J:1244:GLN:HE22	1.48	0.79
6:L:286:LEU:HD23	6:L:340:ALA:HB2	1.64	0.78
4:I:520:PRO:HB2	4:I:794:LEU:HD11	1.66	0.78
4:I:836:LEU:HD13	4:I:1054:LEU:HD13	1.65	0.78
4:I:301:TYR:HB3	4:I:310:ILE:HB	1.64	0.78
4:I:883:LEU:HD11	4:I:1054:LEU:HD11	1.65	0.78
4:I:233:ARG:HD3	4:I:238:GLN:HB2	1.65	0.78
7:O:63:DT:H1'	7:O:64:DT:H5'	1.64	0.78
1:J:218:THR:HA	1:J:221:ILE:HG22	1.66	0.78
6:L:582:VAL:HG21	6:L:587:ILE:HD13	1.64	0.78
1:J:306:LEU:HD13	1:J:307:LEU:HD23	1.66	0.78
4:I:953:LEU:HD22	4:I:1033:ARG:HG3	1.64	0.78
1:J:1167:LYS:HE3	1:J:1170:LYS:HD2	1.66	0.78
4:I:1212:LEU:HD11	4:I:1227:VAL:HG11	1.65	0.77
1:J:399:LYS:HE3	1:J:403:ARG:HH21	1.48	0.77
1:J:288:PRO:HB3	6:L:377:LYS:HG3	1.66	0.77
1:J:348:ASP:OD1	4:I:1246:ARG:NE	2.15	0.77
1:J:112:ALA:HA	1:J:238:ILE:HD13	1.66	0.77
3:M:278:ILE:HG23	3:M:281:LEU:HB3	1.67	0.77
4:I:75:LEU:HD11	4:I:127:ILE:HD11	1.67	0.77
3:G:18:GLN:NE2	3:G:20:SER:O	2.19	0.76
4:I:29:SER:O	4:I:33:ASP:HB2	1.85	0.76
4:I:1314:GLN:HE21	5:K:32:VAL:HG21	1.49	0.76
4:I:255:ILE:HB	4:I:263:VAL:HG12	1.68	0.76
1:J:416:ILE:HG13	1:J:441:LEU:HD21	1.67	0.76
1:J:417:ARG:HG2	1:J:418:GLU:HG2	1.68	0.76
4:I:11:ILE:O	4:I:1149:TYR:OH	2.03	0.76
3:G:14:VAL:HG21	3:G:29:GLU:HB2	1.67	0.76
8:P:29:DA:H1'	8:P:30:DG:H5'	1.67	0.76
3:M:294:ASN:HA	8:P:68:DG:H5''	1.68	0.76
1:J:361:LEU:O	1:J:626:TYR:OH	2.01	0.76
4:I:195:PHE:HB3	4:I:203:LYS:HG3	1.66	0.76
4:I:1078:LYS:HE3	4:I:1080:ASN:HB3	1.67	0.76
1:J:212:THR:HA	1:J:215:LYS:HD2	1.68	0.76
3:H:112:ALA:HB3	3:H:126:PRO:HA	1.65	0.76
1:J:474:LEU:HD13	4:I:1313:HIS:HB2	1.68	0.75
4:I:360:LEU:HD13	4:I:378:ARG:HD3	1.67	0.75
1:J:762:ASN:N	1:J:762:ASN:OD1	2.19	0.75
4:I:180:ARG:NH2	4:I:393:ASP:O	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:516:ASP:HA	1:J:545:HIS:HB2	1.68	0.75
3:H:211:ILE:HG21	3:H:219:ARG:HH22	1.52	0.75
1:J:1346:GLY:O	1:J:1350:ASN:ND2	2.20	0.75
1:J:1357:ILE:HD12	1:J:1359:ALA:HB3	1.69	0.75
4:I:194:LEU:HB3	4:I:206:ALA:HB2	1.68	0.75
4:I:902:LEU:HD12	6:L:607:LEU:HD12	1.68	0.75
1:J:952:VAL:HG13	1:J:1014:GLY:H	1.51	0.75
1:J:813:ASP:OD1	1:J:883:ARG:NH2	2.19	0.74
3:G:35:PHE:HE1	3:H:46:ILE:HG12	1.52	0.74
6:L:142:THR:HA	6:L:145:LEU:HD12	1.69	0.74
4:I:623:LEU:HD22	4:I:627:GLY:HA2	1.70	0.74
1:J:108:ALA:HB2	1:J:280:LYS:HG3	1.68	0.74
4:I:1082:ILE:N	4:I:1082:ILE:HD12	2.02	0.74
6:L:577:GLY:HA2	6:L:582:VAL:HG22	1.69	0.74
1:J:483:LEU:O	1:J:905:ARG:NH1	2.21	0.74
1:J:1265:THR:O	1:J:1303:SER:N	2.19	0.74
6:L:271:ASN:HA	6:L:274:ARG:HD2	1.66	0.74
1:J:34:SER:HB2	1:J:103:GLY:HA2	1.68	0.74
2:N:40:CYS:SG	2:N:42:ASN:ND2	2.60	0.74
3:H:203:ILE:HG21	3:H:217:ILE:HD11	1.69	0.74
4:I:201:ARG:NH1	4:I:370:MET:O	2.19	0.74
4:I:277:LEU:O	4:I:281:ASP:N	2.21	0.74
4:I:1240:ASP:OD1	4:I:1240:ASP:N	2.21	0.74
3:M:292:THR:HG21	3:M:295:LEU:HD13	1.70	0.74
8:P:48:DC:H2''	8:P:49:DT:H71	1.69	0.74
1:J:876:SER:HB3	1:J:990:ARG:HE	1.51	0.74
1:J:702:GLN:HG3	1:J:703:THR:HG23	1.67	0.74
3:G:13:LEU:HD11	3:G:217:ILE:HD11	1.70	0.74
8:P:33:DA:H1'	8:P:34:DT:H5'	1.69	0.73
1:J:475:GLU:OE2	5:K:28:ARG:NH2	2.21	0.73
4:I:303:ASP:N	4:I:308:GLU:O	2.20	0.73
6:L:157:ARG:HD3	6:L:159:SER:H	1.53	0.73
1:J:1215:GLU:HG3	1:J:1220:ILE:HD11	1.69	0.73
3:H:47:LEU:HD13	3:H:183:ILE:HG21	1.69	0.73
1:J:443:GLU:HB2	3:H:196:THR:HG23	1.71	0.73
1:J:1081:VAL:HA	1:J:1088:VAL:H	1.54	0.73
3:M:283:GLN:HE21	3:M:318:LEU:HB2	1.53	0.73
7:O:24:DC:H5''	7:O:24:DC:H6	1.53	0.73
1:J:1005:LYS:HE2	1:J:1017:VAL:HB	1.70	0.73
6:L:278:ASP:OD1	6:L:281:ARG:NH1	2.21	0.73
3:M:259:ASP:O	3:M:310:ARG:NH2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:24:DC:N3	8:P:62:DG:N1	2.37	0.73
1:J:1263:LYS:HE3	1:J:1281:GLU:HG2	1.71	0.73
3:M:255:ARG:HD3	3:M:256:PRO:HD2	1.69	0.73
1:J:210:SER:HB2	1:J:213:LYS:HB2	1.69	0.73
1:J:259:ARG:NH1	6:L:503:GLU:O	2.21	0.73
1:J:1026:PRO:HB2	1:J:1028:ILE:HG23	1.71	0.73
1:J:1115:ILE:HD13	1:J:1119:ASP:HB3	1.70	0.73
1:J:1076:PRO:O	1:J:1101:LEU:N	2.21	0.72
4:I:811:ASN:O	4:I:1099:ASN:ND2	2.21	0.72
4:I:691:PRO:O	4:I:830:THR:OG1	2.05	0.72
1:J:84:ILE:HG22	1:J:91:GLU:HB2	1.71	0.72
4:I:237:LEU:HD13	4:I:289:VAL:HG23	1.72	0.72
4:I:525:THR:HG21	4:I:687:ARG:HD2	1.71	0.72
4:I:745:GLU:HA	4:I:1017:GLN:HG3	1.72	0.72
6:L:287:ILE:HG22	6:L:302:PHE:HE1	1.54	0.72
1:J:741:ALA:O	1:J:762:ASN:ND2	2.22	0.72
1:J:739:GLN:HG2	1:J:744:ARG:HB3	1.71	0.72
2:N:6:ASP:OD1	4:I:678:ARG:NH2	2.23	0.72
7:O:40:DC:H2''	7:O:41:DT:H72	1.70	0.72
1:J:199:GLU:HA	1:J:202:ARG:HD2	1.70	0.72
1:J:1267:VAL:N	1:J:1301:THR:O	2.22	0.72
6:L:123:ILE:HD12	6:L:376:LYS:HG3	1.71	0.72
1:J:534:GLU:OE1	3:H:182:ARG:NH1	2.22	0.72
4:I:176:ILE:HD11	4:I:428:VAL:HG21	1.72	0.72
4:I:230:PHE:HB2	4:I:333:ILE:HB	1.70	0.72
1:J:826:ILE:HG22	1:J:994:SER:HB3	1.71	0.72
4:I:624:ASP:HB3	4:I:630:VAL:HG12	1.70	0.72
4:I:803:ALA:HB2	4:I:1094:VAL:HG11	1.70	0.72
6:L:283:GLN:HB2	6:L:344:LEU:HD21	1.71	0.72
6:L:355:ILE:HG22	6:L:359:LYS:HD2	1.72	0.72
1:J:1005:LYS:HD3	1:J:1017:VAL:HG12	1.71	0.71
1:J:1144:LEU:HD11	1:J:1236:GLU:HB3	1.72	0.71
4:I:629:PHE:HE2	4:I:650:VAL:HG21	1.55	0.71
1:J:603:LYS:O	1:J:607:THR:HG23	1.89	0.71
4:I:1331:ARG:NH2	4:I:1337:ILE:O	2.23	0.71
6:L:234:THR:HB	6:L:244:THR:HB	1.72	0.71
3:M:289:LEU:O	3:M:292:THR:OG1	2.07	0.71
1:J:325:LYS:HG2	1:J:329:ASP:HB2	1.71	0.71
1:J:504:GLN:OE1	1:J:731:ARG:NH1	2.24	0.71
1:J:1179:PRO:HD3	1:J:1184:ASP:HA	1.71	0.71
3:G:222:THR:OG1	3:H:233:ASP:OD1	2.09	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:611:ILE:HG22	1:J:612:LEU:HD12	1.72	0.71
1:J:966:VAL:HG23	1:J:974:VAL:HG23	1.72	0.71
4:I:484:LEU:HB3	4:I:486:THR:HG22	1.72	0.71
4:I:204:LEU:HD11	4:I:369:MET:HE3	1.72	0.71
4:I:685:MET:HE1	4:I:1073:LYS:HG2	1.71	0.71
3:M:260:LEU:HD21	3:M:278:ILE:HD11	1.72	0.71
3:M:298:LYS:NZ	8:P:66:DT:OP1	2.24	0.71
1:J:1023:HIS:HA	1:J:1126:GLN:HE21	1.56	0.71
4:I:826:ASP:OD1	4:I:829:THR:OG1	2.07	0.71
5:K:3:ARG:HH12	5:K:6:VAL:HA	1.55	0.71
4:I:974:ARG:HD3	4:I:1014:LEU:HD21	1.73	0.70
6:L:227:GLN:HG3	6:L:252:LEU:HB2	1.73	0.70
1:J:341:ASN:HD22	4:I:1255:THR:HG21	1.57	0.70
4:I:728:ASP:OD1	4:I:729:ALA:N	2.25	0.70
1:J:848:VAL:HB	1:J:858:VAL:HB	1.74	0.70
3:G:45:ARG:O	3:G:49:SER:OG	2.03	0.70
3:G:165:GLU:HA	3:G:166:ARG:HB3	1.72	0.70
6:L:118:ASP:N	6:L:118:ASP:OD1	2.22	0.70
3:M:278:ILE:HG22	3:M:282:VAL:HG13	1.73	0.70
3:G:29:GLU:OE1	3:G:200:LYS:NZ	2.21	0.70
1:J:1191:PRO:HB2	1:J:1194:ARG:HH11	1.57	0.70
4:I:1008:GLN:O	4:I:1012:GLU:HG2	1.92	0.70
11:J:1506:1N7:C3	11:J:1506:1N7:C18	2.61	0.70
3:G:182:ARG:NH1	4:I:1090:ASN:O	2.25	0.70
4:I:192:ASP:OD2	4:I:436:ARG:NH2	2.25	0.70
4:I:897:PRO:O	4:I:899:GLU:N	2.24	0.70
4:I:10:ARG:NH2	4:I:790:ASP:OD1	2.25	0.69
1:J:77:ARG:HB3	1:J:79:LYS:HG2	1.72	0.69
3:H:180:VAL:HA	3:H:207:THR:HG22	1.75	0.69
4:I:718:ALA:HB2	4:I:783:LEU:HD21	1.74	0.69
4:I:1142:ARG:NH2	4:I:1166:ASP:OD1	2.25	0.69
6:L:311:THR:O	6:L:345:GLN:NE2	2.24	0.69
6:L:31:LEU:HD11	6:L:41:ILE:HG23	1.72	0.69
4:I:886:LYS:NZ	4:I:916:SER:OG	2.25	0.69
7:O:51:DT:H2"	7:O:52:DA:N7	2.06	0.69
4:I:290:GLU:HA	4:I:293:ALA:HB2	1.75	0.69
6:L:456:MET:O	6:L:460:ILE:HG13	1.91	0.69
1:J:1045:THR:HG22	1:J:1071:GLY:HA3	1.73	0.69
4:I:148:GLN:OE1	4:I:454:ARG:NH1	2.25	0.69
4:I:277:LEU:HD22	4:I:282:VAL:HG11	1.75	0.69
4:I:546:GLU:HG3	4:I:547:VAL:HG13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:1069:ARG:NH2	4:I:1114:GLU:OE2	2.25	0.69
6:L:293:GLU:O	6:L:296:LYS:NZ	2.25	0.69
3:M:282:VAL:O	3:M:315:GLY:N	2.26	0.69
1:J:310:GLY:CA	1:J:315:ALA:HB2	2.23	0.69
3:G:6:THR:O	3:G:6:THR:OG1	2.11	0.69
4:I:702:THR:HG22	4:I:1184:THR:O	1.92	0.69
4:I:1146:GLN:NE2	4:I:1150:ASP:OD1	2.26	0.69
1:J:801:VAL:HG12	1:J:920:ALA:HB3	1.75	0.69
1:J:878:ASP:OD1	1:J:878:ASP:N	2.26	0.69
1:J:958:ILE:HB	1:J:1008:GLY:H	1.58	0.69
4:I:992:LEU:HB2	4:I:993:PRO:HD2	1.75	0.68
1:J:654:ILE:HD13	1:J:760:THR:HB	1.74	0.68
3:H:59:VAL:HG11	3:H:85:LEU:HD12	1.75	0.68
4:I:368:ARG:NH1	6:L:33:GLU:OE1	2.25	0.68
6:L:491:GLU:OE1	6:L:495:ARG:NH2	2.26	0.68
1:J:137:ARG:NH2	1:J:143:SER:OG	2.26	0.68
4:I:232:ILE:HB	4:I:331:LYS:HE3	1.73	0.68
4:I:240:GLU:HA	4:I:284:LEU:HD12	1.74	0.68
1:J:331:ILE:HG22	1:J:1328:THR:HG21	1.74	0.68
4:I:101:ARG:NH2	4:I:119:GLU:OE1	2.21	0.68
4:I:732:ILE:HD11	4:I:769:PRO:HB3	1.76	0.68
6:L:358:VAL:HG23	6:L:361:ILE:HD11	1.75	0.68
1:J:958:ILE:HD13	1:J:1005:LYS:HE3	1.76	0.68
1:J:78:LEU:HD23	1:J:81:ARG:HB2	1.74	0.68
3:M:292:THR:HB	3:M:295:LEU:HB3	1.76	0.68
6:L:109:GLU:OE1	6:L:109:GLU:N	2.25	0.68
8:P:24:DG:H1'	8:P:25:DG:H5'	1.75	0.68
4:I:10:ARG:HD2	4:I:1181:PRO:HG2	1.76	0.68
4:I:1061:GLN:HA	4:I:1079:ILE:HD11	1.74	0.68
1:J:965:SER:HA	1:J:975:ILE:HA	1.76	0.68
1:J:996:LYS:HE2	1:J:998:PRO:HA	1.76	0.68
3:H:76:GLU:OE2	3:H:132:HIS:ND1	2.26	0.68
4:I:201:ARG:HA	6:L:28:ASN:HD22	1.58	0.68
1:J:328:ALA:O	1:J:332:LYS:N	2.20	0.67
1:J:974:VAL:HB	1:J:1028:ILE:HD13	1.76	0.67
4:I:746:ALA:CB	4:I:974:ARG:HD2	2.22	0.67
1:J:986:ASP:HB3	1:J:992:LYS:CD	2.24	0.67
6:L:39:ASP:HA	6:L:42:GLU:HG2	1.74	0.67
3:M:255:ARG:HD2	3:M:259:ASP:HB2	1.76	0.67
1:J:883:ARG:NE	1:J:898:CYS:SG	2.68	0.67
4:I:1102:GLY:O	4:I:1106:ARG:HD2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:746:LEU:HD23	1:J:758:PRO:HB3	1.76	0.67
2:N:40:CYS:O	4:I:267:ARG:NH1	2.27	0.67
3:G:8:PHE:HD1	3:G:32:GLU:HG3	1.59	0.67
4:I:183:TRP:N	4:I:199:ASP:OD1	2.27	0.67
4:I:452:ARG:NH2	4:I:458:GLU:OE2	2.20	0.67
4:I:716:ALA:O	4:I:783:LEU:HB2	1.94	0.67
6:L:552:THR:N	6:L:555:GLU:OE2	2.26	0.67
1:J:952:VAL:HG22	1:J:1013:GLY:HA2	1.75	0.67
3:H:140:ILE:HD11	3:H:142:MET:HE2	1.77	0.67
1:J:1349:GLU:O	1:J:1353:VAL:HG12	1.95	0.67
4:I:216:THR:HG22	4:I:219:GLN:HE22	1.60	0.67
1:J:1032:SER:HA	1:J:1115:ILE:O	1.95	0.67
4:I:1168:GLU:OE2	4:I:1171:ARG:NH2	2.28	0.67
11:J:1504:1N7:C3	11:J:1504:1N7:C18	2.67	0.66
4:I:714:VAL:HB	4:I:787:PRO:HD2	1.76	0.66
6:L:23:THR:HG23	6:L:26:GLU:OE1	1.95	0.66
3:M:300:LEU:HA	3:M:303:ILE:HG22	1.75	0.66
1:J:926:PRO:HG2	1:J:1248:ILE:HD11	1.75	0.66
1:J:1358:PRO:HB3	1:J:1366:HIS:HD2	1.60	0.66
4:I:275:ARG:HA	4:I:278:GLU:OE2	1.94	0.66
4:I:469:VAL:O	4:I:472:GLU:HG3	1.95	0.66
6:L:84:LEU:O	6:L:87:VAL:HG12	1.95	0.66
6:L:162:ILE:HG13	6:L:164:GLY:H	1.61	0.66
6:L:464:ASN:O	6:L:468:ARG:HG3	1.96	0.66
7:O:54:DT:H1'	7:O:55:DC:H5'	1.77	0.66
1:J:70:CYS:SG	1:J:71:LEU:N	2.69	0.66
1:J:385:LEU:HD13	1:J:400:MET:HE2	1.75	0.66
1:J:1034:PHE:HA	1:J:1114:GLN:HB3	1.77	0.66
1:J:198:CYS:O	1:J:202:ARG:HG3	1.96	0.66
1:J:962:ASN:HD22	1:J:979:ASN:HB2	1.60	0.66
1:J:1238:GLN:HB3	1:J:1242:ARG:HH21	1.60	0.66
3:H:205:MET:CE	3:H:217:ILE:HG13	2.25	0.66
1:J:242:LEU:HD23	1:J:243:PRO:HD2	1.76	0.66
3:G:45:ARG:NH2	4:I:1216:ARG:HA	2.10	0.66
3:G:96:ASP:OD1	3:G:148:ARG:NH1	2.28	0.66
4:I:895:LEU:HD21	4:I:900:LYS:HE2	1.78	0.66
1:J:888:CYS:SG	1:J:889:ASP:N	2.69	0.66
2:N:67:ARG:HD2	4:I:341:LEU:HG	1.78	0.66
4:I:1246:ARG:NH1	4:I:1265:PHE:O	2.22	0.66
6:L:575:GLU:HA	6:L:578:LYS:HE3	1.78	0.66
1:J:516:ASP:HB3	1:J:573:THR:HG21	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:14:GLN:O	2:N:18:THR:HG22	1.94	0.66
4:I:199:ASP:O	4:I:201:ARG:N	2.28	0.66
1:J:1167:LYS:NZ	1:J:1170:LYS:HB2	2.10	0.66
3:H:46:ILE:CD1	3:H:224:LEU:HB2	2.26	0.66
6:L:454:VAL:HA	6:L:457:ILE:HD12	1.78	0.66
1:J:80:HIS:O	1:J:83:VAL:HG12	1.95	0.65
4:I:159:SER:HB3	4:I:442:VAL:HG11	1.78	0.65
4:I:298:ALA:N	4:I:334:GLU:O	2.26	0.65
4:I:488:MET:HG3	4:I:489:PRO:HD2	1.77	0.65
1:J:262:THR:OG1	1:J:266:ASN:ND2	2.28	0.65
1:J:554:GLU:OE1	1:J:589:TYR:N	2.21	0.65
1:J:697:MET:HE1	1:J:741:ALA:HB3	1.77	0.65
1:J:1163:VAL:HG22	1:J:1175:LEU:HD21	1.79	0.65
3:G:182:ARG:HD2	4:I:1092:THR:HG23	1.79	0.65
6:L:399:LEU:HD21	6:L:446:GLN:HE21	1.62	0.65
4:I:251:ALA:HB2	4:I:269:ILE:HD11	1.77	0.65
6:L:48:ILE:HG13	6:L:84:LEU:HD11	1.79	0.65
1:J:1162:ILE:HA	1:J:1203:ARG:HA	1.78	0.65
1:J:1314:LEU:O	1:J:1326:GLN:NE2	2.29	0.65
1:J:1341:ARG:NH1	1:J:1343:GLU:OE2	2.30	0.65
3:G:61:ILE:HD12	3:G:78:ILE:HD12	1.78	0.65
6:L:347:ILE:HA	6:L:350:GLU:HB2	1.78	0.65
1:J:423:LEU:HB3	1:J:466:MET:HE1	1.79	0.65
4:I:198:ILE:HG22	4:I:199:ASP:H	1.62	0.65
6:L:150:ARG:HG2	6:L:155:GLU:HB2	1.79	0.65
1:J:137:ARG:HE	1:J:143:SER:HB2	1.62	0.65
1:J:557:LYS:HD2	1:J:611:ILE:HG23	1.77	0.65
4:I:331:LYS:HA	4:I:331:LYS:HE2	1.79	0.65
6:L:357:GLN:O	6:L:361:ILE:HG23	1.96	0.65
8:P:49:DT:H1'	8:P:50:DT:H5''	1.78	0.65
1:J:294:ASN:HD22	6:L:406:GLN:HE21	1.42	0.65
1:J:836:ARG:NH2	1:J:870:ASP:OD1	2.29	0.65
3:G:42:ALA:O	3:G:46:ILE:HG12	1.97	0.65
3:G:45:ARG:CD	3:H:38:THR:HB	2.27	0.65
3:G:219:ARG:O	3:G:223:ILE:HG13	1.97	0.65
4:I:185:ASP:HB2	4:I:197:ARG:HG3	1.79	0.65
1:J:853:THR:O	1:J:855:ASP:N	2.24	0.65
4:I:727:VAL:HG23	4:I:732:ILE:HD12	1.78	0.65
1:J:271:ARG:HH11	1:J:316:ILE:HD13	1.62	0.64
1:J:967:VAL:HG22	1:J:973:LEU:HD13	1.78	0.64
1:J:1318:SER:OG	1:J:1342:ASP:OD2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:110:VAL:HG21	3:G:140:ILE:HD11	1.78	0.64
1:J:1061:VAL:HG11	1:J:1076:PRO:HG3	1.79	0.64
4:I:1119:MET:HG2	4:I:1204:LEU:HD13	1.80	0.64
4:I:577:VAL:HG23	4:I:661:VAL:O	1.98	0.64
6:L:163:THR:OG1	6:L:263:PRO:HD3	1.98	0.64
1:J:657:ALA:O	1:J:661:VAL:HG13	1.98	0.64
4:I:1138:VAL:HG21	4:I:1166:ASP:OD2	1.98	0.64
3:M:256:PRO:HG3	3:M:277:TYR:HE1	1.63	0.64
1:J:165:TYR:HE1	1:J:178:ALA:HB3	1.63	0.64
1:J:535:ARG:NH1	3:H:181:GLU:O	2.29	0.64
1:J:726:ALA:HB2	1:J:737:ILE:HD11	1.79	0.64
1:J:1046:ILE:HG21	1:J:1059:LEU:HB3	1.79	0.64
3:G:61:ILE:HB	3:G:64:VAL:HG22	1.79	0.64
6:L:144:LEU:HD11	6:L:224:LEU:HD21	1.79	0.64
6:L:262:VAL:HB	6:L:265:GLN:HG3	1.78	0.64
1:J:1144:LEU:CD1	1:J:1236:GLU:HB3	2.27	0.64
3:H:12:ARG:N	3:H:29:GLU:O	2.27	0.64
1:J:707:ILE:HG22	1:J:708:ASN:H	1.62	0.64
1:J:786:THR:O	1:J:790:THR:HG23	1.97	0.64
4:I:391:SER:HG	4:I:394:ARG:H	1.44	0.64
1:J:849:LEU:HG	1:J:853:THR:HG23	1.78	0.64
1:J:884:SER:OG	1:J:886:VAL:HG12	1.97	0.64
11:J:1505:1N7:C3	11:J:1505:1N7:C2	2.72	0.64
3:G:61:ILE:HB	3:G:64:VAL:CG2	2.28	0.64
4:I:1192:GLU:O	4:I:1196:LYS:HG2	1.98	0.64
6:L:386:LEU:HD11	6:L:390:ILE:HD11	1.79	0.64
3:H:134:THR:HG22	3:H:135:ASP:H	1.62	0.64
4:I:465:ARG:O	4:I:469:VAL:HG23	1.97	0.64
1:J:700:ASN:O	1:J:704:GLU:HB2	1.98	0.63
1:J:1037:PHE:CZ	1:J:1110:GLU:HA	2.32	0.63
3:G:14:VAL:HG12	3:G:15:ASP:H	1.61	0.63
6:L:328:GLU:OE1	6:L:331:HIS:NE2	2.26	0.63
4:I:962:GLU:O	4:I:966:ILE:HG13	1.97	0.63
4:I:643:SER:OG	4:I:644:LEU:N	2.31	0.63
1:J:271:ARG:NH1	1:J:316:ILE:HD13	2.13	0.63
1:J:1266:ILE:HA	1:J:1302:TYR:HA	1.79	0.63
6:L:463:LEU:HD22	6:L:483:LEU:HD23	1.80	0.63
1:J:154:LEU:HD13	1:J:176:PHE:HE1	1.63	0.63
3:G:225:ALA:O	3:G:229:GLU:HG2	1.98	0.63
4:I:56:VAL:HG13	4:I:57:PHE:CD1	2.34	0.63
3:M:289:LEU:HB3	3:M:300:LEU:HD11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:516:ASP:OD2	1:J:547:ARG:NH2	2.32	0.63
1:J:1032:SER:OG	1:J:1117:SER:N	2.32	0.63
3:G:20:SER:OG	3:G:21:SER:N	2.31	0.63
4:I:204:LEU:HD11	4:I:369:MET:CE	2.29	0.63
1:J:104:HIS:HB2	1:J:241:VAL:HG13	1.81	0.63
1:J:998:PRO:HG2	1:J:1020:TRP:CE2	2.34	0.63
11:J:1506:1N7:C3	11:J:1506:1N7:C2	2.71	0.63
4:I:98:VAL:HG21	4:I:124:MET:SD	2.38	0.63
4:I:65:ASN:HB3	4:I:105:TYR:HB2	1.80	0.63
4:I:958:LYS:NZ	4:I:962:GLU:OE1	2.31	0.63
6:L:225:ARG:O	6:L:229:VAL:HG22	1.98	0.63
3:M:285:THR:OG1	3:M:286:GLU:N	2.31	0.63
4:I:617:ALA:N	4:I:652:TYR:O	2.29	0.63
6:L:224:LEU:HD13	6:L:252:LEU:HD11	1.81	0.63
8:P:33:DA:C1'	8:P:34:DT:H5'	2.29	0.63
1:J:510:LEU:HD11	1:J:624:ILE:HG23	1.79	0.62
4:I:615:VAL:N	4:I:651:ASP:OD2	2.20	0.62
4:I:726:TYR:OH	4:I:728:ASP:OD2	2.17	0.62
4:I:1131:MET:CE	4:I:1141:LEU:HA	2.29	0.62
6:L:56:MET:HE1	6:L:60:PRO:O	1.99	0.62
1:J:1275:LEU:HB3	1:J:1278:GLU:HB2	1.80	0.62
3:H:76:GLU:OE1	3:H:76:GLU:N	2.30	0.62
4:I:107:ARG:HD2	8:P:27:DC:H4'	1.82	0.62
4:I:1013:GLN:O	4:I:1017:GLN:NE2	2.31	0.62
1:J:224:LEU:O	1:J:228:VAL:HG23	2.00	0.62
1:J:1001:ALA:HA	1:J:1020:TRP:HB3	1.80	0.62
1:J:1027:VAL:HG11	1:J:1122:ALA:HB3	1.82	0.62
4:I:738:GLU:HA	4:I:741:MET:HE2	1.82	0.62
4:I:928:VAL:HG13	4:I:1052:VAL:HG13	1.80	0.62
6:L:123:ILE:O	6:L:127:ILE:HG23	1.99	0.62
6:L:387:VAL:HG22	6:L:435:ILE:CD1	2.28	0.62
6:L:462:LYS:HB3	6:L:487:MET:HE3	1.81	0.62
1:J:661:VAL:HG12	1:J:685:ILE:HD11	1.82	0.62
3:G:43:LEU:O	3:G:47:LEU:HG	1.99	0.62
4:I:1165:SER:OG	4:I:1167:GLU:N	2.32	0.62
6:L:551:LEU:HD13	6:L:555:GLU:HG3	1.82	0.62
1:J:288:PRO:HD2	1:J:291:ILE:HD11	1.81	0.62
1:J:551:ARG:HB2	1:J:569:LEU:HD12	1.81	0.62
1:J:770:LEU:HD23	4:I:618:GLN:NE2	2.15	0.62
1:J:1196:LEU:HD13	1:J:1210:ILE:HG22	1.81	0.62
1:J:1289:ASN:ND2	1:J:1300:ALA:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1344:LEU:HD12	1:J:1349:GLU:HB3	1.80	0.62
4:I:1131:MET:HE1	4:I:1141:LEU:HA	1.80	0.62
6:L:119:ILE:HG23	6:L:375:ALA:HB1	1.80	0.62
6:L:143:TYR:CG	6:L:269:LEU:HD21	2.33	0.62
1:J:572:THR:OG1	1:J:573:THR:N	2.31	0.62
6:L:110:LEU:HD23	6:L:385:ARG:NE	2.14	0.62
6:L:115:GLY:HA2	6:L:118:ASP:OD2	2.00	0.62
6:L:137:TYR:HB2	6:L:273:MET:HE1	1.82	0.62
6:L:465:ARG:HA	6:L:468:ARG:HE	1.63	0.62
7:O:55:DC:H2''	7:O:56:DC:C5	2.34	0.62
1:J:966:VAL:HG11	1:J:1030:GLU:HA	1.81	0.62
3:H:64:VAL:HG22	3:H:66:HIS:H	1.65	0.62
6:L:534:SER:O	6:L:538:GLU:HG2	1.99	0.62
1:J:140:TYR:OH	1:J:312:ARG:NE	2.32	0.62
1:J:573:THR:OG1	1:J:576:ARG:HD2	1.99	0.62
1:J:630:ALA:O	1:J:634:ARG:HG2	2.00	0.62
1:J:1120:THR:HB	1:J:1123:ARG:CG	2.30	0.62
3:H:48:LEU:HD13	3:H:183:ILE:HD11	1.80	0.62
3:H:96:ASP:OD1	3:H:97:GLU:N	2.31	0.62
4:I:1304:MET:O	4:I:1308:ILE:HG12	2.00	0.62
6:L:394:TYR:HB3	6:L:443:ILE:HD11	1.81	0.62
7:O:25:DA:H2'	7:O:26:DT:C6	2.34	0.62
1:J:1144:LEU:HD21	1:J:1236:GLU:HG2	1.82	0.62
3:H:59:VAL:HB	3:H:144:ILE:HG22	1.82	0.62
4:I:617:ALA:HA	4:I:636:CYS:SG	2.39	0.62
6:L:277:MET:HE3	6:L:281:ARG:NH2	2.15	0.62
7:O:26:DT:H2''	7:O:27:DT:H5'	1.82	0.62
1:J:128:LEU:HB3	1:J:157:GLN:HE22	1.64	0.62
6:L:483:LEU:HB3	6:L:494:ILE:HD13	1.82	0.62
1:J:1143:ASP:OD1	1:J:1148:ARG:HD2	2.00	0.61
4:I:204:LEU:HD21	4:I:369:MET:HG3	1.81	0.61
4:I:303:ASP:HB2	4:I:308:GLU:H	1.65	0.61
4:I:1082:ILE:HD12	4:I:1082:ILE:H	1.64	0.61
6:L:79:ALA:O	6:L:83:VAL:HG23	2.00	0.61
1:J:58:CYS:SG	1:J:61:ILE:HG13	2.39	0.61
1:J:115:TRP:CZ2	1:J:1329:THR:HG22	2.35	0.61
1:J:163:GLU:O	1:J:166:LEU:HG	2.01	0.61
1:J:697:MET:HE1	1:J:737:ILE:HG22	1.80	0.61
1:J:964:LYS:O	1:J:976:THR:OG1	2.11	0.61
4:I:194:LEU:HB3	4:I:206:ALA:CB	2.29	0.61
4:I:314:ASN:OD1	4:I:352:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:960:LEU:HD23	4:I:1029:LEU:HB2	1.82	0.61
6:L:551:LEU:HB3	6:L:555:GLU:HG3	1.82	0.61
7:O:41:DT:H2''	7:O:42:DA:C8	2.35	0.61
1:J:113:HIS:CE1	1:J:115:TRP:HB2	2.35	0.61
1:J:759:ILE:HG21	1:J:767:LEU:HD23	1.81	0.61
3:H:93:GLN:CB	3:H:120:ASP:HB2	2.30	0.61
4:I:452:ARG:NH1	4:I:584:TYR:O	2.33	0.61
6:L:148:TYR:O	6:L:152:GLU:HG2	2.00	0.61
6:L:314:THR:O	6:L:318:ALA:HB3	2.00	0.61
1:J:937:ILE:HD11	1:J:1134:ILE:N	2.15	0.61
4:I:1137:GLU:HG3	4:I:1139:ALA:H	1.64	0.61
1:J:552:ILE:CG1	1:J:570:LYS:HG3	2.31	0.61
1:J:957:SER:HA	1:J:1011:VAL:HG12	1.82	0.61
1:J:981:GLU:HB3	1:J:996:LYS:HA	1.81	0.61
3:H:92:VAL:HG12	3:H:93:GLN:O	2.01	0.61
4:I:255:ILE:O	4:I:262:TYR:N	2.33	0.61
4:I:556:GLY:HA2	4:I:659:GLN:O	2.00	0.61
1:J:91:GLU:HG2	1:J:93:THR:OG1	2.00	0.61
3:H:35:PHE:HA	3:H:38:THR:CG2	2.31	0.61
3:H:95:LYS:HG2	3:H:120:ASP:OD2	2.00	0.61
4:I:171:LEU:O	4:I:188:PHE:HB2	2.00	0.61
4:I:1034:ARG:O	4:I:1038:GLN:HB3	2.01	0.61
8:P:41:DT:H2''	8:P:42:DT:H5''	1.82	0.61
1:J:422:LEU:HD13	1:J:471:PRO:HG3	1.81	0.61
1:J:520:ALA:HB3	1:J:546:ALA:HB2	1.80	0.61
1:J:914:ALA:HB2	1:J:1359:ALA:HB1	1.81	0.61
1:J:965:SER:CB	1:J:975:ILE:HA	2.31	0.61
1:J:1078:LEU:HD21	1:J:1121:LEU:CB	2.30	0.61
6:L:282:THR:HA	6:L:285:ARG:HG2	1.81	0.61
1:J:1265:THR:HG22	1:J:1278:GLU:O	2.00	0.61
3:H:112:ALA:O	3:H:115:ILE:HG13	2.01	0.61
4:I:237:LEU:HD21	4:I:322:LEU:HB2	1.82	0.61
1:J:421:VAL:HG13	1:J:439:PRO:HG3	1.82	0.61
1:J:1284:ARG:O	1:J:1287:ILE:HG13	2.01	0.61
1:J:1360:GLY:HA3	4:I:1282:GLY:HA2	1.81	0.61
4:I:232:ILE:HB	4:I:331:LYS:CE	2.29	0.61
4:I:249:GLU:O	4:I:269:ILE:N	2.23	0.61
3:M:284:ARG:HB3	3:M:288:GLU:HG2	1.82	0.61
8:P:65:DT:H2'	8:P:66:DT:H72	1.82	0.61
1:J:641:ILE:HD13	4:I:1113:LEU:HG	1.82	0.61
1:J:702:GLN:O	1:J:718:SER:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:953:LYS:HE2	1:J:954:ASN:OD1	1.99	0.61
4:I:253:PHE:CE2	4:I:287:VAL:HG12	2.36	0.61
4:I:360:LEU:HB2	4:I:378:ARG:NH1	2.16	0.61
4:I:400:VAL:HG21	4:I:452:ARG:HD2	1.83	0.61
4:I:489:PRO:HA	4:I:492:MET:CG	2.31	0.61
4:I:590:PRO:HB2	4:I:655:VAL:CG2	2.29	0.61
4:I:1111:GLN:HB2	4:I:1230:MET:CE	2.31	0.60
1:J:518:VAL:CG1	1:J:707:ILE:HB	2.31	0.60
1:J:709:ARG:NH1	1:J:710:ASP:OD2	2.34	0.60
1:J:1031:VAL:HG21	1:J:1088:VAL:CG1	2.29	0.60
4:I:607:SER:OG	4:I:608:ALA:N	2.32	0.60
4:I:745:GLU:CA	4:I:1017:GLN:HG3	2.30	0.60
4:I:796:LEU:HB2	4:I:1233:LEU:HD11	1.83	0.60
7:O:36:DA:H1'	7:O:37:DA:H5'	1.82	0.60
1:J:332:LYS:HB2	1:J:1328:THR:HB	1.81	0.60
1:J:801:VAL:O	1:J:805:GLN:HB2	2.01	0.60
1:J:1002:VAL:HB	1:J:1019:ASN:O	2.00	0.60
3:M:278:ILE:HA	3:M:281:LEU:HB2	1.82	0.60
3:G:184:ALA:HB2	4:I:1091:GLY:HA3	1.83	0.60
4:I:898:GLU:HB3	6:L:544:THR:HG21	1.83	0.60
6:L:589:GLN:HE22	7:O:26:DT:H73	1.66	0.60
6:L:291:CYS:HA	6:L:295:CYS:HB3	1.82	0.60
6:L:300:LYS:O	6:L:304:THR:OG1	2.15	0.60
6:L:436:ARG:CZ	8:P:35:DA:H3'	2.32	0.60
3:M:284:ARG:NH1	3:M:288:GLU:OE2	2.32	0.60
1:J:708:ASN:N	1:J:708:ASN:OD1	2.33	0.60
1:J:776:THR:HG22	4:I:550:VAL:HG11	1.84	0.60
1:J:896:ALA:HB1	1:J:909:ILE:HG22	1.84	0.60
4:I:106:GLU:HG3	4:I:108:GLU:OE2	2.02	0.60
4:I:498:ILE:O	4:I:502:VAL:HG12	2.00	0.60
8:P:48:DC:C2'	8:P:49:DT:H71	2.31	0.60
1:J:640:GLY:HA3	4:I:1209:GLN:HE21	1.66	0.60
2:N:36:LEU:HG	2:N:41:GLY:HA2	1.83	0.60
4:I:196:VAL:HG12	4:I:206:ALA:HA	1.82	0.60
1:J:165:TYR:CE1	1:J:178:ALA:HB3	2.37	0.60
1:J:1163:VAL:CG2	1:J:1175:LEU:HD21	2.32	0.60
3:H:228:LEU:O	3:H:232:VAL:HG23	2.01	0.60
4:I:11:ILE:HD11	4:I:1157:GLN:NE2	2.16	0.60
4:I:236:LYS:HA	4:I:237:LEU:HD12	1.84	0.60
4:I:237:LEU:HD13	4:I:289:VAL:CG2	2.31	0.60
5:K:3:ARG:NH1	5:K:5:THR:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:39:VAL:HG13	5:K:53:GLU:HG2	1.84	0.60
6:L:387:VAL:HG21	6:L:412:LEU:HD22	1.84	0.60
1:J:278:ARG:HH21	6:L:446:GLN:HE22	1.49	0.60
1:J:964:LYS:O	1:J:976:THR:N	2.35	0.60
2:N:40:CYS:HB2	4:I:268:ARG:HB3	1.84	0.60
4:I:378:ARG:O	4:I:382:GLU:HG3	2.02	0.60
4:I:819:SER:HB2	4:I:1085:MET:HG3	1.84	0.60
6:L:348:GLU:HG2	6:L:355:ILE:HG12	1.82	0.60
1:J:22:ILE:HD11	1:J:1332:LEU:HD13	1.83	0.60
1:J:189:LEU:HD13	1:J:234:PRO:O	2.02	0.60
1:J:549:LYS:NZ	1:J:571:ASP:OD1	2.25	0.60
1:J:1026:PRO:HA	1:J:1120:THR:HG22	1.82	0.60
1:J:1041:ILE:N	1:J:1045:THR:OG1	2.35	0.60
4:I:152:SER:HB2	4:I:452:ARG:HD3	1.84	0.60
3:G:7:GLU:OE1	3:G:7:GLU:N	2.28	0.59
4:I:500:ALA:O	4:I:504:GLU:HG3	2.01	0.59
4:I:599:VAL:HG21	4:I:623:LEU:HD21	1.83	0.59
6:L:574:GLU:OE2	6:L:584:ARG:HD3	2.02	0.59
3:M:252:ILE:O	3:M:255:ARG:HB3	2.01	0.59
1:J:1005:LYS:CE	1:J:1017:VAL:HB	2.32	0.59
11:J:1505:1N7:H31	11:J:1505:1N7:H5	1.83	0.59
4:I:172:TYR:O	4:I:432:LEU:HD11	2.03	0.59
4:I:207:THR:HG23	4:I:350:THR:HG22	1.85	0.59
6:L:324:LYS:H	6:L:327:SER:HB2	1.65	0.59
1:J:242:LEU:HD23	1:J:243:PRO:CD	2.32	0.59
1:J:338:PHE:CE2	4:I:1326:LEU:HD11	2.38	0.59
4:I:811:ASN:HA	4:I:815:SER:HB2	1.84	0.59
6:L:301:ASN:ND2	6:L:305:LEU:HD13	2.18	0.59
3:M:298:LYS:O	3:M:301:THR:HG22	2.02	0.59
1:J:51:PRO:HB2	1:J:57:PHE:O	2.03	0.59
1:J:105:ILE:HD13	1:J:273:ILE:HG12	1.84	0.59
1:J:809:VAL:HG11	1:J:909:ILE:CG2	2.33	0.59
3:G:8:PHE:CD1	3:G:32:GLU:HG3	2.38	0.59
1:J:370:LYS:HD3	1:J:443:GLU:HG3	1.83	0.59
4:I:105:TYR:HD1	4:I:114:VAL:HA	1.67	0.59
4:I:188:PHE:HE1	4:I:432:LEU:HG	1.67	0.59
6:L:586:ARG:NH2	7:O:24:DC:H3'	2.17	0.59
1:J:232:ASN:ND2	1:J:1337:VAL:O	2.36	0.59
1:J:1368:ASP:O	1:J:1372:ARG:HG2	2.03	0.59
4:I:215:TYR:OH	4:I:422:LYS:HE3	2.03	0.59
6:L:143:TYR:HD2	6:L:269:LEU:HD11	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:419:HIS:NE2	1:J:471:PRO:O	2.28	0.59
1:J:473:THR:HG23	4:I:1289:GLU:OE1	2.03	0.59
1:J:698:MET:O	1:J:702:GLN:HG2	2.03	0.59
1:J:797:THR:O	1:J:801:VAL:HG13	2.03	0.59
1:J:955:LYS:O	1:J:992:LYS:NZ	2.23	0.59
4:I:182:SER:HB2	4:I:389:PHE:HE1	1.68	0.59
4:I:898:GLU:OE2	6:L:541:ARG:HG2	2.03	0.59
7:O:26:DT:H2''	7:O:27:DT:C5'	2.33	0.59
3:H:97:GLU:HG2	3:H:147:GLN:HG2	1.84	0.59
4:I:230:PHE:CE1	4:I:239:MET:HB2	2.38	0.59
4:I:303:ASP:HA	4:I:310:ILE:HD11	1.85	0.59
4:I:936:ARG:HD2	4:I:938:GLY:H	1.68	0.59
11:I:1401:1N7:C3	11:I:1401:1N7:C2	2.71	0.59
6:L:127:ILE:O	6:L:131:GLN:HG3	2.02	0.59
3:G:13:LEU:CD1	3:G:217:ILE:HD11	2.33	0.59
4:I:478:ARG:NE	4:I:487:LEU:HD13	2.18	0.59
4:I:671:LEU:HB3	4:I:1186:VAL:HG12	1.84	0.59
4:I:741:MET:HE3	4:I:974:ARG:HH21	1.68	0.59
1:J:678:ARG:NH1	1:J:756:GLU:OE1	2.33	0.59
1:J:264:ASP:HB3	1:J:324:LEU:HB2	1.85	0.58
1:J:552:ILE:HD11	1:J:570:LYS:HZ3	1.67	0.58
1:J:796:LEU:HD13	1:J:800:LEU:HD13	1.83	0.58
1:J:1026:PRO:CB	1:J:1028:ILE:HG23	2.33	0.58
3:G:76:GLU:HB3	3:G:80:GLU:HB3	1.83	0.58
4:I:230:PHE:CD1	4:I:239:MET:HB2	2.38	0.58
4:I:1002:LEU:HD21	4:I:1007:LYS:HB2	1.85	0.58
6:L:315:TRP:O	6:L:319:ALA:HB2	2.03	0.58
7:O:63:DT:H1'	7:O:64:DT:C5'	2.30	0.58
1:J:720:ASN:O	1:J:723:TYR:N	2.35	0.58
1:J:1030:GLU:OE1	1:J:1091:PRO:HD2	2.03	0.58
6:L:251:LYS:O	6:L:255:VAL:HG12	2.02	0.58
1:J:363:LEU:O	1:J:486:SER:OG	2.21	0.58
1:J:1115:ILE:CG1	1:J:1121:LEU:HD21	2.27	0.58
4:I:253:PHE:CA	4:I:265:LYS:HG3	2.33	0.58
4:I:975:ILE:HG13	4:I:1014:LEU:HD23	1.85	0.58
6:L:144:LEU:HD11	6:L:224:LEU:CD2	2.33	0.58
6:L:595:LEU:O	6:L:599:ARG:HG3	2.03	0.58
1:J:211:GLU:HB3	1:J:215:LYS:NZ	2.19	0.58
1:J:736:GLN:OE1	4:I:1105:SER:HA	2.03	0.58
1:J:1003:LEU:HD23	1:J:1017:VAL:O	2.02	0.58
4:I:631:GLU:OE1	4:I:631:GLU:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:689:ALA:CB	4:I:1233:LEU:HD12	2.33	0.58
4:I:718:ALA:HB2	4:I:783:LEU:CD2	2.34	0.58
6:L:51:MET:HG3	6:L:52:GLY:O	2.03	0.58
1:J:143:SER:O	1:J:180:MET:HE3	2.04	0.58
1:J:836:ARG:HG3	1:J:869:CYS:SG	2.43	0.58
4:I:559:CYS:CB	4:I:662:SER:HG	2.16	0.58
1:J:598:LYS:HA	1:J:601:ILE:HG22	1.84	0.58
1:J:1316:THR:OG1	1:J:1322:ALA:HB2	2.02	0.58
11:J:1504:1N7:C3	11:J:1504:1N7:C2	2.74	0.58
3:H:103:ASN:HA	3:H:141:SER:HA	1.85	0.58
4:I:557:ARG:NH2	4:I:611:GLU:OE1	2.28	0.58
6:L:9:LEU:O	6:L:13:VAL:HG23	2.03	0.58
3:M:283:GLN:HA	3:M:316:MET:O	2.04	0.58
3:G:228:LEU:O	3:G:232:VAL:HG12	2.04	0.58
4:I:360:LEU:HD13	4:I:378:ARG:CD	2.34	0.58
6:L:165:PHE:O	6:L:260:ARG:NH2	2.34	0.58
6:L:369:GLU:O	6:L:373:ARG:HG3	2.04	0.58
6:L:551:LEU:HD11	6:L:598:LEU:CD1	2.33	0.58
1:J:179:LYS:HB3	1:J:184:ALA:HB2	1.84	0.58
1:J:271:ARG:O	1:J:275:ARG:HG3	2.04	0.58
1:J:279:LEU:O	1:J:283:LEU:HG	2.04	0.58
1:J:310:GLY:HA2	1:J:315:ALA:HB2	1.85	0.58
1:J:1045:THR:CG2	1:J:1071:GLY:HA3	2.34	0.58
1:J:1167:LYS:NZ	1:J:1168:GLU:O	2.37	0.58
3:G:133:LEU:HD21	3:G:140:ILE:HG12	1.86	0.58
4:I:253:PHE:CZ	4:I:255:ILE:HG12	2.39	0.58
4:I:861:ALA:O	4:I:862:LEU:HD23	2.03	0.58
6:L:295:CYS:SG	6:L:330:LEU:HA	2.44	0.58
6:L:356:GLU:OE1	6:L:356:GLU:N	2.37	0.58
6:L:384:LEU:HA	6:L:387:VAL:CG2	2.34	0.58
8:P:64:DA:H2 ⁺	8:P:65:DT:H71	1.85	0.58
4:I:59:ILE:HD11	4:I:476:LYS:HD2	1.86	0.58
6:L:584:ARG:NH1	8:P:56:DG:N7	2.51	0.58
1:J:154:LEU:HD23	1:J:158:GLN:NE2	2.18	0.57
3:G:194:GLN:O	3:G:195:ARG:HG2	2.04	0.57
4:I:319:LEU:O	4:I:322:LEU:HG	2.04	0.57
1:J:369:PRO:HA	1:J:442:ILE:O	2.04	0.57
1:J:809:VAL:HG21	1:J:909:ILE:HG13	1.85	0.57
1:J:1173:ARG:HG2	1:J:1190:ILE:O	2.04	0.57
4:I:517:GLN:C	4:I:519:ASN:H	2.08	0.57
4:I:617:ALA:HB3	4:I:653:MET:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:1217:THR:OG1	4:I:1219:GLU:HG2	2.04	0.57
8:P:28:DG:H2''	8:P:29:DA:N7	2.19	0.57
1:J:79:LYS:CB	6:L:569:THR:HG22	2.34	0.57
1:J:531:LYS:NZ	3:H:206:GLU:OE1	2.27	0.57
3:H:77:ASP:O	3:H:81:ILE:HG13	2.04	0.57
3:H:91:ARG:CG	3:H:122:GLU:HB3	2.31	0.57
3:H:104:LYS:HE3	3:H:114:ASP:OD2	2.04	0.57
