Full wwPDB EM Validation Report ⓘ

Mar 10, 2024 – 10:47 PM EDT

PDB ID	:	6PST
EMDB ID	:	EMD-20463
Title	:	Escherichia coli RNA polymerase promoter unwinding intermediate (TRPi1.5b) with TraR and mutant rpsT P2 promoter
Authors	:	Chen, J.; Chiu, C.E.; Campbell, E.A.; Darst, S.A.
Deposited on	:	2019-07-13
Resolution	:	3.00 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:

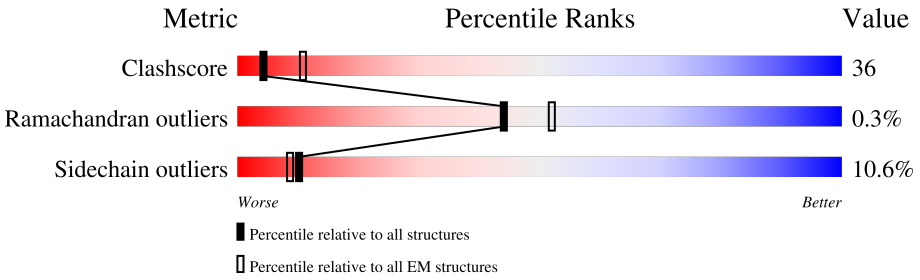
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.00 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 <=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	N	72	7% 56% 39% 6%
2	O	85	13% 9% 49% 41%
3	P	85	13% 13% 47% 40%
4	G	329	5% 33% 30% 7% 29%
4	H	329	29% 33% 5% 34%
4	M	329	22% 5% 17% 78%
5	I	1342	8% 43% 49% 7%
6	J	1430	7% 36% 40% 5% 19%

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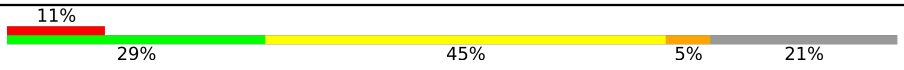
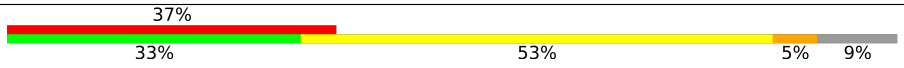
Mol	Chain	Length	Quality of chain
7	K	91	
8	L	616	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 31608 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 Protein TraR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	72	Total	C	N	O	S	0	0
			566	350	103	108	5		

- Molecule 2 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	50	Total	C	N	O	P	0	0
			1026	488	196	292	50		

- Molecule 3 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	51	Total	C	N	O	P	0	0
			1045	499	182	313	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	73	Total	C	N	O	S	0	0
			572	362	100	108	2		
4	G	232	Total	C	N	O	S	0	0
			1769	1106	315	342	6		
4	H	218	Total	C	N	O	S	0	0
			1669	1044	293	326	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	1337	Total	C	N	O	S	0	0
			10512	6598	1831	2040	43		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	1164	Total	C	N	O	S	0	0
			9109	5730	1634	1698	47		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	72	Total	C	N	O	S	0	0
			577	352	110	114	1		

- Molecule 8 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	558	Total	C	N	O	S	0	0
			4495	2804	788	876	27		

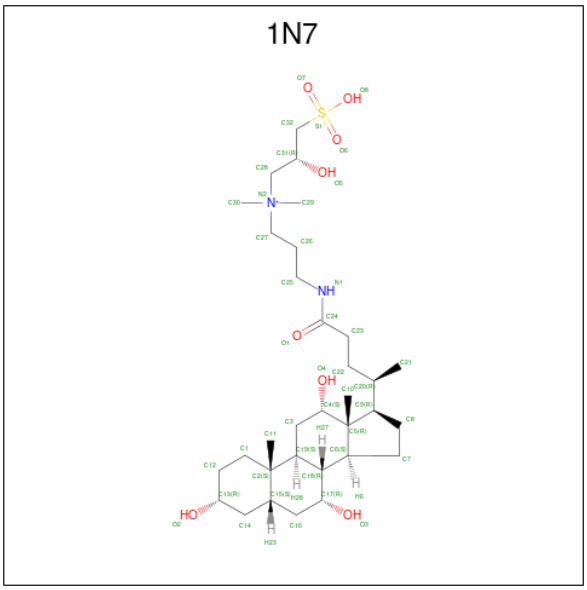
There are 3 discrepancies between the modelled and reference sequences:

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

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

- Molecule 10 is CHAPSO (three-letter code: 1N7) (formula: $C_{32}H_{59}N_2O_8S$).



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

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

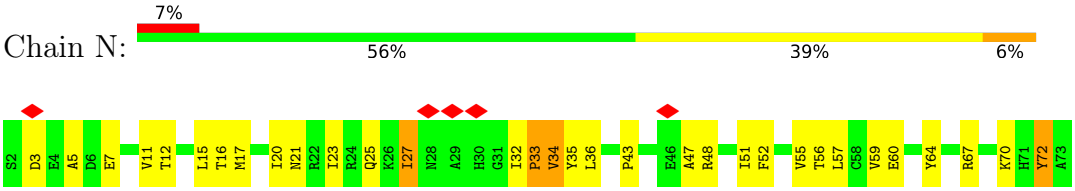
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
11	J	1	1	1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

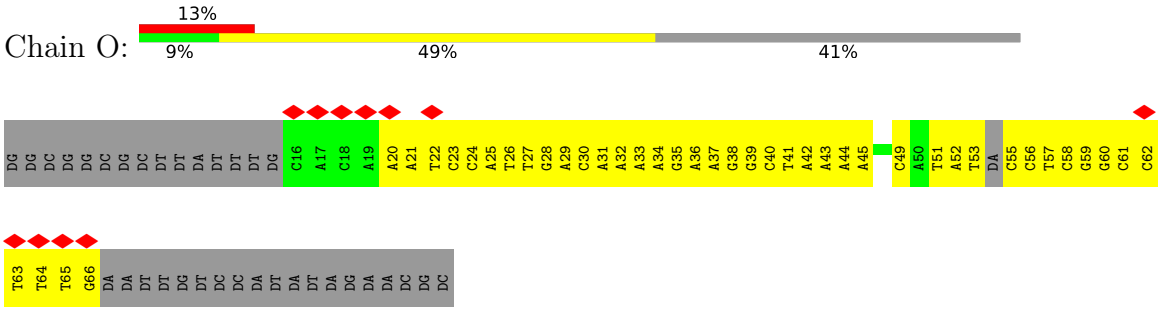
• Molecule 1: Protein TraR

Chain N:



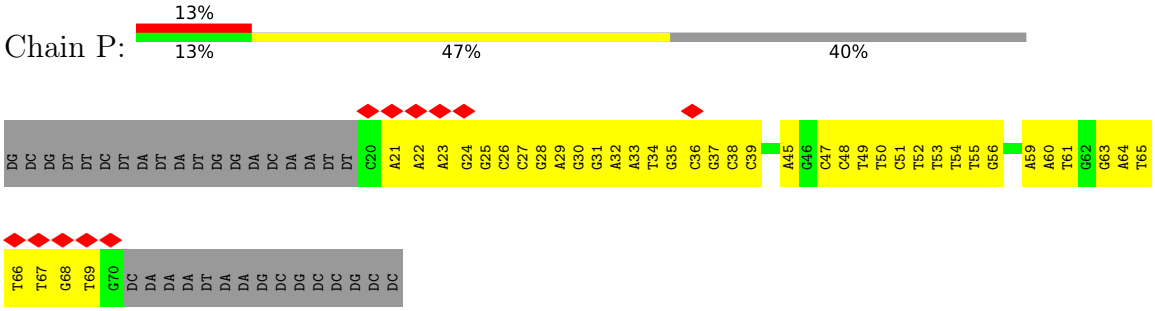
• Molecule 2: DNA (85-MER)

Chain O:



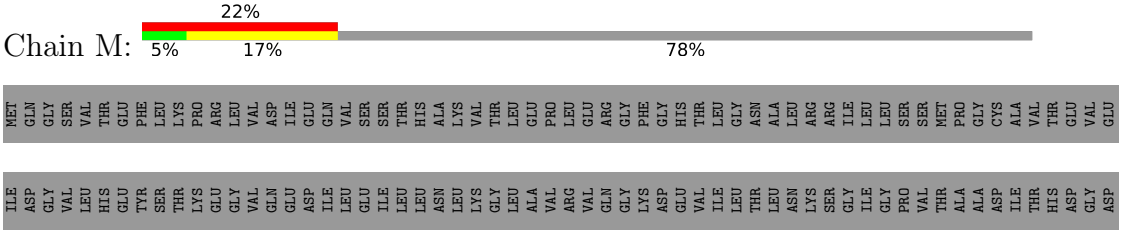
• Molecule 3: DNA (85-MER)

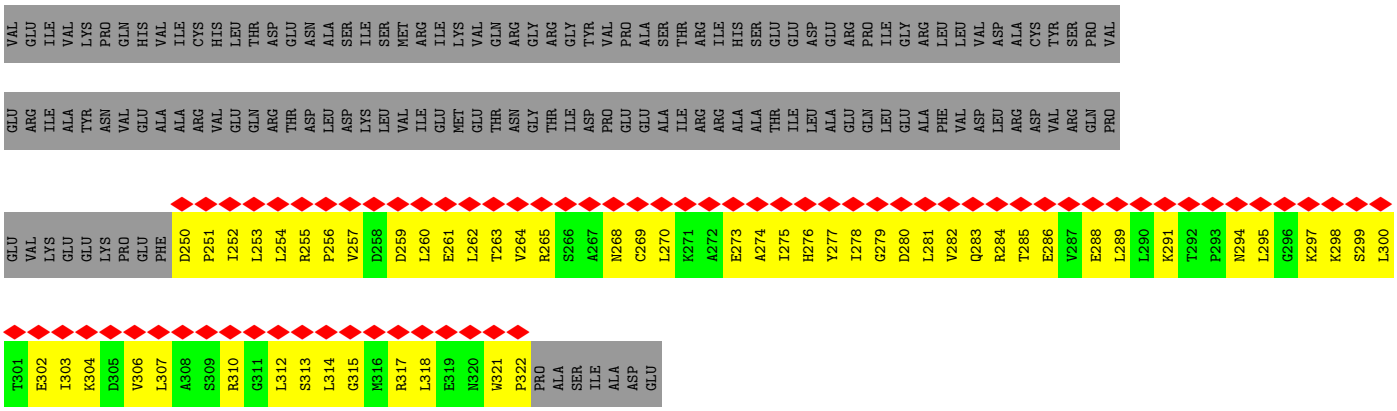
Chain P:



• Molecule 4: DNA-directed RNA polymerase subunit alpha

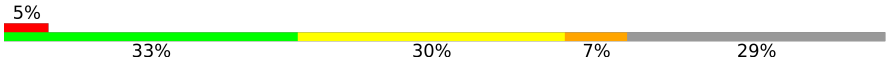
Chain M:

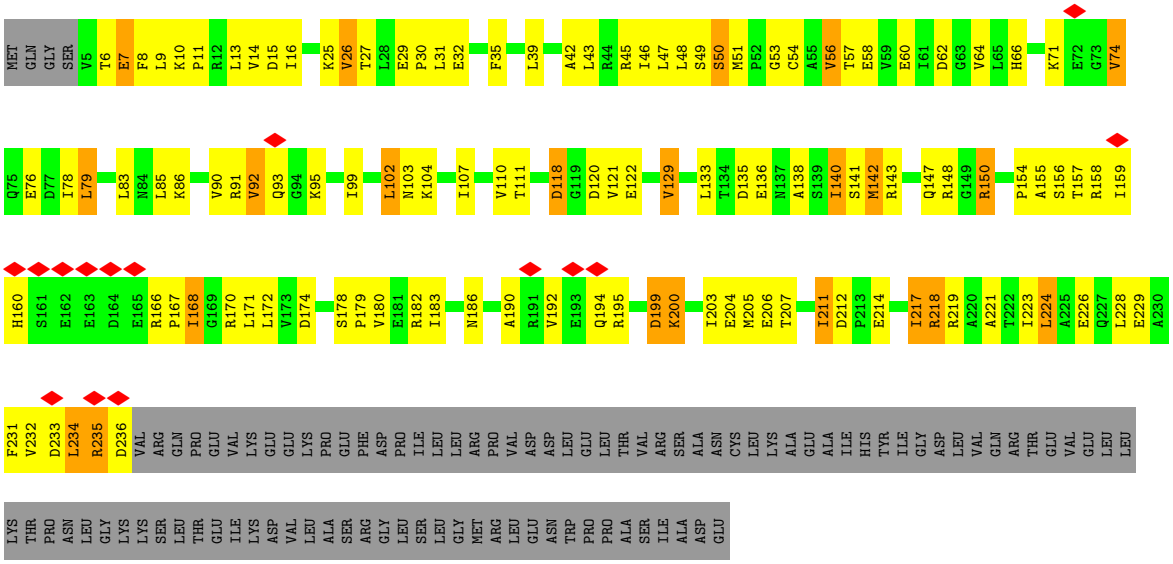




• Molecule 4: DNA-directed RNA polymerase subunit alpha

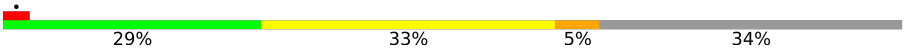
Chain G:

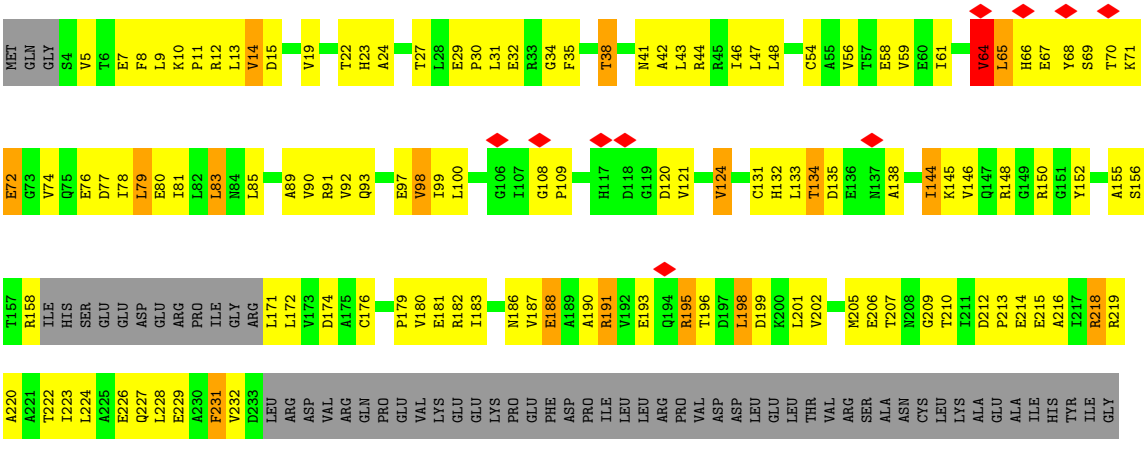




• Molecule 4: DNA-directed RNA polymerase subunit alpha

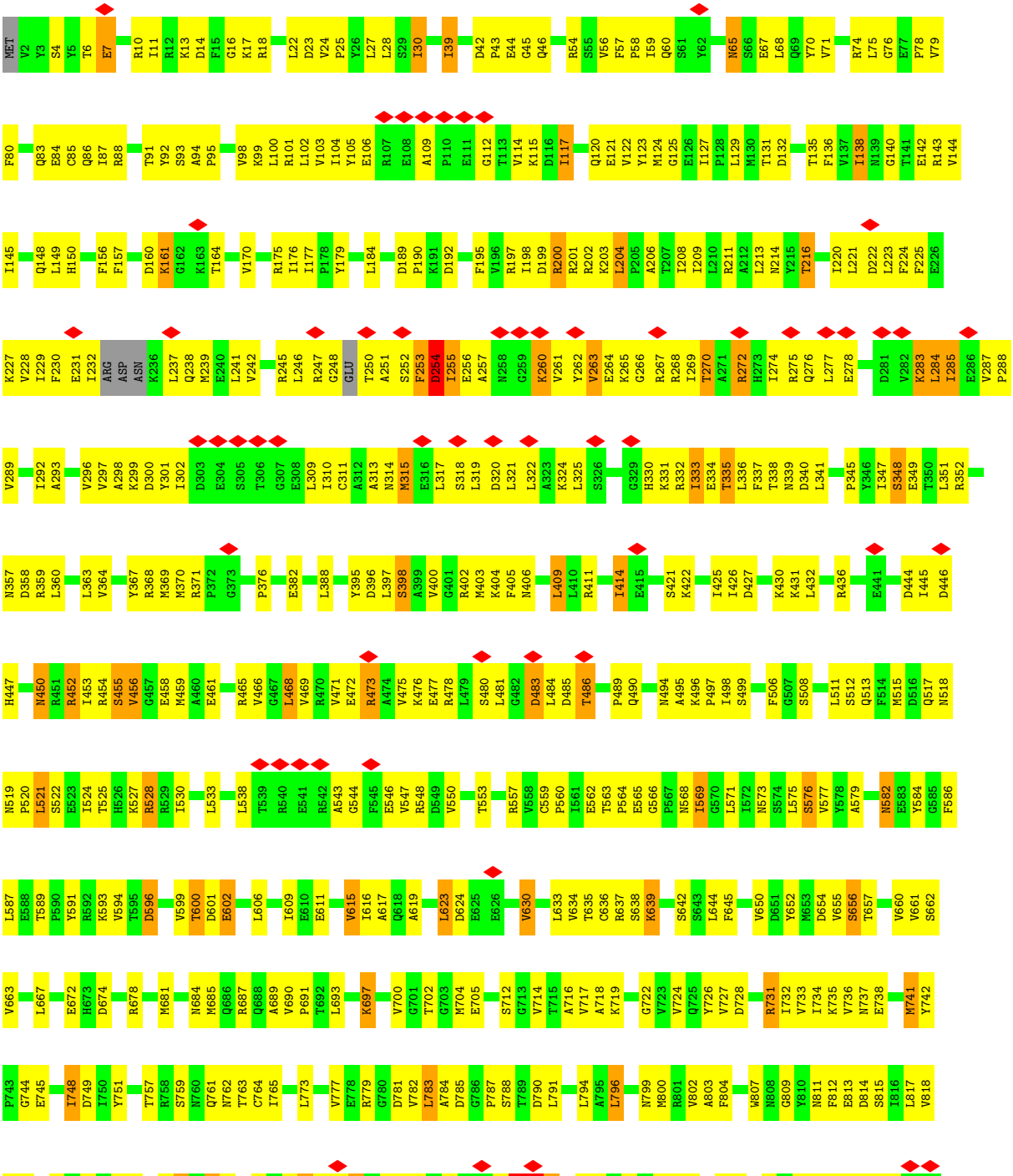
Chain H:

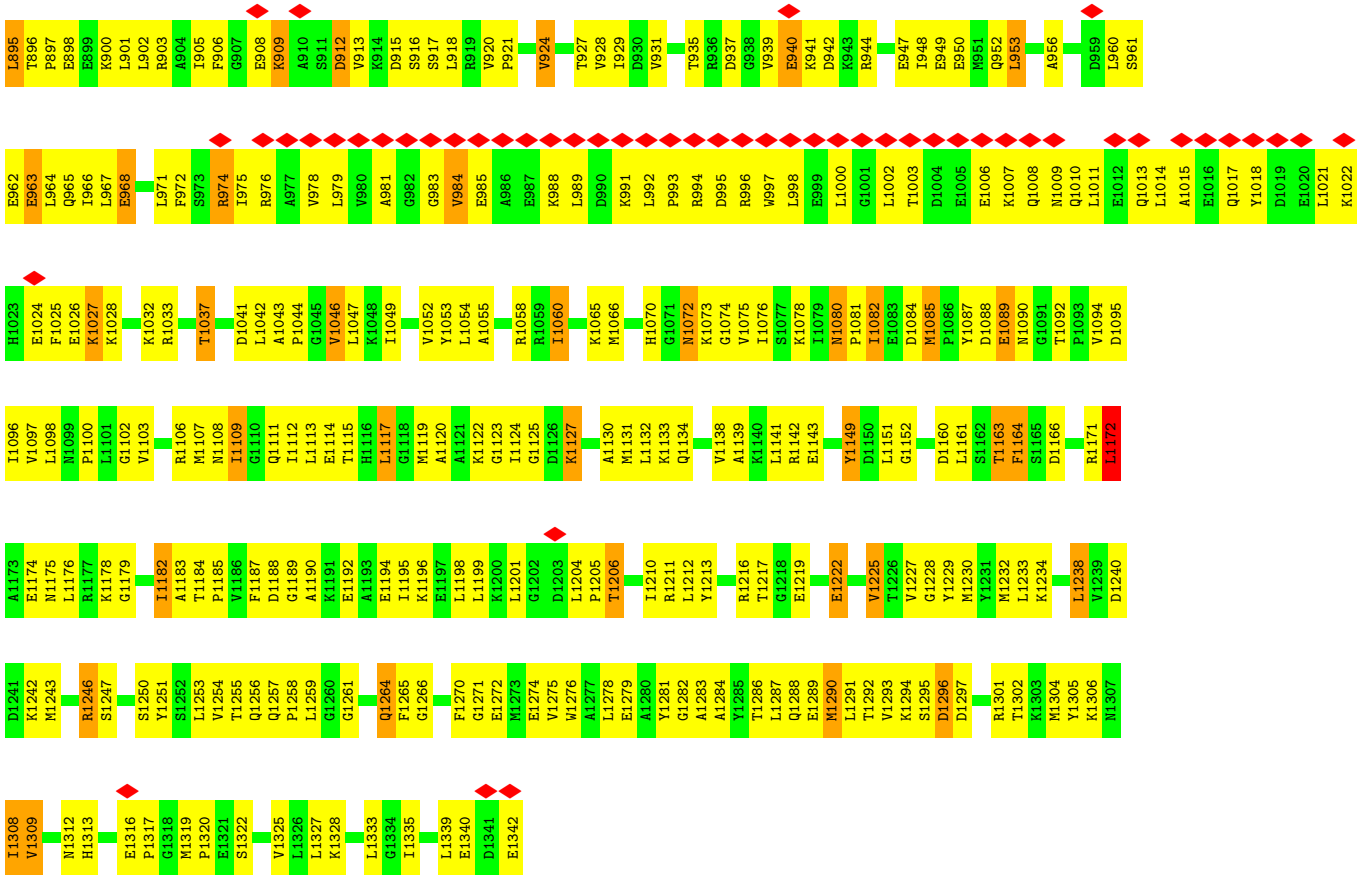




• Molecule 5: DNA-directed RNA polymerase subunit beta

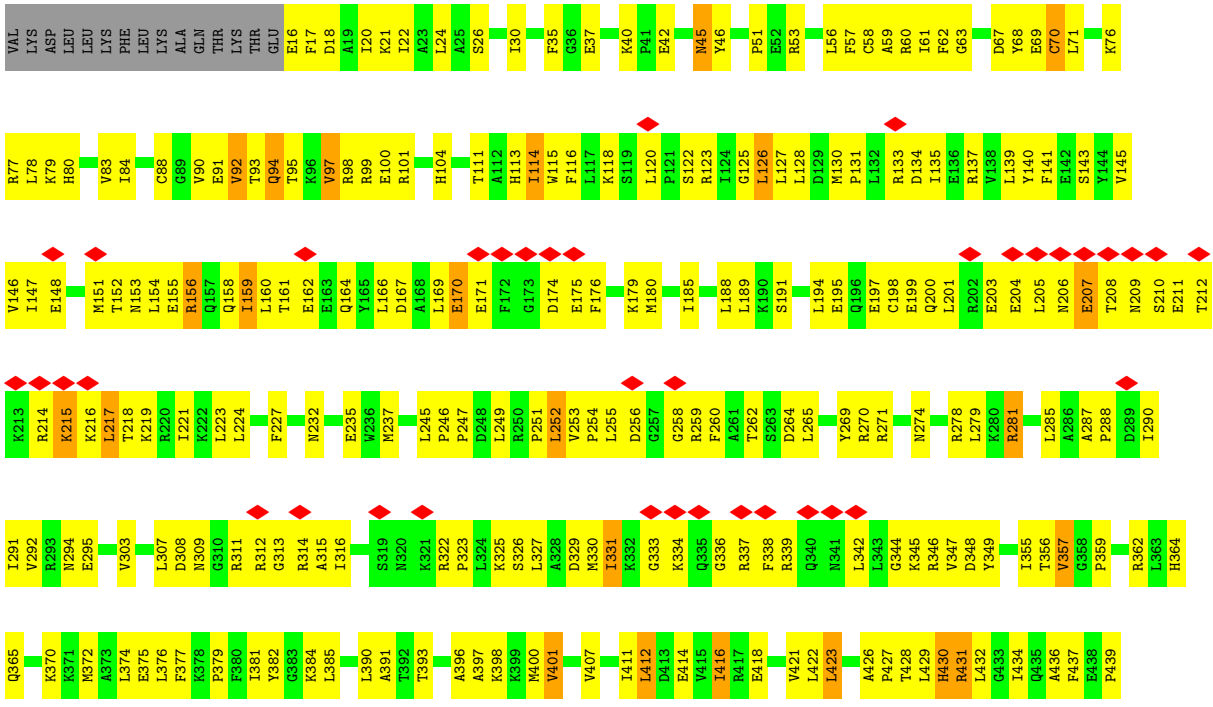
Chain I:

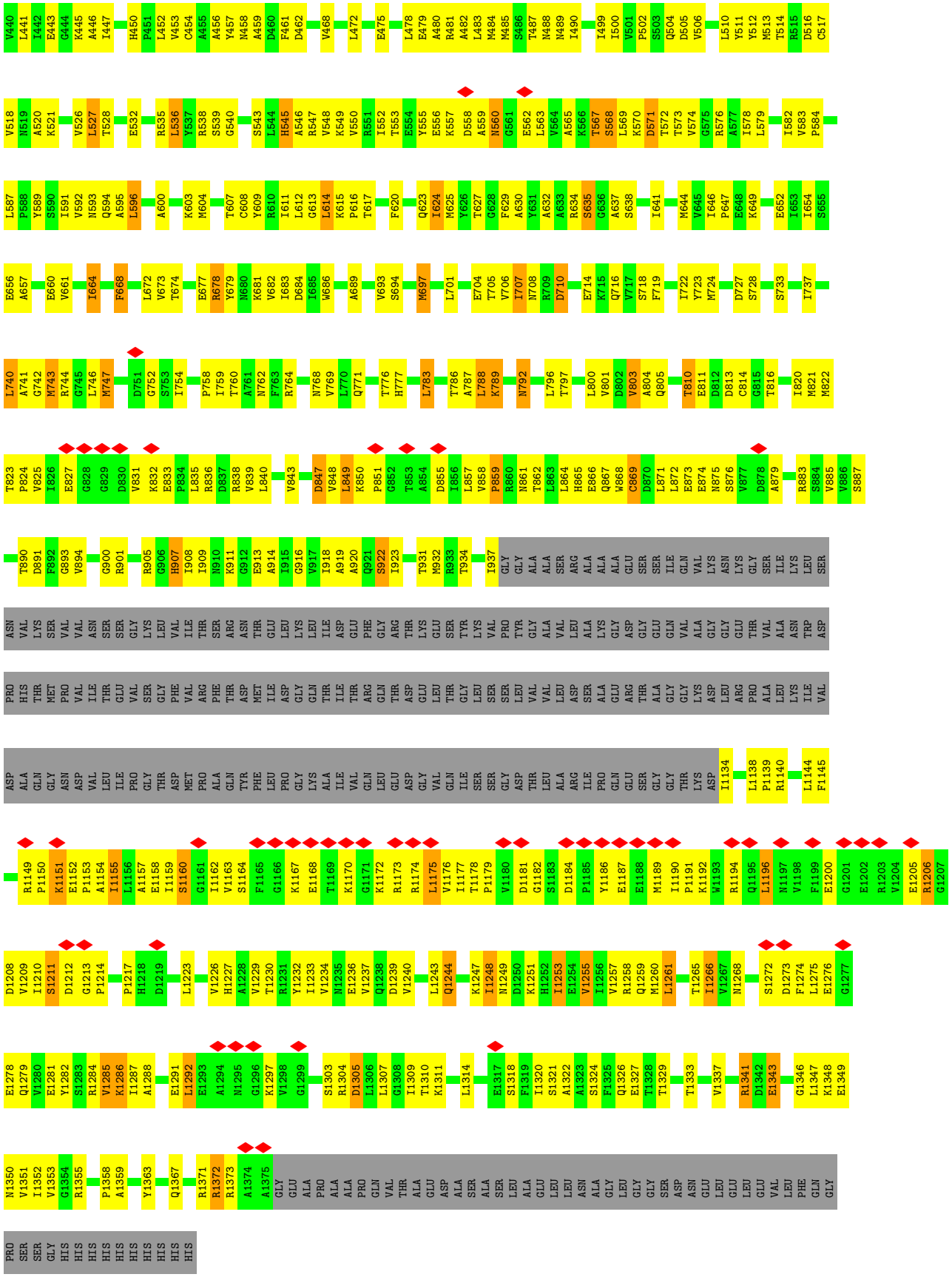




• Molecule 6: DNA-directed RNA polymerase subunit beta'

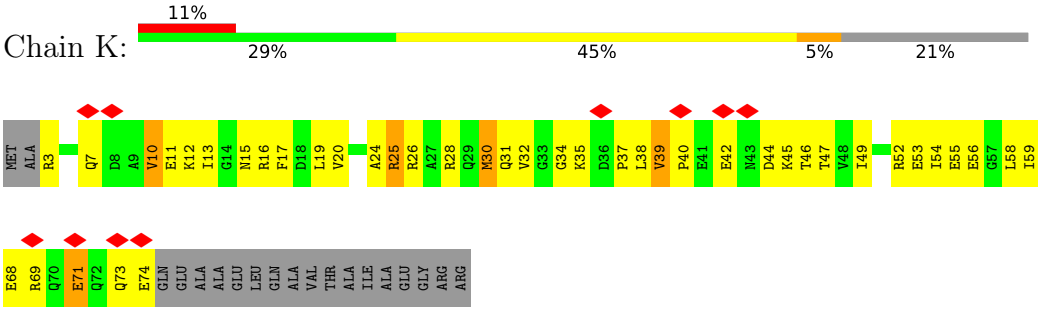
Chain J:





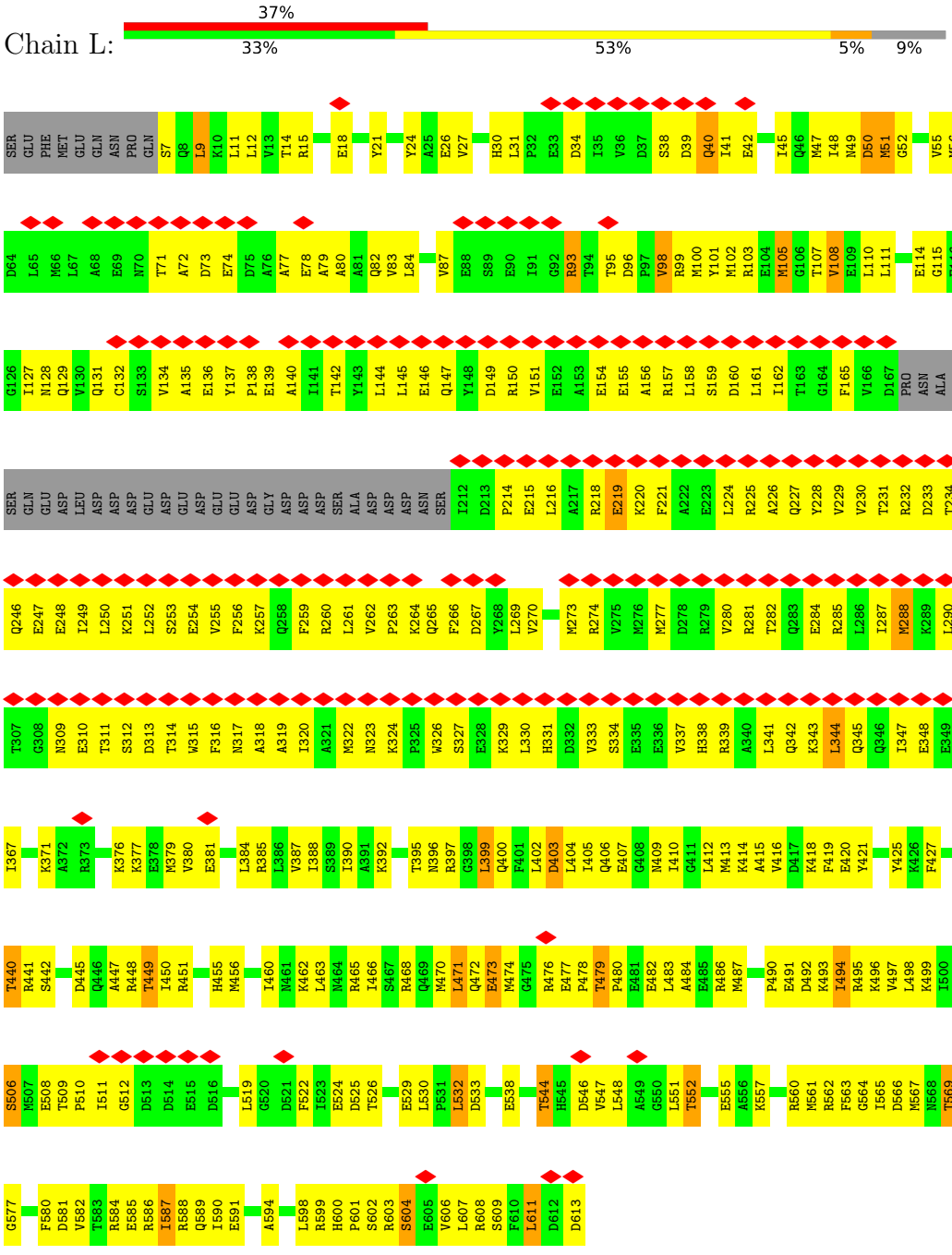
- Molecule 7: DNA-directed RNA polymerase subunit omega

Chain K:



• Molecule 8: RNA polymerase sigma factor RpoD

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	93666	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 ($e^-/Å^2$)	50	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	0.172	Depositor
Minimum map value	-0.120	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	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

5.1 Standard geometry

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

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	N	0.45	0/575	0.53	0/777
2	O	0.72	0/1152	0.92	0/1772
3	P	0.71	0/1169	1.00	0/1803
4	G	0.51	0/1791	0.56	0/2431
4	H	0.44	0/1688	0.53	0/2289
4	M	0.25	0/579	0.43	0/784
5	I	0.53	0/10677	0.54	1/14406 (0.0%)
6	J	0.52	0/9251	0.55	0/12485
7	K	0.36	0/579	0.46	0/779
8	L	0.34	0/4552	0.48	1/6130 (0.0%)
All	All	0.50	0/32013	0.58	2/43656 (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	N	0	1
5	I	0	3
6	J	0	2
8	L	0	1
All	All	0	7

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	1172	LEU	CA-CB-CG	5.35	127.60	115.30
8	L	149	ASP	CB-CG-OD2	5.21	122.99	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	I	254	ASP	Peptide
5	I	855	PRO	Peptide
5	I	857	VAL	Peptide
6	J	1343	GLU	Peptide
6	J	707	ILE	Peptide
8	L	503	GLU	Peptide
1	N	33	PRO	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	N	566	0	552	30	0
2	O	1026	0	562	71	0
3	P	1045	0	579	58	0
4	G	1769	0	1789	134	0
4	H	1669	0	1698	130	0
4	M	572	0	602	87	0
5	I	10512	0	10521	768	0
6	J	9109	0	9308	647	0
7	K	577	0	588	40	0
8	L	4495	0	4517	431	0
9	J	2	0	0	0	0
9	N	1	0	0	0	0
10	I	27	39	37	6	0
10	J	54	78	75	12	0
10	N	27	39	37	6	0
11	J	1	0	0	0	0
All	All	31452	156	30865	2218	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 36.

