



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:20 PM BST

PDB ID : 5FJ8  
EMDB ID: : EMD-3178  
Title : Cryo-EM structure of yeast RNA polymerase III elongation complex at 3.9 Å  
Authors : Hoffmann, N.A.; Jakobi, A.J.; Moreno-Morcillo, M.; Glatt, S.; Kosinski, J.; Hagen, W.J.; Sachse, C.; Muller, C.W.  
Deposited on : 2015-10-06  
Resolution : 3.90 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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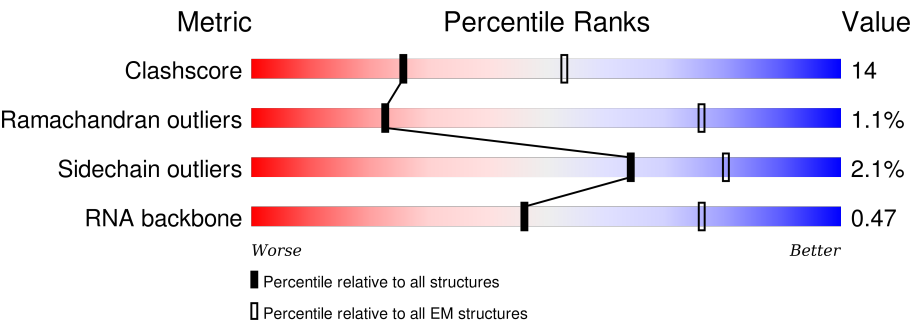
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 Å.

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






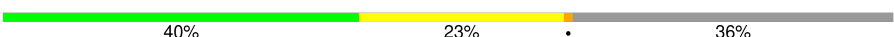
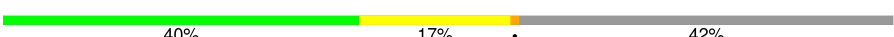





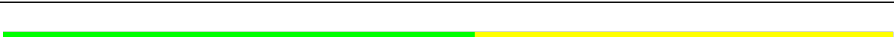
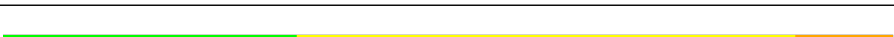
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

Mol	Chain	Length	Quality of chain
1	A	1460	69% 27% ..
2	B	1149	68% 28% ..
3	C	335	70% 28% .
4	D	161	46% 27% . 26%
5	E	215	62% 35% .
6	F	155	44% 8% . 46%
7	G	212	50% 37% . 10%
8	H	146	73% 23% ..

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Mol	Chain	Length	Quality of chain
9	I	110	
10	J	70	
11	K	142	
12	L	70	
13	M	282	
14	N	422	
15	O	654	
16	P	317	
17	Q	104	
18	R	23	
19	S	15	
20	T	9	

## 2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 39284 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1422	Total	C	N	O	S	0	0
			11130	7013	1966	2092	59		

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0
			8788	5558	1516	1654	60		

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	335	Total	C	N	O	S	0	0
			2655	1681	454	511	9		

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	119	Total	C	N	O	S	0	0
			977	628	156	187	6		

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1759	1116	310	321	12		

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			671	429	114	125	3		

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	191	Total	C	N	O	S	0	0
			1544	1007	250	281	6		

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	140	Total	C	N	O	S	0	0
			1120	703	188	224	5		

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	42	Total	C	N	O	S	0	0
			321	204	47	64	6		

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			549	350	95	98	6		

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			792	496	130	161	5		

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	164	Total	C	N	O	S	0	0
			1338	857	227	253	1		

- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	110	Total	C	N	O	S	0	0
			845	536	152	154	3		

- Molecule 15 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	539	Total	C	N	O	S	0	0
			4329	2756	741	813	19		

- Molecule 16 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	89	Total	C	N	O	S	0	0
			738	474	115	146	3		

- Molecule 17 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC7.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	63	Total	C	N	O	0	0
			390	243	73	74		

- Molecule 18 is a DNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	23	Total	C	N	O	P	0	0
			470	224	85	138	23		

- Molecule 19 is a DNA chain called NON-TEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	15	Total	C	N	O	P	0	0
			309	148	56	90	15		