6:L:147:GLN:O	6:L:151:VAL:HG22	2.03	0.57
6:L:550:GLY:O	6:L:551:LEU:HD23	2.04	0.57
6:L:552:THR:O	6:L:555:GLU:HG2	2.03	0.57
3:G:218:ARG:HG3	3:H:231:PHE:O	2.04	0.57
4:I:131:THR:HG22	4:I:132:ASP:H	1.68	0.57
4:I:243:PRO:HB3	4:I:277:LEU:CD1	2.34	0.57
4:I:678:ARG:NH2	4:I:1106:ARG:HG2	2.19	0.57
4:I:720:ARG:NH1	4:I:736:VAL:HG11	2.20	0.57
4:I:1151:LEU:HD22	4:I:1198:LEU:HG	1.86	0.57
6:L:266:PHE:O	6:L:270:VAL:HG23	2.03	0.57
3:M:269:CYS:SG	3:M:295:LEU:HD12	2.44	0.57
3:M:283:GLN:NE2	3:M:318:LEU:HB2	2.19	0.57
1:J:289:ASP:N	1:J:289:ASP:OD1	2.32	0.57
1:J:721:SER:O	1:J:725:MET:HG3	2.05	0.57
1:J:839:VAL:CG1	1:J:864:LEU:HD12	2.33	0.57
3:G:110:VAL:HG11	3:G:140:ILE:HD11	1.86	0.57
4:I:201:ARG:HA	6:L:28:ASN:ND2	2.18	0.57
4:I:1043:ALA:O	4:I:1046:VAL:HG12	2.04	0.57
6:L:358:VAL:O	6:L:362:ASN:ND2	2.36	0.57
7:O:50:DA:H2'	7:O:50:DA:OP2	2.05	0.57
1:J:799:ARG:HG2	1:J:1309:ILE:HD12	1.86	0.57
1:J:839:VAL:HG12	1:J:864:LEU:HD12	1.87	0.57
4:I:144:VAL:CG2	4:I:515:MET:HB2	2.35	0.57
4:I:902:LEU:HD21	6:L:611:LEU:HG	1.87	0.57
1:J:128:LEU:HB3	1:J:157:GLN:NE2	2.19	0.57
4:I:471:VAL:HG21	4:I:498:ILE:HD11	1.85	0.57
4:I:987:GLU:HB2	4:I:990:ASP:OD2	2.05	0.57
6:L:99:ARG:O	6:L:103:ARG:HG3	2.05	0.57
1:J:370:LYS:CE	1:J:443:GLU:HG3	2.35	0.57
1:J:495:ASN:N	1:J:495:ASN:OD1	2.37	0.57
4:I:14:ASP:H	4:I:1157:GLN:HG2	1.69	0.57
5:K:44:ASP:HB3	5:K:49:ILE:HG13	1.87	0.57
6:L:478:PRO:HB2	6:L:483:LEU:CD1	2.35	0.57
8:P:64:DA:H2''	8:P:65:DT:C7	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1036:ARG:HB3	1:J:1079:LYS:HG2	1.86	0.57
3:H:32:GLU:HB3	3:H:35:PHE:HD2	1.69	0.57
4:I:82:VAL:O	4:I:86:GLN:HG3	2.04	0.57
5:K:41:GLU:HB3	5:K:49:ILE:HD11	1.87	0.57
6:L:409:ASN:O	6:L:413:MET:HG3	2.05	0.57
7:O:39:DG:H1'	7:O:40:DC:H5'	1.85	0.57
1:J:121:PRO:HB2	1:J:126:LEU:CD2	2.35	0.57
1:J:147:ILE:HG22	1:J:188:LEU:HG	1.87	0.57
1:J:1322:ALA:O	1:J:1326:GLN:HB2	2.05	0.57
5:K:26:ARG:NH2	5:K:38:LEU:HD23	2.20	0.57
6:L:290:LEU:HB3	6:L:333:VAL:HG21	1.86	0.57
6:L:333:VAL:O	6:L:337:VAL:HG23	2.05	0.57
7:O:40:DC:C2'	7:O:41:DT:H72	2.35	0.57
1:J:1078:LEU:HD21	1:J:1121:LEU:HB2	1.87	0.56
3:H:124:VAL:HG13	3:H:125:LYS:HG3	1.87	0.56
4:I:245:ARG:HB3	4:I:337:PHE:CZ	2.40	0.56
4:I:671:LEU:HD23	4:I:1186:VAL:HG11	1.86	0.56
6:L:143:TYR:CD2	6:L:269:LEU:HD11	2.39	0.56
6:L:378:GLU:HA	6:L:381:GLU:OE2	2.05	0.56
1:J:369:PRO:HB3	1:J:444:GLY:O	2.04	0.56
1:J:935:PHE:HE2	1:J:1243:LEU:HD11	1.70	0.56
1:J:1108:GLN:HB2	1:J:1123:ARG:HH12	1.70	0.56
3:G:179:PRO:HG3	3:G:211:ILE:HG13	1.86	0.56
4:I:975:ILE:CG1	4:I:1014:LEU:HD23	2.35	0.56
6:L:27:VAL:O	6:L:31:LEU:HG	2.05	0.56
6:L:143:TYR:HA	6:L:146:GLU:OE1	2.05	0.56
7:O:29:DA:H1'	7:O:30:DC:H5'	1.87	0.56
8:P:54:DT:C6	8:P:55:DT:H72	2.40	0.56
1:J:661:VAL:HG12	1:J:685:ILE:CD1	2.34	0.56
1:J:1029:THR:OG1	1:J:1118:GLY:N	2.37	0.56
1:J:1266:ILE:CG2	1:J:1300:ALA:HB1	2.35	0.56
1:J:1287:ILE:HG22	1:J:1290:ARG:HH22	1.70	0.56
2:N:64:TYR:HD1	4:I:341:LEU:HD22	1.71	0.56
3:H:44:ARG:HB2	3:H:183:ILE:HD13	1.86	0.56
4:I:56:VAL:HG13	4:I:57:PHE:HD1	1.69	0.56
4:I:104:ILE:CG1	4:I:116:ASP:HB2	2.33	0.56
4:I:239:MET:HB3	4:I:285:ILE:HD11	1.87	0.56
4:I:720:ARG:HH11	4:I:736:VAL:HG11	1.71	0.56
4:I:1117:LEU:HD21	4:I:1182:ILE:HG21	1.88	0.56
4:I:1260:GLY:HA2	4:I:1265:PHE:HB2	1.87	0.56
6:L:358:VAL:CA	6:L:361:ILE:HG12	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:418:GLU:OE1	5:K:2:ALA:HA	2.05	0.56
1:J:965:SER:HB2	1:J:975:ILE:HA	1.87	0.56
1:J:1080:ILE:O	1:J:1088:VAL:HB	2.06	0.56
1:J:1153:PRO:HA	1:J:1214:PRO:O	2.06	0.56
1:J:1171:GLY:O	1:J:1191:PRO:HA	2.06	0.56
3:H:21:SER:O	3:H:21:SER:OG	2.23	0.56
4:I:302:ILE:HA	4:I:310:ILE:H	1.70	0.56
4:I:720:ARG:HG2	4:I:740:GLU:OE1	2.06	0.56
4:I:964:LEU:HD13	4:I:1025:PHE:HD2	1.69	0.56
4:I:1108:ASN:OD1	4:I:1111:GLN:NE2	2.38	0.56
4:I:1119:MET:HG2	4:I:1204:LEU:CD1	2.35	0.56
4:I:1165:SER:OG	4:I:1166:ASP:N	2.37	0.56
6:L:359:LYS:HA	6:L:362:ASN:HD21	1.71	0.56
1:J:594:GLN:HE21	1:J:600:ALA:HB1	1.71	0.56
1:J:1095:MET:HG2	1:J:1096:PRO:O	2.06	0.56
1:J:1152:GLU:O	1:J:1214:PRO:HD2	2.05	0.56
1:J:1172:LYS:CB	1:J:1189:MET:HB3	2.34	0.56
3:G:90:VAL:HG11	3:G:146:VAL:CG2	2.34	0.56
3:G:166:ARG:HB2	3:G:167:PRO:HD2	1.86	0.56
3:H:50:SER:HA	3:H:150:ARG:HG2	1.87	0.56
4:I:422:LYS:O	4:I:426:ILE:HD12	2.06	0.56
4:I:1080:ASN:ND2	4:I:1085:MET:SD	2.78	0.56
4:I:1145:ILE:HD11	4:I:1173:ALA:HB2	1.86	0.56
6:L:544:THR:O	6:L:548:LEU:HG	2.06	0.56
1:J:1174:ARG:HG3	1:J:1189:MET:CE	2.35	0.56
3:G:57:THR:HG22	3:G:175:ALA:HB2	1.87	0.56
1:J:134:ASP:O	1:J:138:VAL:HG23	2.05	0.56
3:G:7:GLU:HG2	3:G:8:PHE:H	1.71	0.56
4:I:1307:ASN:HB3	4:I:1312:ASN:O	2.04	0.56
6:L:262:VAL:HG13	6:L:263:PRO:HD2	1.87	0.56
6:L:287:ILE:HD13	6:L:315:TRP:CH2	2.41	0.56
6:L:484:ALA:CB	6:L:491:GLU:HB2	2.36	0.56
8:P:29:DA:C1'	8:P:30:DG:H5'	2.34	0.56
1:J:147:ILE:CG2	1:J:188:LEU:HG	2.35	0.56
1:J:983:LYS:HE3	1:J:994:SER:CB	2.36	0.56
1:J:1321:SER:O	1:J:1324:SER:OG	2.21	0.56
4:I:50:GLU:O	4:I:54:ARG:HG3	2.05	0.56
4:I:455:SER:O	4:I:459:MET:HG3	2.06	0.56
4:I:1002:LEU:HD23	4:I:1003:THR:O	2.06	0.56
4:I:1078:LYS:CE	4:I:1080:ASN:HB3	2.34	0.56
6:L:141:ILE:O	6:L:144:LEU:HG	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:281:ARG:HA	6:L:284:GLU:OE1	2.06	0.56
6:L:551:LEU:HD11	6:L:598:LEU:HD11	1.87	0.56
1:J:958:ILE:HG12	1:J:1005:LYS:HZ1	1.70	0.56
1:J:1078:LEU:HB3	1:J:1101:LEU:HD11	1.87	0.56
3:G:192:VAL:HG12	3:G:195:ARG:HB2	1.88	0.56
4:I:22:LEU:HD22	4:I:603:ILE:CD1	2.36	0.56
4:I:148:GLN:HB2	4:I:511:LEU:CD1	2.35	0.56
8:P:33:DA:C4'	8:P:34:DT:H5'	2.35	0.56
1:J:22:ILE:HG13	4:I:1337:ILE:HB	1.88	0.56
1:J:218:THR:HA	1:J:221:ILE:CG2	2.34	0.56
1:J:532:GLU:OE2	3:H:86:LYS:NZ	2.25	0.56
1:J:849:LEU:HB3	1:J:853:THR:HG23	1.87	0.56
1:J:870:ASP:O	1:J:874:GLU:HG2	2.05	0.56
1:J:1080:ILE:HD11	1:J:1121:LEU:HD11	1.88	0.56
4:I:98:VAL:O	4:I:122:VAL:HG12	2.06	0.56
4:I:397:LEU:H	4:I:397:LEU:HD12	1.71	0.56
4:I:519:ASN:O	4:I:523:GLU:HG3	2.05	0.56
4:I:1002:LEU:HB3	4:I:1008:GLN:OE1	2.06	0.56
11:I:1401:1N7:C3	11:I:1401:1N7:C18	2.71	0.56
3:M:279:GLY:HA3	3:M:321:TRP:NE1	2.21	0.56
8:P:28:DG:H2''	8:P:29:DA:C8	2.41	0.56
8:P:30:DG:H2''	8:P:31:DG:N7	2.21	0.56
1:J:330:MET:O	1:J:337:ARG:HG2	2.06	0.55
1:J:829:GLY:O	1:J:993:GLU:HG3	2.06	0.55
1:J:849:LEU:CD1	1:J:856:ILE:HA	2.37	0.55
3:G:102:LEU:HD23	3:G:115:ILE:CG1	2.35	0.55
3:G:165:GLU:HA	3:G:166:ARG:CB	2.35	0.55
4:I:1263:ALA:HA	4:I:1264:GLN:HB2	1.88	0.55
5:K:60:ASN:OD1	5:K:63:ILE:HD13	2.06	0.55
6:L:301:ASN:HD21	6:L:305:LEU:HD13	1.70	0.55
6:L:496:LYS:O	6:L:500:ILE:HG12	2.05	0.55
4:I:239:MET:HB3	4:I:285:ILE:CD1	2.35	0.55
6:L:119:ILE:O	6:L:123:ILE:HG12	2.05	0.55
6:L:224:LEU:CD1	6:L:252:LEU:HD11	2.34	0.55
7:O:54:DT:C1'	7:O:55:DC:H5'	2.36	0.55
1:J:45:ASN:HB3	1:J:48:THR:O	2.05	0.55
3:G:190:ALA:HB2	3:G:200:LYS:N	2.21	0.55
4:I:854:ILE:HD11	4:I:885:GLY:HA3	1.89	0.55
1:J:353:SER:OG	1:J:354:VAL:N	2.39	0.55
1:J:958:ILE:HB	1:J:1008:GLY:N	2.20	0.55
1:J:1060:VAL:HA	1:J:1107:VAL:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:287:VAL:HB	4:I:288:PRO:HD2	1.87	0.55
4:I:1174:GLU:HG2	4:I:1177:ARG:HD2	1.87	0.55
6:L:165:PHE:HA	6:L:260:ARG:HB3	1.87	0.55
6:L:484:ALA:HB2	6:L:491:GLU:OE2	2.07	0.55
3:M:295:LEU:HD11	3:M:300:LEU:CD2	2.36	0.55
1:J:77:ARG:HH21	1:J:80:HIS:HE1	1.53	0.55
1:J:384:LYS:HG2	1:J:411:ILE:HG23	1.88	0.55
4:I:596:ASP:OD1	4:I:596:ASP:N	2.40	0.55
4:I:1042:LEU:HB3	4:I:1046:VAL:CG1	2.37	0.55
7:O:30:DC:H2''	7:O:31:DA:C8	2.42	0.55
1:J:551:ARG:HB2	1:J:569:LEU:CD1	2.36	0.55
1:J:552:ILE:HD11	1:J:570:LYS:CE	2.35	0.55
1:J:956:GLY:HA3	1:J:984:LEU:HD11	1.89	0.55
4:I:965:GLN:HA	4:I:968:GLU:OE1	2.07	0.55
4:I:992:LEU:CD1	4:I:1000:LEU:HD11	2.35	0.55
6:L:24:TYR:HA	6:L:27:VAL:HG12	1.87	0.55
6:L:131:GLN:CB	6:L:257:LYS:HE3	2.33	0.55
6:L:292:VAL:HA	6:L:297:MET:HB3	1.89	0.55
1:J:453:VAL:HG12	1:J:457:TYR:HD2	1.70	0.55
3:H:22:THR:OG1	3:H:207:THR:O	2.25	0.55
4:I:478:ARG:CZ	4:I:487:LEU:HD13	2.37	0.55
4:I:995:ASP:OD1	4:I:995:ASP:N	2.39	0.55
6:L:327:SER:HA	6:L:330:LEU:HD12	1.89	0.55
1:J:1050:THR:HA	1:J:1056:LEU:O	2.07	0.55
2:N:46:GLU:OE1	2:N:49:ARG:NH1	2.39	0.55
3:G:11:PRO:HD3	3:H:227:GLN:HG3	1.89	0.55
4:I:11:ILE:HD11	4:I:1157:GLN:HE22	1.72	0.55
4:I:402:ARG:HG2	4:I:416:GLY:H	1.72	0.55
4:I:582:ASN:N	4:I:586:PHE:O	2.27	0.55
1:J:210:SER:O	1:J:214:ARG:HG2	2.05	0.55
1:J:269:TYR:O	1:J:273:ILE:HG13	2.06	0.55
1:J:1072:LYS:NZ	1:J:1168:GLU:HB3	2.21	0.55
4:I:1305:TYR:O	4:I:1309:VAL:HG13	2.06	0.55
5:K:40:PRO:O	5:K:52:ARG:NH2	2.28	0.55
6:L:387:VAL:CG2	6:L:412:LEU:HD22	2.37	0.55
6:L:448:ARG:HH22	6:L:452:ILE:HD13	1.71	0.55
6:L:577:GLY:O	6:L:581:ASP:N	2.39	0.55
8:P:49:DT:H2''	8:P:50:DT:H5''	1.89	0.55
1:J:56:LEU:HD21	1:J:269:TYR:CB	2.37	0.55
1:J:528:THR:CG2	3:H:86:LYS:HE3	2.37	0.55
1:J:1032:SER:CA	1:J:1115:ILE:O	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1090:ILE:HG22	1:J:1095:MET:O	2.07	0.55
3:G:8:PHE:CE1	3:H:150:ARG:HD3	2.42	0.55
4:I:322:LEU:CA	4:I:325:LEU:HD12	2.27	0.55
5:K:15:ASN:OD1	5:K:16:ARG:N	2.39	0.55
6:L:125:ASP:HA	6:L:128:ASN:ND2	2.21	0.55
1:J:1081:VAL:HB	1:J:1086:ASN:O	2.07	0.54
4:I:96:LEU:HD23	4:I:124:MET:O	2.06	0.54
4:I:599:VAL:HG23	4:I:627:GLY:O	2.06	0.54
4:I:887:VAL:CG2	4:I:913:VAL:HG21	2.37	0.54
6:L:355:ILE:HG22	6:L:359:LYS:CD	2.36	0.54
6:L:555:GLU:HB2	6:L:594:ALA:HB2	1.89	0.54
3:M:253:LEU:O	3:M:277:TYR:HB3	2.07	0.54
1:J:72:CYS:SG	1:J:74:LYS:N	2.80	0.54
1:J:576:ARG:HG2	1:J:592:VAL:O	2.07	0.54
1:J:1256:ILE:O	1:J:1260:MET:HG3	2.08	0.54
3:G:231:PHE:CZ	3:H:28:LEU:HD22	2.41	0.54
3:H:208:ASN:OD1	3:H:210:THR:OG1	2.24	0.54
4:I:217:THR:HG23	4:I:351:LEU:HD13	1.88	0.54
4:I:230:PHE:CE1	4:I:292:ILE:HG12	2.42	0.54
4:I:1003:THR:OG1	4:I:1005:GLU:HG3	2.08	0.54
4:I:1066:MET:SD	4:I:1076:ILE:HD11	2.48	0.54
4:I:1078:LYS:HE3	4:I:1080:ASN:CB	2.36	0.54
6:L:38:SER:HA	6:L:41:ILE:CD1	2.37	0.54
6:L:271:ASN:HA	6:L:274:ARG:CD	2.36	0.54
1:J:709:ARG:HD2	1:J:710:ASP:H	1.72	0.54
1:J:759:ILE:HG23	1:J:771:GLN:HB3	1.89	0.54
1:J:965:SER:CA	1:J:975:ILE:HA	2.37	0.54
3:H:61:ILE:HD11	3:H:142:MET:CE	2.38	0.54
3:H:75:GLN:HE22	3:H:132:HIS:HB2	1.72	0.54
1:J:582:ILE:HD13	1:J:627:THR:HG21	1.90	0.54
1:J:709:ARG:HD2	1:J:710:ASP:N	2.22	0.54
4:I:35:PHE:O	4:I:38:PHE:N	2.39	0.54
4:I:517:GLN:O	4:I:519:ASN:N	2.40	0.54
4:I:820:GLU:OE2	4:I:824:GLN:NE2	2.41	0.54
4:I:942:ASP:N	4:I:942:ASP:OD1	2.40	0.54
4:I:976:ARG:O	4:I:980:VAL:HG23	2.07	0.54
6:L:27:VAL:HG11	6:L:55:VAL:HG11	1.88	0.54
6:L:145:LEU:HD22	6:L:225:ARG:HE	1.73	0.54
3:M:255:ARG:HD2	3:M:259:ASP:CB	2.38	0.54
1:J:1138:LEU:HB3	1:J:1139:PRO:HD3	1.89	0.54
1:J:1179:PRO:CD	1:J:1184:ASP:HA	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:158:ARG:HG3	3:G:158:ARG:HH11	1.72	0.54
3:G:181:GLU:O	4:I:821:ARG:NH2	2.40	0.54
4:I:301:TYR:O	4:I:310:ILE:N	2.40	0.54
4:I:692:THR:HG22	4:I:693:LEU:H	1.72	0.54
4:I:989:LEU:HA	4:I:992:LEU:HD21	1.89	0.54
6:L:161:LEU:HD12	6:L:265:GLN:OE1	2.08	0.54
6:L:316:PHE:HZ	6:L:334:SER:HA	1.71	0.54
7:O:62:DC:C6	7:O:63:DT:H72	2.42	0.54
1:J:1079:LYS:NZ	1:J:1081:VAL:HG12	2.22	0.54
1:J:1081:VAL:HB	1:J:1087:ASP:HA	1.90	0.54
3:H:41:ASN:ND2	4:I:1217:THR:HA	2.23	0.54
4:I:1003:THR:O	4:I:1008:GLN:HB2	2.08	0.54
3:M:264:VAL:HB	7:O:23:DC:OP1	2.07	0.54
7:O:33:DA:H5'	7:O:33:DA:C8	2.43	0.54
8:P:40:DC:H2'	8:P:41:DT:H71	1.89	0.54
1:J:146:VAL:HG23	1:J:158:GLN:O	2.08	0.54
1:J:418:GLU:OE2	5:K:2:ALA:N	2.41	0.54
1:J:1263:LYS:HB2	1:J:1307:LEU:HD11	1.90	0.54
2:N:34:VAL:HG21	2:N:56:THR:HA	1.89	0.54
3:G:111:THR:HG22	3:G:129:VAL:HA	1.90	0.54
3:H:13:LEU:HD23	3:H:15:ASP:H	1.71	0.54
3:H:41:ASN:O	3:H:45:ARG:HG3	2.08	0.54
3:H:75:GLN:NE2	3:H:132:HIS:HB2	2.23	0.54
4:I:270:THR:O	4:I:274:ILE:HG13	2.08	0.54
6:L:490:PRO:HD2	6:L:493:LYS:HB3	1.90	0.54
6:L:540:LEU:O	6:L:544:THR:HG23	2.08	0.54
3:M:298:LYS:HB3	8:P:67:DT:OP1	2.07	0.54
7:O:52:DA:C1'	7:O:53:DT:H5''	2.37	0.54
8:P:44:DT:H2''	8:P:45:DA:C8	2.42	0.54
1:J:697:MET:CE	1:J:737:ILE:HG22	2.36	0.54
1:J:836:ARG:NE	1:J:869:CYS:HB3	2.22	0.54
1:J:950:ILE:CG1	1:J:1018:ALA:HB3	2.38	0.54
2:N:51:ILE:O	2:N:53:PRO:HD3	2.08	0.54
3:G:79:LEU:CD1	4:I:693:LEU:HD21	2.38	0.54
4:I:130:MET:SD	4:I:134:GLY:HA2	2.48	0.54
4:I:685:MET:CE	4:I:1073:LYS:HG2	2.38	0.54
4:I:841:ARG:N	4:I:848:GLU:OE1	2.35	0.54
4:I:884:VAL:O	4:I:917:SER:HB2	2.08	0.54
4:I:1103:VAL:CG1	4:I:1112:ILE:HD11	2.31	0.54
4:I:1254:VAL:HG13	4:I:1255:THR:H	1.73	0.54
5:K:19:LEU:HD11	5:K:51:LEU:CD2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:41:GLU:CB	5:K:49:ILE:HD11	2.37	0.54
6:L:344:LEU:O	6:L:348:GLU:HG3	2.07	0.54
6:L:463:LEU:CD2	6:L:483:LEU:HD23	2.38	0.54
3:M:282:VAL:HB	3:M:316:MET:HG2	1.89	0.54
8:P:38:DC:H2''	8:P:39:DC:OP2	2.07	0.54
1:J:552:ILE:HD11	1:J:570:LYS:HE2	1.90	0.54
1:J:950:ILE:HD12	1:J:1018:ALA:HB3	1.89	0.54
4:I:136:PHE:HZ	4:I:456:VAL:HG21	1.73	0.54
4:I:562:GLU:OE1	4:I:574:SER:OG	2.13	0.54
4:I:1236:ASN:HA	4:I:1238:LEU:HD12	1.89	0.54
6:L:402:LEU:HA	6:L:405:ILE:CG1	2.37	0.54
1:J:129:ASP:HB2	1:J:220:ARG:NE	2.23	0.54
1:J:507:VAL:HG12	1:J:601:ILE:HG21	1.89	0.54
4:I:75:LEU:HD12	4:I:94:ALA:HB3	1.90	0.54
4:I:86:GLN:HA	4:I:140:GLY:HA2	1.89	0.54
4:I:253:PHE:N	4:I:265:LYS:HG3	2.23	0.54
4:I:459:MET:SD	4:I:511:LEU:HD12	2.47	0.54
4:I:484:LEU:HB3	4:I:486:THR:H	1.73	0.54
4:I:551:HIS:ND1	4:I:553:THR:HG23	2.22	0.54
6:L:490:PRO:HD2	6:L:493:LYS:CB	2.38	0.54
8:P:35:DA:H1'	8:P:36:DT:C5'	2.37	0.54
1:J:150:GLY:HA3	1:J:175:GLU:O	2.07	0.53
1:J:278:ARG:NH1	1:J:298:MET:HE1	2.23	0.53
1:J:1155:ILE:O	1:J:1210:ILE:HG12	2.08	0.53
6:L:286:LEU:O	6:L:290:LEU:HB2	2.09	0.53
1:J:298:MET:SD	6:L:402:LEU:HB3	2.49	0.53
1:J:514:THR:O	1:J:514:THR:OG1	2.25	0.53
1:J:552:ILE:HD11	1:J:570:LYS:NZ	2.23	0.53
1:J:926:PRO:CG	1:J:1248:ILE:HD11	2.37	0.53
1:J:1037:PHE:HZ	1:J:1110:GLU:HA	1.72	0.53
1:J:1193:TRP:HB2	1:J:1194:ARG:NH1	2.23	0.53
3:H:102:LEU:HD12	3:H:115:ILE:HG12	1.90	0.53
4:I:59:ILE:HD11	4:I:476:LYS:CD	2.37	0.53
4:I:565:GLU:HB3	4:I:680:LEU:HD21	1.91	0.53
4:I:1210:ILE:HG13	4:I:1227:VAL:CG2	2.38	0.53
6:L:478:PRO:HB2	6:L:483:LEU:HD11	1.90	0.53
6:L:503:GLU:OE1	6:L:503:GLU:N	2.33	0.53
1:J:133:ARG:NH1	1:J:136:GLU:OE1	2.41	0.53
1:J:644:MET:CG	1:J:740:LEU:HD23	2.33	0.53
1:J:747:MET:HG3	1:J:759:ILE:CD1	2.38	0.53
1:J:1027:VAL:HG23	1:J:1199:PHE:HE1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1039:ASP:OD1	1:J:1074:LEU:HD12	2.09	0.53
1:J:1069:ALA:HA	1:J:1072:LYS:HB2	1.90	0.53
1:J:320:ASN:O	1:J:321:LYS:HB3	2.09	0.53
2:N:48:ARG:HG3	2:N:48:ARG:HH11	1.74	0.53
3:G:192:VAL:CG1	3:G:195:ARG:HB2	2.38	0.53
4:I:182:SER:HB3	4:I:199:ASP:OD2	2.09	0.53
4:I:396:ASP:HA	4:I:418:GLY:O	2.09	0.53
6:L:130:VAL:O	6:L:134:VAL:HG23	2.08	0.53
6:L:150:ARG:HG2	6:L:155:GLU:CB	2.38	0.53
6:L:291:CYS:O	6:L:295:CYS:HB3	2.08	0.53
6:L:306:PHE:CE1	6:L:310:GLU:HG3	2.43	0.53
6:L:393:LYS:HZ1	6:L:436:ARG:HH22	1.56	0.53
6:L:412:LEU:HB2	6:L:435:ILE:HD11	1.90	0.53
6:L:420:GLU:HB3	6:L:422:ARG:HG2	1.90	0.53
1:J:623:GLN:O	1:J:627:THR:HG22	2.08	0.53
1:J:638:SER:HB2	4:I:804:PHE:O	2.08	0.53
1:J:1056:LEU:HD13	1:J:1108:GLN:NE2	2.24	0.53
3:H:32:GLU:HB3	3:H:35:PHE:CD2	2.43	0.53
3:H:66:HIS:O	3:H:171:LEU:HD21	2.08	0.53
3:H:193:GLU:OE1	3:H:194:GLN:N	2.42	0.53
4:I:384:LEU:HA	4:I:387:ASN:HD21	1.72	0.53
4:I:1212:LEU:HD22	4:I:1225:VAL:CG2	2.33	0.53
6:L:110:LEU:HD23	6:L:385:ARG:CZ	2.39	0.53
6:L:288:MET:HG2	6:L:293:GLU:OE1	2.08	0.53
1:J:235:GLU:OE1	1:J:235:GLU:N	2.37	0.53
1:J:1165:PHE:CD1	1:J:1175:LEU:HG	2.44	0.53
4:I:216:THR:HG22	4:I:219:GLN:NE2	2.23	0.53
6:L:128:ASN:HA	6:L:131:GLN:CG	2.38	0.53
6:L:162:ILE:HG13	6:L:164:GLY:N	2.24	0.53
7:O:38:DG:H2''	7:O:39:DG:N7	2.23	0.53
7:O:40:DC:H2''	7:O:41:DT:C7	2.37	0.53
1:J:935:PHE:O	1:J:1135:THR:HA	2.09	0.53
1:J:1141:VAL:HG21	1:J:1241:TYR:HE1	1.74	0.53
4:I:61:SER:OG	4:I:479:LEU:HB3	2.08	0.53
4:I:122:VAL:HG21	4:I:493:ILE:CG2	2.38	0.53
4:I:245:ARG:HB3	4:I:337:PHE:CE1	2.44	0.53
4:I:299:LYS:HG2	4:I:334:GLU:OE1	2.09	0.53
4:I:700:VAL:HG13	4:I:1117:LEU:HD23	1.89	0.53
4:I:733:VAL:HG21	4:I:966:ILE:HD13	1.89	0.53
6:L:143:TYR:O	6:L:147:GLN:HG2	2.08	0.53
1:J:1167:LYS:HZ1	1:J:1170:LYS:HB2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:256:GLU:HG3	4:I:256:GLU:O	2.08	0.53
4:I:446:ASP:OD2	4:I:551:HIS:HB2	2.09	0.53
6:L:22:LEU:O	6:L:55:VAL:HA	2.08	0.53
8:P:39:DC:OP2	8:P:39:DC:H2'	2.09	0.53
1:J:591:ILE:HG22	1:J:592:VAL:HG13	1.91	0.53
1:J:937:ILE:CG1	1:J:1134:ILE:H	2.21	0.53
2:N:67:ARG:HD2	4:I:341:LEU:CG	2.38	0.53
3:H:101:THR:HG22	3:H:143:ARG:HG2	1.90	0.53
4:I:41:GLN:NE2	4:I:73:TYR:O	2.42	0.53
4:I:197:ARG:NH1	4:I:201:ARG:O	2.41	0.53
4:I:1024:GLU:O	4:I:1027:LYS:HG2	2.09	0.53
5:K:36:ASP:OD1	5:K:37:PRO:HD2	2.09	0.53
6:L:262:VAL:HG12	6:L:265:GLN:H	1.74	0.53
1:J:345:LYS:NZ	4:I:1291:LEU:O	2.32	0.53
1:J:493:PRO:HB3	1:J:904:ALA:HB2	1.89	0.53
1:J:959:LYS:HB2	1:J:985:ILE:HD13	1.90	0.53
6:L:227:GLN:HA	6:L:230:VAL:HG12	1.91	0.53
6:L:551:LEU:HB3	6:L:555:GLU:CG	2.39	0.53
1:J:981:GLU:HB3	1:J:995:TYR:O	2.09	0.52
1:J:1032:SER:HB3	1:J:1116:SER:HA	1.91	0.52
2:N:64:TYR:CE1	4:I:341:LEU:HD13	2.45	0.52
4:I:197:ARG:HB3	4:I:203:LYS:HA	1.90	0.52
4:I:221:LEU:HD21	4:I:351:LEU:HD12	1.90	0.52
4:I:697:LYS:HD2	4:I:1181:PRO:HG3	1.91	0.52
4:I:895:LEU:CD2	4:I:900:LYS:HE2	2.39	0.52
3:M:253:LEU:HB3	3:M:279:GLY:N	2.24	0.52
1:J:287:ALA:HB1	1:J:291:ILE:CD1	2.33	0.52
1:J:340:GLN:HG2	1:J:341:ASN:N	2.24	0.52
1:J:478:LEU:HG	5:K:47:THR:HG22	1.90	0.52
1:J:731:ARG:NE	4:I:1105:SER:OG	2.41	0.52
1:J:967:VAL:HG22	1:J:973:LEU:CD1	2.37	0.52
1:J:1044:GLN:NE2	1:J:1070:GLY:HA3	2.23	0.52
1:J:1151:LYS:C	1:J:1153:PRO:HD3	2.30	0.52
3:G:131:CYS:SG	3:G:132:HIS:N	2.82	0.52
3:H:76:GLU:OE2	3:H:132:HIS:N	2.43	0.52
4:I:257:ALA:HB3	4:I:262:TYR:CE1	2.44	0.52
4:I:469:VAL:O	4:I:473:ARG:HG2	2.09	0.52
4:I:705:GLU:HB3	4:I:794:LEU:H	1.74	0.52
4:I:778:GLU:N	4:I:781:ASP:OD2	2.35	0.52
4:I:935:THR:HG22	4:I:936:ARG:O	2.09	0.52
6:L:38:SER:HA	6:L:41:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:230:SER:OG	1:J:231:GLY:N	2.42	0.52
1:J:426:ALA:HB3	1:J:427:PRO:HD3	1.91	0.52
1:J:1155:ILE:CD1	1:J:1211:SER:HB2	2.40	0.52
1:J:1266:ILE:HG21	1:J:1300:ALA:HB1	1.91	0.52
4:I:11:ILE:HG23	4:I:1149:TYR:OH	2.10	0.52
4:I:1255:THR:O	4:I:1257:GLN:N	2.42	0.52
6:L:320:ILE:HG12	6:L:330:LEU:HB2	1.91	0.52
1:J:306:LEU:HD22	1:J:306:LEU:O	2.09	0.52
1:J:527:LEU:HG	1:J:532:GLU:HG2	1.91	0.52
1:J:586:GLY:O	1:J:587:LEU:HD12	2.09	0.52
1:J:684:ASP:OD2	2:N:27:ILE:HD12	2.10	0.52
1:J:1261:LEU:O	1:J:1304:ARG:NH1	2.42	0.52
2:N:5:ALA:HB3	4:I:678:ARG:NH2	2.24	0.52
5:K:4:VAL:HG22	5:K:5:THR:HG23	1.91	0.52
6:L:162:ILE:N	6:L:262:VAL:HG23	2.24	0.52
8:P:45:DA:H2'	8:P:45:DA:OP2	2.10	0.52
8:P:67:DT:H2''	8:P:68:DG:OP2	2.10	0.52
1:J:530:PRO:HB3	1:J:577:ALA:O	2.10	0.52
1:J:538:ARG:HB3	3:H:44:ARG:NH2	2.24	0.52
1:J:615:LYS:HB2	1:J:616:PRO:HD3	1.90	0.52
1:J:955:LYS:HD3	1:J:956:GLY:N	2.24	0.52
4:I:9:LYS:HG3	4:I:1171:ARG:HH11	1.73	0.52
4:I:144:VAL:HG21	4:I:515:MET:HG3	1.91	0.52
4:I:145:ILE:HA	4:I:511:LEU:O	2.09	0.52
4:I:240:GLU:HA	4:I:284:LEU:CD1	2.38	0.52
4:I:624:ASP:HB3	4:I:630:VAL:CG1	2.38	0.52
1:J:253:VAL:HG11	6:L:523:ILE:HD13	1.91	0.52
1:J:308:ASP:OD2	1:J:311:ARG:NH1	2.43	0.52
1:J:340:GLN:HG2	1:J:341:ASN:H	1.74	0.52
1:J:670:SER:O	1:J:672:LEU:HD12	2.10	0.52
1:J:857:LEU:HG	1:J:858:VAL:HG23	1.91	0.52
1:J:865:HIS:CE1	1:J:867:GLN:HB2	2.44	0.52
1:J:1096:PRO:HD2	1:J:1098:GLN:HE22	1.75	0.52
4:I:290:GLU:HA	4:I:293:ALA:CB	2.40	0.52
4:I:912:ASP:N	4:I:912:ASP:OD1	2.42	0.52
6:L:20:GLY:C	6:L:53:ILE:HG21	2.30	0.52
6:L:41:ILE:O	6:L:45:ILE:HG22	2.10	0.52
6:L:227:GLN:CG	6:L:252:LEU:HD13	2.40	0.52
1:J:325:LYS:HG2	1:J:329:ASP:CB	2.39	0.52
1:J:509:GLY:CA	1:J:632:ALA:HB2	2.40	0.52
1:J:1241:TYR:CE2	1:J:1248:ILE:HD12	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1321:SER:OG	1:J:1348:LYS:HB2	2.08	0.52
3:H:211:ILE:HG21	3:H:219:ARG:NH2	2.22	0.52
6:L:470:MET:SD	6:L:486:ARG:HG3	2.50	0.52
6:L:484:ALA:HB1	6:L:491:GLU:HB2	1.90	0.52
6:L:540:LEU:HD12	6:L:610:PHE:CD2	2.44	0.52
3:M:253:LEU:O	3:M:278:ILE:N	2.43	0.52
1:J:97:VAL:CG1	1:J:101:ARG:HE	2.22	0.52
1:J:569:LEU:HD11	3:H:83:LEU:CD2	2.39	0.52
4:I:135:THR:HG22	4:I:144:VAL:HG22	1.92	0.52
4:I:732:ILE:CD1	4:I:769:PRO:HB3	2.40	0.52
4:I:883:LEU:HD13	4:I:1052:VAL:HG11	1.91	0.52
4:I:896:THR:O	4:I:900:LYS:HE3	2.10	0.52
6:L:530:LEU:H	6:L:530:LEU:HD12	1.75	0.52
1:J:117:LEU:O	1:J:122:SER:OG	2.07	0.52
1:J:478:LEU:HG	5:K:47:THR:CG2	2.39	0.52
1:J:899:TYR:CD2	1:J:909:ILE:HG12	2.45	0.52
1:J:905:ARG:HB3	1:J:907:HIS:CE1	2.45	0.52
2:N:36:LEU:CD2	2:N:41:GLY:HA2	2.39	0.52
3:H:105:SER:OG	3:H:139:SER:HA	2.10	0.52
4:I:10:ARG:HD2	4:I:1181:PRO:CG	2.39	0.52
4:I:273:HIS:O	4:I:277:LEU:HG	2.09	0.52
4:I:823:VAL:HG22	4:I:1060:ILE:CG2	2.39	0.52
4:I:836:LEU:CD1	4:I:1054:LEU:HD13	2.37	0.52
7:O:57:DT:H2'	7:O:57:DT:OP2	2.10	0.52
1:J:147:ILE:O	1:J:177:ASP:HB3	2.09	0.52
1:J:331:ILE:O	1:J:336:GLY:HA3	2.10	0.52
1:J:337:ARG:O	1:J:342:LEU:HB2	2.10	0.52
1:J:899:TYR:CE2	1:J:909:ILE:HG12	2.44	0.52
1:J:1024:THR:CG2	1:J:1123:ARG:HB3	2.30	0.52
3:G:109:PRO:HA	3:G:132:HIS:HD2	1.75	0.52
4:I:74:ARG:NH2	4:I:97:ARG:HG3	2.24	0.52
4:I:231:GLU:OE1	4:I:284:LEU:HD21	2.10	0.52
4:I:271:ALA:O	4:I:274:ILE:HB	2.08	0.52
4:I:936:ARG:HB3	4:I:939:VAL:HG23	1.92	0.52
7:O:44:DA:H2''	7:O:45:DA:O5'	2.08	0.52
1:J:740:LEU:HD21	4:I:1109:ILE:HD11	1.92	0.51
1:J:1029:THR:N	1:J:1118:GLY:HA2	2.25	0.51
1:J:1078:LEU:HD21	1:J:1121:LEU:HB3	1.91	0.51
1:J:1261:LEU:HD12	1:J:1304:ARG:NH1	2.25	0.51
4:I:53:PHE:CE1	4:I:468:LEU:HD11	2.45	0.51
6:L:361:ILE:HG13	6:L:362:ASN:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:303:ILE:HA	3:M:306:VAL:HG12	1.91	0.51
3:M:303:ILE:O	3:M:307:LEU:HG	2.10	0.51
3:M:316:MET:N	3:M:316:MET:SD	2.83	0.51
1:J:68:TYR:CE1	1:J:81:ARG:HG3	2.45	0.51
1:J:399:LYS:O	1:J:403:ARG:HG3	2.09	0.51
1:J:516:ASP:N	1:J:516:ASP:OD1	2.42	0.51
1:J:532:GLU:O	1:J:536:LEU:HG	2.10	0.51
1:J:572:THR:OG1	1:J:576:ARG:HB2	2.10	0.51
1:J:686:TRP:HA	1:J:686:TRP:CE3	2.46	0.51
1:J:861:ASN:OD1	1:J:883:ARG:NH1	2.44	0.51
1:J:1327:GLU:OE1	1:J:1330:ARG:HB2	2.10	0.51
11:J:1506:1N7:H31	11:J:1506:1N7:H5	1.91	0.51
3:G:215:GLU:OE2	3:G:219:ARG:NH2	2.43	0.51
4:I:287:VAL:HG23	4:I:288:PRO:O	2.09	0.51
4:I:685:MET:SD	4:I:1073:LYS:HG2	2.50	0.51
4:I:854:ILE:HD11	4:I:885:GLY:CA	2.40	0.51
1:J:518:VAL:HG11	1:J:707:ILE:HB	1.91	0.51
1:J:786:THR:HG21	2:N:7:GLU:HB2	1.92	0.51
1:J:976:THR:HA	1:J:999:TYR:CE1	2.45	0.51
6:L:292:VAL:HG22	6:L:297:MET:HB3	1.92	0.51
6:L:346:GLN:O	6:L:350:GLU:HG3	2.09	0.51
6:L:448:ARG:HH12	6:L:452:ILE:HD11	1.75	0.51
6:L:573:LEU:HD22	6:L:587:ILE:HG22	1.92	0.51
3:M:270:LEU:O	3:M:274:ALA:N	2.36	0.51
3:M:278:ILE:HA	3:M:281:LEU:CB	2.39	0.51
8:P:32:DA:H1'	8:P:33:DA:H5'	1.91	0.51
4:I:210:LEU:HD13	4:I:220:ILE:HD13	1.92	0.51
4:I:255:ILE:CB	4:I:263:VAL:HG12	2.40	0.51
4:I:696:ASP:O	4:I:697:LYS:HB3	2.11	0.51
4:I:1082:ILE:N	4:I:1082:ILE:CD1	2.73	0.51
1:J:27:PRO:O	1:J:31:ARG:HG3	2.11	0.51
1:J:596:LEU:HA	1:J:600:ALA:HB3	1.93	0.51
1:J:780:ARG:NH2	4:I:560:PRO:O	2.43	0.51
1:J:1115:ILE:HD12	1:J:1116:SER:O	2.10	0.51
1:J:1174:ARG:HG3	1:J:1189:MET:HE1	1.90	0.51
3:H:40:GLY:O	3:H:44:ARG:HG2	2.10	0.51
3:H:92:VAL:HG22	3:H:121:VAL:HG12	1.93	0.51
4:I:135:THR:HG23	4:I:527:LYS:HE2	1.92	0.51
4:I:189:ASP:OD1	4:I:193:ASN:N	2.43	0.51
4:I:317:LEU:HA	4:I:321:LEU:HD12	1.92	0.51
4:I:453:ILE:HD11	4:I:587:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:1099:ASN:OD1	4:I:1101:LEU:HD12	2.10	0.51
6:L:58:GLU:C	6:L:60:PRO:HD2	2.31	0.51
4:I:1060:ILE:HD11	4:I:1076:ILE:HD13	1.92	0.51
6:L:355:ILE:O	6:L:359:LYS:HG3	2.10	0.51
6:L:572:THR:O	6:L:576:VAL:HG23	2.11	0.51
7:O:28:DG:H2''	7:O:29:DA:O5'	2.09	0.51
1:J:755:ILE:HD12	1:J:774:ILE:HG23	1.92	0.51
1:J:789:LYS:HB2	1:J:932:MET:SD	2.51	0.51
4:I:417:SER:OG	4:I:419:ILE:HG12	2.11	0.51
4:I:1080:ASN:OD1	4:I:1085:MET:SD	2.68	0.51
6:L:12:LEU:HB2	6:L:30:HIS:CB	2.41	0.51
6:L:394:TYR:HB3	6:L:443:ILE:CD1	2.39	0.51
1:J:64:PRO:O	1:J:98:ARG:HD2	2.10	0.51
1:J:113:HIS:ND1	1:J:115:TRP:HB2	2.26	0.51
1:J:259:ARG:HD3	11:J:1505:1N7:H23	1.92	0.51
1:J:310:GLY:N	1:J:315:ALA:HB2	2.24	0.51
1:J:840:LEU:HD12	1:J:864:LEU:O	2.11	0.51
3:G:47:LEU:HD23	3:G:220:ALA:HB2	1.92	0.51
3:G:197:ASP:O	3:G:198:LEU:HD23	2.11	0.51
4:I:22:LEU:HB3	4:I:655:VAL:CG1	2.41	0.51
4:I:91:THR:HB	4:I:138:ILE:O	2.10	0.51
4:I:489:PRO:HA	4:I:492:MET:SD	2.51	0.51
4:I:568:ASN:HB2	4:I:571:LEU:HD12	1.92	0.51
4:I:726:TYR:CZ	4:I:728:ASP:HB2	2.46	0.51
6:L:148:TYR:CD2	6:L:221:PHE:HB3	2.46	0.51
6:L:443:ILE:O	6:L:447:ALA:HB2	2.10	0.51
7:O:35:DG:N2	8:P:52:DT:O2	2.44	0.51
8:P:29:DA:C2'	8:P:30:DG:H5'	2.41	0.51
1:J:45:ASN:O	1:J:47:ARG:N	2.40	0.51
1:J:701:LEU:HD11	1:J:720:ASN:ND2	2.26	0.51
1:J:726:ALA:CB	1:J:737:ILE:HD11	2.39	0.51
1:J:845:ALA:HB3	1:J:881:LYS:HG2	1.93	0.51
1:J:845:ALA:N	1:J:881:LYS:O	2.31	0.51
1:J:1047:THR:HB	1:J:1062:LEU:HD12	1.93	0.51
1:J:1079:LYS:CB	1:J:1098:GLN:HA	2.41	0.51
1:J:1082:ASP:N	1:J:1088:VAL:HG23	2.26	0.51
3:G:78:ILE:HD13	3:G:81:ILE:HD12	1.93	0.51
4:I:148:GLN:HB2	4:I:511:LEU:HD11	1.92	0.51
4:I:178:PRO:HG3	4:I:395:TYR:CE2	2.46	0.51
6:L:423:ARG:HB2	6:L:425:TYR:CE1	2.46	0.51
7:O:58:DC:H2''	7:O:59:DG:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:121:PRO:HB2	1:J:126:LEU:HD21	1.93	0.51
1:J:161:THR:OG1	1:J:162:GLU:N	2.44	0.51
1:J:509:GLY:HA3	1:J:632:ALA:HB2	1.92	0.51
1:J:801:VAL:HG12	1:J:920:ALA:CB	2.40	0.51
1:J:1373:ARG:HG2	1:J:1374:ALA:H	1.75	0.51
2:N:7:GLU:O	2:N:11:VAL:HG23	2.12	0.51
4:I:712:SER:OG	4:I:713:GLY:N	2.43	0.51
6:L:247:GLU:O	6:L:251:LYS:HG2	2.11	0.51
1:J:338:PHE:HA	1:J:342:LEU:CD2	2.39	0.50
1:J:418:GLU:CG	5:K:45:LYS:HG3	2.41	0.50
1:J:759:ILE:HG21	1:J:767:LEU:CD2	2.41	0.50
1:J:885:VAL:CG1	1:J:894:VAL:HG21	2.41	0.50
1:J:1027:VAL:CG1	1:J:1122:ALA:H	2.25	0.50
4:I:242:VAL:CG2	4:I:245:ARG:HG3	2.41	0.50
4:I:618:GLN:O	4:I:621:SER:OG	2.15	0.50
4:I:936:ARG:HB2	4:I:1047:LEU:O	2.11	0.50
4:I:1129:ASN:O	4:I:1133:LYS:HB2	2.11	0.50
6:L:21:TYR:HB2	6:L:56:MET:HE3	1.92	0.50
6:L:245:ALA:O	6:L:249:ILE:HG13	2.11	0.50
6:L:322:MET:O	6:L:324:LYS:NZ	2.34	0.50
8:P:68:DG:H1'	8:P:69:DT:C5'	2.42	0.50
1:J:1155:ILE:HD11	1:J:1211:SER:HB2	1.92	0.50
1:J:1176:VAL:HG13	1:J:1186:TYR:O	2.11	0.50
11:J:1504:1N7:H31	11:J:1504:1N7:H5	1.92	0.50
4:I:1256:GLN:O	4:I:1301:ARG:NH2	2.41	0.50
6:L:56:MET:CE	6:L:61:ASP:HB2	2.41	0.50
6:L:381:GLU:O	6:L:384:LEU:HG	2.09	0.50
6:L:600:HIS:O	6:L:604:SER:HB3	2.11	0.50
7:O:49:DC:H2''	7:O:50:DA:H8	1.77	0.50
1:J:199:GLU:O	1:J:202:ARG:HB2	2.11	0.50
1:J:288:PRO:O	1:J:291:ILE:HG12	2.11	0.50
1:J:450:HIS:HE1	1:J:452:LEU:HG	1.76	0.50
1:J:844:THR:CG2	1:J:864:LEU:HD11	2.41	0.50
1:J:1036:ARG:HB3	1:J:1079:LYS:CG	2.41	0.50
1:J:1079:LYS:HE3	1:J:1087:ASP:OD2	2.11	0.50
1:J:1156:LEU:HD13	1:J:1223:LEU:HD23	1.93	0.50
1:J:1360:GLY:HA3	4:I:1282:GLY:CA	2.41	0.50
4:I:205:PRO:HD2	4:I:208:ILE:HD13	1.92	0.50
4:I:243:PRO:HB3	4:I:277:LEU:HB2	1.93	0.50
4:I:842:ASP:OD1	4:I:1047:LEU:HG	2.11	0.50
4:I:1035:LYS:O	4:I:1038:GLN:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:1314:GLN:NE2	5:K:32:VAL:HG21	2.23	0.50
6:L:130:VAL:HG12	6:L:365:MET:O	2.11	0.50
6:L:157:ARG:CD	6:L:159:SER:H	2.21	0.50
6:L:428:SER:O	6:L:432:THR:HG22	2.11	0.50
1:J:337:ARG:O	1:J:342:LEU:HD13	2.10	0.50
1:J:949:SER:HB3	1:J:1019:ASN:OD1	2.11	0.50
1:J:1000:GLY:HA3	1:J:1026:PRO:CG	2.36	0.50
1:J:1165:PHE:HD1	1:J:1175:LEU:HG	1.76	0.50
3:H:44:ARG:O	3:H:48:LEU:HB2	2.11	0.50
4:I:39:ILE:HD11	4:I:75:LEU:HD11	1.93	0.50
4:I:104:ILE:HG23	4:I:116:ASP:O	2.12	0.50
4:I:210:LEU:CB	4:I:220:ILE:HD11	2.42	0.50
4:I:979:LEU:HD11	4:I:1011:LEU:HD11	1.94	0.50
4:I:1259:LEU:HD11	6:L:522:PHE:HA	1.94	0.50
3:G:95:LYS:HE2	3:G:120:ASP:OD2	2.11	0.50
4:I:115:LYS:HG3	4:I:116:ASP:OD2	2.11	0.50
