



Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 01:56 PM EST

PDB ID : 6PSR
EMDB ID : EMD-20461
Title : Escherichia coli RNA polymerase promoter unwinding intermediate (TRPi1) with TraR and rpsT P2 promoter
Authors : Chen, J.; Chiu, C.E.; Campbell, E.A.; Darst, S.A.
Deposited on : 2019-07-13
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

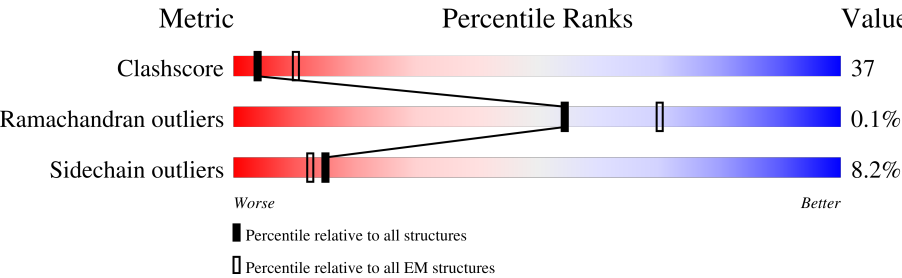
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

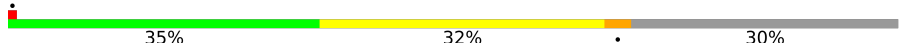
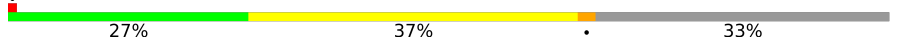

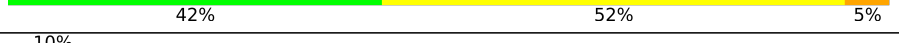
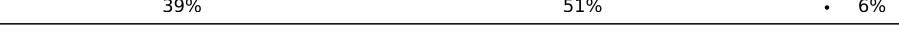
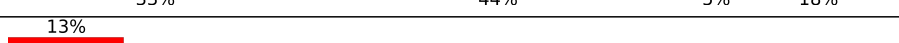


The reported resolution of this entry is 3.40 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

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

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Mol	Chain	Length	Quality of chain
7	O	85	 <div>9%33%58%</div>
8	P	85	 <div>39%59%</div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 32342 atoms, of which 156 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	230	Total	C	N	O	S	0	0
			1771	1106	314	345	6		
1	H	219	Total	C	N	O	S	0	0
			1678	1048	295	329	6		
1	M	73	Total	C	N	O	S	0	0
			572	362	100	108	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	1340	Total	C	N	O	S	0	0
			10559	6627	1841	2048	43		

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

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 4 is a protein called DNA-directed RNA polymerase subunit omega.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	548	Total	C	N	O	S	0	0
			4407	2754	771	855	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 6 is a protein called Protein TraR.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	72	Total	C	N	O	S	0	0
			565	350	102	108	5		

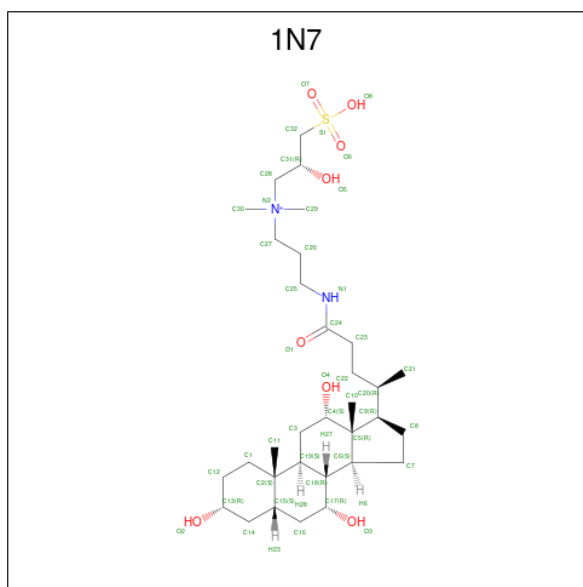
- Molecule 7 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	36	Total	C	N	O	P	0	0
			746	353	154	203	36		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	35	Total	C	N	O	P	0	0
			710	342	111	222	35		

- Molecule 9 is CHAPSO (three-letter code: 1N7) (formula: C₃₂H₅₉N₂O₈S).



Mol	Chain	Residues	Atoms				AltConf
9	I	1	Total	C	H	O	0
			66	24	39	3	
9	J	1	Total	C	H	O	0
			132	48	78	6	
9	J	1	Total	C	H	O	0
			132	48	78	6	
9	L	1	Total	C	H	O	0
			66	24	39	3	

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

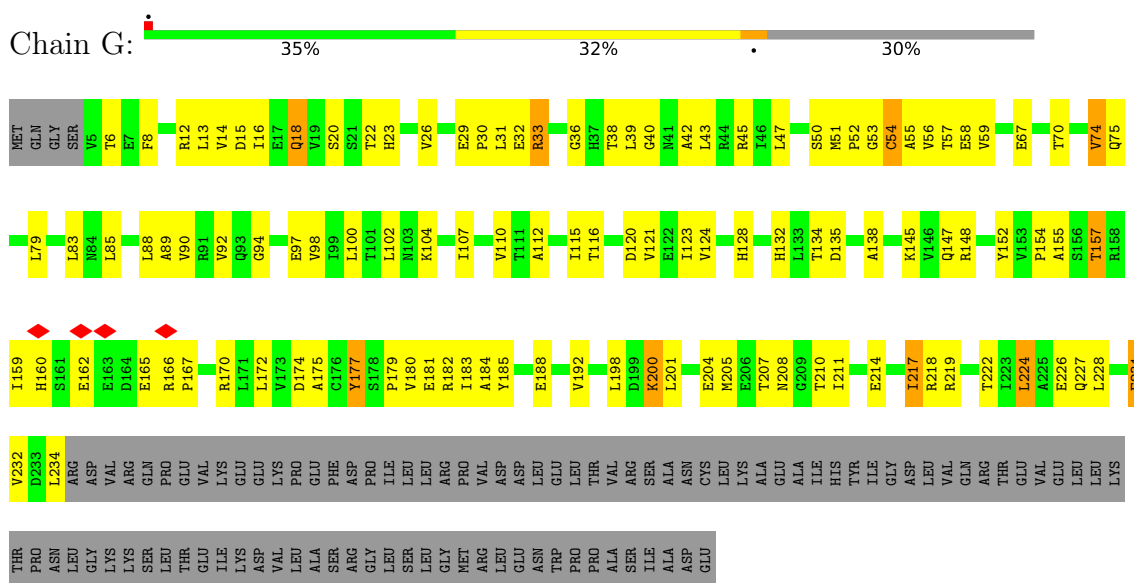
- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

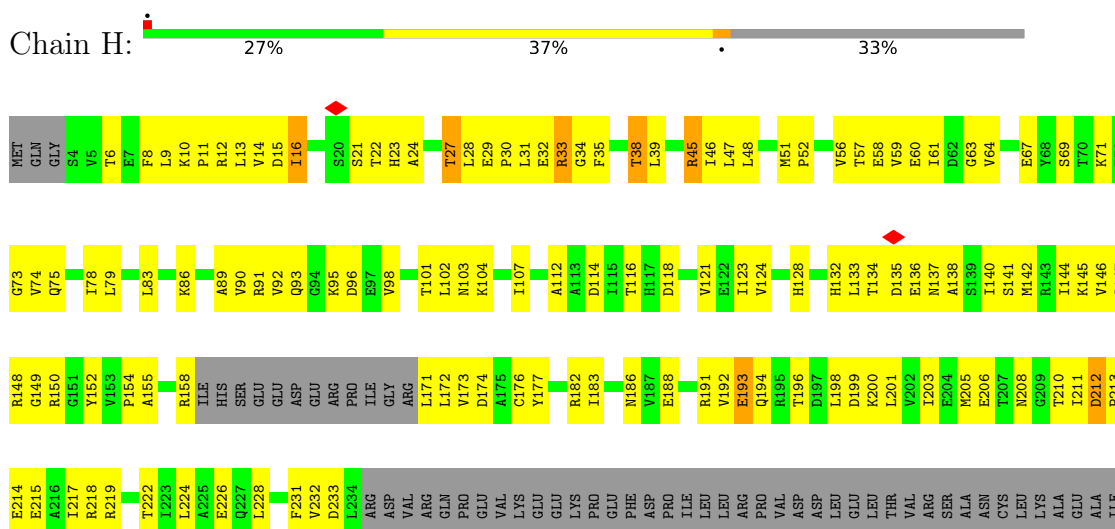
3 Residue-property plots [i](#)

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: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha

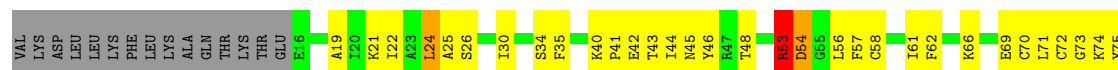


- Molecule 1: DNA-directed RNA polymerase subunit alpha

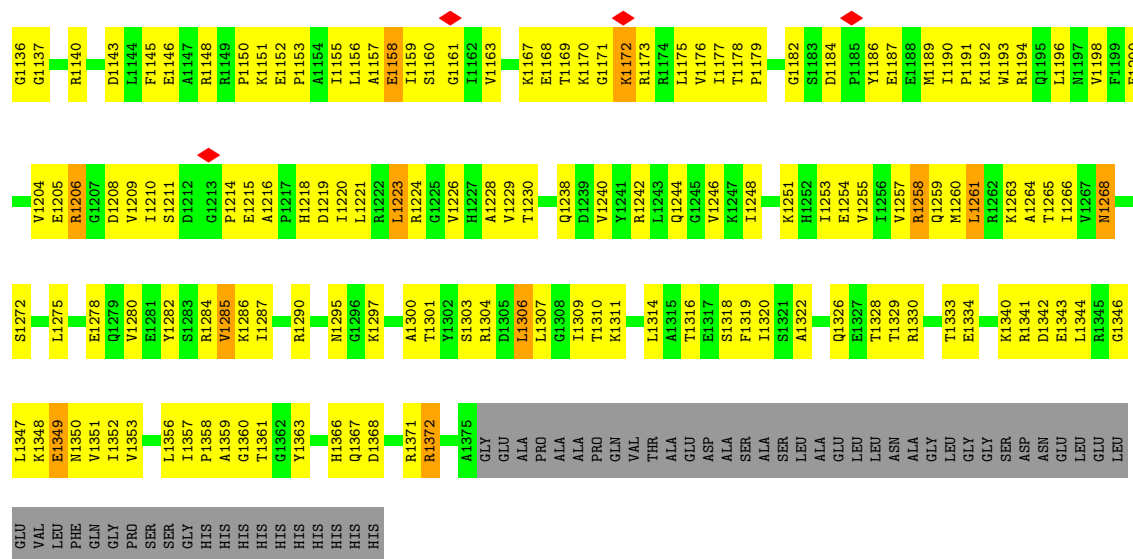
T301	E302	I303	V306	L307	A308	S309	R310	G311	L312	S313	L314	G315	M316	R317	L318	E319	N320	W321	P322	PRO	ALA	SER	ILE	ALA	ASP	GLU
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- Molecule 2: DNA-directed RNA polymerase subunit beta

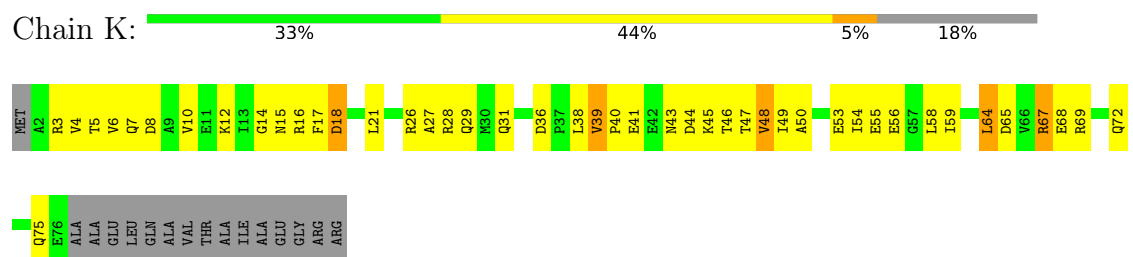
H342	H343	H346	H347	H348	H349	H350	H351	H352	H353	H356	H357	H358	H359	H360	H361	H362	H363	H364	H367	H368	H369	H370	H371	H372	H373	H374	H378	H381	H382	H385	L388	H392	D393	H394	H395	D396	L397	H398	H399	V400	G401	N406	L410	R411	E412	E413	D424	H425
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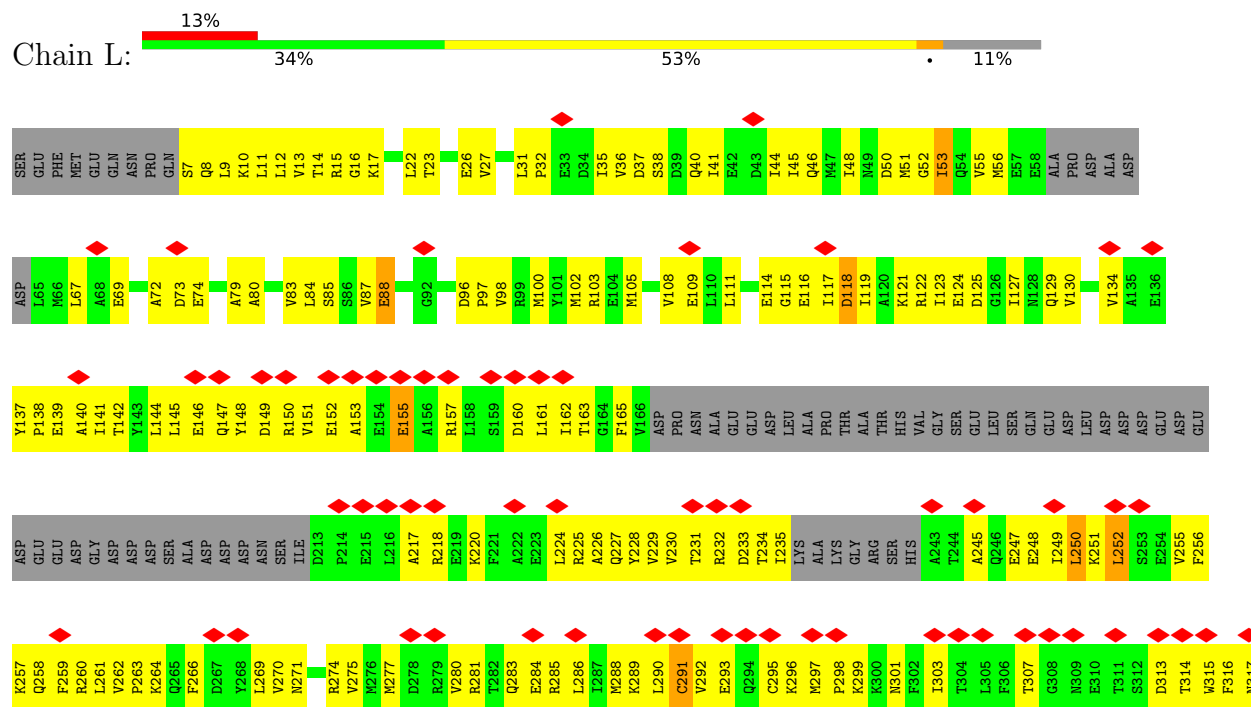


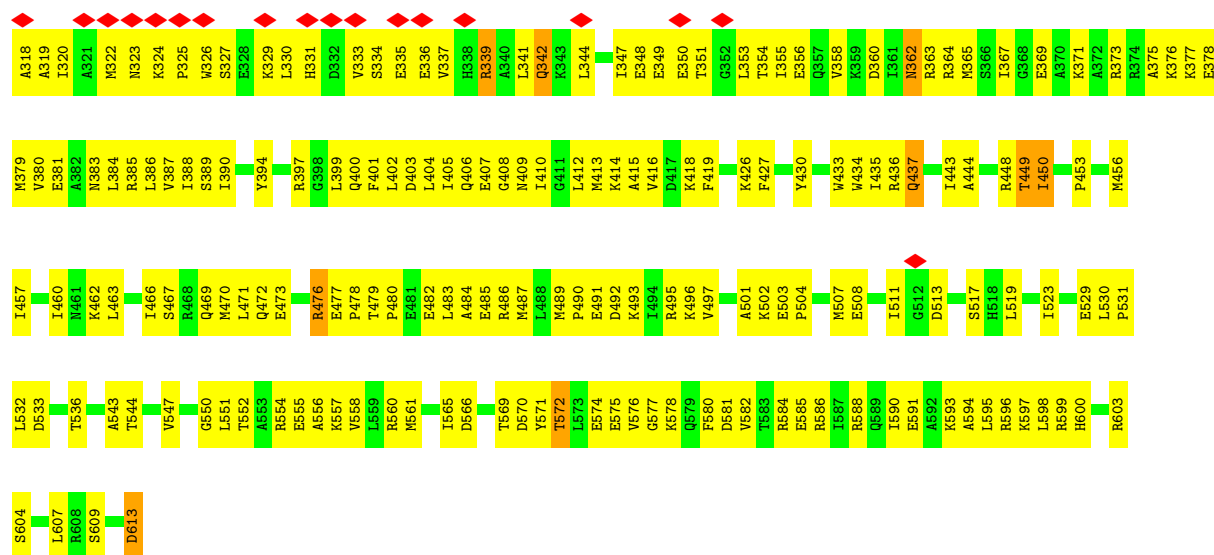


• Molecule 4: DNA-directed RNA polymerase subunit omega

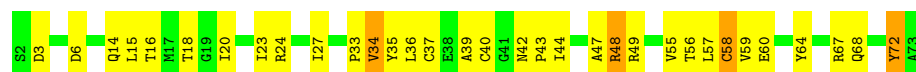


• Molecule 5: RNA polymerase sigma factor RpoD

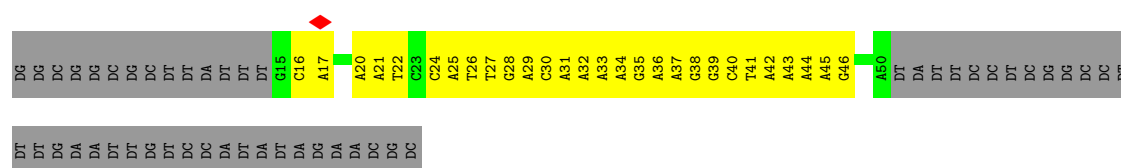




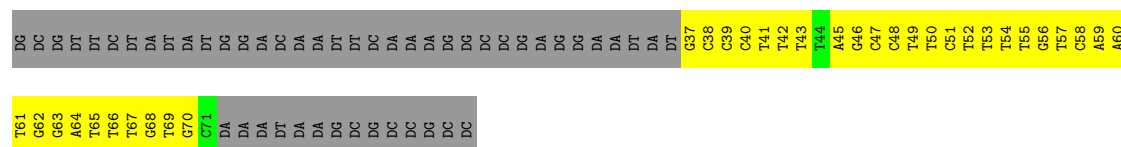
• Molecule 6: Protein TraR



• Molecule 7: DNA (85-MER)



• Molecule 8: DNA (85-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	98324	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.223	Depositor
Minimum map value	-0.124	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality

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	G	0.41	0/1793	0.53	0/2432
1	H	0.37	0/1697	0.54	0/2301
1	M	0.25	0/579	0.47	0/784
2	I	0.43	0/10728	0.52	1/14477 (0.0%)
3	J	0.40	0/10625	0.53	1/14345 (0.0%)
4	K	0.33	0/602	0.49	0/810
5	L	0.29	0/4461	0.48	0/6004
6	N	0.39	0/575	0.49	0/778
7	O	0.61	0/842	0.88	0/1297
8	P	0.58	0/790	1.05	0/1217
All	All	0.41	0/32692	0.55	2/44445 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	I	0	2
3	J	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	53	ARG	CB-CA-C	5.29	120.97	110.40
2	I	15	PHE	C-N-CA	-5.09	111.61	122.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	519	ASN	Peptide
2	I	897	PRO	Peptide
3	J	53	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1771	0	1799	111	0
1	H	1678	0	1698	131	0
1	M	572	0	602	84	0
2	I	10559	0	10577	767	0
3	J	10466	0	10689	868	0
4	K	600	0	607	48	0
5	L	4407	0	4432	414	0
6	N	565	0	545	35	0
7	O	746	0	401	41	0
8	P	710	0	402	50	0
9	I	27	39	39	4	0
9	J	54	78	75	9	0
9	L	27	39	38	4	0
10	J	1	0	0	0	0
11	J	2	0	0	0	0
11	N	1	0	0	0	0
All	All	32186	156	31904	2388	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 37.