All (2218) 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)
10:N:102:1N7:C19	10:N:102:1N7:C3	1.82	1.56
10:I:1401:1N7:C3	10:I:1401:1N7:C19	1.82	1.56
5:I:237:LEU:CD1	5:I:292:ILE:CD1	1.82	1.55
10:J:1505:1N7:C3	10:J:1505:1N7:C19	1.82	1.54
10:J:1504:1N7:C19	10:J:1504:1N7:C3	1.82	1.54
5:I:237:LEU:HD11	5:I:292:ILE:CD1	1.06	1.48
5:I:251:ALA:CB	5:I:269:ILE:HG13	1.51	1.40
5:I:237:LEU:CD1	5:I:292:ILE:HD12	1.45	1.40
5:I:237:LEU:CD2	5:I:288:PRO:O	1.78	1.29
5:I:237:LEU:CD1	5:I:292:ILE:HD11	1.53	1.26
5:I:251:ALA:HB2	5:I:269:ILE:CG1	1.61	1.26
5:I:237:LEU:CD2	5:I:288:PRO:C	2.13	1.16
7:K:25:ARG:HD2	7:K:64:LEU:HD13	1.30	1.12
5:I:237:LEU:HD21	5:I:288:PRO:O	0.93	1.11
5:I:473:ARG:HH11	5:I:473:ARG:HG3	1.12	1.10
8:L:348:GLU:HG3	8:L:355:ILE:HG12	1.36	1.04
2:O:51:DT:H2”	2:O:52:DA:H5”	1.40	1.03
5:I:250:THR:N	5:I:268:ARG:CB	2.20	1.03
4:G:234:LEU:HD21	4:H:214:GLU:HG3	1.41	1.02
5:I:237:LEU:HD21	5:I:288:PRO:C	1.75	1.01
8:L:151:VAL:HG22	8:L:156:ALA:HB3	1.39	1.01
6:J:211:GLU:O	6:J:215:LYS:HB2	1.62	1.00
6:J:1347:LEU:HD11	6:J:1359:ALA:HB2	1.44	0.98
5:I:979:LEU:HD13	5:I:989:LEU:HD11	1.46	0.98
5:I:250:THR:N	5:I:268:ARG:HA	1.80	0.97
5:I:251:ALA:CB	5:I:269:ILE:CG1	2.30	0.97
5:I:237:LEU:HD11	5:I:292:ILE:HD11	0.97	0.97
5:I:964:LEU:HD21	5:I:1022:LYS:HD2	1.48	0.96
6:J:526:VAL:HG12	6:J:549:LYS:HB2	1.46	0.95
6:J:155:GLU:HB2	6:J:158:GLN:HB2	1.47	0.94
6:J:914:ALA:HB2	6:J:1359:ALA:HB1	1.50	0.94
4:G:224:LEU:HD13	4:H:228:LEU:HD11	1.49	0.93
5:I:691:PRO:HB3	5:I:788:SER:HB2	1.50	0.93
5:I:237:LEU:HD13	5:I:292:ILE:HD12	1.49	0.92
5:I:983:GLY:HA3	5:I:1002:LEU:HG	1.51	0.92
6:J:20:ILE:HD12	6:J:1320:ILE:HD11	1.49	0.91
8:L:71:THR:HB	8:L:72:ALA:HB2	1.52	0.91
5:I:473:ARG:HH11	5:I:473:ARG:CG	1.82	0.91
8:L:364:ARG:HA	8:L:367:ILE:HD12	1.50	0.91
5:I:237:LEU:HD23	5:I:288:PRO:C	1.90	0.91
4:G:158:ARG:HD2	4:G:172:LEU:HD23	1.53	0.90
8:L:157:ARG:HG2	8:L:159:SER:H	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:759:ILE:HD13	6:J:771:GLN:HB3	1.52	0.90
8:L:351:THR:HB	8:L:358:VAL:HG21	1.52	0.90
5:I:237:LEU:HD11	5:I:292:ILE:HD12	0.98	0.89
5:I:237:LEU:HD12	5:I:292:ILE:CD1	2.01	0.89
8:L:313:ASP:HB3	8:L:317:ASN:HB2	1.52	0.89
2:O:34:DA:H2"	2:O:35:DG:H5"	1.54	0.89
5:I:176:ILE:HD12	5:I:184:LEU:HD23	1.53	0.89
6:J:77:ARG:HB3	6:J:79:LYS:HG2	1.55	0.89
8:L:311:THR:HA	8:L:344:LEU:HD21	1.54	0.89
2:O:62:DC:H2"	2:O:63:DT:H71	1.55	0.88
6:J:291:ILE:HG12	8:L:409:ASN:HD22	1.37	0.88
4:G:234:LEU:HA	4:G:235:ARG:HB2	1.55	0.88
5:I:250:THR:N	5:I:268:ARG:CA	2.36	0.88
4:G:234:LEU:HA	4:G:235:ARG:CB	2.03	0.87
6:J:1167:LYS:HB3	6:J:1174:ARG:HD2	1.56	0.87
8:L:157:ARG:HB3	8:L:160:ASP:HB2	1.56	0.86
8:L:73:ASP:HB2	8:L:74:GLU:HB3	1.56	0.86
6:J:1176:VAL:HG22	6:J:1187:GLU:HB3	1.55	0.86
5:I:250:THR:N	5:I:268:ARG:HB2	1.89	0.86
8:L:247:GLU:HA	8:L:250:LEU:HD12	1.56	0.86
5:I:314:ASN:HD21	5:I:348:SER:HA	1.41	0.86
4:G:104:LYS:HG2	4:G:110:VAL:HG22	1.57	0.85
6:J:1307:LEU:HD23	6:J:1311:LYS:HG3	1.57	0.85
6:J:204:GLU:HB2	6:J:217:LEU:HD11	1.58	0.85
4:G:236:ASP:HA	4:H:14:VAL:O	1.76	0.85
5:I:237:LEU:HD11	5:I:292:ILE:CG1	2.07	0.84
6:J:114:ILE:HD11	6:J:311:ARG:HB2	1.59	0.84
6:J:338:PHE:HA	6:J:342:LEU:HD22	1.59	0.84
4:M:257:VAL:HG11	4:M:270:LEU:HD22	1.59	0.84
5:I:988:LYS:HA	5:I:991:LYS:HG3	1.59	0.84
8:L:569:THR:HA	8:L:570:ASP:HB2	1.60	0.84
8:L:330:LEU:HA	8:L:333:VAL:HG12	1.60	0.84
6:J:1155:ILE:HG13	6:J:1210:ILE:HB	1.59	0.83
6:J:707:ILE:HA	6:J:708:ASN:HB2	1.61	0.83
4:H:11:PRO:HA	4:H:30:PRO:HD2	1.60	0.83
5:I:237:LEU:HD12	5:I:292:ILE:HD11	1.59	0.82
6:J:478:LEU:HG	7:K:47:THR:HG23	1.61	0.82
8:L:562:ARG:HH11	8:L:573:LEU:HD13	1.44	0.82
4:G:154:PRO:HG2	4:G:157:THR:HG23	1.62	0.81
5:I:255:ILE:HD13	5:I:277:LEU:HD21	1.61	0.81
3:P:68:DG:H5"	4:M:294:ASN:HA	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:100:LEU:HD21	4:H:121:VAL:HG11	1.62	0.80
5:I:1185:PRO:HB2	5:I:1188:ASP:HB3	1.61	0.80
5:I:302:ILE:HG22	5:I:309:LEU:HA	1.61	0.80
6:J:131:PRO:HG2	6:J:134:ASP:HB2	1.63	0.80
8:L:110:LEU:HD13	8:L:385:ARG:HD2	1.62	0.80
5:I:734:ILE:HG13	5:I:751:TYR:HE1	1.47	0.80
6:J:1179:PRO:HB2	6:J:1182:GLY:H	1.45	0.80
6:J:864:LEU:HD22	6:J:872:LEU:HD11	1.64	0.80
8:L:220:LYS:HE3	8:L:259:PHE:HE1	1.46	0.79
4:M:278:ILE:HG21	4:M:312:LEU:HD13	1.65	0.79
5:I:619:ALA:HB2	5:I:654:ASP:HB2	1.63	0.79
8:L:111:LEU:HD11	8:L:119:ILE:HD12	1.65	0.79
5:I:250:THR:N	5:I:268:ARG:CG	2.46	0.79
5:I:1340:GLU:HG3	6:J:1341:ARG:HH21	1.47	0.79
6:J:1167:LYS:HE3	6:J:1170:LYS:HB2	1.64	0.79
5:I:260:LYS:HD3	5:I:261:VAL:H	1.46	0.79
5:I:293:ALA:HB2	5:I:319:LEU:HD21	1.65	0.78
6:J:859:PRO:HD2	6:J:862:THR:HG21	1.66	0.78
5:I:660:VAL:HG11	6:J:769:VAL:HG13	1.65	0.78
5:I:877:VAL:HG21	5:I:920:VAL:HG21	1.64	0.78
5:I:898:GLU:HG2	8:L:544:THR:HG21	1.65	0.78
2:O:29:DA:H1’	2:O:30:DC:H5’	1.65	0.78
5:I:264:GLU:HB2	5:I:267:ARG:HH21	1.50	0.77
8:L:151:VAL:HG12	8:L:158:LEU:HD23	1.67	0.77
4:G:234:LEU:CD2	4:H:214:GLU:OE2	2.33	0.77
4:G:207:THR:HG21	4:G:211:ILE:HG22	1.64	0.77
6:J:209:ASN:HA	6:J:214:ARG:HD3	1.66	0.77
5:I:765:ILE:HG23	5:I:787:PRO:HG3	1.67	0.77
5:I:1243:MET:HE3	6:J:445:LYS:HB3	1.67	0.77
5:I:241:LEU:HD21	5:I:277:LEU:HD23	1.65	0.77
8:L:436:ARG:O	8:L:440:THR:OG1	2.03	0.77
4:G:234:LEU:CA	4:G:235:ARG:HG2	2.14	0.77
8:L:560:ARG:NH1	8:L:566:ASP:OD2	2.17	0.77
6:J:664:ILE:HG13	6:J:681:LYS:HG2	1.65	0.77
5:I:204:LEU:HD11	5:I:369:MET:HE2	1.65	0.76
5:I:242:VAL:HB	5:I:245:ARG:HG3	1.65	0.76
5:I:1103:VAL:HG11	5:I:1112:ILE:HD11	1.65	0.76
5:I:1111:GLN:HB2	5:I:1230:MET:HE2	1.67	0.76
6:J:885:VAL:HG22	6:J:894:VAL:HG11	1.67	0.76
4:G:199:ASP:N	4:G:199:ASP:OD1	2.17	0.76
4:H:35:PHE:HA	4:H:38:THR:HG23	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:108:VAL:O	8:L:385:ARG:NH2	2.19	0.76
4:G:45:ARG:NH2	5:I:1084:ASP:OD1	2.18	0.76
5:I:856:ASN:HB3	8:L:613:ASP:HA	1.64	0.76
5:I:247:ARG:HA	5:I:274:ILE:HD11	1.68	0.76
1:N:47:ALA:HB1	6:J:672:LEU:HD21	1.66	0.76
2:O:38:DG:H1'	2:O:39:DG:H5'	1.67	0.76
5:I:251:ALA:HB1	5:I:269:ILE:HD11	1.66	0.75
5:I:988:LYS:HG2	5:I:991:LYS:HD2	1.66	0.75
5:I:1246:ARG:NH1	5:I:1265:PHE:O	2.19	0.75
6:J:850:LYS:HB2	6:J:855:ASP:HB2	1.66	0.75
8:L:98:VAL:HB	8:L:402:LEU:HD21	1.66	0.75
8:L:296:LYS:HE2	8:L:296:LYS:HA	1.68	0.75
6:J:742:GLY:O	6:J:762:ASN:HB3	1.84	0.75
8:L:218:ARG:HA	8:L:221:PHE:HD2	1.51	0.75
5:I:871:VAL:O	5:I:944:ARG:NH2	2.20	0.75
6:J:148:GLU:OE2	6:J:156:ARG:NE	2.19	0.75
6:J:1160:SER:OG	6:J:1206:ARG:N	2.18	0.75
6:J:452:LEU:HD13	6:J:500:ILE:HG22	1.66	0.75
10:J:1505:1N7:C3	10:J:1505:1N7:C18	2.65	0.75
8:L:552:THR:HG23	8:L:555:GLU:HG3	1.68	0.74
5:I:1256:GLN:O	5:I:1301:ARG:NH2	2.20	0.74
6:J:382:TYR:HE2	8:L:532:LEU:HD11	1.52	0.74
8:L:45:ILE:HD11	8:L:55:VAL:HG11	1.69	0.74
4:G:234:LEU:HD13	4:G:234:LEU:N	2.02	0.74
6:J:647:PRO:HG3	6:J:697:MET:HB3	1.70	0.74
4:M:257:VAL:HA	4:M:260:LEU:HG	1.70	0.74
4:M:262:LEU:HD21	4:M:306:VAL:HG11	1.69	0.74
4:H:64:VAL:HG11	4:H:71:LYS:HB2	1.69	0.74
5:I:562:GLU:OE2	5:I:687:ARG:NH1	2.20	0.74
4:G:8:PHE:HD1	4:G:32:GLU:HG3	1.53	0.73
6:J:147:ILE:HD11	6:J:179:LYS:HG3	1.69	0.73
6:J:334:LYS:HA	6:J:339:ARG:HG2	1.70	0.73
5:I:906:PHE:HD2	8:L:611:LEU:HG	1.53	0.73
6:J:1237:VAL:HG11	6:J:1253:ILE:HG21	1.69	0.73
8:L:51:MET:HE1	8:L:84:LEU:HD12	1.71	0.73
6:J:339:ARG:NH1	6:J:1324:SER:O	2.20	0.73
5:I:175:ARG:HG2	5:I:177:ILE:HG13	1.71	0.73
6:J:1266:ILE:HD12	6:J:1274:PHE:HB3	1.71	0.73
7:K:39:VAL:HG22	7:K:40:PRO:HD2	1.71	0.73
5:I:145:ILE:HG21	5:I:456:VAL:HG13	1.71	0.73
6:J:126:LEU:HD11	6:J:223:LEU:HD23	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:891:ASP:OD1	6:J:1286:LYS:NZ	2.22	0.73
8:L:511:ILE:HG22	8:L:512:GLY:HA2	1.69	0.73
4:H:91:ARG:NH2	4:H:210:THR:O	2.21	0.73
5:I:1109:ILE:HD12	6:J:641:ILE:HD11	1.70	0.73
5:I:148:GLN:OE1	5:I:454:ARG:NH1	2.21	0.72
5:I:251:ALA:CB	5:I:269:ILE:CD1	2.67	0.72
6:J:918:ILE:O	6:J:922:SER:OG	2.04	0.72
6:J:1158:GLU:HA	6:J:1223:LEU:HD11	1.70	0.72
8:L:245:ALA:HA	8:L:248:GLU:HB2	1.70	0.72
8:L:309:ASN:HD21	8:L:312:SER:HB3	1.54	0.72
4:G:234:LEU:HD21	4:H:214:GLU:CG	2.16	0.72
4:G:234:LEU:HD22	4:H:214:GLU:OE2	1.89	0.72
6:J:255:LEU:N	6:J:259:ARG:O	2.20	0.72
6:J:482:ALA:O	7:K:16:ARG:NH1	2.22	0.72
2:O:41:DT:H2"	2:O:42:DA:C8	2.24	0.72
8:L:157:ARG:HE	8:L:159:SER:HB2	1.54	0.72
2:O:42:DA:H1'	2:O:43:DA:H5'	1.70	0.72
5:I:956:ALA:HB1	5:I:1032:LYS:HG2	1.70	0.72
2:O:28:DG:H1'	2:O:29:DA:H5'	1.72	0.72
1:N:32:ILE:HG23	1:N:33:PRO:HD2	1.70	0.72
5:I:135:THR:OG1	5:I:142:GLU:OE2	2.07	0.72
6:J:205:LEU:HG	6:J:217:LEU:HD12	1.71	0.72
4:M:252:ILE:HD11	4:M:310:ARG:HH11	1.54	0.71
5:I:1171:ARG:O	5:I:1175:ASN:ND2	2.23	0.71
2:O:27:DT:H1'	2:O:28:DG:H5'	1.71	0.71
4:G:53:GLY:O	4:G:148:ARG:HA	1.90	0.71
5:I:251:ALA:HB1	5:I:269:ILE:CD1	2.20	0.71
6:J:156:ARG:NH2	6:J:191:SER:OG	2.23	0.71
6:J:611:ILE:HB	6:J:612:LEU:HD12	1.70	0.71
4:M:288:GLU:HA	4:M:291:LYS:HE3	1.71	0.71
7:K:44:ASP:OD2	7:K:52:ARG:NH1	2.23	0.71
5:I:1184:THR:HG23	5:I:1189:GLY:HA3	1.72	0.71
8:L:162:ILE:HA	8:L:262:VAL:HG23	1.71	0.71
8:L:162:ILE:HD11	8:L:221:PHE:HZ	1.54	0.71
5:I:1222:GLU:OE1	6:J:512:TYR:OH	2.05	0.71
6:J:1279:GLN:NE2	6:J:1305:ASP:OD2	2.24	0.71
6:J:84:ILE:HG12	6:J:91:GLU:HB2	1.73	0.71
8:L:287:ILE:HD13	8:L:315:TRP:HH2	1.55	0.71
4:G:234:LEU:HD22	4:G:234:LEU:O	1.91	0.70
10:N:102:1N7:C3	10:N:102:1N7:C18	2.63	0.70
4:G:66:HIS:HB3	5:I:927:THR:HG21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:1225:VAL:HA	6:J:638:SER:HB2	1.73	0.70
5:I:1254:VAL:O	6:J:99:ARG:NH2	2.23	0.70
6:J:206:ASN:ND2	6:J:207:GLU:OE1	2.24	0.70
4:G:58:GLU:OE1	4:G:170:ARG:NH2	2.23	0.70
4:H:61:ILE:HG12	4:H:171:LEU:HD13	1.74	0.70
8:L:473:GLU:OE2	8:L:486:ARG:NH1	2.23	0.70
5:I:314:ASN:O	5:I:352:ARG:NH1	2.21	0.70
5:I:1253:LEU:HD23	8:L:525:ASP:HA	1.74	0.70
6:J:1178:THR:HA	6:J:1184:ASP:HB3	1.73	0.70
5:I:521:LEU:HB2	5:I:794:LEU:HD21	1.74	0.70
6:J:426:ALA:HB3	6:J:427:PRO:HD3	1.72	0.70
2:O:22:DT:OP1	4:M:268:ASN:ND2	2.25	0.70
4:H:41:ASN:OD1	4:H:44:ARG:NH2	2.25	0.70
3:P:51:DC:H2"	3:P:52:DT:H71	1.72	0.70
5:I:237:LEU:HD22	5:I:289:VAL:HA	1.73	0.70
5:I:1058:ARG:HD2	5:I:1238:LEU:HD23	1.74	0.70
6:J:654:ILE:HD11	6:J:743:MET:HE2	1.74	0.70
5:I:314:ASN:OD1	5:I:352:ARG:NH1	2.25	0.69
4:G:234:LEU:HA	4:G:235:ARG:HG2	1.75	0.69
4:H:215:GLU:OE2	4:H:219:ARG:NH2	2.25	0.69
4:M:270:LEU:O	4:M:274:ALA:N	2.20	0.69
5:I:519:ASN:ND2	5:I:689:ALA:O	2.25	0.69
5:I:1271:GLY:N	5:I:1274:GLU:OE1	2.23	0.69
5:I:1335:ILE:HG21	6:J:22:ILE:HD11	1.74	0.69
6:J:874:GLU:OE1	6:J:875:ASN:ND2	2.25	0.69
4:G:48:LEU:HD22	5:I:1082:ILE:HD11	1.73	0.69
5:I:56:VAL:HG21	5:I:468:LEU:HB3	1.75	0.69
5:I:74:ARG:NH1	5:I:121:GLU:OE2	2.26	0.69
6:J:1281:GLU:HG3	6:J:1284:ARG:HB3	1.74	0.69
5:I:11:ILE:O	5:I:1149:TYR:OH	2.10	0.69
6:J:1172:LYS:HG3	6:J:1191:PRO:HA	1.73	0.69
5:I:120:GLN:NE2	5:I:490:GLN:OE1	2.25	0.69
5:I:726:TYR:HA	5:I:773:LEU:HD21	1.75	0.69
7:K:38:LEU:HB3	7:K:58:LEU:HD13	1.75	0.69
8:L:282:THR:HA	8:L:285:ARG:HG2	1.73	0.69
5:I:255:ILE:HG22	5:I:262:TYR:HB2	1.76	0.68
5:I:732:ILE:HD13	5:I:783:LEU:HB3	1.73	0.68
4:G:234:LEU:HA	4:G:235:ARG:CG	2.24	0.68
6:J:1158:GLU:OE1	6:J:1158:GLU:N	2.26	0.68
8:L:585:GLU:OE2	8:L:588:ARG:NH2	2.22	0.68
4:G:155:ALA:O	4:G:159:ILE:HG22	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:1153:PRO:HD2	6:J:1194:ARG:HH21	1.58	0.68
10:I:1401:1N7:C3	10:I:1401:1N7:C2	2.68	0.68
6:J:260:PHE:HB2	8:L:504:PRO:HB3	1.74	0.68
8:L:234:THR:OG1	8:L:248:GLU:OE1	2.11	0.68
4:G:150:ARG:NH1	4:H:5:VAL:O	2.27	0.68
5:I:1238:LEU:O	5:I:1242:LYS:HG3	1.93	0.68
8:L:561:MET:HG2	8:L:576:VAL:HG22	1.75	0.68
2:O:49:DC:N4	8:L:437:GLN:OE1	2.26	0.68
5:I:461:GLU:OE2	5:I:465:ARG:NH2	2.27	0.68
6:J:744:ARG:HB2	6:J:759:ILE:HB	1.76	0.68
6:J:1251:LYS:O	6:J:1255:VAL:HG12	1.94	0.68
6:J:1346:GLY:O	6:J:1350:ASN:ND2	2.27	0.68
5:I:404:LYS:HE3	5:I:450:ASN:HA	1.75	0.68
6:J:416:ILE:HD12	6:J:441:LEU:HD21	1.76	0.68
5:I:1163:THR:O	5:I:1163:THR:OG1	2.06	0.68
5:I:318:SER:OG	5:I:320:ASP:OD1	2.12	0.67
8:L:314:THR:HA	8:L:318:ALA:HB3	1.75	0.67
8:L:334:SER:O	8:L:338:HIS:HB2	1.95	0.67
2:O:44:DA:H2'	8:L:455:HIS:HE1	1.59	0.67
6:J:848:VAL:HB	6:J:858:VAL:HG22	1.77	0.67
4:M:265:ARG:HH21	4:M:294:ASN:HB3	1.59	0.67
6:J:511:TYR:CG	6:J:728:SER:HB3	2.30	0.67
4:M:275:ILE:HG21	4:M:281:LEU:HB2	1.76	0.67
8:L:165:PHE:O	8:L:260:ARG:NH2	2.27	0.67
5:I:473:ARG:CG	5:I:473:ARG:NH1	2.49	0.67
6:J:1149:ARG:HD3	6:J:1150:PRO:HD2	1.77	0.67
5:I:125:GLY:H	5:I:495:ALA:HB1	1.60	0.67
10:J:1504:1N7:C3	10:J:1504:1N7:C2	2.70	0.67
10:N:102:1N7:C3	10:N:102:1N7:C2	2.70	0.66
6:J:218:THR:HA	6:J:221:ILE:HG22	1.76	0.66
6:J:710:ASP:OD1	6:J:710:ASP:N	2.27	0.66
8:L:83:VAL:O	8:L:87:VAL:HG13	1.95	0.66
4:H:11:PRO:HG3	4:H:31:LEU:HD21	1.76	0.66
6:J:211:GLU:O	6:J:215:LYS:CB	2.42	0.66
5:I:411:ARG:NH2	5:I:427:ASP:OD2	2.26	0.66
5:I:515:MET:HE1	5:I:517:GLN:NE2	2.10	0.66
6:J:1140:ARG:NH2	6:J:1236:GLU:OE2	2.28	0.66
6:J:613:GLY:O	6:J:617:THR:OG1	2.11	0.66
4:G:42:ALA:O	4:G:46:ILE:HG12	1.96	0.66
6:J:678:ARG:O	6:J:682:VAL:HG12	1.95	0.66
8:L:145:LEU:HD21	8:L:224:LEU:HD23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:251:ALA:HB2	5:I:269:ILE:HG13	0.71	0.66
5:I:299:LYS:HA	5:I:313:ALA:HB2	1.78	0.66
5:I:1250:SER:OG	8:L:524:GLU:OE1	2.13	0.66
8:L:327:SER:HA	8:L:330:LEU:HD12	1.78	0.66
4:G:13:LEU:HD23	4:G:13:LEU:H	1.61	0.66
4:H:109:PRO:HB3	4:H:132:HIS:CE1	2.31	0.66
5:I:1312:ASN:OD1	7:K:32:VAL:HG21	1.95	0.66
6:J:475:GLU:OE2	7:K:28:ARG:NH1	2.23	0.66
6:J:783:LEU:HA	6:J:786:THR:HG22	1.77	0.66
1:N:60:GLU:OE2	5:I:272:ARG:NH1	2.26	0.65
4:G:234:LEU:CD2	4:H:214:GLU:CD	2.64	0.65
5:I:455:SER:O	5:I:459:MET:HG3	1.96	0.65
6:J:797:THR:O	6:J:801:VAL:HG13	1.95	0.65
5:I:17:LYS:H	5:I:17:LYS:HD2	1.59	0.65
5:I:727:VAL:HG23	5:I:773:LEU:HD23	1.76	0.65
5:I:253:PHE:CE2	5:I:288:PRO:HD3	2.32	0.65
6:J:1145:PHE:HB3	6:J:1309:ILE:HD13	1.78	0.65
8:L:129:GLN:HE22	8:L:367:ILE:HB	1.62	0.65
5:I:221:LEU:HD22	5:I:336:LEU:HD11	1.77	0.65
5:I:800:MET:HE1	5:I:827:ARG:HE	1.61	0.65
6:J:205:LEU:HG	6:J:217:LEU:HB3	1.76	0.65
6:J:516:ASP:HB3	6:J:573:THR:CG2	2.25	0.65
6:J:708:ASN:ND2	6:J:714:GLU:OE1	2.29	0.65
5:I:225:PHE:HE2	5:I:347:ILE:HB	1.62	0.65
5:I:905:ILE:HG22	5:I:906:PHE:CD1	2.32	0.65
2:O:35:DG:H2"	2:O:36:DA:H5'	1.78	0.65
4:H:29:GLU:HB3	4:H:30:PRO:HD3	1.79	0.65
5:I:1151:LEU:HD12	5:I:1198:LEU:HD12	1.79	0.65
8:L:254:GLU:HA	8:L:257:LYS:HD3	1.77	0.65
5:I:192:ASP:OD2	5:I:436:ARG:NH2	2.30	0.65
5:I:1022:LYS:O	5:I:1026:GLU:HG2	1.96	0.65
4:H:35:PHE:HA	4:H:38:THR:CG2	2.27	0.65
6:J:147:ILE:HG22	6:J:188:LEU:CD2	2.27	0.65
6:J:557:LYS:HG2	6:J:563:LEU:HG	1.78	0.65
3:P:33:DA:N7	8:L:396:ASN:ND2	2.43	0.65
4:M:283:GLN:HE21	4:M:318:LEU:HB2	1.62	0.65
4:G:91:ARG:NH2	4:G:122:GLU:OE2	2.30	0.65
8:L:138:PRO:O	8:L:142:THR:HG23	1.96	0.65
4:G:226:GLU:OE2	4:H:10:LYS:NZ	2.30	0.64
6:J:587:LEU:HD11	6:J:608:CYS:HA	1.79	0.64
6:J:931:THR:OG1	6:J:1244:GLN:OE1	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:62:DC:H2"	2:O:63:DT:C7	2.25	0.64
3:P:54:DT:H1'	3:P:55:DT:H5'	1.80	0.64
5:I:985:GLU:O	5:I:989:LEU:HB2	1.97	0.64
6:J:704:GLU:HG2	6:J:718:SER:HA	1.79	0.64
3:P:29:DA:H1'	3:P:30:DG:H5'	1.78	0.64
4:G:102:LEU:HD12	4:G:142:MET:HG3	1.79	0.64
5:I:4:SER:HB3	5:I:7:GLU:HB2	1.79	0.64
5:I:10:ARG:NH1	5:I:790:ASP:OD1	2.24	0.64
5:I:28:LEU:HD21	5:I:524:ILE:HD13	1.79	0.64
6:J:623:GLN:O	6:J:627:THR:HG22	1.98	0.64
6:J:1275:LEU:HD12	6:J:1276:GLU:H	1.63	0.64
8:L:466:ILE:HD12	8:L:487:MET:HG2	1.80	0.64
5:I:689:ALA:HB2	5:I:1233:LEU:HD23	1.78	0.64
6:J:288:PRO:HD2	6:J:291:ILE:HD12	1.78	0.64
8:L:562:ARG:NH2	8:L:572:THR:HA	2.12	0.64
2:O:57:DT:OP1	5:I:476:LYS:NZ	2.28	0.64
5:I:812:PHE:O	6:J:504:GLN:NE2	2.30	0.64
4:H:155:ALA:N	4:H:174:ASP:OD1	2.31	0.64
5:I:968:GLU:HB2	5:I:1018:TYR:CE1	2.32	0.64
10:J:1505:1N7:C3	10:J:1505:1N7:C2	2.71	0.64
7:K:38:LEU:N	7:K:53:GLU:OE2	2.27	0.64
5:I:250:THR:N	5:I:268:ARG:HG3	2.11	0.64
6:J:706:VAL:HG11	6:J:716:GLN:HG2	1.80	0.64
8:L:582:VAL:CG1	8:L:586:ARG:HB3	2.28	0.64
4:G:166:ARG:NH2	5:I:876:GLU:OE1	2.31	0.64
5:I:877:VAL:CG2	5:I:920:VAL:HG21	2.28	0.64
6:J:485:MET:HB3	6:J:488:ASN:ND2	2.14	0.64
6:J:516:ASP:HB3	6:J:573:THR:HG22	1.79	0.64
6:J:1227:HIS:HA	6:J:1230:THR:HG22	1.80	0.64
8:L:235:ILE:HA	8:L:245:ALA:CB	2.27	0.64
6:J:71:LEU:HB2	6:J:90:VAL:HG21	1.80	0.63
6:J:245:LEU:HD12	6:J:246:PRO:HD2	1.79	0.63
4:G:6:THR:HG23	4:G:7:GLU:H	1.61	0.63
6:J:1155:ILE:HG12	6:J:1211:SER:HB3	1.80	0.63
6:J:1310:THR:O	6:J:1314:LEU:HD13	1.98	0.63
8:L:38:SER:O	8:L:41:ILE:HG22	1.97	0.63
5:I:349:GLU:HA	5:I:352:ARG:HG3	1.79	0.63
5:I:1305:TYR:O	5:I:1309:VAL:HG13	1.98	0.63
6:J:68:TYR:HA	6:J:92:VAL:HG23	1.81	0.63
8:L:606:VAL:O	8:L:609:SER:OG	2.13	0.63
1:N:12:THR:O	1:N:16:THR:HG23	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:123:ARG:O	6:J:127:LEU:HB2	1.98	0.63
8:L:231:THR:HG23	8:L:248:GLU:HB3	1.80	0.63
5:I:818:VAL:HG21	5:I:1076:ILE:HG12	1.81	0.63
6:J:555:TYR:HB3	6:J:563:LEU:HD22	1.80	0.63
6:J:848:VAL:O	6:J:857:LEU:N	2.28	0.63
8:L:290:LEU:O	8:L:333:VAL:HG21	1.99	0.63
4:M:289:LEU:HD12	4:M:300:LEU:HD21	1.80	0.63
5:I:811:ASN:HA	5:I:815:SER:HB2	1.79	0.63
6:J:397:ALA:O	6:J:401:VAL:HG13	1.98	0.63
6:J:1167:LYS:CE	6:J:1170:LYS:HB2	2.29	0.63
4:H:83:LEU:HD23	6:J:528:THR:HA	1.80	0.63
5:I:548:ARG:NH1	5:I:568:ASN:HA	2.14	0.63
5:I:909:LYS:HE2	5:I:909:LYS:HA	1.80	0.63
7:K:31:GLN:HG2	7:K:32:VAL:HG23	1.80	0.63
7:K:69:ARG:O	7:K:73:GLN:HG2	1.98	0.63
8:L:290:LEU:O	8:L:294:GLN:HB3	1.99	0.63
4:G:54:CYS:SG	4:G:92:VAL:HG13	2.39	0.63
4:H:47:LEU:HD12	4:H:183:ILE:HD13	1.79	0.63
5:I:24:VAL:HG13	5:I:25:PRO:HD2	1.80	0.63
5:I:521:LEU:O	5:I:525:THR:HG22	1.98	0.63
5:I:890:LYS:HG2	5:I:912:ASP:O	1.99	0.63
6:J:155:GLU:HB2	6:J:158:GLN:CB	2.25	0.63
5:I:229:ILE:HG21	5:I:332:ARG:HH21	1.64	0.63
2:O:45:DA:OP1	8:L:451:ARG:NH2	2.32	0.62
5:I:639:LYS:H	5:I:639:LYS:HD3	1.64	0.62
5:I:1212:LEU:HD22	5:I:1225:VAL:HG22	1.81	0.62
6:J:572:THR:HG21	6:J:589:TYR:OH	1.99	0.62
8:L:347:ILE:HA	8:L:350:GLU:HB2	1.80	0.62
8:L:561:MET:HG3	8:L:571:TYR:CD2	2.34	0.62
3:P:28:DG:OP2	3:P:28:DG:H2'	1.99	0.62
4:H:65:LEU:HD22	4:H:66:HIS:H	1.64	0.62
8:L:248:GLU:HA	8:L:251:LYS:NZ	2.14	0.62
3:P:29:DA:H1'	3:P:30:DG:C5'	2.28	0.62
4:M:277:TYR:HE2	4:M:322:PRO:HB3	1.65	0.62
5:I:928:VAL:HG13	5:I:1052:VAL:HG13	1.81	0.62
8:L:288:MET:HG2	8:L:292:VAL:HG23	1.81	0.62
5:I:91:THR:HB	5:I:138:ILE:O	1.99	0.62
5:I:131:THR:HG22	5:I:132:ASP:H	1.64	0.62
5:I:1161:LEU:O	5:I:1164:PHE:HB2	1.98	0.62
8:L:142:THR:O	8:L:146:GLU:HG3	1.99	0.62
4:G:232:VAL:HG13	4:G:233:ASP:N	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:237:LEU:CD2	5:I:289:VAL:N	2.62	0.62
6:J:161:THR:HG22	6:J:164:GLN:HB3	1.82	0.62
6:J:858:VAL:HG12	6:J:868:TRP:CE3	2.34	0.62
6:J:1167:LYS:NZ	6:J:1168:GLU:O	2.32	0.62
8:L:569:THR:HG23	8:L:571:TYR:N	2.14	0.62
6:J:208:THR:O	6:J:214:ARG:HB3	2.00	0.62
8:L:247:GLU:OE1	8:L:247:GLU:N	2.31	0.62
5:I:106:GLU:HB3	5:I:115:LYS:HD2	1.80	0.62
4:H:172:LEU:HD23	4:H:172:LEU:H	1.64	0.62
5:I:6:THR:HG21	5:I:781:ASP:HB3	1.82	0.62
4:M:254:LEU:HA	4:M:277:TYR:CG	2.35	0.62
5:I:65:ASN:ND2	5:I:483:ASP:OD2	2.33	0.62
5:I:106:GLU:HB3	5:I:115:LYS:CD	2.29	0.62
5:I:748:ILE:HD13	5:I:967:LEU:HD23	1.81	0.62
6:J:77:ARG:CB	6:J:79:LYS:HG2	2.29	0.62
6:J:548:VAL:HG23	6:J:550:VAL:HG23	1.82	0.62
6:J:572:THR:HG22	6:J:593:ASN:OD1	1.99	0.62
3:P:53:DT:H2"	3:P:54:DT:H71	1.82	0.62
5:I:515:MET:HE3	5:I:517:GLN:HG3	1.82	0.62
6:J:372:MET:O	6:J:376:LEU:HG	1.99	0.62
6:J:801:VAL:O	6:J:805:GLN:HB2	2.00	0.62
4:H:98:VAL:HG13	4:H:146:VAL:CG2	2.29	0.61
5:I:145:ILE:CG2	5:I:456:VAL:HG13	2.30	0.61
6:J:200:GLN:O	6:J:204:GLU:HG2	2.00	0.61
1:N:21:ASN:O	1:N:25:GLN:HG2	2.00	0.61
4:H:83:LEU:HD21	6:J:527:LEU:O	2.00	0.61
5:I:230:PHE:HB2	5:I:333:ILE:HD13	1.81	0.61
5:I:997:TRP:HA	5:I:1000:LEU:HG	1.80	0.61
8:L:225:ARG:O	8:L:229:VAL:HG13	2.00	0.61
3:P:67:DT:OP2	4:M:298:LYS:HD3	2.01	0.61
4:G:71:LYS:HB3	4:G:74:VAL:HG13	1.82	0.61
6:J:390:LEU:HD23	6:J:407:VAL:HG21	1.81	0.61
6:J:1230:THR:O	6:J:1234:VAL:HG13	2.01	0.61
8:L:105:MET:O	8:L:108:VAL:HG23	2.00	0.61
4:M:261:GLU:OE1	8:L:600:HIS:ND1	2.28	0.61
5:I:197:ARG:HD2	5:I:200:ARG:HH21	1.64	0.61
5:I:473:ARG:HG3	5:I:473:ARG:NH1	1.95	0.61
6:J:69:GLU:HG3	6:J:76:LYS:HD3	1.82	0.61
6:J:479:GLU:O	6:J:483:LEU:HB2	1.99	0.61
5:I:229:ILE:HG21	5:I:332:ARG:NH2	2.14	0.61
5:I:465:ARG:O	5:I:469:VAL:HG13	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:960:LEU:HB3	5:I:1025:PHE:CE1	2.36	0.61
5:I:976:ARG:HG3	5:I:989:LEU:HD23	1.83	0.61
6:J:245:LEU:HD11	6:J:249:LEU:HD12	1.83	0.61
6:J:603:LYS:O	6:J:607:THR:HG23	2.01	0.61
1:N:47:ALA:CB	6:J:672:LEU:HD21	2.30	0.61
8:L:511:ILE:HG12	8:L:522:PHE:CE2	2.35	0.61
3:P:59:DA:H2"	3:P:60:DA:H5"	1.82	0.61
8:L:251:LYS:O	8:L:255:VAL:HG13	2.01	0.61
5:I:206:ALA:O	5:I:209:ILE:HG22	2.01	0.61
5:I:533:LEU:HD21	5:I:571:LEU:HD13	1.82	0.61
6:J:24:LEU:HD21	6:J:116:PHE:CZ	2.35	0.61
6:J:850:LYS:HG2	6:J:851:PRO:HD2	1.83	0.61
4:H:46:ILE:HD11	4:H:224:LEU:HD13	1.82	0.61
5:I:103:VAL:HG12	5:I:117:ILE:HB	1.82	0.61
5:I:724:VAL:HG11	5:I:727:VAL:HG22	1.83	0.61
5:I:828:PHE:HB3	5:I:1234:LYS:HD3	1.83	0.61
6:J:245:LEU:HD12	6:J:246:PRO:CD	2.31	0.61
8:L:27:VAL:O	8:L:31:LEU:HG	2.00	0.61
8:L:478:PRO:HB2	8:L:483:LEU:CD1	2.31	0.61
2:O:22:DT:H5"	4:M:265:ARG:HD3	1.83	0.61
5:I:251:ALA:HB2	5:I:269:ILE:CD1	2.31	0.61
5:I:856:ASN:CB	8:L:613:ASP:HA	2.31	0.61
5:I:940:GLU:HG3	5:I:941:LYS:H	1.66	0.61
8:L:338:HIS:O	8:L:342:GLN:HG2	2.00	0.61
4:G:234:LEU:HD13	4:G:234:LEU:H	1.66	0.60
5:I:197:ARG:NH1	5:I:201:ARG:O	2.34	0.60
5:I:301:TYR:HB2	5:I:311:CYS:SG	2.41	0.60
5:I:338:THR:CG2	5:I:345:PRO:HB3	2.31	0.60
5:I:564:PRO:HG2	5:I:568:ASN:O	2.01	0.60
6:J:560:ASN:OD1	6:J:560:ASN:N	2.33	0.60
6:J:1178:THR:HG23	6:J:1184:ASP:HB3	1.83	0.60
8:L:582:VAL:HG11	8:L:587:ILE:H	1.66	0.60
4:G:29:GLU:HB3	4:G:30:PRO:HD3	1.83	0.60
5:I:245:ARG:HB3	5:I:337:PHE:CE1	2.37	0.60
6:J:693:VAL:HG21	6:J:743:MET:HE3	1.83	0.60
5:I:657:THR:HG22	5:I:1187:PHE:HB2	1.82	0.60
8:L:561:MET:HE1	8:L:580:PHE:HE1	1.65	0.60
4:G:140:ILE:HD11	4:G:142:MET:HE2	1.82	0.60
5:I:297:VAL:HG12	5:I:315:MET:H	1.66	0.60
5:I:903:ARG:NH1	5:I:908:GLU:O	2.30	0.60
6:J:615:LYS:HB2	6:J:616:PRO:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:697:MET:CE	6:J:741:ALA:HB3	2.30	0.60
6:J:1144:LEU:CD2	6:J:1236:GLU:HG2	2.32	0.60
8:L:144:LEU:HD22	8:L:261:LEU:HD21	1.83	0.60
8:L:315:TRP:CZ3	8:L:316:PHE:HB2	2.37	0.60
5:I:490:GLN:NE2	8:L:473:GLU:HA	2.16	0.60
5:I:732:ILE:CD1	5:I:783:LEU:HB3	2.32	0.60
6:J:552:ILE:HB	6:J:570:LYS:HZ3	1.66	0.60
6:J:1272:SER:OG	6:J:1273:ASP:N	2.35	0.60
4:H:13:LEU:HG	4:H:29:GLU:HB3	1.82	0.60
5:I:528:ARG:NH2	5:I:576:SER:O	2.29	0.60
5:I:736:VAL:HG12	5:I:737:ASN:O	2.02	0.60
8:L:123:ILE:O	8:L:127:ILE:HG23	2.02	0.60
8:L:358:VAL:O	8:L:362:ASN:ND2	2.35	0.60
5:I:254:ASP:HB2	5:I:263:VAL:O	2.01	0.60
8:L:145:LEU:HD13	8:L:225:ARG:HE	1.67	0.60
5:I:854:ILE:HD11	5:I:885:GLY:HA3	1.83	0.60
5:I:935:THR:CG2	5:I:939:VAL:HB	2.32	0.60
5:I:1103:VAL:HG11	5:I:1112:ILE:CD1	2.30	0.60
6:J:1176:VAL:HG22	6:J:1187:GLU:CB	2.28	0.60
8:L:387:VAL:HG11	8:L:409:ASN:OD1	2.02	0.60
8:L:388:ILE:O	8:L:392:LYS:HG3	2.02	0.60
5:I:633:LEU:HB3	5:I:644:LEU:HB3	1.83	0.60
5:I:1333:LEU:HD23	6:J:307:LEU:HD22	1.84	0.60
8:L:562:ARG:NH2	8:L:571:TYR:O	2.35	0.60
8:L:577:GLY:O	8:L:581:ASP:N	2.34	0.60
3:P:34:DT:H71	5:I:497:PRO:HG2	1.84	0.59
6:J:1343:GLU:OE1	6:J:1373:ARG:NH2	2.35	0.59
2:O:23:DC:OP1	4:M:264:VAL:HB	2.02	0.59
5:I:321:LEU:O	5:I:325:LEU:HG	2.02	0.59
5:I:634:VAL:HG13	5:I:636:CYS:SG	2.42	0.59
5:I:983:GLY:CA	5:I:1003:THR:HG23	2.33	0.59
6:J:505:ASP:HB2	6:J:629:PHE:HE1	1.68	0.59
6:J:1172:LYS:HG3	6:J:1191:PRO:CA	2.32	0.59
3:P:31:DG:H5"	3:P:31:DG:H8	1.66	0.59
5:I:1212:LEU:HD22	5:I:1225:VAL:CG2	2.32	0.59
6:J:481:ARG:NH1	7:K:3:ARG:O	2.34	0.59
5:I:230:PHE:HB2	5:I:333:ILE:HG23	1.83	0.59
5:I:714:VAL:HB	5:I:787:PRO:HD2	1.83	0.59
5:I:748:ILE:CD1	5:I:967:LEU:HA	2.32	0.59
5:I:981:ALA:HA	5:I:984:VAL:HB	1.83	0.59
6:J:140:TYR:OH	6:J:312:ARG:HD2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:697:MET:HE1	6:J:741:ALA:HB3	1.84	0.59
6:J:733:SER:O	6:J:737:ILE:HG12	2.02	0.59
6:J:1363:TYR:O	6:J:1367:GLN:HG2	2.03	0.59
8:L:216:LEU:O	8:L:220:LYS:HG2	2.03	0.59
8:L:414:LYS:O	8:L:418:LYS:HG3	2.02	0.59
5:I:1024:GLU:HA	5:I:1027:LYS:HG3	1.85	0.59
6:J:505:ASP:HB2	6:J:629:PHE:CE1	2.38	0.59
6:J:1159:ILE:HD11	6:J:1177:ILE:HB	1.85	0.59
1:N:56:THR:O	1:N:57:LEU:HD23	2.03	0.59
4:G:232:VAL:O	4:H:218:ARG:HB2	2.02	0.59
5:I:577:VAL:HG23	5:I:661:VAL:O	2.03	0.59
5:I:1253:LEU:HA	8:L:525:ASP:HB2	1.85	0.59
8:L:15:ARG:HH22	8:L:26:GLU:HG2	1.67	0.59
8:L:287:ILE:HG12	8:L:337:VAL:HG13	1.85	0.59
8:L:316:PHE:CZ	8:L:334:SER:HA	2.38	0.59
5:I:490:GLN:HE21	8:L:473:GLU:HA	1.68	0.59
6:J:607:THR:O	6:J:611:ILE:HG13	2.03	0.59
6:J:887:SER:HB3	6:J:1227:HIS:HE1	1.67	0.59
4:H:67:GLU:HB3	4:H:68:TYR:HA	1.85	0.59