- Molecule 20 is a RNA chain called TEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	9	Total	C	N	O	P	0	0
			195	87	39	60	9		

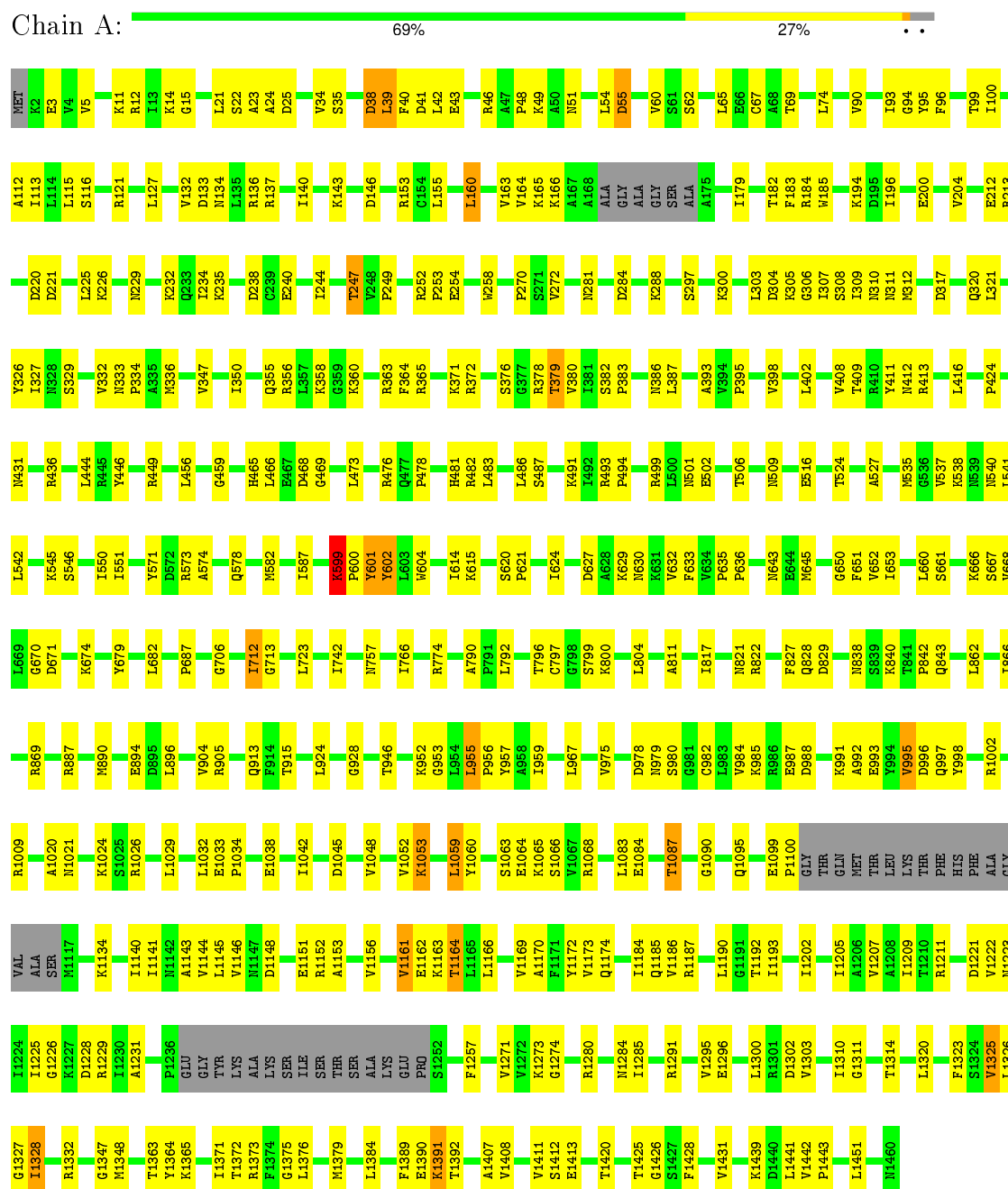
- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
21	B	1	Total	Zn	0
			1	1	
21	A	2	Total	Zn	0
			2	2	
21	L	1	Total	Zn	0
			1	1	
21	J	1	Total	Zn	0
			1	1	
21	I	1	Total	Zn	0
			1	1	