All (2388) 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)
9:L:701:1N7:C19	9:L:701:1N7:C3	1.82	1.58
9:I:1401:1N7:C3	9:I:1401:1N7:C19	1.82	1.56
9:J:1505:1N7:C3	9:J:1505:1N7:C19	1.81	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:1504:1N7:C19	9:J:1504:1N7:C3	1.84	1.50
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.34	1.08
3:J:1025:MET:HB3	3:J:1124:ILE:HB	1.35	1.06
2:I:1002:LEU:HD21	2:I:1008:GLN:HB2	1.37	1.05
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.39	1.04
2:I:985:GLU:HB2	2:I:989:LEU:HB2	1.36	1.04
5:L:45:ILE:HD11	5:L:55:VAL:HG11	1.36	1.03
3:J:1089:LEU:HA	3:J:1096:PRO:HA	1.39	1.01
5:L:37:ASP:HB2	5:L:40:GLN:HG2	1.37	1.01
5:L:394:TYR:HB3	5:L:397:ARG:HG3	1.43	1.00
2:I:745:GLU:HA	2:I:1017:GLN:HG2	1.43	0.99
2:I:207:THR:HA	2:I:210:LEU:HD12	1.42	0.99
3:J:1078:LEU:HD22	3:J:1121:LEU:HD11	1.44	0.98
5:L:364:ARG:HA	5:L:367:ILE:HD12	1.43	0.97
2:I:839:VAL:HG12	2:I:1049:ILE:HG12	1.46	0.97
2:I:372:PRO:HG2	5:L:36:VAL:HG12	1.46	0.96
5:L:145:LEU:HD13	5:L:225:ARG:HG3	1.47	0.96
3:J:201:LEU:HD11	3:J:220:ARG:HD3	1.48	0.95
2:I:142:GLU:HG2	2:I:515:MET:HE2	1.48	0.95
1:M:278:ILE:HG23	1:M:281:LEU:HD23	1.47	0.94
5:L:326:TRP:HA	5:L:329:LYS:HE2	1.49	0.94
2:I:254:ASP:HA	2:I:263:VAL:O	1.68	0.93
2:I:170:VAL:HG23	6:N:72:TYR:HB2	1.47	0.92
5:L:290:LEU:HB3	5:L:333:VAL:HG11	1.51	0.92
5:L:145:LEU:HB3	5:L:225:ARG:HD3	1.53	0.91
3:J:1198:VAL:HG11	3:J:1210:ILE:HD12	1.49	0.91
3:J:975:ILE:HD13	3:J:980:THR:HB	1.50	0.91
3:J:79:LYS:HB2	5:L:569:THR:HB	1.53	0.91
3:J:338:PHE:HA	3:J:342:LEU:HD22	1.53	0.90
3:J:1038:THR:O	3:J:1077:ALA:HB3	1.72	0.90
3:J:1061:VAL:HG21	3:J:1101:LEU:HG	1.51	0.90
3:J:1081:VAL:HG12	3:J:1087:ASP:HA	1.52	0.90
2:I:94:ALA:HB2	2:I:129:LEU:HD11	1.55	0.89
3:J:705:THR:HG22	3:J:707:ILE:HD11	1.53	0.89
3:J:955:LYS:HA	3:J:1012:ALA:HA	1.55	0.89
5:L:119:ILE:HG23	5:L:375:ALA:HB1	1.54	0.88
3:J:129:ASP:HB2	3:J:220:ARG:HH21	1.39	0.88
3:J:809:VAL:HG21	3:J:909:ILE:HG21	1.54	0.88
7:O:40:DC:H2"	7:O:41:DT:H5"	1.55	0.88
5:L:72:ALA:HB1	5:L:73:ASP:HB2	1.56	0.88
2:I:898:GLU:HG3	5:L:565:ILE:HG12	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1333:LEU:HD23	3:J:307:LEU:HD22	1.55	0.88
3:J:958:ILE:HG23	3:J:982:LEU:HD21	1.56	0.88
3:J:1307:LEU:HD23	3:J:1311:LYS:HD2	1.54	0.87
3:J:759:ILE:HG23	3:J:771:GLN:HB3	1.56	0.87
1:G:167:PRO:HG2	1:G:170:ARG:HD2	1.56	0.87
2:I:1103:VAL:HG22	2:I:1111:GLN:HE21	1.40	0.87
5:L:130:VAL:HG12	5:L:365:MET:HG3	1.56	0.87
1:H:61:ILE:HD13	1:H:142:MET:HB3	1.57	0.87
4:K:26:ARG:HD3	4:K:59:ILE:HD12	1.56	0.86
5:L:32:PRO:HB2	5:L:35:ILE:HG13	1.55	0.86
5:L:9:LEU:HD11	5:L:32:PRO:HD3	1.57	0.86
2:I:633:LEU:HD13	2:I:644:LEU:HB3	1.58	0.86
3:J:1104:LYS:HG3	3:J:1124:ILE:HG23	1.58	0.86
1:H:58:GLU:HG3	1:H:145:LYS:HB3	1.57	0.86
2:I:979:LEU:HD23	2:I:989:LEU:HD11	1.55	0.86
2:I:471:VAL:HG11	2:I:498:ILE:HD11	1.59	0.85
3:J:964:LYS:HB3	3:J:977:SER:HB3	1.58	0.85
2:I:106:GLU:HB2	2:I:115:LYS:HG3	1.57	0.85
3:J:398:LYS:HD2	5:L:532:LEU:HD21	1.58	0.85
2:I:1267:GLY:HA3	3:J:347:VAL:O	1.77	0.85
3:J:957:SER:HA	3:J:1010:GLN:HA	1.58	0.85
3:J:163:GLU:HA	3:J:166:LEU:HD12	1.58	0.84
5:L:247:GLU:HA	5:L:250:LEU:HD23	1.58	0.84
3:J:291:ILE:HD13	5:L:409:ASN:HB3	1.58	0.84
5:L:109:GLU:HG3	5:L:111:LEU:HD12	1.59	0.84
2:I:538:LEU:HD21	2:I:547:VAL:HG11	1.57	0.84
5:L:38:SER:HA	5:L:41:ILE:HD12	1.59	0.84
3:J:1135:THR:OG1	3:J:1140:ARG:HG2	1.77	0.83
2:I:993:PRO:HG2	2:I:996:ARG:HB2	1.57	0.83
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.59	0.83
2:I:69:GLN:HE21	2:I:101:ARG:HD2	1.43	0.83
2:I:298:ALA:HB3	2:I:334:GLU:HG2	1.61	0.83
2:I:103:VAL:HG12	2:I:117:ILE:HG13	1.61	0.83
3:J:1079:LYS:HD3	3:J:1098:GLN:HB3	1.61	0.82
1:M:260:LEU:HD11	1:M:310:ARG:HH11	1.43	0.82
5:L:390:ILE:HG21	5:L:435:ILE:HG21	1.61	0.82
1:H:201:LEU:HD21	1:H:203:ILE:HD11	1.61	0.82
3:J:123:ARG:HA	3:J:126:LEU:HD23	1.62	0.82
4:K:5:THR:HG22	4:K:7:GLN:H	1.44	0.82
2:I:1326:LEU:HD22	3:J:342:LEU:HD21	1.62	0.81
3:J:1109:LEU:HD12	3:J:1121:LEU:HD13	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:10:LYS:HE2	5:L:85:SER:HB3	1.63	0.81
3:J:53:ARG:HE	3:J:54:ASP:HB2	1.43	0.81
2:I:9:LYS:HG2	2:I:1171:ARG:HH12	1.45	0.81
3:J:857:LEU:HG	3:J:858:VAL:HG23	1.63	0.81
3:J:553:THR:HG22	3:J:567:THR:HB	1.63	0.80
3:J:823:THR:HG22	3:J:879:ALA:HA	1.62	0.80
2:I:957:LYS:HB2	2:I:1029:LEU:HD11	1.64	0.80
2:I:996:ARG:HA	2:I:996:ARG:HH11	1.46	0.80
3:J:1177:ILE:HB	3:J:1186:TYR:HD2	1.47	0.80
2:I:898:GLU:HG2	5:L:544:THR:HG21	1.63	0.80
2:I:1257:GLN:HE22	3:J:341:ASN:HB2	1.47	0.80
3:J:986:ASP:HB2	3:J:992:LYS:HD3	1.62	0.80
1:H:107:ILE:HG12	1:H:135:ASP:HA	1.62	0.80
3:J:317:THR:H	3:J:318:GLY:HA2	1.45	0.80
2:I:811:ASN:HA	2:I:815:SER:HB2	1.64	0.79
3:J:1176:VAL:HG13	3:J:1187:GLU:HB3	1.63	0.79
9:L:701:1N7:C3	9:L:701:1N7:C18	2.59	0.79
3:J:983:LYS:HE3	3:J:994:SER:HB3	1.64	0.79
2:I:196:VAL:HG23	2:I:206:ALA:HA	1.64	0.79
5:L:118:ASP:N	5:L:118:ASP:OD1	2.15	0.79
1:G:102:LEU:HD11	1:G:110:VAL:HG11	1.62	0.79
3:J:550:VAL:HG23	3:J:552:ILE:HG23	1.63	0.78
2:I:39:ILE:HD11	2:I:75:LEU:HG	1.64	0.78
2:I:303:ASP:HB3	2:I:308:GLU:HB2	1.64	0.78
2:I:746:ALA:HB2	2:I:974:ARG:HD2	1.65	0.78
3:J:278:ARG:HG3	3:J:281:ARG:HH21	1.48	0.78
5:L:316:PHE:HE2	5:L:334:SER:HA	1.48	0.78
1:M:289:LEU:HD13	1:M:300:LEU:HD21	1.65	0.78
5:L:341:LEU:HA	5:L:344:LEU:HD12	1.65	0.78
2:I:242:VAL:HB	2:I:245:ARG:HD3	1.66	0.78
5:L:288:MET:O	5:L:292:VAL:N	2.17	0.78
2:I:528:ARG:NH2	2:I:576:SER:O	2.16	0.78
3:J:1170:LYS:HD3	3:J:1172:LYS:HE3	1.66	0.78
5:L:266:PHE:HA	5:L:269:LEU:HD12	1.63	0.78
1:M:260:LEU:HD23	1:M:306:VAL:HG22	1.65	0.78
5:L:596:ARG:HA	5:L:599:ARG:HD2	1.65	0.77
2:I:300:ASP:HA	2:I:312:ALA:HA	1.65	0.77
3:J:1110:GLU:HB2	3:J:1113:VAL:HG21	1.67	0.77
1:H:64:VAL:HG11	1:H:78:ILE:HD13	1.67	0.77
2:I:538:LEU:HD13	2:I:543:ALA:HB2	1.67	0.77
5:L:588:ARG:NH2	8:P:58:DC:OP2	2.16	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:42:DT:H1'	8:P:43:DT:H5'	1.67	0.77
1:M:269:CYS:HB3	1:M:295:LEU:HD12	1.67	0.76
2:I:826:ASP:OD1	2:I:829:THR:OG1	2.03	0.76
2:I:802:VAL:HG21	2:I:1098:LEU:HD22	1.68	0.76
3:J:973:LEU:HG	3:J:1006:GLY:HA3	1.68	0.76
3:J:804:ALA:HA	3:J:1259:GLN:HG3	1.67	0.76
3:J:888:CYS:SG	3:J:890:THR:OG1	2.44	0.76
1:H:86:LYS:HD3	1:H:174:ASP:HB2	1.68	0.76
3:J:959:LYS:HB3	3:J:983:LYS:HB2	1.68	0.76
1:G:8:PHE:HE1	1:H:150:ARG:HD3	1.51	0.76
3:J:1061:VAL:HG11	3:J:1101:LEU:HB3	1.67	0.76
3:J:108:ALA:H	3:J:276:ASN:HD21	1.30	0.75
5:L:476:ARG:NH2	5:L:482:GLU:OE2	2.20	0.75
2:I:1119:MET:HG2	2:I:1204:LEU:HD13	1.67	0.75
2:I:877:VAL:HG11	2:I:920:VAL:HG21	1.69	0.75
2:I:1242:LYS:HB3	3:J:465:GLN:HE21	1.52	0.75
3:J:288:PRO:HG2	3:J:291:ILE:HD12	1.69	0.75
3:J:1230:THR:HG22	3:J:1257:VAL:HG11	1.68	0.75
1:G:179:PRO:HB3	1:G:210:THR:HG23	1.69	0.75
1:G:14:VAL:HG21	1:G:29:GLU:HB2	1.69	0.75
2:I:341:LEU:HD11	6:N:67:ARG:HD2	1.68	0.75
5:L:449:THR:HG23	5:L:450:ILE:HD13	1.67	0.75
1:G:45:ARG:HG2	1:H:38:THR:HB	1.69	0.74
3:J:1005:LYS:HE3	3:J:1009:GLU:HB3	1.66	0.74
1:G:45:ARG:HH21	2:I:1216:ARG:HA	1.52	0.74
8:P:38:DC:H2''	8:P:39:DC:H5''	1.69	0.74
2:I:484:LEU:HB3	2:I:486:THR:HG22	1.69	0.74
3:J:142:GLU:OE2	5:L:103:ARG:NH2	2.21	0.74
3:J:1172:LYS:HB2	3:J:1189:MET:HB3	1.68	0.74
2:I:1329:GLU:OE1	3:J:337:ARG:NH1	2.21	0.74
3:J:811:GLU:O	3:J:896:ALA:N	2.20	0.74
3:J:412:LEU:HG	3:J:441:LEU:HD11	1.70	0.73
3:J:390:LEU:HD23	3:J:407:VAL:HG21	1.71	0.73
3:J:844:THR:OG1	3:J:860:ARG:O	2.05	0.73
3:J:960:LEU:HD11	3:J:1007:ASP:HA	1.71	0.73
1:H:64:VAL:HG21	1:H:78:ILE:HD11	1.70	0.73
2:I:146:VAL:HG21	2:I:513:GLN:HE21	1.51	0.73
2:I:148:GLN:OE1	2:I:454:ARG:NH1	2.21	0.73
3:J:97:VAL:HG12	3:J:101:ARG:HD2	1.70	0.73
3:J:1046:ILE:HD12	3:J:1059:LEU:HD13	1.70	0.73
5:L:324:LYS:N	5:L:327:SER:OG	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:153:ASN:HB2	3:J:172:PHE:HE2	1.54	0.73
1:G:18:GLN:NE2	1:G:20:SER:O	2.21	0.73
4:K:3:ARG:NH1	4:K:5:THR:O	2.21	0.73
5:L:217:ALA:HA	5:L:220:LYS:HE2	1.69	0.73
8:P:48:DC:H2"	8:P:49:DT:H71	1.70	0.73
3:J:1161:GLY:O	3:J:1204:VAL:N	2.22	0.73
2:I:988:LYS:HA	2:I:991:LYS:HG3	1.71	0.73
1:H:24:ALA:HB3	1:H:213:PRO:HB2	1.70	0.72
2:I:8:LYS:O	2:I:1171:ARG:NH2	2.22	0.72
3:J:895:CYS:SG	3:J:898:CYS:N	2.61	0.72
5:L:401:PHE:HA	5:L:404:LEU:HD12	1.69	0.72
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.72	0.72
2:I:716:ALA:HB3	2:I:784:ALA:HB3	1.70	0.72
3:J:230:SER:OG	3:J:232:ASN:ND2	2.23	0.72
1:H:61:ILE:HG22	1:H:63:GLY:H	1.55	0.72
3:J:893:GLY:O	3:J:1258:ARG:NH2	2.22	0.72
8:P:64:DA:H1'	8:P:65:DT:H5"	1.72	0.72
1:H:47:LEU:HA	1:H:51:MET:HG3	1.71	0.72
2:I:936:ARG:N	2:I:1047:LEU:O	2.23	0.71
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.71	0.71
2:I:897:PRO:O	2:I:899:GLU:N	2.23	0.71
5:L:550:GLY:O	5:L:603:ARG:NH2	2.22	0.71
3:J:264:ASP:HB3	3:J:324:LEU:HD22	1.72	0.71
3:J:1081:VAL:HA	3:J:1088:VAL:HG23	1.72	0.71
2:I:301:TYR:N	2:I:311:CYS:O	2.22	0.71
2:I:1106:ARG:HE	3:J:731:ARG:HH22	1.39	0.71
3:J:53:ARG:HB3	3:J:54:ASP:CB	2.21	0.71
2:I:803:ALA:HB2	2:I:1094:VAL:HG11	1.72	0.71
2:I:990:ASP:N	2:I:990:ASP:OD1	2.22	0.71
5:L:386:LEU:O	5:L:389:SER:OG	2.03	0.71
3:J:809:VAL:HG12	3:J:911:LYS:HA	1.73	0.71
9:J:1505:1N7:C3	9:J:1505:1N7:C18	2.65	0.71
3:J:853:THR:O	3:J:855:ASP:N	2.24	0.71
5:L:463:LEU:HD11	5:L:483:LEU:HD23	1.72	0.71
3:J:1030:GLU:HG3	3:J:1090:ILE:HG23	1.73	0.70
5:L:119:ILE:HA	5:L:122:ARG:HD3	1.72	0.70
2:I:870:ILE:HG21	2:I:931:VAL:HG11	1.74	0.70
5:L:533:ASP:HA	5:L:536:THR:HG22	1.72	0.70
2:I:933:VAL:HG22	2:I:1050:VAL:HG22	1.73	0.70
2:I:1060:ILE:HD12	2:I:1234:LYS:HD2	1.73	0.70
3:J:697:MET:HE3	3:J:741:ALA:HB3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1265:THR:OG1	3:J:1303:SER:O	2.09	0.70
5:L:146:GLU:OE2	5:L:150:ARG:NH1	2.24	0.70
5:L:320:ILE:HD11	5:L:331:HIS:HB3	1.73	0.70
3:J:325:LYS:HD2	5:L:508:GLU:HG3	1.73	0.70
3:J:117:LEU:HG	3:J:124:ILE:HD12	1.72	0.70
5:L:152:GLU:HB3	5:L:218:ARG:HD3	1.74	0.70
5:L:405:ILE:O	5:L:409:ASN:ND2	2.23	0.70
1:H:46:ILE:HD12	1:H:224:LEU:HB2	1.74	0.70
2:I:998:LEU:HG	2:I:1015:ALA:HA	1.74	0.70
1:M:270:LEU:O	1:M:275:ILE:N	2.24	0.70
3:J:1157:ALA:N	3:J:1208:ASP:O	2.25	0.69
5:L:555:GLU:OE2	5:L:597:LYS:NZ	2.24	0.69
3:J:1064:SER:HB3	3:J:1072:LYS:HB2	1.74	0.69
2:I:211:ARG:NH1	2:I:357:ASN:O	2.25	0.69
2:I:253:PHE:CA	2:I:265:LYS:HB3	2.22	0.69
1:G:90:VAL:HG22	1:G:123:ILE:HD13	1.72	0.69
3:J:262:THR:HG23	5:L:504:PRO:HB2	1.74	0.69
2:I:714:VAL:HB	2:I:787:PRO:HD2	1.75	0.69
3:J:961:SER:O	3:J:980:THR:HA	1.92	0.69
5:L:584:ARG:NH2	8:P:56:DG:N7	2.40	0.69
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.75	0.69
2:I:118:LYS:HD3	2:I:488:MET:HG2	1.74	0.69
5:L:319:ALA:HA	5:L:322:MET:HG3	1.75	0.69
2:I:241:LEU:N	2:I:283:LYS:O	2.25	0.69
7:O:26:DT:H2'	7:O:27:DT:H71	1.72	0.69
2:I:685:MET:SD	2:I:1073:LYS:HG2	2.33	0.69
3:J:252:LEU:HD12	3:J:262:THR:HG22	1.75	0.69
3:J:849:LEU:HD12	3:J:856:ILE:HA	1.75	0.69
2:I:517:GLN:HB3	2:I:759:SER:OG	1.93	0.69
2:I:1117:LEU:HD12	2:I:1195:ILE:HG12	1.73	0.69
3:J:749:LYS:HG2	3:J:755:ILE:HD11	1.74	0.69
3:J:1101:LEU:HD12	3:J:1102:PRO:HD2	1.74	0.69
2:I:520:PRO:HG3	2:I:714:VAL:HG21	1.75	0.68
2:I:637:ARG:HA	2:I:642:SER:HA	1.74	0.68
5:L:150:ARG:HB3	5:L:155:GLU:HB2	1.73	0.68
9:L:701:1N7:C3	9:L:701:1N7:C2	2.69	0.68
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.39	0.68
2:I:1288:GLN:O	2:I:1292:THR:HG22	1.93	0.68
5:L:555:GLU:HG2	5:L:594:ALA:HB2	1.74	0.68
5:L:383:ASN:O	5:L:387:VAL:HG23	1.94	0.68
3:J:491:LEU:HB2	3:J:904:ALA:HB1	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1160:SER:OG	3:J:1205:GLU:OE1	2.11	0.68
2:I:361:SER:HA	2:I:364:VAL:HG22	1.75	0.68
1:G:100:LEU:HD23	1:G:115:ILE:HG21	1.76	0.68
3:J:809:VAL:HG23	3:J:915:ILE:HG21	1.74	0.68
2:I:151:ARG:HH11	2:I:445:ILE:HG21	1.59	0.67
2:I:253:PHE:CE2	2:I:255:ILE:HG12	2.28	0.67
2:I:565:GLU:HB3	2:I:680:LEU:HD21	1.73	0.67
5:L:387:VAL:HA	5:L:390:ILE:HG22	1.74	0.67
2:I:1072:ASN:ND2	2:I:1111:GLN:OE1	2.27	0.67
3:J:823:THR:HB	3:J:824:PRO:HD2	1.76	0.67
3:J:1175:LEU:HD13	3:J:1190:ILE:HD11	1.76	0.67
5:L:348:GLU:HG2	5:L:355:ILE:HG23	1.75	0.67
2:I:255:ILE:HD12	2:I:263:VAL:HG21	1.76	0.67
5:L:316:PHE:CE2	5:L:334:SER:HA	2.28	0.67
2:I:142:GLU:HG2	2:I:515:MET:CE	2.21	0.67
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.76	0.67
3:J:534:GLU:O	3:J:538:ARG:HG2	1.94	0.67
3:J:810:THR:OG1	3:J:1363:TYR:OH	2.11	0.67
5:L:72:ALA:CB	5:L:73:ASP:HB2	2.25	0.67
1:M:270:LEU:HB3	1:M:275:ILE:HB	1.76	0.67
3:J:700:ASN:O	3:J:704:GLU:HB2	1.95	0.67
8:P:39:DC:H2''	8:P:40:DC:H5'	1.77	0.67
1:H:182:ARG:NH1	3:J:534:GLU:OE1	2.27	0.67
2:I:253:PHE:HA	2:I:265:LYS:HD2	1.77	0.67
2:I:966:ILE:HG12	9:I:1401:1N7:H26	1.75	0.67
3:J:801:VAL:O	3:J:805:GLN:HB2	1.94	0.67
3:J:950:ILE:HD12	3:J:1017:VAL:HG23	1.75	0.67
2:I:475:VAL:HG22	2:I:492:MET:HE2	1.76	0.67
4:K:38:LEU:N	4:K:53:GLU:OE2	2.27	0.67
5:L:296:LYS:HE2	5:L:296:LYS:HA	1.77	0.67
3:J:253:VAL:HG21	5:L:523:ILE:HD13	1.77	0.67
3:J:842:ARG:HB2	3:J:882:VAL:HG21	1.76	0.67
1:M:307:LEU:O	1:M:311:GLY:N	2.28	0.67
3:J:968:ASN:HD21	3:J:974:VAL:HG13	1.60	0.66
3:J:1357:ILE:HD12	3:J:1359:ALA:HB3	1.76	0.66
2:I:1275:VAL:O	2:I:1279:GLU:HG3	1.95	0.66
5:L:554:ARG:NH2	7:O:25:DA:OP2	2.28	0.66
2:I:982:GLY:O	2:I:1002:LEU:HB2	1.95	0.66
2:I:1151:LEU:HD21	2:I:1198:LEU:HA	1.76	0.66
2:I:1269:ARG:NH2	3:J:344:GLY:O	2.27	0.66
3:J:810:THR:HG1	3:J:1363:TYR:HH	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:381:GLU:O	5:L:384:LEU:HG	1.95	0.66
1:M:294:ASN:N	8:P:69:DT:OP1	2.28	0.66
3:J:1051:ASP:HB2	3:J:1056:LEU:H	1.61	0.66
5:L:577:GLY:O	5:L:581:ASP:N	2.29	0.66
2:I:74:ARG:NH1	2:I:121:GLU:OE2	2.28	0.66
2:I:971:LEU:HD11	2:I:1017:GLN:HG3	1.76	0.66
3:J:314:ARG:H	3:J:314:ARG:HD2	1.61	0.66
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.31	0.66
3:J:886:VAL:HG11	3:J:1230:THR:HG21	1.76	0.66
5:L:335:GLU:O	5:L:339:ARG:HD3	1.96	0.66
5:L:466:ILE:HD11	5:L:486:ARG:HH11	1.61	0.66
5:L:148:TYR:HE1	5:L:218:ARG:HG2	1.59	0.66
3:J:518:VAL:HG11	3:J:707:ILE:HB	1.78	0.66
3:J:789:LYS:NZ	3:J:928:THR:O	2.22	0.66
3:J:1069:ALA:HA	3:J:1072:LYS:HG2	1.76	0.66
5:L:46:GLN:O	5:L:50:ASP:HB2	1.96	0.66
1:M:253:LEU:HD22	1:M:282:VAL:HG21	1.77	0.66
5:L:324:LYS:HB3	5:L:325:PRO:HD2	1.77	0.66
2:I:519:ASN:HB3	2:I:522:SER:H	1.60	0.66
2:I:700:VAL:HG13	2:I:1117:LEU:HD22	1.78	0.66
9:J:1505:1N7:C3	9:J:1505:1N7:C2	2.69	0.66
2:I:120:GLN:NE2	2:I:490:GLN:OE1	2.29	0.65
3:J:1346:GLY:O	3:J:1350:ASN:ND2	2.25	0.65
5:L:448:ARG:NH1	5:L:501:ALA:O	2.28	0.65
1:M:270:LEU:HD22	1:M:275:ILE:HD12	1.78	0.65
2:I:233:ARG:HA	2:I:233:ARG:HE	1.61	0.65
2:I:671:LEU:HB3	2:I:1186:VAL:HG12	1.77	0.65
2:I:977:ALA:HA	2:I:980:VAL:HG23	1.77	0.65
2:I:1065:LYS:HD3	2:I:1235:LEU:HD12	1.77	0.65
2:I:1294:LYS:HD2	3:J:349:TYR:HD2	1.61	0.65
3:J:724:MET:O	3:J:728:SER:OG	2.13	0.65
3:J:803:VAL:HG11	3:J:1309:ILE:HG22	1.77	0.65
5:L:9:LEU:O	5:L:13:VAL:HG23	1.96	0.65
2:I:133:ASN:ND2	2:I:713:GLY:HA3	2.12	0.65
3:J:288:PRO:HG3	5:L:380:VAL:HG21	1.78	0.65
3:J:489:ASN:HD21	3:J:905:ARG:HH11	1.45	0.65
5:L:231:THR:HA	5:L:248:GLU:HG3	1.79	0.65
9:I:1401:1N7:C3	9:I:1401:1N7:C18	2.72	0.65
3:J:198:CYS:O	3:J:202:ARG:HG3	1.95	0.65
8:P:40:DC:H1'	8:P:41:DT:H5'	1.79	0.65
1:G:45:ARG:HD3	2:I:1083:GLU:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:253:PHE:HA	2:I:265:LYS:HB3	1.77	0.65
3:J:1215:GLU:OE1	3:J:1224:ARG:NH2	2.27	0.65
1:M:299:SER:O	1:M:303:ILE:HG13	1.96	0.65
2:I:861:ALA:HB1	2:I:882:ILE:HD11	1.78	0.65
5:L:419:PHE:HA	5:L:430:TYR:HE2	1.60	0.65
3:J:822:MET:SD	3:J:838:ARG:NH2	2.70	0.65
1:G:42:ALA:HB1	1:G:224:LEU:HD11	1.78	0.64
2:I:841:ARG:HA	2:I:1046:VAL:HA	1.79	0.64
9:I:1401:1N7:C3	9:I:1401:1N7:C2	2.71	0.64
1:H:57:THR:OG1	1:H:147:GLN:HB3	1.97	0.64
3:J:308:ASP:OD2	3:J:311:ARG:NH1	2.29	0.64
3:J:137:ARG:HG2	3:J:143:SER:OG	1.97	0.64
5:L:125:ASP:OD2	5:L:371:LYS:NZ	2.31	0.64
5:L:231:THR:HA	5:L:248:GLU:CG	2.27	0.64
1:H:71:LYS:HB3	1:H:74:VAL:HG22	1.78	0.64
2:I:14:ASP:H	2:I:1157:GLN:HG2	1.62	0.64
5:L:460:ILE:HG22	5:L:497:VAL:HG13	1.79	0.64
2:I:813:GLU:HB2	3:J:461:PHE:HD2	1.63	0.64
2:I:886:LYS:H	2:I:917:SER:HB3	1.62	0.64
3:J:1064:SER:CB	3:J:1072:LYS:HB2	2.28	0.64
1:H:33:ARG:NH2	2:I:820:GLU:OE2	2.30	0.64
2:I:57:PHE:CD2	2:I:70:TYR:HB2	2.33	0.64
3:J:937:ILE:HD11	3:J:1134:ILE:HB	1.78	0.64
2:I:529:ARG:HD3	2:I:572:ILE:HG22	1.80	0.64
2:I:742:TYR:HB3	2:I:743:PRO:HD2	1.80	0.64
3:J:364:HIS:HB3	3:J:487:THR:CG2	2.28	0.64
6:N:20:ILE:O	6:N:24:ARG:HG2	1.98	0.64
3:J:518:VAL:O	3:J:547:ARG:NH2	2.31	0.64
3:J:1143:ASP:OD1	5:L:67:LEU:HD22	1.97	0.64
2:I:299:LYS:HG2	2:I:334:GLU:OE1	1.98	0.64
3:J:759:ILE:HD12	3:J:771:GLN:HB3	1.80	0.64
3:J:925:GLU:HB3	3:J:926:PRO:HD3	1.79	0.64
5:L:490:PRO:HG3	5:L:493:LYS:HE3	1.79	0.64
2:I:27:LEU:HD13	2:I:524:ILE:HD11	1.79	0.63
2:I:231:GLU:O	2:I:238:GLN:HG3	1.98	0.63
3:J:417:ARG:NH1	4:K:43:ASN:OD1	2.31	0.63
7:O:25:DA:H2'	7:O:26:DT:H71	1.79	0.63
1:H:215:GLU:OE2	1:H:219:ARG:NH2	2.31	0.63
2:I:130:MET:SD	2:I:134:GLY:HA2	2.38	0.63
2:I:241:LEU:HD21	2:I:277:LEU:HD11	1.80	0.63
5:L:257:LYS:HE2	5:L:258:GLN:HE22	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:490:PRO:HG2	5:L:493:LYS:HG2	1.80	0.63
1:M:262:LEU:HD11	1:M:306:VAL:HG11	1.79	0.63
2:I:1154:ASP:N	2:I:1154:ASP:OD1	2.31	0.63
2:I:1243:MET:HE3	3:J:445:LYS:HB3	1.79	0.63
3:J:596:LEU:HD11	3:J:604:MET:CE	2.28	0.63
5:L:150:ARG:HB3	5:L:155:GLU:CB	2.28	0.63
5:L:377:LYS:O	5:L:381:GLU:HG3	1.98	0.63
1:H:193:GLU:OE1	1:H:194:GLN:N	2.24	0.63
2:I:27:LEU:O	2:I:528:ARG:NH1	2.32	0.63
3:J:73:GLY:O	3:J:76:LYS:NZ	2.24	0.63
3:J:679:TYR:OH	3:J:754:ILE:O	2.12	0.63
1:M:262:LEU:HD11	1:M:306:VAL:CG1	2.28	0.63
1:M:280:ASP:HA	1:M:283:GLN:HG3	1.79	0.63
1:H:59:VAL:O	1:H:171:LEU:HB2	1.98	0.63
2:I:470:ARG:CD	2:I:497:PRO:HB3	2.28	0.63
3:J:826:ILE:HD13	3:J:831:VAL:HG12	1.79	0.63
5:L:266:PHE:O	5:L:270:VAL:HG23	1.97	0.63
3:J:870:ASP:O	3:J:874:GLU:HG2	1.98	0.63
1:H:104:LYS:HG3	1:H:114:ASP:OD1	1.99	0.63
3:J:1075:ARG:HB2	3:J:1100:PHE:HD1	1.64	0.63
3:J:1175:LEU:HD22	3:J:1190:ILE:HD11	1.81	0.63
1:G:8:PHE:CE1	1:H:150:ARG:HD3	2.34	0.63
1:H:228:LEU:O	1:H:232:VAL:HG23	1.97	0.63
2:I:178:PRO:HG3	2:I:395:TYR:CE1	2.33	0.63
1:G:222:THR:OG1	1:H:233:ASP:OD1	2.17	0.63
2:I:1005:GLU:HG2	2:I:1006:GLU:H	1.62	0.63
3:J:252:LEU:HD12	3:J:262:THR:CG2	2.29	0.63
3:J:1329:THR:O	3:J:1333:THR:OG1	2.16	0.63
5:L:484:ALA:HB1	5:L:491:GLU:HG3	1.81	0.63
2:I:12:ARG:HG3	2:I:1181:PRO:HB2	1.79	0.62
2:I:303:ASP:CB	2:I:308:GLU:HB2	2.29	0.62
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.34	0.62
1:H:152:TYR:HE1	1:H:176:CYS:HG	1.45	0.62
2:I:180:ARG:NH2	2:I:393:ASP:O	2.32	0.62
2:I:924:VAL:HG13	2:I:1056:VAL:HG11	1.80	0.62
3:J:423:LEU:HB3	3:J:466:MET:HE2	1.81	0.62
3:J:510:LEU:O	3:J:514:THR:HG23	1.99	0.62
3:J:525:MET:O	3:J:548:VAL:HG22	1.99	0.62
3:J:1035:VAL:HB	3:J:1109:LEU:HD13	1.79	0.62
2:I:216:THR:OG1	2:I:219:GLN:OE1	2.14	0.62
2:I:469:VAL:O	2:I:472:GLU:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1120:ALA:O	2:I:1124:ILE:HG12	1.99	0.62
2:I:1212:LEU:HD22	2:I:1225:VAL:CG2	2.30	0.62
3:J:681:LYS:O	3:J:685:ILE:HG13	1.99	0.62
2:I:225:PHE:HE2	2:I:347:ILE:HB	1.63	0.62
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.80	0.62
2:I:724:VAL:HG11	2:I:727:VAL:HG22	1.81	0.62
3:J:1011:VAL:HG12	3:J:1012:ALA:H	1.63	0.62
5:L:271:ASN:O	5:L:275:VAL:HG23	1.99	0.62
1:M:280:ASP:HB2	1:M:284:ARG:HH21	1.64	0.62
1:G:14:VAL:HG12	1:G:15:ASP:H	1.63	0.62
1:H:73:GLY:CA	1:H:134:THR:HB	2.29	0.62
2:I:796:LEU:HB2	2:I:1233:LEU:HD22	1.81	0.62
3:J:955:LYS:CA	3:J:1012:ALA:HA	2.28	0.62
3:J:1022:PRO:HB2	3:J:1126:GLN:HG2	1.80	0.62
3:J:1079:LYS:HD3	3:J:1098:GLN:CB	2.28	0.62
3:J:1238:GLN:HB3	3:J:1242:ARG:NH2	2.14	0.62
5:L:148:TYR:HE2	5:L:225:ARG:HH21	1.44	0.62
1:G:185:TYR:HB2	1:G:201:LEU:HD11	1.81	0.62
2:I:444:ASP:OD1	2:I:551:HIS:NE2	2.28	0.62
3:J:150:GLY:HA3	3:J:175:GLU:O	1.99	0.62
3:J:609:TYR:HD2	3:J:610:ARG:HD3	1.65	0.62
3:J:664:ILE:HG22	3:J:678:ARG:HG3	1.82	0.62
3:J:1156:LEU:HD23	3:J:1219:ASP:HB3	1.81	0.62
5:L:105:MET:HE1	5:L:385:ARG:HA	1.79	0.62
5:L:119:ILE:O	5:L:123:ILE:HG13	2.00	0.62
5:L:444:ALA:HB1	5:L:457:ILE:HD12	1.81	0.62
1:M:278:ILE:HA	1:M:281:LEU:HB3	1.82	0.62
1:H:205:MET:HE1	1:H:217:ILE:HG13	1.82	0.62
2:I:103:VAL:HG12	2:I:117:ILE:CG1	2.30	0.62
3:J:84:ILE:HD12	3:J:91:GLU:HB2	1.80	0.62
1:G:154:PRO:HG2	1:G:157:THR:HG23	1.81	0.62
1:H:152:TYR:HE2	1:H:154:PRO:HG3	1.65	0.62
2:I:1062:PRO:HA	2:I:1076:ILE:O	2.00	0.62
5:L:109:GLU:HG3	5:L:111:LEU:CD1	2.30	0.62
5:L:409:ASN:O	5:L:413:MET:HG3	1.99	0.62
5:L:551:LEU:HD21	5:L:597:LYS:HD2	1.81	0.62
3:J:930:LEU:HD22	3:J:1244:GLN:HG3	1.80	0.62
3:J:1040:MET:HG2	3:J:1076:PRO:HA	1.82	0.62
3:J:1272:SER:HB2	3:J:1300:ALA:HB2	1.81	0.62
2:I:378:ARG:O	2:I:382:GLU:HG2	1.99	0.61
2:I:1130:ALA:O	2:I:1134:GLN:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1163:VAL:HG13	3:J:1200:GLU:HA	1.82	0.61
2:I:759:SER:OG	2:I:760:ASN:N	2.33	0.61
3:J:337:ARG:HD3	3:J:341:ASN:OD1	2.00	0.61
3:J:816:THR:CG2	3:J:889:ASP:HB2	2.29	0.61
5:L:281:ARG:HG2	5:L:285:ARG:HE	1.64	0.61
5:L:613:ASP:N	5:L:613:ASP:OD1	2.32	0.61
1:G:224:LEU:HD22	1:G:228:LEU:HD23	1.81	0.61
2:I:118:LYS:HD3	2:I:488:MET:HA	1.82	0.61
3:J:848:VAL:CG1	3:J:858:VAL:HB	2.30	0.61
3:J:1156:LEU:HD12	3:J:1209:VAL:HG22	1.81	0.61
1:G:112:ALA:HB1	1:G:123:ILE:HG21	1.82	0.61
2:I:1113:LEU:HD13	3:J:641:ILE:HD13	1.82	0.61
3:J:519:ASN:HA	3:J:523:GLU:OE1	2.00	0.61
3:J:1172:LYS:HD3	3:J:1189:MET:HG3	1.82	0.61
5:L:591:GLU:O	5:L:595:LEU:HG	2.01	0.61
6:N:3:ASP:OD1	6:N:3:ASP:N	2.33	0.61
2:I:262:TYR:O	2:I:273:HIS:NE2	2.32	0.61
2:I:347:ILE:HA	2:I:350:THR:HG22	1.83	0.61
2:I:817:LEU:HD11	2:I:1080:ASN:ND2	2.14	0.61
3:J:859:PRO:HD2	3:J:862:THR:HG21	1.81	0.61
3:J:399:LYS:O	3:J:403:ARG:HG2	2.01	0.61
3:J:427:PRO:O	3:J:429:LEU:HD22	2.01	0.61
5:L:479:THR:HG23	5:L:482:GLU:H	1.65	0.61
5:L:557:LYS:HG3	5:L:561:MET:HE2	1.83	0.61
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.15	0.61
2:I:590:PRO:HG3	2:I:605:TYR:CE1	2.36	0.61
2:I:905:ILE:HD11	5:L:598:LEU:HD12	1.81	0.61
9:J:1504:1N7:C3	9:J:1504:1N7:C2	2.73	0.61
5:L:10:LYS:O	5:L:14:THR:HG22	2.01	0.61
5:L:115:GLY:O	5:L:119:ILE:HG13	2.01	0.61
5:L:147:GLN:CG	5:L:161:LEU:HD13	2.31	0.61
5:L:283:GLN:OE1	5:L:344:LEU:HG	2.01	0.61
1:H:73:GLY:HA2	1:H:134:THR:HB	1.82	0.61
3:J:111:THR:HG23	3:J:300:GLN:OE1	2.00	0.61
3:J:452:LEU:HD13	3:J:500:ILE:CG2	2.30	0.61
5:L:51:MET:HB3	5:L:80:ALA:HB3	1.83	0.61
5:L:470:MET:HE1	5:L:482:GLU:HB3	1.83	0.61
5:L:544:THR:HA	5:L:547:VAL:HG22	1.82	0.61
2:I:1148:ALA:HA	2:I:1201:LEU:HD21	1.82	0.61
3:J:1316:THR:CG2	3:J:1322:ALA:HB2	2.30	0.61
4:K:26:ARG:NH1	4:K:29:GLN:OE1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:155:ALA:N	1:G:174:ASP:OD1	2.27	0.60
2:I:246:LEU:O	2:I:274:ILE:HD11	2.01	0.60
2:I:1289:GLU:OE1	3:J:473:THR:HG22	2.00	0.60
3:J:451:PRO:HG2	3:J:625:MET:HE3	1.83	0.60
3:J:1275:LEU:HB2	3:J:1278:GLU:HB2	1.83	0.60
1:H:214:GLU:O	1:H:218:ARG:NE	2.33	0.60
2:I:1077:SER:HB2	3:J:356:THR:HB	1.82	0.60
3:J:44:ILE:HG13	5:L:450:ILE:HG22	1.82	0.60
3:J:337:ARG:HE	3:J:341:ASN:HD21	1.49	0.60
3:J:1319:PHE:CE1	3:J:1342:ASP:HB2	2.36	0.60
1:G:234:LEU:HD22	1:H:14:VAL:HG11	1.82	0.60
2:I:1263:ALA:N	2:I:1264:GLN:HA	2.16	0.60
3:J:1347:LEU:HD11	3:J:1359:ALA:HB2	1.83	0.60
5:L:51:MET:HB3	5:L:80:ALA:CB	2.31	0.60
5:L:466:ILE:HD11	5:L:486:ARG:HG2	1.83	0.60
2:I:69:GLN:NE2	2:I:101:ARG:HD2	2.15	0.60
2:I:962:GLU:O	2:I:966:ILE:HG13	2.01	0.60
2:I:1070:HIS:NE2	2:I:1114:GLU:OE1	2.28	0.60
2:I:1257:GLN:NE2	3:J:341:ASN:HB2	2.15	0.60
3:J:147:ILE:HD11	3:J:179:LYS:HB2	1.83	0.60
3:J:986:ASP:HB2	3:J:992:LYS:CD	2.31	0.60
3:J:1361:THR:O	4:K:21:LEU:HD11	2.01	0.60
1:M:269:CYS:CB	1:M:295:LEU:HD12	2.30	0.60
8:P:59:DA:H2''	8:P:60:DA:O5'	2.01	0.60
3:J:74:LYS:HG2	3:J:75:TYR:CE2	2.36	0.60
3:J:301:GLU:OE1	5:L:97:PRO:HG2	2.02	0.60
3:J:1023:HIS:HA	3:J:1125:PRO:HA	1.83	0.60
5:L:554:ARG:HD2	5:L:580:PHE:HE1	1.65	0.60
7:O:25:DA:H2'	7:O:26:DT:C6	2.37	0.60
7:O:33:DA:H2''	7:O:34:DA:H5'	1.82	0.60
2:I:471:VAL:HG11	2:I:498:ILE:CD1	2.29	0.60
2:I:903:ARG:HG2	2:I:908:GLU:O	2.02	0.60
3:J:123:ARG:NH2	3:J:1334:GLU:HG2	2.17	0.60
3:J:418:GLU:O	3:J:420:PRO:HD3	2.01	0.60
3:J:1005:LYS:HE2	3:J:1011:VAL:CG2	2.32	0.60
5:L:17:LYS:HG3	5:L:53:ILE:HD11	1.83	0.60
5:L:314:THR:HA	5:L:318:ALA:HB3	1.84	0.60
2:I:204:LEU:H	2:I:204:LEU:HD12	1.67	0.60
2:I:230:PHE:HE1	2:I:239:MET:HG3	1.66	0.60
2:I:240:GLU:HG2	2:I:284:LEU:CD1	2.32	0.60
3:J:147:ILE:CD1	3:J:179:LYS:HB2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:954:ASN:HB2	3:J:992:LYS:NZ	2.17	0.60
9:J:1505:1N7:H31	9:J:1505:1N7:H5	1.84	0.60
1:M:264:VAL:O	1:M:268:ASN:ND2	2.35	0.60
2:I:118:LYS:HG2	2:I:488:MET:HG2	1.82	0.60
2:I:246:LEU:O	2:I:269:ILE:HG21	2.02	0.60
2:I:896:THR:O	2:I:900:LYS:HB2	2.01	0.60
5:L:139:GLU:O	5:L:142:THR:OG1	2.16	0.60
1:G:183:ILE:HD12	1:G:205:MET:HB2	1.84	0.60
2:I:622:ASN:ND2	2:I:631:GLU:OE2	2.34	0.60
3:J:124:ILE:O	3:J:128:LEU:HD12	2.02	0.60
3:J:268:LEU:HB3	3:J:306:LEU:HD23	1.83	0.60
1:M:283:GLN:OE1	1:M:317:ARG:HA	2.02	0.60
2:I:975:ILE:HG13	2:I:1014:LEU:HD23	1.82	0.60
3:J:194:LEU:HD22	3:J:224:LEU:HD22	1.84	0.60
5:L:229:VAL:HB	5:L:232:ARG:NH2	2.16	0.60
5:L:419:PHE:HA	5:L:430:TYR:CE2	2.36	0.60
1:H:215:GLU:HA	1:H:218:ARG:HG2	1.84	0.59
2:I:14:ASP:HA	2:I:1183:ALA:HB3	1.84	0.59
2:I:249:GLU:HB2	2:I:269:ILE:HD13	1.83	0.59
3:J:1171:GLY:O	3:J:1191:PRO:HA	2.02	0.59
5:L:79:ALA:O	5:L:83:VAL:HG23	2.02	0.59
2:I:118:LYS:CG	2:I:488:MET:HG2	2.32	0.59
2:I:210:LEU:HD21	2:I:429:MET:CE	2.32	0.59
3:J:1173:ARG:HH21	3:J:1192:LYS:HB2	1.66	0.59
5:L:280:VAL:O	5:L:283:GLN:HG3	2.01	0.59
7:O:20:DA:H2''	7:O:21:DA:C8	2.37	0.59
1:G:79:LEU:HD21	2:I:693:LEU:HD11	1.85	0.59
2:I:104:ILE:HD11	2:I:116:ASP:HB2	1.85	0.59
2:I:136:PHE:CZ	2:I:456:VAL:HG21	2.36	0.59
2:I:230:PHE:HB2	2:I:333:ILE:HB	1.83	0.59
2:I:1082:ILE:H	2:I:1082:ILE:HD12	1.65	0.59
3:J:899:TYR:CE2	3:J:909:ILE:HD12	2.37	0.59
5:L:298:PRO:HB2	5:L:301:ASN:OD1	2.01	0.59
1:M:253:LEU:HD21	1:M:312:LEU:HD13	1.83	0.59
1:H:89:ALA:HB3	1:H:124:VAL:HG22	1.82	0.59
3:J:656:GLU:O	3:J:660:GLU:HG3	2.01	0.59
3:J:748:ALA:CB	6:N:16:THR:HG22	2.32	0.59
3:J:982:LEU:HB2	3:J:997:VAL:HG21	1.84	0.59
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.83	0.59
8:P:62:DG:H2''	8:P:63:DG:H2'	1.85	0.59
1:H:47:LEU:HA	1:H:51:MET:CG	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:227:LYS:HE3	2:I:298:ALA:HB1	1.84	0.59
3:J:826:ILE:O	3:J:994:SER:OG	2.17	0.59
5:L:235:ILE:HA	5:L:245:ALA:HB2	1.84	0.59
5:L:582:VAL:HG11	5:L:586:ARG:HG2	1.83	0.59
2:I:988:LYS:HA	2:I:991:LYS:CG	2.32	0.59
2:I:1062:PRO:HD3	2:I:1079:ILE:HD13	1.83	0.59
2:I:1103:VAL:HB	2:I:1104:PRO:HD3	1.84	0.59
3:J:418:GLU:HG3	4:K:45:LYS:H	1.66	0.59
3:J:707:ILE:HG22	3:J:708:ASN:H	1.67	0.59
3:J:1061:VAL:O	3:J:1062:LEU:HD23	2.03	0.59
3:J:1284:ARG:O	3:J:1287:ILE:HG13	2.02	0.59
2:I:868:SER:OG	2:I:942:ASP:OD2	2.19	0.59
3:J:491:LEU:O	3:J:904:ALA:HB2	2.03	0.59
3:J:423:LEU:HB3	3:J:466:MET:CE	2.32	0.59
3:J:527:LEU:HB2	3:J:550:VAL:HG12	1.85	0.59
5:L:224:LEU:HD22	5:L:259:PHE:CE2	2.37	0.59
5:L:450:ILE:HD11	5:L:504:PRO:HD3	1.84	0.59
2:I:68:LEU:HD11	2:I:100:LEU:HD13	1.84	0.59
2:I:1121:ALA:HB2	2:I:1182:ILE:HD12	1.84	0.59
3:J:40:LYS:HE3	3:J:42:GLU:HG3	1.84	0.59
3:J:217:LEU:O	3:J:221:ILE:HG13	2.03	0.59
5:L:416:VAL:HG22	5:L:427:PHE:HZ	1.68	0.59
3:J:338:PHE:HA	3:J:342:LEU:CD2	2.30	0.59
3:J:530:PRO:HB2	3:J:581:MET:HG2	1.85	0.59
5:L:256:PHE:CZ	5:L:261:LEU:HD21	2.38	0.59
1:H:222:THR:O	1:H:226:GLU:HG2	2.02	0.58
2:I:349:GLU:OE2	2:I:352:ARG:NH1	2.36	0.58
2:I:808:ASN:H	3:J:633:ALA:HB2	1.66	0.58
3:J:70:CYS:SG	3:J:71:LEU:N	2.76	0.58
3:J:1146:GLU:OE2	3:J:1310:THR:OG1	2.12	0.58
1:H:107:ILE:HG23	1:H:135:ASP:HA	1.84	0.58
2:I:227:LYS:HE2	2:I:334:GLU:HB2	1.85	0.58
3:J:937:ILE:HG13	3:J:1134:ILE:H	1.67	0.58
3:J:1155:ILE:HD11	3:J:1211:SER:HB3	1.85	0.58
5:L:283:GLN:HE22	5:L:344:LEU:HD21	1.68	0.58
1:M:282:VAL:O	1:M:316:MET:N	2.35	0.58
1:H:58:GLU:HA	1:H:173:VAL:HG12	1.84	0.58
2:I:1340:GLU:OE1	3:J:1341:ARG:HD2	2.02	0.58
3:J:201:LEU:CD1	3:J:220:ARG:HD3	2.30	0.58
3:J:1080:ILE:HB	3:J:1097:ALA:O	2.03	0.58
1:M:251:PRO:HA	1:M:254:LEU:HD11	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:285:THR:O	1:M:289:LEU:HD12	2.03	0.58
2:I:298:ALA:HB3	2:I:334:GLU:CG	2.32	0.58
2:I:303:ASP:N	2:I:308:GLU:O	2.29	0.58
2:I:1117:LEU:HD12	2:I:1195:ILE:CG1	2.33	0.58
2:I:1119:MET:HE3	2:I:1210:ILE:HD11	1.86	0.58
3:J:1069:ALA:HA	3:J:1072:LYS:HB3	1.85	0.58
5:L:292:VAL:HA	5:L:297:MET:HB3	1.84	0.58
1:G:16:ILE:CD1	1:G:214:GLU:HB2	2.34	0.58
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.85	0.58
3:J:19:ALA:HB2	3:J:1343:GLU:HA	1.85	0.58
3:J:515:ARG:O	3:J:545:HIS:HB3	2.04	0.58
3:J:865:HIS:HE1	3:J:867:GLN:HB2	1.69	0.58
5:L:511:ILE:CG2	5:L:513:ASP:HB2	2.34	0.58
1:M:287:VAL:O	1:M:291:LYS:HG2	2.02	0.58
7:O:40:DC:C2'	7:O:41:DT:H5''	2.33	0.58
2:I:582:ASN:HA	2:I:588:GLU:OE2	2.03	0.58
2:I:1291:LEU:CD2	3:J:1351:VAL:HG13	2.33	0.58
5:L:557:LYS:HG3	5:L:561:MET:CE	2.34	0.58
7:O:21:DA:H1'	7:O:22:DT:H5'	1.86	0.58
1:H:35:PHE:HA	1:H:38:THR:CG2	2.33	0.58
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	1.86	0.58
2:I:1260:GLY:HA3	2:I:1266:GLY:N	2.18	0.58
5:L:123:ILE:HD11	5:L:379:MET:CE	2.34	0.58
5:L:401:PHE:CZ	5:L:405:ILE:HD11	2.38	0.58
2:I:5:TYR:CE2	2:I:776:PRO:HD2	2.38	0.58
2:I:157:PHE:O	2:I:442:VAL:HB	2.04	0.58
2:I:452:ARG:NH2	2:I:458:GLU:OE2	2.18	0.58
2:I:1124:ILE:HG13	2:I:1198:LEU:HD11	1.86	0.58
3:J:918:ILE:O	3:J:922:SER:OG	2.18	0.58
1:G:135:ASP:HB3	1:G:138:ALA:CB	2.33	0.58
2:I:245:ARG:HH21	2:I:337:PHE:HB2	1.68	0.58
2:I:892:GLU:OE2	2:I:894:GLN:N	2.34	0.58
2:I:1153:ALA:O	2:I:1155:VAL:HG13	2.03	0.58
3:J:282:LEU:HD21	5:L:410:ILE:HG12	1.86	0.58
5:L:493:LYS:HA	5:L:496:LYS:CD	2.34	0.58
7:O:45:DA:H8	7:O:45:DA:H5''	1.68	0.58
2:I:466:VAL:O	2:I:469:VAL:HG12	2.04	0.58
3:J:607:THR:O	3:J:611:ILE:HG13	2.03	0.58
5:L:144:LEU:HD23	5:L:145:LEU:HD23	1.85	0.58
3:J:1116:SER:H	3:J:1119:ASP:HB2	1.69	0.57
5:L:145:LEU:HB3	5:L:225:ARG:CD	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:257:LYS:HE2	5:L:258:GLN:NE2	2.19	0.57
6:N:37:CYS:SG	6:N:39:ALA:N	2.67	0.57
5:L:378:GLU:N	5:L:378:GLU:OE2	2.38	0.57
3:J:201:LEU:HB3	3:J:221:ILE:HG12	1.86	0.57
3:J:350:SER:HA	3:J:468:VAL:O	2.04	0.57
3:J:474:LEU:CD1	4:K:47:THR:HG22	2.34	0.57
3:J:514:THR:OG1	3:J:596:LEU:HB2	2.04	0.57
3:J:958:ILE:HG21	3:J:1006:GLY:O	2.04	0.57
1:M:266:SER:O	1:M:270:LEU:HG	2.04	0.57
1:G:12:ARG:H	1:G:30:PRO:HD2	1.69	0.57
1:H:192:VAL:HG12	1:H:193:GLU:H	1.70	0.57
2:I:255:ILE:HB	2:I:263:VAL:HB	1.85	0.57
2:I:1151:LEU:HD13	2:I:1201:LEU:HD22	1.86	0.57
3:J:205:LEU:HB2	3:J:217:LEU:HD11	1.87	0.57
3:J:397:ALA:O	3:J:401:VAL:HG23	2.05	0.57
3:J:978:ARG:HA	3:J:999:TYR:HD1	1.69	0.57
3:J:1036:ARG:HE	3:J:1081:VAL:HG21	1.70	0.57
5:L:266:PHE:HA	5:L:269:LEU:CD1	2.34	0.57
5:L:322:MET:HB2	5:L:327:SER:CB	2.35	0.57
2:I:866:ASP:OD2	2:I:944:ARG:HG3	2.04	0.57
3:J:842:ARG:HB2	3:J:882:VAL:CG2	2.35	0.57
3:J:1190:ILE:HD13	3:J:1196:LEU:HD11	1.87	0.57
5:L:117:ILE:O	5:L:121:LYS:HG3	2.04	0.57
2:I:289:VAL:HG12	2:I:319:LEU:CD2	2.35	0.57
2:I:1271:GLY:O	2:I:1275:VAL:HG23	2.05	0.57
3:J:474:LEU:HD11	4:K:47:THR:HG22	1.87	0.57
3:J:848:VAL:HG12	3:J:858:VAL:HB	1.86	0.57
5:L:339:ARG:O	5:L:342:GLN:HG3	2.04	0.57
1:M:278:ILE:O	1:M:282:VAL:HG22	2.04	0.57
1:G:208:ASN:OD1	1:G:210:THR:HG22	2.04	0.57
1:H:48:LEU:HD13	1:H:183:ILE:CD1	2.35	0.57
2:I:1119:MET:HE2	2:I:1204:LEU:HB3	1.87	0.57
3:J:203:GLU:O	3:J:207:GLU:HB2	2.05	0.57
3:J:393:THR:HG23	3:J:395:LYS:H	1.70	0.57
3:J:514:THR:OG1	3:J:514:THR:O	2.20	0.57
3:J:772:TYR:O	3:J:776:THR:HG23	2.05	0.57
3:J:975:ILE:N	3:J:1000:GLY:HA2	2.19	0.57
3:J:1251:LYS:O	3:J:1255:VAL:HG23	2.05	0.57
5:L:543:ALA:O	5:L:547:VAL:HG13	2.04	0.57
7:O:46:DG:H3'	7:O:46:DG:OP2	2.04	0.57
2:I:360:LEU:O	2:I:364:VAL:HG13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:835:GLU:HB2	2:I:1053:TYR:CD1	2.39	0.57
3:J:416:ILE:HG13	3:J:441:LEU:HD21	1.85	0.57
3:J:850:LYS:HG2	3:J:851:PRO:HD2	1.87	0.57
3:J:1367:GLN:O	3:J:1371:ARG:HG3	2.05	0.57
5:L:225:ARG:O	5:L:229:VAL:HG13	2.05	0.57
8:P:56:DG:H2'	8:P:57:DT:H71	1.86	0.57
1:G:97:GLU:HG3	1:G:145:LYS:HZ3	1.70	0.57
1:G:135:ASP:HB3	1:G:138:ALA:HB3	1.87	0.57
2:I:168:GLY:O	6:N:72:TYR:HB3	2.05	0.57
2:I:429:MET:O	2:I:433:ILE:HG13	2.05	0.57
2:I:964:LEU:HD13	2:I:1025:PHE:CD2	2.40	0.57
3:J:1109:LEU:HD12	3:J:1121:LEU:CD1	2.33	0.57
3:J:1194:ARG:HD3	3:J:1211:SER:OG	2.05	0.57
3:J:1221:LEU:HD23	3:J:1229:VAL:HG11	1.86	0.57
1:G:155:ALA:O	1:G:159:ILE:HG22	2.04	0.57
2:I:225:PHE:CE2	2:I:347:ILE:HB	2.40	0.57
2:I:930:ASP:HB3	2:I:1053:TYR:HD2	1.70	0.57
3:J:132:LEU:O	3:J:136:GLU:HG2	2.05	0.57
3:J:514:THR:O	3:J:595:ALA:HA	2.05	0.57
3:J:1003:LEU:HA	3:J:1018:ALA:CB	2.35	0.57
3:J:1021:ASP:HB3	3:J:1024:THR:HG23	1.86	0.57
1:G:45:ARG:CD	2:I:1083:GLU:HG3	2.35	0.56
1:H:134:THR:HG22	1:H:138:ALA:HB3	1.88	0.56
2:I:770:CYS:HB3	2:I:785:ASP:OD2	2.05	0.56
2:I:1314:GLN:HB2	4:K:28:ARG:HH11	1.70	0.56
5:L:144:LEU:HD13	5:L:256:PHE:CZ	2.40	0.56
5:L:460:ILE:HG22	5:L:497:VAL:CG1	2.35	0.56
5:L:580:PHE:O	5:L:582:VAL:HG23	2.04	0.56
2:I:231:GLU:HA	2:I:331:LYS:O	2.06	0.56
2:I:271:ALA:O	2:I:275:ARG:HG3	2.04	0.56
2:I:444:ASP:O	2:I:447:HIS:HB2	2.06	0.56
2:I:660:VAL:HG11	3:J:769:VAL:HG13	1.86	0.56
2:I:949:GLU:O	2:I:953:LEU:HG	2.05	0.56
3:J:111:THR:HG21	3:J:303:VAL:HG11	1.86	0.56
3:J:849:LEU:CD1	3:J:856:ILE:HA	2.35	0.56
5:L:9:LEU:HD11	5:L:32:PRO:CD	2.34	0.56
5:L:138:PRO:O	5:L:142:THR:HG23	2.05	0.56
5:L:249:ILE:HG23	5:L:252:LEU:HD22	1.87	0.56
5:L:456:MET:CE	5:L:497:VAL:HG22	2.35	0.56
5:L:467:SER:OG	5:L:478:PRO:HG3	2.06	0.56
2:I:242:VAL:CB	2:I:245:ARG:HD3	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:820:GLU:HB2	2:I:1080:ASN:O	2.05	0.56
2:I:861:ALA:HB1	2:I:882:ILE:CD1	2.35	0.56
2:I:1103:VAL:HG11	2:I:1112:ILE:HD13	1.86	0.56
2:I:1113:LEU:HD13	3:J:641:ILE:CD1	2.35	0.56
3:J:105:ILE:HD13	3:J:273:ILE:HG13	1.87	0.56
3:J:582:ILE:HD12	3:J:627:THR:HG21	1.86	0.56
3:J:809:VAL:HG21	3:J:909:ILE:CG2	2.32	0.56
4:K:41:GLU:HB2	4:K:49:ILE:HD11	1.87	0.56
5:L:137:TYR:CE2	5:L:139:GLU:HB3	2.39	0.56
5:L:493:LYS:O	5:L:496:LYS:HG2	2.05	0.56
5:L:600:HIS:CE1	1:M:259:ASP:HA	2.40	0.56
1:G:89:ALA:O	1:G:124:VAL:HG22	2.05	0.56
1:H:205:MET:CE	1:H:217:ILE:HG13	2.36	0.56
3:J:975:ILE:H	3:J:1000:GLY:HA2	1.70	0.56
1:H:31:LEU:O	1:H:198:LEU:HD22	2.05	0.56
2:I:148:GLN:HB2	2:I:511:LEU:HD11	1.87	0.56
2:I:165:HIS:ND1	2:I:167:SER:HB3	2.21	0.56
2:I:320:ASP:N	2:I:320:ASP:OD1	2.38	0.56
3:J:79:LYS:CB	5:L:569:THR:HB	2.31	0.56
3:J:937:ILE:HG12	3:J:1134:ILE:O	2.06	0.56
1:G:107:ILE:HG23	1:G:134:THR:HA	1.88	0.56
1:H:103:ASN:HA	1:H:140:ILE:O	2.06	0.56
1:H:205:MET:HE3	1:H:213:PRO:HB3	1.87	0.56
3:J:511:TYR:CG	3:J:728:SER:HB3	2.40	0.56
3:J:825:VAL:HG22	3:J:827:GLU:HG3	1.88	0.56
5:L:84:LEU:HA	5:L:87:VAL:HG12	1.88	0.56
1:G:207:THR:HG21	1:G:211:ILE:HG22	1.88	0.56
1:H:14:VAL:HG13	1:H:28:LEU:HD13	1.88	0.56
2:I:197:ARG:HH22	2:I:203:LYS:HD2	1.70	0.56
3:J:126:LEU:HD11	3:J:223:LEU:HD22	1.87	0.56
3:J:156:ARG:NH2	3:J:191:SER:OG	2.39	0.56
3:J:255:LEU:HB2	3:J:259:ARG:O	2.05	0.56
3:J:603:LYS:O	3:J:607:THR:HG23	2.06	0.56
3:J:1287:ILE:HG22	3:J:1290:ARG:HH21	1.70	0.56
2:I:36:GLN:O	2:I:40:GLU:HB2	2.06	0.56
2:I:185:ASP:HB3	2:I:187:GLU:OE2	2.06	0.56
2:I:817:LEU:HB3	2:I:1097:VAL:HB	1.87	0.56
3:J:390:LEU:HD23	3:J:407:VAL:CG2	2.36	0.56
3:J:660:GLU:HB2	3:J:685:ILE:HD13	1.87	0.56
5:L:27:VAL:O	5:L:31:LEU:HG	2.06	0.56
5:L:119:ILE:CG2	5:L:375:ALA:HB1	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:152:GLU:CB	5:L:218:ARG:HD3	2.36	0.56
5:L:256:PHE:HZ	5:L:261:LEU:HD21	1.69	0.56
1:M:255:ARG:O	1:M:278:ILE:HG12	2.06	0.56
1:M:298:LYS:HB2	8:P:67:DT:H3'	1.86	0.56
6:N:48:ARG:HH11	6:N:59:VAL:HG22	1.71	0.56
7:O:34:DA:H4'	7:O:35:DG:OP1	2.06	0.56
2:I:210:LEU:O	2:I:215:TYR:HB2	2.05	0.56
2:I:551:HIS:ND1	2:I:553:THR:HG23	2.21	0.56
3:J:233:LYS:HD2	3:J:235:GLU:OE2	2.06	0.56
4:K:6:VAL:O	4:K:10:VAL:HG23	2.06	0.56
5:L:469:GLN:O	5:L:473:GLU:HG3	2.06	0.56
2:I:484:LEU:HG	2:I:485:ASP:H	1.71	0.56
3:J:189:LEU:HA	3:J:192:MET:HE3	1.88	0.56