5:I:1184:THR:HG23	5:I:1190:ALA:H	1.67	0.59
6:J:514:THR:O	6:J:595:ALA:HA	2.01	0.59
6:J:694:SER:O	6:J:697:MET:HG3	2.03	0.59
8:L:290:LEU:HB3	8:L:333:VAL:CG2	2.33	0.59
5:I:254:ASP:HB3	5:I:265:LYS:HB2	1.84	0.59
5:I:866:ASP:HB3	5:I:872:TYR:CE1	2.38	0.59
6:J:454:CYS:HB3	6:J:459:ALA:O	2.02	0.59
6:J:510:LEU:O	6:J:514:THR:OG1	2.15	0.59
6:J:1265:THR:HG23	6:J:1279:GLN:HG3	1.83	0.59
4:H:54:CYS:SG	4:H:148:ARG:HG3	2.43	0.58
5:I:56:VAL:HG12	5:I:57:PHE:CD1	2.38	0.58
5:I:1281:TYR:CD2	6:J:484:MET:HG2	2.38	0.58
6:J:1217:PRO:HG3	6:J:1232:TYR:CE2	2.38	0.58
8:L:248:GLU:HA	8:L:251:LYS:HZ2	1.67	0.58
2:O:24:DC:H2”	2:O:25:DA:H5”	1.85	0.58
4:M:252:ILE:O	4:M:278:ILE:HD12	2.03	0.58
5:I:109:ALA:HB1	5:I:112:GLY:HA3	1.85	0.58
8:L:313:ASP:HB3	8:L:317:ASN:CB	2.31	0.58
8:L:582:VAL:HG11	8:L:587:ILE:N	2.19	0.58
5:I:237:LEU:CD2	5:I:289:VAL:HA	2.32	0.58
5:I:960:LEU:HB3	5:I:1025:PHE:CD1	2.38	0.58
10:I:1401:1N7:C3	10:I:1401:1N7:C18	2.73	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:448:ARG:NH2	8:L:502:LYS:HA	2.17	0.58
2:O:60:DG:H5'	5:I:371:ARG:NH2	2.19	0.58
5:I:854:ILE:HD11	5:I:885:GLY:CA	2.33	0.58
6:J:214:ARG:HA	6:J:217:LEU:HB2	1.85	0.58
8:L:214:PRO:O	8:L:218:ARG:HG3	2.03	0.58
8:L:233:ASP:O	8:L:236:LYS:NZ	2.33	0.58
4:G:118:ASP:OD1	4:G:118:ASP:N	2.36	0.58
5:I:45:GLY:H	5:I:54:ARG:HH21	1.51	0.58
5:I:452:ARG:NH1	5:I:584:TYR:O	2.36	0.58
5:I:496:LYS:HB3	5:I:497:PRO:HD3	1.84	0.58
5:I:979:LEU:HD13	5:I:1000:LEU:HD13	1.85	0.58
6:J:1190:ILE:HG21	6:J:1196:LEU:HD21	1.84	0.58
8:L:161:LEU:HG	8:L:162:ILE:HG23	1.85	0.58
8:L:355:ILE:O	8:L:359:LYS:HG3	2.04	0.58
8:L:562:ARG:NH1	8:L:573:LEU:HD13	2.15	0.58
3:P:59:DA:H2"	3:P:60:DA:C5'	2.34	0.58
5:I:65:ASN:OD1	5:I:65:ASN:N	2.30	0.58
5:I:444:ASP:O	5:I:450:ASN:ND2	2.37	0.58
5:I:1002:LEU:HD23	5:I:1003:THR:O	2.04	0.58
6:J:56:LEU:HD21	6:J:269:TYR:HB3	1.84	0.58
6:J:407:VAL:O	6:J:411:ILE:HG12	2.03	0.58
8:L:144:LEU:HD13	8:L:261:LEU:HD21	1.85	0.58
8:L:157:ARG:HB3	8:L:160:ASP:CB	2.31	0.58
8:L:256:PHE:HA	8:L:259:PHE:CD2	2.38	0.58
4:G:234:LEU:C	4:G:235:ARG:HH11	2.07	0.58
5:I:667:LEU:CD2	5:I:704:MET:HB3	2.34	0.58
6:J:647:PRO:HG3	6:J:697:MET:CB	2.34	0.58
6:J:724:MET:O	6:J:728:SER:OG	2.16	0.58
8:L:144:LEU:HD21	8:L:261:LEU:HD11	1.85	0.58
8:L:247:GLU:HG3	8:L:250:LEU:HD12	1.84	0.58
4:M:257:VAL:HA	4:M:260:LEU:CG	2.34	0.58
5:I:1282:GLY:O	5:I:1284:ALA:N	2.37	0.58
6:J:485:MET:HB3	6:J:488:ASN:HD22	1.69	0.58
8:L:309:ASN:ND2	8:L:312:SER:HB3	2.19	0.58
5:I:1340:GLU:HG3	6:J:1341:ARG:NH2	2.18	0.58
6:J:152:THR:OG1	6:J:154:LEU:HD13	2.04	0.58
6:J:1226:VAL:O	6:J:1229:VAL:HG12	2.04	0.58
8:L:42:GLU:O	8:L:45:ILE:HG22	2.04	0.58
8:L:146:GLU:O	8:L:150:ARG:HG3	2.04	0.58
4:H:64:VAL:HG23	4:H:65:LEU:H	1.69	0.58
6:J:357:VAL:HG13	6:J:461:PHE:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:548:ARG:HH12	5:I:568:ASN:HA	1.68	0.57
8:L:145:LEU:HB3	8:L:225:ARG:HH21	1.69	0.57
8:L:315:TRP:CH2	8:L:341:LEU:HD11	2.39	0.57
5:I:741:MET:HG2	5:I:974:ARG:HD2	1.86	0.57
5:I:1102:GLY:O	5:I:1106:ARG:HD3	2.04	0.57
5:I:1115:THR:HG22	5:I:1228:GLY:HA3	1.86	0.57
6:J:205:LEU:HG	6:J:217:LEU:CD1	2.33	0.57
8:L:410:ILE:HA	8:L:413:MET:HE3	1.85	0.57
2:O:24:DC:H3'	8:L:586:ARG:HH21	1.68	0.57
4:G:79:LEU:CD1	5:I:693:LEU:HD21	2.34	0.57
5:I:906:PHE:CD2	8:L:611:LEU:HG	2.36	0.57
5:I:981:ALA:CA	5:I:984:VAL:HB	2.34	0.57
5:I:1308:ILE:HG21	6:J:379:PRO:HB2	1.84	0.57
6:J:143:SER:HB2	6:J:159:ILE:HD13	1.86	0.57
6:J:869:CYS:HA	6:J:872:LEU:HD12	1.86	0.57
8:L:162:ILE:HG21	8:L:261:LEU:HG	1.86	0.57
3:P:45:DA:H5'	3:P:45:DA:C8	2.39	0.57
4:G:233:ASP:C	4:G:235:ARG:HG2	2.25	0.57
6:J:385:LEU:CD2	6:J:411:ILE:HG13	2.34	0.57
6:J:689:ALA:O	6:J:693:VAL:HG23	2.05	0.57
8:L:290:LEU:HB3	8:L:333:VAL:HG21	1.87	0.57
8:L:476:ARG:HG3	8:L:477:GLU:H	1.68	0.57
5:I:979:LEU:HG	5:I:1011:LEU:HD21	1.86	0.57
8:L:145:LEU:HD13	8:L:225:ARG:NE	2.18	0.57
8:L:235:ILE:HA	8:L:245:ALA:HB2	1.87	0.57
8:L:476:ARG:O	8:L:477:GLU:HG3	2.04	0.57
4:H:83:LEU:CD2	6:J:528:THR:HA	2.35	0.57
8:L:480:PRO:HA	8:L:483:LEU:HD13	1.86	0.57
1:N:23:ILE:HD13	6:J:679:TYR:HE2	1.69	0.57
4:G:102:LEU:O	4:G:141:SER:HA	2.04	0.57
5:I:229:ILE:HG12	5:I:334:GLU:HG2	1.87	0.57
6:J:203:GLU:O	6:J:206:ASN:HB3	2.05	0.57
6:J:337:ARG:O	6:J:342:LEU:HD13	2.05	0.57
6:J:573:THR:HG23	6:J:576:ARG:HD3	1.87	0.57
4:H:155:ALA:HA	4:H:158:ARG:NH1	2.19	0.57
5:I:1127:LYS:O	5:I:1131:MET:HG3	2.05	0.57
6:J:210:SER:O	6:J:214:ARG:HG2	2.04	0.57
6:J:1152:GLU:O	6:J:1214:PRO:HD2	2.05	0.57
3:P:33:DA:H2'	3:P:35:DG:N7	2.19	0.57
5:I:83:GLN:O	5:I:87:ILE:HG12	2.05	0.57
5:I:1070:HIS:NE2	5:I:1114:GLU:OE1	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:823:THR:HG22	6:J:879:ALA:HA	1.86	0.57
8:L:551:LEU:HD21	8:L:598:LEU:HD21	1.87	0.57
4:H:180:VAL:HG12	4:H:205:MET:HE1	1.86	0.57
6:J:334:LYS:HA	6:J:339:ARG:CG	2.35	0.57
8:L:565:ILE:HG22	8:L:566:ASP:OD2	2.04	0.57
4:H:58:GLU:OE2	4:H:145:LYS:HE2	2.04	0.56
5:I:426:ILE:HG23	5:I:430:LYS:HE3	1.86	0.56
5:I:1251:TYR:OH	6:J:348:ASP:OD2	2.16	0.56
6:J:847:ASP:HA	6:J:859:PRO:O	2.05	0.56
6:J:1288:ALA:O	6:J:1292:LEU:HD22	2.04	0.56
6:J:1350:ASN:HD22	6:J:1358:PRO:HD3	1.70	0.56
8:L:604:SER:O	8:L:604:SER:OG	2.08	0.56
3:P:56:DG:OP2	8:L:573:LEU:HB2	2.05	0.56
4:H:191:ARG:NH2	4:H:193:GLU:O	2.35	0.56
5:I:466:VAL:O	5:I:469:VAL:HG22	2.05	0.56
5:I:1328:LYS:HE2	6:J:100:GLU:O	2.04	0.56
6:J:706:VAL:CG1	6:J:716:GLN:HG2	2.35	0.56
10:N:102:1N7:H5	10:N:102:1N7:H31	1.87	0.56
2:O:44:DA:OP2	8:L:455:HIS:NE2	2.35	0.56
5:I:1132:LEU:HD13	5:I:1141:LEU:HD21	1.87	0.56
5:I:1333:LEU:HD21	6:J:327:LEU:HB2	1.86	0.56
6:J:114:ILE:HD11	6:J:311:ARG:CB	2.32	0.56
6:J:218:THR:HA	6:J:221:ILE:CG2	2.34	0.56
6:J:251:PRO:HB2	6:J:253:VAL:HG13	1.87	0.56
6:J:356:THR:HG23	6:J:446:ALA:HB1	1.87	0.56
6:J:513:MET:HG3	6:J:514:THR:HG23	1.85	0.56
6:J:1348:LYS:O	6:J:1352:ILE:HG12	2.05	0.56
5:I:195:PHE:CG	5:I:203:LYS:HD2	2.40	0.56
5:I:349:GLU:OE1	5:I:349:GLU:N	2.36	0.56
5:I:734:ILE:HG13	5:I:751:TYR:CE1	2.36	0.56
6:J:362:ARG:HG3	6:J:365:GLN:NE2	2.21	0.56
1:N:3:ASP:OD2	5:I:678:ARG:NH1	2.29	0.56
5:I:42:ASP:OD2	5:I:46:GLN:N	2.20	0.56
5:I:887:VAL:HB	5:I:913:VAL:CG2	2.36	0.56
6:J:398:LYS:NZ	8:L:532:LEU:HD22	2.21	0.56
8:L:134:VAL:O	8:L:273:MET:HE1	2.05	0.56
8:L:582:VAL:HB	8:L:587:ILE:HG12	1.88	0.56
5:I:136:PHE:CZ	5:I:456:VAL:HG11	2.41	0.56
5:I:515:MET:HE1	5:I:517:GLN:HE21	1.69	0.56
6:J:235:GLU:OE1	6:J:235:GLU:N	2.28	0.56
8:L:215:GLU:HA	8:L:218:ARG:HE	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:448:ARG:NH1	8:L:450:ILE:O	2.38	0.56
4:M:257:VAL:HG12	4:M:260:LEU:HD12	1.87	0.56
5:I:320:ASP:O	5:I:324:LYS:HG3	2.06	0.56
5:I:684:ASN:OD1	5:I:687:ARG:NH2	2.39	0.56
5:I:979:LEU:CD1	5:I:1000:LEU:HD13	2.35	0.56
6:J:654:ILE:HD13	6:J:760:THR:HB	1.88	0.56
8:L:345:GLN:HA	8:L:348:GLU:OE1	2.06	0.56
8:L:363:ARG:O	8:L:367:ILE:HG13	2.06	0.56
8:L:456:MET:O	8:L:460:ILE:HG13	2.05	0.56
5:I:160:ASP:OD2	5:I:164:THR:OG1	2.24	0.56
5:I:724:VAL:CG1	5:I:727:VAL:HG22	2.36	0.56
6:J:62:PHE:CD1	6:J:247:PRO:HD3	2.40	0.56
6:J:487:THR:O	6:J:614:LEU:HD21	2.06	0.56
6:J:1237:VAL:CG1	6:J:1253:ILE:HD12	2.36	0.56
8:L:462:LYS:HE2	8:L:465:ARG:NH2	2.21	0.56
4:G:192:VAL:HG12	4:G:194:GLN:H	1.70	0.56
5:I:27:LEU:O	5:I:528:ARG:HD2	2.06	0.56
5:I:1308:ILE:CG2	6:J:379:PRO:HB2	2.36	0.56
6:J:265:LEU:HD11	6:J:327:LEU:CD2	2.36	0.56
6:J:516:ASP:HA	6:J:545:HIS:HB2	1.88	0.56
8:L:134:VAL:HG13	8:L:273:MET:HE3	1.87	0.56
8:L:582:VAL:HG11	8:L:586:ARG:HB3	1.88	0.56
4:G:221:ALA:HB3	4:H:231:PHE:HB2	1.88	0.56
4:H:67:GLU:HA	4:H:68:TYR:O	2.05	0.56
5:I:559:CYS:HB2	5:I:662:SER:HB3	1.88	0.56
5:I:785:ASP:OD2	5:I:791:LEU:N	2.36	0.56
5:I:994:ARG:HG2	5:I:997:TRP:CH2	2.40	0.56
5:I:1109:ILE:O	5:I:1113:LEU:HD12	2.05	0.56
6:J:45:ASN:O	6:J:45:ASN:ND2	2.39	0.56
8:L:309:ASN:O	8:L:311:THR:HG23	2.05	0.56
8:L:569:THR:CA	8:L:570:ASP:HB2	2.36	0.56
5:I:43:PRO:HG2	5:I:44:GLU:OE1	2.05	0.55
5:I:256:GLU:O	5:I:285:ILE:HB	2.05	0.55
6:J:843:VAL:CG1	6:J:861:ASN:HA	2.37	0.55
8:L:403:ASP:OD1	8:L:403:ASP:N	2.39	0.55
4:M:251:PRO:O	4:M:254:LEU:HG	2.05	0.55
4:G:8:PHE:CD1	4:G:32:GLU:HG3	2.38	0.55
4:G:133:LEU:HD21	4:G:140:ILE:CG2	2.35	0.55
5:I:997:TRP:O	5:I:1000:LEU:HB2	2.06	0.55
5:I:1013:GLN:O	5:I:1017:GLN:NE2	2.39	0.55
6:J:436:ALA:CB	6:J:480:ALA:HB1	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:79:ALA:O	8:L:83:VAL:HG23	2.05	0.55
8:L:315:TRP:O	8:L:319:ALA:HB2	2.05	0.55
8:L:384:LEU:O	8:L:388:ILE:HG13	2.06	0.55
1:N:67:ARG:HD2	5:I:341:LEU:HD21	1.88	0.55
4:M:302:GLU:O	4:M:306:VAL:HG12	2.06	0.55
5:I:998:LEU:HB3	5:I:1015:ALA:HB1	1.88	0.55
6:J:113:HIS:CE1	6:J:115:TRP:HB2	2.41	0.55
6:J:885:VAL:HG11	6:J:1255:VAL:HA	1.89	0.55
8:L:270:VAL:O	8:L:274:ARG:HG3	2.06	0.55
6:J:568:SER:OG	6:J:569:LEU:N	2.39	0.55
6:J:1152:GLU:HA	6:J:1194:ARG:NH2	2.21	0.55
5:I:615:VAL:HG22	5:I:650:VAL:HA	1.87	0.55
5:I:616:ILE:O	5:I:636:CYS:HB3	2.06	0.55
4:G:10:LYS:NZ	4:H:229:GLU:OE2	2.37	0.55
6:J:115:TRP:CE2	6:J:1329:THR:HG23	2.41	0.55
6:J:205:LEU:CG	6:J:217:LEU:HB3	2.36	0.55
8:L:547:VAL:HG21	8:L:607:LEU:HD22	1.88	0.55
5:I:254:ASP:HB3	5:I:265:LYS:N	2.22	0.55
5:I:905:ILE:O	8:L:599:ARG:NE	2.40	0.55
5:I:1080:ASN:HD22	5:I:1081:PRO:HD2	1.71	0.55
5:I:1281:TYR:CE1	6:J:431:ARG:HD3	2.41	0.55
6:J:596:LEU:HD22	6:J:600:ALA:HB1	1.89	0.55
6:J:1347:LEU:HD12	6:J:1358:PRO:HD2	1.88	0.55
8:L:256:PHE:HA	8:L:259:PHE:CE2	2.42	0.55
8:L:492:ASP:O	8:L:496:LYS:HG2	2.07	0.55
5:I:339:ASN:OD1	5:I:340:ASP:N	2.40	0.55
8:L:145:LEU:HB3	8:L:225:ARG:NH2	2.21	0.55
8:L:445:ASP:OD1	8:L:451:ARG:HD2	2.06	0.55
8:L:470:MET:SD	8:L:478:PRO:HB3	2.47	0.55
5:I:160:ASP:O	5:I:161:LYS:HG2	2.06	0.55
5:I:272:ARG:O	5:I:276:GLN:HG3	2.07	0.55
5:I:311:CYS:HB2	5:I:315:MET:CE	2.37	0.55
5:I:483:ASP:OD1	5:I:483:ASP:N	2.40	0.55
5:I:1008:GLN:OE1	5:I:1011:LEU:HD12	2.07	0.55
5:I:1292:THR:HG21	5:I:1317:PRO:HB2	1.89	0.55
6:J:125:GLY:HA2	6:J:135:ILE:HD11	1.88	0.55
6:J:198:CYS:SG	6:J:224:LEU:HB3	2.47	0.55
8:L:61:ASP:OD1	8:L:62:ALA:N	2.40	0.55
2:O:23:DC:P	4:M:264:VAL:HB	2.47	0.55
5:I:452:ARG:NH2	5:I:458:GLU:OE2	2.40	0.55
5:I:517:GLN:O	5:I:518:ASN:C	2.44	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:895:LEU:HD23	5:I:895:LEU:H	1.71	0.55
5:I:1246:ARG:NE	6:J:348:ASP:OD1	2.29	0.55
8:L:12:LEU:HB2	8:L:30:HIS:HB3	1.88	0.55
2:O:42:DA:H4'	2:O:43:DA:OP1	2.07	0.54
5:I:560:PRO:CB	6:J:776:THR:HG21	2.37	0.54
5:I:1072:ASN:ND2	5:I:1111:GLN:OE1	2.38	0.54
5:I:1319:MET:HG3	5:I:1320:PRO:CD	2.37	0.54
6:J:259:ARG:NH1	8:L:504:PRO:HA	2.21	0.54
6:J:288:PRO:HB3	8:L:377:LYS:HG3	1.89	0.54
6:J:571:ASP:N	6:J:571:ASP:OD1	2.41	0.54
8:L:132:CYS:O	8:L:136:GLU:HG3	2.07	0.54
8:L:551:LEU:HD11	8:L:598:LEU:HD11	1.88	0.54
4:G:133:LEU:HD21	4:G:140:ILE:HG23	1.89	0.54
4:G:236:ASP:CA	4:H:14:VAL:O	2.52	0.54
4:H:186:ASN:ND2	4:H:188:GLU:OE2	2.39	0.54
5:I:245:ARG:HB3	5:I:337:PHE:CZ	2.42	0.54
5:I:1294:LYS:HD3	6:J:472:LEU:CD1	2.36	0.54
8:L:236:LYS:H	8:L:236:LYS:HD2	1.71	0.54
8:L:320:ILE:HG21	8:L:331:HIS:CE1	2.42	0.54
8:L:339:ARG:HA	8:L:342:GLN:HG2	1.88	0.54
8:L:561:MET:HG3	8:L:571:TYR:HD2	1.72	0.54
4:M:285:THR:O	4:M:289:LEU:HG	2.07	0.54
5:I:135:THR:CG2	5:I:527:LYS:HE2	2.36	0.54
5:I:297:VAL:HG12	5:I:315:MET:O	2.08	0.54
5:I:898:GLU:O	5:I:902:LEU:HB2	2.07	0.54
6:J:204:GLU:HB2	6:J:217:LEU:CD1	2.35	0.54
8:L:491:GLU:OE2	8:L:495:ARG:NH2	2.34	0.54
4:G:92:VAL:HG21	4:G:95:LYS:O	2.07	0.54
5:I:459:MET:SD	5:I:511:LEU:HD13	2.47	0.54
6:J:154:LEU:HD11	6:J:176:PHE:CE2	2.43	0.54
5:I:568:ASN:HB2	5:I:571:LEU:HB2	1.89	0.54
5:I:966:ILE:HD11	10:I:1401:1N7:H15	1.89	0.54
5:I:994:ARG:HG2	5:I:997:TRP:CZ3	2.42	0.54
6:J:478:LEU:CG	7:K:47:THR:HG23	2.34	0.54
8:L:448:ARG:HH21	8:L:502:LYS:HA	1.71	0.54
5:I:402:ARG:HD2	5:I:406:ASN:ND2	2.22	0.54
5:I:1276:TRP:CE2	6:J:801:VAL:HG21	2.43	0.54
6:J:197:GLU:O	6:J:201:LEU:HD23	2.07	0.54
8:L:14:THR:O	8:L:18:GLU:HG2	2.07	0.54
4:H:24:ALA:HB3	4:H:213:PRO:HB2	1.89	0.54
5:I:135:THR:HG23	5:I:527:LYS:HE2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:275:ARG:O	5:I:278:GLU:HG2	2.08	0.54
5:I:803:ALA:HA	5:I:1227:VAL:HG12	1.90	0.54
5:I:1082:ILE:O	5:I:1082:ILE:HG12	2.08	0.54
5:I:1130:ALA:O	5:I:1134:GLN:HG3	2.07	0.54
4:G:228:LEU:HD11	4:H:224:LEU:HG	1.88	0.54
5:I:1138:VAL:O	5:I:1142:ARG:HB2	2.08	0.54
6:J:53:ARG:CZ	6:J:60:ARG:HD2	2.38	0.54
6:J:1253:ILE:O	6:J:1257:VAL:HG23	2.08	0.54
8:L:21:TYR:HB2	8:L:56:MET:CE	2.37	0.54
8:L:359:LYS:HA	8:L:362:ASN:HD21	1.73	0.54
8:L:463:LEU:HD12	8:L:497:VAL:HG11	1.89	0.54
1:N:67:ARG:O	1:N:70:LYS:HB3	2.07	0.54
3:P:63:DG:H2"	3:P:64:DA:C8	2.43	0.54
4:G:57:THR:HG22	4:G:58:GLU:HG3	1.89	0.54
4:H:77:ASP:O	4:H:80:GLU:HB3	2.07	0.54
5:I:521:LEU:O	5:I:521:LEU:HD22	2.07	0.54
5:I:565:GLU:HA	5:I:569:ILE:CD1	2.37	0.54
5:I:759:SER:HG	5:I:763:THR:HG1	1.54	0.54
6:J:573:THR:HG23	6:J:576:ARG:NH1	2.23	0.54
8:L:98:VAL:O	8:L:102:MET:HG2	2.08	0.54
8:L:339:ARG:HB3	8:L:343:LYS:NZ	2.23	0.54
8:L:351:THR:CB	8:L:358:VAL:HG21	2.34	0.54
8:L:586:ARG:O	8:L:590:ILE:HG13	2.07	0.54
4:M:252:ILE:HD11	4:M:310:ARG:NH1	2.22	0.54
4:G:107:ILE:HG13	4:G:136:GLU:HA	1.90	0.54
5:I:125:GLY:HA3	5:I:499:SER:HB2	1.90	0.54
5:I:637:ARG:HA	5:I:642:SER:HA	1.90	0.54
5:I:1246:ARG:NH2	5:I:1258:PRO:HB3	2.23	0.54
6:J:511:TYR:OH	6:J:727:ASP:OD2	2.17	0.54
6:J:905:ARG:HB2	6:J:907:HIS:CE1	2.43	0.54
6:J:1233:ILE:O	6:J:1237:VAL:HG12	2.08	0.54
8:L:245:ALA:HA	8:L:248:GLU:CB	2.37	0.54
5:I:515:MET:CE	5:I:517:GLN:CG	2.86	0.53
5:I:963:GLU:OE1	5:I:964:LEU:N	2.41	0.53
5:I:994:ARG:HA	5:I:997:TRP:CD2	2.42	0.53
6:J:154:LEU:HD21	6:J:176:PHE:CD2	2.42	0.53
6:J:265:LEU:HD11	6:J:327:LEU:HD23	1.89	0.53
8:L:7:SER:O	8:L:11:LEU:HG	2.08	0.53
8:L:40:GLN:OE1	8:L:93:ARG:HB3	2.08	0.53
4:M:260:LEU:HD21	4:M:278:ILE:CD1	2.38	0.53
4:G:9:LEU:N	4:G:32:GLU:OE2	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:617:ALA:HA	5:I:636:CYS:SG	2.49	0.53
5:I:828:PHE:O	5:I:1234:LYS:HE2	2.07	0.53
5:I:968:GLU:HB2	5:I:1018:TYR:HE1	1.71	0.53
5:I:1308:ILE:HD12	5:I:1313:HIS:CD2	2.44	0.53
6:J:51:PRO:HB3	6:J:57:PHE:O	2.07	0.53
6:J:517:CYS:HB3	6:J:719:PHE:CZ	2.44	0.53
6:J:801:VAL:HG12	6:J:920:ALA:HB3	1.91	0.53
2:O:59:DG:C3'	5:I:371:ARG:HH12	2.22	0.53
4:G:221:ALA:CB	4:H:231:PHE:HB2	2.39	0.53
4:G:233:ASP:N	4:G:233:ASP:OD1	2.41	0.53
4:H:135:ASP:HB2	4:H:138:ALA:HB2	1.89	0.53
5:I:983:GLY:HA2	5:I:1003:THR:HG23	1.89	0.53
5:I:1002:LEU:HD13	5:I:1011:LEU:HD11	1.90	0.53
6:J:133:ARG:O	6:J:137:ARG:HG3	2.08	0.53
8:L:151:VAL:CG1	8:L:158:LEU:HD23	2.38	0.53
3:P:31:DG:H2"	3:P:32:DA:C8	2.44	0.53
4:M:265:ARG:HA	4:M:268:ASN:ND2	2.23	0.53
4:H:222:THR:O	4:H:226:GLU:HG3	2.08	0.53
5:I:67:GLU:O	5:I:102:LEU:HD12	2.08	0.53
5:I:1100:PRO:HG3	6:J:637:ALA:O	2.07	0.53
6:J:1196:LEU:HD13	6:J:1210:ILE:HG23	1.91	0.53
1:N:20:ILE:HG13	6:J:754:ILE:CD1	2.39	0.53
4:M:278:ILE:CG2	4:M:312:LEU:HD13	2.36	0.53
5:I:942:ASP:OD1	5:I:942:ASP:N	2.42	0.53
6:J:572:THR:HG21	6:J:589:TYR:CE2	2.44	0.53
8:L:39:ASP:HB2	8:L:99:ARG:HH12	1.73	0.53
4:G:234:LEU:CA	4:G:235:ARG:CB	2.84	0.53
5:I:544:GLY:HA3	5:I:546:GLU:N	2.23	0.53
5:I:961:SER:O	5:I:965:GLN:HG2	2.08	0.53
5:I:1305:TYR:CE2	6:J:379:PRO:HG3	2.42	0.53
6:J:362:ARG:HD3	6:J:364:HIS:HE1	1.73	0.53
6:J:822:MET:SD	6:J:838:ARG:NH2	2.81	0.53
6:J:1164:SER:O	6:J:1175:LEU:HG	2.09	0.53
6:J:1265:THR:CG2	6:J:1279:GLN:HG3	2.38	0.53
6:J:1292:LEU:O	6:J:1297:LYS:HB2	2.09	0.53
8:L:470:MET:HE1	8:L:486:ARG:HB2	1.89	0.53
4:M:278:ILE:O	4:M:282:VAL:HG13	2.09	0.53
4:H:11:PRO:HG3	4:H:31:LEU:CD2	2.38	0.53
5:I:189:ASP:HB2	5:I:195:PHE:CE2	2.44	0.53
5:I:253:PHE:CZ	5:I:288:PRO:HD3	2.44	0.53
5:I:254:ASP:HB3	5:I:265:LYS:CA	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:591:TYR:OH	5:I:611:GLU:OE1	2.22	0.53
6:J:288:PRO:O	6:J:292:VAL:HG22	2.08	0.53
6:J:1211:SER:OG	6:J:1212:ASP:N	2.39	0.53
8:L:326:TRP:HA	8:L:329:LYS:HD2	1.90	0.53
4:G:93:GLN:N	4:G:120:ASP:O	2.42	0.53
5:I:71:VAL:HB	5:I:99:LYS:O	2.09	0.53
5:I:103:VAL:HG12	5:I:117:ILE:CG2	2.39	0.53
5:I:1247:SER:HB3	6:J:375:GLU:O	2.09	0.53
5:I:1339:LEU:HB3	6:J:17:PHE:HB3	1.91	0.53
6:J:483:LEU:CD2	7:K:16:ARG:HG2	2.38	0.53
8:L:129:GLN:NE2	8:L:367:ILE:HB	2.24	0.53
4:H:191:ARG:CB	4:H:196:THR:HG22	2.39	0.53
5:I:814:ASP:CB	6:J:462:ASP:HB3	2.39	0.53
5:I:1325:VAL:HG22	6:J:249:LEU:HD22	1.91	0.53
6:J:169:LEU:O	6:J:169:LEU:HD13	2.09	0.53
6:J:391:ALA:HB2	6:J:400:MET:SD	2.49	0.53
8:L:601:PRO:O	8:L:602:SER:OG	2.26	0.53
2:O:57:DT:H6	2:O:57:DT:H5'	1.74	0.53
5:I:88:ARG:NH1	5:I:88:ARG:HB2	2.24	0.53
6:J:502:PRO:HB3	6:J:506:VAL:HG11	1.89	0.53
6:J:587:LEU:HD21	6:J:608:CYS:HB2	1.91	0.53
6:J:686:TRP:CD2	6:J:758:PRO:HG2	2.44	0.53
8:L:119:ILE:HG21	8:L:379:MET:HB2	1.90	0.53
8:L:162:ILE:CG2	8:L:261:LEU:HG	2.39	0.53
8:L:264:LYS:HA	8:L:267:ASP:OD2	2.09	0.53
4:H:109:PRO:HB3	4:H:132:HIS:NE2	2.25	0.52
4:H:124:VAL:HG21	4:H:209:GLY:HA3	1.90	0.52
5:I:742:TYR:O	5:I:744:GLY:N	2.42	0.52
6:J:327:LEU:O	6:J:331:ILE:HG13	2.09	0.52
6:J:1265:THR:O	6:J:1303:SER:N	2.33	0.52
2:O:36:DA:H2"	2:O:37:DA:H5"	1.90	0.52
2:O:56:DC:C2'	2:O:57:DT:H71	2.40	0.52
3:P:67:DT:H2"	3:P:68:DG:OP2	2.09	0.52
4:G:234:LEU:N	4:G:235:ARG:HG2	2.24	0.52
4:H:42:ALA:O	4:H:46:ILE:HG13	2.09	0.52
5:I:70:TYR:HA	5:I:100:LEU:CD2	2.39	0.52
5:I:148:GLN:O	5:I:453:ILE:HA	2.08	0.52
5:I:844:LYS:N	5:I:844:LYS:HD2	2.23	0.52
5:I:974:ARG:O	5:I:978:VAL:HG23	2.09	0.52
6:J:254:PRO:HG3	6:J:260:PHE:CE1	2.45	0.52
3:P:63:DG:H2"	3:P:64:DA:N7	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:229:GLU:O	4:G:232:VAL:HG12	2.10	0.52
5:I:885:GLY:HA2	5:I:917:SER:HB2	1.90	0.52
5:I:1120:ALA:O	5:I:1124:ILE:HG12	2.10	0.52
6:J:1333:THR:O	6:J:1337:VAL:HG22	2.09	0.52
1:N:64:TYR:OH	5:I:340:ASP:OD2	2.28	0.52
5:I:298:ALA:HB3	5:I:334:GLU:HB2	1.90	0.52
5:I:421:SER:O	5:I:425:ILE:HG13	2.10	0.52
5:I:575:LEU:HG	5:I:579:ALA:HB3	1.91	0.52
5:I:1256:GLN:HB3	5:I:1301:ARG:HH22	1.75	0.52
5:I:1257:GLN:HG3	5:I:1296:ASP:OD1	2.10	0.52
6:J:97:VAL:O	6:J:101:ARG:HG3	2.10	0.52
6:J:355:ILE:HA	6:J:447:ILE:O	2.09	0.52
6:J:823:THR:HB	6:J:824:PRO:HD2	1.90	0.52
6:J:1167:LYS:HB3	6:J:1174:ARG:CD	2.32	0.52
8:L:128:ASN:HA	8:L:131:GLN:OE1	2.08	0.52
8:L:165:PHE:CE1	8:L:259:PHE:HB3	2.44	0.52
5:I:325:LEU:O	5:I:330:HIS:HB2	2.09	0.52
5:I:803:ALA:CB	5:I:1094:VAL:HG11	2.39	0.52
5:I:953:LEU:HD21	5:I:1033:ARG:HG3	1.92	0.52
6:J:747:MET:SD	6:J:759:ILE:HG13	2.49	0.52
8:L:320:ILE:HG23	8:L:327:SER:O	2.10	0.52
8:L:419:PHE:CE2	8:L:427:PHE:HA	2.45	0.52
5:I:58:PRO:HB2	5:I:67:GLU:OE2	2.08	0.52
5:I:794:LEU:HG	5:I:796:LEU:HD13	1.91	0.52
5:I:898:GLU:HA	5:I:901:LEU:HB3	1.91	0.52
5:I:1261:GLY:O	5:I:1266:GLY:N	2.40	0.52
5:I:1319:MET:HG3	5:I:1320:PRO:HD2	1.91	0.52
6:J:258:GLY:O	8:L:501:ALA:HB2	2.10	0.52
6:J:421:VAL:HG13	6:J:439:PRO:HG3	1.92	0.52
6:J:825:VAL:CG2	6:J:833:GLU:HB3	2.38	0.52
1:N:15:LEU:HD21	6:J:752:GLY:HA2	1.90	0.52
3:P:25:DG:H2"	3:P:26:DC:H5'	1.92	0.52
4:M:253:LEU:HB3	4:M:279:GLY:HA3	1.92	0.52
4:M:269:CYS:CB	4:M:295:LEU:HD12	2.39	0.52
5:I:320:ASP:OD1	5:I:321:LEU:N	2.42	0.52
6:J:649:LYS:HD2	6:J:652:GLU:OE1	2.09	0.52
6:J:1341:ARG:HD3	6:J:1343:GLU:HG2	1.92	0.52
8:L:245:ALA:HA	8:L:248:GLU:CG	2.39	0.52
5:I:868:SER:OG	5:I:942:ASP:OD2	2.27	0.52
5:I:1225:VAL:HA	6:J:638:SER:CB	2.38	0.52
8:L:51:MET:N	8:L:52:GLY:HA2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:26:DT:H2"	2:O:27:DT:O5'	2.09	0.52
4:H:23:HIS:ND1	4:H:206:GLU:HG2	2.24	0.52
5:I:477:GLU:O	5:I:480:SER:HB3	2.10	0.52
5:I:565:GLU:HA	5:I:569:ILE:HD13	1.92	0.52
5:I:1106:ARG:O	5:I:1108:ASN:N	2.39	0.52
5:I:1109:ILE:HD12	6:J:641:ILE:CD1	2.39	0.52
5:I:1184:THR:CG2	5:I:1189:GLY:HA3	2.39	0.52
6:J:56:LEU:CD2	6:J:269:TYR:HB3	2.40	0.52
6:J:115:TRP:HB3	6:J:1333:THR:HG22	1.90	0.52
6:J:215:LYS:HE2	6:J:216:LYS:HG2	1.92	0.52
6:J:287:ALA:HB1	6:J:288:PRO:HD2	1.92	0.52
8:L:334:SER:O	8:L:338:HIS:CB	2.58	0.52
1:N:64:TYR:CD1	5:I:341:LEU:HD22	2.45	0.52
4:G:232:VAL:CG1	4:G:233:ASP:N	2.73	0.52
5:I:231:GLU:HA	5:I:331:LYS:O	2.08	0.52
5:I:292:ILE:HB	5:I:322:LEU:HD11	1.91	0.52
5:I:1291:LEU:CD1	6:J:1351:VAL:HG13	2.40	0.52
6:J:483:LEU:HD21	7:K:16:ARG:HG2	1.92	0.52
6:J:1327:GLU:OE2	6:J:1329:THR:HB	2.10	0.52
8:L:96:ASP:O	8:L:100:MET:HG3	2.10	0.52
5:I:832:HIS:CD2	5:I:1058:ARG:HG3	2.45	0.51
5:I:1002:LEU:HB3	5:I:1008:GLN:OE1	2.10	0.51
6:J:333:GLY:O	6:J:336:GLY:N	2.35	0.51
6:J:657:ALA:O	6:J:661:VAL:HG13	2.10	0.51
6:J:1367:GLN:O	6:J:1371:ARG:HG2	2.10	0.51
8:L:122:ARG:CG	8:L:371:LYS:HE2	2.40	0.51
2:O:26:DT:C7	8:L:586:ARG:HB2	2.41	0.51
2:O:56:DC:H2'	2:O:57:DT:H71	1.92	0.51
2:O:60:DG:H1'	2:O:61:DC:H5'	1.92	0.51
4:M:288:GLU:HA	4:M:291:LYS:HG3	1.92	0.51
4:G:26:VAL:HG11	4:G:217:ILE:CD1	2.41	0.51
4:G:47:LEU:HD23	4:G:51:MET:HE3	1.91	0.51
4:H:214:GLU:OE2	4:H:218:ARG:NH2	2.44	0.51
5:I:447:HIS:CD2	5:I:553:THR:HG21	2.45	0.51
5:I:1292:THR:HG21	5:I:1317:PRO:CB	2.39	0.51
6:J:804:ALA:HA	6:J:1259:GLN:HG3	1.93	0.51
6:J:1151:LYS:H	6:J:1151:LYS:HD2	1.75	0.51
6:J:1282:TYR:HA	6:J:1285:VAL:CG1	2.41	0.51
8:L:24:TYR:CE2	8:L:57:GLU:HB2	2.45	0.51
8:L:51:MET:CE	8:L:84:LEU:HD12	2.40	0.51
8:L:585:GLU:O	8:L:589:GLN:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:35:DG:H2”	8:L:397:ARG:NH2	2.25	0.51
4:M:285:THR:OG1	4:M:286:GLU:N	2.44	0.51
4:G:234:LEU:N	4:G:234:LEU:CD1	2.73	0.51
5:I:803:ALA:CB	5:I:1227:VAL:HG12	2.40	0.51
5:I:888:THR:HG22	5:I:889:PRO:HD2	1.92	0.51
6:J:762:ASN:OD1	6:J:762:ASN:N	2.42	0.51
6:J:1155:ILE:HG12	6:J:1211:SER:H	1.75	0.51
6:J:1167:LYS:HG2	6:J:1168:GLU:N	2.26	0.51
8:L:215:GLU:HA	8:L:218:ARG:NE	2.24	0.51
8:L:265:GLN:O	8:L:269:LEU:HG	2.10	0.51
8:L:316:PHE:HZ	8:L:334:SER:HA	1.74	0.51
3:P:60:DA:H2’	3:P:61:DT:H71	1.92	0.51
4:M:284:ARG:HD2	4:M:288:GLU:OE2	2.10	0.51
5:I:956:ALA:CB	5:I:1032:LYS:HG2	2.39	0.51
5:I:1243:MET:HE3	6:J:445:LYS:CB	2.37	0.51
6:J:591:ILE:CG2	6:J:592:VAL:HG13	2.41	0.51
6:J:611:ILE:CB	6:J:612:LEU:HD12	2.39	0.51
7:K:64:LEU:O	7:K:68:GLU:HG2	2.10	0.51
8:L:50:ASP:OD2	8:L:80:ALA:HB2	2.11	0.51
3:P:36:DC:O4’	8:L:397:ARG:NH1	2.38	0.51
4:G:179:PRO:HG3	4:G:211:ILE:HG13	1.93	0.51
5:I:156:PHE:CD2	5:I:177:ILE:HD12	2.45	0.51
5:I:195:PHE:CD2	5:I:203:LYS:HD2	2.46	0.51
5:I:363:LEU:HD13	5:I:382:GLU:HA	1.93	0.51
5:I:975:ILE:HD11	5:I:1014:LEU:HB3	1.91	0.51
10:I:1401:1N7:C19	10:I:1401:1N7:C4	2.85	0.51
6:J:664:ILE:CD1	6:J:678:ARG:HB2	2.40	0.51
6:J:850:LYS:N	6:J:855:ASP:O	2.40	0.51
8:L:47:MET:SD	8:L:80:ALA:HA	2.51	0.51
4:H:191:ARG:HB2	4:H:196:THR:HG22	1.92	0.51
5:I:76:GLY:O	5:I:94:ALA:HB1	2.11	0.51
5:I:125:GLY:N	5:I:495:ALA:HB1	2.24	0.51
5:I:241:LEU:CD2	5:I:277:LEU:HD23	2.39	0.51
5:I:360:LEU:O	5:I:364:VAL:HG23	2.11	0.51
6:J:573:THR:HG23	6:J:576:ARG:HH11	1.75	0.51
6:J:1261:LEU:O	6:J:1304:ARG:NH1	2.44	0.51
2:O:32:DA:H2”	2:O:33:DA:C8	2.46	0.51
4:M:262:LEU:HD12	4:M:270:LEU:HD11	1.92	0.51
4:H:64:VAL:CG1	4:H:71:LYS:HD3	2.41	0.51
4:H:152:TYR:OH	6:J:532:GLU:OE2	2.24	0.51
4:H:181:GLU:O	6:J:535:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:338:THR:HB	5:I:345:PRO:HB3	1.93	0.51
5:I:685:MET:SD	5:I:1073:LYS:HB3	2.50	0.51
5:I:1122:LYS:HG2	5:I:1229:TYR:CE1	2.46	0.51
5:I:1339:LEU:HD23	6:J:17:PHE:CD1	2.46	0.51
6:J:288:PRO:CD	6:J:291:ILE:HD12	2.40	0.51
8:L:147:GLN:O	8:L:151:VAL:HG23	2.11	0.51
8:L:244:THR:O	8:L:248:GLU:HG3	2.10	0.51
8:L:244:THR:O	8:L:248:GLU:N	2.39	0.51
8:L:356:GLU:O	8:L:359:LYS:HB2	2.11	0.51
2:O:59:DG:H2"	2:O:60:DG:C8	2.46	0.51
5:I:144:VAL:HG23	5:I:515:MET:HB2	1.91	0.51
5:I:204:LEU:HD11	5:I:369:MET:CE	2.38	0.51
6:J:398:LYS:HE2	8:L:532:LEU:CD1	2.41	0.51
6:J:527:LEU:CD2	6:J:548:VAL:HG21	2.40	0.51
6:J:646:ILE:HD13	6:J:762:ASN:HD21	1.75	0.51
6:J:1163:VAL:HG13	6:J:1200:GLU:O	2.10	0.51
8:L:150:ARG:HB3	8:L:155:GLU:OE1	2.10	0.51
8:L:462:LYS:HE2	8:L:465:ARG:HH21	1.76	0.51
8:L:471:LEU:HD12	8:L:477:GLU:CG	2.41	0.51
4:H:64:VAL:HG13	4:H:71:LYS:HD3	1.93	0.51
4:H:83:LEU:HD11	6:J:526:VAL:HB	1.92	0.51
5:I:284:LEU:HD12	5:I:284:LEU:O	2.11	0.51
5:I:1043:ALA:HB1	5:I:1044:PRO:HD2	1.93	0.51
5:I:1342:GLU:HB3	6:J:16:GLU:O	2.11	0.51
6:J:115:TRP:HB3	6:J:1333:THR:CG2	2.40	0.51
6:J:128:LEU:HD21	6:J:189:LEU:HD23	1.93	0.51
6:J:146:VAL:HG23	6:J:158:GLN:O	2.10	0.51
8:L:407:GLU:HG3	8:L:442:SER:OG	2.11	0.51
8:L:463:LEU:HD12	8:L:497:VAL:CG1	2.40	0.51
10:N:102:1N7:H25	6:J:937:ILE:HG21	1.92	0.51
5:I:949:GLU:OE2	5:I:1037:THR:HA	2.11	0.51
5:I:983:GLY:CA	5:I:1002:LEU:HG	2.34	0.51
5:I:1142:ARG:HH22	5:I:1166:ASP:HA	1.75	0.51
5:I:1152:GLY:HA2	5:I:1194:GLU:HG2	1.92	0.51
6:J:26:SER:O	6:J:30:ILE:HG13	2.11	0.51
8:L:48:ILE:O	8:L:51:MET:HB2	2.10	0.51
8:L:56:MET:CE	8:L:60:PRO:HD3	2.41	0.51
8:L:134:VAL:HG22	8:L:273:MET:HE3	1.92	0.51
8:L:277:MET:HE2	8:L:281:ARG:NH2	2.26	0.51
4:G:25:LYS:HD2	4:G:204:GLU:HG2	1.92	0.50
5:I:6:THR:HG23	5:I:781:ASP:OD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:660:VAL:HG11	6:J:769:VAL:CG1	2.40	0.50
5:I:983:GLY:HA3	5:I:1003:THR:H	1.76	0.50
6:J:450:HIS:HB3	6:J:453:VAL:HG23	1.92	0.50
8:L:390:ILE:HD12	8:L:435:ILE:HG21	1.92	0.50