4:I:263:VAL:HG23	4:I:273:HIS:NE2	2.26	0.50
4:I:488:MET:CG	4:I:489:PRO:HD2	2.40	0.50
4:I:602:GLU:O	4:I:602:GLU:HG3	2.12	0.50
4:I:1111:GLN:HB2	4:I:1230:MET:HE1	1.93	0.50
4:I:1119:MET:HB2	4:I:1228:GLY:HA2	1.93	0.50
6:L:23:THR:O	6:L:27:VAL:HG12	2.11	0.50
6:L:147:GLN:HA	6:L:150:ARG:CB	2.39	0.50
1:J:385:LEU:HD23	1:J:411:ILE:HG13	1.93	0.50
4:I:1312:ASN:OD1	4:I:1314:GLN:HG3	2.12	0.50
1:J:26:SER:O	1:J:30:ILE:HG13	2.11	0.50
1:J:84:ILE:O	1:J:84:ILE:HG13	2.12	0.50
1:J:132:LEU:O	1:J:135:ILE:HG12	2.11	0.50
1:J:388:ARG:NH2	1:J:414:GLU:OE1	2.40	0.50
1:J:519:ASN:CG	1:J:709:ARG:HD3	2.32	0.50
4:I:22:LEU:HB3	4:I:655:VAL:HG13	1.94	0.50
4:I:1282:GLY:HA3	5:K:17:PHE:CE1	2.46	0.50
6:L:320:ILE:HG12	6:L:330:LEU:CB	2.42	0.50
6:L:436:ARG:NH1	8:P:35:DA:H3'	2.27	0.50
3:M:254:LEU:HA	3:M:277:TYR:HB3	1.92	0.50
1:J:62:PHE:O	1:J:98:ARG:HG3	2.11	0.50
1:J:534:GLU:HA	1:J:578:ILE:HD11	1.94	0.50
1:J:809:VAL:HG11	1:J:909:ILE:HG23	1.93	0.50
1:J:935:PHE:HD2	1:J:1136:GLY:HA3	1.77	0.50
1:J:962:ASN:HD22	1:J:979:ASN:CB	2.22	0.50
1:J:983:LYS:HE3	1:J:994:SER:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:31:LEU:HB2	3:G:199:ASP:O	2.11	0.50
4:I:130:MET:HG3	4:I:134:GLY:HA2	1.93	0.50
4:I:303:ASP:OD2	4:I:308:GLU:HB3	2.12	0.50
4:I:383:SER:O	4:I:387:ASN:ND2	2.45	0.50
4:I:715:THR:CG2	4:I:782:VAL:HG13	2.41	0.50
4:I:928:VAL:HG13	4:I:1052:VAL:CG1	2.41	0.50
6:L:16:GLY:C	6:L:53:ILE:HD13	2.31	0.50
6:L:23:THR:OG1	6:L:25:ALA:N	2.45	0.50
1:J:611:ILE:CG2	1:J:612:LEU:HD12	2.41	0.50
1:J:849:LEU:CB	1:J:853:THR:HG23	2.42	0.50
1:J:1358:PRO:HB3	1:J:1366:HIS:CD2	2.43	0.50
3:G:98:VAL:HG22	3:G:100:LEU:HD23	1.93	0.50
3:H:36:GLY:N	3:H:199:ASP:OD2	2.22	0.50
3:H:192:VAL:HG12	3:H:193:GLU:H	1.76	0.50
4:I:582:ASN:HA	4:I:588:GLU:OE2	2.11	0.50
6:L:123:ILE:CD1	6:L:375:ALA:HB3	2.41	0.50
6:L:291:CYS:HA	6:L:295:CYS:CB	2.42	0.50
6:L:507:MET:O	6:L:520:GLY:N	2.44	0.50
1:J:1028:ILE:HG22	1:J:1118:GLY:O	2.12	0.49
1:J:1072:LYS:HZ3	1:J:1168:GLU:HB3	1.78	0.49
1:J:1350:ASN:HD22	1:J:1358:PRO:HD3	1.76	0.49
3:H:134:THR:HG22	3:H:135:ASP:OD1	2.12	0.49
4:I:1002:LEU:HD21	4:I:1007:LYS:CB	2.41	0.49
6:L:277:MET:HE1	6:L:359:LYS:HE3	1.92	0.49
6:L:436:ARG:O	6:L:440:THR:HG22	2.11	0.49
1:J:842:ARG:HB2	1:J:882:VAL:HG21	1.94	0.49
1:J:1197:ASN:HB2	1:J:1210:ILE:O	2.13	0.49
1:J:1226:VAL:O	1:J:1229:VAL:HG12	2.12	0.49
4:I:330:HIS:O	4:I:331:LYS:HD2	2.12	0.49
4:I:484:LEU:HD22	4:I:485:ASP:H	1.76	0.49
4:I:902:LEU:HD11	6:L:607:LEU:O	2.12	0.49
6:L:292:VAL:HG21	6:L:302:PHE:CG	2.47	0.49
1:J:124:ILE:HG23	1:J:189:LEU:HD11	1.94	0.49
1:J:255:LEU:HB2	1:J:259:ARG:O	2.11	0.49
1:J:926:PRO:HB2	1:J:1248:ILE:HD11	1.94	0.49
1:J:955:LYS:HE2	1:J:955:LYS:HA	1.94	0.49
1:J:1030:GLU:OE1	1:J:1090:ILE:HG13	2.12	0.49
1:J:1096:PRO:HB2	1:J:1098:GLN:OE1	2.13	0.49
1:J:1155:ILE:HG12	1:J:1211:SER:H	1.77	0.49
1:J:1236:GLU:HA	1:J:1239:ASP:OD2	2.12	0.49
4:I:150:HIS:CD2	4:I:454:ARG:HG3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:470:ARG:HA	4:I:473:ARG:HG2	1.94	0.49
4:I:699:LEU:HD12	4:I:1121:ALA:HB3	1.94	0.49
4:I:745:GLU:N	4:I:1017:GLN:HG3	2.27	0.49
4:I:811:ASN:ND2	4:I:1097:VAL:HG12	2.26	0.49
3:M:255:ARG:HD3	3:M:256:PRO:CD	2.38	0.49
1:J:886:VAL:HA	1:J:1258:ARG:HB2	1.95	0.49
1:J:999:TYR:CE2	1:J:1026:PRO:HG2	2.48	0.49
1:J:1061:VAL:HG21	1:J:1076:PRO:HB2	1.93	0.49
3:H:73:GLY:O	3:H:134:THR:N	2.45	0.49
4:I:14:ASP:HA	4:I:1183:ALA:HB3	1.94	0.49
4:I:759:SER:OG	4:I:763:THR:OG1	2.26	0.49
4:I:797:GLY:O	4:I:798:GLN:HG2	2.13	0.49
4:I:993:PRO:HG2	4:I:996:ARG:CB	2.38	0.49
3:M:260:LEU:HB3	3:M:306:VAL:HG21	1.94	0.49
3:H:35:PHE:HA	3:H:38:THR:HG22	1.93	0.49
4:I:360:LEU:HD22	4:I:378:ARG:HH11	1.78	0.49
4:I:470:ARG:O	4:I:473:ARG:HG3	2.11	0.49
6:L:145:LEU:HB3	6:L:225:ARG:NH2	2.28	0.49
3:M:303:ILE:HA	3:M:306:VAL:CG1	2.43	0.49
7:O:62:DC:H2'	7:O:63:DT:H72	1.94	0.49
1:J:364:HIS:HB3	1:J:487:THR:HG23	1.93	0.49
1:J:797:THR:HB	1:J:924:GLY:HA3	1.93	0.49
1:J:823:THR:HG23	1:J:878:ASP:O	2.13	0.49
1:J:823:THR:HG22	1:J:824:PRO:HD2	1.93	0.49
1:J:1251:LYS:O	1:J:1255:VAL:HG12	2.13	0.49
3:G:73:GLY:O	3:G:134:THR:HG22	2.13	0.49
4:I:163:LYS:HD3	6:L:62:ALA:CB	2.42	0.49
4:I:233:ARG:HD2	4:I:284:LEU:HD23	1.93	0.49
4:I:524:ILE:O	4:I:528:ARG:HG3	2.13	0.49
4:I:905:ILE:HA	6:L:595:LEU:HD22	1.94	0.49
4:I:927:THR:O	4:I:929:ILE:HG23	2.13	0.49
5:K:18:ASP:O	5:K:22:VAL:HG23	2.12	0.49
6:L:290:LEU:CD2	6:L:336:GLU:HB3	2.42	0.49
6:L:362:ASN:O	6:L:365:MET:HB3	2.12	0.49
1:J:697:MET:CE	1:J:741:ALA:HB3	2.43	0.49
1:J:833:GLU:HG3	1:J:834:PRO:HD2	1.94	0.49
1:J:1372:ARG:O	1:J:1375:ALA:HB3	2.12	0.49
3:H:59:VAL:CG2	3:H:144:ILE:HG22	2.42	0.49
4:I:615:VAL:HG12	4:I:650:VAL:HA	1.93	0.49
4:I:689:ALA:HB2	4:I:1233:LEU:HD12	1.95	0.49
4:I:802:VAL:HG21	4:I:1098:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:19:LEU:HD11	5:K:51:LEU:HD23	1.93	0.49
6:L:21:TYR:HA	6:L:53:ILE:CG2	2.43	0.49
7:O:54:DT:OP2	7:O:54:DT:H2'	2.12	0.49
8:P:34:DT:H4'	8:P:35:DA:H5'	1.95	0.49
1:J:1167:LYS:CE	1:J:1170:LYS:HB2	2.42	0.49
4:I:12:ARG:NH2	4:I:793:GLU:OE2	2.40	0.49
4:I:277:LEU:HB3	4:I:282:VAL:HG12	1.93	0.49
4:I:292:ILE:HG22	4:I:317:LEU:CD1	2.39	0.49
4:I:599:VAL:HG11	4:I:653:MET:SD	2.53	0.49
4:I:1132:LEU:HD13	4:I:1173:ALA:O	2.12	0.49
3:M:254:LEU:HD23	3:M:321:TRP:HH2	1.77	0.49
7:O:49:DC:H2''	7:O:50:DA:C8	2.47	0.49
8:P:21:DA:H1'	8:P:22:DA:C8	2.48	0.49
1:J:275:ARG:HD3	1:J:298:MET:HE3	1.95	0.49
1:J:364:HIS:HB3	1:J:487:THR:CG2	2.43	0.49
3:G:13:LEU:HD21	3:G:16:ILE:HD11	1.95	0.49
3:G:190:ALA:HA	3:G:200:LYS:HE2	1.94	0.49
3:H:58:GLU:OE2	3:H:145:LYS:HD3	2.12	0.49
4:I:478:ARG:NH2	4:I:487:LEU:HD22	2.28	0.49
4:I:748:ILE:CD1	4:I:966:ILE:HG22	2.39	0.49
4:I:948:ILE:O	4:I:952:GLN:HG3	2.13	0.49
6:L:119:ILE:O	6:L:122:ARG:HB2	2.13	0.49
6:L:290:LEU:HB3	6:L:333:VAL:CG2	2.43	0.49
6:L:334:SER:O	6:L:338:HIS:HB2	2.13	0.49
1:J:166:LEU:O	1:J:170:GLU:HG3	2.13	0.49
1:J:826:ILE:HG12	1:J:831:VAL:HA	1.94	0.49
1:J:1109:LEU:HD22	1:J:1115:ILE:HG21	1.95	0.49
3:H:133:LEU:HD21	3:H:140:ILE:HG22	1.95	0.49
4:I:238:GLN:CD	4:I:286:GLU:HB3	2.33	0.49
4:I:277:LEU:HB3	4:I:282:VAL:CG1	2.43	0.49
5:K:26:ARG:HH22	5:K:38:LEU:HD23	1.78	0.49
6:L:386:LEU:O	6:L:389:SER:OG	2.23	0.49
3:M:260:LEU:CB	3:M:262:LEU:HD23	2.43	0.49
1:J:309:ASN:HD22	1:J:324:LEU:HD12	1.78	0.48
1:J:337:ARG:HB3	1:J:342:LEU:HD13	1.95	0.48
1:J:787:ALA:CB	4:I:569:ILE:HD11	2.42	0.48
1:J:794:GLY:O	1:J:798:ARG:HB3	2.13	0.48
3:G:190:ALA:HB2	3:G:200:LYS:HB3	1.94	0.48
3:H:39:LEU:O	3:H:43:LEU:HG	2.13	0.48
4:I:239:MET:HG2	4:I:240:GLU:O	2.13	0.48
4:I:934:PHE:HE2	4:I:1051:LYS:HD2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:996:ARG:O	4:I:1000:LEU:HG	2.13	0.48
4:I:1106:ARG:O	4:I:1108:ASN:N	2.44	0.48
6:L:94:THR:HA	6:L:100:MET:SD	2.53	0.48
6:L:554:ARG:O	6:L:558:VAL:HG23	2.12	0.48
7:O:35:DG:H2''	7:O:36:DA:C8	2.47	0.48
7:O:39:DG:H2''	7:O:40:DC:H5'	1.94	0.48
8:P:34:DT:P	8:P:34:DT:H3'	2.52	0.48
1:J:360:TYR:OH	1:J:442:ILE:HD11	2.14	0.48
1:J:687:ALA:HB1	2:N:24:ARG:HH22	1.78	0.48
1:J:952:VAL:CG2	1:J:1013:GLY:HA2	2.42	0.48
3:G:223:ILE:HD13	3:H:8:PHE:CZ	2.48	0.48
4:I:887:VAL:HG23	4:I:913:VAL:HG21	1.94	0.48
5:K:38:LEU:HB3	5:K:58:LEU:HD11	1.95	0.48
6:L:157:ARG:HD2	6:L:159:SER:HB2	1.94	0.48
1:J:355:ILE:HG21	1:J:466:MET:HG3	1.94	0.48
1:J:370:LYS:CD	1:J:443:GLU:HG3	2.43	0.48
3:G:110:VAL:HG11	3:G:140:ILE:CD1	2.44	0.48
3:H:27:THR:CG2	3:H:200:LYS:HE3	2.43	0.48
4:I:239:MET:O	4:I:284:LEU:HG	2.13	0.48
4:I:470:ARG:CZ	4:I:497:PRO:HB3	2.43	0.48
1:J:152:THR:OG1	1:J:153:ASN:N	2.45	0.48
1:J:697:MET:HG3	1:J:698:MET:N	2.28	0.48
1:J:908:ILE:HG23	1:J:909:ILE:O	2.13	0.48
1:J:935:PHE:HZ	11:J:1506:1N7:H27	1.78	0.48
1:J:1031:VAL:HB	1:J:1080:ILE:HG21	1.94	0.48
1:J:1342:ASP:OD1	1:J:1344:LEU:HD13	2.14	0.48
3:H:102:LEU:HD21	3:H:110:VAL:CG1	2.43	0.48
4:I:104:ILE:HG12	4:I:116:ASP:O	2.14	0.48
4:I:189:ASP:HB3	4:I:195:PHE:HE2	1.77	0.48
4:I:243:PRO:HB3	4:I:277:LEU:HD13	1.94	0.48
4:I:285:ILE:HD13	4:I:287:VAL:HG13	1.95	0.48
4:I:745:GLU:H	4:I:1017:GLN:HG3	1.77	0.48
4:I:797:GLY:C	4:I:798:GLN:HG2	2.34	0.48
4:I:977:ALA:HA	4:I:980:VAL:HG23	1.96	0.48
6:L:56:MET:SD	6:L:60:PRO:HG2	2.53	0.48
6:L:147:GLN:OE1	6:L:150:ARG:NE	2.46	0.48
6:L:384:LEU:HA	6:L:387:VAL:HG23	1.96	0.48
3:M:295:LEU:HD21	3:M:300:LEU:CD2	2.43	0.48
1:J:1120:THR:HB	1:J:1123:ARG:CD	2.43	0.48
1:J:1241:TYR:CD2	1:J:1248:ILE:HD12	2.49	0.48
3:G:229:GLU:HA	3:G:232:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:144:VAL:HG23	4:I:515:MET:HB2	1.95	0.48
4:I:646:SER:OG	4:I:649:GLN:HG3	2.14	0.48
4:I:1236:ASN:HA	4:I:1238:LEU:CD1	2.43	0.48
6:L:117:ILE:HG13	6:L:118:ASP:OD1	2.13	0.48
8:P:25:DG:H2''	8:P:26:DC:C5	2.49	0.48
1:J:126:LEU:HD12	1:J:223:LEU:CD2	2.44	0.48
1:J:512:TYR:OH	4:I:1222:GLU:HG3	2.13	0.48
1:J:526:VAL:HA	1:J:549:LYS:O	2.14	0.48
1:J:849:LEU:CG	1:J:853:THR:HG23	2.43	0.48
4:I:638:SER:HB3	4:I:645:PHE:CE2	2.48	0.48
7:O:56:DC:C2'	7:O:57:DT:H71	2.43	0.48
1:J:145:VAL:CG1	1:J:184:ALA:HB1	2.44	0.48
1:J:814:CYS:HB3	1:J:890:THR:HG23	1.95	0.48
1:J:909:ILE:HD12	1:J:909:ILE:HA	1.59	0.48
1:J:1247:LYS:HB3	1:J:1247:LYS:HE3	1.56	0.48
3:G:58:GLU:CG	3:G:172:LEU:HD23	2.44	0.48
4:I:75:LEU:HD11	4:I:127:ILE:CD1	2.42	0.48
4:I:253:PHE:CZ	4:I:287:VAL:HG12	2.49	0.48
4:I:265:LYS:HG2	4:I:266:GLY:N	2.28	0.48
4:I:1004:ASP:OD1	4:I:1004:ASP:N	2.45	0.48
4:I:1253:LEU:O	4:I:1253:LEU:HD22	2.12	0.48
3:M:267:ALA:O	3:M:271:LYS:HG3	2.13	0.48
1:J:569:LEU:HD11	3:H:83:LEU:HD22	1.96	0.48
1:J:1265:THR:HG23	1:J:1279:GLN:HG3	1.95	0.48
2:N:16:THR:O	2:N:20:ILE:HG13	2.13	0.48
3:H:112:ALA:HB1	3:H:123:ILE:HG21	1.95	0.48
4:I:563:THR:HG21	4:I:570:GLY:N	2.22	0.48
4:I:632:ASP:HA	4:I:647:ARG:HD2	1.94	0.48
4:I:1247:SER:O	4:I:1248:THR:OG1	2.32	0.48
6:L:40:GLN:O	6:L:44:ILE:HG23	2.14	0.48
6:L:290:LEU:O	6:L:333:VAL:HG21	2.14	0.48
6:L:313:ASP:O	6:L:317:ASN:HB2	2.13	0.48
3:M:295:LEU:HD11	3:M:300:LEU:HD21	1.95	0.48
8:P:65:DT:H2''	8:P:66:DT:C6	2.49	0.48
1:J:278:ARG:NH2	6:L:403:ASP:OD1	2.33	0.48
1:J:474:LEU:HD13	4:I:1313:HIS:CB	2.42	0.48
1:J:937:ILE:HG12	1:J:1134:ILE:O	2.14	0.48
1:J:1027:VAL:HG23	1:J:1199:PHE:CE1	2.49	0.48
1:J:1156:LEU:HA	1:J:1208:ASP:O	2.14	0.48
1:J:1350:ASN:ND2	1:J:1358:PRO:HD3	2.28	0.48
4:I:170:VAL:O	4:I:171:LEU:HD23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:802:VAL:HA	4:I:1096:ILE:O	2.13	0.48
1:J:553:THR:HB	1:J:567:THR:HG22	1.96	0.48
1:J:779:ALA:HB1	4:I:677:ASN:OD1	2.13	0.48
1:J:1041:ILE:CG2	1:J:1044:GLN:HB2	2.43	0.48
3:G:16:ILE:HD11	3:G:214:GLU:HB3	1.96	0.48
3:H:133:LEU:HD21	3:H:140:ILE:CG2	2.44	0.48
6:L:213:ASP:OD1	6:L:214:PRO:HD2	2.13	0.48
6:L:214:PRO:O	6:L:218:ARG:HG3	2.13	0.48
6:L:376:LYS:NZ	6:L:417:ASP:OD1	2.23	0.48
7:O:24:DC:H5''	7:O:24:DC:C6	2.41	0.48
1:J:53:ARG:HA	1:J:54:ASP:HA	1.61	0.47
1:J:850:LYS:HB3	1:J:851:PRO:HD2	1.96	0.47
1:J:966:VAL:CG2	1:J:974:VAL:HG23	2.43	0.47
1:J:1143:ASP:CG	1:J:1148:ARG:HD2	2.34	0.47
4:I:103:VAL:HG12	4:I:117:ILE:HB	1.96	0.47
4:I:568:ASN:CB	4:I:571:LEU:HD12	2.44	0.47
8:P:62:DG:H2''	8:P:63:DG:C8	2.49	0.47
1:J:126:LEU:HD12	1:J:126:LEU:O	2.14	0.47
1:J:189:LEU:O	1:J:234:PRO:HB2	2.13	0.47
1:J:1373:ARG:HG2	1:J:1373:ARG:HH11	1.79	0.47
3:H:93:GLN:CG	3:H:120:ASP:HB2	2.42	0.47
4:I:82:VAL:CG2	4:I:137:VAL:HG21	2.44	0.47
4:I:82:VAL:HG23	4:I:137:VAL:HG21	1.95	0.47
4:I:165:HIS:ND1	4:I:167:SER:HB3	2.29	0.47
4:I:296:VAL:O	4:I:335:THR:HA	2.14	0.47
4:I:811:ASN:HD21	4:I:1097:VAL:HG12	1.79	0.47
4:I:836:LEU:CD2	4:I:921:PRO:HD3	2.39	0.47
4:I:878:THR:OG1	4:I:879:GLY:N	2.43	0.47
4:I:1314:GLN:HG2	5:K:28:ARG:NH1	2.29	0.47
6:L:377:LYS:O	6:L:381:GLU:HG3	2.14	0.47
3:M:260:LEU:HB2	3:M:262:LEU:HD23	1.95	0.47
8:P:60:DA:C8	8:P:61:DT:H72	2.49	0.47
8:P:66:DT:C2'	8:P:67:DT:H72	2.44	0.47
1:J:390:LEU:HD23	1:J:407:VAL:HG21	1.95	0.47
3:G:228:LEU:HD11	3:H:43:LEU:HD21	1.97	0.47
3:H:86:LYS:HD3	3:H:174:ASP:O	2.14	0.47
4:I:104:ILE:HD11	4:I:116:ASP:OD2	2.15	0.47
4:I:1210:ILE:HG22	4:I:1211:ARG:N	2.29	0.47
8:P:68:DG:P	8:P:68:DG:H2'	2.54	0.47
1:J:343:LEU:CD2	1:J:1352:ILE:HD11	2.44	0.47
4:I:24:VAL:HG13	4:I:25:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:453:PRO:O	6:L:457:ILE:HG13	2.15	0.47
6:L:463:LEU:HD23	6:L:463:LEU:HA	1.61	0.47
3:M:284:ARG:O	3:M:314:LEU:HB3	2.15	0.47
7:O:24:DC:N4	8:P:62:DG:O6	2.46	0.47
8:P:49:DT:C2'	8:P:50:DT:H5''	2.44	0.47
1:J:1167:LYS:HE3	1:J:1170:LYS:HB2	1.96	0.47
3:G:213:PRO:O	3:G:217:ILE:HG23	2.15	0.47
3:G:226:GLU:OE1	3:H:10:LYS:HD3	2.15	0.47
4:I:136:PHE:CZ	4:I:456:VAL:HG21	2.49	0.47
4:I:165:HIS:CE1	4:I:167:SER:HB3	2.49	0.47
4:I:242:VAL:HG23	4:I:245:ARG:HG3	1.96	0.47
4:I:425:ILE:O	4:I:429:MET:HG3	2.15	0.47
4:I:593:LYS:HD3	4:I:652:TYR:CE1	2.50	0.47
4:I:836:LEU:HD13	4:I:1054:LEU:CD1	2.41	0.47
4:I:1134:GLN:O	4:I:1136:GLN:NE2	2.48	0.47
11:I:1401:1N7:H31	11:I:1401:1N7:H5	1.95	0.47
3:M:313:SER:OG	3:M:314:LEU:N	2.47	0.47
7:O:31:DA:H2''	7:O:32:DA:C8	2.50	0.47
1:J:56:LEU:HD21	1:J:269:TYR:HB3	1.97	0.47
1:J:58:CYS:HB3	1:J:61:ILE:HG13	1.97	0.47
1:J:70:CYS:SG	1:J:90:VAL:HB	2.53	0.47
1:J:261:ALA:HA	6:L:505:ILE:O	2.14	0.47
1:J:1167:LYS:HG2	1:J:1168:GLU:N	2.29	0.47
3:G:48:LEU:HG	3:G:183:ILE:HG13	1.96	0.47
4:I:122:VAL:HG21	4:I:493:ILE:HG21	1.96	0.47
4:I:303:ASP:HB2	4:I:308:GLU:N	2.29	0.47
4:I:1288:GLN:O	4:I:1292:THR:OG1	2.29	0.47
1:J:141:PHE:HA	1:J:180:MET:HE2	1.96	0.47
1:J:1022:PRO:O	1:J:1126:GLN:HG2	2.15	0.47
1:J:1089:LEU:HA	1:J:1096:PRO:CA	2.32	0.47
1:J:1135:THR:OG1	1:J:1140:ARG:HD3	2.15	0.47
1:J:1226:VAL:O	1:J:1230:THR:HG22	2.14	0.47
3:G:88:LEU:HD13	3:G:130:ILE:HD11	1.96	0.47
4:I:146:VAL:HG13	4:I:529:ARG:HB3	1.96	0.47
4:I:995:ASP:O	4:I:996:ARG:NH1	2.47	0.47
4:I:1124:ILE:HD11	4:I:1198:LEU:CD2	2.45	0.47
4:I:1264:GLN:HE21	4:I:1266:GLY:HA3	1.79	0.47
6:L:281:ARG:O	6:L:285:ARG:HG2	2.15	0.47
6:L:604:SER:O	6:L:604:SER:OG	2.32	0.47
6:L:606:VAL:O	6:L:609:SER:OG	2.27	0.47
3:M:256:PRO:HG3	3:M:277:TYR:CE1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:264:VAL:O	3:M:267:ALA:HB3	2.15	0.47
7:O:24:DC:H2''	7:O:25:DA:C5'	2.45	0.47
8:P:26:DC:H2''	8:P:27:DC:C6	2.49	0.47
1:J:800:LEU:HD23	1:J:1256:ILE:CD1	2.45	0.47
1:J:1138:LEU:O	1:J:1141:VAL:HB	2.15	0.47
1:J:1372:ARG:NE	1:J:1372:ARG:HA	2.30	0.47
2:N:67:ARG:HD2	4:I:341:LEU:CD1	2.44	0.47
3:G:133:LEU:HD13	3:G:133:LEU:HA	1.55	0.47
3:G:137:ASN:N	3:G:137:ASN:OD1	2.48	0.47
7:O:57:DT:H2''	7:O:58:DC:OP2	2.14	0.47
1:J:445:LYS:HD3	4:I:1243:MET:CE	2.45	0.47
1:J:647:PRO:HG3	1:J:697:MET:HA	1.96	0.47
1:J:1035:VAL:CG2	1:J:1113:VAL:H	2.27	0.47
1:J:1162:ILE:HG22	1:J:1178:THR:O	2.15	0.47
4:I:384:LEU:HA	4:I:387:ASN:ND2	2.30	0.47
4:I:759:SER:HG	4:I:763:THR:HG1	1.52	0.47
4:I:1124:ILE:HD11	4:I:1198:LEU:HD22	1.97	0.47
6:L:290:LEU:HD23	6:L:336:GLU:HB3	1.96	0.47
6:L:389:SER:HA	6:L:392:LYS:CE	2.37	0.47
6:L:460:ILE:HD13	6:L:501:ALA:CB	2.45	0.47
6:L:582:VAL:HG23	6:L:583:THR:O	2.15	0.47
7:O:24:DC:H2''	7:O:25:DA:O4'	2.14	0.47
7:O:30:DC:H2''	7:O:31:DA:H8	1.79	0.47
1:J:115:TRP:HB3	1:J:1333:THR:CG2	2.45	0.47
1:J:137:ARG:HB3	1:J:143:SER:HB2	1.97	0.47
1:J:951:GLN:HG2	1:J:1016:THR:OG1	2.15	0.47
1:J:962:ASN:HB2	1:J:979:ASN:O	2.15	0.47
1:J:1033:GLY:O	1:J:1080:ILE:HD12	2.15	0.47
3:G:11:PRO:HD2	3:H:227:GLN:O	2.15	0.47
3:H:13:LEU:HD23	3:H:15:ASP:N	2.30	0.47
3:H:61:ILE:HD11	3:H:142:MET:HE1	1.97	0.47
4:I:175:ARG:HE	4:I:175:ARG:HB2	1.58	0.47
4:I:184:LEU:HD13	4:I:389:PHE:CZ	2.49	0.47
4:I:221:LEU:HD13	4:I:336:LEU:HD11	1.97	0.47
4:I:377:THR:HB	4:I:380:ALA:HB3	1.97	0.47
4:I:727:VAL:HG22	4:I:728:ASP:H	1.80	0.47
4:I:738:GLU:OE1	4:I:738:GLU:N	2.48	0.47
4:I:1151:LEU:O	4:I:1151:LEU:HD23	2.14	0.47
6:L:339:ARG:HA	6:L:342:GLN:HG3	1.96	0.47
3:M:260:LEU:HD21	3:M:278:ILE:CD1	2.40	0.47
1:J:77:ARG:HG2	1:J:79:LYS:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:500:ILE:HG22	1:J:500:ILE:O	2.14	0.46
1:J:615:LYS:HB2	1:J:615:LYS:HE2	1.64	0.46
1:J:735:ALA:O	1:J:738:ARG:HB3	2.14	0.46
1:J:788:LEU:HD11	4:I:548:ARG:HH12	1.80	0.46
1:J:954:ASN:HB2	1:J:984:LEU:CD2	2.45	0.46
1:J:965:SER:HA	1:J:976:THR:H	1.80	0.46
1:J:1155:ILE:HG13	1:J:1210:ILE:HB	1.97	0.46
3:G:110:VAL:HG21	3:G:133:LEU:HD23	1.97	0.46
3:H:67:GLU:OE1	3:H:67:GLU:N	2.46	0.46
3:H:190:ALA:HB2	3:H:200:LYS:HB2	1.97	0.46
4:I:102:LEU:HD12	4:I:102:LEU:HA	1.59	0.46
4:I:421:SER:O	4:I:425:ILE:HG13	2.14	0.46
4:I:496:LYS:HB3	4:I:497:PRO:HD3	1.98	0.46
4:I:667:LEU:HA	4:I:702:THR:OG1	2.15	0.46
4:I:816:ILE:HG21	4:I:1066:MET:CE	2.45	0.46
4:I:1297:ASP:OD2	4:I:1318:GLY:HA3	2.15	0.46
6:L:44:ILE:HG13	6:L:45:ILE:N	2.29	0.46
6:L:419:PHE:CZ	6:L:427:PHE:HB2	2.50	0.46
3:M:300:LEU:O	3:M:303:ILE:HG22	2.15	0.46
8:P:23:DA:H2''	8:P:24:DG:OP2	2.15	0.46
1:J:195:GLU:HG3	1:J:196:GLN:N	2.29	0.46
1:J:211:GLU:HB3	1:J:215:LYS:HZ1	1.79	0.46
1:J:337:ARG:HB3	1:J:342:LEU:CD1	2.45	0.46
1:J:337:ARG:C	1:J:342:LEU:HD13	2.35	0.46
1:J:392:THR:OG1	1:J:393:THR:HG23	2.15	0.46
1:J:973:LEU:HD12	1:J:973:LEU:HA	1.75	0.46
1:J:983:LYS:HE3	1:J:994:SER:HA	1.98	0.46
1:J:1075:ARG:HH12	1:J:1165:PHE:HB2	1.80	0.46
1:J:1333:THR:O	1:J:1337:VAL:HG13	2.16	0.46
4:I:94:ALA:HB2	4:I:129:LEU:HD11	1.98	0.46
4:I:518:ASN:O	4:I:691:PRO:HD3	2.16	0.46
4:I:772:SER:O	4:I:775:GLU:HB3	2.16	0.46
4:I:975:ILE:CD1	4:I:1014:LEU:HB3	2.34	0.46
6:L:348:GLU:HG2	6:L:355:ILE:CD1	2.45	0.46
7:O:37:DA:H2''	7:O:38:DG:OP2	2.15	0.46
8:P:68:DG:H1'	8:P:69:DT:H5'	1.97	0.46
1:J:572:THR:HG1	1:J:576:ARG:HB2	1.80	0.46
1:J:646:ILE:HD12	1:J:762:ASN:ND2	2.30	0.46
1:J:937:ILE:HD11	1:J:1134:ILE:H	1.80	0.46
3:G:7:GLU:HG2	3:G:8:PHE:N	2.30	0.46
3:H:93:GLN:HB2	3:H:120:ASP:CB	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:140:ILE:HD11	3:H:142:MET:CE	2.43	0.46
6:L:376:LYS:O	6:L:380:VAL:HG23	2.15	0.46
8:P:49:DT:C1'	8:P:50:DT:H5''	2.46	0.46
1:J:683:ILE:HG21	2:N:23:ILE:HG21	1.96	0.46
1:J:1031:VAL:HB	1:J:1080:ILE:CG2	2.45	0.46
3:G:71:LYS:O	3:G:74:VAL:HG22	2.14	0.46
3:H:91:ARG:HD3	3:H:122:GLU:OE2	2.15	0.46
4:I:22:LEU:HD22	4:I:603:ILE:HD13	1.97	0.46
4:I:521:LEU:HB2	4:I:794:LEU:HD21	1.97	0.46
6:L:277:MET:CE	6:L:359:LYS:HE3	2.45	0.46
6:L:444:ALA:HB1	6:L:454:VAL:HG12	1.97	0.46
6:L:452:ILE:O	6:L:452:ILE:HG13	2.15	0.46
7:O:48:DG:H2''	7:O:49:DC:C6	2.50	0.46
1:J:194:LEU:HB3	1:J:228:VAL:HG22	1.97	0.46
1:J:1027:VAL:CG1	1:J:1122:ALA:HB3	2.45	0.46
3:H:47:LEU:CD2	3:H:180:VAL:HG21	2.42	0.46
3:H:149:GLY:HA3	3:H:177:TYR:CD2	2.50	0.46
4:I:103:VAL:HG12	4:I:117:ILE:CG2	2.46	0.46
4:I:161:LYS:H	4:I:161:LYS:HG2	1.52	0.46
4:I:233:ARG:CD	4:I:238:GLN:HB2	2.39	0.46
4:I:620:ASN:O	4:I:620:ASN:ND2	2.49	0.46
4:I:1264:GLN:NE2	4:I:1266:GLY:HA3	2.31	0.46
6:L:235:ILE:H	6:L:235:ILE:HG13	1.42	0.46
6:L:348:GLU:HB3	6:L:354:THR:HA	1.98	0.46
7:O:50:DA:C8	7:O:51:DT:H72	2.50	0.46
1:J:56:LEU:HD12	1:J:56:LEU:HA	1.50	0.46
1:J:115:TRP:O	1:J:119:SER:HB3	2.15	0.46
1:J:132:LEU:O	1:J:132:LEU:HD12	2.16	0.46
1:J:474:LEU:HD21	5:K:31:GLN:OE1	2.16	0.46
1:J:555:TYR:O	1:J:556:GLU:HG3	2.15	0.46
1:J:647:PRO:HG3	1:J:697:MET:CA	2.45	0.46
1:J:1310:THR:O	1:J:1314:LEU:HD13	2.16	0.46
3:G:39:LEU:HD23	3:G:39:LEU:HA	1.66	0.46
3:G:189:ALA:HA	3:G:199:ASP:OD1	2.15	0.46
3:H:54:CYS:HA	3:H:147:GLN:O	2.16	0.46
4:I:741:MET:HE3	4:I:974:ARG:NH2	2.29	0.46
4:I:896:THR:HG22	4:I:897:PRO:N	2.31	0.46
6:L:135:ALA:HA	6:L:256:PHE:CE2	2.51	0.46
6:L:381:GLU:HA	6:L:384:LEU:CD2	2.46	0.46
6:L:476:ARG:O	6:L:477:GLU:HG3	2.15	0.46
1:J:309:ASN:ND2	1:J:324:LEU:HD12	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:335:GLN:O	1:J:340:GLN:NE2	2.27	0.46
1:J:552:ILE:HD11	1:J:570:LYS:HG3	1.97	0.46
1:J:934:THR:OG1	1:J:935:PHE:N	2.47	0.46
1:J:956:GLY:CA	1:J:984:LEU:HD11	2.46	0.46
1:J:1027:VAL:HG12	1:J:1122:ALA:H	1.80	0.46
1:J:1238:GLN:OE1	1:J:1238:GLN:HA	2.15	0.46
3:H:61:ILE:CD1	3:H:142:MET:HB3	2.46	0.46
4:I:26:TYR:HE2	4:I:32:LEU:HD12	1.80	0.46
6:L:607:LEU:O	6:L:610:PHE:HB2	2.16	0.46
1:J:210:SER:O	1:J:214:ARG:N	2.32	0.46
1:J:355:ILE:CG2	1:J:466:MET:HB2	2.46	0.46
1:J:686:TRP:CD2	1:J:758:PRO:HG3	2.51	0.46
1:J:707:ILE:O	1:J:714:GLU:N	2.43	0.46
1:J:925:GLU:HG3	1:J:926:PRO:CD	2.45	0.46
1:J:975:ILE:HG22	1:J:977:SER:H	1.80	0.46
1:J:1163:VAL:HG13	1:J:1200:GLU:O	2.16	0.46
3:G:11:PRO:HB3	3:G:31:LEU:CD2	2.46	0.46
3:G:25:LYS:HA	3:G:203:ILE:O	2.15	0.46
4:I:123:TYR:O	4:I:495:ALA:HB2	2.16	0.46
4:I:1264:GLN:HG2	4:I:1266:GLY:H	1.80	0.46
3:M:296:GLY:N	8:P:67:DT:H3'	2.31	0.46
1:J:137:ARG:HH21	1:J:143:SER:HG	1.61	0.46
1:J:359:PRO:HD2	4:I:810:TYR:CE1	2.51	0.46
1:J:849:LEU:HD12	1:J:855:ASP:O	2.15	0.46
1:J:985:ILE:HG23	1:J:989:GLY:O	2.15	0.46
4:I:49:LEU:HD22	4:I:464:PHE:CE2	2.51	0.46
4:I:253:PHE:O	4:I:265:LYS:HA	2.16	0.46
4:I:257:ALA:O	4:I:260:LYS:HB3	2.16	0.46
4:I:272:ARG:O	4:I:276:GLN:HG2	2.15	0.46
4:I:979:LEU:HD11	4:I:1011:LEU:CD1	2.46	0.46
5:K:29:GLN:HE22	5:K:64:LEU:HD22	1.81	0.46
6:L:23:THR:HA	6:L:56:MET:O	2.16	0.46
6:L:247:GLU:HG2	6:L:248:GLU:N	2.31	0.46
6:L:252:LEU:O	6:L:255:VAL:HG13	2.16	0.46
6:L:429:THR:HA	6:L:432:THR:HG22	1.96	0.46
3:M:254:LEU:HB3	3:M:321:TRP:CZ2	2.50	0.46
8:P:62:DG:H2''	8:P:63:DG:H8	1.81	0.46
1:J:128:LEU:HD21	1:J:189:LEU:HD23	1.98	0.46
1:J:566:LYS:O	1:J:566:LYS:HG3	2.15	0.46
1:J:652:GLU:O	1:J:656:GLU:HG3	2.16	0.46
1:J:1044:GLN:CD	1:J:1070:GLY:HA3	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1077:ALA:HB2	1:J:1100:PHE:CD1	2.51	0.46
1:J:1275:LEU:HD23	1:J:1277:GLY:N	2.31	0.46
3:H:46:ILE:HD12	3:H:224:LEU:HB2	1.98	0.46
4:I:189:ASP:HB3	4:I:195:PHE:CE2	2.50	0.46
6:L:145:LEU:HD21	6:L:224:LEU:HG	1.97	0.46
6:L:479:THR:CG2	6:L:480:PRO:HD2	2.45	0.46
6:L:498:LEU:HD12	6:L:498:LEU:HA	1.59	0.46
1:J:101:ARG:O	1:J:246:PRO:HG3	2.17	0.45
1:J:113:HIS:HD1	1:J:115:TRP:HB2	1.80	0.45
1:J:425:ARG:HG2	1:J:426:ALA:H	1.81	0.45
1:J:664:ILE:CD1	1:J:681:LYS:HG2	2.46	0.45
1:J:914:ALA:HB2	1:J:1359:ALA:CB	2.47	0.45
4:I:12:ARG:NH1	4:I:1181:PRO:HB3	2.31	0.45
4:I:151:ARG:HD3	4:I:156:PHE:CE2	2.51	0.45
4:I:407:ARG:HH11	4:I:609:ILE:HD11	1.80	0.45
4:I:548:ARG:HD3	4:I:569:ILE:O	2.16	0.45
4:I:671:LEU:HD12	4:I:671:LEU:O	2.15	0.45
6:L:399:LEU:HD11	6:L:446:GLN:O	2.16	0.45
1:J:804:ALA:O	1:J:916:GLY:HA3	2.15	0.45
1:J:969:SER:CB	1:J:1116:SER:HB3	2.46	0.45
1:J:1151:LYS:HA	1:J:1151:LYS:HE3	1.98	0.45
3:G:22:THR:HB	3:G:207:THR:O	2.16	0.45
4:I:239:MET:SD	4:I:285:ILE:HD11	2.57	0.45
4:I:494:ASN:ND2	4:I:496:LYS:HB3	2.31	0.45
4:I:692:THR:HG21	4:I:798:GLN:HE21	1.81	0.45
4:I:861:ALA:C	4:I:862:LEU:HD23	2.36	0.45
4:I:1111:GLN:HB2	4:I:1230:MET:HE2	1.99	0.45
4:I:1119:MET:CE	4:I:1210:ILE:HD11	2.46	0.45
6:L:316:PHE:CZ	6:L:334:SER:HA	2.50	0.45
6:L:343:LYS:O	6:L:347:ILE:HG13	2.16	0.45
6:L:582:VAL:CG2	6:L:587:ILE:HD13	2.40	0.45
6:L:596:ARG:HB3	6:L:596:ARG:NH1	2.31	0.45
3:M:253:LEU:O	3:M:279:GLY:N	2.44	0.45
7:O:25:DA:H2''	7:O:26:DT:O5'	2.16	0.45
7:O:38:DG:H2''	7:O:39:DG:C8	2.51	0.45
1:J:931:THR:HG23	1:J:1244:GLN:NE2	2.24	0.45
1:J:1144:LEU:HD21	1:J:1236:GLU:CG	2.45	0.45
4:I:475:VAL:HG22	4:I:492:MET:HE2	1.98	0.45
4:I:716:ALA:HB3	4:I:784:ALA:HB3	1.98	0.45
4:I:996:ARG:HA	4:I:996:ARG:HH11	1.81	0.45
1:J:16:GLU:HG3	1:J:17:PHE:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:390:LEU:HD23	1:J:407:VAL:CG2	2.47	0.45
1:J:790:THR:O	1:J:793:SER:HB3	2.16	0.45
1:J:809:VAL:HG11	1:J:909:ILE:HG21	1.99	0.45
1:J:975:ILE:H	1:J:975:ILE:HD12	1.81	0.45
1:J:1355:ARG:HH12	1:J:1369:ARG:HH21	1.65	0.45
2:N:64:TYR:CD1	4:I:341:LEU:HD13	2.51	0.45
3:G:58:GLU:HG2	3:G:172:LEU:HD23	1.98	0.45
3:G:90:VAL:CG2	3:G:123:ILE:HD13	2.40	0.45
4:I:672:GLU:OE1	4:I:672:GLU:N	2.35	0.45
4:I:1145:ILE:CD1	4:I:1173:ALA:HB2	2.45	0.45
4:I:1198:LEU:HA	4:I:1198:LEU:HD23	1.56	0.45
5:K:3:ARG:HH21	5:K:55:GLU:CD	2.20	0.45
6:L:292:VAL:HG13	6:L:297:MET:O	2.17	0.45
6:L:442:SER:OG	6:L:443:ILE:N	2.48	0.45
7:O:53:DT:H6	7:O:53:DT:H5'	1.81	0.45
1:J:84:ILE:HG22	1:J:91:GLU:CB	2.43	0.45
1:J:445:LYS:HD3	4:I:1243:MET:HE3	1.99	0.45
1:J:739:GLN:CG	1:J:744:ARG:HB3	2.40	0.45
1:J:754:ILE:HG22	1:J:755:ILE:O	2.17	0.45
1:J:893:GLY:O	1:J:894:VAL:HG23	2.16	0.45
4:I:360:LEU:O	4:I:364:VAL:HG23	2.16	0.45
4:I:417:SER:OG	4:I:418:GLY:N	2.49	0.45
4:I:802:VAL:HG23	4:I:1096:ILE:O	2.16	0.45
6:L:135:ALA:HA	6:L:256:PHE:HE2	1.82	0.45
8:P:33:DA:H4'	8:P:34:DT:H5'	1.99	0.45
1:J:453:VAL:HG12	1:J:457:TYR:CD2	2.50	0.45
1:J:570:LYS:HE2	1:J:589:TYR:HB3	1.98	0.45
1:J:747:MET:HG3	1:J:759:ILE:HD12	1.98	0.45
1:J:1041:ILE:HG21	1:J:1044:GLN:HB2	1.99	0.45
2:N:36:LEU:CG	2:N:41:GLY:HA2	2.45	0.45
3:G:67:GLU:HB2	3:G:79:LEU:HD23	1.99	0.45
4:I:99:LYS:NZ	4:I:121:GLU:OE1	2.50	0.45
4:I:202:ARG:NH1	4:I:369:MET:HA	2.31	0.45
4:I:543:ALA:HB2	4:I:546:GLU:OE2	2.17	0.45
4:I:961:SER:O	4:I:965:GLN:HG3	2.16	0.45
6:L:292:VAL:HA	6:L:297:MET:CB	2.47	0.45
3:M:253:LEU:HB3	3:M:279:GLY:CA	2.46	0.45
1:J:1060:VAL:HA	1:J:1107:VAL:CG1	2.46	0.45
4:I:406:ASN:HB3	4:I:411:ARG:HB2	1.97	0.45
4:I:517:GLN:C	4:I:519:ASN:N	2.70	0.45
6:L:130:VAL:HB	6:L:365:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:142:THR:HG23	6:L:228:TYR:OH	2.17	0.45
6:L:224:LEU:HD12	6:L:224:LEU:O	2.16	0.45
3:M:257:VAL:HA	3:M:260:LEU:CG	2.40	0.45
8:P:41:DT:H2'	8:P:42:DT:H72	1.98	0.45
1:J:520:ALA:HB3	1:J:546:ALA:CB	2.46	0.45
1:J:527:LEU:HD13	1:J:548:VAL:CG1	2.46	0.45
1:J:835:LEU:HG	1:J:839:VAL:CG2	2.47	0.45
1:J:977:SER:HB2	1:J:980:THR:OG1	2.16	0.45
1:J:1161:GLY:O	1:J:1204:VAL:N	2.48	0.45
3:H:61:ILE:HD11	3:H:142:MET:HE2	1.99	0.45
3:H:84:ASN:HB3	3:H:130:ILE:HA	1.98	0.45
4:I:346:TYR:OH	4:I:436:ARG:NH1	2.49	0.45
4:I:521:LEU:O	4:I:521:LEU:HD22	2.17	0.45
4:I:905:ILE:HA	6:L:595:LEU:CD2	2.46	0.45
4:I:1018:TYR:O	4:I:1022:LYS:HG2	2.17	0.45
6:L:152:GLU:CD	6:L:218:ARG:HG2	2.37	0.45
6:L:393:LYS:NZ	6:L:436:ARG:HH22	2.14	0.45
7:O:54:DT:H4'	7:O:55:DC:OP1	2.16	0.45
1:J:33:TRP:CZ3	4:I:1331:ARG:HG3	2.51	0.45
1:J:99:ARG:NH2	4:I:1254:VAL:O	2.22	0.45
1:J:825:VAL:HG23	1:J:833:GLU:N	2.32	0.45
1:J:1275:LEU:HD23	1:J:1277:GLY:H	1.81	0.45
4:I:57:PHE:CE2	4:I:100:LEU:HD22	2.52	0.45
4:I:149:LEU:HD12	4:I:452:ARG:O	2.17	0.45
4:I:296:VAL:HA	4:I:315:MET:O	2.16	0.45
4:I:520:PRO:CB	4:I:794:LEU:HD11	2.41	0.45
4:I:960:LEU:HA	4:I:960:LEU:HD12	1.63	0.45
4:I:989:LEU:HA	4:I:992:LEU:CD2	2.47	0.45
4:I:1263:ALA:N	4:I:1264:GLN:HA	2.31	0.45
5:K:62:GLN:OE1	5:K:66:VAL:HG23	2.16	0.45
6:L:456:MET:O	6:L:459:THR:OG1	2.30	0.45
6:L:597:LYS:O	6:L:603:ARG:NH2	2.50	0.45
3:M:262:LEU:HD21	3:M:306:VAL:CG1	2.28	0.45
1:J:97:VAL:HG12	1:J:101:ARG:HE	1.82	0.45
1:J:465:GLN:NE2	4:I:1242:LYS:HD2	2.32	0.45
1:J:731:ARG:NH2	4:I:1106:ARG:HE	2.15	0.45
1:J:770:LEU:HD23	4:I:618:GLN:HE22	1.79	0.45
1:J:1041:ILE:HB	1:J:1045:THR:CG2	2.34	0.45
1:J:1155:ILE:HG12	1:J:1155:ILE:H	1.51	0.45
2:N:5:ALA:HB3	4:I:678:ARG:CZ	2.47	0.45
3:H:36:GLY:HA3	3:H:187:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:6:THR:HG22	4:I:781:ASP:OD1	2.16	0.45
4:I:671:LEU:HD23	4:I:1186:VAL:CG1	2.46	0.45
6:L:93:ARG:CB	6:L:99:ARG:HH22	2.29	0.45
6:L:298:PRO:O	6:L:301:ASN:HB3	2.17	0.45
6:L:471:LEU:O	6:L:471:LEU:HD23	2.17	0.45
6:L:493:LYS:O	6:L:497:VAL:HG12	2.16	0.45
6:L:559:LEU:HA	6:L:559:LEU:HD12	1.68	0.45
7:O:26:DT:H2''	7:O:27:DT:O5'	2.17	0.45
7:O:31:DA:H2''	7:O:32:DA:O5'	2.17	0.45
1:J:56:LEU:HD21	1:J:269:TYR:HB2	1.99	0.44
1:J:478:LEU:HD22	5:K:23:ALA:HB3	1.98	0.44
1:J:844:THR:HG23	1:J:864:LEU:HD21	1.98	0.44
1:J:926:PRO:HB3	1:J:1246:VAL:CG1	2.47	0.44
1:J:1155:ILE:CG1	1:J:1211:SER:H	2.30	0.44
3:G:184:ALA:HB2	4:I:1091:GLY:CA	2.47	0.44
3:H:9:LEU:HA	3:H:9:LEU:HD23	1.65	0.44
3:H:64:VAL:HG11	3:H:78:ILE:HD13	1.98	0.44
4:I:68:LEU:HD13	4:I:102:LEU:HD13	1.98	0.44
4:I:503:LYS:HE3	4:I:503:LYS:HB3	1.67	0.44
4:I:543:ALA:HA	4:I:544:GLY:HA3	1.56	0.44
4:I:837:ALA:O	4:I:918:LEU:HD22	2.16	0.44
4:I:902:LEU:HD12	6:L:607:LEU:CD1	2.42	0.44
4:I:996:ARG:HA	4:I:996:ARG:HD3	1.62	0.44
8:P:51:DC:H1'	8:P:52:DT:O4'	2.17	0.44