3:J:369:PRO:HD2	3:J:372:MET:HE2	1.87	0.56
5:L:479:THR:CG2	5:L:482:GLU:H	2.19	0.56
2:I:118:LYS:CD	2:I:488:MET:HG2	2.36	0.55
2:I:196:VAL:CG2	2:I:206:ALA:HA	2.36	0.55
2:I:231:GLU:HB2	2:I:238:GLN:NE2	2.20	0.55
3:J:22:ILE:HG22	3:J:1340:LYS:O	2.06	0.55
3:J:1040:MET:HE2	3:J:1078:LEU:HG	1.88	0.55
3:J:1177:ILE:O	3:J:1179:PRO:HD3	2.06	0.55
4:K:26:ARG:HD3	4:K:59:ILE:CD1	2.33	0.55
5:L:419:PHE:CE1	5:L:427:PHE:HA	2.41	0.55
5:L:503:GLU:CD	5:L:504:PRO:HD2	2.26	0.55
1:G:58:GLU:OE1	1:G:170:ARG:NH1	2.36	0.55
2:I:107:ARG:NH2	2:I:108:GLU:HA	2.21	0.55
2:I:227:LYS:HE3	2:I:298:ALA:CB	2.36	0.55
3:J:516:ASP:HA	3:J:545:HIS:HB2	1.88	0.55
3:J:664:ILE:CG2	3:J:678:ARG:HG3	2.35	0.55
3:J:719:PHE:HA	3:J:724:MET:HE2	1.89	0.55
3:J:914:ALA:O	3:J:918:ILE:HG13	2.06	0.55
3:J:1272:SER:CB	3:J:1300:ALA:HB2	2.36	0.55
5:L:96:ASP:OD1	5:L:98:VAL:HG12	2.05	0.55
1:M:283:GLN:O	1:M:315:GLY:HA2	2.05	0.55
7:O:21:DA:H1'	7:O:22:DT:C5'	2.36	0.55
1:H:71:LYS:HB3	1:H:74:VAL:CG2	2.36	0.55
2:I:6:THR:O	2:I:6:THR:OG1	2.24	0.55
2:I:76:GLY:N	2:I:95:PRO:O	2.33	0.55
2:I:270:THR:HG22	6:N:42:ASN:HD21	1.72	0.55
2:I:629:PHE:HB2	2:I:647:ARG:HD2	1.88	0.55
2:I:1332:SER:CB	3:J:245:LEU:HD13	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:123:ARG:HA	3:J:126:LEU:CD2	2.35	0.55
3:J:140:TYR:O	3:J:297:ARG:NH1	2.39	0.55
3:J:511:TYR:CE2	3:J:724:MET:HG2	2.41	0.55
3:J:1177:ILE:N	3:J:1186:TYR:O	2.26	0.55
1:G:22:THR:HB	1:G:207:THR:O	2.07	0.55
2:I:192:ASP:OD2	2:I:436:ARG:NH2	2.39	0.55
2:I:1033:ARG:O	2:I:1037:THR:HG22	2.07	0.55
3:J:645:VAL:HG22	3:J:700:ASN:HD21	1.70	0.55
5:L:41:ILE:O	5:L:45:ILE:HG22	2.05	0.55
5:L:406:GLN:O	5:L:410:ILE:HG13	2.06	0.55
5:L:572:THR:O	5:L:576:VAL:HG23	2.07	0.55
1:H:182:ARG:O	1:H:205:MET:HA	2.07	0.55
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.88	0.55
2:I:690:VAL:HG23	2:I:763:THR:HG21	1.89	0.55
2:I:697:LYS:HD2	2:I:1181:PRO:HG3	1.87	0.55
3:J:683:ILE:HD12	6:N:23:ILE:HD13	1.89	0.55
3:J:816:THR:HG23	3:J:889:ASP:HB2	1.88	0.55
5:L:375:ALA:O	5:L:379:MET:HG2	2.06	0.55
8:P:42:DT:H1'	8:P:43:DT:C5'	2.35	0.55
2:I:65:ASN:HB3	2:I:105:TYR:CB	2.37	0.55
2:I:231:GLU:HB2	2:I:238:GLN:HE21	1.71	0.55
2:I:1127:LYS:O	2:I:1131:MET:HG3	2.06	0.55
3:J:127:LEU:CD2	3:J:234:PRO:HB3	2.37	0.55
3:J:975:ILE:HB	3:J:1000:GLY:H	1.70	0.55
4:K:8:ASP:HB2	4:K:55:GLU:HG3	1.88	0.55
5:L:141:ILE:O	5:L:145:LEU:HG	2.07	0.55
5:L:387:VAL:HG22	5:L:435:ILE:CD1	2.37	0.55
5:L:511:ILE:HG23	5:L:513:ASP:HB2	1.89	0.55
1:H:208:ASN:N	1:H:208:ASN:OD1	2.39	0.55
2:I:70:TYR:HA	2:I:100:LEU:CD2	2.37	0.55
2:I:232:ILE:HG13	2:I:237:LEU:HD23	1.87	0.55
2:I:359:ARG:O	2:I:363:LEU:HD12	2.07	0.55
2:I:470:ARG:HD2	2:I:497:PRO:HB3	1.88	0.55
2:I:618:GLN:HE22	3:J:770:LEU:HD23	1.72	0.55
3:J:381:ILE:HD11	3:J:412:LEU:HD13	1.89	0.55
3:J:1116:SER:N	3:J:1119:ASP:HB2	2.21	0.55
3:J:1163:VAL:O	3:J:1200:GLU:HG2	2.07	0.55
3:J:1194:ARG:HD3	3:J:1211:SER:CB	2.37	0.55
3:J:239:LEU:HD11	3:J:307:LEU:HD11	1.87	0.55
5:L:270:VAL:O	5:L:274:ARG:HG2	2.06	0.55
2:I:75:LEU:HD11	2:I:127:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:411:ARG:NH2	2:I:424:ASP:OD1	2.39	0.55
2:I:728:ASP:OD1	2:I:729:ALA:N	2.39	0.55
3:J:385:LEU:CD2	3:J:411:ILE:HG13	2.37	0.55
3:J:454:CYS:HB3	3:J:459:ALA:O	2.07	0.55
3:J:872:LEU:O	3:J:877:VAL:HG23	2.07	0.55
2:I:829:THR:HG22	2:I:1057:LYS:HG2	1.89	0.55
3:J:124:ILE:HG22	3:J:135:ILE:HD13	1.89	0.55
3:J:259:ARG:HH21	5:L:502:LYS:HD3	1.72	0.55
3:J:388:ARG:HB2	3:J:390:LEU:HD13	1.88	0.55
3:J:391:ALA:HB2	3:J:400:MET:SD	2.47	0.55
2:I:1067:ALA:HB3	2:I:1235:LEU:HD21	1.89	0.54
2:I:1104:PRO:HG2	3:J:725:MET:SD	2.47	0.54
3:J:297:ARG:HD3	5:L:100:MET:HE2	1.88	0.54
3:J:1198:VAL:CG1	3:J:1210:ILE:HG23	2.37	0.54
5:L:565:ILE:HG22	5:L:566:ASP:OD2	2.07	0.54
1:H:107:ILE:HA	1:H:134:THR:O	2.07	0.54
2:I:71:VAL:HB	2:I:99:LYS:O	2.07	0.54
3:J:596:LEU:HD11	3:J:604:MET:HE1	1.87	0.54
3:J:1061:VAL:HG11	3:J:1101:LEU:CB	2.37	0.54
5:L:289:LYS:HA	5:L:293:GLU:CB	2.36	0.54
5:L:574:GLU:O	5:L:578:LYS:HG3	2.07	0.54
8:P:38:DC:C2'	8:P:39:DC:H5''	2.36	0.54
2:I:303:ASP:HB2	2:I:310:ILE:HD11	1.90	0.54
2:I:453:ILE:HG22	2:I:585:GLY:O	2.07	0.54
2:I:508:SER:O	2:I:508:SER:OG	2.25	0.54
2:I:898:GLU:CG	5:L:544:THR:HG21	2.35	0.54
2:I:1304:MET:CE	2:I:1315:MET:HB3	2.38	0.54
3:J:559:ALA:HB3	3:J:562:GLU:O	2.07	0.54
3:J:985:ILE:HD13	3:J:991:THR:HA	1.89	0.54
4:K:72:GLN:HA	4:K:75:GLN:OE1	2.07	0.54
5:L:570:ASP:OD1	5:L:570:ASP:N	2.40	0.54
1:M:318:LEU:HD23	1:M:321:TRP:CG	2.42	0.54
2:I:84:GLU:O	2:I:88:ARG:HG3	2.07	0.54
2:I:170:VAL:HG23	6:N:72:TYR:CB	2.30	0.54
2:I:539:THR:HG22	2:I:541:GLU:H	1.72	0.54
2:I:548:ARG:HD2	2:I:569:ILE:O	2.06	0.54
3:J:491:LEU:HB2	3:J:904:ALA:CB	2.37	0.54
3:J:1023:HIS:O	3:J:1125:PRO:HA	2.08	0.54
2:I:877:VAL:HG13	2:I:881:ASP:HB2	1.90	0.54
3:J:146:VAL:HA	3:J:178:ALA:HA	1.88	0.54
3:J:646:ILE:HD11	3:J:762:ASN:HD21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:50:ALA:O	4:K:54:ILE:HG13	2.07	0.54
5:L:130:VAL:CG1	5:L:365:MET:HG3	2.34	0.54
1:H:107:ILE:CG2	1:H:135:ASP:HA	2.37	0.54
2:I:194:LEU:HB3	2:I:206:ALA:CB	2.38	0.54
2:I:594:VAL:HG11	2:I:650:VAL:HG23	1.89	0.54
3:J:826:ILE:HD11	3:J:992:LYS:O	2.08	0.54
3:J:1027:VAL:CG2	3:J:1122:ALA:HB3	2.38	0.54
3:J:1090:ILE:HG12	3:J:1097:ALA:HA	1.89	0.54
3:J:1310:THR:O	3:J:1314:LEU:HD13	2.07	0.54
5:L:9:LEU:CD2	5:L:44:ILE:HD11	2.38	0.54
5:L:137:TYR:OH	5:L:351:THR:HA	2.08	0.54
5:L:228:TYR:CD1	5:L:252:LEU:HD12	2.43	0.54
5:L:554:ARG:HD2	5:L:580:PHE:CE1	2.41	0.54
1:M:283:GLN:NE2	1:M:318:LEU:HB2	2.22	0.54
2:I:153:PRO:HB2	2:I:401:GLY:HA3	1.88	0.54
2:I:478:ARG:HH22	2:I:483:ASP:HB2	1.73	0.54
2:I:661:VAL:HG11	2:I:671:LEU:CD2	2.37	0.54
2:I:961:SER:O	2:I:965:GLN:HG3	2.07	0.54
3:J:385:LEU:HD23	3:J:411:ILE:HG13	1.89	0.54
3:J:511:TYR:HE2	3:J:724:MET:HG2	1.72	0.54
3:J:952:VAL:CG2	3:J:984:LEU:HD22	2.38	0.54
3:J:1178:THR:HA	3:J:1184:ASP:O	2.08	0.54
3:J:1268:ASN:HB3	3:J:1301:THR:OG1	2.07	0.54
2:I:136:PHE:HB3	2:I:138:ILE:HD13	1.88	0.54
2:I:268:ARG:HB3	6:N:40:CYS:CB	2.37	0.54
2:I:556:GLY:HA2	2:I:659:GLN:O	2.07	0.54
2:I:738:GLU:HA	2:I:741:MET:CE	2.37	0.54
2:I:1340:GLU:HG3	3:J:21:LYS:HB2	1.89	0.54
3:J:697:MET:CE	3:J:741:ALA:HB3	2.37	0.54
3:J:1152:GLU:O	3:J:1214:PRO:HD2	2.08	0.54
5:L:470:MET:CE	5:L:482:GLU:HB3	2.38	0.54
1:G:40:GLY:HA2	1:G:201:LEU:HD21	1.90	0.54
2:I:11:ILE:O	2:I:1149:TYR:OH	2.24	0.54
2:I:268:ARG:HB3	6:N:40:CYS:HB2	1.89	0.54
2:I:494:ASN:HB3	2:I:497:PRO:HD2	1.90	0.54
2:I:958:LYS:HD3	2:I:962:GLU:OE2	2.07	0.54
3:J:762:ASN:N	3:J:762:ASN:OD1	2.39	0.54
3:J:1023:HIS:CA	3:J:1125:PRO:HA	2.38	0.54
5:L:415:ALA:O	5:L:419:PHE:N	2.41	0.54
1:M:275:ILE:HG12	1:M:284:ARG:HH12	1.73	0.54
1:M:296:GLY:N	8:P:68:DG:OP1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:58:CYS:SG	6:N:60:GLU:HG2	2.48	0.54
7:O:44:DA:H4'	7:O:45:DA:OP1	2.08	0.54
1:G:152:TYR:CD2	1:G:154:PRO:HD3	2.43	0.54
1:H:56:VAL:HG22	1:H:146:VAL:HG23	1.90	0.54
2:I:448:LEU:HB2	2:I:553:THR:OG1	2.08	0.54
2:I:753:LEU:HD11	2:I:769:PRO:HG3	1.90	0.54
2:I:846:GLY:O	2:I:889:PRO:HG3	2.07	0.54
2:I:1141:LEU:HD21	2:I:1173:ALA:HB1	1.90	0.54
3:J:1170:LYS:CD	3:J:1172:LYS:HE3	2.36	0.54
3:J:1368:ASP:O	3:J:1372:ARG:HG2	2.08	0.54
5:L:105:MET:CE	5:L:388:ILE:HD12	2.38	0.54
7:O:40:DC:H2''	7:O:41:DT:C6	2.43	0.54
3:J:1049:GLN:O	3:J:1058:SER:HB2	2.08	0.53
5:L:322:MET:HB3	5:L:324:LYS:HG2	1.90	0.53
5:L:376:LYS:O	5:L:380:VAL:HG22	2.08	0.53
2:I:529:ARG:HD3	2:I:572:ILE:CG2	2.38	0.53
2:I:854:ILE:HG22	2:I:855:PRO:HD2	1.91	0.53
2:I:1132:LEU:HD13	2:I:1177:ARG:NH1	2.23	0.53
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.07	0.53
2:I:1275:VAL:HG13	2:I:1287:LEU:HD21	1.89	0.53
3:J:325:LYS:HE2	3:J:329:ASP:OD2	2.08	0.53
3:J:1175:LEU:HD13	3:J:1190:ILE:CD1	2.37	0.53
5:L:123:ILE:HD11	5:L:379:MET:HE2	1.90	0.53
5:L:228:TYR:HD1	5:L:252:LEU:HD12	1.73	0.53
5:L:571:TYR:HB3	5:L:575:GLU:HB3	1.89	0.53
8:P:59:DA:H2''	8:P:60:DA:C5'	2.38	0.53
2:I:559:CYS:SG	2:I:662:SER:OG	2.51	0.53
2:I:883:LEU:HG	2:I:920:VAL:HG23	1.89	0.53
3:J:1109:LEU:HD22	3:J:1113:VAL:HB	1.90	0.53
1:H:29:GLU:HG2	1:H:30:PRO:CA	2.39	0.53
3:J:179:LYS:HB3	3:J:184:ALA:HB2	1.89	0.53
3:J:331:ILE:HG22	3:J:1328:THR:HG21	1.90	0.53
3:J:1035:VAL:N	3:J:1113:VAL:O	2.32	0.53
5:L:232:ARG:O	5:L:235:ILE:HG23	2.08	0.53
5:L:493:LYS:O	5:L:497:VAL:HG23	2.08	0.53
5:L:593:LYS:HG2	5:L:596:ARG:HH21	1.74	0.53
1:M:253:LEU:HD22	1:M:282:VAL:HG11	1.90	0.53
2:I:39:ILE:CD1	2:I:75:LEU:HG	2.37	0.53
3:J:844:THR:CG2	3:J:864:LEU:HD11	2.38	0.53
5:L:9:LEU:HD13	5:L:88:GLU:HG2	1.90	0.53
2:I:246:LEU:HD22	2:I:249:GLU:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:519:ASN:OD1	2:I:796:LEU:HD22	2.09	0.53
2:I:671:LEU:CB	2:I:1186:VAL:HG12	2.38	0.53
2:I:813:GLU:HB2	3:J:461:PHE:CD2	2.43	0.53
2:I:877:VAL:CG1	2:I:920:VAL:HG21	2.37	0.53
3:J:422:LEU:HD13	3:J:471:PRO:HG3	1.89	0.53
3:J:1167:LYS:O	3:J:1173:ARG:HA	2.09	0.53
5:L:383:ASN:HA	5:L:386:LEU:HB3	1.90	0.53
1:M:283:GLN:C	1:M:315:GLY:HA2	2.29	0.53
8:P:64:DA:C1'	8:P:65:DT:H5''	2.38	0.53
1:H:23:HIS:ND1	1:H:206:GLU:HG2	2.24	0.53
2:I:241:LEU:HD21	2:I:277:LEU:CD1	2.39	0.53
2:I:598:VAL:HA	2:I:627:GLY:O	2.08	0.53
3:J:205:LEU:HB2	3:J:217:LEU:CD1	2.38	0.53
3:J:553:THR:HG22	3:J:567:THR:CB	2.36	0.53
3:J:827:GLU:HB2	3:J:832:LYS:HE2	1.90	0.53
3:J:842:ARG:NH2	3:J:1254:GLU:OE1	2.28	0.53
5:L:37:ASP:HB2	5:L:40:GLN:CG	2.25	0.53
5:L:162:ILE:N	5:L:262:VAL:HG23	2.24	0.53
6:N:44:ILE:O	6:N:49:ARG:NH2	2.33	0.53
2:I:221:LEU:HD23	2:I:336:LEU:HD21	1.91	0.53
8:P:53:DT:H2''	8:P:54:DT:H5'	1.91	0.53
2:I:253:PHE:CE2	2:I:287:VAL:HG12	2.43	0.53
2:I:255:ILE:HG23	2:I:285:ILE:HD12	1.90	0.53
2:I:454:ARG:HD2	2:I:459:MET:HG2	1.91	0.53
2:I:1107:MET:HG2	3:J:740:LEU:HD13	1.91	0.53
3:J:481:ARG:NH1	4:K:3:ARG:O	2.42	0.53
3:J:495:ASN:OD1	3:J:497:GLU:HB2	2.09	0.53
3:J:705:THR:OG1	3:J:718:SER:HA	2.09	0.53
3:J:1021:ASP:HB3	3:J:1024:THR:CG2	2.39	0.53
3:J:1226:VAL:HG23	3:J:1261:LEU:CD2	2.39	0.53
5:L:600:HIS:HB3	1:M:261:GLU:OE2	2.09	0.53
1:G:13:LEU:HD21	1:G:26:VAL:HG13	1.90	0.53
1:G:51:MET:CE	1:G:211:ILE:HD13	2.39	0.53
2:I:192:ASP:HB3	2:I:346:TYR:CD1	2.44	0.53
2:I:349:GLU:O	2:I:353:VAL:HG23	2.09	0.53
3:J:40:LYS:HE2	3:J:53:ARG:HG3	1.91	0.53
3:J:138:VAL:HG21	3:J:145:VAL:HG12	1.91	0.53
3:J:388:ARG:NH2	3:J:414:GLU:OE1	2.39	0.53
3:J:1150:PRO:O	3:J:1153:PRO:HG3	2.09	0.53
3:J:1157:ALA:HB1	3:J:1204:VAL:CG1	2.39	0.53
1:G:183:ILE:CD1	1:G:205:MET:HB2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:812:PHE:CD2	2:I:813:GLU:HG2	2.43	0.52
3:J:438:GLU:OE2	3:J:481:ARG:NH2	2.21	0.52
5:L:369:GLU:O	5:L:373:ARG:HG3	2.09	0.52
1:M:270:LEU:CB	1:M:275:ILE:HB	2.37	0.52
1:G:207:THR:HG21	1:G:211:ILE:CG2	2.39	0.52
1:H:134:THR:HG23	1:H:136:GLU:N	2.23	0.52
2:I:1243:MET:CE	3:J:445:LYS:HD2	2.40	0.52
5:L:229:VAL:HB	5:L:232:ARG:HH21	1.72	0.52
2:I:356:THR:HG23	2:I:361:SER:HB2	1.90	0.52
3:J:124:ILE:HG22	3:J:135:ILE:CD1	2.39	0.52
3:J:523:GLU:OE2	3:J:547:ARG:NH2	2.42	0.52
3:J:781:LYS:HE3	3:J:785:ASP:OD1	2.08	0.52
5:L:125:ASP:O	5:L:129:GLN:HG3	2.10	0.52
7:O:39:DG:H5''	7:O:39:DG:C8	2.45	0.52
1:H:32:GLU:HB3	1:H:35:PHE:CD1	2.45	0.52
1:H:95:LYS:HD2	1:H:96:ASP:H	1.74	0.52
2:I:520:PRO:HB2	2:I:794:LEU:HD13	1.92	0.52
2:I:803:ALA:HB2	2:I:1227:VAL:HG12	1.92	0.52
3:J:56:LEU:HD21	3:J:269:TYR:HB2	1.91	0.52
3:J:201:LEU:HB3	3:J:221:ILE:CD1	2.39	0.52
3:J:361:LEU:HD13	3:J:366:CYS:HA	1.90	0.52
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.92	0.52
3:J:1178:THR:HG23	3:J:1184:ASP:HB3	1.90	0.52
5:L:102:MET:O	5:L:105:MET:HG3	2.10	0.52
5:L:285:ARG:O	5:L:289:LYS:HG2	2.10	0.52
5:L:400:GLN:HB2	5:L:403:ASP:OD1	2.08	0.52
7:O:41:DT:H1'	7:O:42:DA:H5'	1.90	0.52
2:I:95:PRO:HG3	2:I:126:GLU:OE2	2.10	0.52
2:I:228:VAL:HB	2:I:335:THR:OG1	2.10	0.52
2:I:240:GLU:HG2	2:I:284:LEU:HD11	1.92	0.52
3:J:331:ILE:CG2	3:J:1328:THR:HG21	2.39	0.52
3:J:341:ASN:O	3:J:345:LYS:HE2	2.10	0.52
3:J:518:VAL:CG1	3:J:707:ILE:HB	2.37	0.52
3:J:686:TRP:CD2	3:J:758:PRO:HG3	2.44	0.52
3:J:807:LEU:HD11	3:J:1259:GLN:HG2	1.90	0.52
3:J:1348:LYS:O	3:J:1352:ILE:HD12	2.09	0.52
5:L:247:GLU:O	5:L:250:LEU:HG	2.09	0.52
5:L:313:ASP:O	5:L:317:ASN:N	2.41	0.52
1:M:264:VAL:HG22	1:M:268:ASN:HD21	1.74	0.52
2:I:1145:ILE:HG22	2:I:1161:LEU:HD11	1.92	0.52
2:I:1304:MET:O	2:I:1308:ILE:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:43:THR:HG21	5:L:449:THR:OG1	2.09	0.52
3:J:163:GLU:HA	3:J:166:LEU:CD1	2.36	0.52
3:J:654:ILE:HD13	3:J:760:THR:HB	1.92	0.52
3:J:975:ILE:HD13	3:J:980:THR:CB	2.32	0.52
4:K:44:ASP:HB3	4:K:48:VAL:HG23	1.91	0.52
1:M:270:LEU:CA	1:M:275:ILE:HB	2.40	0.52
1:G:23:HIS:HE1	1:G:204:GLU:HG3	1.74	0.52
1:H:27:THR:O	1:H:27:THR:OG1	2.23	0.52
2:I:61:SER:HB3	2:I:65:ASN:N	2.24	0.52
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.92	0.52
2:I:1325:VAL:O	2:I:1329:GLU:HG3	2.09	0.52
3:J:71:LEU:HB2	3:J:90:VAL:HG21	1.90	0.52
3:J:320:ASN:HD22	3:J:322:ARG:HH21	1.58	0.52
3:J:491:LEU:HD22	3:J:496:GLY:O	2.09	0.52
3:J:660:GLU:CB	3:J:685:ILE:HD13	2.39	0.52
3:J:1034:PHE:CD2	3:J:1083:ALA:HA	2.45	0.52
5:L:226:ALA:O	5:L:230:VAL:HG22	2.09	0.52
5:L:285:ARG:HA	5:L:289:LYS:HE2	1.92	0.52
2:I:292:ILE:HG22	2:I:317:LEU:HD12	1.90	0.52
2:I:1148:ALA:HA	2:I:1201:LEU:CD2	2.39	0.52
3:J:984:LEU:HB3	3:J:993:GLU:HB2	1.92	0.52
3:J:1155:ILE:HD12	3:J:1155:ILE:O	2.10	0.52
5:L:456:MET:HE3	5:L:497:VAL:HG22	1.92	0.52
1:G:45:ARG:HH22	2:I:1216:ARG:HG2	1.75	0.52
2:I:205:PRO:O	2:I:208:ILE:HG22	2.10	0.52
2:I:958:LYS:O	2:I:962:GLU:HG3	2.09	0.52
3:J:53:ARG:HB3	3:J:54:ASP:HB3	1.92	0.52
3:J:268:LEU:CB	3:J:306:LEU:HD23	2.39	0.52
3:J:275:ARG:NH2	5:L:403:ASP:OD1	2.40	0.52
3:J:349:TYR:CD2	3:J:472:LEU:HD11	2.44	0.52
3:J:812:ASP:O	3:J:897:HIS:ND1	2.37	0.52
3:J:1221:LEU:HD23	3:J:1229:VAL:CG1	2.39	0.52
8:P:46:DG:H2"	8:P:47:DC:C6	2.45	0.52
1:G:226:GLU:OE2	1:H:10:LYS:NZ	2.35	0.52
2:I:230:PHE:O	2:I:231:GLU:HG3	2.10	0.52
2:I:596:ASP:OD1	2:I:596:ASP:N	2.42	0.52
2:I:1289:GLU:O	2:I:1294:LYS:HG3	2.10	0.52
3:J:443:GLU:OE2	3:J:444:GLY:N	2.43	0.52
3:J:653:ILE:HG12	3:J:692:ARG:NH2	2.25	0.52
3:J:799:ARG:HD3	3:J:1310:THR:CG2	2.40	0.52
3:J:934:THR:HA	3:J:1137:GLY:HA3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1040:MET:CE	3:J:1078:LEU:HG	2.39	0.52
5:L:381:GLU:HA	5:L:384:LEU:CD2	2.39	0.52
5:L:503:GLU:OE2	5:L:504:PRO:HD2	2.10	0.52
1:M:270:LEU:HD22	1:M:275:ILE:CD1	2.39	0.52
1:M:280:ASP:O	1:M:283:GLN:HB2	2.09	0.52
7:O:38:DG:H1'	7:O:39:DG:H5''	1.92	0.52
2:I:470:ARG:HD3	2:I:497:PRO:HB3	1.91	0.51
2:I:736:VAL:HG12	2:I:737:ASN:O	2.10	0.51
3:J:66:LYS:HE2	3:J:69:GLU:OE1	2.09	0.51
3:J:421:VAL:HG13	3:J:439:PRO:HG3	1.92	0.51
3:J:625:MET:HE3	3:J:629:PHE:HE2	1.76	0.51
3:J:1005:LYS:HG3	3:J:1009:GLU:HB2	1.91	0.51
3:J:1104:LYS:O	3:J:1124:ILE:HA	2.11	0.51
4:K:65:ASP:O	4:K:69:ARG:HG2	2.10	0.51
2:I:136:PHE:CE2	2:I:456:VAL:HG21	2.46	0.51
2:I:198:ILE:HG22	2:I:199:ASP:OD1	2.09	0.51
3:J:596:LEU:HD13	3:J:601:ILE:HG13	1.91	0.51
3:J:847:ASP:OD1	3:J:860:ARG:N	2.43	0.51
3:J:919:ALA:O	3:J:923:ILE:HG13	2.11	0.51
3:J:973:LEU:HB3	3:J:1003:LEU:HD12	1.92	0.51
5:L:363:ARG:O	5:L:367:ILE:HG13	2.10	0.51
2:I:21:VAL:HG21	2:I:592:ARG:CZ	2.40	0.51
2:I:347:ILE:HA	2:I:350:THR:CG2	2.39	0.51
2:I:754:THR:O	2:I:766:ASN:HA	2.10	0.51
3:J:343:LEU:HD21	3:J:1352:ILE:HD11	1.91	0.51
3:J:1009:GLU:O	3:J:1011:VAL:HG23	2.11	0.51
5:L:124:GLU:O	5:L:127:ILE:HG13	2.10	0.51
5:L:137:TYR:HE1	5:L:351:THR:HB	1.75	0.51
5:L:484:ALA:CB	5:L:491:GLU:HG3	2.41	0.51
2:I:237:LEU:HD12	2:I:322:LEU:HD23	1.92	0.51
2:I:905:ILE:HG22	2:I:906:PHE:CD1	2.46	0.51
2:I:993:PRO:HB2	2:I:995:ASP:OD2	2.10	0.51
2:I:1305:TYR:CE1	3:J:379:PRO:HG3	2.45	0.51
3:J:123:ARG:HH22	3:J:1334:GLU:HG2	1.76	0.51
3:J:483:LEU:CD2	4:K:16:ARG:HG2	2.41	0.51
5:L:140:ALA:HB1	5:L:269:LEU:CD2	2.39	0.51
5:L:147:GLN:HG2	5:L:161:LEU:HD13	1.92	0.51
5:L:234:THR:OG1	5:L:248:GLU:HG2	2.10	0.51
5:L:479:THR:HG22	5:L:482:GLU:CG	2.41	0.51
2:I:65:ASN:O	2:I:105:TYR:HB2	2.11	0.51
2:I:131:THR:HG23	2:I:135:THR:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:360:LEU:HA	2:I:363:LEU:HD12	1.93	0.51
2:I:618:GLN:NE2	3:J:770:LEU:HD23	2.26	0.51
2:I:1242:LYS:HB3	3:J:465:GLN:NE2	2.24	0.51
2:I:1293:VAL:HG11	2:I:1304:MET:SD	2.51	0.51
3:J:53:ARG:HB3	3:J:54:ASP:CA	2.40	0.51
3:J:194:LEU:HD22	3:J:224:LEU:CD2	2.41	0.51
3:J:650:LYS:O	3:J:654:ILE:HG13	2.10	0.51
3:J:1004:ALA:H	3:J:1018:ALA:HA	1.75	0.51
3:J:1175:LEU:HB2	3:J:1190:ILE:HG13	1.92	0.51
1:G:98:VAL:HG21	1:G:121:VAL:HG21	1.92	0.51
2:I:264:GLU:O	2:I:267:ARG:HB2	2.09	0.51
2:I:424:ASP:O	2:I:428:VAL:HG23	2.11	0.51
2:I:582:ASN:N	2:I:586:PHE:O	2.28	0.51
2:I:1008:GLN:NE2	2:I:1008:GLN:O	2.43	0.51
2:I:1222:GLU:OE1	3:J:512:TYR:OH	2.22	0.51
2:I:1327:LEU:HD21	2:I:1339:LEU:HD21	1.92	0.51
3:J:1226:VAL:HG23	3:J:1261:LEU:HD22	1.93	0.51
8:P:41:DT:H2"	8:P:42:DT:OP2	2.10	0.51
1:G:179:PRO:HB3	1:G:210:THR:CG2	2.38	0.51
3:J:162:GLU:O	3:J:166:LEU:HG	2.11	0.51
3:J:969:SER:HB2	3:J:1116:SER:HB2	1.93	0.51
5:L:248:GLU:OE2	5:L:251:LYS:HD2	2.10	0.51
1:G:54:CYS:HB3	1:G:90:VAL:O	2.10	0.51
2:I:1076:ILE:HD11	2:I:1079:ILE:HD11	1.93	0.51
3:J:133:ARG:HD2	3:J:136:GLU:OE1	2.11	0.51
3:J:436:ALA:HB1	3:J:480:ALA:HB1	1.91	0.51
3:J:1257:VAL:HA	3:J:1260:MET:HB2	1.93	0.51
3:J:1314:LEU:HA	3:J:1326:GLN:NE2	2.26	0.51
1:G:6:THR:CG2	1:H:148:ARG:HD3	2.41	0.51
1:H:158:ARG:HB2	1:H:172:LEU:HD23	1.92	0.51
2:I:270:THR:HA	6:N:60:GLU:OE1	2.11	0.51
2:I:816:ILE:HG23	2:I:1098:LEU:HD12	1.92	0.51
2:I:877:VAL:CG1	2:I:881:ASP:HB2	2.41	0.51
3:J:490:ILE:HB	3:J:500:ILE:HG13	1.92	0.51
5:L:251:LYS:O	5:L:255:VAL:HG22	2.11	0.51
5:L:456:MET:O	5:L:460:ILE:HG23	2.11	0.51
2:I:110:PRO:HD2	2:I:113:THR:HB	1.93	0.51
2:I:738:GLU:HA	2:I:741:MET:HE3	1.93	0.51
2:I:1002:LEU:HG	2:I:1003:THR:O	2.11	0.51
2:I:1027:LYS:HE2	2:I:1027:LYS:HA	1.93	0.51
3:J:105:ILE:N	3:J:242:LEU:O	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1264:ALA:HB3	3:J:1285:VAL:HG11	1.91	0.51
1:G:192:VAL:HG11	1:G:198:LEU:HD12	1.93	0.50
2:I:303:ASP:CB	2:I:310:ILE:HD11	2.41	0.50
3:J:1025:MET:CB	3:J:1124:ILE:HB	2.25	0.50
3:J:1260:MET:HE3	3:J:1307:LEU:O	2.11	0.50
1:M:253:LEU:O	1:M:279:GLY:N	2.44	0.50
7:O:30:DC:H2''	7:O:31:DA:C8	2.46	0.50
1:H:14:VAL:HG13	1:H:28:LEU:CD1	2.40	0.50
2:I:699:LEU:HD13	2:I:1121:ALA:HB3	1.92	0.50
3:J:78:LEU:O	3:J:81:ARG:HB2	2.11	0.50
3:J:233:LYS:HB3	3:J:235:GLU:OE1	2.11	0.50
3:J:309:ASN:OD1	3:J:315:ALA:HA	2.11	0.50
3:J:885:VAL:HG23	3:J:894:VAL:CG1	2.42	0.50
4:K:45:LYS:O	4:K:49:ILE:HG13	2.11	0.50
5:L:11:LEU:HA	5:L:14:THR:CG2	2.41	0.50
1:M:260:LEU:HD23	1:M:306:VAL:CG2	2.39	0.50
2:I:228:VAL:CG2	2:I:337:PHE:HB2	2.40	0.50
2:I:840:SER:O	2:I:840:SER:OG	2.26	0.50
2:I:1314:GLN:HB2	4:K:28:ARG:NH1	2.26	0.50
3:J:844:THR:HG22	3:J:864:LEU:HD11	1.93	0.50
3:J:888:CYS:HB2	3:J:898:CYS:CB	2.41	0.50
3:J:1000:GLY:O	3:J:1026:PRO:HG3	2.11	0.50
5:L:299:LYS:O	5:L:303:ILE:HG12	2.11	0.50
1:H:73:GLY:O	1:H:134:THR:N	2.44	0.50
2:I:297:VAL:HG13	2:I:313:ALA:HA	1.94	0.50
2:I:1246:ARG:HG2	2:I:1247:SER:N	2.27	0.50
3:J:201:LEU:HB3	3:J:221:ILE:HD11	1.92	0.50
4:K:58:LEU:HD23	4:K:58:LEU:H	1.76	0.50
1:G:13:LEU:CD1	1:G:217:ILE:HD11	2.42	0.50
1:G:13:LEU:HD22	1:G:16:ILE:HD11	1.94	0.50
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.94	0.50
3:J:56:LEU:HD21	3:J:269:TYR:CB	2.42	0.50
3:J:322:ARG:HG3	3:J:323:PRO:HD2	1.94	0.50
3:J:438:GLU:HG3	3:J:485:MET:CE	2.42	0.50
8:P:64:DA:C2'	8:P:65:DT:H5''	2.41	0.50
1:H:212:ASP:OD1	1:H:212:ASP:N	2.35	0.50
2:I:127:ILE:HG13	2:I:127:ILE:O	2.11	0.50
2:I:478:ARG:HD2	2:I:492:MET:HB3	1.92	0.50
2:I:631:GLU:OE1	2:I:631:GLU:N	2.45	0.50
2:I:696:ASP:O	2:I:795:ALA:HB1	2.12	0.50
2:I:971:LEU:HD13	2:I:1018:TYR:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1061:VAL:O	3:J:1103:GLY:HA2	2.11	0.50
5:L:145:LEU:O	5:L:149:ASP:OD1	2.30	0.50
5:L:150:ARG:O	5:L:155:GLU:N	2.42	0.50
5:L:381:GLU:HA	5:L:384:LEU:HD23	1.94	0.50
5:L:405:ILE:HG22	5:L:409:ASN:HD21	1.76	0.50
5:L:492:ASP:O	5:L:495:ARG:HB2	2.12	0.50
2:I:81:ASP:HB3	2:I:84:GLU:OE1	2.12	0.50
2:I:726:TYR:OH	2:I:728:ASP:OD2	2.26	0.50
3:J:130:MET:HE2	3:J:134:ASP:C	2.31	0.50
3:J:138:VAL:HG21	3:J:145:VAL:CG1	2.41	0.50
3:J:364:HIS:HB3	3:J:487:THR:HG21	1.94	0.50
3:J:398:LYS:HD2	5:L:532:LEU:CD2	2.35	0.50
3:J:748:ALA:HB3	6:N:16:THR:HG22	1.92	0.50
3:J:1064:SER:OG	3:J:1072:LYS:HB2	2.12	0.50
5:L:286:LEU:HD23	5:L:290:LEU:HD22	1.93	0.50
1:M:252:ILE:CG2	1:M:312:LEU:HD11	2.42	0.50
1:M:284:ARG:HD2	1:M:288:GLU:OE2	2.12	0.50
2:I:339:ASN:ND2	2:I:343:HIS:HB2	2.27	0.50
2:I:724:VAL:CG1	2:I:727:VAL:HG22	2.41	0.50
2:I:803:ALA:CB	2:I:1227:VAL:HG12	2.42	0.50
2:I:911:SER:OG	2:I:913:VAL:HG12	2.11	0.50
2:I:1167:GLU:O	2:I:1171:ARG:HG3	2.11	0.50
3:J:436:ALA:N	3:J:484:MET:O	2.37	0.50
3:J:528:THR:O	3:J:528:THR:OG1	2.29	0.50
3:J:858:VAL:HG22	3:J:868:TRP:CE3	2.47	0.50
3:J:1040:MET:HG2	3:J:1076:PRO:CA	2.42	0.50
3:J:1110:GLU:HB2	3:J:1113:VAL:CG2	2.38	0.50
5:L:116:GLU:OE1	5:L:116:GLU:N	2.45	0.50
1:G:59:VAL:HG21	1:G:85:LEU:HD12	1.94	0.50
1:H:29:GLU:HG2	1:H:30:PRO:N	2.26	0.50
2:I:496:LYS:O	2:I:500:ALA:CB	2.60	0.50
2:I:1201:LEU:O	2:I:1201:LEU:HD12	2.12	0.50
2:I:1247:SER:O	3:J:348:ASP:HB3	2.12	0.50
3:J:1229:VAL:HG21	3:J:1306:LEU:CD1	2.41	0.50
3:J:1229:VAL:HG21	3:J:1306:LEU:HD13	1.94	0.50
5:L:403:ASP:O	5:L:407:GLU:HG2	2.12	0.50
1:M:285:THR:HG22	1:M:286:GLU:H	1.77	0.50
2:I:82:VAL:HG13	2:I:83:GLN:HG3	1.94	0.49
2:I:136:PHE:HB3	2:I:138:ILE:CD1	2.42	0.49
2:I:314:ASN:ND2	2:I:351:LEU:HB2	2.26	0.49
2:I:319:LEU:HA	2:I:322:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:488:MET:HB3	2:I:489:PRO:HD2	1.94	0.49
2:I:1107:MET:HG2	3:J:740:LEU:CD1	2.42	0.49
2:I:1323:PHE:CZ	3:J:1353:VAL:HG12	2.47	0.49
3:J:107:LEU:HA	3:J:276:ASN:ND2	2.27	0.49
3:J:473:THR:OG1	3:J:475:GLU:OE1	2.20	0.49
3:J:572:THR:OG1	3:J:573:THR:N	2.45	0.49
3:J:1123:ARG:O	3:J:1125:PRO:HD3	2.11	0.49
5:L:12:LEU:HD11	5:L:22:LEU:HD13	1.94	0.49
8:P:59:DA:H4'	8:P:60:DA:OP1	2.11	0.49
1:G:39:LEU:O	1:G:43:LEU:HG	2.12	0.49
1:H:31:LEU:HD11	1:H:39:LEU:HD12	1.94	0.49
1:H:48:LEU:HD13	1:H:183:ILE:HD13	1.92	0.49
1:H:112:ALA:N	1:H:128:HIS:O	2.45	0.49
2:I:788:SER:O	2:I:795:ALA:N	2.29	0.49
2:I:1248:THR:HG1	2:I:1305:TYR:HE1	1.58	0.49
3:J:127:LEU:HD21	3:J:234:PRO:HB3	1.94	0.49
3:J:452:LEU:HD13	3:J:500:ILE:HG23	1.93	0.49
3:J:1307:LEU:HD23	3:J:1311:LYS:CD	2.34	0.49
6:N:36:LEU:HA	6:N:43:PRO:HA	1.94	0.49
6:N:56:THR:HG23	6:N:57:LEU:HG	1.93	0.49
1:H:34:GLY:N	1:H:199:ASP:OD2	2.45	0.49
1:H:101:THR:HG22	1:H:116:THR:OG1	2.12	0.49
2:I:1340:GLU:OE1	3:J:21:LYS:HD3	2.13	0.49
3:J:812:ASP:HA	3:J:896:ALA:HB3	1.93	0.49
3:J:1322:ALA:O	3:J:1326:GLN:HB2	2.12	0.49
4:K:38:LEU:HD11	4:K:67:ARG:HH12	1.77	0.49
5:L:36:VAL:HG23	5:L:37:ASP:OD1	2.11	0.49
7:O:38:DG:H2''	7:O:39:DG:OP2	2.13	0.49
1:G:14:VAL:HG21	1:G:29:GLU:HG3	1.95	0.49
1:G:165:GLU:OE2	1:G:172:LEU:HD11	2.12	0.49
1:H:52:PRO:HG3	1:H:150:ARG:NH1	2.26	0.49
2:I:833:ILE:HA	2:I:1054:LEU:O	2.12	0.49
3:J:143:SER:HB2	3:J:160:LEU:O	2.13	0.49
3:J:337:ARG:O	3:J:342:LEU:HD13	2.12	0.49
3:J:1061:VAL:HG21	3:J:1101:LEU:CG	2.34	0.49
3:J:1061:VAL:HG22	3:J:1105:ALA:O	2.12	0.49
4:K:38:LEU:HD11	4:K:67:ARG:HH22	1.77	0.49
5:L:449:THR:HG21	5:L:504:PRO:HG3	1.93	0.49
1:M:292:THR:OG1	1:M:295:LEU:HB3	2.12	0.49
2:I:287:VAL:HB	2:I:288:PRO:HD2	1.93	0.49
2:I:475:VAL:CG2	2:I:492:MET:HE2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:672:GLU:HG3	2:I:673:HIS:CD2	2.47	0.49
2:I:754:THR:N	2:I:767:GLN:OE1	2.24	0.49
2:I:1151:LEU:HD21	2:I:1198:LEU:CA	2.42	0.49
2:I:1326:LEU:HD21	3:J:338:PHE:CZ	2.47	0.49
3:J:115:TRP:O	3:J:119:SER:HB3	2.12	0.49
3:J:117:LEU:CD1	3:J:139:LEU:HD11	2.42	0.49
3:J:610:ARG:HG3	3:J:866:GLU:OE2	2.11	0.49
5:L:314:THR:HG23	5:L:318:ALA:HB3	1.94	0.49
5:L:507:MET:SD	5:L:523:ILE:HD12	2.52	0.49
2:I:455:SER:O	2:I:459:MET:HG3	2.13	0.49
2:I:660:VAL:HG11	3:J:769:VAL:CG1	2.43	0.49
3:J:214:ARG:HA	3:J:217:LEU:HB3	1.94	0.49
3:J:276:ASN:O	3:J:280:LYS:HG3	2.12	0.49
3:J:646:ILE:HG23	3:J:647:PRO:HD2	1.94	0.49
5:L:105:MET:O	5:L:108:VAL:HG12	2.13	0.49
1:M:250:ASP:OD1	1:M:251:PRO:HD2	2.12	0.49
7:O:28:DG:H2"	7:O:29:DA:H8	1.78	0.49
1:G:98:VAL:HG21	1:G:121:VAL:CG2	2.42	0.49
1:H:14:VAL:HG22	1:H:28:LEU:HD12	1.95	0.49
2:I:60:GLN:HB3	2:I:67:GLU:OE2	2.13	0.49
2:I:65:ASN:HB3	2:I:105:TYR:HB3	1.95	0.49
2:I:232:ILE:HG12	2:I:237:LEU:H	1.77	0.49
2:I:237:LEU:CD1	2:I:322:LEU:HD23	2.43	0.49
2:I:690:VAL:HG12	2:I:1234:LYS:O	2.12	0.49
2:I:995:ASP:O	2:I:996:ARG:NH1	2.46	0.49
3:J:318:GLY:N	3:J:322:ARG:O	2.45	0.49
3:J:1036:ARG:NE	3:J:1081:VAL:HG21	2.28	0.49
3:J:1061:VAL:HG11	3:J:1101:LEU:HD23	1.95	0.49
4:K:5:THR:HG22	4:K:7:GLN:N	2.21	0.49
5:L:286:LEU:O	5:L:290:LEU:HD22	2.13	0.49
1:M:280:ASP:O	1:M:284:ARG:NE	2.45	0.49
3:J:46:TYR:CE1	5:L:453:PRO:HD3	2.47	0.49
3:J:750:PRO:HB3	3:J:781:LYS:HD3	1.95	0.49
3:J:955:LYS:NZ	3:J:986:ASP:OD1	2.26	0.49
3:J:1047:THR:HG22	3:J:1060:VAL:O	2.13	0.49
2:I:145:ILE:HA	2:I:511:LEU:O	2.13	0.49
2:I:1296:ASP:OD2	2:I:1322:SER:HB3	2.13	0.49
3:J:201:LEU:HB3	3:J:221:ILE:CG1	2.42	0.49
3:J:372:MET:O	3:J:376:LEU:HG	2.13	0.49
5:L:148:TYR:CE1	5:L:218:ARG:HG2	2.45	0.49
5:L:249:ILE:HD13	5:L:353:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:530:LEU:O	5:L:533:ASP:N	2.36	0.49
1:M:269:CYS:SG	1:M:295:LEU:HB2	2.53	0.49
2:I:852:ALA:HB2	2:I:869:GLY:HA2	1.95	0.49
3:J:316:ILE:O	3:J:316:ILE:HG13	2.13	0.49
3:J:957:SER:OG	3:J:1010:GLN:HB3	2.13	0.49
3:J:1005:LYS:CE	3:J:1009:GLU:HB3	2.39	0.49
5:L:235:ILE:O	5:L:245:ALA:HB2	2.12	0.49
5:L:482:GLU:O	5:L:485:GLU:HB3	2.13	0.49
1:H:11:PRO:HG3	1:H:28:LEU:HD21	1.95	0.48
1:H:92:VAL:HG12	1:H:121:VAL:HG22	1.95	0.48
2:I:207:THR:CG2	2:I:350:THR:HG23	2.43	0.48
2:I:545:PHE:HE2	3:J:788:LEU:HD11	1.77	0.48
2:I:812:PHE:CE2	2:I:813:GLU:HG2	2.48	0.48
2:I:975:ILE:CG1	2:I:1014:LEU:HD23	2.42	0.48
3:J:104:HIS:HA	3:J:243:PRO:HA	1.95	0.48
3:J:251:PRO:HG2	5:L:507:MET:CE	2.42	0.48
3:J:622:ASP:OD2	3:J:622:ASP:N	2.46	0.48
3:J:793:SER:OG	3:J:794:GLY:N	2.46	0.48
3:J:959:LYS:O	3:J:982:LEU:HA	2.13	0.48
3:J:1075:ARG:HB2	3:J:1100:PHE:CD1	2.45	0.48
5:L:157:ARG:O	5:L:160:ASP:HB2	2.12	0.48
5:L:277:MET:HG2	5:L:281:ARG:HH12	1.77	0.48
5:L:383:ASN:O	5:L:386:LEU:HB3	2.13	0.48
1:M:251:PRO:HA	1:M:254:LEU:CG	2.42	0.48
8:P:60:DA:C8	8:P:61:DT:H72	2.48	0.48
1:G:31:LEU:HD11	1:G:201:LEU:HB2	1.95	0.48
2:I:221:LEU:HD23	2:I:336:LEU:CD2	2.43	0.48
2:I:264:GLU:HB3	2:I:267:ARG:HG3	1.94	0.48
2:I:689:ALA:HB3	2:I:796:LEU:HB3	1.94	0.48
3:J:215:LYS:O	3:J:218:THR:HG22	2.13	0.48
3:J:748:ALA:HB2	6:N:16:THR:HG22	1.95	0.48
3:J:1053:LEU:O	3:J:1053:LEU:HD23	2.13	0.48
3:J:1069:ALA:CA	3:J:1072:LYS:HG2	2.44	0.48
3:J:1177:ILE:HB	3:J:1186:TYR:CD2	2.38	0.48
5:L:415:ALA:HB2	5:L:434:TRP:CB	2.43	0.48
1:M:255:ARG:HD2	1:M:256:PRO:HD3	1.95	0.48
1:G:52:PRO:HG2	1:G:219:ARG:NH1	2.28	0.48
2:I:875:ALA:O	2:I:877:VAL:HG23	2.14	0.48
3:J:204:GLU:O	3:J:208:THR:HB	2.13	0.48
3:J:954:ASN:O	3:J:984:LEU:HD21	2.13	0.48
3:J:1011:VAL:HG11	3:J:1015:GLU:CD	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:66:SER:HB3	2:I:479:LEU:HD22	1.95	0.48
2:I:247:ARG:HH12	2:I:271:ALA:HA	1.78	0.48
2:I:490:GLN:NE2	5:L:472:GLN:O	2.47	0.48
3:J:978:ARG:HA	3:J:999:TYR:CD1	2.47	0.48
3:J:1046:ILE:CD1	3:J:1059:LEU:HD13	2.40	0.48
3:J:1176:VAL:HA	3:J:1187:GLU:HA	1.93	0.48
5:L:108:VAL:HG21	5:L:381:GLU:CD	2.34	0.48
5:L:147:GLN:HB3	5:L:161:LEU:HD13	1.94	0.48
5:L:288:MET:HA	5:L:292:VAL:HG23	1.95	0.48
5:L:292:VAL:HG22	5:L:297:MET:HB3	1.94	0.48
5:L:552:THR:OG1	5:L:555:GLU:OE1	2.16	0.48
2:I:58:PRO:HB3	2:I:69:GLN:CB	2.44	0.48
2:I:1234:LYS:HE3	2:I:1238:LEU:HD21	1.94	0.48
2:I:1262:LYS:HE2	2:I:1262:LYS:HA	1.96	0.48
4:K:64:LEU:HD23	4:K:64:LEU:HA	1.68	0.48
5:L:247:GLU:HA	5:L:250:LEU:CD2	2.39	0.48
1:M:260:LEU:HB3	1:M:306:VAL:HG21	1.95	0.48
1:M:264:VAL:HG22	1:M:268:ASN:ND2	2.28	0.48
1:H:206:GLU:OE1	3:J:531:LYS:NZ	2.40	0.48
2:I:238:GLN:HB2	2:I:285:ILE:O	2.14	0.48
2:I:254:ASP:CA	2:I:263:VAL:O	2.53	0.48
2:I:478:ARG:HH22	2:I:483:ASP:CB	2.27	0.48
2:I:538:LEU:HD13	2:I:543:ALA:CB	2.41	0.48
2:I:866:ASP:HB3	2:I:872:TYR:CE1	2.49	0.48
3:J:436:ALA:CB	3:J:480:ALA:HB1	2.43	0.48
3:J:978:ARG:HG3	3:J:979:ASN:OD1	2.13	0.48
3:J:1172:LYS:HB2	3:J:1189:MET:CB	2.39	0.48
5:L:163:THR:CG2	5:L:263:PRO:HD3	2.44	0.48
5:L:289:LYS:HA	5:L:293:GLU:HB3	1.94	0.48
1:M:251:PRO:HA	1:M:254:LEU:CD1	2.42	0.48
2:I:230:PHE:CE2	2:I:292:ILE:HG23	2.49	0.48
2:I:781:ASP:OD2	2:I:782:VAL:N	2.47	0.48
3:J:1220:ILE:HG22	3:J:1228:ALA:HB1	1.95	0.48
5:L:415:ALA:HB2	5:L:434:TRP:HB2	1.95	0.48
7:O:44:DA:H1'	7:O:45:DA:C8	2.49	0.48
1:G:90:VAL:HG22	1:G:123:ILE:CD1	2.43	0.48
2:I:7:GLU:OE1	2:I:7:GLU:HA	2.12	0.48
2:I:619:ALA:HB2	2:I:654:ASP:HB2	1.95	0.48
2:I:883:LEU:HD11	2:I:1054:LEU:HD11	1.95	0.48
3:J:357:VAL:HG13	3:J:358:GLY:H	1.78	0.48
3:J:438:GLU:HG3	3:J:485:MET:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:507:VAL:HA	3:J:601:ILE:CD1	2.44	0.48
5:L:109:GLU:HB2	5:L:111:LEU:HG	1.95	0.48
2:I:545:PHE:CE2	3:J:788:LEU:HD11	2.49	0.48
2:I:548:ARG:O	3:J:780:ARG:HD3	2.13	0.48
2:I:865:LEU:HD22	2:I:869:GLY:O	2.14	0.48
3:J:553:THR:CG2	3:J:567:THR:HB	2.40	0.48
3:J:954:ASN:HB2	3:J:992:LYS:CE	2.44	0.48
5:L:152:GLU:HG3	5:L:218:ARG:HG2	1.96	0.48
5:L:316:PHE:CE2	5:L:337:VAL:HB	2.49	0.48
8:P:55:DT:H2''	8:P:56:DG:H8	1.78	0.48
1:G:94:GLY:H	1:G:120:ASP:HB3	1.78	0.48
1:H:192:VAL:HG23	1:H:198:LEU:CD1	2.44	0.48
2:I:993:PRO:HG2	2:I:996:ARG:CB	2.36	0.48
3:J:955:LYS:CB	3:J:1012:ALA:HA	2.44	0.48
3:J:958:ILE:HB	3:J:1008:GLY:N	2.29	0.48
3:J:968:ASN:HD21	3:J:974:VAL:CG1	2.26	0.48
3:J:1226:VAL:O	3:J:1230:THR:HG23	2.14	0.48
3:J:1263:LYS:HB2	3:J:1307:LEU:HD11	1.96	0.48
5:L:295:CYS:HB3	5:L:329:LYS:HB3	1.96	0.48
5:L:437:GLN:HG3	8:P:37:DG:O6	2.14	0.48
5:L:560:ARG:HD3	5:L:566:ASP:OD2	2.14	0.48
7:O:41:DT:H4'	7:O:41:DT:OP1	2.13	0.48
1:G:8:PHE:HB3	1:G:32:GLU:HG3	1.94	0.47
2:I:130:MET:HE1	2:I:456:VAL:HG11	1.96	0.47
2:I:231:GLU:O	2:I:238:GLN:N	2.47	0.47
2:I:272:ARG:O	2:I:276:GLN:HG2	2.14	0.47
2:I:324:LYS:HA	2:I:327:GLN:HG2	1.95	0.47
2:I:1010:GLN:O	2:I:1014:LEU:HD13	2.14	0.47
3:J:1047:THR:CG2	3:J:1060:VAL:HB	2.44	0.47
9:J:1504:1N7:C3	9:J:1504:1N7:C18	2.76	0.47
5:L:130:VAL:O	5:L:134:VAL:HG23	2.14	0.47
5:L:316:PHE:CD1	5:L:337:VAL:HG11	2.49	0.47
5:L:317:ASN:O	5:L:320:ILE:HG22	2.14	0.47
2:I:53:PHE:CD1	2:I:468:LEU:HD11	2.49	0.47
2:I:255:ILE:CB	2:I:263:VAL:HB	2.44	0.47
2:I:1032:LYS:O	2:I:1036:ILE:HG13	2.14	0.47
3:J:591:ILE:HD12	3:J:591:ILE:HA	1.74	0.47
3:J:1030:GLU:HG3	3:J:1090:ILE:CG2	2.43	0.47
4:K:65:ASP:O	4:K:68:GLU:HB2	2.14	0.47
5:L:9:LEU:HD22	5:L:44:ILE:HD11	1.95	0.47
5:L:118:ASP:O	5:L:122:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:251:LYS:O	5:L:255:VAL:HG13	2.13	0.47
8:P:45:DA:H2''	8:P:46:DG:H8	1.79	0.47
2:I:8:LYS:HB3	2:I:11:ILE:HD11	1.96	0.47
2:I:133:ASN:HD21	2:I:713:GLY:HA3	1.78	0.47
2:I:182:SER:HB2	2:I:199:ASP:OD1	2.14	0.47
2:I:521:LEU:HD23	2:I:521:LEU:HA	1.72	0.47
3:J:45:ASN:HB3	3:J:48:THR:O	2.13	0.47
3:J:1318:SER:HB3	3:J:1342:ASP:OD2	2.14	0.47
1:G:67:GLU:H	1:G:67:GLU:HG2	1.45	0.47
1:H:107:ILE:HG12	1:H:135:ASP:CA	2.38	0.47
1:H:140:ILE:HD12	1:H:141:SER:H	1.80	0.47
2:I:360:LEU:O	2:I:360:LEU:HD23	2.13	0.47
2:I:1212:LEU:HD21	2:I:1227:VAL:HG11	1.96	0.47
3:J:126:LEU:CD1	3:J:223:LEU:HD22	2.44	0.47
3:J:474:LEU:HD23	4:K:31:GLN:NE2	2.30	0.47
3:J:646:ILE:CD1	3:J:762:ASN:HD21	2.28	0.47
3:J:1069:ALA:HA	3:J:1072:LYS:CG	2.44	0.47
4:K:53:GLU:O	4:K:58:LEU:HD23	2.14	0.47
5:L:123:ILE:O	5:L:127:ILE:HG23	2.14	0.47
5:L:142:THR:HG22	5:L:228:TYR:HE2	1.78	0.47
5:L:419:PHE:HD1	5:L:430:TYR:HD2	1.62	0.47
6:N:14:GLN:O	6:N:18:THR:HG22	2.14	0.47
1:H:149:GLY:HA3	1:H:177:TYR:CD1	2.50	0.47
1:H:152:TYR:CE2	1:H:154:PRO:HG3	2.45	0.47
2:I:210:LEU:HD21	2:I:429:MET:HE1	1.96	0.47
2:I:972:PHE:CE2	2:I:994:ARG:HB3	2.50	0.47
2:I:1086:PRO:HB3	2:I:1221:PHE:HE2	1.80	0.47
3:J:875:ASN:N	3:J:875:ASN:OD1	2.46	0.47
3:J:1115:ILE:HB	3:J:1119:ASP:HB3	1.97	0.47
5:L:449:THR:HG23	5:L:450:ILE:CD1	2.41	0.47
5:L:551:LEU:HD13	5:L:555:GLU:HB3	1.94	0.47
5:L:560:ARG:NH1	5:L:566:ASP:OD2	2.45	0.47
8:P:51:DC:C6	8:P:52:DT:H72	2.50	0.47
1:G:14:VAL:HG21	1:G:29:GLU:CB	2.41	0.47
1:G:53:GLY:O	1:G:148:ARG:HA	2.15	0.47
1:H:52:PRO:HA	1:H:150:ARG:HA	1.95	0.47
1:H:75:GLN:OE1	1:H:75:GLN:N	2.43	0.47
2:I:197:ARG:HG3	2:I:201:ARG:O	2.15	0.47
2:I:246:LEU:HA	2:I:249:GLU:CD	2.35	0.47
2:I:669:PRO:HG3	2:I:1069:ARG:NH2	2.30	0.47
2:I:890:LYS:HD2	2:I:890:LYS:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1210:ILE:HG22	2:I:1211:ARG:O	2.15	0.47
2:I:1282:GLY:HA3	4:K:17:PHE:CE1	2.50	0.47
3:J:209:ASN:HA	3:J:214:ARG:HD3	1.95	0.47
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	1.97	0.47
5:L:286:LEU:HD23	5:L:286:LEU:O	2.15	0.47
5:L:529:GLU:OE1	5:L:529:GLU:HA	2.14	0.47
5:L:560:ARG:HA	5:L:565:ILE:HB	1.95	0.47
1:G:13:LEU:HD21	1:G:26:VAL:CG1	2.44	0.47
1:G:234:LEU:HD22	1:H:14:VAL:CG1	2.45	0.47
1:H:158:ARG:HB2	1:H:172:LEU:CD2	2.45	0.47
2:I:195:PHE:CE2	2:I:203:LYS:HE2	2.50	0.47
2:I:218:GLU:CD	2:I:299:LYS:HB2	2.35	0.47
2:I:629:PHE:HB2	2:I:647:ARG:CD	2.44	0.47
2:I:849:GLU:O	2:I:886:LYS:HG3	2.14	0.47
2:I:1043:ALA:HB1	2:I:1044:PRO:HD2	1.97	0.47
2:I:1282:GLY:CA	3:J:1360:GLY:HA3	2.44	0.47
3:J:322:ARG:HB3	3:J:322:ARG:CZ	2.44	0.47
3:J:357:VAL:CG2	3:J:451:PRO:HG3	2.45	0.47
3:J:952:VAL:HG11	3:J:1017:VAL:HG13	1.97	0.47
3:J:1059:LEU:HD12	3:J:1059:LEU:O	2.15	0.47
3:J:1140:ARG:HA	3:J:1140:ARG:HD2	1.54	0.47
3:J:1257:VAL:O	3:J:1260:MET:N	2.48	0.47
4:K:10:VAL:O	4:K:14:GLY:N	2.45	0.47
5:L:9:LEU:CD1	5:L:88:GLU:HG2	2.44	0.47
5:L:16:GLY:HA3	5:L:22:LEU:HG	1.96	0.47
5:L:23:THR:HA	5:L:56:MET:O	2.14	0.47
5:L:163:THR:OG1	5:L:261:LEU:O	2.28	0.47
5:L:281:ARG:O	5:L:285:ARG:HG2	2.14	0.47
5:L:348:GLU:OE1	5:L:355:ILE:HG12	2.14	0.47
5:L:412:LEU:O	5:L:416:VAL:HG23	2.15	0.47
7:O:32:DA:H2"	7:O:33:DA:C8	2.49	0.47
2:I:102:LEU:N	2:I:118:LYS:O	2.40	0.47
2:I:197:ARG:NH2	2:I:203:LYS:HB3	2.30	0.47
2:I:479:LEU:CD1	2:I:492:MET:HE1	2.45	0.47
2:I:1304:MET:HE1	2:I:1315:MET:HB3	1.95	0.47
3:J:128:LEU:O	3:J:157:GLN:NE2	2.45	0.47
3:J:264:ASP:CB	3:J:324:LEU:HD22	2.41	0.47
3:J:1005:LYS:HE3	3:J:1009:GLU:CB	2.40	0.47
3:J:1101:LEU:HD12	3:J:1102:PRO:CD	2.42	0.47
1:H:92:VAL:HG23	1:H:93:GLN:O	2.15	0.47
1:H:191:ARG:NH1	1:H:193:GLU:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:346:TYR:O	2:I:350:THR:HG22	2.14	0.47
2:I:887:VAL:CG2	2:I:913:VAL:HG21	2.44	0.47
2:I:1073:LYS:H	2:I:1073:LYS:HG3	1.38	0.47
2:I:1103:VAL:HG22	2:I:1111:GLN:NE2	2.20	0.47
2:I:1120:ALA:HB1	2:I:1198:LEU:HG	1.97	0.47
3:J:349:TYR:CE2	3:J:472:LEU:HD11	2.50	0.47
5:L:326:TRP:O	5:L:329:LYS:HB2	2.15	0.47
1:G:218:ARG:HG3	1:H:231:PHE:O	2.15	0.47
1:H:16:ILE:HD12	1:H:214:GLU:HB3	1.96	0.47
2:I:178:PRO:HB3	2:I:397:LEU:CD1	2.45	0.47
2:I:198:ILE:HG13	2:I:369:MET:HE2	1.97	0.47
2:I:829:THR:CG2	2:I:1057:LYS:HG2	2.45	0.47
2:I:1117:LEU:HD21	2:I:1182:ILE:HG21	1.96	0.47
2:I:1129:ASN:OD1	2:I:1177:ARG:NE	2.48	0.47
3:J:141:PHE:HA	3:J:180:MET:CG	2.44	0.47
3:J:797:THR:O	3:J:801:VAL:HG23	2.15	0.47
3:J:803:VAL:HG11	3:J:1309:ILE:CG2	2.45	0.47
3:J:810:THR:O	3:J:811:GLU:HG2	2.15	0.47
3:J:1061:VAL:HG12	3:J:1076:PRO:CG	2.45	0.47
3:J:1136:GLY:HA2	3:J:1240:VAL:HG23	1.97	0.47
5:L:551:LEU:HD23	5:L:551:LEU:HA	1.69	0.47
7:O:40:DC:C6	7:O:41:DT:H72	2.49	0.47
1:G:38:THR:OG1	1:H:45:ARG:HD3	2.15	0.46
2:I:10:ARG:HD2	2:I:697:LYS:HD3	1.96	0.46
2:I:106:GLU:O	2:I:115:LYS:HE2	2.15	0.46
2:I:453:ILE:HD11	2:I:530:ILE:CD1	2.44	0.46
3:J:1036:ARG:CD	3:J:1081:VAL:HG21	2.46	0.46
5:L:227:GLN:NE2	5:L:255:VAL:HG11	2.30	0.46
2:I:67:GLU:HB3	2:I:103:VAL:CG2	2.45	0.46
2:I:230:PHE:CE2	2:I:292:ILE:HG12	2.49	0.46
2:I:230:PHE:CE1	2:I:239:MET:HG3	2.49	0.46
2:I:1323:PHE:CE2	3:J:1353:VAL:HG12	2.49	0.46
3:J:442:ILE:HD13	3:J:448:GLN:HG3	1.98	0.46
3:J:584:PRO:HG2	3:J:587:LEU:CD1	2.46	0.46
3:J:1198:VAL:HG12	3:J:1210:ILE:HG23	1.97	0.46
3:J:1295:ASN:OD1	3:J:1297:LYS:HE3	2.15	0.46
5:L:137:TYR:HD2	5:L:140:ALA:HB2	1.80	0.46
5:L:490:PRO:CG	5:L:493:LYS:HG2	2.44	0.46
1:H:60:GLU:OE1	1:H:171:LEU:N	2.48	0.46
2:I:106:GLU:CB	2:I:115:LYS:HG3	2.37	0.46
2:I:144:VAL:HG23	2:I:515:MET:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:453:ILE:HD11	2:I:530:ILE:HD12	1.97	0.46