1:N:36:LEU:HD23	1:N:43:PRO:HA	1.94	0.50
4:G:57:THR:HG21	4:G:147:GLN:NE2	2.27	0.50
5:I:255:ILE:HG22	5:I:262:TYR:CB	2.40	0.50
5:I:582:ASN:HB2	5:I:586:PHE:O	2.11	0.50
3:P:23:DA:H1'	3:P:24:DG:O4'	2.11	0.50
4:G:14:VAL:HG23	4:G:15:ASP:OD1	2.11	0.50
5:I:1095:ASP:O	5:I:1096:ILE:HG13	2.11	0.50
5:I:1296:ASP:OD2	5:I:1322:SER:N	2.44	0.50
6:J:139:LEU:HD13	6:J:185:ILE:HG13	1.92	0.50
6:J:783:LEU:HA	6:J:786:THR:CG2	2.41	0.50
3:P:47:DC:H4'	3:P:48:DC:OP1	2.10	0.50
4:H:90:VAL:CG1	4:H:121:VAL:HG13	2.41	0.50
8:L:548:LEU:CD1	8:L:560:ARG:HG3	2.41	0.50
8:L:555:GLU:HB3	8:L:594:ALA:HB2	1.92	0.50
2:O:37:DA:H2"	2:O:38:DG:C8	2.46	0.50
4:H:46:ILE:CD1	4:H:224:LEU:HB2	2.41	0.50
5:I:909:LYS:HA	5:I:909:LYS:CE	2.41	0.50
5:I:1271:GLY:O	5:I:1275:VAL:HG23	2.11	0.50
6:J:259:ARG:NH2	8:L:504:PRO:O	2.44	0.50
6:J:792:ASN:OD1	6:J:792:ASN:N	2.44	0.50
2:O:44:DA:H2'	8:L:455:HIS:CE1	2.42	0.50
4:M:269:CYS:HB3	4:M:295:LEU:HD12	1.94	0.50
4:G:16:ILE:HD12	4:G:214:GLU:HB2	1.94	0.50
6:J:53:ARG:NH1	6:J:88:CYS:O	2.41	0.50
6:J:154:LEU:HD21	6:J:176:PHE:CG	2.46	0.50
6:J:746:LEU:H	6:J:746:LEU:HD12	1.77	0.50
5:I:157:PHE:CZ	5:I:431:LYS:HG2	2.46	0.50
5:I:311:CYS:HB2	5:I:315:MET:HE2	1.92	0.50
5:I:667:LEU:HD23	5:I:704:MET:HB3	1.92	0.50
5:I:823:VAL:HG23	5:I:1060:ILE:HG22	1.93	0.50
5:I:1138:VAL:HG21	5:I:1166:ASP:OD1	2.12	0.50
8:L:567:MET:HG3	8:L:569:THR:O	2.11	0.50
3:P:22:DA:H1'	3:P:23:DA:H5'	1.93	0.50
3:P:59:DA:H4'	3:P:60:DA:OP1	2.12	0.50
4:M:250:ASP:OD2	4:M:252:ILE:HG22	2.12	0.50
4:M:321:TRP:HA	4:M:322:PRO:O	2.11	0.50
4:G:13:LEU:HA	4:G:27:THR:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:79:LEU:HD11	5:I:693:LEU:HD21	1.93	0.50
4:G:205:MET:HE1	4:G:217:ILE:HD12	1.94	0.50
5:I:22:LEU:HD13	5:I:23:ASP:O	2.12	0.50
5:I:109:ALA:HB1	5:I:112:GLY:CA	2.42	0.50
5:I:1073:LYS:NZ	6:J:462:ASP:OD2	2.43	0.50
8:L:280:VAL:HG11	8:L:355:ILE:HG23	1.93	0.50
2:O:22:DT:H5'	4:M:265:ARG:NH1	2.26	0.50
2:O:42:DA:H1'	2:O:43:DA:C5'	2.41	0.50
3:P:37:DG:O6	8:L:437:GLN:HB2	2.12	0.50
4:M:260:LEU:HD21	4:M:278:ILE:HG12	1.94	0.50
4:H:56:VAL:HG22	4:H:144:ILE:HG13	1.94	0.50
4:H:74:VAL:HG11	4:H:81:ILE:HD11	1.93	0.50
6:J:141:PHE:HA	6:J:180:MET:HE2	1.93	0.50
6:J:264:ASP:OD1	8:L:506:SER:HB2	2.12	0.50
7:K:71:GLU:O	7:K:74:GLU:HB3	2.11	0.50
8:L:39:ASP:OD2	8:L:99:ARG:NH1	2.44	0.50
8:L:45:ILE:HA	8:L:48:ILE:HG22	1.93	0.50
8:L:56:MET:HE1	8:L:60:PRO:HD3	1.94	0.50
8:L:493:LYS:O	8:L:497:VAL:HG23	2.11	0.50
4:G:35:PHE:CE1	4:H:227:GLN:HG3	2.47	0.49
4:G:49:SER:HG	4:G:50:SER:HG	1.55	0.49
5:I:575:LEU:HD11	5:I:587:LEU:HD21	1.92	0.49
6:J:146:VAL:HG11	6:J:154:LEU:HB3	1.94	0.49
6:J:801:VAL:HG12	6:J:920:ALA:CB	2.42	0.49
6:J:1275:LEU:HB3	6:J:1278:GLU:OE1	2.12	0.49
8:L:466:ILE:CD1	8:L:487:MET:HG2	2.41	0.49
8:L:511:ILE:HD13	8:L:519:LEU:HA	1.92	0.49
8:L:573:LEU:HB3	8:L:584:ARG:HD3	1.94	0.49
1:N:52:PHE:O	1:N:55:VAL:HG23	2.11	0.49
4:G:29:GLU:OE2	4:G:190:ALA:HB1	2.10	0.49
5:I:254:ASP:N	5:I:254:ASP:OD1	2.42	0.49
5:I:804:PHE:CE1	5:I:1098:LEU:HD23	2.48	0.49
5:I:1010:GLN:O	5:I:1014:LEU:HD13	2.12	0.49
6:J:40:LYS:HD3	6:J:42:GLU:OE2	2.12	0.49
6:J:322:ARG:NH1	8:L:510:PRO:HD3	2.27	0.49
6:J:831:VAL:HG22	6:J:833:GLU:H	1.77	0.49
6:J:1162:ILE:HG22	6:J:1178:THR:O	2.12	0.49
1:N:5:ALA:HB3	5:I:678:ARG:NH2	2.28	0.49
4:G:29:GLU:HA	4:G:200:LYS:HB2	1.94	0.49
4:G:66:HIS:CB	5:I:927:THR:HG21	2.41	0.49
5:I:135:THR:HG22	5:I:144:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:700:VAL:HG13	5:I:1117:LEU:HD13	1.93	0.49
6:J:518:VAL:HG11	6:J:706:VAL:HG13	1.94	0.49
6:J:707:ILE:HA	6:J:708:ASN:CB	2.39	0.49
6:J:833:GLU:HG2	6:J:838:ARG:HG3	1.94	0.49
8:L:127:ILE:O	8:L:131:GLN:HG3	2.11	0.49
8:L:227:GLN:HA	8:L:230:VAL:HG12	1.93	0.49
8:L:561:MET:CG	8:L:576:VAL:HG22	2.41	0.49
2:O:23:DC:H5"	2:O:23:DC:H6	1.77	0.49
4:M:269:CYS:SG	4:M:295:LEU:HD12	2.53	0.49
4:M:284:ARG:HD2	4:M:288:GLU:CD	2.33	0.49
5:I:222:ASP:HA	5:I:227:LYS:HZ1	1.77	0.49
5:I:225:PHE:CB	5:I:336:LEU:HD22	2.42	0.49
5:I:1138:VAL:HG21	5:I:1166:ASP:OD2	2.12	0.49
6:J:821:MET:HE3	6:J:879:ALA:HB1	1.93	0.49
7:K:26:ARG:NH2	7:K:38:LEU:HD13	2.28	0.49
8:L:277:MET:HE2	8:L:281:ARG:HH21	1.78	0.49
8:L:511:ILE:HG12	8:L:522:PHE:HE2	1.78	0.49
2:O:30:DC:H4'	2:O:31:DA:OP1	2.11	0.49
3:P:48:DC:H2"	3:P:49:DT:OP2	2.13	0.49
4:G:233:ASP:O	4:G:235:ARG:HG2	2.13	0.49
4:H:98:VAL:O	4:H:146:VAL:HG22	2.12	0.49
4:H:158:ARG:HH11	4:H:172:LEU:HD12	1.78	0.49
5:I:237:LEU:HD22	5:I:289:VAL:CA	2.39	0.49
5:I:515:MET:HE1	5:I:517:GLN:CG	2.42	0.49
5:I:1271:GLY:HA2	6:J:344:GLY:HA2	1.94	0.49
6:J:288:PRO:CG	6:J:291:ILE:HD12	2.43	0.49
6:J:803:VAL:HG11	6:J:1309:ILE:HB	1.93	0.49
8:L:226:ALA:O	8:L:229:VAL:HG22	2.13	0.49
5:I:414:ILE:HD11	5:I:584:TYR:OH	2.12	0.49
5:I:916:SER:O	5:I:916:SER:OG	2.26	0.49
5:I:1211:ARG:NH2	5:I:1213:TYR:OH	2.43	0.49
5:I:1283:ALA:HB1	5:I:1286:THR:OG1	2.12	0.49
5:I:1327:LEU:HD11	5:I:1339:LEU:HD11	1.94	0.49
6:J:114:ILE:O	6:J:114:ILE:HG12	2.12	0.49
6:J:164:GLN:HA	6:J:167:ASP:OD2	2.12	0.49
6:J:170:GLU:O	6:J:171:GLU:HB2	2.12	0.49
6:J:1236:GLU:O	6:J:1239:ASP:HB2	2.12	0.49
8:L:253:SER:O	8:L:257:LYS:HG3	2.13	0.49
2:O:26:DT:H2'	2:O:27:DT:H72	1.95	0.49
3:P:48:DC:C6	3:P:49:DT:H72	2.47	0.49
4:M:253:LEU:HD12	4:M:318:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:136:PHE:CE1	5:I:456:VAL:HG11	2.47	0.49
6:J:162:GLU:O	6:J:166:LEU:HD23	2.13	0.49
6:J:679:TYR:OH	6:J:754:ILE:O	2.23	0.49
8:L:78:GLU:O	8:L:82:GLN:HG2	2.12	0.49
8:L:103:ARG:O	8:L:107:THR:HG23	2.12	0.49
8:L:231:THR:HA	8:L:248:GLU:OE1	2.12	0.49
8:L:252:LEU:O	8:L:255:VAL:HG22	2.13	0.49
2:O:23:DC:H2"	2:O:24:DC:H5'	1.95	0.49
2:O:52:DA:C8	2:O:53:DT:H72	2.48	0.49
4:G:10:LYS:HE2	4:H:226:GLU:HB3	1.94	0.49
4:G:234:LEU:CA	4:G:235:ARG:CG	2.86	0.49
4:H:155:ALA:HA	4:H:158:ARG:HH12	1.77	0.49
5:I:1295:SER:OG	6:J:345:LYS:HB3	2.13	0.49
6:J:333:GLY:O	6:J:339:ARG:HD3	2.12	0.49
6:J:836:ARG:HB2	6:J:873:GLU:HG3	1.93	0.49
3:P:31:DG:H5"	3:P:31:DG:C8	2.46	0.49
4:H:9:LEU:O	4:H:10:LYS:HG3	2.13	0.49
5:I:30:ILE:HD11	5:I:528:ARG:HA	1.94	0.49
5:I:68:LEU:HD12	5:I:101:ARG:O	2.13	0.49
5:I:138:ILE:HG12	5:I:143:ARG:HG3	1.95	0.49
5:I:741:MET:O	5:I:745:GLU:HB2	2.13	0.49
5:I:812:PHE:CE2	5:I:813:GLU:HG2	2.48	0.49
6:J:199:GLU:O	6:J:203:GLU:HG3	2.12	0.49
6:J:1167:LYS:CD	6:J:1170:LYS:HB2	2.43	0.49
7:K:10:VAL:HG23	7:K:19:LEU:HD22	1.94	0.49
7:K:54:ILE:HG12	7:K:59:ILE:HG22	1.95	0.49
8:L:137:TYR:HD2	8:L:140:ALA:HB2	1.78	0.49
8:L:315:TRP:CE3	8:L:316:PHE:HB2	2.47	0.49
4:G:233:ASP:HB2	4:G:235:ARG:CZ	2.43	0.49
5:I:28:LEU:HD22	5:I:527:LYS:HD2	1.94	0.49
5:I:1292:THR:HG23	5:I:1297:ASP:HB2	1.95	0.49
6:J:527:LEU:HB2	6:J:550:VAL:HG22	1.94	0.49
6:J:630:ALA:O	6:J:634:ARG:HG3	2.12	0.49
6:J:668:PHE:HA	6:J:673:VAL:HG22	1.95	0.49
8:L:12:LEU:HB2	8:L:30:HIS:CB	2.43	0.49
8:L:552:THR:HG23	8:L:555:GLU:CG	2.41	0.49
4:H:100:LEU:O	4:H:144:ILE:HG23	2.12	0.48
5:I:222:ASP:HA	5:I:227:LYS:NZ	2.28	0.48
5:I:865:LEU:HD11	5:I:882:ILE:O	2.13	0.48
6:J:309:ASN:OD1	6:J:315:ALA:HA	2.12	0.48
6:J:583:VAL:HG22	6:J:620:PHE:CZ	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:678:ARG:HG3	6:J:679:TYR:N	2.27	0.48
8:L:135:ALA:O	8:L:253:SER:OG	2.26	0.48
8:L:147:GLN:HB3	8:L:161:LEU:CD1	2.43	0.48
8:L:230:VAL:O	8:L:234:THR:OG1	2.14	0.48
8:L:470:MET:SD	8:L:482:GLU:HG3	2.53	0.48
8:L:519:LEU:O	8:L:519:LEU:HD23	2.12	0.48
4:G:50:SER:HB3	4:H:8:PHE:HE1	1.77	0.48
5:I:257:ALA:HB3	5:I:262:TYR:CE1	2.48	0.48
5:I:311:CYS:HB2	5:I:315:MET:SD	2.53	0.48
5:I:525:THR:HG21	5:I:687:ARG:HD3	1.94	0.48
5:I:851:THR:HG22	5:I:887:VAL:HG22	1.94	0.48
5:I:947:GLU:O	5:I:950:GLU:HG2	2.13	0.48
6:J:126:LEU:CD1	6:J:223:LEU:HD23	2.43	0.48
6:J:609:TYR:HE1	6:J:614:LEU:HD12	1.78	0.48
6:J:1275:LEU:HD12	6:J:1276:GLU:N	2.28	0.48
8:L:84:LEU:O	8:L:87:VAL:HG22	2.13	0.48
5:I:242:VAL:HB	5:I:245:ARG:CG	2.40	0.48
5:I:599:VAL:HG21	5:I:623:LEU:CD2	2.42	0.48
5:I:823:VAL:CG2	5:I:1060:ILE:HG22	2.43	0.48
5:I:920:VAL:HG13	5:I:921:PRO:HD2	1.95	0.48
6:J:661:VAL:O	6:J:664:ILE:HG22	2.13	0.48
6:J:840:LEU:HD12	6:J:864:LEU:O	2.13	0.48
8:L:134:VAL:HG22	8:L:273:MET:SD	2.53	0.48
4:M:307:LEU:HD22	4:M:312:LEU:CB	2.43	0.48
5:I:255:ILE:HG21	5:I:277:LEU:HD11	1.96	0.48
5:I:727:VAL:HG12	5:I:728:ASP:H	1.77	0.48
5:I:757:THR:HG23	5:I:765:ILE:HB	1.95	0.48
6:J:1179:PRO:HB2	6:J:1182:GLY:N	2.21	0.48
3:P:21:DA:H1'	3:P:22:DA:H5'	1.94	0.48
3:P:68:DG:H3'	3:P:68:DG:OP1	2.12	0.48
4:M:257:VAL:HA	4:M:260:LEU:CD1	2.44	0.48
4:H:190:ALA:O	4:H:198:LEU:HB2	2.12	0.48
5:I:214:ASN:HB2	5:I:359:ARG:HH21	1.79	0.48
5:I:265:LYS:HG2	5:I:266:GLY:N	2.29	0.48
5:I:624:ASP:OD1	5:I:630:VAL:HG23	2.13	0.48
5:I:835:GLU:HB3	5:I:1053:TYR:CE2	2.48	0.48
5:I:1065:LYS:HG3	5:I:1074:GLY:O	2.13	0.48
5:I:1340:GLU:OE2	6:J:21:LYS:HE3	2.14	0.48
6:J:338:PHE:CA	6:J:342:LEU:HD22	2.39	0.48
6:J:789:LYS:HE3	6:J:932:MET:HB3	1.94	0.48
6:J:850:LYS:CB	6:J:855:ASP:HB2	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:15:ARG:O	8:L:18:GLU:HG3	2.13	0.48
8:L:157:ARG:HG2	8:L:159:SER:N	2.18	0.48
8:L:479:THR:O	8:L:482:GLU:N	2.47	0.48
4:M:253:LEU:O	4:M:278:ILE:N	2.47	0.48
4:M:289:LEU:HD12	4:M:300:LEU:CD2	2.44	0.48
5:I:245:ARG:HD3	5:I:337:PHE:CE1	2.47	0.48
5:I:738:GLU:HG2	5:I:741:MET:HE2	1.95	0.48
5:I:820:GLU:N	5:I:1080:ASN:O	2.46	0.48
6:J:385:LEU:HD23	6:J:411:ILE:HG13	1.96	0.48
6:J:1157:ALA:N	6:J:1208:ASP:O	2.47	0.48
8:L:216:LEU:HD12	8:L:219:GLU:CD	2.34	0.48
5:I:563:THR:OG1	5:I:564:PRO:HD2	2.14	0.48
5:I:689:ALA:CB	5:I:1233:LEU:HD23	2.44	0.48
5:I:1080:ASN:HB3	5:I:1085:MET:SD	2.54	0.48
5:I:1240:ASP:OD1	5:I:1240:ASP:N	2.34	0.48
6:J:35:PHE:CD2	6:J:101:ARG:HB3	2.48	0.48
6:J:143:SER:HB3	6:J:160:LEU:O	2.14	0.48
8:L:471:LEU:HD23	8:L:472:GLN:N	2.28	0.48
8:L:504:PRO:O	8:L:505:ILE:HG23	2.13	0.48
5:I:99:LYS:HA	5:I:121:GLU:HA	1.95	0.48
5:I:149:LEU:HB2	5:I:530:ILE:HG22	1.95	0.48
6:J:252:LEU:HD12	6:J:262:THR:HG22	1.96	0.48
6:J:313:GLY:HA2	6:J:314:ARG:HA	1.42	0.48
6:J:1153:PRO:HD2	6:J:1194:ARG:NH2	2.27	0.48
6:J:1159:ILE:CD1	6:J:1177:ILE:HB	2.43	0.48
8:L:123:ILE:HD13	8:L:376:LYS:HG2	1.96	0.48
8:L:419:PHE:HE2	8:L:427:PHE:HA	1.78	0.48
8:L:471:LEU:HD12	8:L:477:GLU:HG3	1.94	0.48
5:I:735:LYS:HD3	5:I:748:ILE:HG22	1.95	0.48
5:I:966:ILE:HG13	10:I:1401:1N7:H26	1.95	0.48
5:I:1275:VAL:HG13	5:I:1287:LEU:HD11	1.96	0.48
6:J:615:LYS:NZ	7:K:7:GLN:HB3	2.28	0.48
8:L:144:LEU:CD2	8:L:261:LEU:HD11	2.43	0.48
8:L:287:ILE:HD11	8:L:341:LEU:HD12	1.95	0.48
2:O:60:DG:H2"	2:O:61:DC:H5'	1.95	0.48
5:I:847:PRO:HB3	5:I:1047:LEU:HD11	1.95	0.48
6:J:385:LEU:HD21	6:J:411:ILE:HG13	1.95	0.48
6:J:857:LEU:HD11	6:J:871:LEU:HD11	1.96	0.48
7:K:12:LYS:HE3	7:K:55:GLU:O	2.14	0.48
8:L:478:PRO:HB2	8:L:483:LEU:HD11	1.95	0.48
4:M:285:THR:HA	4:M:314:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:103:VAL:HG12	5:I:117:ILE:CB	2.42	0.47
5:I:638:SER:HB2	5:I:645:PHE:CZ	2.48	0.47
5:I:749:ASP:OD1	5:I:749:ASP:N	2.47	0.47
5:I:759:SER:HB3	5:I:765:ILE:HD11	1.96	0.47
5:I:895:LEU:HD12	5:I:900:LYS:N	2.28	0.47
5:I:1306:LYS:HD3	8:L:538:GLU:OE1	2.14	0.47
6:J:396:ALA:O	6:J:400:MET:HG3	2.13	0.47
6:J:553:THR:OG1	6:J:567:THR:HB	2.13	0.47
6:J:803:VAL:HG23	6:J:1259:GLN:HB3	1.96	0.47
6:J:1174:ARG:HG2	6:J:1189:MET:SD	2.54	0.47
4:M:315:GLY:O	4:M:317:ARG:HG3	2.14	0.47
4:H:97:GLU:CD	4:H:145:LYS:HD2	2.35	0.47
5:I:971:LEU:HD21	5:I:1014:LEU:HB3	1.96	0.47
6:J:62:PHE:O	6:J:98:ARG:HA	2.14	0.47
6:J:1155:ILE:CD1	6:J:1211:SER:HB3	2.44	0.47
6:J:1350:ASN:HA	6:J:1353:VAL:HG12	1.95	0.47
7:K:52:ARG:O	7:K:56:GLU:HG2	2.15	0.47
7:K:60:ASN:OD1	7:K:63:ILE:HD13	2.15	0.47
8:L:122:ARG:HG3	8:L:371:LYS:HE2	1.95	0.47
8:L:490:PRO:HD2	8:L:493:LYS:HB2	1.96	0.47
8:L:561:MET:SD	8:L:576:VAL:HG22	2.54	0.47
3:P:24:DG:H2"	3:P:25:DG:C8	2.49	0.47
4:M:280:ASP:HA	4:M:283:GLN:OE1	2.14	0.47
5:I:179:TYR:HB3	5:I:396:ASP:O	2.13	0.47
5:I:224:PHE:CG	5:I:347:ILE:HG13	2.50	0.47
5:I:262:TYR:O	5:I:263:VAL:HG23	2.14	0.47
5:I:928:VAL:HG22	5:I:1054:LEU:HD12	1.95	0.47
6:J:625:MET:HG2	6:J:629:PHE:CE2	2.49	0.47
8:L:147:GLN:HB3	8:L:161:LEU:HD11	1.96	0.47
8:L:330:LEU:HD23	8:L:333:VAL:HG11	1.96	0.47
8:L:437:GLN:O	8:L:441:ARG:HG2	2.14	0.47
5:I:265:LYS:HG2	5:I:266:GLY:H	1.79	0.47
5:I:336:LEU:HD23	5:I:336:LEU:HA	1.61	0.47
6:J:174:ASP:OD2	6:J:175:GLU:HG2	2.14	0.47
6:J:516:ASP:HB3	6:J:573:THR:HG21	1.97	0.47
6:J:1167:LYS:HD2	6:J:1174:ARG:NH1	2.29	0.47
6:J:1237:VAL:HG13	6:J:1253:ILE:HD12	1.95	0.47
8:L:162:ILE:HD11	8:L:221:PHE:CZ	2.43	0.47
4:M:321:TRP:CD2	4:M:322:PRO:HA	2.49	0.47
4:G:71:LYS:HB3	4:G:74:VAL:CG1	2.44	0.47
5:I:127:ILE:O	5:I:127:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:213:LEU:HD13	5:I:422:LYS:HA	1.96	0.47
5:I:237:LEU:CD2	5:I:289:VAL:CA	2.93	0.47
6:J:315:ALA:HB1	6:J:323:PRO:HB3	1.96	0.47
2:O:35:DG:OP1	2:O:35:DG:H4'	2.14	0.47
4:M:253:LEU:HD22	4:M:279:GLY:HA2	1.97	0.47
4:M:254:LEU:HB3	4:M:321:TRP:CZ2	2.50	0.47
4:M:288:GLU:HA	4:M:291:LYS:CE	2.42	0.47
4:M:303:ILE:O	4:M:307:LEU:HG	2.14	0.47
4:M:307:LEU:HD22	4:M:312:LEU:HB2	1.96	0.47
4:G:219:ARG:O	4:G:223:ILE:HG13	2.15	0.47
4:G:234:LEU:CD2	4:H:214:GLU:HG3	2.29	0.47
4:H:9:LEU:HD11	4:H:195:ARG:NH2	2.30	0.47
4:H:100:LEU:HD13	4:H:146:VAL:HG13	1.97	0.47
4:H:228:LEU:O	4:H:232:VAL:HG23	2.15	0.47
5:I:176:ILE:CD1	5:I:184:LEU:HD23	2.36	0.47
5:I:211:ARG:NH1	5:I:357:ASN:O	2.47	0.47
5:I:260:LYS:HD3	5:I:261:VAL:O	2.14	0.47
5:I:301:TYR:O	5:I:309:LEU:HD12	2.15	0.47
5:I:317:LEU:HD21	5:I:322:LEU:HD21	1.96	0.47
5:I:538:LEU:HD21	5:I:547:VAL:HG21	1.96	0.47
5:I:906:PHE:CE2	8:L:608:ARG:HA	2.49	0.47
5:I:924:VAL:HG21	5:I:1054:LEU:HD23	1.96	0.47
5:I:1024:GLU:O	5:I:1028:LYS:HG3	2.14	0.47
5:I:1119:MET:HG2	5:I:1204:LEU:HD13	1.95	0.47
5:I:1138:VAL:HG11	5:I:1166:ASP:OD1	2.15	0.47
5:I:1160:ASP:OD1	5:I:1160:ASP:N	2.47	0.47
6:J:20:ILE:HD12	6:J:1320:ILE:CD1	2.33	0.47
6:J:123:ARG:O	6:J:127:LEU:CB	2.62	0.47
6:J:668:PHE:HB2	6:J:673:VAL:CG2	2.45	0.47
6:J:1307:LEU:HD23	6:J:1311:LYS:CG	2.36	0.47
8:L:21:TYR:HB2	8:L:56:MET:HE1	1.97	0.47
8:L:449:THR:CG2	8:L:504:PRO:HD2	2.44	0.47
8:L:470:MET:HE2	8:L:486:ARG:NH1	2.30	0.47
4:H:191:ARG:O	4:H:191:ARG:HD3	2.14	0.47
5:I:525:THR:HG21	5:I:687:ARG:CD	2.45	0.47
5:I:594:VAL:HG11	5:I:650:VAL:HG23	1.96	0.47
5:I:814:ASP:HB2	6:J:462:ASP:HB3	1.96	0.47
5:I:855:PRO:O	5:I:857:VAL:N	2.48	0.47
6:J:259:ARG:HD3	10:J:1505:1N7:C16	2.45	0.47
6:J:848:VAL:HB	6:J:858:VAL:CG2	2.44	0.47
8:L:470:MET:O	8:L:474:MET:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:582:VAL:HG12	8:L:584:ARG:N	2.29	0.47
4:G:64:VAL:HG11	4:G:78:ILE:HG13	1.97	0.47
4:G:79:LEU:HD12	5:I:693:LEU:HD21	1.97	0.47
4:G:223:ILE:HG12	4:H:8:PHE:CE2	2.50	0.47
4:H:9:LEU:HB2	4:H:32:GLU:HG2	1.96	0.47
5:I:145:ILE:CB	5:I:456:VAL:HG13	2.45	0.47
5:I:179:TYR:HB2	5:I:398:SER:OG	2.15	0.47
6:J:84:ILE:HA	6:J:91:GLU:HA	1.97	0.47
6:J:315:ALA:CB	6:J:323:PRO:HB3	2.45	0.47
6:J:1172:LYS:HG2	6:J:1189:MET:O	2.14	0.47
8:L:137:TYR:HB3	8:L:273:MET:HE1	1.97	0.47
5:I:70:TYR:HA	5:I:100:LEU:HD22	1.96	0.47
5:I:156:PHE:CE2	5:I:177:ILE:HD12	2.49	0.47
5:I:566:GLY:O	6:J:787:ALA:HB1	2.15	0.47
5:I:602:GLU:OE1	5:I:602:GLU:N	2.48	0.47
5:I:741:MET:HG2	5:I:974:ARG:HH11	1.79	0.47
6:J:326:SER:H	6:J:329:ASP:HB2	1.79	0.47
6:J:416:ILE:HG23	6:J:439:PRO:HG2	1.97	0.47
6:J:511:TYR:CD2	6:J:728:SER:HB3	2.50	0.47
6:J:546:ALA:O	6:J:548:VAL:HG13	2.14	0.47
6:J:1144:LEU:HD21	6:J:1236:GLU:HG2	1.96	0.47
6:J:1155:ILE:HG13	6:J:1210:ILE:CB	2.39	0.47
7:K:42:GLU:OE1	7:K:52:ARG:NH2	2.48	0.47
8:L:509:THR:HG22	8:L:510:PRO:O	2.14	0.47
2:O:64:DT:C6	2:O:65:DT:H72	2.50	0.46
3:P:34:DT:H71	5:I:497:PRO:CG	2.44	0.46
3:P:38:DC:H2”	3:P:39:DC:C6	2.50	0.46
3:P:59:DA:H2”	3:P:60:DA:O5’	2.15	0.46
4:M:300:LEU:HD13	4:M:304:LYS:HG3	1.97	0.46
4:H:22:THR:OG1	4:H:207:THR:O	2.32	0.46
4:H:135:ASP:HB2	4:H:138:ALA:CB	2.44	0.46
5:I:254:ASP:O	5:I:255:ILE:HG13	2.15	0.46
5:I:367:TYR:CD2	5:I:376:PRO:HB3	2.50	0.46
5:I:722:GLY:HA2	5:I:737:ASN:OD1	2.15	0.46
5:I:843:THR:OG1	5:I:845:LEU:HD12	2.15	0.46
5:I:972:PHE:HD2	5:I:994:ARG:HH21	1.62	0.46
5:I:1075:VAL:HB	6:J:461:PHE:O	2.14	0.46
5:I:1250:SER:HB3	5:I:1259:LEU:HD12	1.96	0.46
6:J:423:LEU:HD22	6:J:437:PHE:CD1	2.49	0.46
6:J:475:GLU:HG3	7:K:24:ALA:HB1	1.96	0.46
6:J:555:TYR:CE2	6:J:565:ALA:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:111:THR:HA	4:G:129:VAL:HA	1.97	0.46
4:G:135:ASP:HB3	4:G:138:ALA:CB	2.46	0.46
5:I:248:GLY:O	5:I:268:ARG:NH2	2.49	0.46
5:I:888:THR:O	5:I:913:VAL:HG23	2.15	0.46
5:I:1085:MET:HE2	5:I:1085:MET:HB3	1.90	0.46
6:J:334:LYS:HA	6:J:339:ARG:CB	2.45	0.46
6:J:374:LEU:HG	6:J:374:LEU:O	2.15	0.46
6:J:827:GLU:HB3	6:J:832:LYS:HE2	1.97	0.46
6:J:1144:LEU:HD22	6:J:1236:GLU:HG2	1.98	0.46
8:L:561:MET:HG2	8:L:576:VAL:CG2	2.43	0.46
1:N:3:ASP:OD1	5:I:1073:LYS:NZ	2.29	0.46
4:M:303:ILE:HA	4:M:306:VAL:HG12	1.97	0.46
5:I:16:GLY:HA2	5:I:1188:ASP:O	2.16	0.46
5:I:296:VAL:O	5:I:335:THR:HA	2.15	0.46
5:I:320:ASP:OD1	5:I:321:LEU:HG	2.16	0.46
5:I:702:THR:HA	5:I:1184:THR:H	1.79	0.46
6:J:810:THR:HG23	6:J:893:GLY:HA3	1.97	0.46
8:L:247:GLU:HA	8:L:250:LEU:CD1	2.36	0.46
4:M:253:LEU:HD13	4:M:279:GLY:CA	2.45	0.46
5:I:870:ILE:HG21	5:I:931:VAL:HG11	1.97	0.46
6:J:126:LEU:HD11	6:J:223:LEU:CD2	2.42	0.46
6:J:281:ARG:O	6:J:285:LEU:HD13	2.16	0.46
6:J:909:ILE:HD11	6:J:913:GLU:HG2	1.97	0.46
4:H:120:ASP:OD1	4:H:120:ASP:N	2.49	0.46
5:I:1254:VAL:HG13	5:I:1255:THR:HG23	1.97	0.46
8:L:101:TYR:CE2	8:L:405:ILE:HG21	2.50	0.46
8:L:134:VAL:HG13	8:L:273:MET:CE	2.45	0.46
8:L:142:THR:HG22	8:L:228:TYR:OH	2.15	0.46
8:L:157:ARG:NE	8:L:159:SER:HB2	2.27	0.46
4:G:47:LEU:HD12	4:G:183:ILE:HD12	1.98	0.46
5:I:11:ILE:HB	5:I:1149:TYR:OH	2.16	0.46
5:I:559:CYS:SG	5:I:662:SER:N	2.88	0.46
5:I:888:THR:CG2	5:I:889:PRO:HD2	2.45	0.46
5:I:1290:MET:HG3	6:J:347:VAL:HG21	1.97	0.46
6:J:114:ILE:HD13	6:J:308:ASP:HB3	1.96	0.46
6:J:120:LEU:HD13	6:J:120:LEU:HA	1.60	0.46
6:J:490:ILE:O	6:J:499:ILE:N	2.33	0.46
6:J:900:GLY:HA3	6:J:1251:LYS:HE2	1.97	0.46
8:L:322:MET:HB2	8:L:327:SER:OG	2.15	0.46
5:I:10:ARG:NH1	5:I:697:LYS:HG2	2.30	0.46
5:I:150:HIS:CD2	5:I:454:ARG:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:161:LYS:HB3	5:I:161:LYS:HE3	1.50	0.46
5:I:201:ARG:HD2	5:I:370:MET:SD	2.56	0.46
5:I:238:GLN:HG2	5:I:239:MET:N	2.30	0.46
5:I:515:MET:HE3	5:I:517:GLN:CG	2.45	0.46
5:I:818:VAL:CG2	5:I:1076:ILE:HG12	2.45	0.46
5:I:898:GLU:HG2	8:L:544:THR:CG2	2.39	0.46
5:I:1243:MET:HE3	6:J:445:LYS:HD3	1.96	0.46
6:J:294:ASN:OD1	8:L:406:GLN:NE2	2.48	0.46
8:L:250:LEU:O	8:L:254:GLU:HG2	2.16	0.46
8:L:310:GLU:O	8:L:344:LEU:HD11	2.16	0.46
4:M:286:GLU:HG3	4:M:300:LEU:CD1	2.46	0.46
5:I:211:ARG:HD3	5:I:357:ASN:O	2.16	0.46
5:I:320:ASP:HB2	5:I:324:LYS:HE3	1.98	0.46
5:I:544:GLY:HA3	5:I:546:GLU:H	1.81	0.46
5:I:557:ARG:NH2	5:I:611:GLU:OE1	2.40	0.46
5:I:560:PRO:HB2	6:J:776:THR:HG21	1.97	0.46
5:I:929:ILE:HD13	5:I:1055:ALA:HB2	1.96	0.46
5:I:1002:LEU:HD22	5:I:1008:GLN:N	2.31	0.46
5:I:1123:GLY:HA3	5:I:1204:LEU:HD11	1.98	0.46
6:J:256:ASP:OD2	10:J:1504:1N7:O2	2.33	0.46
6:J:556:GLU:HB3	6:J:558:ASP:OD1	2.15	0.46
6:J:583:VAL:HG13	6:J:584:PRO:HD2	1.98	0.46
6:J:583:VAL:HG13	6:J:587:LEU:HD22	1.98	0.46
6:J:647:PRO:HG3	6:J:697:MET:CA	2.45	0.46
8:L:557:LYS:HD3	8:L:580:PHE:CZ	2.51	0.46
4:H:67:GLU:HA	4:H:68:TYR:C	2.36	0.46
5:I:10:ARG:CZ	5:I:697:LYS:HG2	2.46	0.46
5:I:86:GLN:HG2	5:I:140:GLY:O	2.16	0.46
5:I:293:ALA:HB2	5:I:319:LEU:CD2	2.40	0.46
5:I:485:ASP:O	5:I:486:THR:HG22	2.16	0.46
5:I:619:ALA:HB2	5:I:654:ASP:CB	2.41	0.46
5:I:748:ILE:CD1	5:I:967:LEU:HD23	2.45	0.46
5:I:1072:ASN:OD1	5:I:1072:ASN:N	2.41	0.46
5:I:1288:GLN:O	5:I:1292:THR:HB	2.16	0.46
6:J:1265:THR:OG1	6:J:1303:SER:OG	2.31	0.46
8:L:280:VAL:HG21	8:L:355:ILE:HD12	1.97	0.46
8:L:555:GLU:H	8:L:555:GLU:HG2	1.60	0.46
4:G:167:PRO:HG2	4:G:170:ARG:HD3	1.97	0.46
5:I:1199:LEU:HD13	5:I:1205:PRO:O	2.16	0.46
5:I:1275:VAL:O	5:I:1279:GLU:HG3	2.16	0.46
6:J:161:THR:HG22	6:J:164:GLN:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:1138:LEU:HB3	6:J:1139:PRO:HD3	1.97	0.46
6:J:1181:ASP:N	6:J:1181:ASP:OD1	2.48	0.46
4:M:265:ARG:HA	4:M:268:ASN:HD22	1.81	0.45
4:G:182:ARG:NH1	5:I:1090:ASN:O	2.45	0.45
4:H:92:VAL:HG22	4:H:121:VAL:HG22	1.98	0.45
5:I:39:ILE:HG13	5:I:75:LEU:HD21	1.98	0.45
5:I:254:ASP:HB3	5:I:265:LYS:CB	2.46	0.45
5:I:310:ILE:HG21	5:I:325:LEU:HD23	1.97	0.45
5:I:854:ILE:HG23	5:I:915:ASP:OD1	2.16	0.45
5:I:896:THR:HB	5:I:897:PRO:HD2	1.99	0.45
5:I:979:LEU:HG	5:I:1011:LEU:CD2	2.46	0.45
6:J:131:PRO:HG2	6:J:134:ASP:CB	2.39	0.45
6:J:134:ASP:OD1	6:J:159:ILE:HG13	2.15	0.45
6:J:201:LEU:CD1	6:J:217:LEU:HD22	2.46	0.45
6:J:432:LEU:HB3	6:J:456:ALA:HB1	1.98	0.45
6:J:1227:HIS:HA	6:J:1230:THR:CG2	2.45	0.45
6:J:1322:ALA:O	6:J:1326:GLN:HB2	2.16	0.45
8:L:145:LEU:HD21	8:L:224:LEU:CD2	2.46	0.45
3:P:53:DT:H2"	3:P:54:DT:C7	2.47	0.45
4:M:253:LEU:HD22	4:M:279:GLY:CA	2.47	0.45
4:G:45:ARG:NH1	4:H:38:THR:HG22	2.32	0.45
4:H:205:MET:HG3	4:H:213:PRO:HB3	1.98	0.45
5:I:85:CYS:SG	5:I:92:TYR:HB2	2.57	0.45
6:J:693:VAL:HG21	6:J:743:MET:CE	2.47	0.45
8:L:162:ILE:HD12	8:L:165:PHE:HE1	1.82	0.45
8:L:220:LYS:HB3	8:L:259:PHE:CE1	2.51	0.45
8:L:330:LEU:O	8:L:334:SER:OG	2.16	0.45
4:M:300:LEU:HD13	4:M:300:LEU:O	2.16	0.45
4:H:65:LEU:HD22	4:H:66:HIS:N	2.31	0.45
5:I:225:PHE:CE2	5:I:347:ILE:HB	2.48	0.45
5:I:847:PRO:CB	5:I:1047:LEU:HD11	2.46	0.45
5:I:935:THR:HG23	5:I:939:VAL:HB	1.98	0.45
5:I:1293:VAL:HG11	5:I:1304:MET:HG2	1.98	0.45
6:J:147:ILE:HG22	6:J:188:LEU:HD21	1.99	0.45
6:J:215:LYS:HE2	6:J:216:LYS:N	2.32	0.45
6:J:574:VAL:O	6:J:578:ILE:HG13	2.17	0.45
6:J:654:ILE:CD1	6:J:760:THR:HB	2.47	0.45
6:J:821:MET:CE	6:J:879:ALA:HB1	2.46	0.45
6:J:1208:ASP:OD1	6:J:1209:VAL:N	2.45	0.45
8:L:316:PHE:CZ	8:L:337:VAL:HB	2.52	0.45
8:L:463:LEU:CD2	8:L:483:LEU:HD23	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:484:ALA:HA	8:L:494:ILE:HD12	1.97	0.45
8:L:582:VAL:HG12	8:L:584:ARG:H	1.81	0.45
3:P:35:DG:OP1	8:L:468:ARG:NH1	2.49	0.45
7:K:60:ASN:OD1	7:K:63:ILE:HB	2.16	0.45
8:L:105:MET:HB3	8:L:105:MET:HE2	1.69	0.45
8:L:137:TYR:CE2	8:L:139:GLU:HB2	2.51	0.45
4:H:191:ARG:HB3	4:H:196:THR:HA	1.97	0.45
4:H:212:ASP:OD1	4:H:212:ASP:N	2.49	0.45
5:I:1219:GLU:OE2	6:J:634:ARG:NH2	2.50	0.45
5:I:1264:GLN:HE21	5:I:1264:GLN:HA	1.82	0.45
6:J:1284:ARG:O	6:J:1287:ILE:HG12	2.16	0.45
8:L:355:ILE:HA	8:L:355:ILE:HD13	1.76	0.45
8:L:377:LYS:HG2	8:L:381:GLU:OE2	2.16	0.45
4:G:16:ILE:CD1	4:G:214:GLU:HB2	2.46	0.45
5:I:1254:VAL:HG13	5:I:1255:THR:H	1.82	0.45
6:J:198:CYS:HA	6:J:221:ILE:HD13	1.97	0.45
6:J:683:ILE:HD12	6:J:746:LEU:CD2	2.47	0.45
7:K:31:GLN:HB2	7:K:46:THR:HG21	1.97	0.45
8:L:288:MET:HG2	8:L:292:VAL:CG2	2.46	0.45
8:L:379:MET:SD	8:L:416:VAL:HG13	2.57	0.45
3:P:37:DG:H4'	3:P:38:DC:OP1	2.15	0.45
4:G:234:LEU:CD2	4:H:214:GLU:CG	2.87	0.45
4:H:32:GLU:HB2	4:H:35:PHE:CD1	2.52	0.45
5:I:76:GLY:O	5:I:95:PRO:HD2	2.17	0.45
5:I:478:ARG:NH1	5:I:481:LEU:O	2.50	0.45
5:I:731:ARG:NH1	5:I:962:GLU:OE2	2.50	0.45
5:I:1122:LYS:HD2	5:I:1178:LYS:O	2.15	0.45
8:L:470:MET:HE2	8:L:486:ARG:HH11	1.81	0.45
1:N:48:ARG:NH2	6:J:677:GLU:OE2	2.49	0.45
4:M:262:LEU:CD2	4:M:306:VAL:HG11	2.43	0.45
4:G:13:LEU:HD11	4:G:214:GLU:HG3	1.98	0.45
4:H:93:GLN:N	4:H:120:ASP:O	2.40	0.45
5:I:762:ASN:O	5:I:833:ILE:N	2.34	0.45
5:I:944:ARG:O	5:I:948:ILE:HG13	2.16	0.45
6:J:201:LEU:HD12	6:J:217:LEU:HD22	1.99	0.45
6:J:804:ALA:O	6:J:916:GLY:HA3	2.17	0.45
2:O:55:DC:H2"	2:O:56:DC:C6	2.52	0.45
3:P:64:DA:C2'	3:P:65:DT:H72	2.46	0.45
5:I:453:ILE:HD13	5:I:530:ILE:HD12	1.99	0.45
5:I:803:ALA:HB2	5:I:1094:VAL:HG11	1.99	0.45
5:I:948:ILE:O	5:I:952:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:997:TRP:HB3	5:I:1000:LEU:HD12	1.97	0.45
6:J:147:ILE:O	6:J:147:ILE:HG13	2.16	0.45
8:L:74:GLU:O	8:L:77:ALA:HB3	2.17	0.45
8:L:347:ILE:O	8:L:351:THR:HG23	2.16	0.45
4:M:259:ASP:OD2	4:M:310:ARG:NH1	2.37	0.45
5:I:426:ILE:CG2	5:I:430:LYS:HE3	2.47	0.45
5:I:809:GLY:O	6:J:359:PRO:HG3	2.17	0.45
5:I:1272:GLU:HG2	5:I:1276:TRP:CZ2	2.52	0.45
6:J:635:SER:OG	6:J:637:ALA:HB2	2.16	0.45
6:J:937:ILE:HG12	6:J:1134:ILE:O	2.17	0.45
6:J:1154:ALA:HB2	6:J:1213:GLY:N	2.31	0.45
6:J:1258:ARG:O	6:J:1258:ARG:HG2	2.17	0.45
8:L:291:CYS:O	8:L:295:CYS:HB2	2.17	0.45
2:O:36:DA:C2'	2:O:37:DA:H5"	2.47	0.44
4:M:263:THR:HG23	4:M:302:GLU:OE2	2.17	0.44
4:H:24:ALA:HB3	4:H:213:PRO:CB	2.47	0.44
4:H:47:LEU:HD21	4:H:216:ALA:O	2.16	0.44
4:H:65:LEU:HD13	4:H:66:HIS:N	2.33	0.44
4:H:187:VAL:HG13	4:H:199:ASP:OD1	2.16	0.44
5:I:255:ILE:HD13	5:I:277:LEU:CD2	2.41	0.44
5:I:275:ARG:HA	5:I:278:GLU:CD	2.37	0.44
5:I:992:LEU:HB2	5:I:993:PRO:HD2	1.99	0.44
6:J:521:LYS:NZ	6:J:540:GLY:O	2.41	0.44
6:J:1196:LEU:CD1	6:J:1210:ILE:HG23	2.47	0.44
8:L:114:GLU:HG3	8:L:115:GLY:N	2.32	0.44
8:L:151:VAL:HG21	8:L:161:LEU:HB2	1.99	0.44
8:L:162:ILE:CA	8:L:262:VAL:HG23	2.42	0.44
8:L:228:TYR:HA	8:L:252:LEU:HD22	1.98	0.44
2:O:22:DT:H5'	4:M:265:ARG:HH11	1.82	0.44