1:J:146:VAL:HG22	1:J:160:LEU:HD11	1.99	0.44
1:J:245:LEU:HD12	1:J:246:PRO:HD3	1.98	0.44
1:J:379:PRO:HG3	4:I:1305:TYR:CE2	2.52	0.44
1:J:649:LYS:HD2	1:J:652:GLU:OE1	2.18	0.44
1:J:952:VAL:HG11	1:J:1012:ALA:O	2.17	0.44
1:J:1080:ILE:HD13	1:J:1080:ILE:HA	1.86	0.44
1:J:1287:ILE:HG22	1:J:1290:ARG:NH2	2.32	0.44
3:H:219:ARG:HB2	3:H:219:ARG:HH11	1.81	0.44
4:I:21:VAL:HG21	4:I:592:ARG:CZ	2.46	0.44
4:I:936:ARG:NH2	4:I:1047:LEU:HD23	2.32	0.44
4:I:964:LEU:HD12	4:I:964:LEU:O	2.18	0.44
4:I:1082:ILE:H	4:I:1082:ILE:CD1	2.29	0.44
6:L:114:GLU:OE2	6:L:114:GLU:HA	2.17	0.44
6:L:244:THR:O	6:L:248:GLU:HG2	2.17	0.44
6:L:287:ILE:HD13	6:L:315:TRP:HH2	1.82	0.44
6:L:295:CYS:HB2	6:L:333:VAL:HG11	1.99	0.44
6:L:456:MET:HE2	6:L:497:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:540:LEU:HD12	6:L:610:PHE:HD2	1.81	0.44
3:M:295:LEU:HD21	3:M:300:LEU:HD23	1.99	0.44
1:J:19:ALA:HB3	1:J:1341:ARG:NH2	2.32	0.44
1:J:925:GLU:HG3	1:J:926:PRO:HD3	2.00	0.44
1:J:984:LEU:HG	1:J:992:LYS:HB2	2.00	0.44
4:I:49:LEU:HD12	4:I:73:TYR:CE2	2.53	0.44
4:I:216:THR:H	4:I:219:GLN:NE2	2.15	0.44
4:I:339:ASN:O	4:I:344:GLY:HA2	2.18	0.44
4:I:594:VAL:HG13	4:I:594:VAL:O	2.17	0.44
4:I:936:ARG:HH21	4:I:1047:LEU:HD23	1.82	0.44
6:L:456:MET:CE	6:L:497:VAL:HG23	2.47	0.44
6:L:510:PRO:HA	6:L:518:HIS:HA	1.99	0.44
1:J:278:ARG:NH2	6:L:446:GLN:HE22	2.15	0.44
1:J:926:PRO:HB3	1:J:1246:VAL:HG11	1.99	0.44
1:J:950:ILE:HB	1:J:1018:ALA:HB3	2.00	0.44
1:J:975:ILE:HD13	1:J:997:VAL:CG1	2.48	0.44
1:J:1275:LEU:HD23	1:J:1276:GLU:N	2.32	0.44
1:J:1344:LEU:HB3	1:J:1350:ASN:OD1	2.18	0.44
3:G:102:LEU:HB3	3:G:142:MET:CG	2.48	0.44
3:G:158:ARG:NH2	3:G:173:VAL:O	2.51	0.44
4:I:195:PHE:HD1	4:I:205:PRO:HA	1.82	0.44
4:I:678:ARG:HA	4:I:678:ARG:HD3	1.71	0.44
4:I:685:MET:SD	4:I:1235:LEU:HD21	2.58	0.44
6:L:128:ASN:O	6:L:131:GLN:HB2	2.17	0.44
6:L:450:ILE:HG13	6:L:450:ILE:O	2.17	0.44
1:J:85:CYS:O	1:J:89:GLY:N	2.45	0.44
1:J:312:ARG:HG3	1:J:313:GLY:N	2.33	0.44
1:J:316:ILE:CD1	1:J:324:LEU:HD11	2.42	0.44
4:I:161:LYS:HA	4:I:170:VAL:HG12	1.98	0.44
4:I:237:LEU:HD23	4:I:333:ILE:HD11	2.00	0.44
4:I:1125:GLY:HA3	4:I:1179:GLY:HA2	2.00	0.44
6:L:226:ALA:O	6:L:229:VAL:HG23	2.18	0.44
6:L:281:ARG:HG2	6:L:285:ARG:HE	1.83	0.44
3:M:278:ILE:CG2	3:M:282:VAL:HG13	2.46	0.44
8:P:47:DC:H4'	8:P:48:DC:OP1	2.16	0.44
1:J:421:VAL:HG13	1:J:439:PRO:CG	2.46	0.44
1:J:601:ILE:O	1:J:601:ILE:HG12	2.17	0.44
2:N:52:PHE:O	2:N:55:VAL:HG12	2.18	0.44
3:G:29:GLU:HB3	3:G:30:PRO:HD3	1.99	0.44
3:G:207:THR:HG21	3:G:211:ILE:HG22	1.98	0.44
3:G:234:LEU:HD23	3:G:234:LEU:HA	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:346:TYR:HE2	4:I:437:ASN:HD21	1.66	0.44
4:I:484:LEU:HD12	4:I:486:THR:CB	2.41	0.44
4:I:696:ASP:HB3	4:I:697:LYS:H	1.64	0.44
8:P:33:DA:H2'	8:P:34:DT:H2'	2.00	0.44
1:J:146:VAL:HA	1:J:178:ALA:HA	2.00	0.44
1:J:501:VAL:CG1	1:J:602:SER:HB2	2.48	0.44
1:J:850:LYS:HD2	1:J:855:ASP:OD1	2.18	0.44
1:J:1190:ILE:HG21	1:J:1196:LEU:CD2	2.39	0.44
3:G:29:GLU:HA	3:G:200:LYS:CB	2.37	0.44
3:G:166:ARG:HH22	4:I:876:GLU:CD	2.21	0.44
3:G:229:GLU:HA	3:G:232:VAL:CG1	2.48	0.44
3:H:39:LEU:HD23	3:H:39:LEU:HA	1.88	0.44
3:H:66:HIS:HB3	3:H:68:TYR:CE1	2.53	0.44
3:H:92:VAL:HG13	3:H:120:ASP:OD2	2.17	0.44
4:I:273:HIS:HA	4:I:276:GLN:HG2	1.98	0.44
4:I:302:ILE:HA	4:I:309:LEU:HA	1.99	0.44
4:I:823:VAL:HG21	4:I:1079:ILE:HD13	1.99	0.44
4:I:1066:MET:HB2	4:I:1066:MET:HE2	1.89	0.44
6:L:125:ASP:HA	6:L:128:ASN:CG	2.38	0.44
1:J:84:ILE:HG22	1:J:91:GLU:HA	1.99	0.44
1:J:189:LEU:HD23	1:J:189:LEU:HA	1.82	0.44
1:J:195:GLU:HA	1:J:198:CYS:SG	2.58	0.44
1:J:479:GLU:OE1	4:I:1286:THR:OG1	2.14	0.44
1:J:687:ALA:HB1	2:N:24:ARG:NH2	2.32	0.44
1:J:896:ALA:CB	1:J:909:ILE:HG22	2.48	0.44
1:J:1227:HIS:HA	1:J:1230:THR:CG2	2.48	0.44
1:J:1351:VAL:HG13	4:I:1291:LEU:CD1	2.47	0.44
2:N:24:ARG:HG2	2:N:24:ARG:O	2.18	0.44
4:I:118:LYS:HB3	4:I:488:MET:SD	2.58	0.44
4:I:238:GLN:CG	4:I:286:GLU:HB3	2.48	0.44
4:I:591:TYR:HB3	4:I:652:TYR:HB3	1.99	0.44
4:I:731:ARG:NH1	4:I:750:ILE:HD11	2.33	0.44
4:I:1087:TYR:HA	4:I:1093:PRO:HA	2.00	0.44
6:L:58:GLU:HB2	6:L:60:PRO:HD2	2.00	0.44
6:L:157:ARG:HD3	6:L:158:LEU:N	2.33	0.44
6:L:224:LEU:O	6:L:228:TYR:HB2	2.17	0.44
6:L:252:LEU:HD12	6:L:255:VAL:HG13	1.98	0.44
1:J:44:ILE:HG12	6:L:450:ILE:HG22	2.00	0.44
1:J:335:GLN:OE1	1:J:340:GLN:NE2	2.51	0.44
1:J:461:PHE:HD2	4:I:813:GLU:HB2	1.83	0.44
1:J:932:MET:HG3	1:J:933:ARG:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:40:CYS:CB	4:I:268:ARG:HB3	2.47	0.44
3:H:32:GLU:O	3:H:35:PHE:HB2	2.18	0.44
4:I:15:PHE:CD2	4:I:1190:ALA:HB2	2.53	0.44
4:I:189:ASP:OD1	4:I:193:ASN:HB2	2.18	0.44
4:I:699:LEU:HD23	4:I:799:ASN:ND2	2.33	0.44
4:I:854:ILE:HG23	4:I:855:PRO:HD2	1.99	0.44
4:I:964:LEU:HB2	4:I:1025:PHE:CD2	2.53	0.44
7:O:58:DC:H2''	7:O:59:DG:H8	1.82	0.44
1:J:638:SER:OG	1:J:639:VAL:N	2.50	0.43
1:J:1175:LEU:HD23	1:J:1176:VAL:N	2.32	0.43
3:G:14:VAL:HG12	3:G:15:ASP:OD2	2.18	0.43
4:I:198:ILE:HG23	4:I:389:PHE:HZ	1.83	0.43
4:I:201:ARG:HH22	4:I:370:MET:CE	2.31	0.43
4:I:429:MET:O	4:I:433:ILE:HG12	2.18	0.43
4:I:588:GLU:OE1	4:I:605:TYR:HB3	2.18	0.43
4:I:1270:PHE:CE1	4:I:1274:GLU:HB3	2.54	0.43
3:M:302:GLU:O	3:M:306:VAL:HG12	2.18	0.43
1:J:37:GLU:HB2	1:J:104:HIS:NE2	2.33	0.43
1:J:268:LEU:HD23	1:J:268:LEU:HA	1.79	0.43
1:J:528:THR:HG23	3:H:86:LYS:HE3	2.00	0.43
1:J:594:GLN:NE2	1:J:600:ALA:HB1	2.32	0.43
2:N:48:ARG:NH1	2:N:59:VAL:HB	2.33	0.43
3:H:48:LEU:HD13	3:H:183:ILE:CD1	2.45	0.43
4:I:12:ARG:HG3	4:I:1181:PRO:HB2	2.00	0.43
4:I:243:PRO:HB3	4:I:277:LEU:CB	2.49	0.43
4:I:255:ILE:HD11	4:I:269:ILE:HD11	1.99	0.43
4:I:285:ILE:HD13	4:I:287:VAL:CG1	2.49	0.43
4:I:1331:ARG:HA	4:I:1335:ILE:O	2.17	0.43
5:K:22:VAL:HG12	5:K:54:ILE:HD11	2.00	0.43
6:L:27:VAL:O	6:L:27:VAL:HG22	2.18	0.43
6:L:136:GLU:O	6:L:138:PRO:HD3	2.18	0.43
1:J:199:GLU:HA	1:J:202:ARG:CD	2.43	0.43
1:J:268:LEU:HD13	1:J:306:LEU:HA	1.99	0.43
1:J:385:LEU:HD13	1:J:400:MET:CE	2.47	0.43
1:J:490:ILE:HD11	1:J:609:TYR:CE1	2.53	0.43
1:J:646:ILE:HG22	1:J:647:PRO:HD2	1.99	0.43
1:J:647:PRO:HG3	1:J:697:MET:HB3	2.00	0.43
1:J:1075:ARG:HB2	1:J:1100:PHE:CD1	2.54	0.43
1:J:1172:LYS:O	1:J:1189:MET:HE3	2.18	0.43
3:G:51:MET:HE3	3:G:52:PRO:HD2	1.99	0.43
4:I:255:ILE:HD12	4:I:263:VAL:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:770:CYS:HB2	4:I:791:LEU:CD2	2.47	0.43
6:L:123:ILE:HD11	6:L:375:ALA:HB3	2.00	0.43
6:L:479:THR:O	6:L:482:GLU:N	2.51	0.43
1:J:31:ARG:NE	1:J:241:VAL:HG21	2.33	0.43
1:J:501:VAL:HG11	1:J:602:SER:HB2	2.01	0.43
1:J:1034:PHE:CD2	1:J:1083:ALA:HA	2.53	0.43
1:J:1286:LYS:O	1:J:1286:LYS:HG2	2.19	0.43
4:I:135:THR:HG21	4:I:515:MET:SD	2.59	0.43
4:I:229:ILE:HD13	4:I:229:ILE:HA	1.80	0.43
4:I:636:CYS:SG	4:I:650:VAL:HG12	2.58	0.43
4:I:998:LEU:HD23	4:I:1015:ALA:HB1	2.00	0.43
4:I:1096:ILE:HG22	4:I:1098:LEU:HD13	1.99	0.43
6:L:98:VAL:HA	6:L:402:LEU:HD21	2.00	0.43
6:L:465:ARG:O	6:L:469:GLN:HG3	2.19	0.43
6:L:579:GLN:OE1	6:L:579:GLN:HA	2.19	0.43
3:M:257:VAL:CA	3:M:260:LEU:HG	2.39	0.43
1:J:553:THR:O	1:J:553:THR:OG1	2.33	0.43
1:J:1037:PHE:HB3	1:J:1040:MET:HB2	2.00	0.43
1:J:1044:GLN:HG2	1:J:1070:GLY:HA3	2.01	0.43
11:J:1504:1N7:C19	11:J:1504:1N7:C4	2.90	0.43
3:H:95:LYS:NZ	3:H:98:VAL:HG12	2.33	0.43
4:I:799:ASN:OD1	4:I:799:ASN:N	2.49	0.43
6:L:384:LEU:HA	6:L:387:VAL:HB	1.99	0.43
1:J:17:PHE:HZ	1:J:1353:VAL:CG2	2.32	0.43
1:J:331:ILE:CG2	1:J:1328:THR:HG21	2.46	0.43
1:J:332:LYS:HA	1:J:1328:THR:OG1	2.18	0.43
1:J:342:LEU:O	1:J:343:LEU:HD23	2.18	0.43
1:J:516:ASP:HB3	1:J:573:THR:CG2	2.48	0.43
1:J:615:LYS:O	1:J:618:VAL:HG22	2.18	0.43
1:J:975:ILE:HD11	1:J:1003:LEU:CD1	2.39	0.43
1:J:1230:THR:O	1:J:1234:VAL:HG23	2.17	0.43
3:G:179:PRO:CG	3:G:211:ILE:HG13	2.48	0.43
3:H:102:LEU:HB3	3:H:142:MET:CG	2.49	0.43
4:I:105:TYR:CD1	4:I:114:VAL:HA	2.49	0.43
4:I:829:THR:CG2	4:I:1057:LYS:HD3	2.49	0.43
6:L:37:ASP:OD1	6:L:39:ASP:HB2	2.18	0.43
6:L:146:GLU:O	6:L:150:ARG:HB2	2.18	0.43
1:J:31:ARG:HE	1:J:241:VAL:HG21	1.82	0.43
1:J:198:CYS:HB2	1:J:221:ILE:HD12	2.01	0.43
1:J:392:THR:OG1	1:J:393:THR:N	2.50	0.43
1:J:418:GLU:O	1:J:420:PRO:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:596:LEU:HD21	1:J:604:MET:HE1	2.01	0.43
1:J:950:ILE:CD1	1:J:1018:ALA:HB3	2.48	0.43
1:J:1077:ALA:HB2	1:J:1100:PHE:CE1	2.54	0.43
1:J:1359:ALA:O	1:J:1363:TYR:HB2	2.18	0.43
3:H:136:GLU:HG2	3:H:137:ASN:H	1.84	0.43
4:I:231:GLU:HA	4:I:331:LYS:O	2.19	0.43
4:I:420:LEU:HD23	4:I:420:LEU:HA	1.78	0.43
4:I:514:PHE:HD1	4:I:514:PHE:HA	1.69	0.43
4:I:515:MET:HE2	4:I:515:MET:HB3	1.83	0.43
6:L:587:ILE:HD12	6:L:587:ILE:HA	1.65	0.43
8:P:21:DA:H2''	8:P:22:DA:OP2	2.18	0.43
8:P:29:DA:H2''	8:P:30:DG:H5'	2.00	0.43
1:J:107:LEU:HA	1:J:107:LEU:HD23	1.58	0.43
1:J:355:ILE:HD13	1:J:466:MET:HG3	2.01	0.43
1:J:426:ALA:HB3	1:J:427:PRO:CD	2.48	0.43
1:J:560:ASN:OD1	1:J:560:ASN:N	2.40	0.43
1:J:955:LYS:NZ	1:J:1011:VAL:O	2.40	0.43
1:J:976:THR:HA	1:J:999:TYR:HE1	1.83	0.43
1:J:1107:VAL:HG13	1:J:1107:VAL:O	2.19	0.43
1:J:1189:MET:O	1:J:1191:PRO:HD3	2.19	0.43
3:G:17:GLU:OE1	3:G:25:LYS:HD2	2.19	0.43
3:G:66:HIS:HB3	4:I:927:THR:HG21	2.01	0.43
3:G:192:VAL:HB	3:G:198:LEU:HD12	2.00	0.43
4:I:77:GLU:HG3	4:I:78:PRO:HD2	2.01	0.43
4:I:210:LEU:HB2	4:I:220:ILE:HD11	2.01	0.43
4:I:519:ASN:OD1	4:I:520:PRO:HD2	2.18	0.43
4:I:1073:LYS:H	4:I:1073:LYS:HG3	1.44	0.43
5:K:49:ILE:O	5:K:53:GLU:HG3	2.18	0.43
6:L:128:ASN:HA	6:L:131:GLN:HG3	2.00	0.43
6:L:270:VAL:CG1	6:L:365:MET:HE3	2.40	0.43
6:L:402:LEU:HA	6:L:405:ILE:HG12	2.00	0.43
1:J:809:VAL:HG21	1:J:909:ILE:CG1	2.48	0.43
1:J:1061:VAL:CG1	1:J:1076:PRO:HG3	2.48	0.43
1:J:1079:LYS:HB3	1:J:1098:GLN:HA	1.99	0.43
3:H:24:ALA:HB3	3:H:213:PRO:HB2	2.00	0.43
3:H:59:VAL:CB	3:H:144:ILE:HG22	2.46	0.43
4:I:21:VAL:HG21	4:I:592:ARG:NH1	2.34	0.43
4:I:517:GLN:O	4:I:517:GLN:HG2	2.19	0.43
4:I:655:VAL:H	4:I:659:GLN:NE2	2.17	0.43
4:I:890:LYS:HD2	4:I:890:LYS:HA	1.64	0.43
4:I:941:LYS:HB3	4:I:945:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:1271:GLY:N	4:I:1274:GLU:OE1	2.52	0.43
6:L:103:ARG:O	6:L:107:THR:HG23	2.18	0.43
6:L:298:PRO:HD2	6:L:301:ASN:HB3	2.01	0.43
6:L:380:VAL:O	6:L:412:LEU:HD21	2.17	0.43
7:O:25:DA:H2'	7:O:26:DT:H6	1.79	0.43
1:J:95:THR:O	1:J:95:THR:OG1	2.36	0.43
1:J:373:ALA:CB	1:J:441:LEU:HD11	2.49	0.43
1:J:399:LYS:HE3	1:J:403:ARG:NH2	2.24	0.43
1:J:473:THR:HG22	4:I:1304:MET:HE2	2.01	0.43
1:J:526:VAL:HG23	3:H:83:LEU:HD11	2.01	0.43
1:J:536:LEU:HD21	3:H:152:TYR:CZ	2.53	0.43
1:J:683:ILE:HG21	2:N:23:ILE:CG2	2.49	0.43
4:I:210:LEU:HD13	4:I:220:ILE:CD1	2.48	0.43
4:I:270:THR:OG1	4:I:272:ARG:HB3	2.19	0.43
4:I:484:LEU:HD13	4:I:485:ASP:OD1	2.19	0.43
4:I:560:PRO:HD3	4:I:660:VAL:O	2.18	0.43
4:I:905:ILE:HG22	4:I:906:PHE:CG	2.54	0.43
4:I:1032:LYS:HB2	4:I:1032:LYS:HE3	1.71	0.43
4:I:1256:GLN:OE1	6:L:528:LEU:HD11	2.19	0.43
6:L:10:LYS:O	6:L:14:THR:HG23	2.19	0.43
6:L:280:VAL:O	6:L:284:GLU:HG3	2.19	0.43
6:L:418:LYS:HD3	6:L:434:TRP:HZ2	1.84	0.43
1:J:268:LEU:HD21	1:J:324:LEU:HD11	2.00	0.42
1:J:493:PRO:O	1:J:903:LEU:HD13	2.19	0.42
1:J:581:MET:HE3	3:H:182:ARG:HD2	2.00	0.42
1:J:926:PRO:CB	1:J:1248:ILE:HD11	2.49	0.42
1:J:1141:VAL:HG23	1:J:1240:VAL:HG11	2.00	0.42
1:J:1292:LEU:HA	1:J:1292:LEU:HD23	1.46	0.42
3:G:61:ILE:HB	3:G:64:VAL:HG21	2.00	0.42
3:G:88:LEU:HD12	3:G:128:HIS:HD2	1.84	0.42
3:H:64:VAL:HG22	3:H:66:HIS:N	2.33	0.42
4:I:13:LYS:HB2	4:I:1180:MET:CE	2.49	0.42
4:I:57:PHE:HE2	4:I:100:LEU:HD22	1.83	0.42
4:I:120:GLN:NE2	4:I:490:GLN:HB3	2.34	0.42
4:I:195:PHE:CD1	4:I:205:PRO:HA	2.54	0.42
4:I:255:ILE:HD12	4:I:263:VAL:HG11	2.01	0.42
4:I:404:LYS:HD2	4:I:404:LYS:HA	1.83	0.42
4:I:898:GLU:CB	6:L:544:THR:HG21	2.47	0.42
6:L:73:ASP:HA	6:L:74:GLU:HA	1.63	0.42
6:L:348:GLU:HG2	6:L:355:ILE:CG1	2.48	0.42
6:L:456:MET:CE	6:L:497:VAL:HA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:468:ARG:CZ	6:L:468:ARG:HB2	2.49	0.42
6:L:494:ILE:HA	6:L:497:VAL:HG12	1.99	0.42
8:P:52:DT:H2"	8:P:53:DT:C6	2.54	0.42
1:J:1344:LEU:HD12	1:J:1349:GLU:CB	2.46	0.42
3:G:47:LEU:CD2	3:G:220:ALA:HB2	2.49	0.42
3:G:95:LYS:HE3	3:G:95:LYS:HB2	1.84	0.42
4:I:689:ALA:HB1	4:I:1233:LEU:HD12	2.00	0.42
4:I:819:SER:OG	4:I:820:GLU:N	2.53	0.42
4:I:829:THR:HG21	4:I:1057:LYS:HD3	2.02	0.42
6:L:101:TYR:O	6:L:105:MET:HG3	2.19	0.42
6:L:366:SER:O	6:L:369:GLU:HG3	2.19	0.42
1:J:984:LEU:CG	1:J:992:LYS:HB2	2.50	0.42
2:N:44:ILE:H	2:N:44:ILE:HG13	1.64	0.42
3:G:8:PHE:HE1	3:H:150:ARG:HD3	1.84	0.42
3:G:51:MET:HA	3:G:52:PRO:HD3	1.88	0.42
3:G:232:VAL:O	3:H:218:ARG:HG3	2.20	0.42
4:I:30:ILE:H	4:I:30:ILE:HG13	1.27	0.42
4:I:848:GLU:HG2	4:I:888:THR:HG22	2.00	0.42
5:K:9:ALA:HB1	5:K:19:LEU:CD1	2.49	0.42
6:L:231:THR:HA	6:L:248:GLU:HB2	2.01	0.42
1:J:188:LEU:HD23	1:J:188:LEU:HA	1.86	0.42
1:J:401:VAL:HA	1:J:408:VAL:HG21	2.01	0.42
1:J:438:GLU:HA	1:J:439:PRO:HD3	1.92	0.42
1:J:568:SER:OG	1:J:569:LEU:N	2.52	0.42
1:J:847:ASP:OD2	1:J:856:ILE:HD13	2.19	0.42
1:J:902:ASP:HB2	1:J:909:ILE:HD13	2.02	0.42
3:G:159:ILE:HD12	3:G:159:ILE:HA	1.86	0.42
3:G:182:ARG:C	3:G:183:ILE:HG12	2.39	0.42
3:H:8:PHE:O	3:H:10:LYS:NZ	2.32	0.42
4:I:70:TYR:CZ	4:I:72:SER:HA	2.55	0.42
4:I:251:ALA:HB2	4:I:269:ILE:CD1	2.46	0.42
4:I:699:LEU:HB2	4:I:799:ASN:HD22	1.85	0.42
4:I:905:ILE:HG22	4:I:906:PHE:CD1	2.54	0.42
6:L:123:ILE:HD12	6:L:376:LYS:CG	2.44	0.42
6:L:315:TRP:CH2	6:L:341:LEU:HD11	2.54	0.42
6:L:457:ILE:O	6:L:461:ASN:ND2	2.52	0.42
1:J:816:THR:HG21	1:J:889:ASP:HB2	2.01	0.42
1:J:1108:GLN:HB2	1:J:1123:ARG:NH1	2.33	0.42
3:G:58:GLU:CD	3:G:170:ARG:HD2	2.40	0.42
3:G:92:VAL:HG23	3:G:148:ARG:NH2	2.34	0.42
4:I:115:LYS:HG3	4:I:116:ASP:CG	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:198:ILE:HG22	4:I:199:ASP:N	2.32	0.42
4:I:283:LYS:HD3	4:I:283:LYS:HA	1.78	0.42
4:I:589:THR:OG1	4:I:659:GLN:OE1	2.33	0.42
4:I:850:ILE:O	4:I:850:ILE:HG22	2.19	0.42
4:I:1160:ASP:OD1	4:I:1160:ASP:N	2.51	0.42
5:K:58:LEU:HD12	5:K:58:LEU:O	2.20	0.42
6:L:253:SER:O	6:L:257:LYS:HG2	2.20	0.42
6:L:423:ARG:HB2	6:L:425:TYR:CD1	2.54	0.42
7:O:24:DC:H2''	7:O:25:DA:H5''	2.01	0.42
8:P:33:DA:H1'	8:P:34:DT:O4'	2.19	0.42
8:P:51:DC:H5'	8:P:51:DC:C6	2.55	0.42
1:J:26:SER:OG	1:J:28:ASP:N	2.52	0.42
1:J:54:ASP:OD1	1:J:54:ASP:N	2.52	0.42
1:J:121:PRO:HB2	1:J:126:LEU:HD23	2.02	0.42
1:J:487:THR:HG21	5:K:4:VAL:HG23	2.00	0.42
1:J:647:PRO:HG3	1:J:697:MET:CB	2.48	0.42
1:J:708:ASN:HB3	1:J:713:GLU:HA	2.01	0.42
1:J:1079:LYS:HE2	1:J:1098:GLN:HB3	2.02	0.42
3:G:194:GLN:HA	3:G:194:GLN:OE1	2.20	0.42
4:I:208:ILE:HG22	4:I:354:ASP:OD1	2.20	0.42
4:I:839:VAL:HG12	4:I:1049:ILE:HG23	2.01	0.42
4:I:1148:ALA:HA	4:I:1201:LEU:HD21	2.01	0.42
6:L:24:TYR:HA	6:L:27:VAL:CG1	2.50	0.42
6:L:150:ARG:CG	6:L:155:GLU:HB2	2.48	0.42
3:M:307:LEU:HD12	3:M:313:SER:HA	2.00	0.42
1:J:22:ILE:CD1	1:J:1332:LEU:HD13	2.49	0.42
1:J:327:LEU:HB2	4:I:1333:LEU:HD21	2.01	0.42
1:J:450:HIS:CE1	1:J:452:LEU:HG	2.53	0.42
1:J:574:VAL:O	1:J:578:ILE:HG13	2.20	0.42
1:J:730:ALA:O	1:J:731:ARG:HG2	2.20	0.42
1:J:1005:LYS:HD3	1:J:1017:VAL:CG1	2.46	0.42
3:G:185:TYR:HB2	3:G:201:LEU:HD11	2.01	0.42
3:H:31:LEU:HD13	3:H:39:LEU:HD12	2.02	0.42
3:H:146:VAL:O	3:H:147:GLN:HG3	2.19	0.42
4:I:475:VAL:HG22	4:I:492:MET:CE	2.50	0.42
5:K:38:LEU:CB	5:K:58:LEU:HD11	2.49	0.42
6:L:252:LEU:HA	6:L:255:VAL:CG1	2.50	0.42
7:O:39:DG:C2'	7:O:40:DC:H5'	2.50	0.42
1:J:544:LEU:HD12	1:J:544:LEU:HA	1.65	0.42
1:J:707:ILE:HG22	1:J:708:ASN:N	2.33	0.42
1:J:776:THR:HG21	4:I:560:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1195:GLN:H	1:J:1195:GLN:HG3	1.62	0.42
2:N:56:THR:O	2:N:57:LEU:HG	2.20	0.42
4:I:135:THR:HG23	4:I:527:LYS:CE	2.50	0.42
5:K:16:ARG:O	5:K:16:ARG:HG2	2.19	0.42
7:O:62:DC:H2''	7:O:63:DT:C6	2.55	0.42
8:P:59:DA:H2''	8:P:60:DA:O5'	2.19	0.42
1:J:341:ASN:HD22	4:I:1255:THR:CG2	2.30	0.42
3:G:106:GLY:O	3:G:133:LEU:HB3	2.20	0.42
3:G:112:ALA:HB1	3:G:123:ILE:HG21	2.02	0.42
4:I:14:ASP:HB3	4:I:1157:GLN:HB2	2.01	0.42
4:I:407:ARG:NH1	4:I:609:ILE:HD11	2.34	0.42
4:I:838:CYS:HB2	4:I:918:LEU:HD22	2.01	0.42
4:I:1000:LEU:HD23	4:I:1000:LEU:HA	1.75	0.42
4:I:1290:MET:HG3	4:I:1290:MET:O	2.20	0.42
6:L:115:GLY:HA2	6:L:118:ASP:CG	2.40	0.42
6:L:390:ILE:HD13	6:L:432:THR:OG1	2.19	0.42
1:J:84:ILE:HA	1:J:90:VAL:O	2.20	0.42
1:J:117:LEU:HD13	1:J:124:ILE:HD12	2.01	0.42
1:J:949:SER:HB2	1:J:1016:THR:HG21	2.01	0.42
1:J:1026:PRO:HB3	1:J:1120:THR:CG2	2.50	0.42
1:J:1227:HIS:HA	1:J:1230:THR:HG22	2.02	0.42
1:J:1285:VAL:HG11	1:J:1302:TYR:HB3	2.02	0.42
3:H:64:VAL:HG23	3:H:69:SER:HB3	2.02	0.42
4:I:306:THR:HG22	4:I:306:THR:O	2.20	0.42
4:I:598:VAL:HA	4:I:627:GLY:O	2.20	0.42
4:I:835:GLU:HB2	4:I:1053:TYR:CE1	2.55	0.42
4:I:1145:ILE:HD11	4:I:1173:ALA:CB	2.50	0.42
4:I:1301:ARG:HG3	4:I:1302:THR:N	2.34	0.42
6:L:8:GLN:OE1	6:L:8:GLN:HA	2.20	0.42
6:L:316:PHE:CZ	6:L:337:VAL:HB	2.54	0.42
6:L:316:PHE:HA	6:L:319:ALA:CB	2.50	0.42
3:M:313:SER:HB3	3:M:316:MET:HE1	2.00	0.42
1:J:194:LEU:HD13	1:J:227:PHE:HB3	2.01	0.41
3:G:217:ILE:O	3:G:217:ILE:HG13	2.20	0.41
4:I:253:PHE:HA	4:I:265:LYS:HG3	2.01	0.41
4:I:470:ARG:HA	4:I:473:ARG:CG	2.49	0.41
4:I:671:LEU:HB3	4:I:1186:VAL:CG1	2.49	0.41
4:I:916:SER:OG	4:I:916:SER:O	2.38	0.41
6:L:286:LEU:HA	6:L:290:LEU:HD13	2.02	0.41
7:O:16:DC:H6	7:O:16:DC:H2'	1.71	0.41
1:J:320:ASN:OD1	1:J:320:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:385:LEU:CD1	1:J:400:MET:HE2	2.47	0.41
1:J:887:SER:HB3	1:J:1227:HIS:HE1	1.84	0.41
1:J:960:LEU:HD21	1:J:1003:LEU:HD11	2.02	0.41
1:J:1141:VAL:HG21	1:J:1241:TYR:CE1	2.54	0.41
1:J:1169:THR:HG22	1:J:1169:THR:O	2.21	0.41
4:I:62:TYR:O	4:I:63:SER:OG	2.26	0.41
4:I:130:MET:CG	4:I:134:GLY:HA2	2.49	0.41
4:I:471:VAL:CG2	4:I:498:ILE:HD11	2.49	0.41
4:I:1031:ALA:O	4:I:1034:ARG:HG2	2.20	0.41
6:L:290:LEU:O	6:L:333:VAL:HG11	2.20	0.41
6:L:310:GLU:OE2	6:L:355:ILE:HG21	2.20	0.41
3:M:257:VAL:HG12	3:M:260:LEU:CD1	2.43	0.41
1:J:25:ALA:HB2	4:I:1336:ASN:HB2	2.01	0.41
1:J:33:TRP:CH2	4:I:1331:ARG:HG3	2.54	0.41
1:J:132:LEU:HA	1:J:135:ILE:HD11	2.02	0.41
1:J:170:GLU:HG3	1:J:170:GLU:H	1.65	0.41
1:J:324:LEU:HD12	1:J:324:LEU:O	2.21	0.41
1:J:332:LYS:HG2	1:J:333:GLY:N	2.34	0.41
1:J:1034:PHE:O	1:J:1080:ILE:HA	2.19	0.41
3:H:48:LEU:HD12	3:H:48:LEU:HA	1.85	0.41
3:H:102:LEU:O	3:H:102:LEU:HD23	2.20	0.41
4:I:194:LEU:HD12	4:I:194:LEU:HA	1.87	0.41
4:I:789:THR:HA	4:I:793:GLU:O	2.19	0.41
4:I:870:ILE:HG12	4:I:1050:VAL:HG11	2.03	0.41
8:P:66:DT:H2 ⁷	8:P:67:DT:H72	2.02	0.41
1:J:133:ARG:HD2	1:J:133:ARG:HA	1.71	0.41
1:J:465:GLN:HE22	4:I:1242:LYS:HD2	1.84	0.41
1:J:515:ARG:O	1:J:573:THR:HG21	2.21	0.41
1:J:1163:VAL:HG12	1:J:1202:GLU:N	2.35	0.41
1:J:1191:PRO:HB2	1:J:1194:ARG:NH1	2.28	0.41
3:H:127:GLN:O	3:H:127:GLN:HG2	2.20	0.41
4:I:183:TRP:CZ3	4:I:200:ARG:HD3	2.56	0.41
4:I:669:PRO:O	4:I:1070:HIS:HE1	2.03	0.41
4:I:1084:ASP:OD1	4:I:1216:ARG:HG2	2.20	0.41
4:I:1268:GLN:NE2	4:I:1268:GLN:HA	2.35	0.41
6:L:143:TYR:CB	6:L:269:LEU:HD21	2.50	0.41
6:L:320:ILE:HA	6:L:327:SER:O	2.20	0.41
6:L:499:LYS:HE2	6:L:499:LYS:HB3	1.81	0.41
1:J:346:ARG:HA	4:I:1268:GLN:O	2.21	0.41
1:J:810:THR:CG2	1:J:893:GLY:HA3	2.50	0.41
3:H:183:ILE:HD12	3:H:183:ILE:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:31:GLN:HE21	4:I:31:GLN:HB3	1.66	0.41
4:I:618:GLN:HB2	4:I:635:THR:O	2.20	0.41
4:I:724:VAL:HG22	4:I:734:ILE:CD1	2.51	0.41
4:I:865:LEU:HD21	4:I:882:ILE:O	2.20	0.41
6:L:73:ASP:CB	6:L:74:GLU:HB2	2.51	0.41
6:L:316:PHE:O	6:L:319:ALA:HB3	2.21	0.41
1:J:20:ILE:HD13	1:J:1320:ILE:HD11	2.01	0.41
1:J:30:ILE:HG21	1:J:241:VAL:HG12	2.02	0.41
1:J:79:LYS:HB2	6:L:569:THR:HG22	2.02	0.41
1:J:198:CYS:O	1:J:221:ILE:HD13	2.20	0.41
1:J:353:SER:HB2	4:I:1243:MET:HG2	2.03	0.41
1:J:467:ALA:HB1	4:I:1268:GLN:HG3	2.02	0.41
1:J:532:GLU:O	1:J:532:GLU:HG3	2.21	0.41
1:J:644:MET:SD	4:I:1109:ILE:HG12	2.61	0.41
1:J:840:LEU:HD13	1:J:869:CYS:SG	2.61	0.41
1:J:966:VAL:HG23	1:J:974:VAL:CG2	2.46	0.41
1:J:1040:MET:HG3	1:J:1077:ALA:H	1.85	0.41
3:G:101:THR:O	3:G:115:ILE:HG23	2.20	0.41
4:I:145:ILE:O	4:I:145:ILE:HG22	2.20	0.41
4:I:170:VAL:C	4:I:171:LEU:HD23	2.41	0.41
4:I:174:ALA:HB3	4:I:432:LEU:HD22	2.02	0.41
4:I:518:ASN:OD1	4:I:518:ASN:N	2.52	0.41
4:I:551:HIS:CE1	4:I:553:THR:HG23	2.55	0.41
4:I:578:TYR:HH	4:I:656:SER:HG	1.66	0.41
5:K:3:ARG:HH12	5:K:6:VAL:HG12	1.84	0.41
6:L:20:GLY:O	6:L:53:ILE:HG21	2.20	0.41
6:L:286:LEU:O	6:L:290:LEU:HD22	2.20	0.41
6:L:506:SER:O	6:L:509:THR:HG22	2.20	0.41
7:O:45:DA:H2'	7:O:46:DG:O5'	2.20	0.41
8:P:38:DC:H1'	8:P:39:DC:O5'	2.21	0.41
1:J:21:LYS:O	4:I:1337:ILE:HA	2.21	0.41
3:H:61:ILE:HD13	3:H:142:MET:HB3	2.02	0.41
3:H:85:LEU:HD23	3:H:85:LEU:HA	1.83	0.41
4:I:95:PRO:HB3	4:I:123:TYR:HE2	1.85	0.41
4:I:538:LEU:HD11	4:I:547:VAL:HG21	2.03	0.41
4:I:891:GLY:HA2	4:I:892:GLU:HA	1.58	0.41
4:I:1122:LYS:HD2	4:I:1178:LYS:O	2.21	0.41
6:L:99:ARG:HB3	6:L:99:ARG:HH11	1.86	0.41
6:L:314:THR:C	6:L:318:ALA:HB3	2.40	0.41
3:M:260:LEU:HD23	3:M:310:ARG:HH12	1.85	0.41
3:M:300:LEU:HD13	3:M:303:ILE:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:57:PHE:HB3	1:J:98:ARG:HH22	1.86	0.41
1:J:811:GLU:O	1:J:895:CYS:HA	2.21	0.41
1:J:996:LYS:HZ3	1:J:998:PRO:HG3	1.86	0.41
1:J:1189:MET:N	1:J:1189:MET:SD	2.94	0.41
3:G:8:PHE:CZ	3:H:150:ARG:HD3	2.56	0.41
3:G:14:VAL:CG2	3:G:29:GLU:HB2	2.44	0.41
4:I:12:ARG:HH22	4:I:698:PRO:HD2	1.86	0.41
4:I:27:LEU:HD23	4:I:27:LEU:HA	1.78	0.41
4:I:141:THR:HB	4:I:514:PHE:CE1	2.55	0.41
4:I:211:ARG:HA	4:I:215:TYR:O	2.21	0.41
4:I:391:SER:OG	4:I:394:ARG:N	2.38	0.41
4:I:466:VAL:O	4:I:470:ARG:HG2	2.21	0.41
4:I:578:TYR:HD2	4:I:659:GLN:HB2	1.86	0.41
4:I:636:CYS:HB2	4:I:645:PHE:CD2	2.56	0.41
5:K:22:VAL:CG1	5:K:54:ILE:HD11	2.51	0.41
6:L:277:MET:SD	6:L:359:LYS:HG2	2.61	0.41
6:L:298:PRO:HB2	6:L:301:ASN:HB2	2.03	0.41
6:L:303:ILE:O	6:L:307:THR:HB	2.20	0.41
6:L:340:ALA:HA	6:L:343:LYS:HE2	2.03	0.41
6:L:355:ILE:CG2	6:L:359:LYS:HD2	2.48	0.41
6:L:384:LEU:O	6:L:388:ILE:HG13	2.20	0.41
6:L:511:ILE:HD12	6:L:512:GLY:N	2.36	0.41
6:L:517:SER:HB2	6:L:521:ASP:OD2	2.20	0.41
6:L:558:VAL:O	6:L:562:ARG:HB2	2.21	0.41
6:L:571:TYR:CD1	6:L:575:GLU:HG2	2.55	0.41
1:J:120:LEU:HA	1:J:120:LEU:HD22	1.79	0.41
1:J:198:CYS:HB2	1:J:221:ILE:CD1	2.50	0.41
1:J:245:LEU:HD12	1:J:246:PRO:CD	2.50	0.41
1:J:338:PHE:HB3	1:J:1324:SER:HA	2.02	0.41
1:J:356:THR:HG22	4:I:1075:VAL:HG11	2.02	0.41
1:J:553:THR:HA	1:J:567:THR:HA	2.02	0.41
1:J:744:ARG:HE	1:J:744:ARG:HB2	1.28	0.41
1:J:865:HIS:HE1	1:J:867:GLN:HB2	1.84	0.41
1:J:950:ILE:HD12	1:J:1018:ALA:CB	2.51	0.41
1:J:951:GLN:HA	1:J:1016:THR:HA	2.02	0.41
1:J:986:ASP:HB3	1:J:992:LYS:CE	2.50	0.41
1:J:1024:THR:HG21	1:J:1123:ARG:HD2	2.02	0.41
1:J:1193:TRP:HB2	1:J:1194:ARG:CZ	2.51	0.41
1:J:1368:ASP:N	1:J:1368:ASP:OD1	2.53	0.41
2:N:67:ARG:HD2	4:I:341:LEU:HD11	2.03	0.41
3:G:179:PRO:O	3:G:207:THR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:224:LEU:O	3:G:228:LEU:HD23	2.21	0.41
3:G:231:PHE:CE2	3:H:28:LEU:HD22	2.56	0.41
4:I:22:LEU:HD22	4:I:603:ILE:HD12	2.02	0.41
4:I:207:THR:OG1	4:I:354:ASP:OD2	2.39	0.41
4:I:533:LEU:HD23	4:I:538:LEU:O	2.21	0.41
4:I:803:ALA:CB	4:I:1227:VAL:HG12	2.51	0.41
4:I:905:ILE:HD11	6:L:598:LEU:CD2	2.40	0.41
4:I:1072:ASN:ND2	4:I:1111:GLN:OE1	2.42	0.41
4:I:1157:GLN:HG3	4:I:1157:GLN:O	2.21	0.41
6:L:405:ILE:HG12	6:L:405:ILE:H	1.63	0.41
6:L:462:LYS:HB3	6:L:487:MET:CE	2.49	0.41
8:P:47:DC:H1'	8:P:48:DC:C5	2.55	0.41
1:J:275:ARG:HD3	1:J:298:MET:HB3	2.02	0.41
1:J:835:LEU:HG	1:J:839:VAL:HG21	2.03	0.41
1:J:982:LEU:HD23	1:J:1017:VAL:HG21	2.02	0.41
4:I:144:VAL:CG2	4:I:515:MET:CB	2.99	0.41
4:I:182:SER:HB2	4:I:389:PHE:CE1	2.52	0.41
4:I:243:PRO:HG2	4:I:278:GLU:HB3	2.03	0.41
4:I:367:TYR:CD2	4:I:384:LEU:HD22	2.56	0.41
4:I:582:ASN:HB2	4:I:586:PHE:O	2.21	0.41
4:I:1081:PRO:HD2	4:I:1084:ASP:HB2	2.03	0.41
6:L:39:ASP:HA	6:L:42:GLU:CG	2.49	0.41
3:M:280:ASP:O	3:M:284:ARG:HG2	2.22	0.41
3:M:282:VAL:O	3:M:316:MET:N	2.54	0.41
1:J:68:TYR:CD1	1:J:81:ARG:HG3	2.56	0.40
1:J:514:THR:HB	1:J:576:ARG:HG3	2.03	0.40
1:J:805:GLN:NE2	4:I:1279:GLU:OE1	2.54	0.40
1:J:982:LEU:C	1:J:983:LYS:HD2	2.41	0.40
1:J:1001:ALA:HA	1:J:1020:TRP:CB	2.49	0.40
1:J:1079:LYS:HE2	1:J:1098:GLN:OE1	2.20	0.40
1:J:1373:ARG:HG2	1:J:1374:ALA:N	2.35	0.40
3:G:53:GLY:O	3:G:148:ARG:HA	2.21	0.40
3:H:91:ARG:HG2	3:H:122:GLU:O	2.21	0.40
3:H:96:ASP:OD2	3:H:148:ARG:HB3	2.21	0.40
4:I:27:LEU:HD22	4:I:663:VAL:HG11	2.03	0.40
4:I:28:LEU:HD21	4:I:527:LYS:HD3	2.02	0.40
4:I:100:LEU:CD1	4:I:122:VAL:HG11	2.51	0.40
4:I:402:ARG:HG2	4:I:416:GLY:N	2.36	0.40
4:I:494:ASN:HD21	4:I:496:LYS:HB3	1.86	0.40
4:I:538:LEU:HD13	4:I:543:ALA:CB	2.29	0.40
4:I:541:GLU:HG2	4:I:542:ARG:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:746:ALA:HB2	4:I:974:ARG:CD	2.37	0.40
4:I:800:MET:CE	4:I:822:VAL:HG22	2.51	0.40
6:L:53:ILE:N	6:L:53:ILE:HD12	2.36	0.40
6:L:315:TRP:CZ3	6:L:316:PHE:HB2	2.56	0.40
1:J:194:LEU:CB	1:J:228:VAL:HG22	2.52	0.40
1:J:259:ARG:HE	6:L:505:ILE:HD11	1.86	0.40
1:J:264:ASP:CB	1:J:324:LEU:HB2	2.49	0.40
1:J:337:ARG:HD3	1:J:341:ASN:HD21	1.86	0.40
1:J:374:LEU:HD11	1:J:401:VAL:HG13	2.03	0.40
1:J:520:ALA:HB1	1:J:543:SER:HB3	2.03	0.40
3:G:176:CYS:O	3:G:178:SER:N	2.55	0.40
3:H:137:ASN:OD1	3:H:137:ASN:N	2.54	0.40
4:I:180:ARG:NH2	4:I:394:ARG:O	2.54	0.40
4:I:233:ARG:HD2	4:I:284:LEU:CD2	2.51	0.40
4:I:356:THR:HB	4:I:361:SER:CB	2.51	0.40
4:I:528:ARG:NH2	4:I:575:LEU:HD23	2.35	0.40
4:I:758:ARG:HB3	4:I:833:ILE:HB	2.04	0.40
4:I:1014:LEU:HA	4:I:1014:LEU:HD12	1.77	0.40
6:L:226:ALA:HA	6:L:229:VAL:CG2	2.51	0.40
3:M:265:ARG:HA	3:M:268:ASN:ND2	2.36	0.40
7:O:38:DG:OP2	7:O:38:DG:H2'	2.21	0.40
8:P:40:DC:H2''	8:P:41:DT:O5'	2.21	0.40
1:J:598:LYS:HA	1:J:601:ILE:CG2	2.51	0.40
1:J:680:ASN:HD22	1:J:680:ASN:HA	1.67	0.40
1:J:1142:ALA:O	1:J:1146:GLU:HG2	2.21	0.40
1:J:1221:LEU:CD2	1:J:1226:VAL:HA	2.51	0.40
4:I:217:THR:HG23	4:I:351:LEU:CD1	2.50	0.40
4:I:870:ILE:HG21	4:I:931:VAL:HG11	2.02	0.40
6:L:589:GLN:NE2	7:O:26:DT:H73	2.36	0.40
7:O:52:DA:H2''	7:O:53:DT:OP2	2.22	0.40
1:J:139:LEU:HD23	1:J:139:LEU:HA	1.92	0.40
1:J:461:PHE:CD2	4:I:813:GLU:HB2	2.55	0.40
1:J:519:ASN:HA	1:J:523:GLU:OE1	2.21	0.40
1:J:787:ALA:HB2	4:I:569:ILE:HD11	2.04	0.40
1:J:975:ILE:HG21	1:J:980:THR:HG21	2.04	0.40
1:J:982:LEU:CD2	1:J:1017:VAL:HG21	2.51	0.40
1:J:1027:VAL:HG12	1:J:1122:ALA:O	2.21	0.40
3:G:79:LEU:HD23	3:G:79:LEU:HA	1.59	0.40
4:I:294:GLY:HA2	4:I:316:GLU:OE2	2.22	0.40
4:I:559:CYS:HG	4:I:662:SER:H	1.70	0.40
4:I:884:VAL:HB	4:I:918:LEU:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:989:LEU:O	4:I:989:LEU:HG	2.21	0.40
4:I:1022:LYS:HE3	4:I:1022:LYS:HA	2.02	0.40
11:I:1401:1N7:C19	11:I:1401:1N7:C4	2.92	0.40
6:L:381:GLU:HA	6:L:384:LEU:HD23	2.02	0.40
6:L:448:ARG:HH12	6:L:452:ILE:CD1	2.34	0.40
1:J:44:ILE:CG1	6:L:450:ILE:HG22	2.51	0.40
1:J:423:LEU:HD23	1:J:466:MET:HE2	2.03	0.40
1:J:683:ILE:HD12	2:N:23:ILE:HD13	2.03	0.40
1:J:1218:HIS:CD2	1:J:1218:HIS:H	2.40	0.40
3:G:5:VAL:N	3:G:7:GLU:OE1	2.54	0.40
4:I:142:GLU:HB3	4:I:515:MET:HE2	2.04	0.40
4:I:205:PRO:HG2	4:I:355:PRO:HD2	2.03	0.40
4:I:594:VAL:HG12	4:I:652:TYR:HA	2.03	0.40
4:I:1253:LEU:HB2	6:L:523:ILE:O	2.21	0.40
5:K:59:ILE:HD13	5:K:59:ILE:HA	1.84	0.40
6:L:509:THR:HA	6:L:510:PRO:HD3	1.90	0.40
3:M:260:LEU:HA	3:M:310:ARG:HH22	1.86	0.40
3:M:300:LEU:HD13	3:M:303:ILE:HG21	2.03	0.40
8:P:39:DC:H2'	8:P:39:DC:P	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	J	1339/1430 (94%)	1190 (89%)	146 (11%)	3 (0%)	47	78
2	N	70/72 (97%)	65 (93%)	5 (7%)	0	100	100
3	G	228/329 (69%)	209 (92%)	19 (8%)	0	100	100
3	H	215/329 (65%)	193 (90%)	22 (10%)	0	100	100
3	M	71/329 (22%)	68 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	I	1337/1342 (100%)	1172 (88%)	158 (12%)	7 (0%)	29	61
5	K	73/91 (80%)	70 (96%)	3 (4%)	0	100	100
6	L	543/616 (88%)	501 (92%)	41 (8%)	1 (0%)	47	78
All	All	3876/4538 (85%)	3468 (90%)	397 (10%)	11 (0%)	44	72