2:I:542:ARG:HD3	2:I:543:ALA:N	2.30	0.46
2:I:680:LEU:HD13	3:J:783:LEU:HD12	1.97	0.46
2:I:964:LEU:HB2	2:I:1025:PHE:CD2	2.51	0.46
2:I:1119:MET:CE	2:I:1210:ILE:HD11	2.44	0.46
3:J:759:ILE:HD12	3:J:771:GLN:CB	2.45	0.46
3:J:1034:PHE:CE2	3:J:1083:ALA:HA	2.50	0.46
5:L:15:ARG:NH2	5:L:26:GLU:OE2	2.49	0.46
5:L:105:MET:HE2	5:L:388:ILE:HD12	1.97	0.46
5:L:291:CYS:O	5:L:297:MET:N	2.41	0.46
5:L:533:ASP:HA	5:L:536:THR:CG2	2.42	0.46
1:M:257:VAL:HB	1:M:270:LEU:HD12	1.98	0.46
2:I:814:ASP:O	2:I:1074:GLY:HA3	2.14	0.46
3:J:98:ARG:O	3:J:247:PRO:HD2	2.15	0.46
3:J:516:ASP:HA	3:J:545:HIS:CB	2.45	0.46
3:J:952:VAL:HG22	3:J:984:LEU:HD22	1.97	0.46
8:P:65:DT:H1'	8:P:66:DT:H5'	1.97	0.46
1:H:79:LEU:HD12	3:J:526:VAL:HG11	1.98	0.46
2:I:122:VAL:HG21	2:I:493:ILE:HG21	1.98	0.46
2:I:146:VAL:CG2	2:I:513:GLN:HE21	2.24	0.46
2:I:1328:LYS:HD3	2:I:1328:LYS:HA	1.61	0.46
3:J:26:SER:HB2	3:J:236:TRP:CZ2	2.51	0.46
3:J:128:LEU:HD21	3:J:189:LEU:HD23	1.98	0.46
3:J:205:LEU:HD12	3:J:217:LEU:CD1	2.46	0.46
3:J:510:LEU:HD11	3:J:624:ILE:HG23	1.97	0.46
3:J:644:MET:HB2	3:J:764:ARG:HD2	1.97	0.46
3:J:1003:LEU:HA	3:J:1018:ALA:HB1	1.97	0.46
3:J:1023:HIS:HA	3:J:1126:GLN:N	2.31	0.46
3:J:1221:LEU:O	3:J:1221:LEU:HD22	2.16	0.46
5:L:84:LEU:O	5:L:87:VAL:HG12	2.16	0.46
5:L:144:LEU:HD13	5:L:256:PHE:HZ	1.78	0.46
8:P:64:DA:H2''	8:P:65:DT:H5''	1.97	0.46
2:I:478:ARG:O	2:I:478:ARG:NH1	2.46	0.46
2:I:479:LEU:HG	2:I:492:MET:CE	2.46	0.46
3:J:500:ILE:HG22	3:J:500:ILE:O	2.15	0.46
3:J:664:ILE:HD11	3:J:681:LYS:HG2	1.97	0.46
3:J:708:ASN:N	3:J:708:ASN:OD1	2.49	0.46
3:J:756:GLU:O	3:J:758:PRO:HD3	2.15	0.46
3:J:895:CYS:SG	3:J:897:HIS:N	2.88	0.46
3:J:1031:VAL:HG21	3:J:1088:VAL:HG11	1.96	0.46
5:L:556:ALA:O	5:L:560:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:29:DA:H2''	7:O:30:DC:O5'	2.15	0.46
1:G:51:MET:HE3	1:G:211:ILE:HD13	1.98	0.46
1:G:192:VAL:HG21	1:G:198:LEU:HD13	1.97	0.46
2:I:46:GLN:OE1	2:I:47:TYR:N	2.47	0.46
2:I:1138:VAL:O	2:I:1142:ARG:HB3	2.15	0.46
3:J:510:LEU:HB2	3:J:601:ILE:HD11	1.98	0.46
3:J:1005:LYS:HE2	3:J:1011:VAL:HG22	1.97	0.46
3:J:1179:PRO:HD2	3:J:1184:ASP:CA	2.24	0.46
3:J:1275:LEU:HD23	3:J:1278:GLU:OE1	2.16	0.46
5:L:235:ILE:C	5:L:245:ALA:HB2	2.36	0.46
8:P:50:DT:H5'	8:P:50:DT:C6	2.51	0.46
2:I:144:VAL:CG2	2:I:515:MET:HB2	2.46	0.46
2:I:805:MET:HE3	3:J:636:GLY:HA2	1.98	0.46
2:I:1182:ILE:HD11	2:I:1198:LEU:HD21	1.98	0.46
2:I:1243:MET:HE1	3:J:445:LYS:HD2	1.98	0.46
3:J:318:GLY:H	3:J:322:ARG:H	1.63	0.46
3:J:355:ILE:HG21	3:J:466:MET:HG3	1.98	0.46
3:J:663:GLU:O	3:J:667:GLN:HG3	2.15	0.46
3:J:848:VAL:O	3:J:857:LEU:HB3	2.16	0.46
3:J:1104:LYS:O	3:J:1124:ILE:HG23	2.16	0.46
3:J:1137:GLY:O	3:J:1140:ARG:N	2.47	0.46
3:J:1169:THR:HG22	3:J:1169:THR:O	2.16	0.46
5:L:344:LEU:O	5:L:348:GLU:HG3	2.16	0.46
5:L:360:ASP:HA	5:L:363:ARG:HB3	1.97	0.46
5:L:586:ARG:O	5:L:590:ILE:HG13	2.15	0.46
8:P:55:DT:H2''	8:P:56:DG:C8	2.50	0.46
1:H:155:ALA:HA	1:H:158:ARG:HG2	1.97	0.46
2:I:14:ASP:HB3	2:I:1157:GLN:HB2	1.98	0.46
2:I:27:LEU:HD22	2:I:663:VAL:HG21	1.97	0.46
2:I:835:GLU:HB2	2:I:1053:TYR:HD1	1.80	0.46
2:I:1096:ILE:HG22	2:I:1098:LEU:HD13	1.97	0.46
2:I:1148:ALA:CA	2:I:1201:LEU:HD21	2.45	0.46
3:J:320:ASN:HD22	3:J:322:ARG:NH2	2.13	0.46
3:J:378:LYS:HE3	3:J:382:TYR:OH	2.16	0.46
3:J:1357:ILE:HG13	3:J:1357:ILE:O	2.16	0.46
5:L:108:VAL:HG21	5:L:381:GLU:OE1	2.16	0.46
7:O:42:DA:H2''	7:O:43:DA:C8	2.51	0.46
1:H:16:ILE:O	1:H:16:ILE:HG12	2.16	0.46
2:I:256:GLU:HB2	2:I:261:VAL:HA	1.98	0.46
2:I:359:ARG:O	2:I:362:ALA:HB3	2.15	0.46
2:I:371:ARG:HB3	2:I:374:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:819:SER:HB2	2:I:1085:MET:CG	2.46	0.46
2:I:839:VAL:HG12	2:I:1049:ILE:CG1	2.31	0.46
3:J:278:ARG:HG3	3:J:281:ARG:NH2	2.23	0.46
3:J:526:VAL:HG12	3:J:549:LYS:HB2	1.97	0.46
5:L:477:GLU:CD	5:L:478:PRO:HD2	2.37	0.46
5:L:511:ILE:HG21	5:L:517:SER:HB3	1.97	0.46
1:H:46:ILE:CD1	1:H:224:LEU:HB2	2.44	0.45
2:I:9:LYS:HG2	2:I:1171:ARG:NH1	2.23	0.45
2:I:755:LYS:NZ	2:I:767:GLN:O	2.41	0.45
3:J:58:CYS:SG	3:J:61:ILE:HG13	2.56	0.45
3:J:859:PRO:HB2	3:J:862:THR:HG23	1.97	0.45
2:I:148:GLN:NE2	2:I:535:PRO:O	2.45	0.45
2:I:255:ILE:HG23	2:I:285:ILE:CD1	2.46	0.45
2:I:336:LEU:H	2:I:336:LEU:HG	1.56	0.45
2:I:1141:LEU:HD21	2:I:1173:ALA:CB	2.47	0.45
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.97	0.45
5:L:594:ALA:O	5:L:598:LEU:HG	2.16	0.45
1:G:74:VAL:HA	1:G:132:HIS:O	2.16	0.45
2:I:15:PHE:CD2	2:I:1190:ALA:HB2	2.52	0.45
2:I:122:VAL:HG21	2:I:493:ILE:CG2	2.46	0.45
2:I:142:GLU:CG	2:I:515:MET:HE2	2.33	0.45
2:I:816:ILE:HG23	2:I:1098:LEU:CD1	2.45	0.45
3:J:146:VAL:HA	3:J:178:ALA:CB	2.46	0.45
3:J:552:ILE:HG12	3:J:570:LYS:HG3	1.98	0.45
3:J:1003:LEU:HD23	3:J:1018:ALA:CB	2.46	0.45
3:J:1361:THR:CG2	4:K:21:LEU:HD21	2.46	0.45
5:L:323:ASN:N	5:L:327:SER:OG	2.50	0.45
2:I:356:THR:HG23	2:I:361:SER:CB	2.46	0.45
2:I:715:THR:HG21	2:I:782:VAL:HG12	1.98	0.45
2:I:854:ILE:HB	2:I:857:VAL:HG21	1.99	0.45
2:I:1128:ILE:HG23	2:I:1141:LEU:HD11	1.98	0.45
3:J:128:LEU:HD11	3:J:189:LEU:HD21	1.98	0.45
3:J:201:LEU:HD12	3:J:221:ILE:HG12	1.98	0.45
3:J:816:THR:HG21	3:J:889:ASP:HB2	1.98	0.45
3:J:1068:THR:HG22	3:J:1069:ALA:H	1.81	0.45
5:L:401:PHE:CE2	5:L:405:ILE:HD11	2.51	0.45
7:O:21:DA:C8	7:O:21:DA:H5'	2.51	0.45
2:I:69:GLN:O	2:I:100:LEU:HD22	2.17	0.45
2:I:233:ARG:HB3	2:I:238:GLN:HG2	1.99	0.45
2:I:388:LEU:HD12	2:I:388:LEU:HA	1.79	0.45
2:I:446:ASP:OD2	2:I:551:HIS:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:727:VAL:HG12	2:I:728:ASP:H	1.82	0.45
2:I:882:ILE:H	2:I:882:ILE:HD12	1.80	0.45
3:J:474:LEU:HD23	4:K:31:GLN:HE22	1.82	0.45
3:J:1170:LYS:CE	3:J:1172:LYS:HE3	2.47	0.45
1:H:211:ILE:HD12	1:H:212:ASP:H	1.81	0.45
2:I:1245:ALA:HA	3:J:351:GLY:HA2	1.97	0.45
3:J:56:LEU:HD12	3:J:56:LEU:HA	1.62	0.45
3:J:1027:VAL:HG21	3:J:1122:ALA:HB3	1.98	0.45
3:J:1105:ALA:HB1	3:J:1122:ALA:HB1	1.99	0.45
5:L:313:ASP:HB3	5:L:317:ASN:OD1	2.15	0.45
1:M:252:ILE:HG21	1:M:312:LEU:HD11	1.98	0.45
1:M:253:LEU:CD2	1:M:282:VAL:HG11	2.46	0.45
8:P:45:DA:H2''	8:P:46:DG:OP2	2.16	0.45
1:H:9:LEU:HD21	1:H:192:VAL:HG21	1.98	0.45
2:I:75:LEU:HD12	2:I:94:ALA:HB3	1.98	0.45
3:J:420:PRO:O	3:J:471:PRO:HD2	2.17	0.45
3:J:490:ILE:HB	3:J:500:ILE:CG1	2.46	0.45
3:J:925:GLU:HB3	3:J:926:PRO:CD	2.47	0.45
3:J:1047:THR:HB	3:J:1062:LEU:CD1	2.47	0.45
3:J:1191:PRO:HB3	3:J:1193:TRP:CZ3	2.52	0.45
5:L:73:ASP:OD1	5:L:74:GLU:N	2.50	0.45
8:P:67:DT:H2''	8:P:68:DG:O5'	2.16	0.45
2:I:255:ILE:HG13	2:I:263:VAL:HG11	1.98	0.45
2:I:1284:ALA:HB1	3:J:1356:LEU:HD23	1.98	0.45
2:I:1298:VAL:HB	2:I:1321:GLU:OE2	2.17	0.45
3:J:1029:THR:HA	3:J:1099:TYR:OH	2.16	0.45
5:L:22:LEU:HD23	5:L:22:LEU:HA	1.78	0.45
5:L:38:SER:CA	5:L:41:ILE:HD12	2.41	0.45
5:L:230:VAL:HA	5:L:233:ASP:HB2	1.99	0.45
5:L:349:GLU:OE2	5:L:350:GLU:HG3	2.17	0.45
5:L:414:LYS:O	5:L:418:LYS:HG3	2.17	0.45
2:I:107:ARG:CZ	2:I:108:GLU:HA	2.46	0.45
2:I:251:ALA:CB	2:I:265:LYS:HA	2.47	0.45
3:J:985:ILE:HD13	3:J:991:THR:CB	2.47	0.45
3:J:1120:THR:HB	3:J:1123:ARG:HD3	1.98	0.45
5:L:532:LEU:O	5:L:536:THR:HB	2.16	0.45
1:M:289:LEU:HD13	1:M:300:LEU:CD2	2.40	0.45
1:G:159:ILE:O	1:G:159:ILE:HG23	2.17	0.45
1:H:211:ILE:HD12	1:H:212:ASP:OD1	2.16	0.45
2:I:277:LEU:CD2	2:I:282:VAL:HB	2.47	0.45
2:I:719:LYS:HB2	2:I:719:LYS:HE3	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:815:SER:HB3	2:I:1077:SER:HB3	1.99	0.45
2:I:1064:ASP:OD1	2:I:1239:VAL:HG12	2.17	0.45
3:J:137:ARG:O	3:J:142:GLU:HB2	2.17	0.45
3:J:959:LYS:CB	3:J:983:LYS:HB2	2.43	0.45
3:J:974:VAL:HB	3:J:1028:ILE:HD13	1.99	0.45
3:J:978:ARG:HG3	3:J:979:ASN:CG	2.38	0.45
3:J:1029:THR:OG1	3:J:1030:GLU:N	2.49	0.45
3:J:1060:VAL:HG13	3:J:1106:ILE:HA	1.99	0.45
1:G:152:TYR:CE2	1:G:154:PRO:HD3	2.52	0.44
2:I:361:SER:O	2:I:364:VAL:HG22	2.17	0.44
2:I:611:GLU:HG2	2:I:611:GLU:O	2.18	0.44
3:J:107:LEU:HA	3:J:276:ASN:HD21	1.82	0.44
3:J:958:ILE:HG22	3:J:960:LEU:HD12	1.99	0.44
3:J:1346:GLY:HA3	3:J:1349:GLU:OE2	2.18	0.44
5:L:31:LEU:HD23	5:L:31:LEU:HA	1.76	0.44
5:L:141:ILE:CD1	5:L:252:LEU:HD11	2.46	0.44
5:L:162:ILE:HD12	5:L:165:PHE:CE2	2.51	0.44
5:L:320:ILE:HD13	5:L:330:LEU:HD12	1.97	0.44
1:M:298:LYS:HB2	8:P:67:DT:C3'	2.47	0.44
7:O:45:DA:H5''	7:O:45:DA:C8	2.50	0.44
1:G:50:SER:HB3	1:H:8:PHE:CZ	2.52	0.44
2:I:34:SER:O	2:I:37:LYS:HB2	2.17	0.44
2:I:902:LEU:HD12	5:L:607:LEU:HB3	1.99	0.44
3:J:849:LEU:HG	3:J:853:THR:HG23	2.00	0.44
4:K:26:ARG:NH2	4:K:36:ASP:O	2.50	0.44
5:L:53:ILE:H	5:L:53:ILE:HD12	1.82	0.44
5:L:277:MET:CE	5:L:362:ASN:HD21	2.30	0.44
5:L:376:LYS:HA	5:L:379:MET:HE3	1.99	0.44
5:L:557:LYS:O	5:L:561:MET:HE2	2.17	0.44
1:M:253:LEU:HD22	1:M:282:VAL:CG2	2.47	0.44
2:I:10:ARG:HD2	2:I:697:LYS:CD	2.47	0.44
2:I:58:PRO:HB3	2:I:69:GLN:HB3	2.00	0.44
2:I:59:ILE:CD1	2:I:472:GLU:HB2	2.47	0.44
2:I:196:VAL:O	2:I:203:LYS:HA	2.18	0.44
2:I:341:LEU:HD22	6:N:64:TYR:HD1	1.81	0.44
2:I:561:ILE:HG21	3:J:772:TYR:HE2	1.83	0.44
3:J:141:PHE:CD1	3:J:180:MET:HG2	2.52	0.44
3:J:516:ASP:HB3	3:J:573:THR:HG21	1.99	0.44
3:J:931:THR:OG1	3:J:1244:GLN:NE2	2.45	0.44
3:J:975:ILE:HB	3:J:1000:GLY:N	2.32	0.44
3:J:1060:VAL:HG22	3:J:1106:ILE:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:324:LYS:N	5:L:327:SER:HG	2.12	0.44
5:L:416:VAL:HG22	5:L:427:PHE:CZ	2.50	0.44
1:G:231:PHE:CE2	1:H:28:LEU:HD22	2.52	0.44
3:J:161:THR:OG1	3:J:162:GLU:N	2.50	0.44
3:J:396:ALA:O	3:J:400:MET:HG3	2.18	0.44
3:J:606:ASN:OD1	3:J:610:ARG:NH1	2.49	0.44
3:J:825:VAL:CG2	3:J:827:GLU:HG3	2.46	0.44
3:J:968:ASN:HA	3:J:1117:SER:O	2.17	0.44
3:J:1023:HIS:CD2	3:J:1126:GLN:HG3	2.52	0.44
3:J:1023:HIS:C	3:J:1125:PRO:HA	2.37	0.44
3:J:1151:LYS:C	3:J:1153:PRO:HD3	2.38	0.44
5:L:463:LEU:HD12	5:L:487:MET:SD	2.57	0.44
5:L:551:LEU:HD13	5:L:555:GLU:CB	2.47	0.44
1:M:280:ASP:CB	1:M:284:ARG:HH21	2.29	0.44
7:O:16:DC:H2"	7:O:17:DA:OP2	2.18	0.44
1:H:69:SER:HB2	1:H:78:ILE:CD1	2.47	0.44
1:H:133:LEU:HD12	1:H:133:LEU:HA	1.79	0.44
2:I:848:GLU:OE1	2:I:886:LYS:NZ	2.29	0.44
3:J:152:THR:OG1	3:J:153:ASN:N	2.50	0.44
3:J:203:GLU:HG2	3:J:207:GLU:OE2	2.17	0.44
3:J:707:ILE:HG22	3:J:708:ASN:N	2.32	0.44
3:J:1170:LYS:HE2	3:J:1172:LYS:HE3	2.00	0.44
1:M:275:ILE:HG12	1:M:284:ARG:NH1	2.31	0.44
1:M:298:LYS:HB2	8:P:68:DG:P	2.57	0.44
1:H:91:ARG:HD2	1:H:124:VAL:CG1	2.47	0.44
2:I:66:SER:O	2:I:479:LEU:HD13	2.17	0.44
2:I:270:THR:OG1	2:I:273:HIS:N	2.46	0.44
2:I:594:VAL:HG11	2:I:650:VAL:CG2	2.47	0.44
2:I:891:GLY:HA2	2:I:892:GLU:HA	1.70	0.44
3:J:975:ILE:HG22	3:J:977:SER:O	2.18	0.44
5:L:123:ILE:HD11	5:L:379:MET:HE1	2.00	0.44
5:L:147:GLN:CB	5:L:161:LEU:HD13	2.48	0.44
7:O:22:DT:O2	8:P:64:DA:N1	2.51	0.44
1:G:16:ILE:HG12	1:G:26:VAL:HG13	1.98	0.44
1:G:75:GLN:HE21	1:G:132:HIS:CB	2.31	0.44
2:I:240:GLU:HG2	2:I:284:LEU:HD12	1.99	0.44
2:I:255:ILE:HG13	2:I:263:VAL:CG1	2.47	0.44
2:I:672:GLU:H	2:I:672:GLU:HG2	1.51	0.44
2:I:1322:SER:HB2	3:J:342:LEU:HD12	2.00	0.44
3:J:136:GLU:HA	3:J:139:LEU:HB2	1.98	0.44
3:J:204:GLU:O	3:J:204:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:265:LEU:HD11	3:J:327:LEU:HD23	1.99	0.44
3:J:707:ILE:N	3:J:707:ILE:HD12	2.33	0.44
3:J:721:SER:O	3:J:725:MET:HG3	2.18	0.44
3:J:999:TYR:O	3:J:1026:PRO:HD2	2.17	0.44
3:J:1190:ILE:CG2	3:J:1196:LEU:HD21	2.48	0.44
5:L:149:ASP:O	5:L:153:ALA:CB	2.66	0.44
1:M:298:LYS:O	1:M:301:THR:HG22	2.18	0.44
1:G:227:GLN:HB3	1:H:39:LEU:HD11	1.99	0.44
2:I:70:TYR:HA	2:I:100:LEU:HD23	2.00	0.44
2:I:93:SER:HB3	2:I:126:GLU:HB3	2.00	0.44
2:I:148:GLN:HB2	2:I:511:LEU:CD1	2.46	0.44
2:I:231:GLU:O	2:I:237:LEU:HA	2.18	0.44
2:I:538:LEU:HD22	2:I:547:VAL:HG21	2.00	0.44
2:I:724:VAL:HG22	2:I:734:ILE:HD11	2.00	0.44
2:I:877:VAL:HG11	2:I:920:VAL:CG2	2.44	0.44
2:I:896:THR:HB	2:I:897:PRO:HD2	2.00	0.44
3:J:245:LEU:HD12	3:J:245:LEU:HA	1.87	0.44
3:J:352:ARG:HA	3:J:466:MET:O	2.17	0.44
3:J:1155:ILE:HD11	3:J:1211:SER:CB	2.47	0.44
3:J:1158:GLU:HG3	3:J:1186:TYR:OH	2.17	0.44
3:J:1358:PRO:HB3	3:J:1366:HIS:CG	2.53	0.44
5:L:313:ASP:HB3	5:L:317:ASN:HB2	1.99	0.44
5:L:453:PRO:HG2	7:O:44:DA:OP2	2.17	0.44
1:M:280:ASP:HA	1:M:283:GLN:CG	2.46	0.44
1:G:33:ARG:HB3	1:G:33:ARG:CZ	2.48	0.44
1:G:50:SER:HB3	1:H:8:PHE:HZ	1.83	0.44
2:I:4:SER:OG	2:I:7:GLU:HB2	2.18	0.44
2:I:360:LEU:HD23	2:I:364:VAL:HG13	1.99	0.44
2:I:563:THR:OG1	2:I:564:PRO:HD2	2.18	0.44
2:I:800:MET:HE1	2:I:822:VAL:HG22	2.00	0.44
2:I:1125:GLY:HA3	2:I:1179:GLY:HA2	1.99	0.44
3:J:118:LYS:NZ	3:J:312:ARG:HB2	2.32	0.44
3:J:929:GLN:HB2	3:J:1246:VAL:HG21	2.00	0.44
5:L:235:ILE:CA	5:L:245:ALA:HB2	2.45	0.44
1:H:16:ILE:CD1	1:H:214:GLU:HB3	2.48	0.43
1:H:35:PHE:HA	1:H:38:THR:HG22	1.98	0.43
2:I:228:VAL:HG22	2:I:245:ARG:HH21	1.82	0.43
2:I:974:ARG:HG2	2:I:1014:LEU:HD21	1.99	0.43
3:J:201:LEU:CD1	3:J:221:ILE:HG12	2.48	0.43
3:J:347:VAL:HG12	3:J:348:ASP:O	2.18	0.43
3:J:783:LEU:HD23	3:J:783:LEU:HA	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1361:THR:HG22	4:K:21:LEU:HD21	1.99	0.43
5:L:336:GLU:HA	5:L:339:ARG:NE	2.33	0.43
1:G:55:ALA:HB3	1:G:177:TYR:CD1	2.54	0.43
1:H:103:ASN:HB3	1:H:141:SER:HB2	1.99	0.43
2:I:61:SER:HB3	2:I:65:ASN:H	1.83	0.43
3:J:25:ALA:HB3	3:J:30:ILE:HD11	1.99	0.43
3:J:705:THR:CG2	3:J:707:ILE:HD11	2.37	0.43
3:J:706:VAL:HG12	3:J:713:GLU:HG2	2.00	0.43
3:J:747:MET:CG	3:J:774:ILE:HG22	2.47	0.43
7:O:35:DG:H2''	7:O:36:DA:OP2	2.17	0.43
8:P:42:DT:OP2	8:P:42:DT:H2'	2.17	0.43
1:G:234:LEU:HB2	1:H:218:ARG:NH2	2.34	0.43
2:I:600:THR:CG2	2:I:602:GLU:HG2	2.49	0.43
2:I:1340:GLU:CD	3:J:1341:ARG:HD2	2.39	0.43
3:J:645:VAL:CG2	3:J:700:ASN:HD21	2.31	0.43
3:J:1005:LYS:HE2	3:J:1011:VAL:HG21	1.98	0.43
3:J:1206:ARG:O	3:J:1206:ARG:HG3	2.18	0.43
5:L:137:TYR:CZ	5:L:139:GLU:HB3	2.54	0.43
5:L:405:ILE:HG22	5:L:409:ASN:ND2	2.33	0.43
5:L:462:LYS:HE3	5:L:489:MET:CE	2.47	0.43
6:N:3:ASP:OD1	6:N:6:ASP:HB2	2.19	0.43
1:G:79:LEU:HD11	2:I:1057:LYS:NZ	2.33	0.43
1:H:102:LEU:HD12	1:H:144:ILE:HD11	1.99	0.43
1:H:205:MET:HE3	1:H:213:PRO:CB	2.49	0.43
2:I:74:ARG:NH2	2:I:97:ARG:HG3	2.33	0.43
2:I:219:GLN:HA	2:I:222:ASP:HB2	2.00	0.43
2:I:865:LEU:HD21	2:I:882:ILE:O	2.18	0.43
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.51	0.43
2:I:1131:MET:HE2	2:I:1141:LEU:HA	2.01	0.43
3:J:41:PRO:HG3	3:J:274:ASN:OD1	2.18	0.43
3:J:108:ALA:N	3:J:276:ASN:HD21	2.08	0.43
3:J:432:LEU:HD21	3:J:489:ASN:HB3	2.01	0.43
3:J:500:ILE:HG23	3:J:500:ILE:HD12	1.82	0.43
3:J:507:VAL:HA	3:J:601:ILE:HD12	2.00	0.43
3:J:664:ILE:CD1	3:J:681:LYS:HG2	2.48	0.43
3:J:1078:LEU:CD2	3:J:1121:LEU:HD11	2.32	0.43
3:J:1172:LYS:CB	3:J:1189:MET:HB3	2.45	0.43
5:L:147:GLN:OE1	5:L:151:VAL:HG23	2.19	0.43
5:L:152:GLU:CG	5:L:218:ARG:HD3	2.47	0.43
5:L:476:ARG:HE	5:L:476:ARG:HB3	1.47	0.43
5:L:511:ILE:CG2	5:L:517:SER:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:153:PRO:HA	2:I:177:ILE:O	2.18	0.43
2:I:957:LYS:CB	2:I:1029:LEU:HD11	2.42	0.43
3:J:131:PRO:HG2	3:J:134:ASP:OD2	2.18	0.43
3:J:596:LEU:HD22	3:J:596:LEU:HA	1.73	0.43
3:J:707:ILE:O	3:J:714:GLU:N	2.52	0.43
3:J:1216:ALA:O	3:J:1220:ILE:HG12	2.18	0.43
5:L:586:ARG:NE	7:O:24:DC:H2'	2.33	0.43
1:M:257:VAL:HG11	1:M:275:ILE:HG22	2.01	0.43
1:M:294:ASN:HA	8:P:68:DG:O3'	2.18	0.43
1:G:167:PRO:CG	1:G:170:ARG:HD2	2.39	0.43
1:H:134:THR:HG23	1:H:136:GLU:H	1.83	0.43
2:I:57:PHE:HD1	2:I:59:ILE:HG13	1.83	0.43
2:I:66:SER:CB	2:I:479:LEU:HD22	2.49	0.43
2:I:468:LEU:HA	2:I:471:VAL:HG22	2.00	0.43
2:I:618:GLN:O	2:I:621:SER:OG	2.17	0.43
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.84	0.43
3:J:137:ARG:HG3	3:J:142:GLU:HB2	2.01	0.43
3:J:190:LYS:HE3	3:J:190:LYS:HB2	1.67	0.43
3:J:809:VAL:HG23	3:J:915:ILE:CG2	2.43	0.43
3:J:974:VAL:HB	3:J:1028:ILE:CD1	2.49	0.43
3:J:1143:ASP:OD1	3:J:1148:ARG:NH1	2.43	0.43
3:J:1223:LEU:HD13	3:J:1223:LEU:HA	1.80	0.43
4:K:64:LEU:O	4:K:68:GLU:HG2	2.18	0.43
5:L:72:ALA:CA	5:L:73:ASP:HB2	2.49	0.43
5:L:121:LYS:HA	5:L:124:GLU:OE1	2.19	0.43
5:L:281:ARG:O	5:L:284:GLU:HB2	2.18	0.43
2:I:218:GLU:OE1	2:I:299:LYS:HB2	2.18	0.43
2:I:241:LEU:HD12	2:I:242:VAL:H	1.84	0.43
2:I:667:LEU:CD1	2:I:794:LEU:HD23	2.49	0.43
3:J:146:VAL:HG13	3:J:156:ARG:O	2.18	0.43
3:J:188:LEU:HA	3:J:188:LEU:HD23	1.79	0.43
3:J:672:LEU:CD2	6:N:47:ALA:HB1	2.48	0.43
3:J:812:ASP:HA	3:J:896:ALA:CB	2.48	0.43
3:J:868:TRP:O	3:J:872:LEU:HG	2.19	0.43
3:J:1159:ILE:HD12	3:J:1186:TYR:CG	2.54	0.43
9:J:1505:1N7:C19	9:J:1505:1N7:C4	2.85	0.43
5:L:399:LEU:HD12	5:L:399:LEU:HA	1.86	0.43
1:M:257:VAL:HG13	1:M:276:HIS:C	2.39	0.43
6:N:48:ARG:NH1	6:N:59:VAL:HG22	2.34	0.43
6:N:56:THR:O	6:N:57:LEU:HD23	2.18	0.43
1:G:88:LEU:HD12	1:G:128:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:100:LEU:HD23	2:I:100:LEU:HA	1.61	0.43
2:I:223:LEU:HD23	2:I:223:LEU:HA	1.84	0.43
3:J:512:TYR:CD2	3:J:635:SER:HB2	2.53	0.43
3:J:1189:MET:N	3:J:1189:MET:SD	2.91	0.43
4:K:15:ASN:HB2	4:K:18:ASP:HB2	1.99	0.43
4:K:15:ASN:CB	4:K:18:ASP:HB2	2.49	0.43
5:L:45:ILE:O	5:L:48:ILE:HG22	2.19	0.43
5:L:449:THR:HG23	5:L:450:ILE:H	1.84	0.43
1:G:175:ALA:HB1	1:G:177:TYR:CZ	2.53	0.43
1:H:186:ASN:O	1:H:188:GLU:HG2	2.19	0.43
2:I:57:PHE:HD2	2:I:70:TYR:HB2	1.81	0.43
2:I:253:PHE:O	2:I:263:VAL:HG12	2.19	0.43
2:I:448:LEU:HA	2:I:448:LEU:HD23	1.70	0.43
2:I:903:ARG:NH1	2:I:910:ALA:HA	2.33	0.43
3:J:530:PRO:CB	3:J:581:MET:HG2	2.48	0.43
3:J:857:LEU:HD22	3:J:875:ASN:HD22	1.83	0.43
3:J:958:ILE:HG12	3:J:1009:GLU:O	2.19	0.43
4:K:41:GLU:HG3	4:K:41:GLU:O	2.18	0.43
6:N:64:TYR:O	6:N:68:GLN:HG2	2.19	0.43
1:G:188:GLU:HG2	1:G:200:LYS:HD2	2.01	0.43
2:I:18:ARG:HD3	2:I:18:ARG:HA	1.75	0.43
2:I:1301:ARG:HG3	2:I:1302:THR:N	2.33	0.43
3:J:317:THR:N	3:J:318:GLY:HA2	2.16	0.43
3:J:432:LEU:CD2	3:J:489:ASN:HB3	2.49	0.43
3:J:474:LEU:HA	3:J:474:LEU:HD13	1.77	0.43
3:J:800:LEU:HA	3:J:803:VAL:HG12	2.01	0.43
3:J:850:LYS:HD3	3:J:854:ALA:CB	2.49	0.43
3:J:888:CYS:HB2	3:J:898:CYS:HB3	2.01	0.43
3:J:1172:LYS:HD2	3:J:1172:LYS:O	2.19	0.43
5:L:40:GLN:O	5:L:44:ILE:HG22	2.18	0.43
5:L:148:TYR:O	5:L:152:GLU:HG2	2.19	0.43
1:M:256:PRO:O	1:M:278:ILE:HD11	2.19	0.43
8:P:58:DC:H2''	8:P:59:DA:H8	1.83	0.43
8:P:62:DG:H2''	8:P:63:DG:H5'	2.01	0.43
2:I:213:LEU:HD23	2:I:385:PHE:HE2	1.83	0.42
2:I:215:TYR:HB3	2:I:220:ILE:HG13	2.00	0.42
2:I:223:LEU:HD13	2:I:426:ILE:HG21	2.01	0.42
2:I:233:ARG:CB	2:I:238:GLN:HG2	2.49	0.42
2:I:277:LEU:HD23	2:I:277:LEU:HA	1.81	0.42
2:I:516:ASP:HB3	2:I:522:SER:HB3	2.01	0.42
2:I:800:MET:CE	2:I:822:VAL:HG22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1211:ARG:O	2:I:1212:LEU:HD12	2.19	0.42
3:J:189:LEU:HD13	3:J:234:PRO:O	2.19	0.42
3:J:332:LYS:O	3:J:336:GLY:HA3	2.19	0.42
3:J:694:SER:HA	3:J:697:MET:HG3	2.01	0.42
3:J:1089:LEU:CD2	3:J:1094:ASP:HA	2.48	0.42
1:G:13:LEU:CD2	1:G:16:ILE:HD11	2.49	0.42
2:I:185:ASP:N	2:I:185:ASP:OD1	2.52	0.42
2:I:398:SER:OG	2:I:399:ALA:N	2.53	0.42
2:I:745:GLU:HA	2:I:1017:GLN:CG	2.31	0.42
3:J:153:ASN:HB2	3:J:172:PHE:CE2	2.43	0.42
3:J:382:TYR:HB3	3:J:394:ILE:CD1	2.49	0.42
3:J:400:MET:HB3	3:J:405:GLU:HG3	2.00	0.42
3:J:1163:VAL:HG13	3:J:1200:GLU:O	2.19	0.42
3:J:1286:LYS:HD2	3:J:1286:LYS:HA	1.76	0.42
2:I:39:ILE:O	2:I:39:ILE:HG23	2.19	0.42
2:I:314:ASN:ND2	2:I:352:ARG:HG2	2.34	0.42
2:I:361:SER:CA	2:I:364:VAL:HG22	2.48	0.42
2:I:561:ILE:CD1	2:I:661:VAL:HG12	2.50	0.42
2:I:804:PHE:O	3:J:638:SER:HB2	2.19	0.42
2:I:817:LEU:CD2	2:I:1078:LYS:HB3	2.49	0.42
2:I:871:VAL:CG1	2:I:928:VAL:HG11	2.50	0.42
2:I:1287:LEU:O	2:I:1291:LEU:HG	2.20	0.42
3:J:316:ILE:HA	3:J:317:THR:HA	1.59	0.42
3:J:374:LEU:HD23	3:J:381:ILE:CD1	2.49	0.42
3:J:839:VAL:HG12	3:J:864:LEU:HD12	2.00	0.42
3:J:1320:ILE:HG12	3:J:1342:ASP:OD2	2.19	0.42
1:M:255:ARG:HD2	1:M:256:PRO:CD	2.49	0.42
8:P:46:DG:OP2	8:P:46:DG:H2'	2.19	0.42
1:G:192:VAL:HG11	1:G:198:LEU:CD1	2.49	0.42
1:H:39:LEU:HA	1:H:39:LEU:HD23	1.71	0.42
2:I:920:VAL:HG13	2:I:921:PRO:HD2	2.01	0.42
2:I:1151:LEU:CD2	2:I:1198:LEU:HD13	2.49	0.42
3:J:185:ILE:O	3:J:189:LEU:HG	2.19	0.42
5:L:316:PHE:CE1	5:L:330:LEU:HD13	2.53	0.42
2:I:39:ILE:HG13	2:I:75:LEU:CD2	2.49	0.42
2:I:1016:GLU:N	2:I:1016:GLU:OE1	2.51	0.42
2:I:1100:PRO:HG2	3:J:637:ALA:O	2.20	0.42
3:J:287:ALA:HB1	3:J:288:PRO:HD2	2.01	0.42
3:J:357:VAL:HG13	3:J:358:GLY:N	2.34	0.42
3:J:748:ALA:HB2	3:J:754:ILE:HD13	2.00	0.42
3:J:844:THR:HA	3:J:882:VAL:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:114:GLU:HA	5:L:114:GLU:OE1	2.19	0.42
5:L:227:GLN:HE21	5:L:255:VAL:HG11	1.84	0.42
5:L:584:ARG:HG3	5:L:585:GLU:OE2	2.20	0.42
7:O:39:DG:H5''	7:O:39:DG:H8	1.84	0.42
8:P:69:DT:H2''	8:P:70:DG:C8	2.53	0.42
1:H:11:PRO:CG	1:H:28:LEU:HD11	2.49	0.42
1:H:90:VAL:HG22	1:H:123:ILE:CD1	2.50	0.42
2:I:12:ARG:CZ	2:I:1181:PRO:HB3	2.49	0.42
2:I:324:LYS:HA	2:I:327:GLN:CG	2.49	0.42
2:I:324:LYS:O	2:I:327:GLN:HG3	2.20	0.42
2:I:638:SER:HB2	2:I:645:PHE:CZ	2.55	0.42
2:I:1255:THR:O	2:I:1255:THR:OG1	2.32	0.42
3:J:949:SER:HB3	3:J:1016:THR:HG21	2.01	0.42
3:J:954:ASN:HB2	3:J:992:LYS:HZ1	1.81	0.42
3:J:1021:ASP:OD1	3:J:1023:HIS:N	2.49	0.42
3:J:1061:VAL:HG12	3:J:1076:PRO:HG3	2.01	0.42
5:L:45:ILE:HA	5:L:48:ILE:HG22	2.01	0.42
5:L:387:VAL:HG11	5:L:408:GLY:HA3	2.00	0.42
5:L:582:VAL:HG13	7:O:25:DA:H5'	2.01	0.42
1:M:262:LEU:HD13	1:M:302:GLU:OE1	2.20	0.42
1:M:284:ARG:HB2	1:M:289:LEU:HD11	2.02	0.42
1:M:307:LEU:CD2	1:M:312:LEU:HD12	2.50	0.42
8:P:53:DT:H2'	8:P:54:DT:H71	2.02	0.42
1:G:75:GLN:O	2:I:729:ALA:HB2	2.20	0.42
1:G:228:LEU:HD13	1:G:228:LEU:HA	1.91	0.42
2:I:533:LEU:HD21	2:I:571:LEU:CD1	2.50	0.42
2:I:720:ARG:NH2	2:I:749:ASP:OD1	2.53	0.42
2:I:988:LYS:O	2:I:992:LEU:HG	2.20	0.42
2:I:992:LEU:HB3	2:I:993:PRO:HD2	2.02	0.42
2:I:1211:ARG:HD3	2:I:1220:GLN:OE1	2.20	0.42
3:J:259:ARG:HD2	9:J:1504:1N7:O2	2.19	0.42
3:J:374:LEU:O	3:J:378:LYS:HG3	2.20	0.42
3:J:930:LEU:CD2	3:J:1244:GLN:HG3	2.48	0.42
3:J:1061:VAL:HG23	3:J:1103:GLY:HA2	2.02	0.42
5:L:8:GLN:OE1	5:L:11:LEU:HD13	2.20	0.42
5:L:264:LYS:H	5:L:264:LYS:HZ3	1.68	0.42
5:L:554:ARG:O	5:L:558:VAL:HG23	2.20	0.42
6:N:34:VAL:CG2	6:N:44:ILE:HD12	2.49	0.42
1:G:42:ALA:CB	1:G:224:LEU:HD11	2.48	0.42
1:H:136:GLU:HG2	1:H:137:ASN:H	1.85	0.42
2:I:498:ILE:H	2:I:498:ILE:HD12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:616:ILE:HG13	2:I:652:TYR:HB2	2.02	0.42
2:I:870:ILE:H	2:I:870:ILE:HD12	1.84	0.42
3:J:78:LEU:O	3:J:78:LEU:HD23	2.19	0.42
3:J:166:LEU:O	3:J:170:GLU:HG2	2.19	0.42
4:K:12:LYS:HA	4:K:12:LYS:HD3	1.86	0.42
1:H:67:GLU:HG3	1:H:171:LEU:HD22	2.01	0.42
2:I:53:PHE:CE1	2:I:468:LEU:HD11	2.54	0.42
2:I:83:GLN:HG3	2:I:83:GLN:H	1.73	0.42
2:I:107:ARG:NH1	2:I:108:GLU:O	2.52	0.42
3:J:424:ASN:HB2	3:J:434:ILE:HG12	2.02	0.42
3:J:910:ASN:HB2	4:K:15:ASN:OD1	2.19	0.42
5:L:227:GLN:HG2	5:L:255:VAL:HG21	2.00	0.42
5:L:313:ASP:O	5:L:317:ASN:HB2	2.20	0.42
5:L:327:SER:HA	5:L:330:LEU:CD2	2.50	0.42
5:L:457:ILE:O	5:L:460:ILE:HG12	2.20	0.42
5:L:600:HIS:NE2	1:M:259:ASP:O	2.53	0.42
1:G:54:CYS:SG	1:G:92:VAL:HG22	2.59	0.42
1:G:102:LEU:HD11	1:G:110:VAL:CG1	2.40	0.42
1:H:46:ILE:HD11	1:H:224:LEU:HD13	2.01	0.42
1:H:90:VAL:HG21	1:H:146:VAL:HG21	2.01	0.42
2:I:561:ILE:O	2:I:680:LEU:HA	2.20	0.42
2:I:1303:LYS:HB2	2:I:1303:LYS:HE3	1.57	0.42
2:I:1331:ARG:HA	2:I:1335:ILE:O	2.19	0.42
3:J:324:LEU:HD23	3:J:324:LEU:HA	1.76	0.42
3:J:337:ARG:O	3:J:342:LEU:HB2	2.20	0.42
3:J:596:LEU:HD11	3:J:604:MET:HE3	1.99	0.42
3:J:603:LYS:HE2	3:J:603:LYS:HB2	1.51	0.42
3:J:1282:TYR:HA	3:J:1285:VAL:HG13	2.02	0.42
5:L:316:PHE:CZ	5:L:337:VAL:HB	2.55	0.42
5:L:413:MET:HG3	5:L:413:MET:H	1.68	0.42
6:N:35:TYR:O	6:N:43:PRO:HA	2.19	0.42
1:G:135:ASP:HB3	1:G:138:ALA:HB2	2.02	0.41
2:I:192:ASP:HB3	2:I:346:TYR:CE1	2.55	0.41
2:I:233:ARG:HA	2:I:233:ARG:NE	2.29	0.41
2:I:299:LYS:HB2	2:I:299:LYS:HE3	1.80	0.41
2:I:560:PRO:HG3	3:J:773:PHE:CD1	2.55	0.41
2:I:562:GLU:HG3	2:I:683:ALA:HB1	2.02	0.41
2:I:590:PRO:HB2	2:I:655:VAL:HG21	2.01	0.41
2:I:616:ILE:O	2:I:636:CYS:HB3	2.19	0.41
2:I:1017:GLN:NE2	2:I:1021:LEU:HG	2.35	0.41
3:J:84:ILE:CD1	3:J:91:GLU:HB2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:111:THR:HG21	3:J:303:VAL:CG1	2.50	0.41
3:J:245:LEU:HD12	3:J:246:PRO:HD3	2.01	0.41
3:J:367:GLY:O	3:J:447:ILE:HG23	2.20	0.41
3:J:672:LEU:HD21	6:N:47:ALA:HB1	2.02	0.41
3:J:705:THR:HG22	3:J:707:ILE:CD1	2.37	0.41
3:J:1179:PRO:HB2	3:J:1182:GLY:H	1.85	0.41
5:L:102:MET:HA	5:L:105:MET:CG	2.50	0.41
5:L:347:ILE:HA	5:L:350:GLU:OE1	2.19	0.41
1:H:118:ASP:N	1:H:118:ASP:OD1	2.53	0.41
1:H:188:GLU:HB2	1:H:200:LYS:HB3	2.02	0.41
2:I:49:LEU:HD23	2:I:49:LEU:HA	1.87	0.41
2:I:130:MET:CG	2:I:134:GLY:HA2	2.50	0.41
2:I:153:PRO:HG2	2:I:400:VAL:HG12	2.01	0.41
2:I:155:VAL:HA	2:I:175:ARG:O	2.20	0.41
2:I:156:PHE:CE2	2:I:177:ILE:HD12	2.56	0.41
2:I:192:ASP:HB3	2:I:346:TYR:HD1	1.86	0.41
2:I:406:ASN:ND2	2:I:413:GLU:O	2.31	0.41
2:I:496:LYS:O	2:I:500:ALA:HB2	2.20	0.41
2:I:1124:ILE:HD11	2:I:1198:LEU:HD12	2.02	0.41
2:I:1131:MET:CE	2:I:1141:LEU:HA	2.50	0.41
2:I:1255:THR:O	2:I:1257:GLN:N	2.54	0.41
2:I:1268:GLN:HG3	3:J:467:ALA:HB1	2.00	0.41
3:J:117:LEU:HD23	3:J:117:LEU:HA	1.71	0.41
3:J:224:LEU:HA	3:J:224:LEU:HD23	1.73	0.41
3:J:1266:ILE:HD13	3:J:1266:ILE:HA	1.87	0.41
5:L:341:LEU:O	5:L:344:LEU:HB2	2.20	0.41
5:L:466:ILE:HG21	5:L:487:MET:SD	2.60	0.41
1:M:268:ASN:HA	1:M:271:LYS:NZ	2.35	0.41
8:P:47:DC:H2''	8:P:48:DC:C6	2.56	0.41
1:G:47:LEU:O	1:G:180:VAL:HG21	2.19	0.41
1:G:57:THR:HB	1:G:147:GLN:HE21	1.84	0.41
1:H:24:ALA:N	1:H:213:PRO:HG2	2.35	0.41
1:H:61:ILE:HD13	1:H:142:MET:CB	2.39	0.41
2:I:296:VAL:HG21	2:I:352:ARG:HH22	1.85	0.41
2:I:974:ARG:HD3	2:I:1014:LEU:HD11	2.02	0.41
3:J:24:LEU:HB2	3:J:232:ASN:OD1	2.19	0.41
3:J:35:PHE:CD2	3:J:101:ARG:HG2	2.56	0.41
3:J:203:GLU:HA	3:J:207:GLU:OE1	2.20	0.41
3:J:260:PHE:O	5:L:504:PRO:HA	2.19	0.41
3:J:410:ASP:O	3:J:414:GLU:HG3	2.20	0.41
3:J:510:LEU:HD23	3:J:513:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:738:ARG:O	3:J:742:GLY:N	2.50	0.41
3:J:911:LYS:HB2	3:J:911:LYS:HE3	1.80	0.41
3:J:1121:LEU:O	3:J:1123:ARG:NH1	2.53	0.41
3:J:1192:LYS:HB2	3:J:1192:LYS:HE2	1.84	0.41
5:L:470:MET:SD	5:L:483:LEU:HD12	2.60	0.41
1:M:313:SER:HB3	1:M:316:MET:CE	2.50	0.41
7:O:36:DA:H2''	7:O:37:DA:O5'	2.19	0.41
1:G:47:LEU:HD12	1:G:183:ILE:HG21	2.01	0.41
2:I:53:PHE:HE1	2:I:468:LEU:HD21	1.85	0.41
2:I:173:ASN:CB	2:I:187:GLU:HG3	2.51	0.41
2:I:463:GLN:HG3	2:I:505:PHE:HB2	2.02	0.41
2:I:839:VAL:HG21	2:I:841:ARG:NH1	2.35	0.41
2:I:1225:VAL:HA	3:J:638:SER:HB3	2.01	0.41
3:J:62:PHE:CD1	3:J:247:PRO:HD3	2.54	0.41
3:J:245:LEU:HD12	3:J:246:PRO:CD	2.50	0.41
3:J:878:ASP:OD2	3:J:991:THR:HG22	2.21	0.41
3:J:1155:ILE:H	3:J:1155:ILE:HG13	1.68	0.41
3:J:1311:LYS:HG2	3:J:1311:LYS:O	2.21	0.41
5:L:298:PRO:HG2	5:L:326:TRP:CD1	2.55	0.41
1:H:91:ARG:HD2	1:H:124:VAL:HG12	2.03	0.41
2:I:76:GLY:O	2:I:94:ALA:HB1	2.21	0.41
2:I:270:THR:HG22	6:N:42:ASN:ND2	2.35	0.41
2:I:311:CYS:SG	2:I:315:MET:HB3	2.60	0.41
2:I:544:GLY:O	2:I:548:ARG:HG2	2.20	0.41
2:I:551:HIS:CG	2:I:552:PRO:HD2	2.55	0.41
2:I:741:MET:SD	2:I:974:ARG:NH2	2.91	0.41
2:I:832:HIS:HB2	2:I:1056:VAL:HG23	2.02	0.41
2:I:1248:THR:HG21	2:I:1305:TYR:CD1	2.56	0.41
2:I:1291:LEU:HD21	3:J:1351:VAL:HG13	2.02	0.41
2:I:1298:VAL:HB	2:I:1321:GLU:CD	2.41	0.41
2:I:1332:SER:HB2	3:J:245:LEU:HD13	2.02	0.41
3:J:294:ASN:ND2	5:L:406:GLN:HE21	2.17	0.41
3:J:672:LEU:O	6:N:48:ARG:HG3	2.20	0.41
3:J:694:SER:O	3:J:697:MET:HG3	2.20	0.41
3:J:1104:LYS:HD2	3:J:1104:LYS:HA	1.61	0.41
3:J:1172:LYS:HB2	3:J:1189:MET:CG	2.51	0.41
3:J:1177:ILE:O	3:J:1186:TYR:HB3	2.21	0.41
5:L:149:ASP:OD1	5:L:149:ASP:N	2.52	0.41
5:L:399:LEU:HD22	5:L:443:ILE:HA	2.02	0.41
5:L:401:PHE:O	5:L:405:ILE:HG13	2.20	0.41
7:O:26:DT:H2'	7:O:27:DT:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:THR:CB	1:G:147:GLN:HE21	2.34	0.41
1:H:215:GLU:HA	1:H:218:ARG:CG	2.50	0.41
2:I:83:GLN:O	2:I:87:ILE:HD13	2.21	0.41
2:I:135:THR:HG21	2:I:142:GLU:OE2	2.21	0.41
2:I:702:THR:O	2:I:702:THR:OG1	2.39	0.41
2:I:1223:ARG:NH1	2:I:1223:ARG:HB3	2.36	0.41
3:J:550:VAL:HG22	3:J:572:THR:CG2	2.51	0.41
3:J:1115:ILE:HD12	3:J:1115:ILE:O	2.20	0.41
3:J:1145:PHE:CE1	3:J:1253:ILE:HG23	2.55	0.41
3:J:1218:HIS:CD2	3:J:1218:HIS:H	2.39	0.41
5:L:52:GLY:HA2	5:L:53:ILE:C	2.40	0.41
5:L:354:THR:HB	5:L:356:GLU:OE2	2.21	0.41
5:L:412:LEU:HB2	5:L:435:ILE:HD11	2.02	0.41
1:M:284:ARG:CB	1:M:289:LEU:HG	2.51	0.41
8:P:38:DC:OP1	8:P:38:DC:H3'	2.20	0.41
8:P:39:DC:C2'	8:P:40:DC:H5'	2.48	0.41
8:P:66:DT:H2''	8:P:67:DT:C6	2.55	0.41
1:G:180:VAL:HA	1:G:207:THR:HA	2.03	0.41
1:H:69:SER:HB2	1:H:78:ILE:HD12	2.01	0.41
1:H:95:LYS:CG	1:H:98:VAL:HG22	2.51	0.41
2:I:296:VAL:HA	2:I:316:GLU:HA	2.02	0.41
2:I:998:LEU:HG	2:I:1015:ALA:CA	2.45	0.41
2:I:1042:LEU:HD13	2:I:1049:ILE:HG13	2.02	0.41
2:I:1101:LEU:HD23	3:J:725:MET:SD	2.60	0.41
2:I:1302:THR:O	2:I:1306:LYS:HG3	2.20	0.41
3:J:506:VAL:HG11	3:J:625:MET:HA	2.01	0.41
3:J:572:THR:OG1	3:J:576:ARG:HB2	2.21	0.41
3:J:1151:LYS:O	3:J:1153:PRO:HD3	2.21	0.41
5:L:430:TYR:O	5:L:433:TRP:HB3	2.21	0.41
5:L:456:MET:HE1	5:L:497:VAL:HG22	2.01	0.41
1:M:253:LEU:CD2	1:M:312:LEU:HD13	2.50	0.41
8:P:41:DT:H2''	8:P:42:DT:C6	2.55	0.41
1:G:98:VAL:HG11	1:G:121:VAL:HG22	2.03	0.41
1:G:134:THR:HB	2:I:773:LEU:HD12	2.02	0.41
1:H:12:ARG:CG	1:H:13:LEU:HD23	2.51	0.41
2:I:101:ARG:HA	2:I:118:LYS:O	2.20	0.41
2:I:149:LEU:HD21	2:I:451:ARG:CZ	2.50	0.41
2:I:346:TYR:HE2	2:I:437:ASN:HD21	1.68	0.41
2:I:816:ILE:HG22	2:I:1096:ILE:HG23	2.03	0.41
2:I:1262:LYS:HB2	2:I:1265:PHE:HB2	2.02	0.41
3:J:454:CYS:HG	3:J:461:PHE:HZ	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:858:VAL:HG22	3:J:868:TRP:HE3	1.85	0.41
3:J:923:ILE:HA	3:J:1248:ILE:HD12	2.02	0.41
3:J:1046:ILE:HG21	3:J:1059:LEU:HD13	2.02	0.41
5:L:151:VAL:HG13	5:L:157:ARG:O	2.20	0.41
5:L:163:THR:HG21	5:L:263:PRO:HD3	2.02	0.41
1:G:79:LEU:O	1:G:83:LEU:HG	2.21	0.41
2:I:5:TYR:HB3	2:I:778:GLU:OE1	2.20	0.41
2:I:13:LYS:O	2:I:13:LYS:HG3	2.20	0.41
2:I:199:ASP:O	2:I:200:ARG:HD3	2.21	0.41
2:I:297:VAL:HG22	2:I:298:ALA:H	1.86	0.41
2:I:410:LEU:HD23	2:I:410:LEU:HA	1.82	0.41
2:I:467:GLY:O	2:I:471:VAL:HG22	2.21	0.41
2:I:598:VAL:HG12	2:I:628:HIS:CD2	2.56	0.41
2:I:685:MET:HE3	2:I:1067:ALA:HB1	2.02	0.41
2:I:854:ILE:HD12	2:I:862:LEU:HD21	2.02	0.41
2:I:901:LEU:O	2:I:905:ILE:HG13	2.21	0.41
2:I:998:LEU:HG	2:I:1015:ALA:CB	2.51	0.41
2:I:1106:ARG:O	2:I:1108:ASN:N	2.53	0.41
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.85	0.41
3:J:34:SER:HA	3:J:102:MET:O	2.21	0.41
3:J:253:VAL:HG21	5:L:523:ILE:CD1	2.49	0.41
3:J:364:HIS:HB3	3:J:487:THR:HG23	2.02	0.41
3:J:806:ASP:N	3:J:806:ASP:OD1	2.54	0.41
3:J:1032:SER:OG	3:J:1116:SER:HA	2.21	0.41
3:J:1109:LEU:HD23	3:J:1109:LEU:HA	1.88	0.41
3:J:1198:VAL:HG11	3:J:1210:ILE:HG23	2.03	0.41
3:J:1220:ILE:CG2	3:J:1228:ALA:HB1	2.51	0.41
5:L:7:SER:CB	5:L:88:GLU:HG3	2.50	0.41
5:L:148:TYR:CE1	5:L:152:GLU:HG3	2.56	0.41
5:L:162:ILE:HA	5:L:261:LEU:HA	2.02	0.41
5:L:478:PRO:HB3	5:L:483:LEU:HD11	2.02	0.41
5:L:490:PRO:HD2	5:L:493:LYS:CG	2.50	0.41
1:M:257:VAL:CG1	1:M:275:ILE:HG22	2.51	0.41
6:N:33:PRO:HB2	6:N:35:TYR:CE2	2.55	0.41
6:N:36:LEU:HA	6:N:42:ASN:O	2.20	0.41
6:N:48:ARG:HH11	6:N:48:ARG:HG3	1.86	0.41
2:I:98:VAL:HG21	2:I:124:MET:SD	2.61	0.41
2:I:178:PRO:HG3	2:I:395:TYR:CZ	2.56	0.41
2:I:607:SER:HB3	2:I:610:GLU:OE2	2.21	0.41
2:I:757:THR:HG23	2:I:765:ILE:HB	2.02	0.41
2:I:841:ARG:H	2:I:841:ARG:HG2	1.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:975:ILE:CD1	2:I:998:LEU:HD12	2.51	0.41
2:I:1243:MET:HE3	3:J:445:LYS:HD2	2.03	0.41
3:J:270:ARG:O	3:J:274:ASN:ND2	2.54	0.41
3:J:300:GLN:NE2	3:J:304:ASP:OD1	2.54	0.41
3:J:487:THR:OG1	4:K:4:VAL:O	2.28	0.41
3:J:826:ILE:O	3:J:826:ILE:HG23	2.21	0.41
3:J:1029:THR:HA	3:J:1099:TYR:CE2	2.56	0.41
3:J:1036:ARG:NH2	3:J:1079:LYS:HG3	2.36	0.41
1:G:162:GLU:CD	1:G:165:GLU:HB3	2.41	0.40
1:H:193:GLU:H	1:H:193:GLU:HG3	1.58	0.40
2:I:561:ILE:HD11	2:I:665:ALA:HB1	2.03	0.40
2:I:715:THR:HG21	2:I:782:VAL:CG1	2.51	0.40
2:I:717:VAL:HG12	2:I:782:VAL:HG12	2.03	0.40
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.51	0.40
2:I:1075:VAL:HG11	3:J:463:GLY:HA2	2.02	0.40
3:J:393:THR:HG22	5:L:609:SER:OG	2.21	0.40
3:J:845:ALA:HB3	3:J:881:LYS:HD3	2.03	0.40
3:J:1158:GLU:H	3:J:1158:GLU:HG2	1.54	0.40
4:K:6:VAL:O	4:K:6:VAL:HG23	2.21	0.40
5:L:17:LYS:HB3	5:L:17:LYS:HE2	1.92	0.40
5:L:224:LEU:HD21	5:L:256:PHE:CD1	2.57	0.40
5:L:327:SER:HA	5:L:330:LEU:HD23	2.03	0.40
5:L:390:ILE:HD11	5:L:436:ARG:NH2	2.37	0.40
8:P:47:DC:H4'	8:P:48:DC:OP1	2.21	0.40
1:G:58:GLU:OE1	1:G:145:LYS:HD2	2.20	0.40
1:H:21:SER:OG	1:H:22:THR:HG23	2.21	0.40
2:I:561:ILE:HD11	2:I:665:ALA:CB	2.51	0.40
2:I:724:VAL:HG23	2:I:777:VAL:HG13	2.03	0.40
2:I:738:GLU:HA	2:I:741:MET:HE2	2.03	0.40
2:I:1322:SER:CB	3:J:342:LEU:HD12	2.50	0.40
3:J:230:SER:OG	3:J:231:GLY:N	2.54	0.40
3:J:510:LEU:CD1	3:J:601:ILE:HD11	2.51	0.40
3:J:1033:GLY:O	3:J:1115:ILE:HG13	2.21	0.40
4:K:27:ALA:HB1	4:K:46:THR:HB	2.03	0.40
1:M:251:PRO:HA	1:M:254:LEU:HG	2.03	0.40
2:I:170:VAL:HG12	2:I:171:LEU:O	2.20	0.40
2:I:347:ILE:CA	2:I:350:THR:HG22	2.49	0.40
2:I:400:VAL:HG22	2:I:584:TYR:HB3	2.03	0.40
2:I:615:VAL:HB	2:I:650:VAL:HA	2.02	0.40
2:I:885:GLY:HA2	2:I:917:SER:CB	2.51	0.40
3:J:53:ARG:HB3	3:J:54:ASP:C	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:105:ILE:HG13	3:J:244:VAL:CG1	2.52	0.40
3:J:300:GLN:HG3	3:J:312:ARG:HH12	1.86	0.40
3:J:733:SER:O	3:J:737:ILE:HG12	2.22	0.40
3:J:809:VAL:HG11	3:J:909:ILE:HG23	2.02	0.40
3:J:1025:MET:HB3	3:J:1124:ILE:CB	2.27	0.40
3:J:1038:THR:HB	3:J:1079:LYS:HG2	2.03	0.40
4:K:15:ASN:HB3	4:K:18:ASP:H	1.86	0.40
5:L:11:LEU:HA	5:L:14:THR:HG22	2.03	0.40
5:L:165:PHE:HE1	5:L:260:ARG:H	1.69	0.40
5:L:354:THR:O	5:L:358:VAL:HG22	2.21	0.40
5:L:426:LYS:HB2	5:L:426:LYS:HE2	1.84	0.40
7:O:37:DA:H2''	7:O:38:DG:O5'	2.21	0.40
1:H:90:VAL:HG22	1:H:123:ILE:HD13	2.03	0.40
2:I:27:LEU:HD13	2:I:524:ILE:CD1	2.48	0.40
2:I:179:TYR:HB3	2:I:396:ASP:O	2.21	0.40
2:I:629:PHE:O	2:I:647:ARG:HD2	2.21	0.40
2:I:896:THR:HB	2:I:897:PRO:CD	2.52	0.40
2:I:1225:VAL:HG12	3:J:638:SER:HB3	2.04	0.40
3:J:62:PHE:O	3:J:98:ARG:HA	2.22	0.40
3:J:72:CYS:SG	3:J:73:GLY:N	2.93	0.40
3:J:137:ARG:HG3	3:J:142:GLU:CB	2.51	0.40
3:J:515:ARG:C	3:J:545:HIS:HB3	2.42	0.40
3:J:605:LEU:HA	3:J:605:LEU:HD23	1.90	0.40
3:J:707:ILE:O	3:J:713:GLU:HA	2.22	0.40
3:J:982:LEU:HB2	3:J:997:VAL:CG2	2.49	0.40
3:J:1042:ASP:OD2	3:J:1046:ILE:HG13	2.22	0.40
3:J:1280:VAL:HG13	3:J:1285:VAL:HG12	2.03	0.40
5:L:277:MET:CE	5:L:281:ARG:HH22	2.35	0.40
1:M:255:ARG:HD3	1:M:255:ARG:HA	1.73	0.40
7:O:21:DA:H2''	7:O:22:DT:H71	2.04	0.40
1:G:217:ILE:HG13	1:G:218:ARG:N	2.35	0.40
2:I:43:PRO:O	2:I:44:GLU:HG3	2.22	0.40
2:I:230:PHE:HD1	2:I:239:MET:HA	1.86	0.40
2:I:277:LEU:HD22	2:I:282:VAL:HB	2.04	0.40
2:I:533:LEU:HD21	2:I:571:LEU:HD13	2.03	0.40
2:I:578:TYR:HD2	2:I:659:GLN:HG3	1.87	0.40
2:I:606:LEU:HD21	2:I:652:TYR:CE2	2.57	0.40
2:I:849:GLU:HB3	2:I:851:THR:HG23	2.03	0.40
2:I:1096:ILE:HD12	2:I:1232:MET:SD	2.61	0.40
2:I:1305:TYR:CG	5:L:531:PRO:HB2	2.56	0.40
3:J:265:LEU:HD23	3:J:265:LEU:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:393:THR:OG1	3:J:394:ILE:N	2.54	0.40
3:J:505:ASP:HB2	3:J:629:PHE:HE1	1.85	0.40
3:J:555:TYR:HB3	3:J:563:LEU:HB3	2.03	0.40
3:J:904:ALA:O	3:J:906:GLY:N	2.55	0.40
5:L:479:THR:OG1	5:L:480:PRO:HD2	2.21	0.40
5:L:511:ILE:HD11	9:L:701:1N7:C10	2.51	0.40
7:O:35:DG:H2''	7:O:36:DA:H8	1.87	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	G	228/329 (69%)	205 (90%)	23 (10%)	0	100	100
1	H	215/329 (65%)	189 (88%)	26 (12%)	0	100	100
1	M	71/329 (22%)	68 (96%)	3 (4%)	0	100	100
2	I	1338/1342 (100%)	1179 (88%)	157 (12%)	2 (0%)	51	82
3	J	1339/1430 (94%)	1197 (89%)	141 (10%)	1 (0%)	51	82
4	K	73/91 (80%)	68 (93%)	5 (7%)	0	100	100
5	L	540/616 (88%)	500 (93%)	40 (7%)	0	100	100
6	N	70/72 (97%)	65 (93%)	5 (7%)	0	100	100
All	All	3874/4538 (85%)	3471 (90%)	400 (10%)	3 (0%)	54	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	898	GLU
3	J	854	ALA
2	I	897	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	G	195/286 (68%)	177 (91%)	18 (9%)	9	31
1	H	184/286 (64%)	171 (93%)	13 (7%)	14	44
1	M	65/286 (23%)	62 (95%)	3 (5%)	27	57
2	I	1153/1157 (100%)	1043 (90%)	110 (10%)	8	29
3	J	1128/1189 (95%)	1036 (92%)	92 (8%)	11	37
4	K	65/75 (87%)	59 (91%)	6 (9%)	9	31
5	L	479/543 (88%)	456 (95%)	23 (5%)	25	56
6	N	60/61 (98%)	53 (88%)	7 (12%)	5	20
All	All	3329/3883 (86%)	3057 (92%)	272 (8%)	15	37