2:O:22:DT:C5'	4:M:265:ARG:HD3	2.47	0.44
5:I:202:ARG:NH2	5:I:369:MET:HA	2.32	0.44
5:I:719:LYS:HB2	5:I:719:LYS:HE3	1.68	0.44
6:J:145:VAL:HG12	6:J:179:LYS:O	2.17	0.44
6:J:866:GLU:N	6:J:866:GLU:OE1	2.49	0.44
7:K:34:GLY:O	7:K:35:LYS:HG2	2.16	0.44
8:L:162:ILE:CG2	8:L:261:LEU:HA	2.47	0.44
1:N:55:VAL:HG12	1:N:57:LEU:H	1.81	0.44
2:O:23:DC:H2"	2:O:24:DC:OP2	2.16	0.44
4:G:57:THR:HG21	4:G:147:GLN:HE21	1.83	0.44
4:G:167:PRO:HG2	4:G:170:ARG:CD	2.47	0.44
5:I:59:ILE:HD12	5:I:475:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:817:LEU:CD2	5:I:1078:LYS:HB3	2.47	0.44
5:I:825:GLU:HB2	5:I:827:ARG:HG3	1.98	0.44
5:I:849:GLU:O	5:I:886:LYS:HG3	2.17	0.44
5:I:997:TRP:HA	5:I:1000:LEU:CG	2.44	0.44
5:I:1294:LYS:HD3	6:J:472:LEU:HD12	1.98	0.44
6:J:596:LEU:HA	6:J:600:ALA:HB3	1.98	0.44
6:J:796:LEU:O	6:J:800:LEU:HD13	2.18	0.44
6:J:810:THR:CG2	6:J:893:GLY:HA3	2.47	0.44
6:J:905:ARG:HB2	6:J:907:HIS:ND1	2.32	0.44
6:J:1248:ILE:HG12	6:J:1249:ASN:N	2.30	0.44
8:L:96:ASP:HB3	8:L:98:VAL:HG13	1.99	0.44
2:O:60:DG:H5'	5:I:371:ARG:HH22	1.82	0.44
3:P:25:DG:H1'	3:P:26:DC:C5'	2.47	0.44
4:G:90:VAL:HG23	4:G:121:VAL:HG13	1.98	0.44
4:H:67:GLU:CB	4:H:68:TYR:HA	2.46	0.44
5:I:189:ASP:HB2	5:I:195:PHE:HE2	1.82	0.44
5:I:596:ASP:OD1	5:I:596:ASP:N	2.49	0.44
5:I:1089:GLU:H	5:I:1089:GLU:HG2	1.40	0.44
6:J:42:GLU:H	6:J:42:GLU:HG2	1.55	0.44
6:J:644:MET:HG3	6:J:722:ILE:CD1	2.48	0.44
6:J:813:ASP:OD1	6:J:883:ARG:NH2	2.38	0.44
8:L:165:PHE:CD1	8:L:259:PHE:HB3	2.52	0.44
4:G:62:ASP:O	4:G:71:LYS:NZ	2.50	0.44
5:I:633:LEU:O	5:I:644:LEU:HD12	2.18	0.44
5:I:800:MET:HE2	5:I:828:PHE:CE2	2.53	0.44
5:I:905:ILE:HD11	8:L:598:LEU:HD12	2.00	0.44
5:I:964:LEU:HD21	5:I:1022:LYS:CD	2.33	0.44
6:J:215:LYS:CE	6:J:216:LYS:HG2	2.48	0.44
6:J:418:GLU:HG3	7:K:45:LYS:HG2	1.99	0.44
6:J:559:ALA:HB1	6:J:562:GLU:CD	2.37	0.44
10:J:1505:1N7:H31	10:J:1505:1N7:H5	1.99	0.44
8:L:280:VAL:CG2	8:L:347:ILE:HG21	2.47	0.44
8:L:399:LEU:HD13	8:L:447:ALA:HB2	1.99	0.44
8:L:551:LEU:HD21	8:L:598:LEU:CD2	2.47	0.44
2:O:24:DC:H3'	8:L:586:ARG:NH2	2.32	0.44
4:M:284:ARG:O	4:M:314:LEU:HD22	2.18	0.44
4:G:135:ASP:HB3	4:G:138:ALA:HB2	2.00	0.44
5:I:135:THR:HG21	5:I:515:MET:SD	2.58	0.44
5:I:733:VAL:HG21	5:I:966:ILE:HD13	1.99	0.44
5:I:1199:LEU:HA	5:I:1199:LEU:HD23	1.81	0.44
5:I:1270:PHE:CE1	5:I:1274:GLU:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:98:ARG:O	6:J:247:PRO:HD2	2.17	0.44
6:J:259:ARG:HD3	10:J:1505:1N7:H24	2.00	0.44
10:J:1504:1N7:H16	8:L:519:LEU:HD21	2.00	0.44
8:L:45:ILE:O	8:L:48:ILE:HG22	2.18	0.44
8:L:162:ILE:HG22	8:L:261:LEU:HA	1.98	0.44
2:O:58:DC:H2"	2:O:59:DG:C8	2.53	0.44
2:O:63:DT:C2'	2:O:64:DT:H71	2.47	0.44
4:H:179:PRO:O	4:H:207:THR:HB	2.17	0.44
5:I:216:THR:O	5:I:220:ILE:HG13	2.17	0.44
5:I:519:ASN:HB2	5:I:520:PRO:CD	2.48	0.44
6:J:125:GLY:HA2	6:J:135:ILE:CD1	2.47	0.44
6:J:154:LEU:HD21	6:J:176:PHE:CE2	2.53	0.44
6:J:278:ARG:HD2	6:J:295:GLU:OE1	2.18	0.44
6:J:326:SER:O	6:J:330:MET:HG3	2.17	0.44
6:J:741:ALA:O	6:J:762:ASN:ND2	2.51	0.44
6:J:1159:ILE:HD11	6:J:1177:ILE:C	2.38	0.44
6:J:1350:ASN:ND2	6:J:1358:PRO:HD3	2.33	0.44
7:K:59:ILE:HA	7:K:59:ILE:HD13	1.75	0.44
1:N:7:GLU:O	1:N:11:VAL:HG23	2.18	0.44
4:H:13:LEU:HD11	4:H:29:GLU:HB2	1.98	0.44
4:H:72:GLU:H	4:H:72:GLU:HG2	1.57	0.44
4:H:223:ILE:O	4:H:227:GLN:HG2	2.18	0.44
5:I:432:LEU:HA	5:I:432:LEU:HD12	1.73	0.44
5:I:718:ALA:HB2	5:I:783:LEU:HD21	2.00	0.44
8:L:314:THR:O	8:L:318:ALA:HB3	2.17	0.44
8:L:353:LEU:HD13	8:L:357:GLN:OE1	2.18	0.44
1:N:17:MET:HE2	10:N:102:1N7:H3	2.00	0.44
2:O:21:DA:H2"	2:O:22:DT:OP2	2.18	0.44
3:P:33:DA:H4'	3:P:34:DT:OP1	2.17	0.44
4:G:102:LEU:O	4:G:102:LEU:HD13	2.18	0.44
5:I:395:TYR:CE1	5:I:397:LEU:HD13	2.53	0.44
5:I:726:TYR:HA	5:I:773:LEU:CD2	2.43	0.44
5:I:993:PRO:HD2	5:I:996:ARG:HB2	2.00	0.44
5:I:1210:ILE:HD11	5:I:1212:LEU:HD11	2.00	0.44
5:I:1278:LEU:HD23	5:I:1278:LEU:HA	1.58	0.44
6:J:68:TYR:CA	6:J:92:VAL:HG23	2.47	0.44
6:J:657:ALA:HB2	6:J:689:ALA:HB2	2.00	0.44
6:J:1145:PHE:HZ	6:J:1253:ILE:HG23	1.83	0.44
8:L:134:VAL:HG22	8:L:273:MET:CE	2.48	0.44
1:N:47:ALA:O	1:N:51:ILE:HG13	2.18	0.43
3:P:68:DG:H2"	3:P:69:DT:O5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:307:LEU:O	4:M:312:LEU:N	2.51	0.43
4:H:68:TYR:O	4:H:69:SER:OG	2.26	0.43
5:I:105:TYR:CE1	5:I:114:VAL:HG12	2.53	0.43
6:J:422:LEU:O	6:J:468:VAL:HA	2.18	0.43
6:J:452:LEU:HD13	6:J:500:ILE:CG2	2.44	0.43
6:J:516:ASP:OD1	6:J:516:ASP:N	2.50	0.43
6:J:646:ILE:HD11	6:J:764:ARG:HD3	2.00	0.43
6:J:1266:ILE:HD12	6:J:1274:PHE:CB	2.46	0.43
10:J:1504:1N7:H24	10:J:1505:1N7:H17	2.00	0.43
3:P:34:DT:H5'	3:P:34:DT:H6	1.83	0.43
4:H:46:ILE:HD12	4:H:224:LEU:HB2	2.00	0.43
4:H:48:LEU:HD21	6:J:539:SER:HB3	2.00	0.43
5:I:189:ASP:OD1	5:I:190:PRO:HD2	2.17	0.43
5:I:887:VAL:HB	5:I:913:VAL:HG21	2.00	0.43
5:I:994:ARG:HA	5:I:997:TRP:CE3	2.54	0.43
6:J:111:THR:HG21	6:J:303:VAL:HB	2.00	0.43
6:J:205:LEU:CD2	6:J:217:LEU:HB3	2.48	0.43
6:J:1244:GLN:HE21	6:J:1244:GLN:HB2	1.50	0.43
8:L:162:ILE:HD12	8:L:165:PHE:CE1	2.53	0.43
8:L:573:LEU:HD12	8:L:573:LEU:HA	1.61	0.43
4:G:168:ILE:H	4:G:168:ILE:HG12	1.43	0.43
5:I:887:VAL:HB	5:I:913:VAL:HG22	2.00	0.43
5:I:1066:MET:HG3	5:I:1076:ILE:HD11	2.00	0.43
5:I:1182:ILE:HD11	5:I:1198:LEU:HD21	2.00	0.43
6:J:201:LEU:O	6:J:205:LEU:HD12	2.18	0.43
6:J:255:LEU:HD12	10:J:1504:1N7:H23	2.00	0.43
6:J:362:ARG:HB2	6:J:364:HIS:CE1	2.54	0.43
4:M:253:LEU:HD22	4:M:279:GLY:N	2.33	0.43
5:I:242:VAL:O	5:I:245:ARG:HG3	2.19	0.43
5:I:656:SER:OG	5:I:657:THR:N	2.52	0.43
5:I:1007:LYS:HA	5:I:1010:GLN:HB2	1.99	0.43
6:J:245:LEU:CD1	6:J:249:LEU:HD12	2.47	0.43
6:J:516:ASP:HA	6:J:545:HIS:CB	2.48	0.43
7:K:7:GLN:O	7:K:11:GLU:HG2	2.19	0.43
7:K:37:PRO:HB3	7:K:49:ILE:HG21	2.01	0.43
8:L:330:LEU:HD23	8:L:333:VAL:CG1	2.48	0.43
8:L:406:GLN:O	8:L:410:ILE:HG13	2.18	0.43
3:P:50:DT:H2"	3:P:51:DC:OP2	2.18	0.43
4:M:286:GLU:HG3	4:M:300:LEU:HD12	2.00	0.43
5:I:800:MET:O	5:I:1229:TYR:HA	2.18	0.43
5:I:1127:LYS:HE2	5:I:1127:LYS:HB2	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:1138:VAL:HG21	5:I:1166:ASP:CG	2.38	0.43
5:I:1192:GLU:HA	5:I:1195:ILE:HD12	2.00	0.43
6:J:99:ARG:O	6:J:99:ARG:HG2	2.19	0.43
6:J:427:PRO:O	6:J:429:LEU:HD22	2.18	0.43
6:J:673:VAL:HG23	6:J:674:THR:O	2.18	0.43
7:K:45:LYS:O	7:K:49:ILE:HG13	2.18	0.43
8:L:98:VAL:HB	8:L:402:LEU:CD2	2.44	0.43
2:O:56:DC:H2"	2:O:57:DT:C5'	2.48	0.43
4:G:182:ARG:HB3	4:G:206:GLU:HB3	2.00	0.43
4:H:59:VAL:O	4:H:171:LEU:HB2	2.18	0.43
4:H:69:SER:OG	4:H:78:ILE:HD12	2.19	0.43
5:I:18:ARG:HB2	5:I:1188:ASP:OD2	2.18	0.43
5:I:667:LEU:HD21	5:I:704:MET:HB3	1.99	0.43
5:I:1124:ILE:HD11	5:I:1201:LEU:HB3	2.00	0.43
6:J:204:GLU:CB	6:J:217:LEU:HD11	2.38	0.43
6:J:412:LEU:HD22	6:J:416:ILE:HG13	2.00	0.43
6:J:632:ALA:O	6:J:635:SER:HB3	2.18	0.43
6:J:664:ILE:HG13	6:J:681:LYS:CG	2.43	0.43
6:J:788:LEU:HD21	6:J:932:MET:HE1	2.00	0.43
8:L:73:ASP:HB2	8:L:74:GLU:CB	2.38	0.43
8:L:231:THR:CG2	8:L:249:ILE:HG12	2.49	0.43
8:L:511:ILE:HD12	8:L:511:ILE:HA	1.87	0.43
5:I:351:LEU:HA	5:I:351:LEU:HD23	1.74	0.43
5:I:447:HIS:NE2	5:I:553:THR:HG21	2.34	0.43
5:I:716:ALA:HB3	5:I:784:ALA:HB3	2.00	0.43
5:I:1125:GLY:HA3	5:I:1179:GLY:HA2	2.00	0.43
5:I:1192:GLU:O	5:I:1196:LYS:HG2	2.18	0.43
5:I:1243:MET:CE	6:J:445:LYS:HD3	2.49	0.43
5:I:1342:GLU:O	6:J:1372:ARG:NH1	2.45	0.43
6:J:326:SER:O	6:J:330:MET:N	2.51	0.43
6:J:827:GLU:CB	6:J:832:LYS:HE2	2.48	0.43
6:J:1173:ARG:HD2	6:J:1174:ARG:N	2.33	0.43
8:L:96:ASP:HB2	8:L:99:ARG:HD2	2.00	0.43
5:I:388:LEU:HD23	5:I:388:LEU:HA	1.68	0.43
5:I:550:VAL:HG13	6:J:777:HIS:ND1	2.34	0.43
6:J:58:CYS:CB	6:J:61:ILE:HD12	2.49	0.43
6:J:147:ILE:HG22	6:J:188:LEU:HD23	2.00	0.43
6:J:170:GLU:OE2	6:J:170:GLU:HA	2.18	0.43
6:J:219:LYS:HD3	6:J:219:LYS:O	2.18	0.43
6:J:252:LEU:HD12	6:J:262:THR:CG2	2.48	0.43
6:J:398:LYS:HE2	8:L:532:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:591:ILE:HG23	6:J:592:VAL:HG13	2.01	0.43
8:L:118:ASP:HA	8:L:121:LYS:HG2	2.01	0.43
8:L:564:GLY:HA2	8:L:569:THR:O	2.18	0.43
1:N:72:TYR:HB2	5:I:170:VAL:HG23	2.00	0.43
4:H:64:VAL:CG1	4:H:71:LYS:HB2	2.44	0.43
4:H:188:GLU:OE2	4:H:202:VAL:HG21	2.18	0.43
5:I:302:ILE:HG22	5:I:309:LEU:CA	2.40	0.43
5:I:422:LYS:HE2	5:I:422:LYS:HB3	1.72	0.43
5:I:494:ASN:OD1	5:I:497:PRO:HD3	2.19	0.43
6:J:37:GLU:HB2	6:J:104:HIS:CE1	2.54	0.43
6:J:122:SER:O	6:J:125:GLY:N	2.51	0.43
6:J:290:ILE:H	6:J:290:ILE:HD12	1.84	0.43
6:J:741:ALA:HA	6:J:762:ASN:HD22	1.83	0.43
6:J:759:ILE:CD1	6:J:771:GLN:HB3	2.35	0.43
6:J:1348:LYS:HB2	6:J:1348:LYS:HE3	1.85	0.43
8:L:281:ARG:O	8:L:285:ARG:HG2	2.18	0.43
8:L:415:ALA:HB2	8:L:434:TRP:HB2	2.00	0.43
8:L:562:ARG:HG2	8:L:591:GLU:CD	2.39	0.43
1:N:34:VAL:O	1:N:35:TYR:HB2	2.19	0.43
4:G:56:VAL:HG11	4:G:85:LEU:O	2.19	0.43
5:I:93:SER:HB2	5:I:127:ILE:O	2.19	0.43
5:I:109:ALA:HB1	5:I:112:GLY:C	2.39	0.43
5:I:593:LYS:HG3	5:I:594:VAL:N	2.34	0.43
5:I:972:PHE:HD1	5:I:972:PHE:HA	1.74	0.43
5:I:1289:GLU:O	5:I:1294:LYS:HG3	2.19	0.43
6:J:143:SER:HB2	6:J:159:ILE:CD1	2.49	0.43
6:J:514:THR:OG1	6:J:595:ALA:O	2.37	0.43
6:J:520:ALA:HB1	6:J:543:SER:HB3	2.00	0.43
6:J:559:ALA:CB	6:J:562:GLU:HB2	2.49	0.43
6:J:572:THR:HG21	6:J:589:TYR:CZ	2.54	0.43
6:J:1155:ILE:CG1	6:J:1211:SER:HB3	2.46	0.43
6:J:1257:VAL:O	6:J:1260:MET:N	2.50	0.43
8:L:71:THR:HA	8:L:72:ALA:HA	1.75	0.43
8:L:117:ILE:HG22	8:L:121:LYS:HE3	2.01	0.43
8:L:162:ILE:HB	8:L:261:LEU:HA	2.01	0.43
8:L:287:ILE:HA	8:L:337:VAL:HG22	2.00	0.43
8:L:377:LYS:O	8:L:381:GLU:HG3	2.19	0.43
2:O:63:DT:C6	2:O:63:DT:H5'	2.53	0.42
5:I:997:TRP:CB	5:I:1000:LEU:HD12	2.49	0.42
5:I:1028:LYS:HE2	5:I:1028:LYS:HB3	1.78	0.42
5:I:1232:MET:HB3	5:I:1232:MET:HE3	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:59:ALA:HA	6:J:63:GLY:O	2.19	0.42
6:J:453:VAL:HG12	6:J:457:TYR:CD2	2.54	0.42
6:J:579:LEU:O	6:J:582:ILE:HG12	2.19	0.42
6:J:811:GLU:OE1	6:J:890:THR:HG23	2.19	0.42
6:J:1151:LYS:HG2	6:J:1152:GLU:N	2.33	0.42
7:K:38:LEU:HD21	7:K:67:ARG:HH22	1.83	0.42
2:O:51:DT:H5"	8:L:425:TYR:CE1	2.54	0.42
3:P:49:DT:C2'	3:P:50:DT:H71	2.49	0.42
4:M:252:ILE:O	4:M:255:ARG:HB3	2.19	0.42
5:I:886:LYS:H	5:I:917:SER:CB	2.32	0.42
5:I:1027:LYS:HE3	5:I:1027:LYS:HB2	1.85	0.42
5:I:1085:MET:HE1	5:I:1097:VAL:HG23	2.00	0.42
5:I:1163:THR:O	5:I:1164:PHE:HD1	2.02	0.42
6:J:919:ALA:O	6:J:923:ILE:HG13	2.19	0.42
8:L:231:THR:HG23	8:L:248:GLU:CB	2.47	0.42
8:L:306:PHE:CE1	8:L:310:GLU:HG3	2.53	0.42
8:L:499:LYS:HB2	8:L:499:LYS:NZ	2.34	0.42
2:O:57:DT:H2"	2:O:58:DC:C6	2.54	0.42
3:P:27:DC:H2"	3:P:28:DG:OP2	2.19	0.42
4:G:48:LEU:HD22	5:I:1082:ILE:CD1	2.45	0.42
5:I:122:VAL:HB	5:I:489:PRO:O	2.19	0.42
5:I:1087:TYR:HD2	5:I:1088:ASP:O	2.02	0.42
6:J:152:THR:O	6:J:153:ASN:HB3	2.19	0.42
6:J:325:LYS:HD2	8:L:508:GLU:HG2	2.01	0.42
6:J:552:ILE:HG21	6:J:589:TYR:CD1	2.54	0.42
6:J:615:LYS:HZ1	7:K:7:GLN:HB3	1.84	0.42
6:J:875:ASN:O	6:J:876:SER:OG	2.30	0.42
6:J:1237:VAL:HG11	6:J:1253:ILE:HD12	2.00	0.42
8:L:47:MET:HG3	8:L:80:ALA:HB1	2.01	0.42
8:L:150:ARG:O	8:L:155:GLU:HB2	2.20	0.42
8:L:395:THR:HA	8:L:404:LEU:HD11	2.01	0.42
5:I:591:TYR:CD2	5:I:606:LEU:HD22	2.54	0.42
5:I:616:ILE:HG12	5:I:652:TYR:HB2	2.01	0.42
5:I:886:LYS:HE2	5:I:916:SER:O	2.19	0.42
5:I:964:LEU:CD1	5:I:1021:LEU:HB3	2.49	0.42
5:I:1139:ALA:O	5:I:1143:GLU:HG3	2.19	0.42
6:J:70:CYS:SG	6:J:71:LEU:N	2.92	0.42
6:J:143:SER:CB	6:J:159:ILE:HD13	2.50	0.42
6:J:428:THR:HG22	6:J:430:HIS:O	2.19	0.42
6:J:849:LEU:HA	6:J:855:ASP:O	2.19	0.42
6:J:865:HIS:CD2	6:J:867:GLN:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:227:GLN:HG3	8:L:252:LEU:HD13	2.00	0.42
8:L:264:LYS:HB2	8:L:264:LYS:NZ	2.34	0.42
8:L:310:GLU:O	8:L:344:LEU:HD21	2.20	0.42
8:L:546:ASP:N	8:L:546:ASP:OD1	2.51	0.42
2:O:23:DC:H1'	2:O:24:DC:C5'	2.48	0.42
4:M:269:CYS:O	4:M:273:GLU:HG2	2.20	0.42
4:G:103:ASN:OD1	4:G:141:SER:HB2	2.20	0.42
4:H:76:GLU:OE1	4:H:131:CYS:HA	2.19	0.42
5:I:103:VAL:HG12	5:I:117:ILE:HG22	2.00	0.42
5:I:283:LYS:HE3	5:I:283:LYS:HA	2.01	0.42
5:I:317:LEU:CD2	5:I:322:LEU:HD21	2.49	0.42
5:I:405:PHE:O	5:I:409:LEU:HD22	2.19	0.42
5:I:506:PHE:O	5:I:512:SER:OG	2.24	0.42
5:I:717:VAL:HG22	5:I:782:VAL:HG12	2.01	0.42
5:I:921:PRO:HG2	5:I:924:VAL:HG11	2.02	0.42
5:I:1196:LYS:HD2	5:I:1206:THR:HG23	2.01	0.42
6:J:349:TYR:CD2	6:J:472:LEU:HD11	2.55	0.42
6:J:475:GLU:O	6:J:479:GLU:HG3	2.18	0.42
7:K:15:ASN:OD1	7:K:16:ARG:N	2.52	0.42
8:L:359:LYS:HE2	8:L:359:LYS:HB3	1.70	0.42
8:L:494:ILE:O	8:L:498:LEU:HD13	2.20	0.42
8:L:572:THR:HG23	8:L:575:GLU:HG3	2.02	0.42
8:L:587:ILE:HA	8:L:587:ILE:HD13	1.69	0.42
2:O:22:DT:H2"	2:O:23:DC:C5	2.53	0.42
4:G:224:LEU:HD13	4:H:228:LEU:CD1	2.36	0.42
4:G:228:LEU:HD23	4:G:228:LEU:HA	1.87	0.42
5:I:231:GLU:C	5:I:232:ILE:HG13	2.40	0.42
5:I:519:ASN:HB2	5:I:520:PRO:HD2	2.01	0.42
5:I:697:LYS:H	5:I:697:LYS:HG3	1.71	0.42
5:I:836:LEU:HD21	5:I:921:PRO:CD	2.50	0.42
5:I:836:LEU:HD21	5:I:921:PRO:HD3	2.01	0.42
5:I:1240:ASP:HB3	6:J:445:LYS:NZ	2.35	0.42
6:J:381:ILE:O	6:J:385:LEU:HG	2.20	0.42
6:J:500:ILE:HD12	6:J:500:ILE:HG23	1.74	0.42
6:J:528:THR:HG22	6:J:532:GLU:CB	2.50	0.42
6:J:701:LEU:HG	6:J:723:TYR:HB2	2.01	0.42
6:J:1159:ILE:HD11	6:J:1177:ILE:O	2.20	0.42
8:L:246:GLN:O	8:L:250:LEU:HG	2.19	0.42
1:N:60:GLU:OE2	5:I:270:THR:HB	2.20	0.42
3:P:55:DT:H2"	3:P:56:DG:C8	2.55	0.42
4:M:282:VAL:HB	4:M:313:SER:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:233:ASP:HB2	4:G:235:ARG:NH2	2.35	0.42
4:H:89:ALA:HB3	4:H:124:VAL:HG13	2.00	0.42
5:I:98:VAL:HG21	5:I:124:MET:SD	2.60	0.42
5:I:228:VAL:HG23	5:I:245:ARG:NH1	2.35	0.42
5:I:953:LEU:HD13	5:I:953:LEU:HA	1.85	0.42
6:J:1158:GLU:HB2	6:J:1186:TYR:CE2	2.54	0.42
8:L:530:LEU:O	8:L:533:ASP:N	2.50	0.42
4:G:14:VAL:HG11	4:G:29:GLU:HB2	2.02	0.42
4:G:26:VAL:HG21	4:G:217:ILE:CD1	2.50	0.42
4:G:48:LEU:HG	4:G:183:ILE:HG13	2.02	0.42
4:H:158:ARG:HD2	4:H:172:LEU:HD12	2.02	0.42
5:I:524:ILE:HG12	5:I:712:SER:HB2	2.01	0.42
6:J:482:ALA:HB3	7:K:20:VAL:HG22	2.02	0.42
6:J:1227:HIS:CA	6:J:1230:THR:HG22	2.48	0.42
8:L:344:LEU:HG	8:L:348:GLU:OE2	2.20	0.42
4:H:47:LEU:CD2	4:H:220:ALA:HB2	2.50	0.42
4:H:93:GLN:HB2	4:H:120:ASP:HA	2.02	0.42
4:H:133:LEU:O	4:H:134:THR:HG22	2.20	0.42
5:I:515:MET:CE	5:I:517:GLN:HG3	2.47	0.42
5:I:681:MET:CE	5:I:1073:LYS:HE3	2.50	0.42
5:I:903:ARG:HH12	5:I:908:GLU:HG3	1.85	0.42
5:I:962:GLU:HA	5:I:965:GLN:HG2	2.02	0.42
5:I:1308:ILE:HD12	5:I:1313:HIS:HD2	1.83	0.42
6:J:128:LEU:HD23	6:J:128:LEU:HA	1.79	0.42
6:J:743:MET:HE3	6:J:743:MET:HB3	1.89	0.42
6:J:768:ASN:OD1	6:J:768:ASN:N	2.33	0.42
6:J:1167:LYS:HG2	6:J:1168:GLU:H	1.84	0.42
8:L:299:LYS:O	8:L:302:PHE:HB3	2.20	0.42
2:O:56:DC:H2”	2:O:57:DT:H5’	2.01	0.42
2:O:65:DT:H2”	2:O:66:DG:O5’	2.20	0.42
5:I:13:LYS:O	5:I:1183:ALA:N	2.47	0.42
5:I:246:LEU:O	5:I:269:ILE:HG21	2.20	0.42
5:I:524:ILE:HG21	5:I:663:VAL:HG21	2.01	0.42
5:I:929:ILE:HG12	5:I:1053:TYR:O	2.20	0.42
5:I:1250:SER:CB	5:I:1259:LEU:HD12	2.50	0.42
6:J:94:GLN:O	6:J:97:VAL:HB	2.19	0.42
6:J:113:HIS:HB3	6:J:116:PHE:HD2	1.85	0.42
6:J:674:THR:OG1	6:J:677:GLU:HB2	2.19	0.42
6:J:1240:VAL:O	6:J:1243:LEU:HB3	2.20	0.42
8:L:551:LEU:CG	8:L:598:LEU:HD21	2.50	0.42
8:L:551:LEU:CD2	8:L:598:LEU:HD21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:594:ALA:O	8:L:598:LEU:HG	2.20	0.42
2:O:24:DC:H2"	2:O:25:DA:C5'	2.50	0.41
3:P:50:DT:H6	3:P:50:DT:H2'	1.67	0.41
4:M:252:ILE:HD11	4:M:310:ARG:HD3	2.02	0.41
4:M:253:LEU:HD13	4:M:279:GLY:HA3	2.02	0.41
4:M:303:ILE:HA	4:M:306:VAL:CG1	2.49	0.41
4:G:234:LEU:HD23	4:H:214:GLU:CD	2.40	0.41
4:H:85:LEU:HD23	4:H:85:LEU:HA	1.75	0.41
5:I:260:LYS:CD	5:I:261:VAL:H	2.26	0.41
5:I:600:THR:HG22	5:I:601:ASP:H	1.85	0.41
5:I:616:ILE:C	5:I:636:CYS:HB3	2.40	0.41
5:I:854:ILE:HG23	5:I:855:PRO:HD2	2.01	0.41
5:I:901:LEU:HA	8:L:563:PHE:CE2	2.55	0.41
5:I:1325:VAL:HG11	6:J:337:ARG:NH1	2.35	0.41
6:J:92:VAL:O	6:J:92:VAL:HG22	2.20	0.41
6:J:384:LYS:HA	6:J:384:LYS:HD2	1.46	0.41
6:J:526:VAL:HA	6:J:549:LYS:O	2.19	0.41
8:L:9:LEU:HD23	8:L:9:LEU:O	2.20	0.41
8:L:281:ARG:O	8:L:284:GLU:HB2	2.20	0.41
8:L:412:LEU:HD12	8:L:412:LEU:O	2.20	0.41
8:L:529:GLU:OE2	8:L:533:ASP:HB3	2.19	0.41
2:O:40:DC:H2"	2:O:41:DT:C6	2.55	0.41
4:G:205:MET:HE1	4:G:217:ILE:CD1	2.51	0.41
4:H:27:THR:HA	4:H:201:LEU:O	2.19	0.41
4:H:29:GLU:CB	4:H:30:PRO:HD3	2.49	0.41
5:I:223:LEU:HD23	5:I:223:LEU:HA	1.77	0.41
5:I:338:THR:CB	5:I:345:PRO:HB3	2.49	0.41
5:I:575:LEU:CD1	5:I:587:LEU:HD21	2.50	0.41
5:I:803:ALA:CA	5:I:1227:VAL:HG12	2.50	0.41
5:I:1006:GLU:HA	5:I:1009:ASN:HB2	2.02	0.41
6:J:80:HIS:O	6:J:83:VAL:HG12	2.19	0.41
6:J:398:LYS:HZ3	8:L:532:LEU:HD22	1.84	0.41
6:J:563:LEU:HA	6:J:563:LEU:HD23	1.67	0.41
6:J:768:ASN:OD1	6:J:771:GLN:HG3	2.21	0.41
8:L:603:ARG:O	8:L:603:ARG:HG3	2.19	0.41
1:N:20:ILE:HG13	6:J:754:ILE:HD13	2.01	0.41
3:P:30:DG:H2"	3:P:31:DG:OP2	2.20	0.41
4:G:43:LEU:O	4:G:47:LEU:HG	2.20	0.41
4:G:79:LEU:O	4:G:83:LEU:HD13	2.20	0.41
5:I:211:ARG:HH21	5:I:351:LEU:HD22	1.84	0.41
5:I:1080:ASN:HD22	5:I:1081:PRO:CD	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:1115:THR:HG22	5:I:1228:GLY:CA	2.50	0.41
6:J:536:LEU:HD12	6:J:536:LEU:HA	1.69	0.41
6:J:843:VAL:HG12	6:J:861:ASN:HA	2.02	0.41
8:L:353:LEU:HB3	8:L:357:GLN:OE1	2.20	0.41
8:L:582:VAL:HG13	8:L:586:ARG:HB3	2.02	0.41
2:O:63:DT:H1'	2:O:64:DT:H5'	2.02	0.41
3:P:34:DT:H71	5:I:497:PRO:HB2	2.00	0.41
4:H:64:VAL:O	4:H:65:LEU:HB2	2.20	0.41
5:I:287:VAL:HB	5:I:288:PRO:HD2	2.03	0.41
5:I:734:ILE:HD12	5:I:777:VAL:HG21	2.02	0.41
6:J:53:ARG:NH1	6:J:60:ARG:HD2	2.35	0.41
6:J:450:HIS:HB3	6:J:453:VAL:CG2	2.50	0.41
6:J:604:MET:CE	6:J:624:ILE:HD11	2.51	0.41
6:J:1227:HIS:O	6:J:1230:THR:HG22	2.20	0.41
8:L:45:ILE:CD1	8:L:55:VAL:HG11	2.45	0.41
8:L:266:PHE:O	8:L:270:VAL:HG23	2.20	0.41
8:L:414:LYS:HE2	8:L:434:TRP:CZ3	2.55	0.41
8:L:476:ARG:HG3	8:L:477:GLU:N	2.32	0.41
1:N:27:ILE:HD12	6:J:684:ASP:OD2	2.20	0.41
2:O:51:DT:C2'	2:O:52:DA:H5"	2.29	0.41
3:P:60:DA:H2"	3:P:61:DT:C6	2.55	0.41
3:P:67:DT:H1'	3:P:68:DG:O5'	2.21	0.41
5:I:1217:THR:OG1	5:I:1219:GLU:HG2	2.20	0.41
6:J:95:THR:O	6:J:95:THR:OG1	2.34	0.41
6:J:596:LEU:CD2	6:J:600:ALA:HB1	2.49	0.41
6:J:664:ILE:HD13	6:J:664:ILE:O	2.20	0.41
6:J:816:THR:HG21	6:J:887:SER:O	2.20	0.41
7:K:30:MET:HE2	7:K:30:MET:HB2	1.81	0.41
8:L:140:ALA:HB2	8:L:273:MET:HE2	2.03	0.41
8:L:493:LYS:HE2	8:L:493:LYS:HB3	1.59	0.41
8:L:529:GLU:HG3	8:L:533:ASP:HB2	2.02	0.41
5:I:230:PHE:CE1	5:I:239:MET:HB2	2.56	0.41
5:I:560:PRO:HB3	6:J:776:THR:HG21	2.02	0.41
5:I:1042:LEU:HD22	5:I:1049:ILE:CD1	2.51	0.41
5:I:1212:LEU:HD21	5:I:1227:VAL:HG11	2.03	0.41
6:J:118:LYS:HD3	6:J:312:ARG:HH22	1.84	0.41
6:J:265:LEU:HD23	6:J:265:LEU:HA	1.58	0.41
6:J:370:LYS:NZ	6:J:443:GLU:OE2	2.35	0.41
6:J:377:PHE:O	6:J:381:ILE:HG13	2.20	0.41
8:L:236:LYS:HD2	8:L:236:LYS:N	2.33	0.41
8:L:333:VAL:HG22	8:L:337:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:339:ARG:HB3	8:L:343:LYS:HZ3	1.86	0.41
4:M:286:GLU:N	4:M:314:LEU:HD13	2.36	0.41
4:G:180:VAL:HA	4:G:207:THR:HA	2.01	0.41
5:I:75:LEU:HD11	5:I:127:ILE:CD1	2.51	0.41
5:I:854:ILE:HG22	5:I:857:VAL:HG22	2.03	0.41
5:I:884:VAL:HG23	5:I:918:LEU:HD23	2.03	0.41
5:I:939:VAL:HG21	5:I:1047:LEU:HB3	2.02	0.41
5:I:956:ALA:HB1	5:I:1032:LYS:NZ	2.36	0.41
5:I:1172:LEU:HD22	5:I:1176:LEU:HG	2.03	0.41
5:I:1304:MET:CE	5:I:1308:ILE:HD11	2.51	0.41
6:J:130:MET:CG	6:J:131:PRO:HD2	2.51	0.41
6:J:686:TRP:CE3	6:J:686:TRP:HA	2.55	0.41
6:J:1172:LYS:HE3	6:J:1191:PRO:HG3	2.02	0.41
8:L:84:LEU:HA	8:L:87:VAL:HG22	2.02	0.41
4:G:26:VAL:HG21	4:G:217:ILE:HD13	2.01	0.41
4:H:78:ILE:O	4:H:79:LEU:HB3	2.20	0.41
5:I:757:THR:HG22	5:I:765:ILE:O	2.21	0.41
5:I:1006:GLU:OE1	5:I:1006:GLU:N	2.51	0.41
5:I:1122:LYS:HG2	5:I:1229:TYR:CZ	2.56	0.41
5:I:1282:GLY:HA3	7:K:17:PHE:CE1	2.56	0.41
6:J:1247:LYS:HE3	6:J:1247:LYS:HB2	1.83	0.41
8:L:287:ILE:CD1	8:L:341:LEU:HD12	2.51	0.41
8:L:376:LYS:O	8:L:380:VAL:HG23	2.21	0.41
1:N:33:PRO:O	1:N:35:TYR:N	2.54	0.41
2:O:25:DA:C2'	2:O:26:DT:H72	2.51	0.41
2:O:60:DG:C2'	2:O:61:DC:H5'	2.51	0.41
3:P:25:DG:H1'	3:P:26:DC:H5'	2.03	0.41
4:G:218:ARG:NH1	4:H:231:PHE:O	2.54	0.41
4:H:59:VAL:HG21	4:H:85:LEU:HD12	2.02	0.41
5:I:198:ILE:HG22	5:I:199:ASP:OD2	2.21	0.41
5:I:400:VAL:HG13	5:I:586:PHE:HE2	1.86	0.41
5:I:524:ILE:O	5:I:528:ARG:HG3	2.20	0.41
5:I:803:ALA:HB2	5:I:1227:VAL:HG12	2.02	0.41
5:I:1178:LYS:HD3	5:I:1178:LYS:HA	1.60	0.41
5:I:1259:LEU:HD23	5:I:1259:LEU:HA	1.91	0.41
6:J:24:LEU:HA	6:J:24:LEU:HD23	1.85	0.41
6:J:205:LEU:HD21	6:J:218:THR:N	2.36	0.41
6:J:270:ARG:O	6:J:274:ASN:ND2	2.54	0.41
6:J:384:LYS:NZ	6:J:414:GLU:OE2	2.52	0.41
6:J:490:ILE:HB	6:J:500:ILE:HG13	2.03	0.41
6:J:557:LYS:HG2	6:J:563:LEU:CG	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:1160:SER:OG	6:J:1205:GLU:OE1	2.23	0.41
6:J:1206:ARG:HH21	6:J:1223:LEU:HD13	1.85	0.41
8:L:313:ASP:O	8:L:317:ASN:HB2	2.20	0.41
8:L:319:ALA:O	8:L:322:MET:HG3	2.20	0.41
2:O:20:DA:H2"	2:O:21:DA:OP2	2.20	0.41
4:M:279:GLY:HA2	4:M:282:VAL:HG22	2.03	0.41
4:G:7:GLU:OE1	4:G:8:PHE:N	2.41	0.41
4:G:92:VAL:HG22	4:G:148:ARG:NH2	2.36	0.41
5:I:6:THR:CG2	5:I:781:ASP:HB3	2.49	0.41
5:I:56:VAL:CG2	5:I:468:LEU:HB3	2.48	0.41
5:I:80:PHE:HB3	5:I:84:GLU:HB2	2.02	0.41
5:I:538:LEU:HD13	5:I:543:ALA:HB2	2.02	0.41
5:I:1172:LEU:HD22	5:I:1172:LEU:O	2.21	0.41
6:J:434:ILE:HG21	6:J:434:ILE:HD13	1.83	0.41
6:J:1321:SER:HB2	6:J:1349:GLU:HG3	2.03	0.41
3:P:66:DT:H3'	4:M:298:LYS:NZ	2.35	0.40
4:M:297:LYS:HB2	4:M:297:LYS:HE3	1.80	0.40
4:M:307:LEU:HB3	4:M:312:LEU:C	2.41	0.40
4:G:11:PRO:HB3	4:G:31:LEU:CD2	2.51	0.40
5:I:39:ILE:O	5:I:39:ILE:HG23	2.21	0.40
5:I:444:ASP:HB2	5:I:447:HIS:HB2	2.02	0.40
5:I:498:ILE:H	5:I:498:ILE:HD12	1.85	0.40
5:I:674:ASP:HA	5:I:1108:ASN:HA	2.03	0.40
6:J:67:ASP:HB3	6:J:68:TYR:HD1	1.86	0.40
6:J:1291:GLU:HG2	6:J:1292:LEU:HD13	2.03	0.40
8:L:262:VAL:HG13	8:L:263:PRO:HD2	2.02	0.40
8:L:292:VAL:O	8:L:296:LYS:HA	2.21	0.40
8:L:385:ARG:H	8:L:385:ARG:HG3	1.67	0.40
4:G:60:GLU:HG2	4:G:143:ARG:HH21	1.84	0.40
4:G:86:LYS:HE3	4:G:174:ASP:O	2.20	0.40
5:I:39:ILE:HD11	5:I:75:LEU:HG	2.02	0.40
5:I:898:GLU:CG	8:L:544:THR:HG21	2.42	0.40
5:I:993:PRO:HB2	5:I:995:ASP:OD1	2.21	0.40
5:I:998:LEU:CB	5:I:1015:ALA:HB1	2.48	0.40
6:J:161:THR:HG23	6:J:164:GLN:H	1.86	0.40
6:J:338:PHE:HA	6:J:342:LEU:CD2	2.42	0.40
6:J:454:CYS:O	6:J:458:ASN:N	2.55	0.40
6:J:641:ILE:HD12	6:J:641:ILE:HA	1.88	0.40
6:J:839:VAL:HG12	6:J:864:LEU:HD13	2.02	0.40
8:L:105:MET:O	8:L:105:MET:HG2	2.21	0.40
8:L:228:TYR:CZ	8:L:232:ARG:HD3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:339:ARG:O	8:L:342:GLN:HB2	2.21	0.40
4:G:39:LEU:HD23	4:G:39:LEU:HA	1.84	0.40
5:I:364:VAL:O	5:I:368:ARG:HG3	2.22	0.40
5:I:819:SER:HB2	5:I:1085:MET:SD	2.61	0.40
5:I:841:ARG:HA	5:I:1046:VAL:HA	2.02	0.40
6:J:254:PRO:HG3	6:J:260:PHE:HE1	1.87	0.40
6:J:271:ARG:NH1	6:J:316:ILE:HD12	2.37	0.40
6:J:436:ALA:HB2	6:J:480:ALA:HB1	2.02	0.40
8:L:281:ARG:HG2	8:L:285:ARG:HE	1.86	0.40
8:L:323:ASN:O	8:L:324:LYS:HD3	2.21	0.40
8:L:463:LEU:HD22	8:L:483:LEU:HD23	2.03	0.40
4:G:54:CYS:HB2	4:G:90:VAL:O	2.21	0.40
4:G:232:VAL:HG13	4:G:233:ASP:OD1	2.21	0.40
4:H:108:GLY:HA2	4:H:109:PRO:HD3	1.98	0.40
5:I:357:ASN:OD1	5:I:358:ASP:N	2.55	0.40
5:I:842:ASP:HA	5:I:847:PRO:HA	2.03	0.40
5:I:1042:LEU:HD22	5:I:1049:ILE:HD11	2.03	0.40
6:J:24:LEU:HB2	6:J:232:ASN:OD1	2.21	0.40
6:J:58:CYS:SG	6:J:59:ALA:N	2.94	0.40
6:J:259:ARG:HA	6:J:259:ARG:HE	1.86	0.40
6:J:656:GLU:O	6:J:660:GLU:HG2	2.21	0.40
6:J:858:VAL:O	6:J:858:VAL:HG23	2.22	0.40
6:J:1253:ILE:H	6:J:1253:ILE:HG12	1.48	0.40
6:J:1261:LEU:O	6:J:1261:LEU:HD12	2.20	0.40
8:L:311:THR:HG22	8:L:348:GLU:OE2	2.22	0.40
3:P:32:DA:H2"	3:P:33:DA:O4'	2.22	0.40
4:M:256:PRO:HA	4:M:276:HIS:O	2.21	0.40
4:M:295:LEU:HD23	4:M:299:SER:HB2	2.03	0.40
4:G:154:PRO:HG2	4:G:157:THR:CG2	2.41	0.40
4:H:34:GLY:O	4:H:38:THR:HG22	2.21	0.40
5:I:78:PRO:HB3	5:I:93:SER:O	2.22	0.40
5:I:403:MET:HE3	5:I:586:PHE:CE2	2.57	0.40
5:I:599:VAL:HG21	5:I:623:LEU:HD22	2.02	0.40
5:I:812:PHE:CD2	5:I:813:GLU:HG2	2.57	0.40
5:I:1033:ARG:O	5:I:1037:THR:HB	2.21	0.40
5:I:1041:ASP:OD1	5:I:1041:ASP:N	2.51	0.40
5:I:1199:LEU:HD22	5:I:1204:LEU:HB2	2.03	0.40
5:I:1258:PRO:HD2	6:J:346:ARG:O	2.21	0.40
6:J:557:LYS:HB3	6:J:557:LYS:HE2	1.90	0.40
6:J:740:LEU:HA	6:J:740:LEU:HD12	1.83	0.40
8:L:121:LYS:HB3	8:L:421:TYR:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:154:GLU:OE1	8:L:154:GLU:HA	2.22	0.40
8:L:269:LEU:O	8:L:273:MET:HG3	2.22	0.40
8:L:400:GLN:O	8:L:404:LEU:HG	2.21	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	N	70/72 (97%)	60 (86%)	9 (13%)	1 (1%)	11 43
4	G	230/329 (70%)	210 (91%)	19 (8%)	1 (0%)	34 72
4	H	214/329 (65%)	184 (86%)	29 (14%)	1 (0%)	29 68
4	M	71/329 (22%)	68 (96%)	3 (4%)	0	100 100
5	I	1331/1342 (99%)	1218 (92%)	107 (8%)	6 (0%)	29 68
6	J	1160/1430 (81%)	1065 (92%)	94 (8%)	1 (0%)	51 85
7	K	70/91 (77%)	65 (93%)	5 (7%)	0	100 100
8	L	552/616 (90%)	520 (94%)	31 (6%)	1 (0%)	47 82
All	All	3698/4538 (82%)	3390 (92%)	297 (8%)	11 (0%)	44 76