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	854	ALA
4	I	200	ARG
4	I	518	ASN
4	I	898	GLU
4	I	199	ASP
4	I	897	PRO
1	J	855	ASP
1	J	46	TYR
4	I	1081	PRO
4	I	697	LYS
6	L	60	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	J	1128/1189 (95%)	1025 (91%)	103 (9%)	9	32
2	N	61/61 (100%)	54 (88%)	7 (12%)	5	20
3	G	193/286 (68%)	170 (88%)	23 (12%)	5	19
3	H	185/286 (65%)	174 (94%)	11 (6%)	19	49
3	M	65/286 (23%)	60 (92%)	5 (8%)	13	40
4	I	1152/1157 (100%)	1037 (90%)	115 (10%)	7	27
5	K	65/75 (87%)	60 (92%)	5 (8%)	13	40
6	L	475/543 (88%)	433 (91%)	42 (9%)	10	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3324/3883 (86%)	3013 (91%)	311 (9%)	12	30

All (311) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	24	LEU
1	J	26	SER
1	J	37	GLU
1	J	46	TYR
1	J	56	LEU
1	J	60	ARG
1	J	67	ASP
1	J	76	LYS
1	J	77	ARG
1	J	93	THR
1	J	95	THR
1	J	109	SER
1	J	120	LEU
1	J	161	THR
1	J	199	GLU
1	J	212	THR
1	J	217	LEU
1	J	227	PHE
1	J	252	LEU
1	J	264	ASP
1	J	284	ASP
1	J	289	ASP
1	J	292	VAL
1	J	306	LEU
1	J	320	ASN
1	J	321	LYS
1	J	324	LEU
1	J	326	SER
1	J	332	LYS
1	J	365	GLN
1	J	374	LEU
1	J	393	THR
1	J	442	ILE
1	J	473	THR
1	J	478	LEU
1	J	489	ASN
1	J	492	SER