All (272) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	18	GLN
1	G	33	ARG
1	G	54	CYS
1	G	56	VAL
1	G	70	THR
1	G	74	VAL
1	G	116	THR
1	G	157	THR
1	G	160	HIS
1	G	166	ARG
1	G	177	TYR
1	G	181	GLU
1	G	182	ARG
1	G	200	LYS
1	G	217	ILE
1	G	224	LEU
1	G	231	PHE
1	G	232	VAL
1	H	6	THR

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Mol	Chain	Res	Type
1	H	15	ASP
1	H	16	ILE
1	H	27	THR
1	H	33	ARG
1	H	38	THR
1	H	45	ARG
1	H	83	LEU
1	H	132	HIS
1	H	193	GLU
1	H	196	THR
1	H	210	THR
1	H	212	ASP
2	I	6	THR
2	I	55	SER
2	I	56	VAL
2	I	60	GLN
2	I	62	TYR
2	I	66	SER
2	I	75	LEU
2	I	91	THR
2	I	104	ILE
2	I	105	TYR
2	I	107	ARG
2	I	138	ILE
2	I	147	SER
2	I	149	LEU
2	I	158	ASP
2	I	159	SER
2	I	161	LYS
2	I	185	ASP
2	I	189	ASP
2	I	194	LEU
2	I	199	ASP
2	I	202	ARG
2	I	233	ARG
2	I	250	THR
2	I	277	LEU
2	I	301	TYR
2	I	320	ASP
2	I	321	LEU
2	I	322	LEU
2	I	367	TYR