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	252	SER
5	I	254	ASP
5	I	856	ASN
8	L	504	PRO
1	N	34	VAL
4	G	235	ARG
5	I	255	ILE

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Mol	Chain	Res	Type
5	I	940	GLU
6	J	859	PRO
5	I	855	PRO
4	H	64	VAL

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	N	60/61 (98%)	57 (95%)	3 (5%)	24 60
4	G	192/286 (67%)	160 (83%)	32 (17%)	2 11
4	H	184/286 (64%)	156 (85%)	28 (15%)	3 14
4	M	65/286 (23%)	65 (100%)	0	100 100
5	I	1145/1157 (99%)	1011 (88%)	134 (12%)	5 22
6	J	976/1189 (82%)	876 (90%)	100 (10%)	7 28
7	K	63/75 (84%)	57 (90%)	6 (10%)	8 32
8	L	491/543 (90%)	457 (93%)	34 (7%)	15 48
All	All	3176/3883 (82%)	2839 (89%)	337 (11%)	10 26

All (337) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	27	ILE
1	N	59	VAL
1	N	72	TYR
4	G	7	GLU
4	G	26	VAL
4	G	50	SER
4	G	56	VAL
4	G	74	VAL
4	G	76	GLU
4	G	79	LEU
4	G	92	VAL