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Mol	Chain	Res	Type
1	J	506	VAL
1	J	517	CYS
1	J	543	SER
1	J	545	HIS
1	J	553	THR
1	J	558	ASP
1	J	571	ASP
1	J	572	THR
1	J	638	SER
1	J	674	THR
1	J	678	ARG
1	J	683	ILE
1	J	717	VAL
1	J	722	ILE
1	J	744	ARG
1	J	762	ASN
1	J	770	LEU
1	J	783	LEU
1	J	788	LEU
1	J	796	LEU
1	J	797	THR
1	J	823	THR
1	J	825	VAL
1	J	835	LEU
1	J	869	CYS
1	J	878	ASP
1	J	882	VAL
1	J	891	ASP
1	J	903	LEU
1	J	909	ILE
1	J	918	ILE
1	J	928	THR
1	J	931	THR
1	J	1034	PHE
1	J	1120	THR
1	J	1148	ARG
1	J	1155	ILE
1	J	1164	SER
1	J	1181	ASP
1	J	1188	GLU
1	J	1194	ARG
1	J	1196	LEU

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Mol	Chain	Res	Type
1	J	1198	VAL
1	J	1206	ARG
1	J	1220	ILE
1	J	1223	LEU
1	J	1230	THR
1	J	1236	GLU
1	J	1242	ARG
1	J	1243	LEU
1	J	1258	ARG
1	J	1261	LEU
1	J	1262	ARG
1	J	1266	ILE
1	J	1273	ASP
1	J	1284	ARG
1	J	1304	ARG
1	J	1307	LEU
1	J	1310	THR
1	J	1332	LEU
1	J	1333	THR
1	J	1342	ASP
1	J	1345	ARG
1	J	1355	ARG
1	J	1366	HIS
1	J	1368	ASP
2	N	10	SER
2	N	21	ASN
2	N	22	ARG
2	N	27	ILE
2	N	43	PRO
2	N	48	ARG
2	N	61	CYS
3	G	6	THR
3	G	12	ARG
3	G	13	LEU
3	G	29	GLU
3	G	33	ARG
3	G	70	THR
3	G	71	LYS
3	G	79	LEU
3	G	92	VAL
3	G	125	LYS
3	G	128	HIS