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Mol	Chain	Res	Type
2	I	392	GLU
2	I	393	ASP
2	I	397	LEU
2	I	443	ASP
2	I	447	HIS
2	I	461	GLU
2	I	472	GLU
2	I	475	VAL
2	I	478	ARG
2	I	493	ILE
2	I	494	ASN
2	I	508	SER
2	I	514	PHE
2	I	521	LEU
2	I	524	ILE
2	I	525	THR
2	I	542	ARG
2	I	550	VAL
2	I	561	ILE
2	I	573	ASN
2	I	604	HIS
2	I	630	VAL
2	I	653	MET
2	I	692	THR
2	I	699	LEU
2	I	702	THR
2	I	711	ASP
2	I	731	ARG
2	I	750	ILE
2	I	757	THR
2	I	759	SER
2	I	766	ASN
2	I	789	THR
2	I	799	ASN
2	I	800	MET
2	I	807	TRP
2	I	815	SER
2	I	816	ILE
2	I	819	SER
2	I	821	ARG
2	I	826	ASP
2	I	827	ARG

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Mol	Chain	Res	Type
2	I	841	ARG
2	I	857	VAL
2	I	878	THR
2	I	888	THR
2	I	890	LYS
2	I	895	LEU
2	I	902	LEU
2	I	944	ARG
2	I	951	MET
2	I	958	LYS
2	I	990	ASP
2	I	996	ARG
2	I	1002	LEU
2	I	1003	THR
2	I	1016	GLU
2	I	1054	LEU
2	I	1056	VAL
2	I	1073	LYS
2	I	1076	ILE
2	I	1092	THR
2	I	1106	ARG
2	I	1107	MET
2	I	1109	ILE
2	I	1117	LEU
2	I	1149	TYR
2	I	1156	ARG
2	I	1163	THR
2	I	1167	GLU
2	I	1186	VAL
2	I	1211	ARG
2	I	1222	GLU
2	I	1235	LEU
2	I	1253	LEU
2	I	1265	PHE
2	I	1269	ARG
2	I	1287	LEU
2	I	1296	ASP
2	I	1301	ARG
3	J	24	LEU
3	J	53	ARG
3	J	54	ASP
3	J	77	ARG