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Mol	Chain	Res	Type
4	G	99	ILE
4	G	102	LEU
4	G	118	ASP
4	G	129	VAL
4	G	140	ILE
4	G	142	MET
4	G	150	ARG
4	G	156	SER
4	G	160	HIS
4	G	168	ILE
4	G	171	LEU
4	G	178	SER
4	G	186	ASN
4	G	195	ARG
4	G	199	ASP
4	G	200	LYS
4	G	203	ILE
4	G	211	ILE
4	G	212	ASP
4	G	217	ILE
4	G	218	ARG
4	G	224	LEU
4	G	231	PHE
4	G	234	LEU
4	H	7	GLU
4	H	12	ARG
4	H	14	VAL
4	H	15	ASP
4	H	19	VAL
4	H	38	THR
4	H	43	LEU
4	H	64	VAL
4	H	65	LEU
4	H	70	THR
4	H	72	GLU
4	H	79	LEU
4	H	83	LEU
4	H	98	VAL
4	H	99	ILE
4	H	124	VAL
4	H	134	THR
4	H	144	ILE

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Mol	Chain	Res	Type
4	H	150	ARG
4	H	156	SER
4	H	176	CYS
4	H	182	ARG
4	H	188	GLU
4	H	191	ARG
4	H	195	ARG
4	H	198	LEU
4	H	218	ARG
4	H	231	PHE
5	I	7	GLU
5	I	14	ASP
5	I	30	ILE
5	I	39	ILE
5	I	60	GLN
5	I	65	ASN
5	I	79	VAL
5	I	104	ILE
5	I	117	ILE
5	I	123	TYR
5	I	129	LEU
5	I	138	ILE
5	I	161	LYS
5	I	200	ARG
5	I	204	LEU
5	I	208	ILE
5	I	216	THR
5	I	253	PHE
5	I	254	ASP
5	I	260	LYS
5	I	263	VAL
5	I	270	THR
5	I	272	ARG
5	I	283	LYS
5	I	284	LEU
5	I	285	ILE
5	I	300	ASP
5	I	315	MET
5	I	333	ILE
5	I	335	THR
5	I	348	SER
5	I	398	SER

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Mol	Chain	Res	Type
5	I	409	LEU
5	I	414	ILE
5	I	445	ILE
5	I	446	ASP
5	I	450	ASN
5	I	452	ARG
5	I	455	SER
5	I	456	VAL
5	I	468	LEU
5	I	471	VAL
5	I	472	GLU
5	I	473	ARG
5	I	483	ASP
5	I	484	LEU
5	I	486	THR
5	I	508	SER
5	I	513	GLN
5	I	521	LEU
5	I	522	SER
5	I	528	ARG
5	I	569	ILE
5	I	573	ASN
5	I	576	SER
5	I	582	ASN
5	I	589	THR
5	I	596	ASP
5	I	600	THR
5	I	602	GLU
5	I	609	ILE
5	I	615	VAL
5	I	623	LEU
5	I	630	VAL
5	I	635	THR
5	I	639	LYS
5	I	655	VAL
5	I	656	SER
5	I	672	GLU
5	I	690	VAL
5	I	697	LYS
5	I	705	GLU
5	I	731	ARG
5	I	741	MET

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Mol	Chain	Res	Type
5	I	748	ILE
5	I	761	GLN
5	I	764	CYS
5	I	779	ARG
5	I	783	LEU
5	I	796	LEU
5	I	799	ASN
5	I	802	VAL
5	I	807	TRP
5	I	833	ILE
5	I	835	GLU
5	I	839	VAL
5	I	842	ASP
5	I	845	LEU
5	I	848	GLU
5	I	856	ASN
5	I	895	LEU
5	I	909	LYS
5	I	912	ASP
5	I	924	VAL
5	I	937	ASP
5	I	953	LEU
5	I	963	GLU
5	I	968	GLU
5	I	974	ARG
5	I	984	VAL
5	I	1027	LYS
5	I	1037	THR
5	I	1046	VAL
5	I	1060	ILE
5	I	1072	ASN
5	I	1080	ASN
5	I	1082	ILE
5	I	1085	MET
5	I	1089	GLU
5	I	1092	THR
5	I	1107	MET
5	I	1109	ILE
5	I	1117	LEU
5	I	1127	LYS
5	I	1133	LYS
5	I	1149	TYR

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Mol	Chain	Res	Type
5	I	1163	THR
5	I	1164	PHE
5	I	1172	LEU
5	I	1174	GLU
5	I	1182	ILE
5	I	1206	THR
5	I	1216	ARG
5	I	1222	GLU
5	I	1225	VAL
5	I	1238	LEU
5	I	1246	ARG
5	I	1264	GLN
5	I	1290	MET
5	I	1296	ASP
5	I	1302	THR
5	I	1308	ILE
5	I	1309	VAL
5	I	1316	GLU
6	J	18	ASP
6	J	45	ASN
6	J	46	TYR
6	J	70	CYS
6	J	78	LEU
6	J	92	VAL
6	J	93	THR
6	J	94	GLN
6	J	97	VAL
6	J	114	ILE
6	J	126	LEU
6	J	151	MET
6	J	156	ARG
6	J	159	ILE
6	J	170	GLU
6	J	194	LEU
6	J	195	GLU
6	J	207	GLU
6	J	212	THR
6	J	215	LYS
6	J	217	LEU
6	J	227	PHE
6	J	237	MET
6	J	252	LEU

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Mol	Chain	Res	Type
6	J	279	LEU
6	J	281	ARG
6	J	331	ILE
6	J	357	VAL
6	J	393	THR
6	J	401	VAL
6	J	412	LEU
6	J	416	ILE
6	J	423	LEU
6	J	430	HIS
6	J	431	ARG
6	J	489	ASN
6	J	527	LEU
6	J	536	LEU
6	J	538	ARG
6	J	545	HIS
6	J	547	ARG
6	J	560	ASN
6	J	567	THR
6	J	568	SER
6	J	571	ASP
6	J	594	GLN
6	J	596	LEU
6	J	614	LEU
6	J	624	ILE
6	J	635	SER
6	J	664	ILE
6	J	668	PHE
6	J	678	ARG
6	J	697	MET
6	J	705	THR
6	J	710	ASP
6	J	740	LEU
6	J	743	MET
6	J	747	MET
6	J	783	LEU
6	J	788	LEU
6	J	789	LYS
6	J	792	ASN
6	J	803	VAL
6	J	810	THR
6	J	814	CYS

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Mol	Chain	Res	Type
6	J	820	ILE
6	J	835	LEU
6	J	847	ASP
6	J	849	LEU
6	J	869	CYS
6	J	901	ARG
6	J	907	HIS
6	J	908	ILE
6	J	911	LYS
6	J	922	SER
6	J	934	THR
6	J	1151	LYS
6	J	1155	ILE
6	J	1160	SER
6	J	1175	LEU
6	J	1192	LYS
6	J	1196	LEU
6	J	1206	ARG
6	J	1211	SER
6	J	1244	GLN
6	J	1248	ILE
6	J	1253	ILE
6	J	1255	VAL
6	J	1261	LEU
6	J	1266	ILE
6	J	1268	ASN
6	J	1285	VAL
6	J	1286	LYS
6	J	1292	LEU
6	J	1305	ASP
6	J	1318	SER
6	J	1341	ARG
6	J	1355	ARG
6	J	1372	ARG
7	K	10	VAL
7	K	13	ILE
7	K	25	ARG
7	K	30	MET
7	K	39	VAL
7	K	71	GLU
8	L	9	LEU
8	L	34	ASP

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Mol	Chain	Res	Type
8	L	40	GLN
8	L	49	ASN
8	L	50	ASP
8	L	51	MET
8	L	93	ARG
8	L	95	THR
8	L	98	VAL
8	L	105	MET
8	L	108	VAL
8	L	219	GLU
8	L	288	MET
8	L	344	LEU
8	L	399	LEU
8	L	403	ASP
8	L	420	GLU
8	L	440	THR
8	L	449	THR
8	L	471	LEU
8	L	473	GLU
8	L	479	THR
8	L	494	ILE
8	L	505	ILE
8	L	506	SER
8	L	526	THR
8	L	532	LEU
8	L	544	THR
8	L	552	THR
8	L	569	THR
8	L	573	LEU
8	L	587	ILE
8	L	604	SER
8	L	611	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	21	ASN
1	N	25	GLN
1	N	28	ASN
1	N	71	HIS
4	M	268	ASN
4	M	320	ASN

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Mol	Chain	Res	Type
4	G	18	GLN
4	H	93	GLN
4	H	227	GLN
5	I	343	HIS
5	I	554	HIS
5	I	582	ASN
5	I	620	ASN
5	I	628	HIS
5	I	811	ASN
5	I	932	GLN
5	I	965	GLN
5	I	1017	GLN
5	I	1080	ASN
5	I	1116	HIS
5	I	1237	HIS
5	I	1264	GLN
5	I	1313	HIS
6	J	153	ASN
6	J	206	ASN
6	J	229	GLN
6	J	364	HIS
6	J	450	HIS
6	J	488	ASN
6	J	665	GLN
6	J	720	ASN
6	J	875	ASN
6	J	1227	HIS
6	J	1244	GLN
6	J	1268	ASN
6	J	1279	GLN
6	J	1350	ASN
8	L	19	GLN
8	L	129	GLN
8	L	227	GLN
8	L	246	GLN
8	L	309	ASN
8	L	331	HIS
8	L	338	HIS
8	L	362	ASN
8	L	409	ASN
8	L	464	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
10	1N7	I	1401	-	30,30,46	4.82	15 (50%)	47,48,72	2.43	13 (27%)
10	1N7	J	1504	-	30,30,46	4.88	15 (50%)	47,48,72	2.51	14 (29%)
10	1N7	J	1505	-	30,30,46	4.84	14 (46%)	47,48,72	2.31	16 (34%)
10	1N7	N	102	-	30,30,46	4.91	15 (50%)	47,48,72	2.26	19 (40%)

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
10	1N7	I	1401	-	-	2/7/72/92	0/4/4/4
10	1N7	J	1504	-	-	4/7/72/92	0/4/4/4
10	1N7	J	1505	-	-	2/7/72/92	0/4/4/4
10	1N7	N	102	-	-	1/7/72/92	0/4/4/4

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	1505	1N7	C3-C19	17.48	1.82	1.53
10	I	1401	1N7	C3-C19	17.31	1.82	1.53
10	N	102	1N7	C3-C19	17.29	1.82	1.53
10	J	1504	1N7	C3-C19	17.22	1.82	1.53
10	N	102	1N7	C3-C4	11.45	1.72	1.53
10	J	1505	1N7	C3-C4	11.20	1.72	1.53
10	I	1401	1N7	C3-C4	11.04	1.71	1.53
10	J	1504	1N7	C3-C4	10.75	1.71	1.53
10	J	1504	1N7	C5-C4	-9.40	1.39	1.54
10	N	102	1N7	C5-C4	-9.13	1.40	1.54
10	J	1505	1N7	C5-C4	-8.90	1.40	1.54
10	I	1401	1N7	C5-C4	-8.74	1.40	1.54
10	I	1401	1N7	C2-C19	-7.42	1.42	1.56
10	J	1504	1N7	C2-C19	-7.40	1.42	1.56
10	N	102	1N7	C2-C19	-7.39	1.42	1.56
10	J	1505	1N7	C2-C19	-6.86	1.43	1.56
10	J	1504	1N7	C8-C7	6.22	1.71	1.54
10	I	1401	1N7	C8-C7	5.82	1.70	1.54
10	N	102	1N7	C8-C7	5.66	1.69	1.54
10	J	1505	1N7	C8-C7	5.56	1.69	1.54
10	J	1504	1N7	O4-C4	-4.23	1.36	1.43
10	N	102	1N7	C5-C9	4.15	1.62	1.55
10	N	102	1N7	O4-C4	-4.10	1.36	1.43
10	I	1401	1N7	C5-C9	4.08	1.62	1.55
10	I	1401	1N7	O4-C4	-4.08	1.36	1.43
10	J	1504	1N7	C5-C6	-4.08	1.48	1.55
10	J	1505	1N7	O4-C4	-4.05	1.36	1.43
10	J	1505	1N7	C5-C9	3.80	1.62	1.55
10	J	1504	1N7	C7-C6	3.72	1.62	1.54
10	N	102	1N7	C2-C15	3.62	1.61	1.55
10	J	1505	1N7	C2-C15	3.60	1.61	1.55
10	N	102	1N7	C5-C6	-3.55	1.49	1.55
10	I	1401	1N7	C18-C6	-3.53	1.47	1.53
10	I	1401	1N7	C5-C6	-3.43	1.49	1.55
10	J	1504	1N7	C18-C6	-3.37	1.47	1.53
10	N	102	1N7	C14-C15	-3.32	1.48	1.53
10	J	1505	1N7	C5-C6	-3.31	1.49	1.55
10	J	1504	1N7	C2-C15	3.28	1.60	1.55
10	J	1505	1N7	C18-C6	-3.14	1.47	1.53
10	J	1504	1N7	C5-C9	3.06	1.60	1.55
10	N	102	1N7	C18-C6	-3.06	1.47	1.53
10	I	1401	1N7	C7-C6	3.05	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	1505	1N7	C7-C6	2.94	1.60	1.54
10	J	1504	1N7	C14-C15	-2.92	1.49	1.53
10	J	1505	1N7	C14-C15	-2.88	1.49	1.53
10	N	102	1N7	C7-C6	2.74	1.60	1.54
10	I	1401	1N7	C14-C15	-2.67	1.49	1.53
10	J	1504	1N7	O2-C13	-2.46	1.36	1.43
10	I	1401	1N7	O2-C13	-2.42	1.36	1.43
10	J	1504	1N7	C10-C5	2.35	1.58	1.54
10	J	1505	1N7	C1-C2	2.33	1.58	1.54
10	J	1504	1N7	C1-C2	2.32	1.58	1.54
10	I	1401	1N7	C10-C5	2.28	1.58	1.54
10	J	1505	1N7	O2-C13	-2.27	1.36	1.43
10	N	102	1N7	C1-C2	2.27	1.58	1.54
10	N	102	1N7	O2-C13	-2.25	1.36	1.43
10	I	1401	1N7	C16-C15	2.19	1.57	1.53
10	I	1401	1N7	C2-C15	2.13	1.58	1.55
10	N	102	1N7	C10-C5	2.02	1.57	1.54

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	1504	1N7	C9-C5-C4	-9.15	109.31	117.67
10	I	1401	1N7	C9-C5-C4	-7.16	111.13	117.67
10	J	1505	1N7	C9-C5-C4	-5.40	112.74	117.67
10	J	1505	1N7	C7-C6-C18	-5.32	110.89	118.33
10	N	102	1N7	C9-C5-C6	5.26	105.40	100.09
10	I	1401	1N7	C19-C3-C4	-5.21	107.42	114.30
10	I	1401	1N7	C7-C6-C18	-5.08	111.23	118.33
10	N	102	1N7	C9-C5-C4	-5.05	113.06	117.67
10	N	102	1N7	C7-C6-C18	-5.05	111.28	118.33
10	J	1504	1N7	C6-C5-C4	4.97	112.03	107.40
10	N	102	1N7	C3-C19-C18	-4.95	103.62	110.88
10	J	1505	1N7	C3-C19-C18	-4.48	104.32	110.88
10	J	1504	1N7	C7-C6-C18	-4.47	112.08	118.33
10	I	1401	1N7	C21-C20-C22	-4.43	103.42	110.36
10	J	1504	1N7	C21-C20-C9	-4.37	106.23	112.92
10	J	1504	1N7	C5-C9-C20	-4.32	114.34	119.50
10	I	1401	1N7	C6-C5-C4	4.18	111.29	107.40
10	N	102	1N7	C2-C19-C18	4.16	116.28	111.82
10	J	1505	1N7	C9-C5-C6	4.13	104.26	100.09
10	J	1504	1N7	C19-C18-C17	-4.05	107.03	111.88
10	I	1401	1N7	C19-C18-C17	-4.02	107.06	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	N	102	1N7	C16-C15-C14	-4.02	106.56	111.19
10	J	1505	1N7	C2-C19-C18	3.96	116.07	111.82
10	J	1505	1N7	C5-C6-C18	3.95	119.79	114.74
10	J	1505	1N7	C21-C20-C22	-3.77	104.45	110.36
10	I	1401	1N7	C9-C5-C6	3.77	103.90	100.09
10	J	1504	1N7	C16-C17-C18	-3.74	107.48	111.48
10	N	102	1N7	C5-C6-C18	3.68	119.44	114.74
10	J	1505	1N7	C14-C13-C12	-3.59	106.27	110.55
10	J	1505	1N7	C6-C5-C4	3.49	110.66	107.40
10	I	1401	1N7	C16-C15-C2	-3.47	108.97	112.66
10	I	1401	1N7	C5-C6-C18	3.46	119.15	114.74
10	I	1401	1N7	C8-C7-C6	-3.44	98.32	105.13
10	J	1504	1N7	C8-C9-C20	3.43	117.46	112.15
10	J	1505	1N7	C19-C18-C17	-3.40	107.81	111.88
10	I	1401	1N7	C1-C12-C13	-3.24	106.30	110.47
10	J	1505	1N7	C11-C2-C1	-3.23	103.05	108.26
10	N	102	1N7	C21-C20-C22	-3.03	105.62	110.36
10	J	1505	1N7	C1-C12-C13	-3.01	106.60	110.47
10	J	1504	1N7	C19-C3-C4	-3.01	110.32	114.30
10	I	1401	1N7	C2-C19-C18	2.94	114.97	111.82
10	J	1504	1N7	C22-C20-C9	2.87	116.21	110.28
10	J	1505	1N7	C16-C15-C2	-2.86	109.62	112.66
10	J	1505	1N7	C8-C9-C20	-2.77	107.86	112.15
10	I	1401	1N7	C3-C19-C2	-2.73	110.91	113.73
10	J	1504	1N7	C9-C5-C6	2.61	102.73	100.09
10	N	102	1N7	C14-C15-C2	2.59	115.40	112.66
10	N	102	1N7	C21-C20-C9	-2.57	108.98	112.92
10	N	102	1N7	C14-C13-C12	-2.54	107.53	110.55
10	J	1505	1N7	C10-C5-C9	-2.53	107.25	111.21
10	J	1504	1N7	C1-C12-C13	-2.51	107.24	110.47
10	J	1504	1N7	C16-C15-C14	-2.49	108.33	111.19
10	N	102	1N7	C19-C2-C15	2.41	111.97	108.58
10	J	1504	1N7	C14-C13-C12	-2.34	107.76	110.55
10	N	102	1N7	C22-C20-C9	2.32	115.08	110.28
10	N	102	1N7	C1-C12-C13	-2.25	107.58	110.47
10	N	102	1N7	C8-C9-C20	-2.25	108.67	112.15
10	N	102	1N7	C19-C18-C17	-2.18	109.27	111.88
10	N	102	1N7	C19-C3-C4	-2.13	111.49	114.30
10	N	102	1N7	C11-C2-C1	-2.13	104.83	108.26
10	N	102	1N7	C10-C5-C9	-2.12	107.89	111.21
10	J	1505	1N7	C19-C2-C15	2.05	111.46	108.58

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	J	1504	1N7	C21-C20-C9-C5
10	J	1504	1N7	C21-C20-C9-C8
10	J	1504	1N7	C22-C20-C9-C8
10	J	1504	1N7	C22-C20-C9-C5
10	J	1505	1N7	C9-C20-C22-C23
10	J	1505	1N7	C21-C20-C22-C23
10	I	1401	1N7	C9-C20-C22-C23
10	N	102	1N7	C20-C22-C23-C24
10	I	1401	1N7	C21-C20-C22-C23

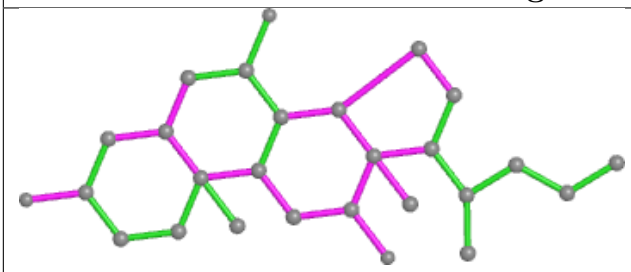
There are no ring outliers.