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Mol	Chain	Res	Type
3	G	133	LEU
3	G	158	ARG
3	G	177	TYR
3	G	182	ARG
3	G	191	ARG
3	G	192	VAL
3	G	200	LYS
3	G	211	ILE
3	G	214	GLU
3	G	217	ILE
3	G	226	GLU
3	G	231	PHE
3	H	29	GLU
3	H	38	THR
3	H	79	LEU
3	H	83	LEU
3	H	99	ILE
3	H	117	HIS
3	H	172	LEU
3	H	183	ILE
3	H	193	GLU
3	H	212	ASP
3	H	219	ARG
4	I	3	TYR
4	I	11	ILE
4	I	30	ILE
4	I	33	ASP
4	I	37	LYS
4	I	70	TYR
4	I	91	THR
4	I	104	ILE
4	I	105	TYR
4	I	107	ARG
4	I	133	ASN
4	I	147	SER
4	I	158	ASP
4	I	197	ARG
4	I	220	ILE
4	I	268	ARG
4	I	286	GLU
4	I	289	VAL
4	I	301	TYR

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Mol	Chain	Res	Type
4	I	319	LEU
4	I	391	SER
4	I	397	LEU
4	I	398	SER
4	I	413	GLU
4	I	417	SER
4	I	461	GLU
4	I	470	ARG
4	I	471	VAL
4	I	478	ARG
4	I	484	LEU
4	I	487	LEU
4	I	514	PHE
4	I	515	MET
4	I	518	ASN
4	I	521	LEU
4	I	524	ILE
4	I	528	ARG
4	I	531	SER
4	I	539	THR
4	I	553	THR
4	I	554	HIS
4	I	561	ILE
4	I	563	THR
4	I	573	ASN
4	I	576	SER
4	I	581	THR
4	I	589	THR
4	I	596	ASP
4	I	600	THR
4	I	602	GLU
4	I	604	HIS
4	I	606	LEU
4	I	609	ILE
4	I	633	LEU
4	I	635	THR
4	I	643	SER
4	I	647	ARG
4	I	657	THR
4	I	658	GLN
4	I	663	VAL
4	I	690	VAL

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Mol	Chain	Res	Type
4	I	699	LEU
4	I	750	ILE
4	I	764	CYS
4	I	765	ILE
4	I	770	CYS
4	I	773	LEU
4	I	783	LEU
4	I	799	ASN
4	I	800	MET
4	I	801	ARG
4	I	807	TRP
4	I	813	GLU
4	I	819	SER
4	I	827	ARG
4	I	841	ARG
4	I	878	THR
4	I	895	LEU
4	I	909	LYS
4	I	911	SER
4	I	914	LYS
4	I	919	ARG
4	I	922	ASN
4	I	943	LYS
4	I	944	ARG
4	I	960	LEU
4	I	976	ARG
4	I	992	LEU
4	I	1002	LEU
4	I	1003	THR
4	I	1004	ASP
4	I	1014	LEU
4	I	1041	ASP
4	I	1061	GLN
4	I	1065	LYS
4	I	1073	LYS
4	I	1083	GLU
4	I	1107	MET
4	I	1134	GLN
4	I	1135	GLN
4	I	1149	TYR
4	I	1151	LEU
4	I	1165	SER

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Mol	Chain	Res	Type
4	I	1198	LEU
4	I	1201	LEU
4	I	1220	GLN
4	I	1240	ASP
4	I	1247	SER
4	I	1254	VAL
4	I	1255	THR
4	I	1295	SER
4	I	1296	ASP
4	I	1322	SER
4	I	1327	LEU
4	I	1341	ASP
5	K	13	ILE
5	K	42	GLU
5	K	46	THR
5	K	47	THR
5	K	52	ARG
6	L	15	ARG
6	L	23	THR
6	L	24	TYR
6	L	110	LEU
6	L	118	ASP
6	L	132	CYS
6	L	144	LEU
6	L	148	TYR
6	L	150	ARG
6	L	157	ARG
6	L	162	ILE
6	L	165	PHE
6	L	229	VAL
6	L	231	THR
6	L	255	VAL
6	L	273	MET
6	L	276	MET
6	L	289	LYS
6	L	314	THR
6	L	330	LEU
6	L	357	GLN
6	L	360	ASP
6	L	366	SER
6	L	386	LEU
6	L	389	SER

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Mol	Chain	Res	Type
6	L	395	THR
6	L	402	LEU
6	L	403	ASP
6	L	405	ILE
6	L	442	SER
6	L	454	VAL
6	L	467	SER
6	L	472	GLN
6	L	498	LEU
6	L	517	SER
6	L	519	LEU
6	L	530	LEU
6	L	585	GLU
6	L	587	ILE
6	L	593	LYS
6	L	603	ARG
6	L	604	SER
3	M	252	ILE
3	M	262	LEU
3	M	285	THR
3	M	297	LYS
3	M	300	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	80	HIS
1	J	266	ASN
1	J	450	HIS
1	J	545	HIS
1	J	777	HIS
1	J	792	ASN
1	J	962	ASN
1	J	1010	GLN
1	J	1126	GLN
1	J	1218	HIS
1	J	1227	HIS
1	J	1244	GLN
1	J	1249	ASN
3	G	18	GLN
3	G	23	HIS
3	G	128	HIS

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Mol	Chain	Res	Type
3	G	132	HIS
3	H	84	ASN
4	I	31	GLN
4	I	150	HIS
4	I	357	ASN
4	I	437	ASN
4	I	463	GLN
4	I	618	GLN
4	I	688	GLN
4	I	811	ASN
4	I	834	GLN
4	I	1116	HIS
4	I	1134	GLN
4	I	1136	GLN
4	I	1209	GLN
4	I	1237	HIS
4	I	1264	GLN
4	I	1314	GLN
5	K	29	GLN
5	K	61	ASN
6	L	28	ASN
6	L	227	GLN
6	L	323	ASN
6	L	338	HIS
6	L	362	ASN
6	L	406	GLN
6	L	409	ASN
6	L	446	GLN
6	L	461	ASN
6	L	518	HIS
3	M	268	ASN
3	M	283	GLN
3	M	320	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	1N7	J	1505	-	30,30,46	4.95	17 (56%)	47,48,72	2.31	16 (34%)
11	1N7	I	1401	-	30,30,46	4.82	13 (43%)	47,48,72	2.31	19 (40%)
11	1N7	J	1506	-	30,30,46	4.87	14 (46%)	47,48,72	2.16	15 (31%)
11	1N7	J	1504	-	30,30,46	4.92	15 (50%)	47,48,72	2.37	20 (42%)

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
11	1N7	J	1505	-	-	1/7/72/92	0/4/4/4
11	1N7	I	1401	-	-	0/7/72/92	0/4/4/4
11	1N7	J	1506	-	-	0/7/72/92	0/4/4/4
11	1N7	J	1504	-	-	0/7/72/92	0/4/4/4

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	J	1504	1N7	C3-C19	17.72	1.83	1.53
11	J	1506	1N7	C3-C19	17.51	1.82	1.53
11	J	1505	1N7	C3-C19	17.35	1.82	1.53
11	I	1401	1N7	C3-C19	17.22	1.82	1.53
11	J	1504	1N7	C3-C4	11.92	1.73	1.53
11	J	1505	1N7	C3-C4	11.37	1.72	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	1401	1N7	C3-C4	11.27	1.72	1.53
11	J	1506	1N7	C3-C4	11.22	1.72	1.53
11	J	1505	1N7	C5-C4	-9.11	1.40	1.54
11	I	1401	1N7	C5-C4	-9.01	1.40	1.54
11	J	1506	1N7	C5-C4	-8.89	1.40	1.54
11	J	1504	1N7	C5-C4	-8.41	1.41	1.54
11	J	1506	1N7	C2-C19	-7.51	1.42	1.56
11	I	1401	1N7	C2-C19	-7.51	1.42	1.56
11	J	1505	1N7	C2-C19	-7.17	1.42	1.56
11	J	1504	1N7	C2-C19	-7.10	1.43	1.56
11	J	1505	1N7	C8-C7	5.96	1.70	1.54
11	J	1504	1N7	C8-C7	5.72	1.69	1.54
11	J	1506	1N7	C8-C7	5.42	1.68	1.54
11	I	1401	1N7	C8-C7	5.36	1.68	1.54
11	J	1505	1N7	O4-C4	-4.43	1.36	1.43
11	J	1506	1N7	O4-C4	-4.30	1.36	1.43
11	J	1506	1N7	C5-C9	4.26	1.62	1.55
11	J	1504	1N7	C5-C9	4.24	1.62	1.55
11	I	1401	1N7	O4-C4	-4.24	1.36	1.43
11	J	1505	1N7	C5-C9	3.86	1.62	1.55
11	J	1505	1N7	C5-C6	-3.73	1.49	1.55
11	I	1401	1N7	C5-C6	-3.68	1.49	1.55
11	J	1505	1N7	C2-C15	3.64	1.61	1.55
11	I	1401	1N7	C18-C6	-3.59	1.46	1.53
11	J	1504	1N7	O4-C4	-3.59	1.37	1.43
11	I	1401	1N7	C5-C9	3.56	1.61	1.55
11	J	1504	1N7	C14-C15	-3.51	1.48	1.53
11	J	1505	1N7	C18-C6	-3.42	1.47	1.53
11	J	1506	1N7	C5-C6	-3.40	1.49	1.55
11	J	1504	1N7	C18-C6	-3.33	1.47	1.53
11	J	1505	1N7	C1-C2	3.26	1.60	1.54
11	J	1505	1N7	C7-C6	3.21	1.61	1.54
11	J	1504	1N7	C5-C6	-3.19	1.50	1.55
11	J	1506	1N7	C18-C6	-3.11	1.47	1.53
11	J	1506	1N7	C14-C15	-3.10	1.48	1.53
11	J	1504	1N7	C7-C6	3.09	1.60	1.54
11	I	1401	1N7	C14-C15	-2.98	1.49	1.53
11	J	1505	1N7	C14-C15	-2.97	1.49	1.53
11	J	1506	1N7	C2-C15	2.93	1.60	1.55
11	J	1504	1N7	C2-C15	2.74	1.59	1.55
11	J	1506	1N7	C7-C6	2.57	1.59	1.54
11	I	1401	1N7	C7-C6	2.54	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	1401	1N7	C2-C15	2.51	1.59	1.55
11	J	1505	1N7	C16-C15	2.49	1.57	1.53
11	J	1504	1N7	C10-C5	2.38	1.58	1.54
11	J	1506	1N7	O2-C13	-2.33	1.36	1.43
11	J	1505	1N7	O2-C13	-2.25	1.36	1.43
11	I	1401	1N7	O2-C13	-2.24	1.36	1.43
11	J	1505	1N7	C14-C13	2.15	1.55	1.51
11	J	1504	1N7	C1-C2	2.13	1.58	1.54
11	J	1505	1N7	C10-C5	2.06	1.57	1.54
11	J	1506	1N7	C10-C5	2.06	1.57	1.54
11	J	1504	1N7	O2-C13	-2.01	1.37	1.43

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	1401	1N7	C7-C6-C18	-7.13	108.36	118.33
11	J	1505	1N7	C7-C6-C18	-6.50	109.24	118.33
11	J	1504	1N7	C7-C6-C18	-6.04	109.89	118.33
11	J	1506	1N7	C3-C19-C18	-5.64	102.62	110.88
11	J	1505	1N7	C9-C5-C4	-5.50	112.65	117.67
11	J	1505	1N7	C19-C18-C17	-5.40	105.42	111.88
11	I	1401	1N7	C19-C18-C17	-5.39	105.43	111.88
11	J	1506	1N7	C7-C6-C18	-5.10	111.20	118.33
11	J	1504	1N7	C19-C18-C17	-4.90	106.01	111.88
11	J	1504	1N7	C5-C6-C18	4.82	120.89	114.74
11	J	1506	1N7	C9-C5-C4	-4.61	113.45	117.67
11	I	1401	1N7	C9-C5-C4	-4.56	113.50	117.67
11	J	1506	1N7	C9-C5-C6	4.52	104.66	100.09
11	I	1401	1N7	C21-C20-C22	-4.10	103.93	110.36
11	I	1401	1N7	C5-C6-C18	3.95	119.79	114.74
11	J	1504	1N7	C19-C3-C4	-3.77	109.32	114.30
11	J	1505	1N7	C14-C13-C12	-3.64	106.20	110.55
11	J	1506	1N7	C2-C19-C18	3.60	115.68	111.82
11	J	1505	1N7	C1-C12-C13	-3.52	105.95	110.47
11	J	1504	1N7	C3-C19-C18	-3.51	105.73	110.88
11	J	1504	1N7	C14-C13-C12	-3.42	106.47	110.55
11	J	1504	1N7	C9-C5-C4	-3.42	114.54	117.67
11	J	1505	1N7	C6-C5-C4	3.41	110.58	107.40
11	I	1401	1N7	C1-C12-C13	-3.40	106.11	110.47
11	J	1506	1N7	C21-C20-C22	-3.37	105.08	110.36
11	J	1504	1N7	C1-C12-C13	-3.34	106.19	110.47
11	I	1401	1N7	C6-C5-C4	3.32	110.50	107.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	J	1504	1N7	C21-C20-C22	-3.30	105.19	110.36
11	J	1504	1N7	C9-C5-C6	3.27	103.39	100.09
11	J	1505	1N7	C19-C18-C6	3.25	114.17	109.71
11	J	1504	1N7	C6-C5-C4	3.22	110.40	107.40
11	J	1506	1N7	C16-C15-C2	-3.21	109.25	112.66
11	J	1506	1N7	C5-C6-C18	3.19	118.81	114.74
11	I	1401	1N7	C14-C13-C12	-3.17	106.77	110.55
11	J	1504	1N7	C16-C15-C14	-3.15	107.56	111.19
11	J	1505	1N7	C9-C5-C6	3.14	103.26	100.09
11	J	1505	1N7	C5-C6-C18	3.13	118.74	114.74
11	J	1505	1N7	C8-C9-C20	-3.10	107.34	112.15
11	I	1401	1N7	C8-C9-C20	-3.06	107.41	112.15
11	J	1504	1N7	C8-C9-C20	-3.00	107.50	112.15
11	J	1504	1N7	C11-C2-C15	-2.99	105.29	110.36
11	J	1505	1N7	C11-C2-C15	-2.94	105.37	110.36
11	J	1506	1N7	C14-C13-C12	-2.82	107.18	110.55
11	J	1505	1N7	C21-C20-C22	-2.78	106.01	110.36
11	J	1504	1N7	C16-C17-C18	2.77	114.44	111.48
11	J	1504	1N7	C10-C5-C9	-2.72	106.95	111.21
11	I	1401	1N7	C9-C5-C6	2.71	102.82	100.09
11	J	1505	1N7	C15-C14-C13	-2.71	108.78	112.76
11	I	1401	1N7	C11-C2-C15	-2.69	105.80	110.36
11	I	1401	1N7	C2-C19-C18	2.64	114.66	111.82
11	J	1505	1N7	C16-C15-C14	-2.64	108.15	111.19
11	J	1504	1N7	C2-C19-C18	2.62	114.63	111.82
11	J	1505	1N7	C16-C17-C18	-2.62	108.69	111.48
11	I	1401	1N7	C19-C3-C4	-2.43	111.09	114.30
11	J	1506	1N7	C8-C9-C20	-2.34	108.53	112.15
11	J	1506	1N7	C19-C2-C15	2.33	111.85	108.58
11	J	1506	1N7	C11-C2-C15	-2.25	106.55	110.36
11	I	1401	1N7	C11-C2-C1	-2.24	104.66	108.26
11	J	1504	1N7	C3-C4-C5	-2.18	109.00	111.24
11	J	1505	1N7	C2-C19-C18	2.18	114.16	111.82
11	J	1506	1N7	C16-C15-C14	-2.16	108.70	111.19
11	I	1401	1N7	C16-C15-C2	-2.13	110.39	112.66
11	J	1504	1N7	C8-C7-C6	-2.12	100.93	105.13
11	J	1506	1N7	C10-C5-C9	-2.12	107.90	111.21
11	I	1401	1N7	C11-C2-C19	2.08	114.06	111.18
11	J	1504	1N7	O4-C4-C5	2.08	114.55	111.03
11	I	1401	1N7	C8-C7-C6	-2.06	101.06	105.13
11	J	1506	1N7	C11-C2-C19	2.04	113.99	111.18
11	I	1401	1N7	C1-C2-C19	2.03	114.55	111.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	1401	1N7	C3-C19-C18	-2.01	107.94	110.88

There are no chirality outliers.

All (1) torsion outliers are listed below:

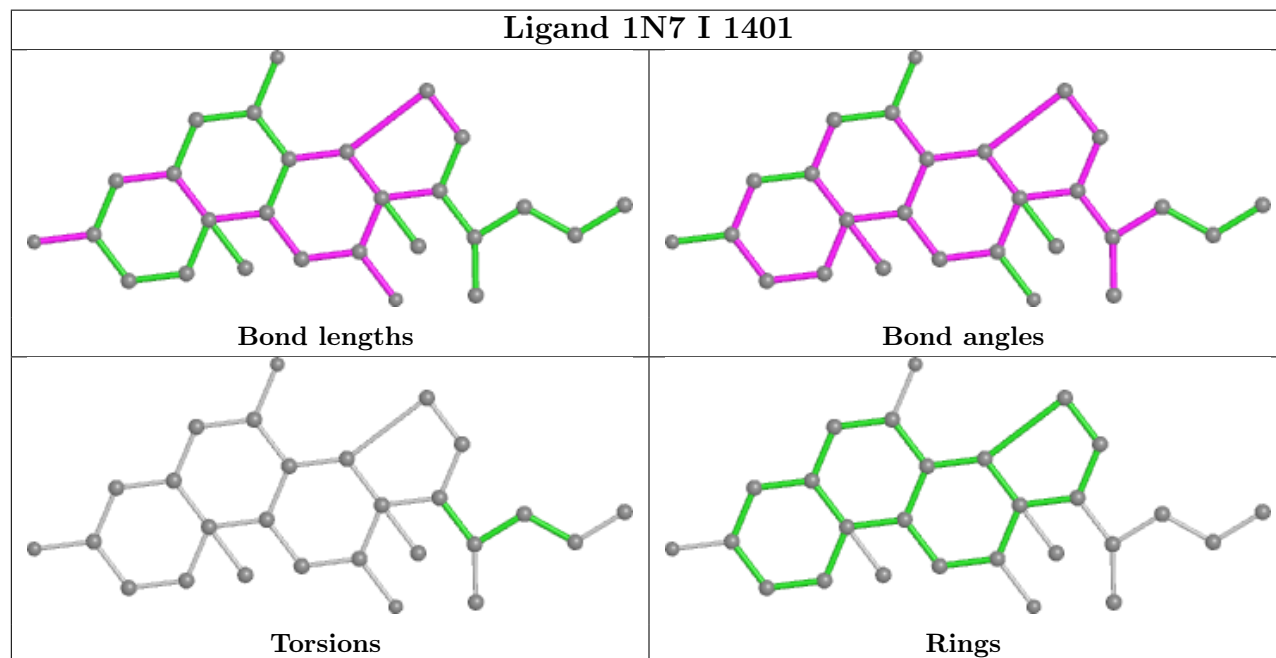
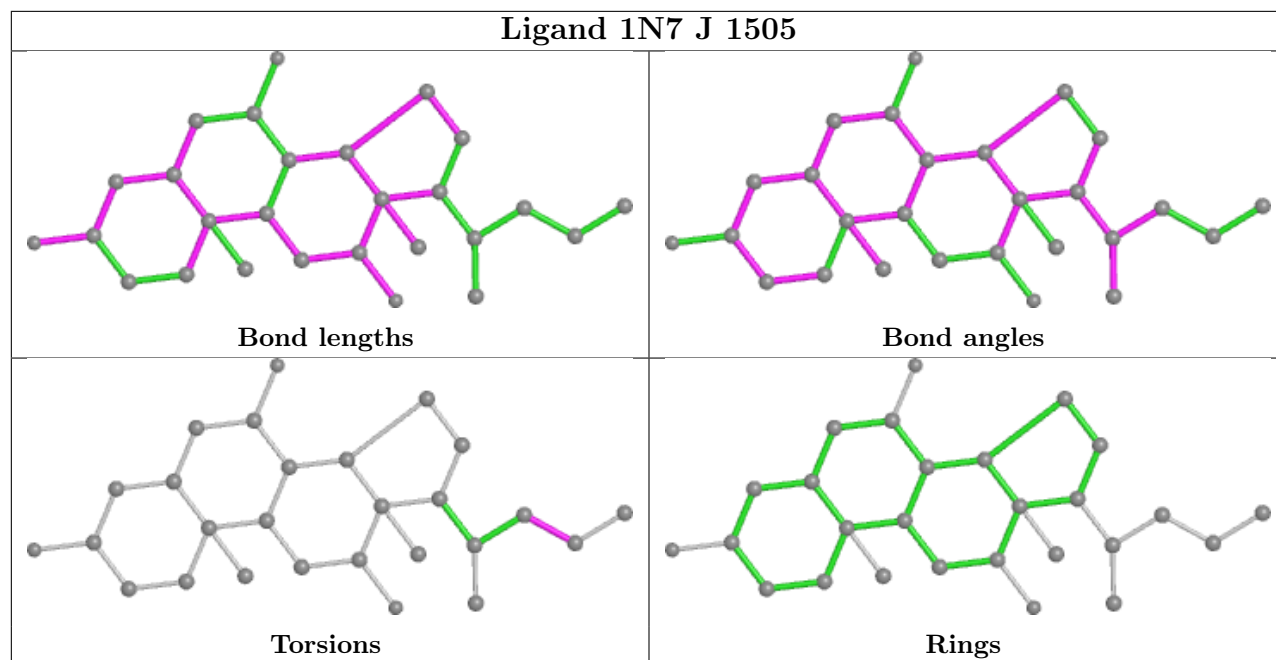
Mol	Chain	Res	Type	Atoms
11	J	1505	1N7	C20-C22-C23-C24

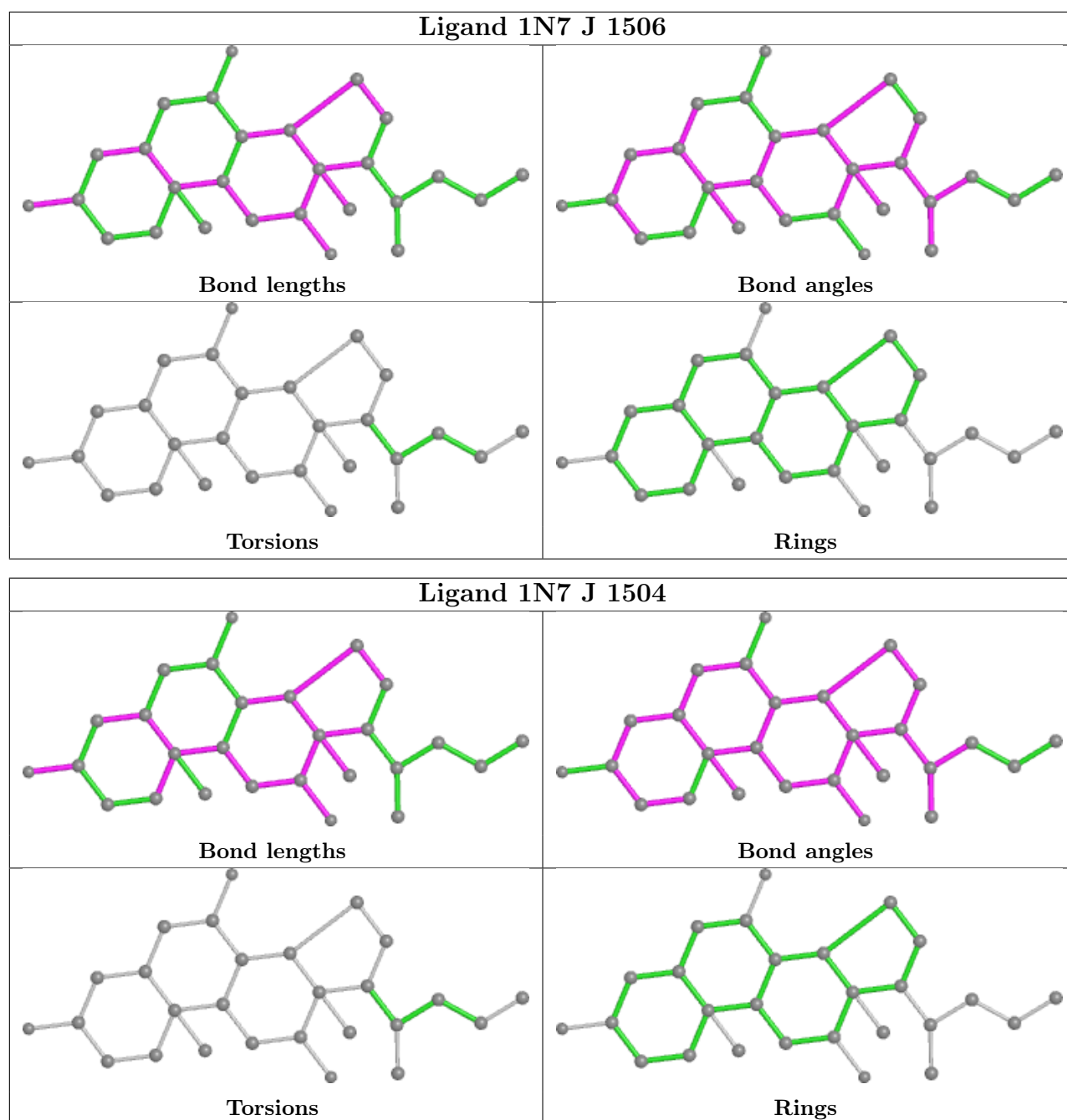
There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	J	1505	1N7	4	0
11	I	1401	1N7	5	0
11	J	1506	1N7	5	0
11	J	1504	1N7	5	0

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





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

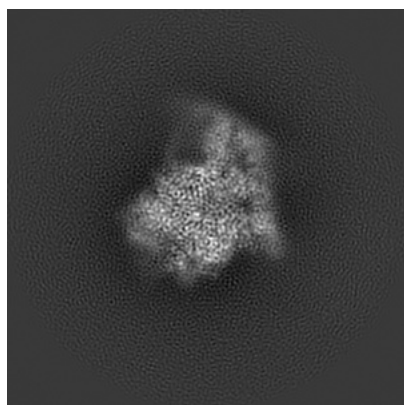
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20460. These allow visual inspection of the internal detail of the map and identification of artifacts.