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Mol	Chain	Res	Type
3	J	88	CYS
3	J	126	LEU
3	J	128	LEU
3	J	129	ASP
3	J	154	LEU
3	J	159	ILE
3	J	161	THR
3	J	163	GLU
3	J	176	PHE
3	J	192	MET
3	J	227	PHE
3	J	230	SER
3	J	240	THR
3	J	252	LEU
3	J	253	VAL
3	J	255	LEU
3	J	299	LEU
3	J	314	ARG
3	J	317	THR
3	J	320	ASN
3	J	353	SER
3	J	374	LEU
3	J	384	LYS
3	J	403	ARG
3	J	416	ILE
3	J	428	THR
3	J	429	LEU
3	J	430	HIS
3	J	431	ARG
3	J	442	ILE
3	J	474	LEU
3	J	478	LEU
3	J	486	SER
3	J	490	ILE
3	J	514	THR
3	J	515	ARG
3	J	526	VAL
3	J	545	HIS
3	J	548	VAL
3	J	567	THR
3	J	569	LEU
3	J	582	ILE

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Mol	Chain	Res	Type
3	J	596	LEU
3	J	601	ILE
3	J	610	ARG
3	J	622	ASP
3	J	635	SER
3	J	638	SER
3	J	644	MET
3	J	655	SER
3	J	674	THR
3	J	708	ASN
3	J	712	GLN
3	J	720	ASN
3	J	740	LEU
3	J	746	LEU
3	J	762	ASN
3	J	770	LEU
3	J	786	THR
3	J	806	ASP
3	J	837	ASP
3	J	875	ASN
3	J	882	VAL
3	J	884	SER
3	J	890	THR
3	J	895	CYS
3	J	902	ASP
3	J	903	LEU
3	J	907	HIS
3	J	922	SER
3	J	985	ILE
3	J	1068	THR
3	J	1072	LYS
3	J	1158	GLU
3	J	1168	GLU
3	J	1172	LYS
3	J	1206	ARG
3	J	1223	LEU
3	J	1258	ARG
3	J	1261	LEU
3	J	1268	ASN
3	J	1285	VAL
3	J	1304	ARG
3	J	1306	LEU

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Mol	Chain	Res	Type
3	J	1330	ARG
3	J	1344	LEU
3	J	1349	GLU
3	J	1372	ARG
4	K	18	ASP
4	K	39	VAL
4	K	48	VAL
4	K	56	GLU
4	K	64	LEU
4	K	67	ARG
5	L	53	ILE
5	L	69	GLU
5	L	88	GLU
5	L	118	ASP
5	L	155	GLU
5	L	250	LEU
5	L	252	LEU
5	L	291	CYS
5	L	307	THR
5	L	315	TRP
5	L	339	ARG
5	L	342	GLN
5	L	362	ASN
5	L	402	LEU
5	L	437	GLN
5	L	449	THR
5	L	450	ILE
5	L	471	LEU
5	L	476	ARG
5	L	519	LEU
5	L	572	THR
5	L	604	SER
5	L	613	ASP
1	M	265	ARG
1	M	285	THR
1	M	317	ARG
6	N	15	LEU
6	N	27	ILE
6	N	34	VAL
6	N	48	ARG
6	N	55	VAL
6	N	58	CYS

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Mol	Chain	Res	Type
6	N	72	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	23	HIS
1	G	147	GLN
1	H	84	ASN
2	I	31	GLN
2	I	69	GLN
2	I	120	GLN
2	I	258	ASN
2	I	437	ASN
2	I	513	GLN
2	I	618	GLN
2	I	659	GLN
2	I	686	GLN
2	I	1009	ASN
2	I	1061	GLN
2	I	1116	HIS
2	I	1244	HIS
2	I	1257	GLN
2	I	1268	GLN
3	J	276	ASN
3	J	294	ASN
3	J	320	ASN
3	J	340	GLN
3	J	465	GLN
3	J	477	GLN
3	J	489	ASN
3	J	680	ASN
3	J	700	ASN
3	J	777	HIS
3	J	1108	GLN
3	J	1114	GLN
3	J	1235	ASN
3	J	1279	GLN
4	K	7	GLN
4	K	31	GLN
5	L	40	GLN
5	L	129	GLN
5	L	227	GLN

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Mol	Chain	Res	Type
5	L	258	GLN
5	L	342	GLN
5	L	362	ASN
5	L	437	GLN
5	L	464	ASN
1	M	268	ASN
1	M	276	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	1N7	J	1505	-	30,30,46	4.80	14 (46%)	47,48,72	2.11	15 (31%)
9	1N7	L	701	-	30,30,46	4.86	15 (50%)	47,48,72	2.48	20 (42%)
9	1N7	I	1401	-	30,30,46	4.93	16 (53%)	47,48,72	2.08	10 (21%)
9	1N7	J	1504	-	30,30,46	5.06	16 (53%)	47,48,72	2.39	17 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	1N7	J	1505	-	-	0/7/72/92	0/4/4/4
9	1N7	L	701	-	-	5/7/72/92	0/4/4/4
9	1N7	I	1401	-	-	5/7/72/92	0/4/4/4
9	1N7	J	1504	-	-	7/7/72/92	0/4/4/4

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	1504	1N7	C3-C19	18.21	1.84	1.53
9	I	1401	1N7	C3-C19	17.49	1.82	1.53
9	L	701	1N7	C3-C19	17.01	1.82	1.53
9	J	1505	1N7	C3-C19	16.93	1.81	1.53
9	J	1504	1N7	C3-C4	11.93	1.73	1.53
9	I	1401	1N7	C3-C4	11.66	1.73	1.53
9	J	1505	1N7	C3-C4	11.22	1.72	1.53
9	L	701	1N7	C3-C4	10.90	1.71	1.53
9	L	701	1N7	C5-C4	-9.30	1.40	1.54
9	J	1504	1N7	C5-C4	-9.21	1.40	1.54
9	I	1401	1N7	C5-C4	-9.05	1.40	1.54
9	J	1505	1N7	C5-C4	-8.54	1.41	1.54
9	J	1505	1N7	C2-C19	-7.57	1.42	1.56
9	L	701	1N7	C2-C19	-7.31	1.42	1.56
9	J	1504	1N7	C2-C19	-7.14	1.43	1.56
9	I	1401	1N7	C2-C19	-7.11	1.43	1.56
9	L	701	1N7	C8-C7	6.40	1.71	1.54
9	J	1505	1N7	C8-C7	5.99	1.70	1.54
9	J	1504	1N7	C8-C7	5.84	1.70	1.54
9	I	1401	1N7	C8-C7	5.78	1.69	1.54
9	J	1505	1N7	C5-C9	4.32	1.62	1.55
9	L	701	1N7	O4-C4	-4.32	1.36	1.43
9	J	1504	1N7	O4-C4	-4.26	1.36	1.43
9	J	1505	1N7	O4-C4	-4.20	1.36	1.43
9	I	1401	1N7	O4-C4	-4.03	1.36	1.43
9	L	701	1N7	C5-C9	3.91	1.62	1.55
9	J	1504	1N7	C5-C6	-3.83	1.49	1.55
9	I	1401	1N7	C5-C6	-3.76	1.49	1.55
9	L	701	1N7	C5-C6	-3.68	1.49	1.55
9	L	701	1N7	C7-C6	3.67	1.62	1.54
9	I	1401	1N7	C5-C9	3.63	1.61	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	1504	1N7	C2-C15	3.56	1.61	1.55
9	I	1401	1N7	C7-C6	3.51	1.61	1.54
9	I	1401	1N7	C18-C6	-3.46	1.47	1.53
9	J	1505	1N7	C5-C6	-3.46	1.49	1.55
9	J	1504	1N7	C5-C9	3.44	1.61	1.55
9	J	1504	1N7	C7-C6	3.39	1.61	1.54
9	J	1504	1N7	C10-C5	3.25	1.59	1.54
9	J	1505	1N7	C18-C6	-3.08	1.47	1.53
9	L	701	1N7	C14-C15	-3.05	1.48	1.53
9	I	1401	1N7	C14-C15	-3.01	1.49	1.53
9	L	701	1N7	C2-C15	3.01	1.60	1.55
9	J	1504	1N7	C18-C6	-3.00	1.48	1.53
9	J	1505	1N7	C14-C15	-2.92	1.49	1.53
9	I	1401	1N7	C2-C15	2.89	1.60	1.55
9	L	701	1N7	C18-C6	-2.85	1.48	1.53
9	J	1505	1N7	C7-C6	2.77	1.60	1.54
9	J	1505	1N7	C2-C15	2.76	1.59	1.55
9	L	701	1N7	C10-C5	2.71	1.58	1.54
9	I	1401	1N7	C10-C5	2.59	1.58	1.54
9	J	1504	1N7	C14-C15	-2.50	1.49	1.53
9	I	1401	1N7	C1-C2	2.50	1.58	1.54
9	J	1504	1N7	C1-C2	2.32	1.58	1.54
9	J	1505	1N7	O2-C13	-2.31	1.36	1.43
9	J	1504	1N7	C14-C13	2.23	1.56	1.51
9	J	1505	1N7	C10-C5	2.13	1.57	1.54
9	I	1401	1N7	O2-C13	-2.13	1.37	1.43
9	J	1504	1N7	O2-C13	-2.13	1.37	1.43
9	L	701	1N7	C1-C2	2.13	1.58	1.54
9	I	1401	1N7	C14-C13	2.12	1.55	1.51
9	L	701	1N7	O2-C13	-2.11	1.37	1.43

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	701	1N7	C9-C5-C4	-7.75	110.59	117.67
9	J	1504	1N7	C9-C5-C4	-7.62	110.71	117.67
9	I	1401	1N7	C9-C5-C4	-6.66	111.58	117.67
9	L	701	1N7	C3-C19-C18	-6.35	101.58	110.88
9	J	1505	1N7	C19-C3-C4	-4.95	107.77	114.30
9	J	1504	1N7	C19-C18-C17	-4.74	106.21	111.88
9	L	701	1N7	C2-C19-C18	4.74	116.90	111.82
9	J	1505	1N7	C9-C5-C4	-4.63	113.44	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	1505	1N7	C7-C6-C18	-4.63	111.86	118.33
9	J	1504	1N7	C14-C13-C12	-4.60	105.06	110.55
9	I	1401	1N7	C6-C5-C4	4.59	111.68	107.40
9	J	1504	1N7	C7-C6-C18	-4.55	111.97	118.33
9	L	701	1N7	C6-C5-C4	4.48	111.58	107.40
9	I	1401	1N7	C19-C18-C17	-4.21	106.84	111.88
9	J	1505	1N7	C3-C19-C18	-4.15	104.80	110.88
9	J	1504	1N7	C21-C20-C22	-4.12	103.90	110.36
9	J	1505	1N7	C2-C19-C18	4.04	116.16	111.82
9	I	1401	1N7	C7-C6-C18	-4.03	112.70	118.33
9	I	1401	1N7	C21-C20-C9	-3.98	106.83	112.92
9	J	1505	1N7	C6-C5-C4	3.76	110.91	107.40
9	I	1401	1N7	C19-C3-C4	-3.57	109.59	114.30
9	L	701	1N7	C14-C13-C12	-3.49	106.38	110.55
9	J	1504	1N7	C6-C5-C4	3.49	110.65	107.40
9	L	701	1N7	C16-C15-C2	-3.49	108.95	112.66
9	L	701	1N7	C19-C3-C4	-3.47	109.72	114.30
9	J	1504	1N7	C22-C20-C9	3.35	117.20	110.28
9	L	701	1N7	C21-C20-C22	-3.33	105.15	110.36
9	J	1504	1N7	C16-C15-C14	-3.29	107.40	111.19
9	J	1504	1N7	C16-C17-C18	-3.26	108.00	111.48
9	J	1504	1N7	C1-C12-C13	-3.15	106.42	110.47
9	J	1505	1N7	C21-C20-C22	-3.07	105.55	110.36
9	J	1505	1N7	C16-C15-C2	-3.04	109.43	112.66
9	L	701	1N7	C5-C6-C18	2.99	118.56	114.74
9	J	1504	1N7	C5-C9-C20	-2.94	115.99	119.50
9	L	701	1N7	C1-C12-C13	-2.90	106.75	110.47
9	J	1505	1N7	C5-C6-C18	2.88	118.42	114.74
9	L	701	1N7	C7-C6-C18	-2.86	114.33	118.33
9	I	1401	1N7	C1-C12-C13	-2.86	106.80	110.47
9	J	1505	1N7	C11-C2-C1	-2.83	103.70	108.26
9	I	1401	1N7	C16-C15-C14	-2.79	107.98	111.19
9	I	1401	1N7	C2-C19-C18	2.72	114.74	111.82
9	J	1505	1N7	C16-C17-C18	2.68	114.34	111.48
9	J	1505	1N7	C9-C5-C6	2.65	102.76	100.09
9	L	701	1N7	C9-C5-C6	2.58	102.69	100.09
9	J	1505	1N7	C22-C20-C9	2.53	115.51	110.28
9	L	701	1N7	C8-C9-C20	2.50	116.01	112.15
9	L	701	1N7	C11-C2-C1	-2.49	104.25	108.26
9	J	1504	1N7	C8-C9-C20	2.46	115.95	112.15
9	L	701	1N7	C5-C9-C20	-2.44	116.58	119.50
9	L	701	1N7	C22-C20-C9	2.37	115.18	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	1504	1N7	C9-C5-C6	2.33	102.44	100.09
9	J	1504	1N7	C11-C2-C15	-2.28	106.50	110.36
9	L	701	1N7	C19-C2-C15	2.27	111.78	108.58
9	I	1401	1N7	C8-C9-C20	2.19	115.53	112.15
9	J	1505	1N7	C8-C7-C6	-2.17	100.83	105.13
9	J	1504	1N7	C14-C15-C2	2.17	114.96	112.66
9	J	1504	1N7	C21-C20-C9	-2.15	109.63	112.92
9	L	701	1N7	C15-C14-C13	-2.12	109.64	112.76
9	L	701	1N7	C11-C2-C15	-2.06	106.86	110.36
9	L	701	1N7	C8-C9-C5	-2.05	101.54	103.55
9	J	1504	1N7	C7-C8-C9	-2.02	101.13	105.13
9	J	1505	1N7	C11-C2-C19	2.00	113.94	111.18

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	1504	1N7	C21-C20-C9-C5
9	J	1504	1N7	C21-C20-C9-C8
9	I	1401	1N7	C21-C20-C9-C5
9	I	1401	1N7	C21-C20-C9-C8
9	I	1401	1N7	C22-C20-C9-C5
9	J	1504	1N7	C22-C20-C9-C5
9	I	1401	1N7	C22-C20-C9-C8
9	J	1504	1N7	C22-C20-C9-C8
9	J	1504	1N7	C9-C20-C22-C23
9	L	701	1N7	C20-C22-C23-C24
9	J	1504	1N7	C21-C20-C22-C23
9	I	1401	1N7	C20-C22-C23-C24
9	L	701	1N7	C21-C20-C9-C5
9	J	1504	1N7	C20-C22-C23-C24
9	L	701	1N7	C21-C20-C9-C8
9	L	701	1N7	C22-C20-C9-C5
9	L	701	1N7	C22-C20-C9-C8

There are no ring outliers.

4 monomers are involved in 17 short contacts:

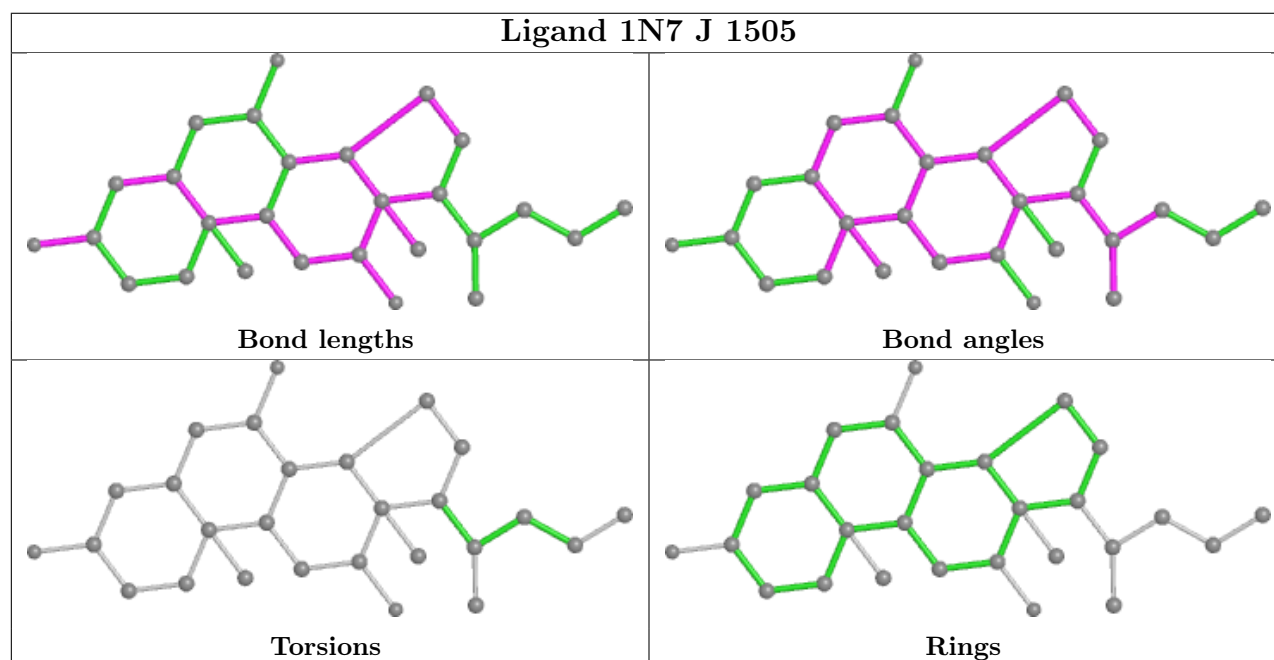
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	J	1505	1N7	5	0
9	L	701	1N7	4	0

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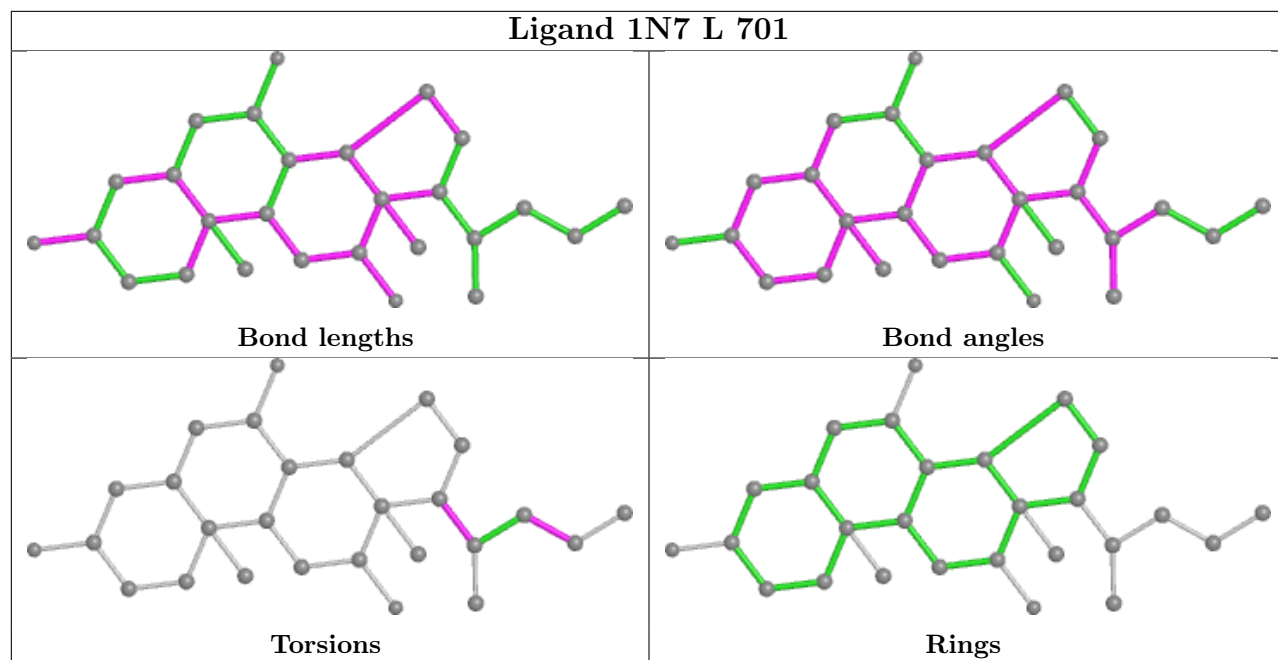
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	1401	1N7	4	0
9	J	1504	1N7	4	0

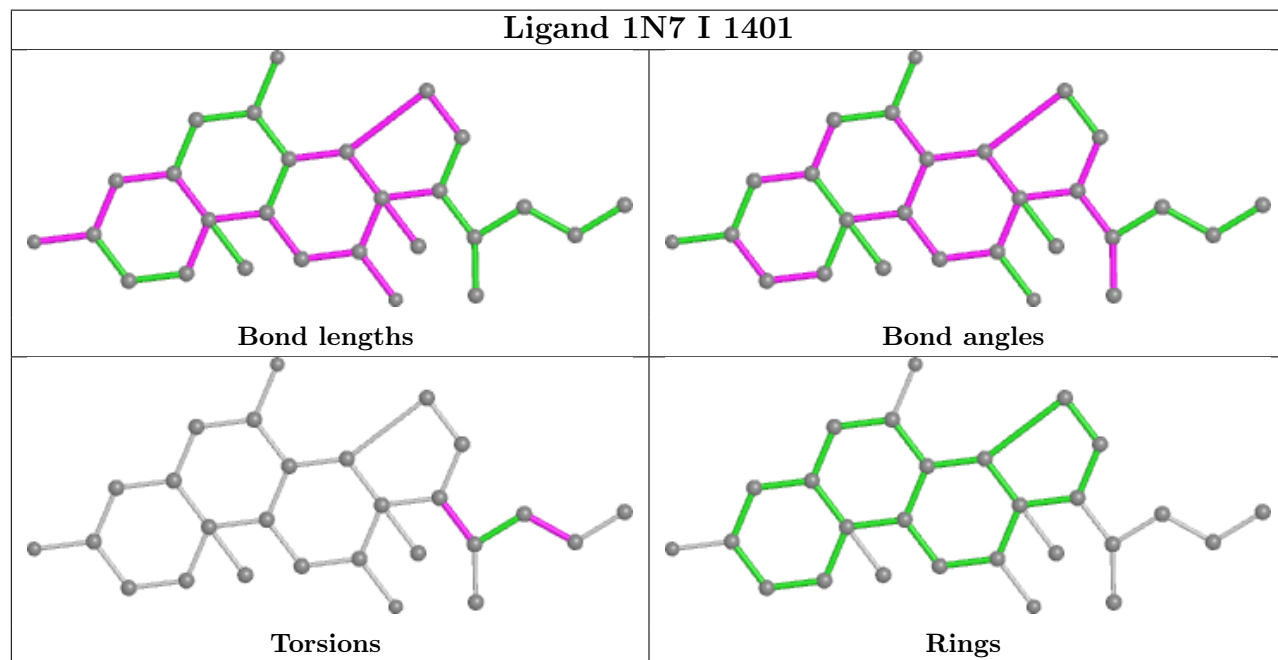
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

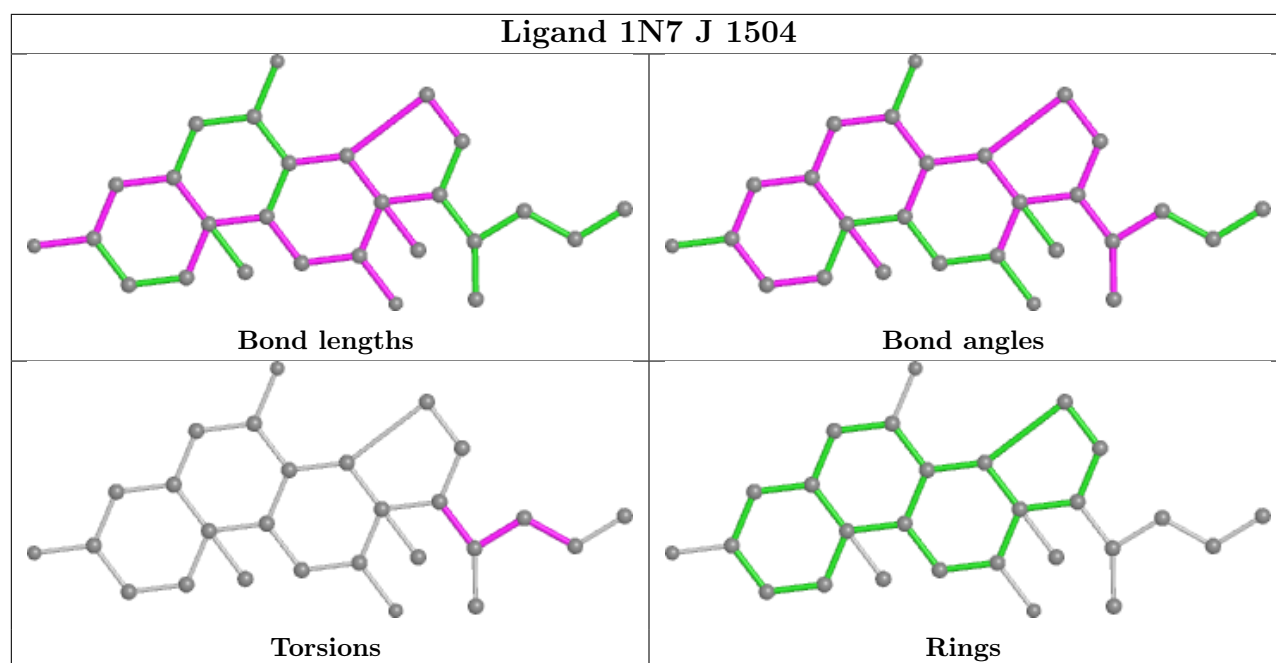


Ligand 1N7 L 701



Ligand 1N7 I 1401





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

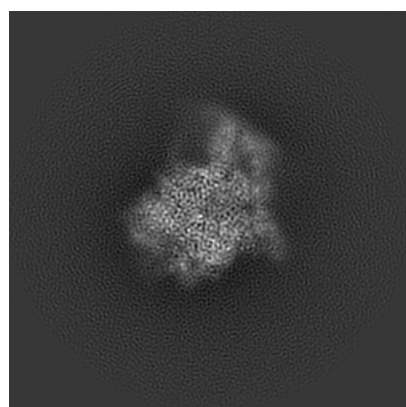
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20461. These allow visual inspection of the internal detail of the map and identification of artifacts.