4 monomers are involved in 24 short contacts:

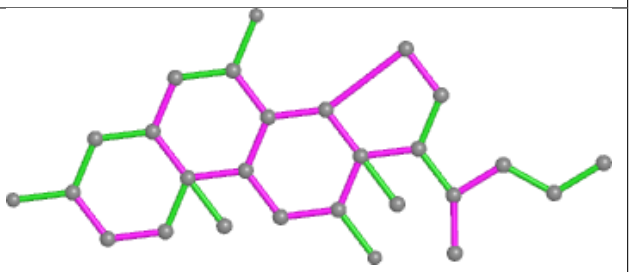
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	I	1401	1N7	6	0
10	J	1504	1N7	6	0
10	J	1505	1N7	7	0
10	N	102	1N7	6	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

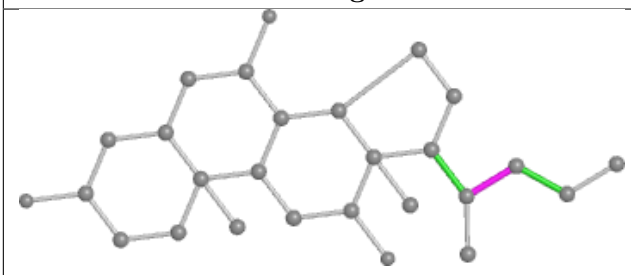
Ligand 1N7 I 1401



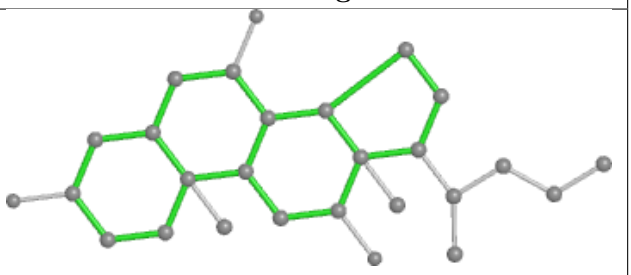
Bond lengths



Bond angles

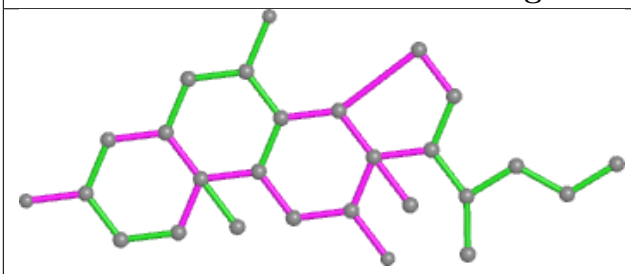


Torsions

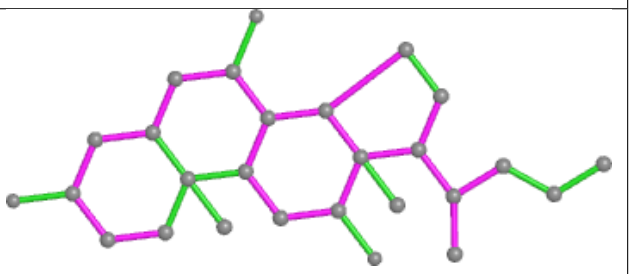


Rings

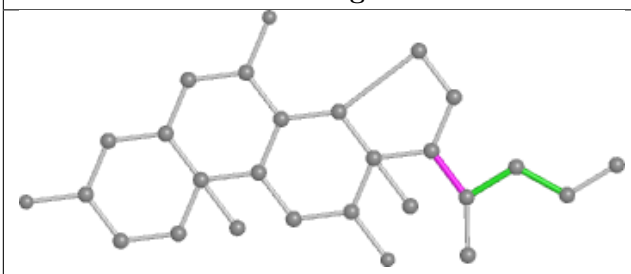
Ligand 1N7 J 1504



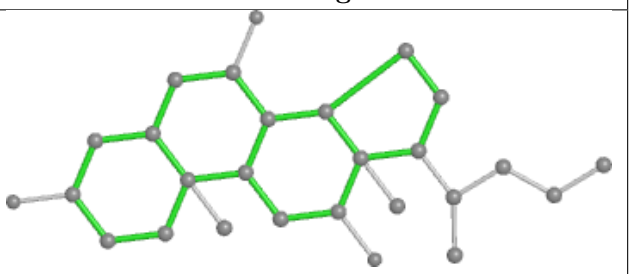
Bond lengths



Bond angles

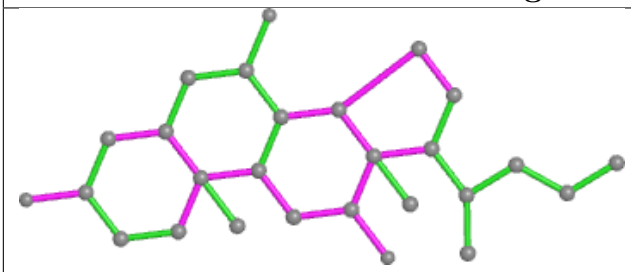


Torsions

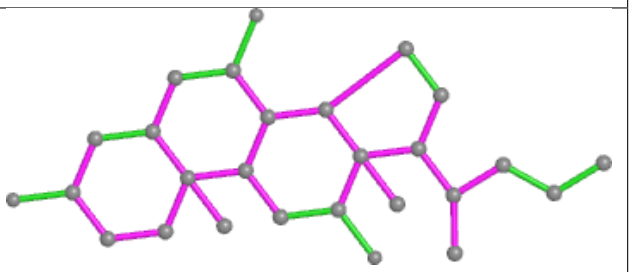


Rings

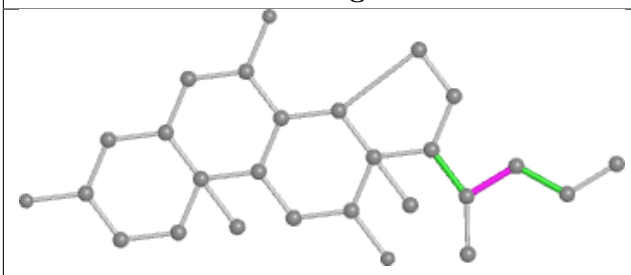
Ligand 1N7 J 1505



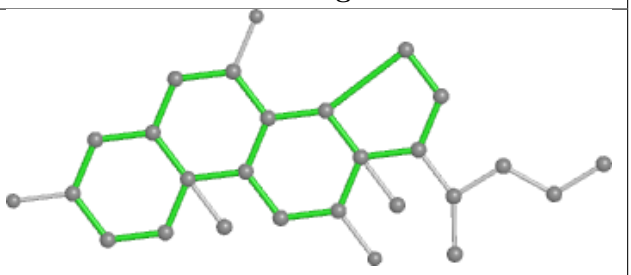
Bond lengths



Bond angles

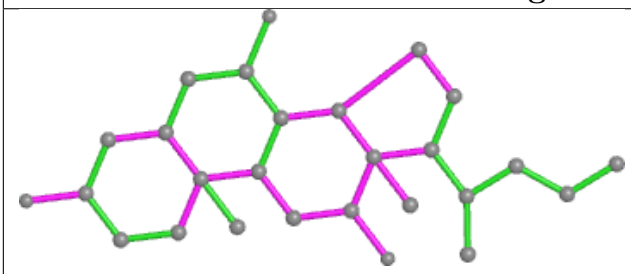


Torsions

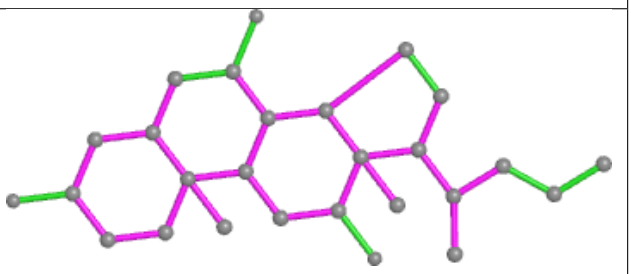


Rings

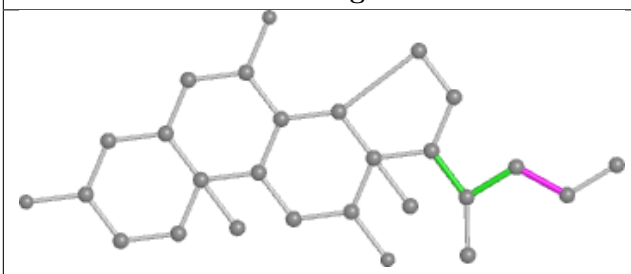
Ligand 1N7 N 102



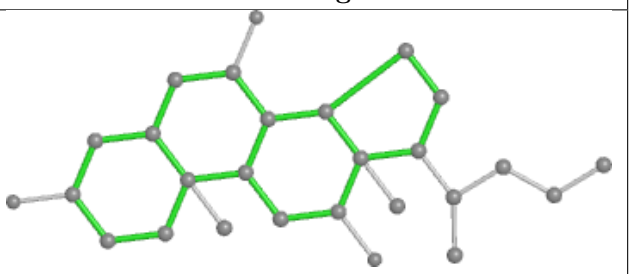
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

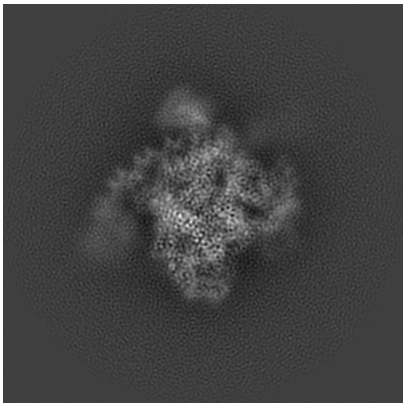
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20463. These allow visual inspection of the internal detail of the map and identification of artifacts.

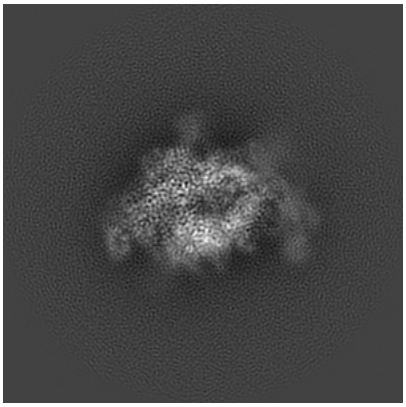
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

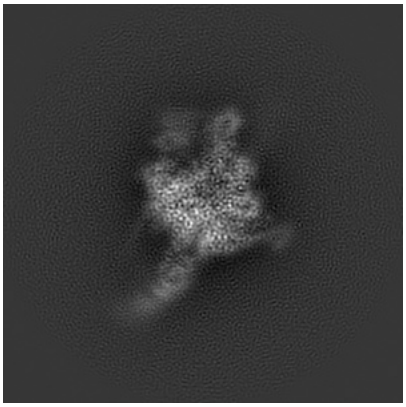
6.1.1 Primary map



X



Y

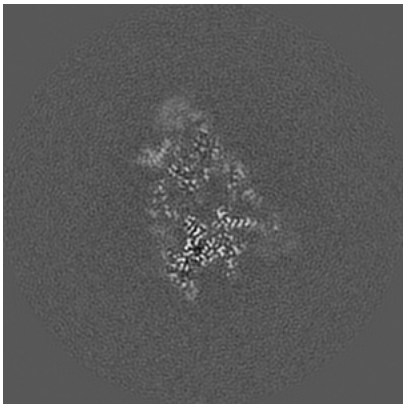


Z

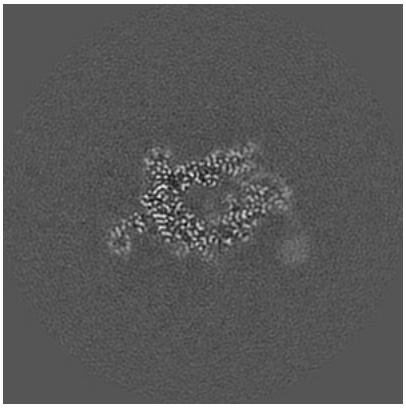
The images above show the map projected in three orthogonal directions.

6.2 Central slices

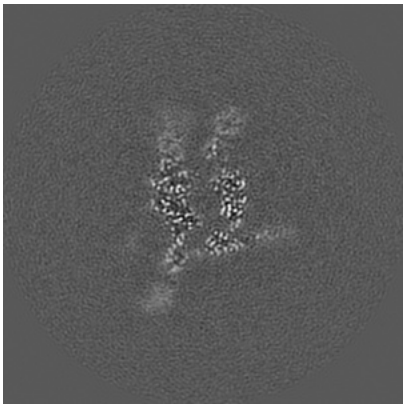
6.2.1 Primary map



X Index: 128



Y Index: 128

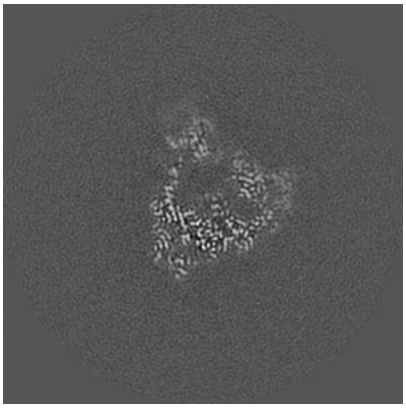


Z Index: 128

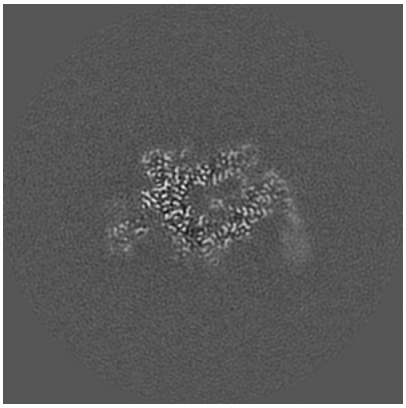
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

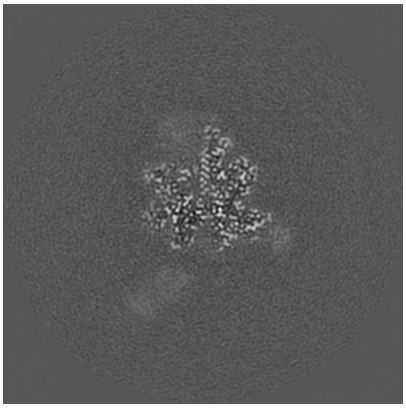
6.3.1 Primary map



X Index: 138



Y Index: 124

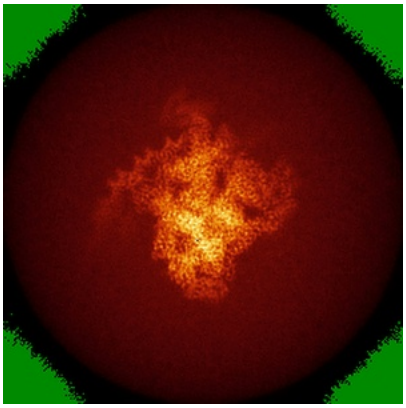


Z Index: 115

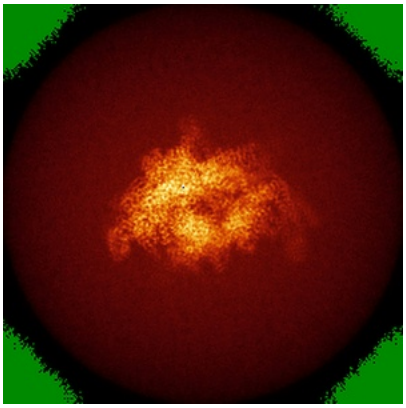
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

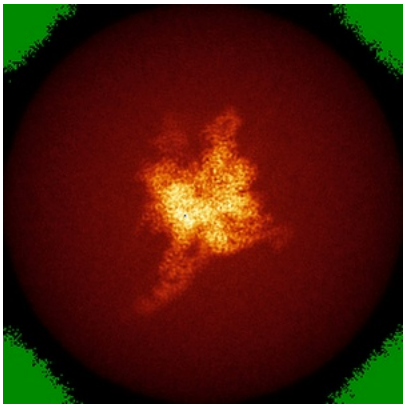
6.4.1 Primary map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

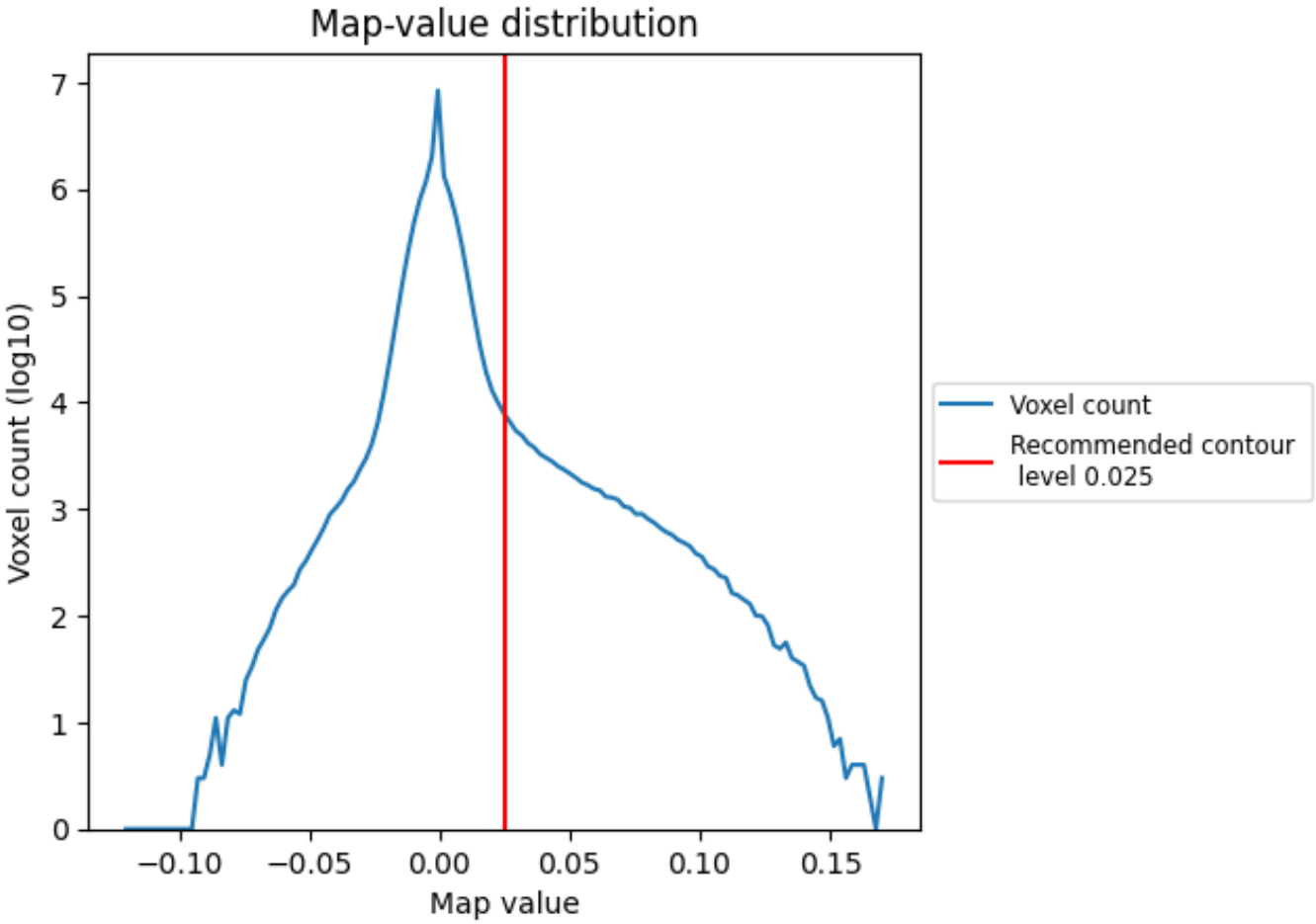
6.6 Mask visualisation (i)

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

7 Map analysis

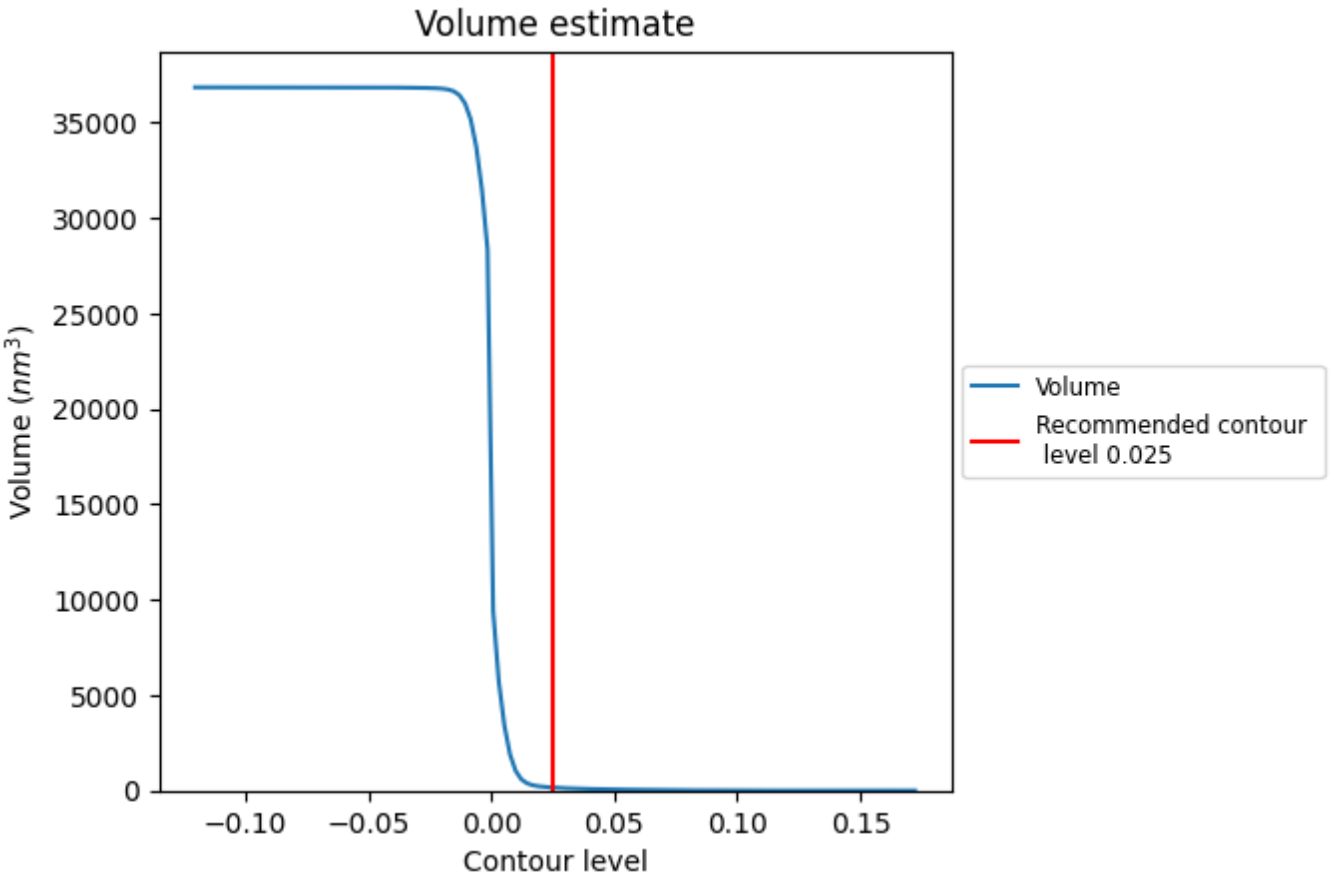
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

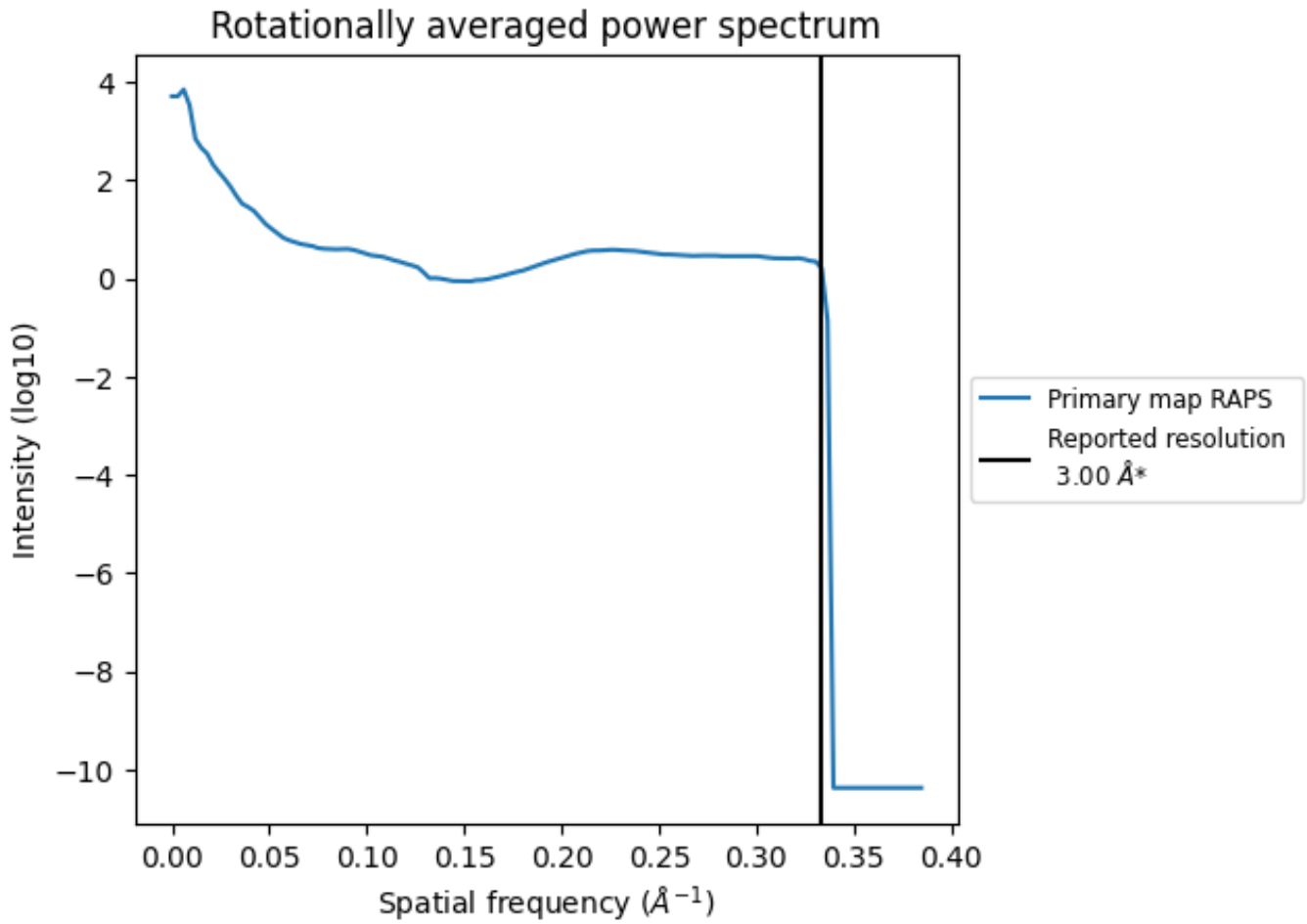
7.2 Volume estimate



The volume at the recommended contour level is 159 nm^3; this corresponds to an approximate mass of 143 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)

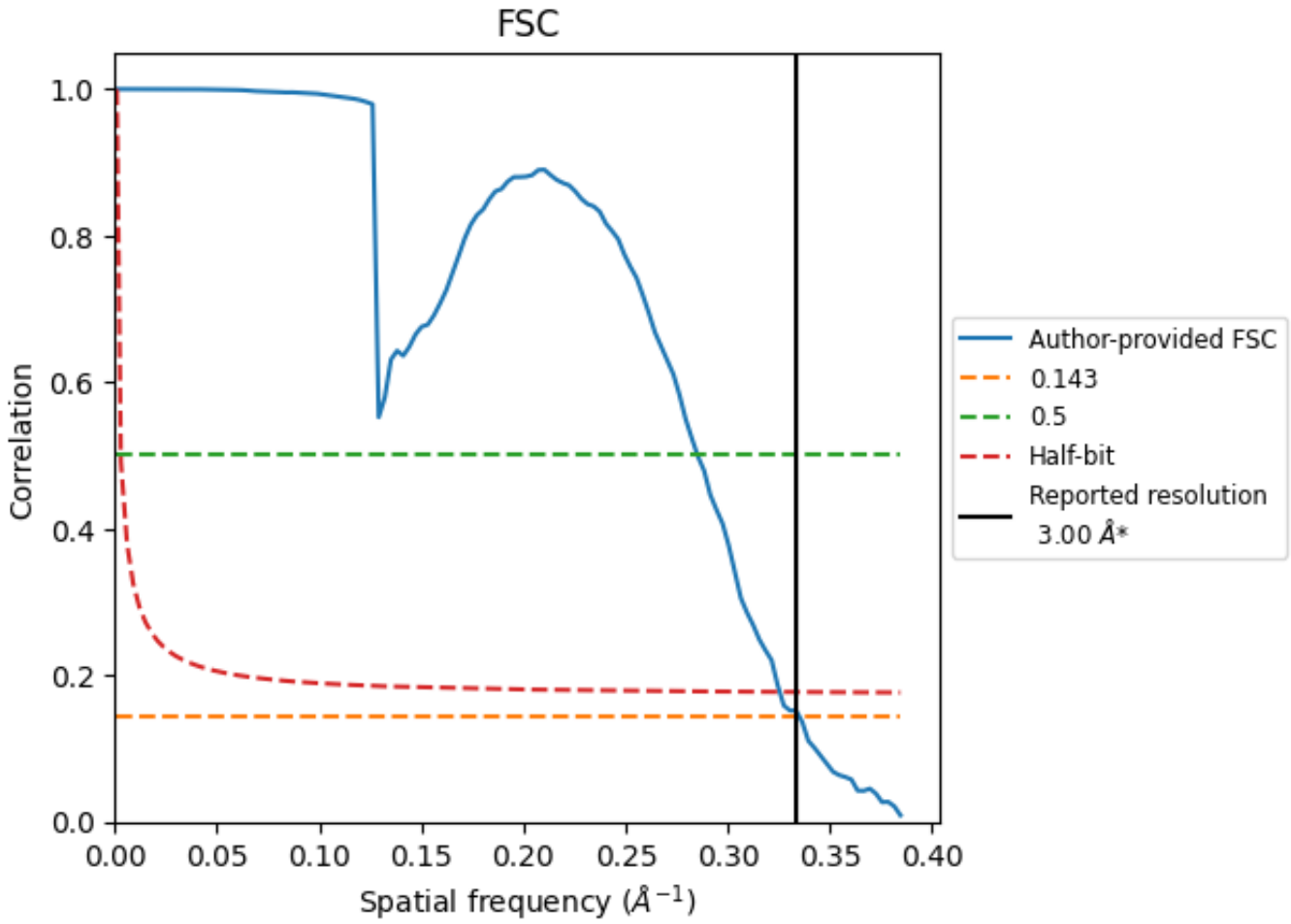


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

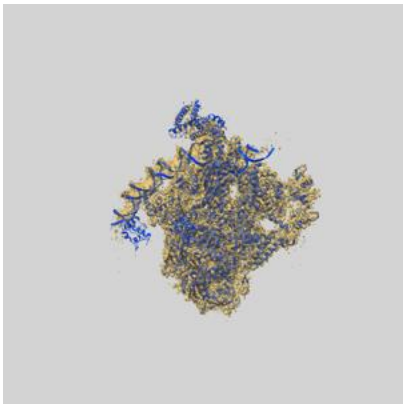
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.98	3.51	3.07
Unmasked-calculated*	-	-	-

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

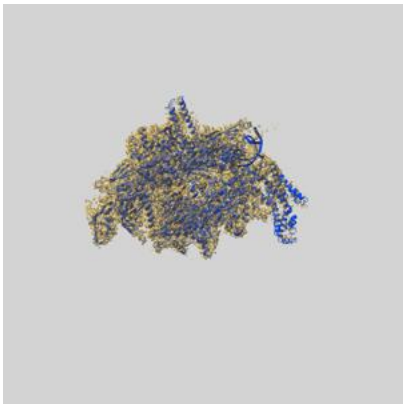
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20463 and PDB model 6PST. Per-residue inclusion information can be found in section 3 on page 8.

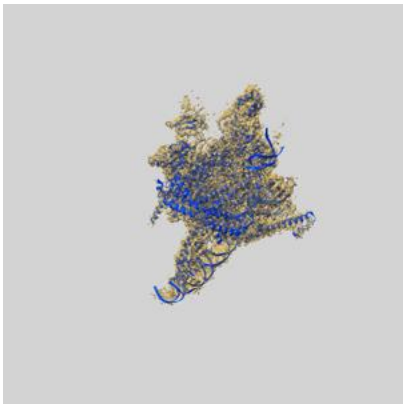
9.1 Map-model overlay



X



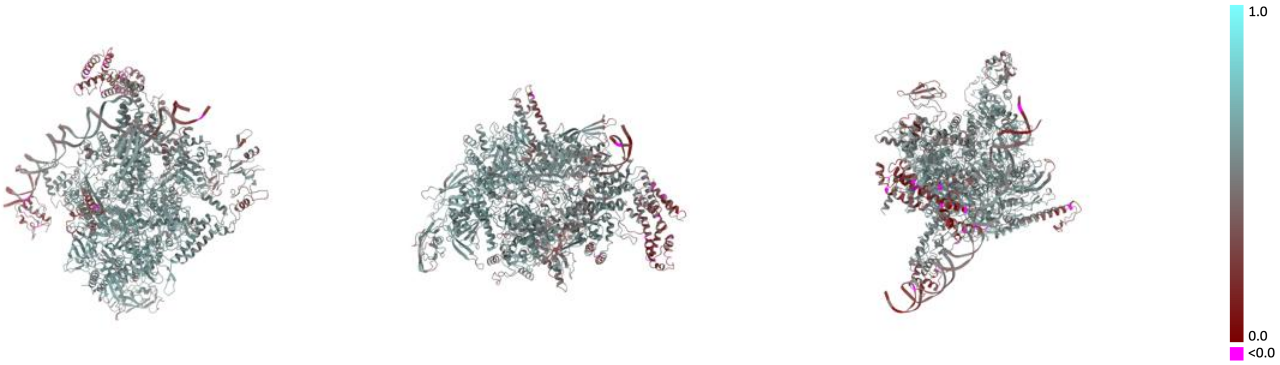
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

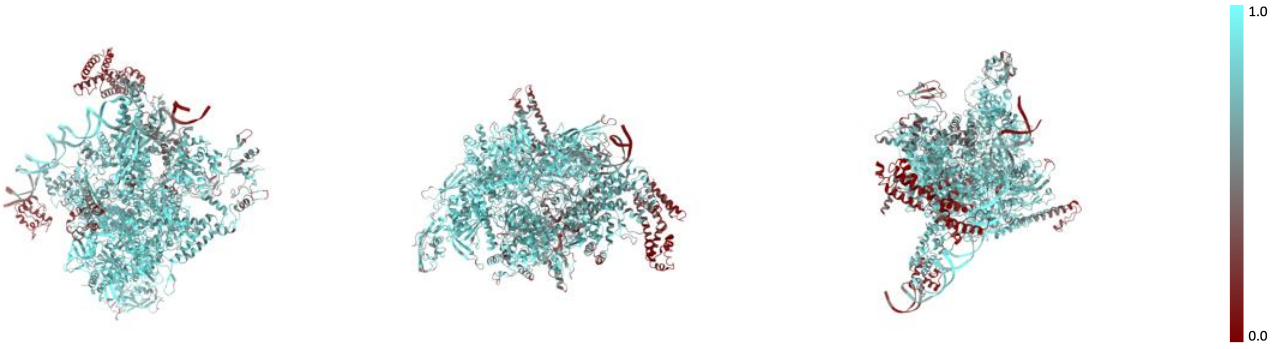
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

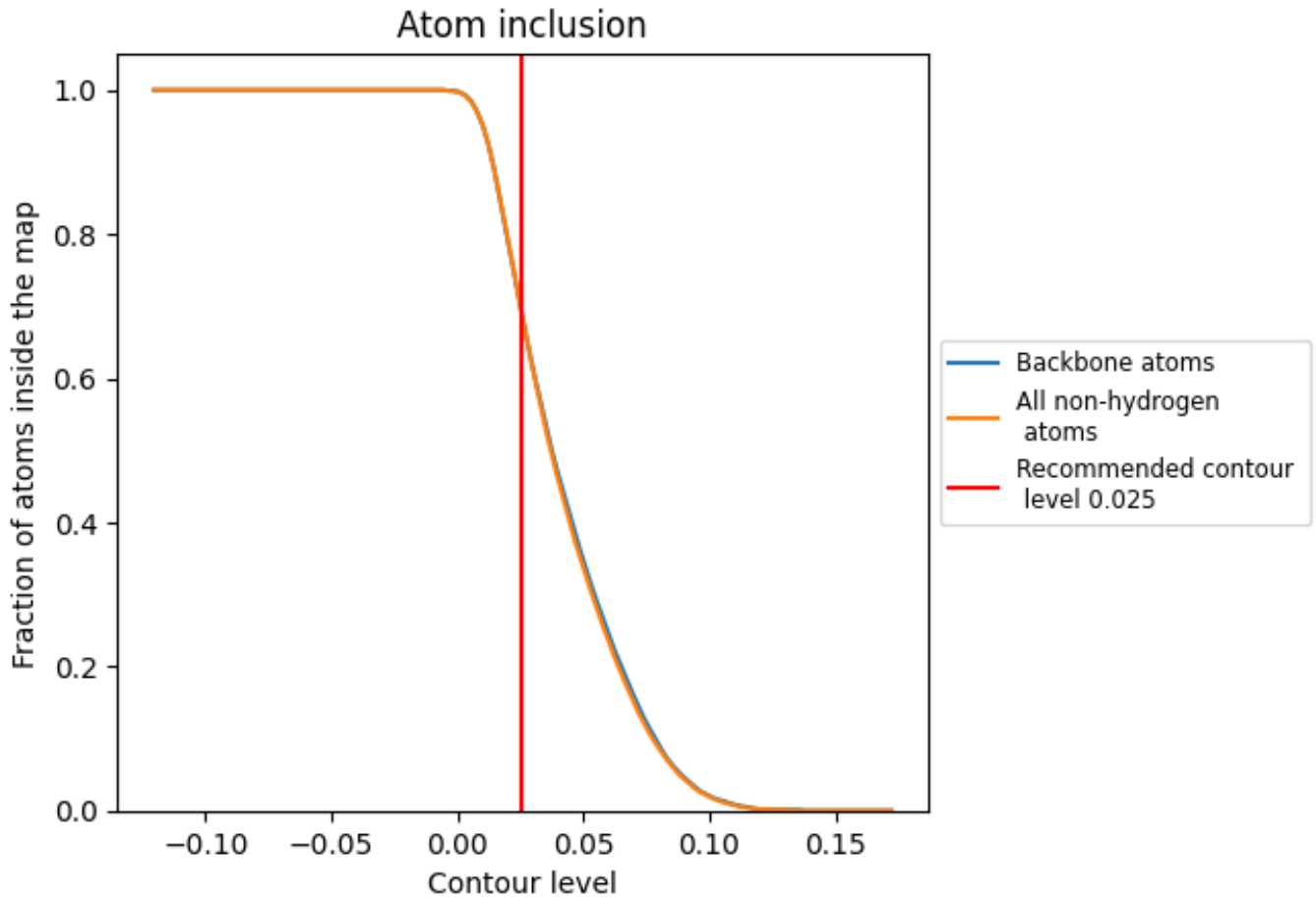
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 70% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6980	0.5140
G	0.8030	0.5640
H	0.7580	0.5390
I	0.7720	0.5510
J	0.7720	0.5470
K	0.6540	0.5560
L	0.4760	0.4160
M	0.0390	0.2480
N	0.7560	0.5270
O	0.6370	0.4080
P	0.6060	0.3850