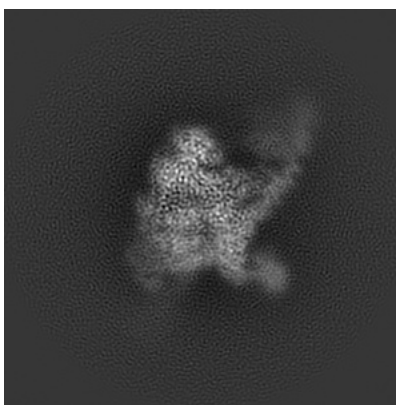
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

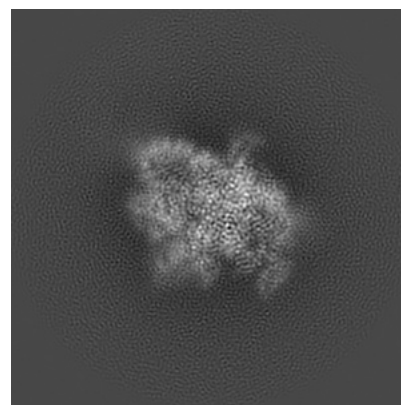
6.1.1 Primary map



X



Y

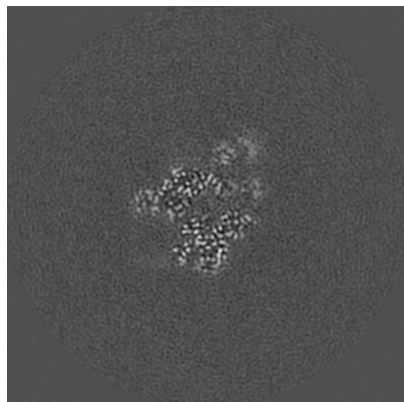


Z

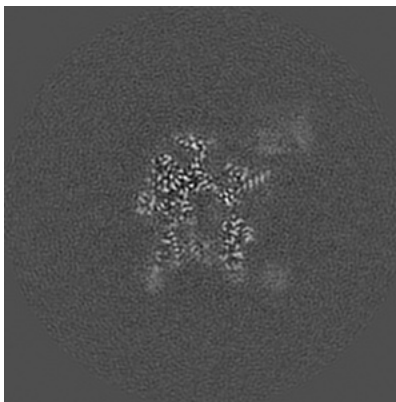
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

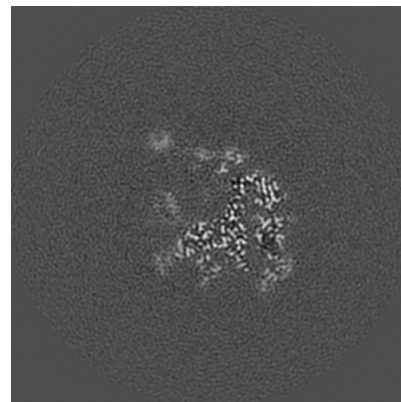
6.2.1 Primary map



X Index: 128



Y Index: 128

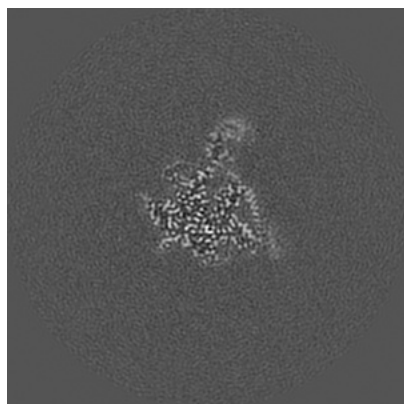


Z Index: 128

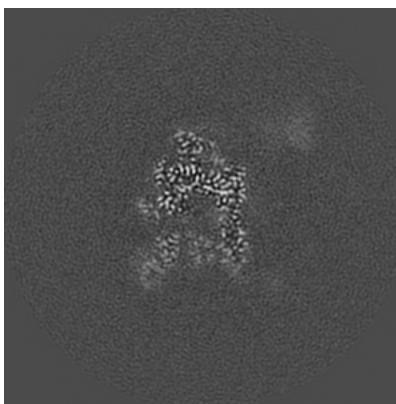
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

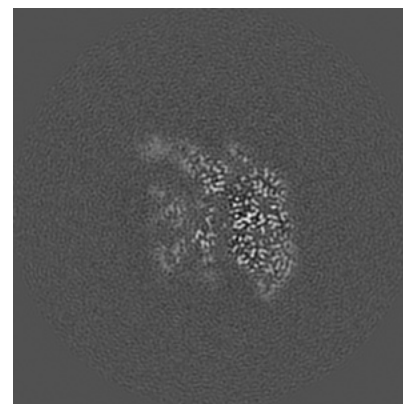
6.3.1 Primary map



X Index: 146



Y Index: 123

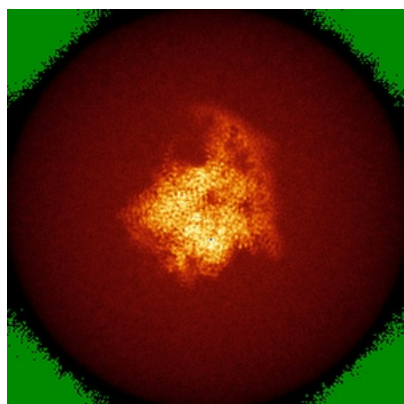


Z Index: 121

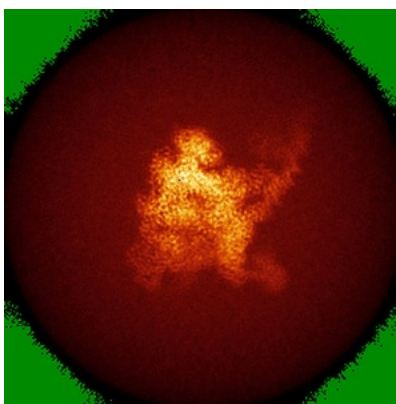
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

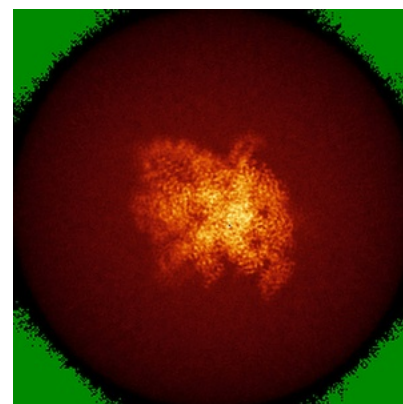
6.4.1 Primary map



X



Y

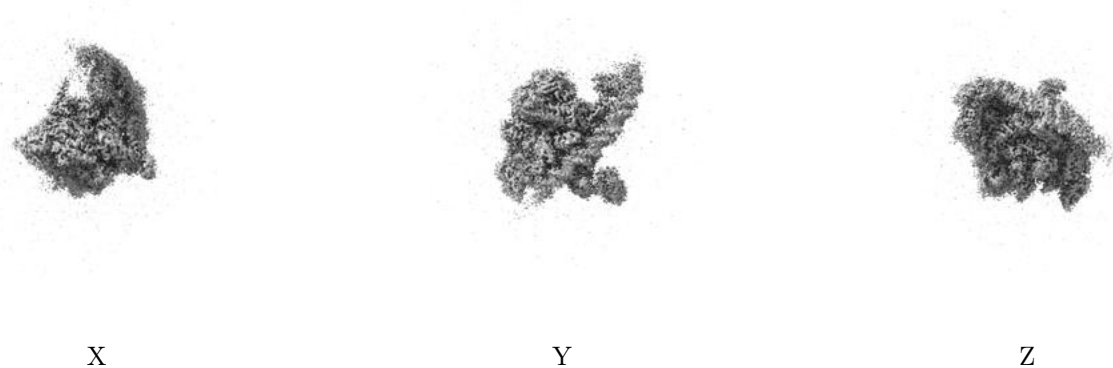


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

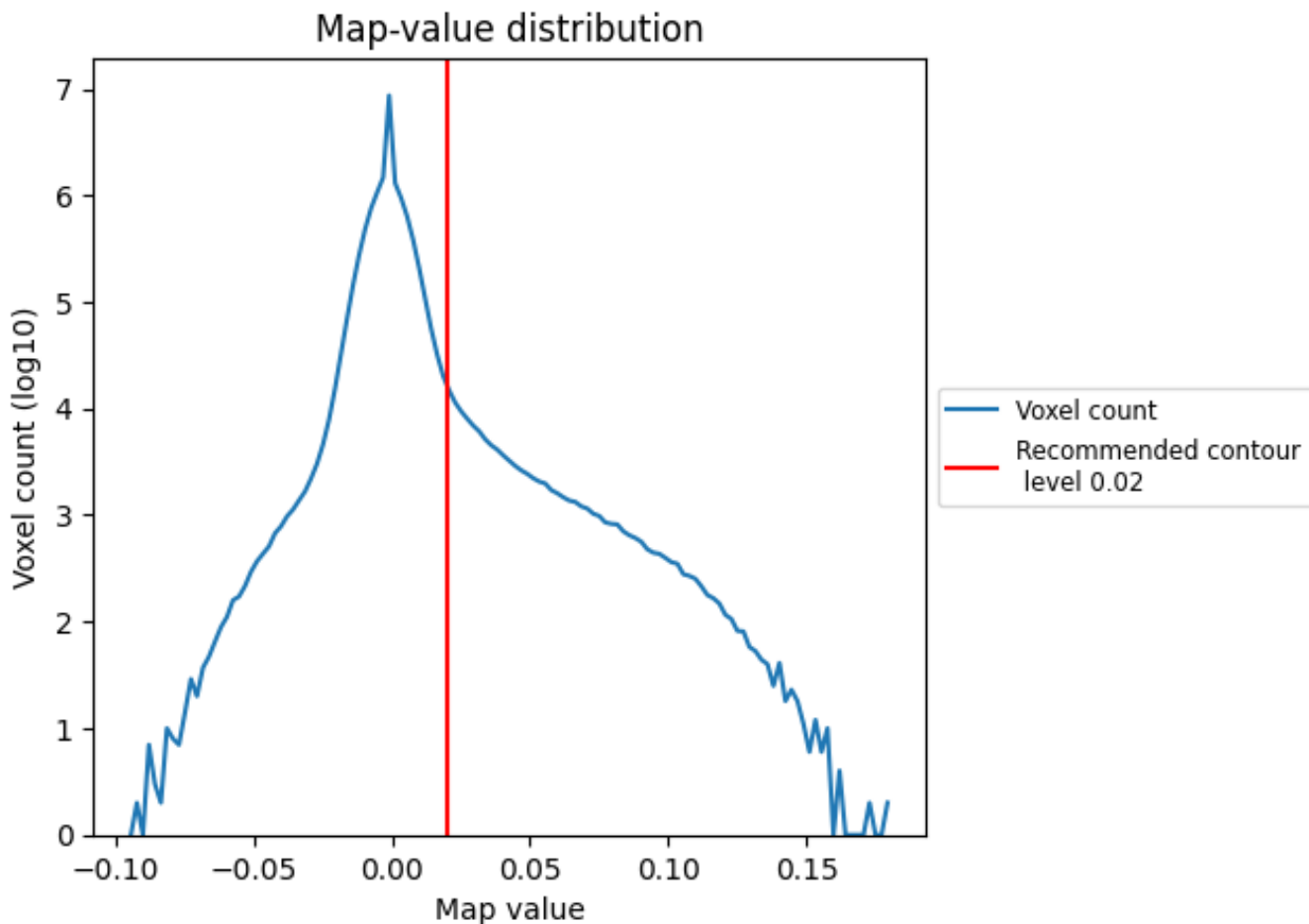
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

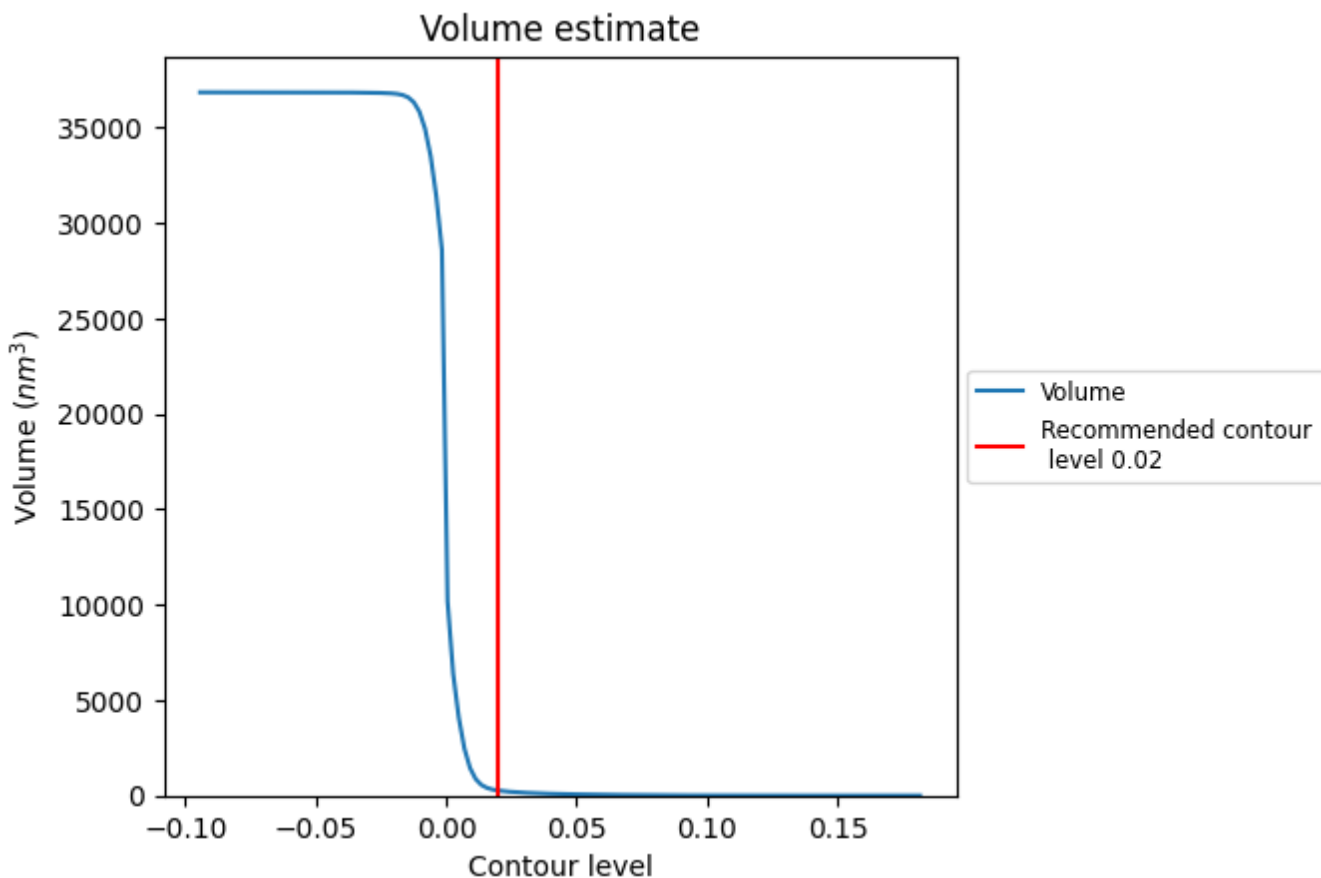
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

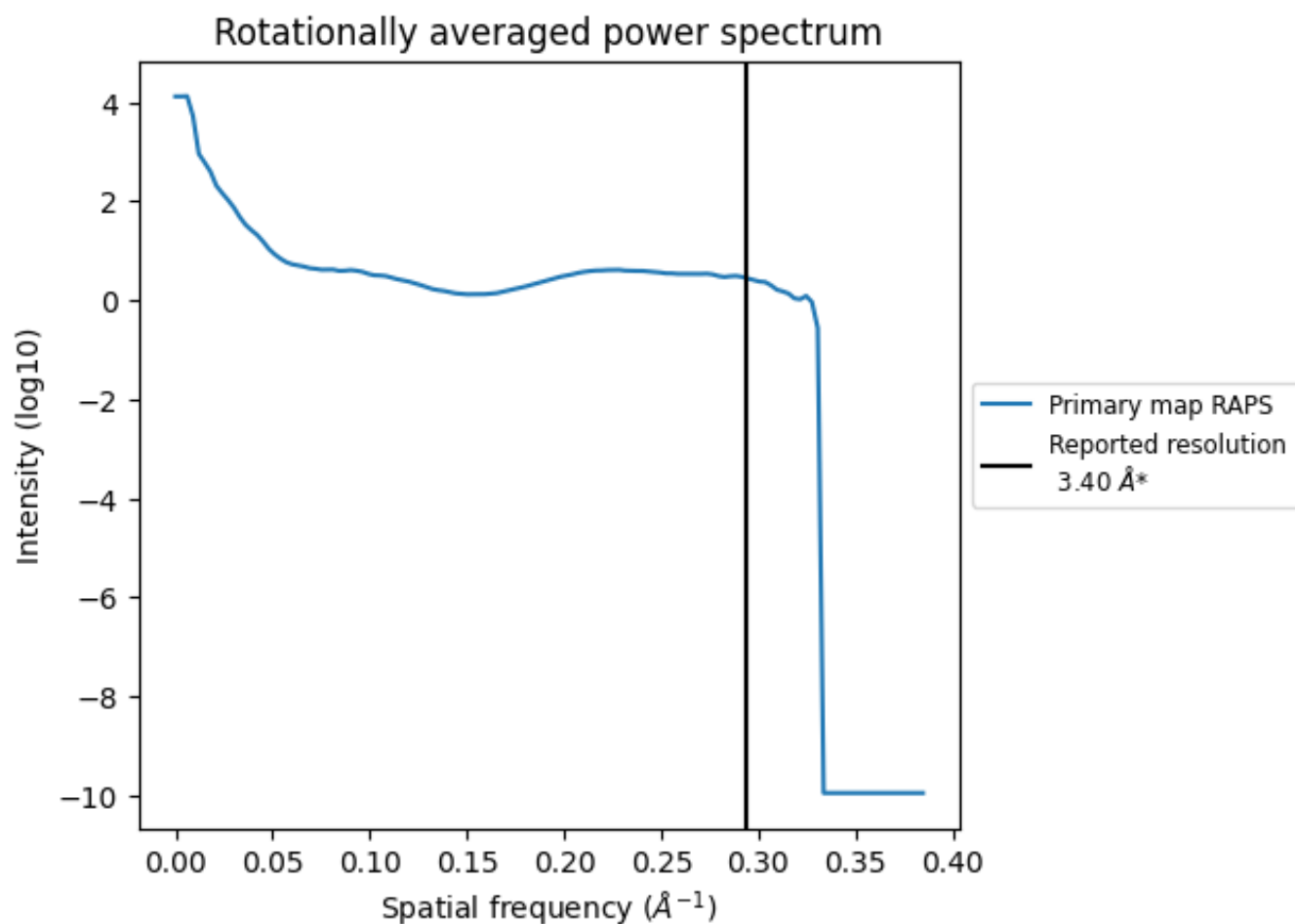
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 264 nm^3 ; this corresponds to an approximate mass of 238 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

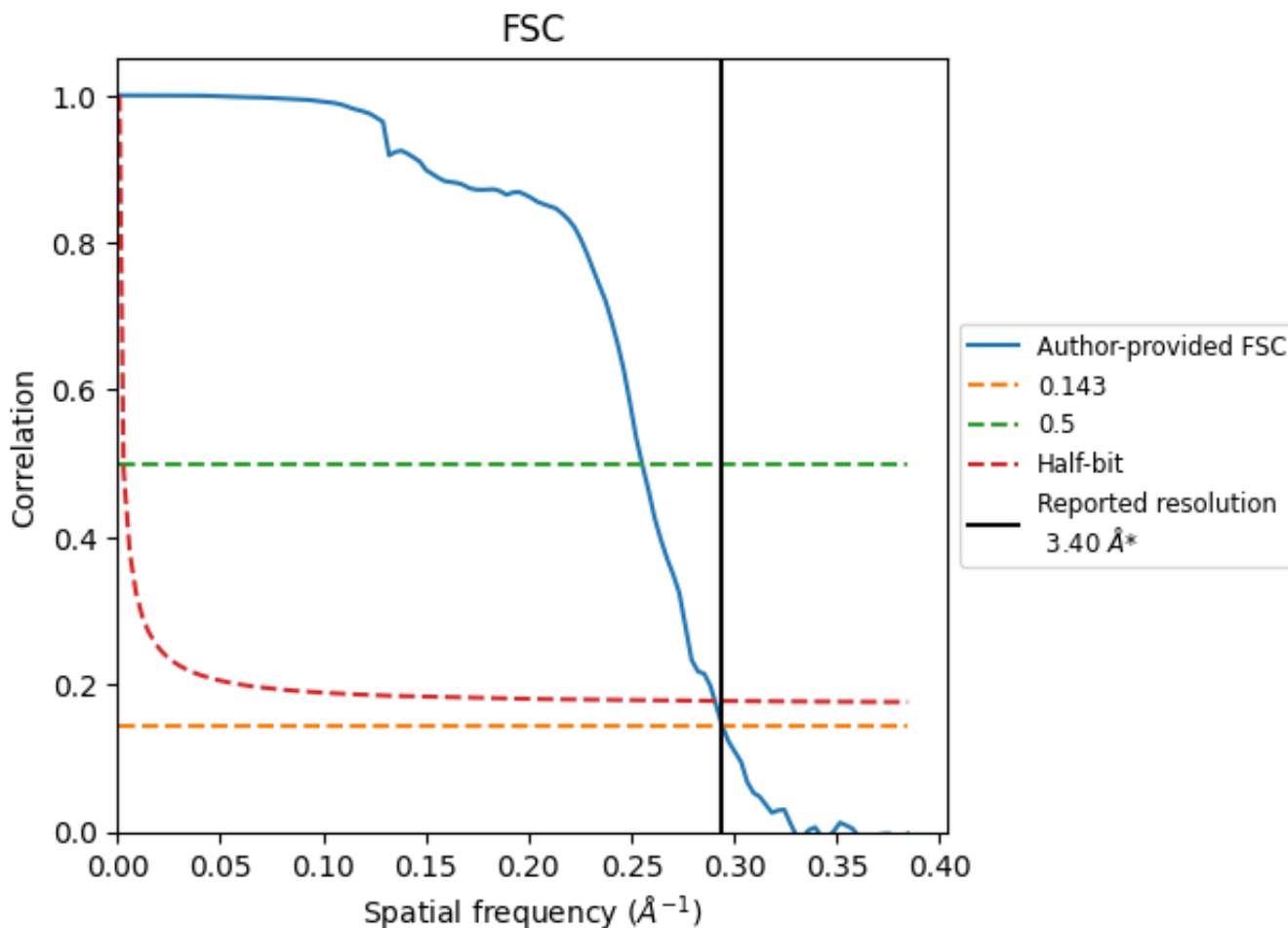


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [\(i\)](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

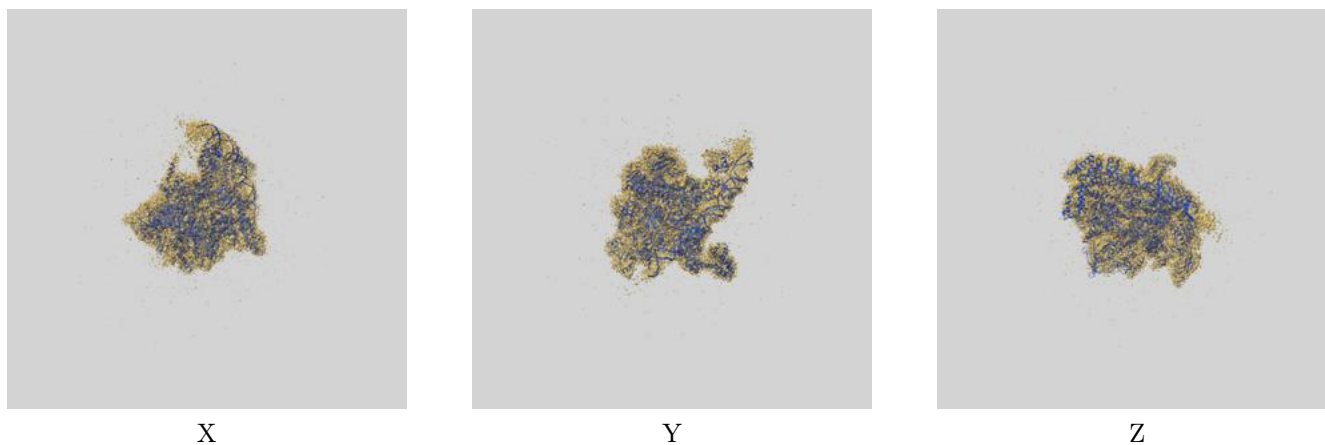
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.92	3.44
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

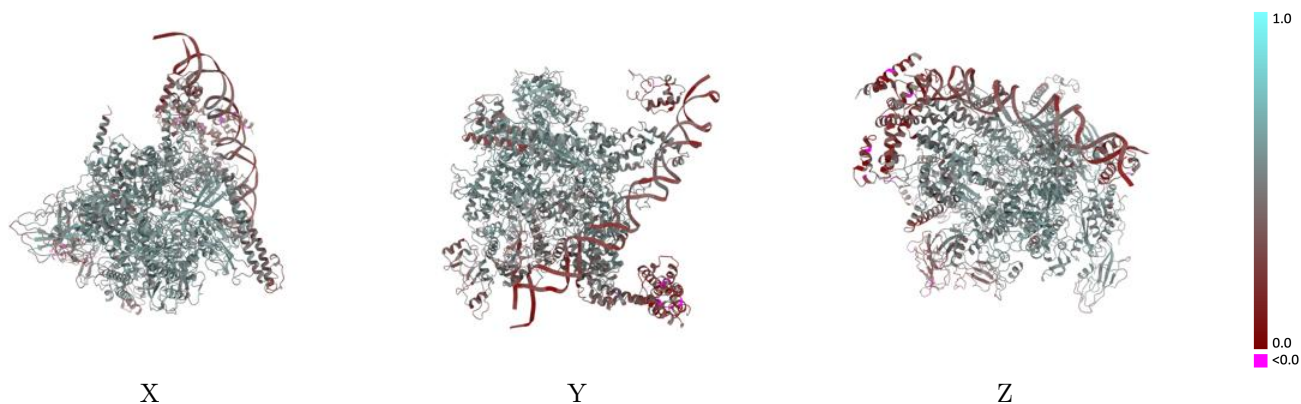
This section contains information regarding the fit between EMDB map EMD-20460 and PDB model 6PSQ. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



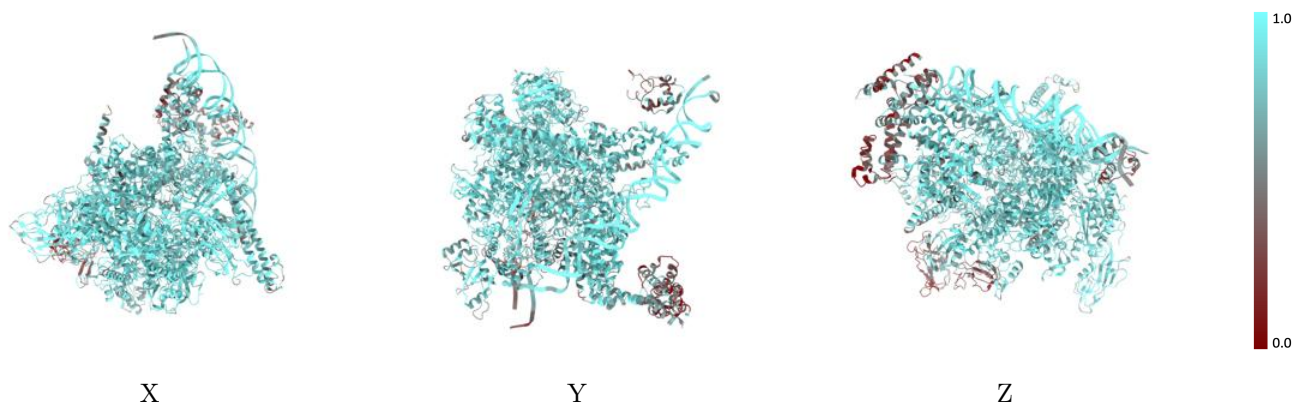
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



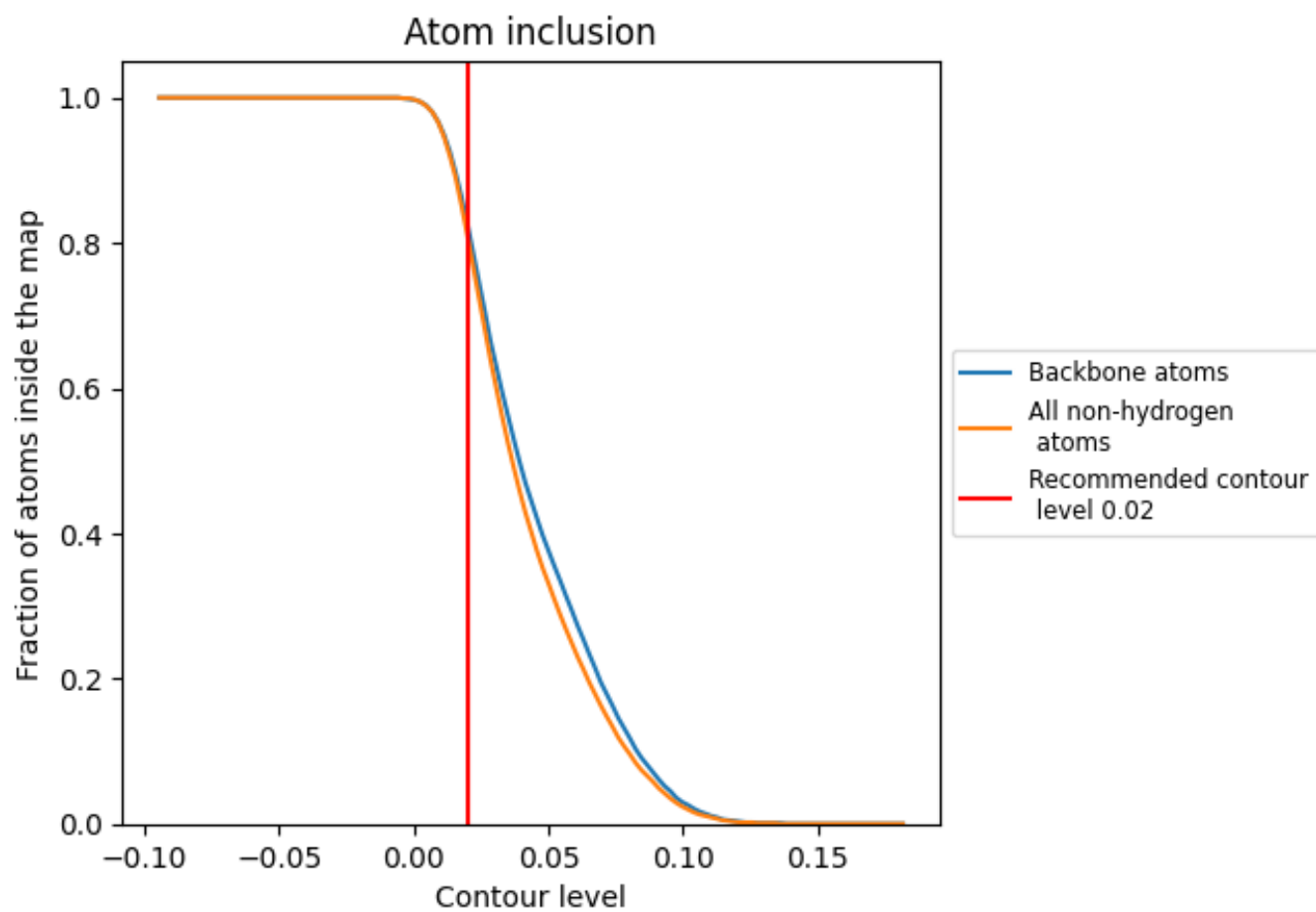
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).























9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8100	 0.4790
G	 0.8920	 0.5500
H	 0.8720	 0.5180
I	 0.8760	 0.5230
J	 0.7990	 0.4970
K	 0.7790	 0.5300
L	 0.6740	 0.3920
M	 0.4660	 0.3170
N	 0.8710	 0.5140
O	 0.8230	 0.2800
P	 0.8250	 0.2730