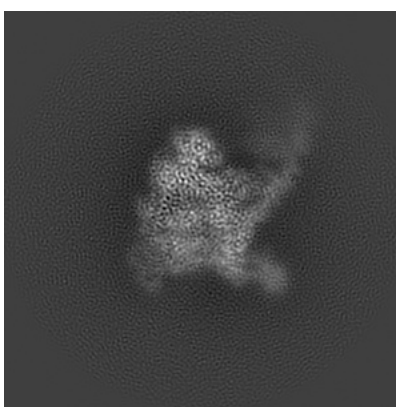
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

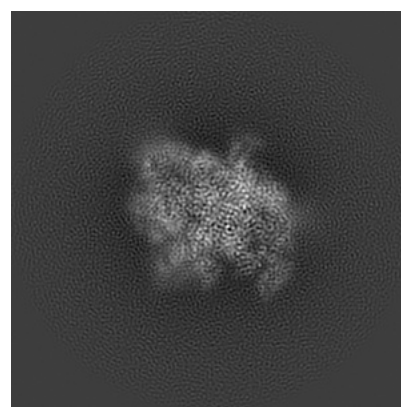
6.1.1 Primary map



X



Y

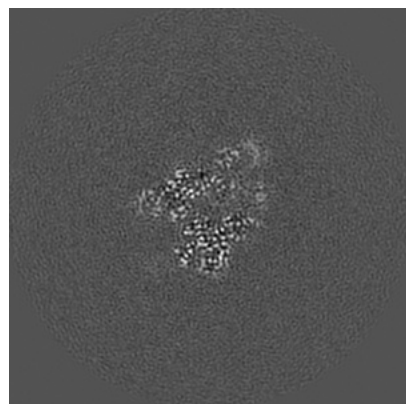


Z

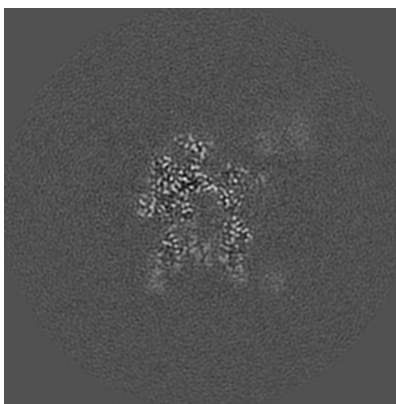
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

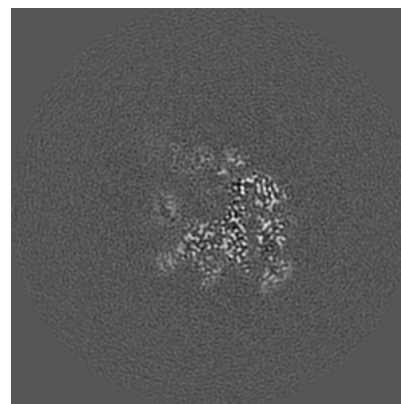
6.2.1 Primary map



X Index: 128



Y Index: 128

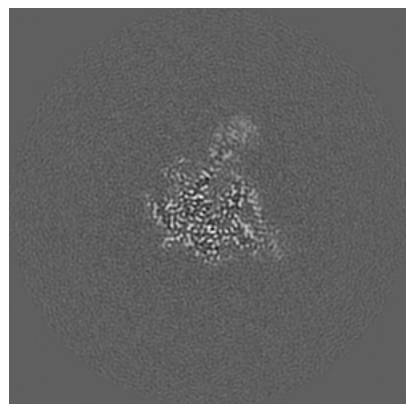


Z Index: 128

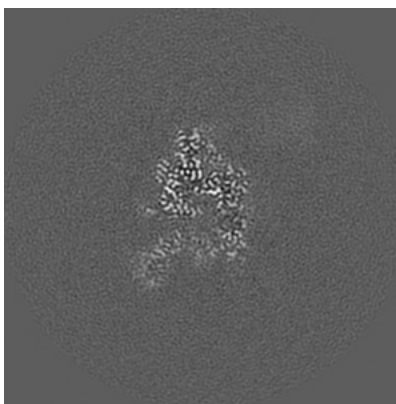
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

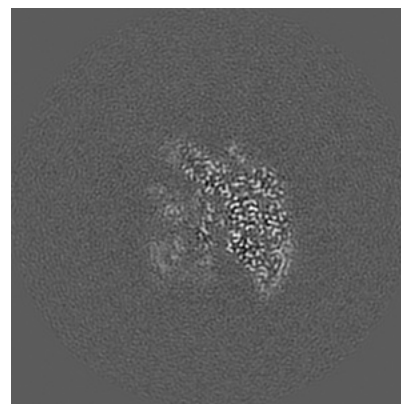
6.3.1 Primary map



X Index: 146



Y Index: 121

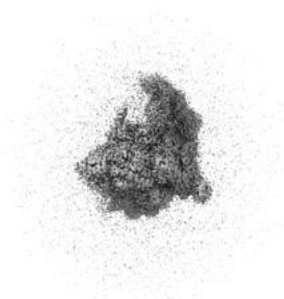


Z Index: 120

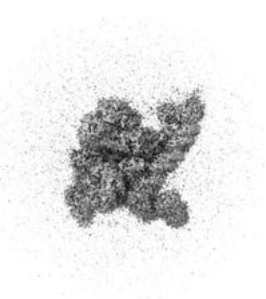
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

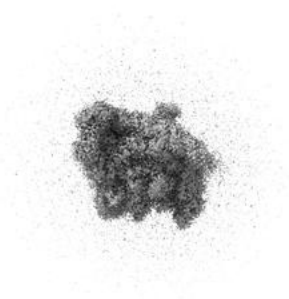
6.4.1 Primary map



X



Y



Z

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

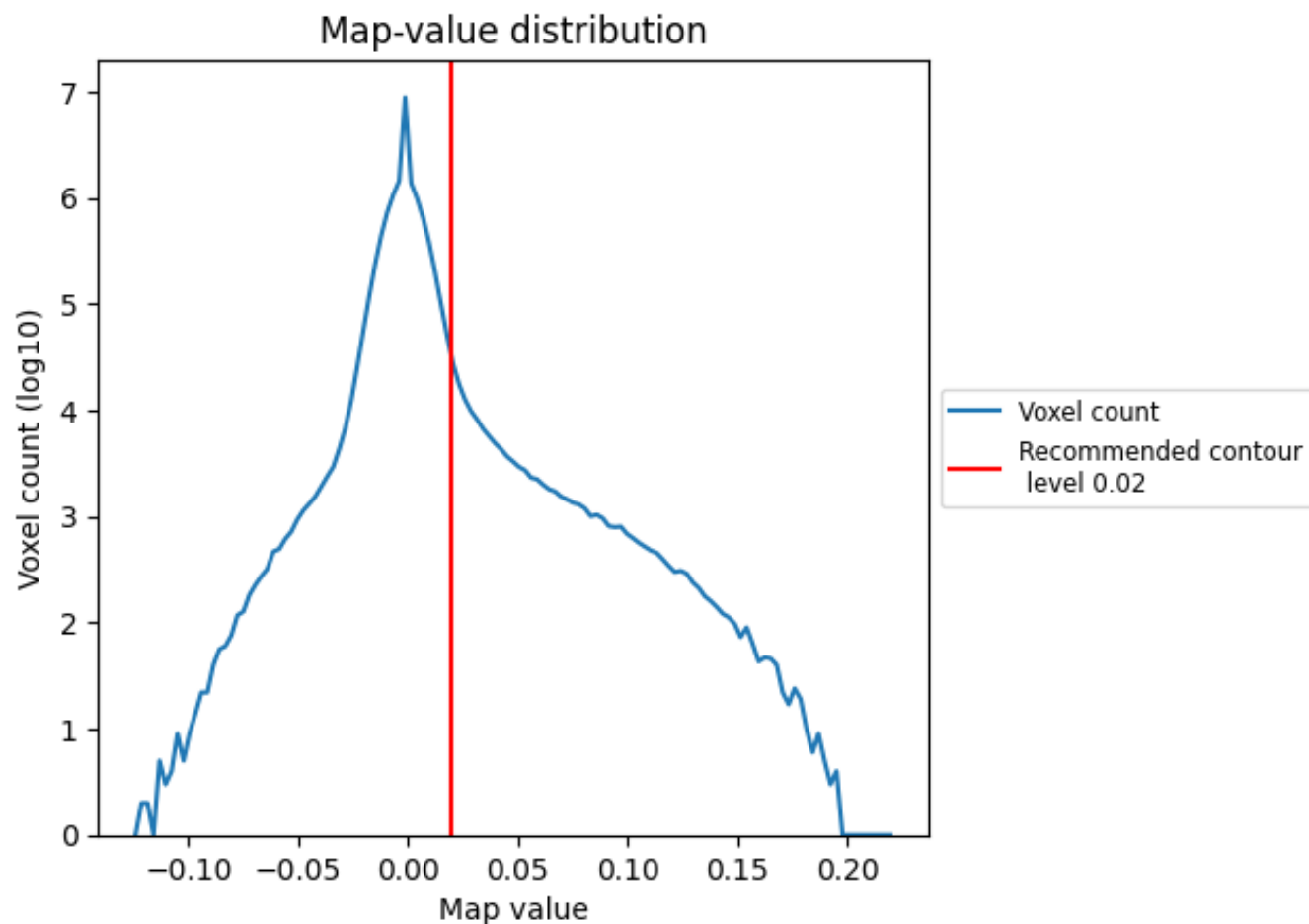
6.5 Mask visualisation

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

7 Map analysis [i](#)

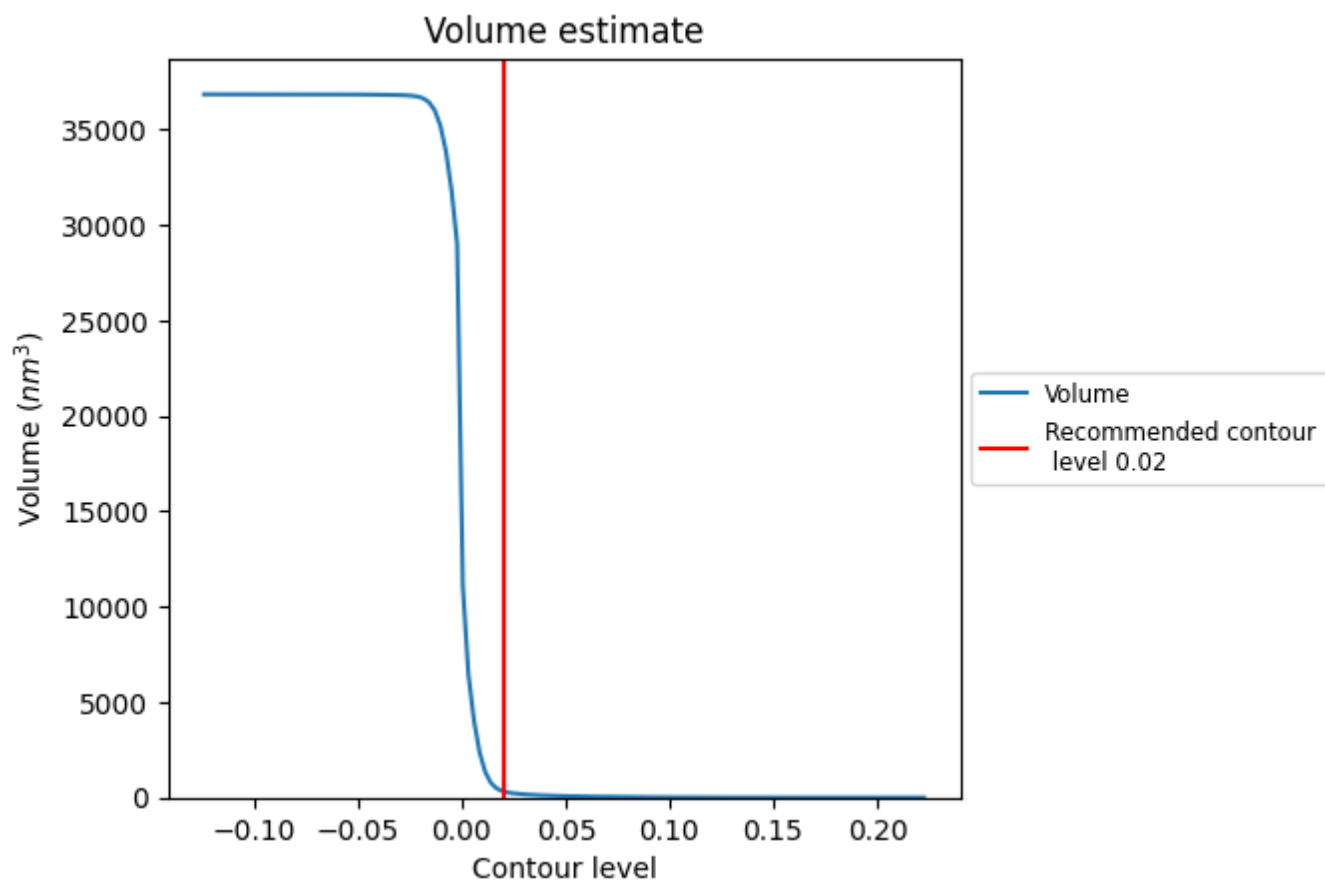
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

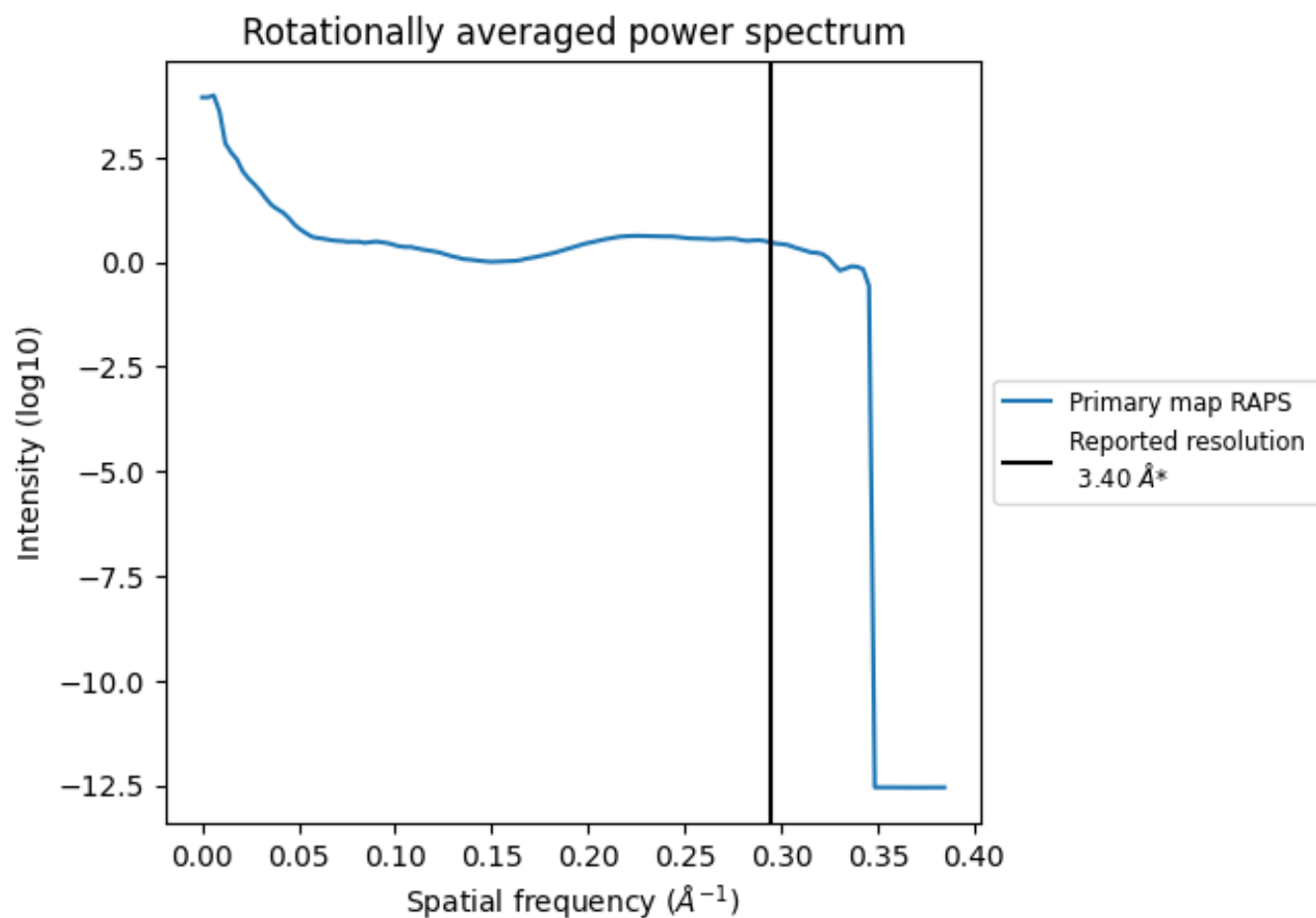
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 325 nm³; this corresponds to an approximate mass of 294 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 ⓘ

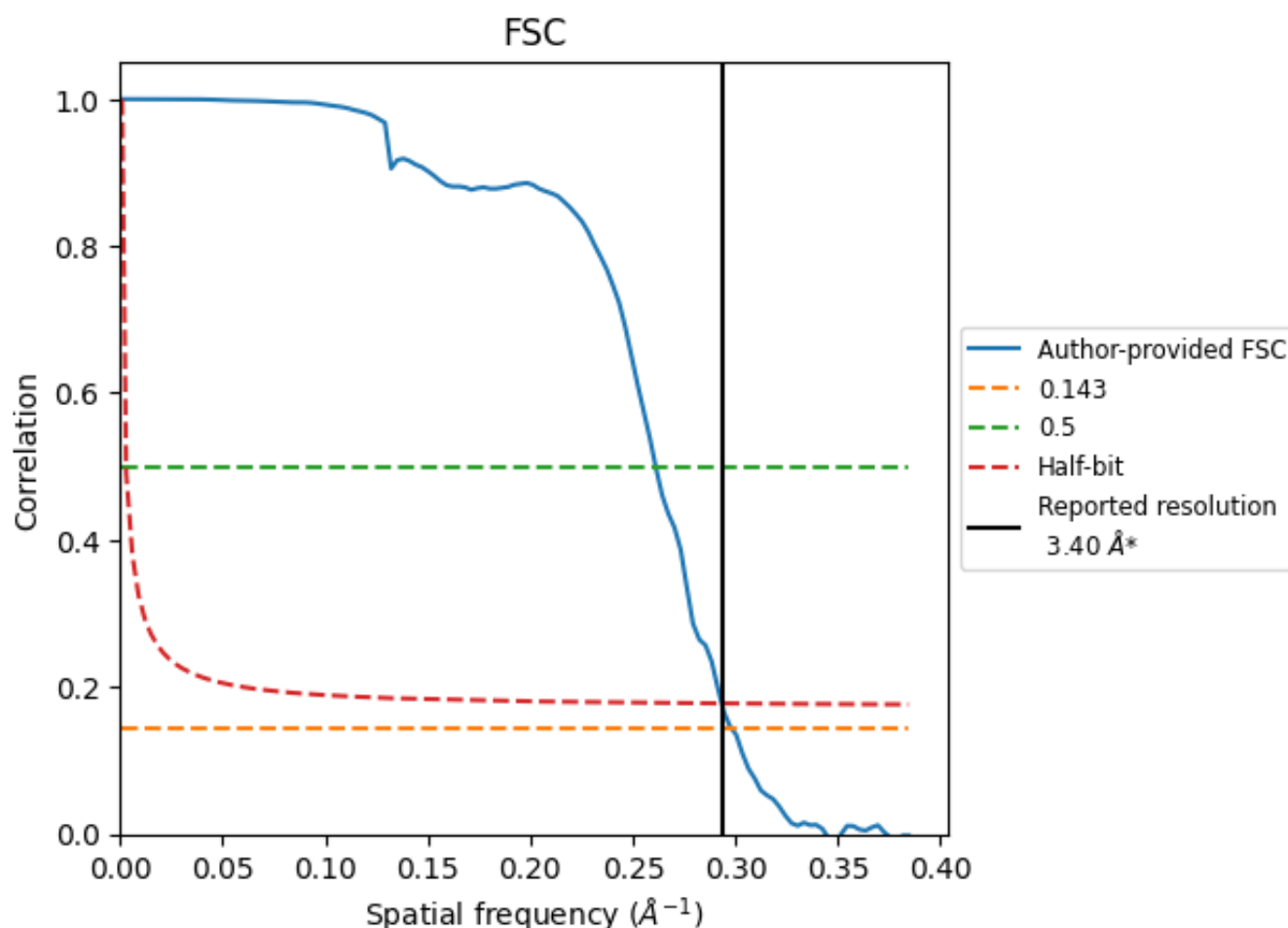


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

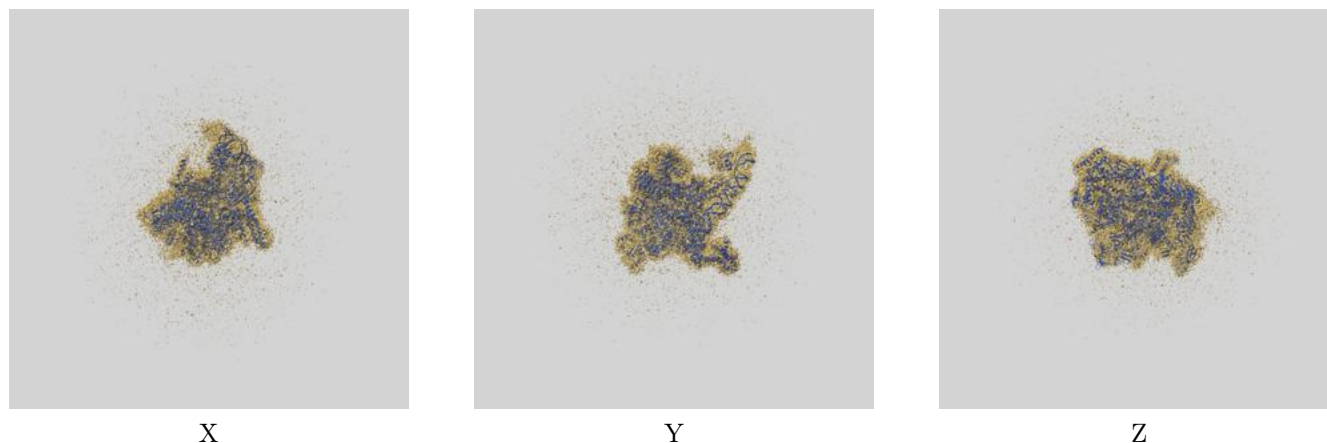
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.35	3.83	3.41
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

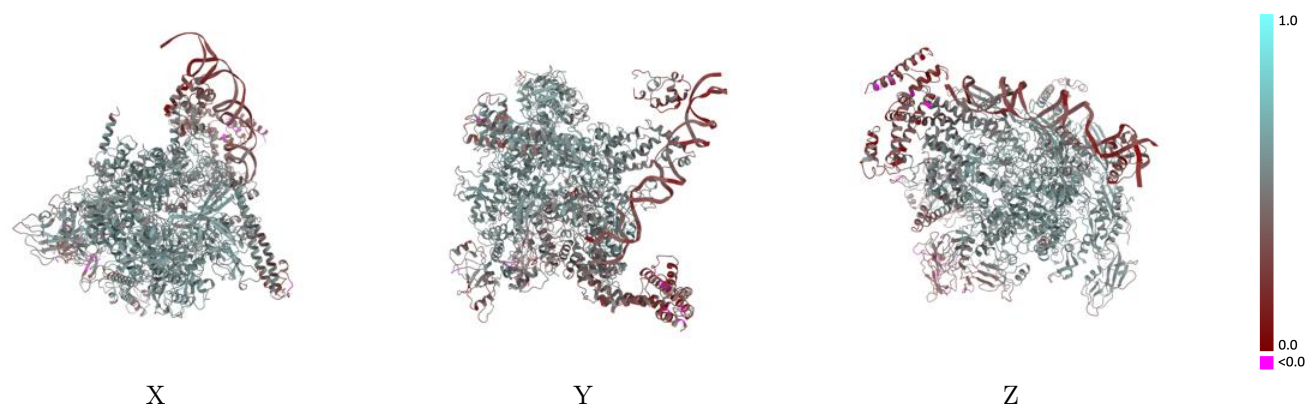
This section contains information regarding the fit between EMDB map EMD-20461 and PDB model 6PSR. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



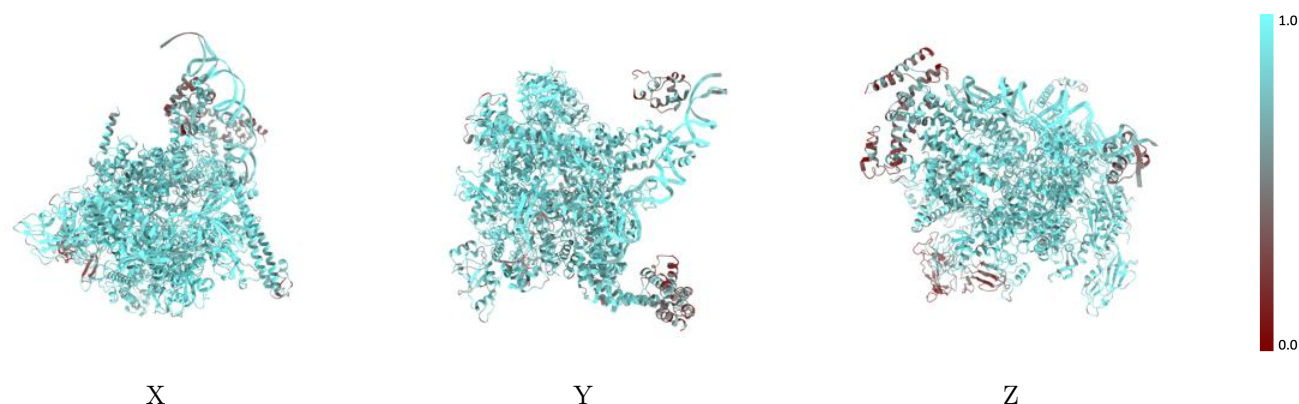
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



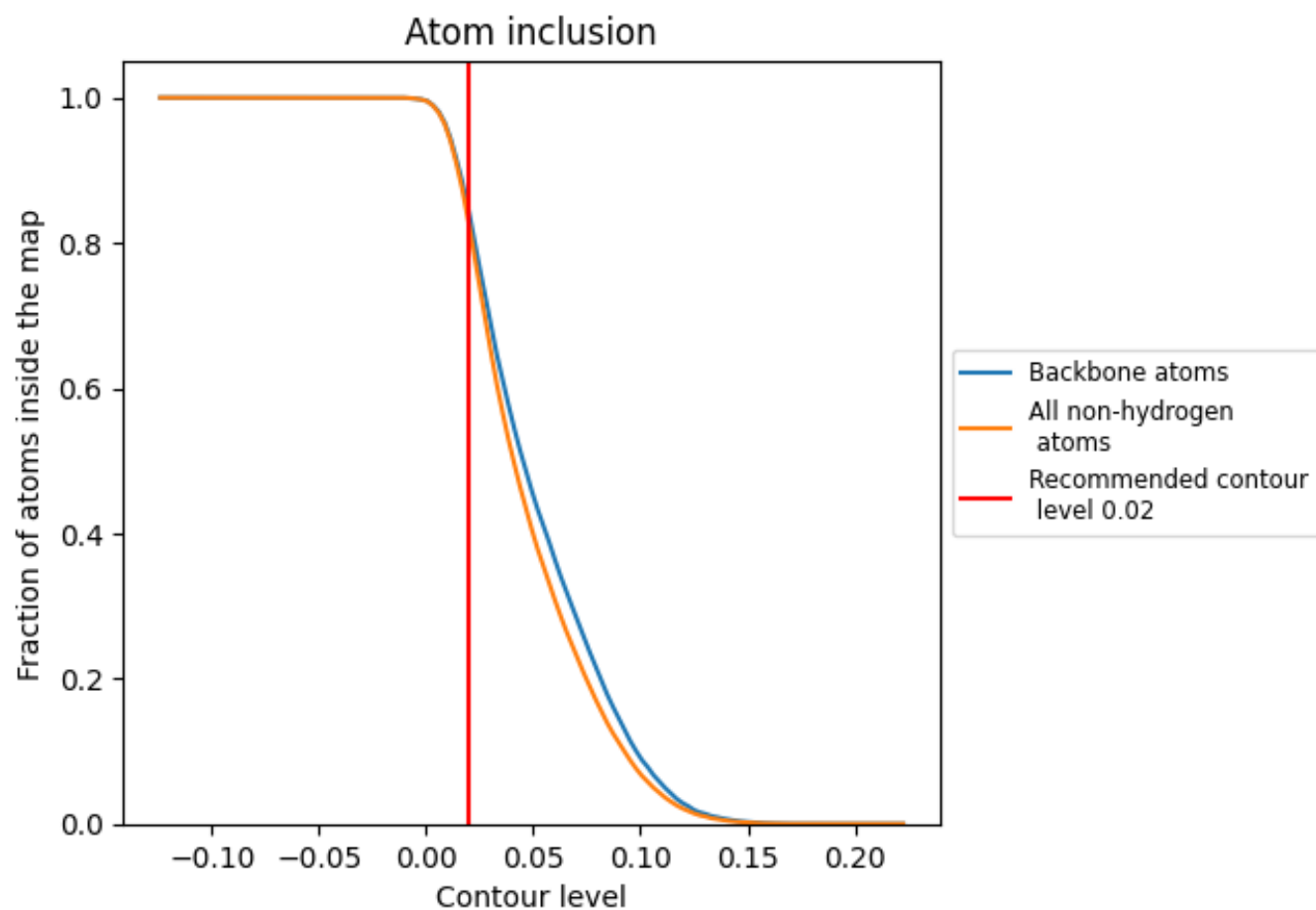
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	<div></div> 0.8245	<div></div> 0.4800
G	<div></div> 0.9003	<div></div> 0.5390
H	<div></div> 0.8870	<div></div> 0.5150
I	<div></div> 0.8861	<div></div> 0.5260
J	<div></div> 0.8125	<div></div> 0.4940
K	<div></div> 0.8236	<div></div> 0.5280
L	<div></div> 0.7078	<div></div> 0.3850
M	<div></div> 0.4554	<div></div> 0.3030
N	<div></div> 0.9149	<div></div> 0.5220
O	<div></div> 0.8056	<div></div> 0.2790
P	<div></div> 0.8113	<div></div> 0.2510

1.0

0.0

<0.0