### 3 Residue-property plots

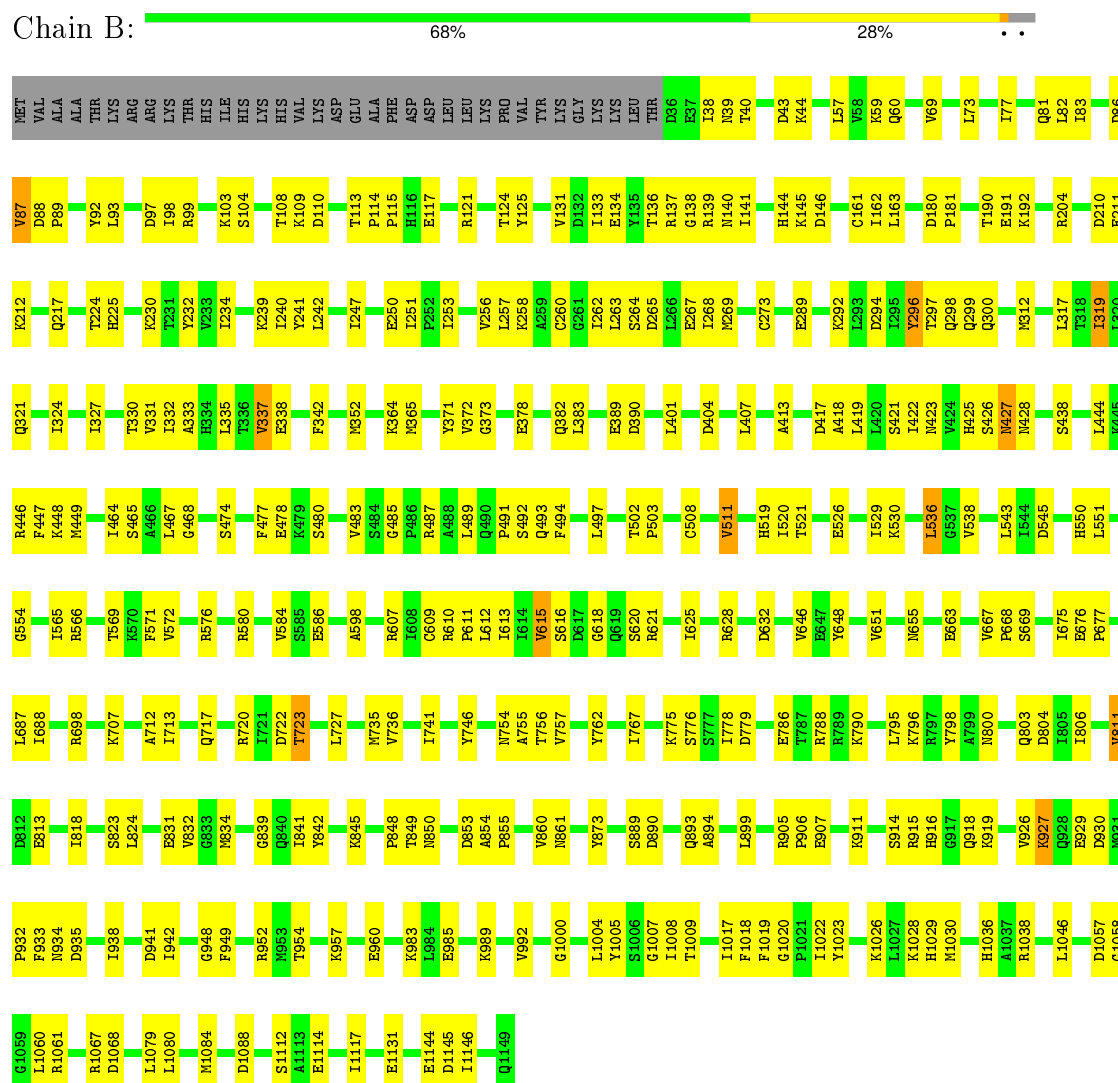
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric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

- Molecule 1: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC1

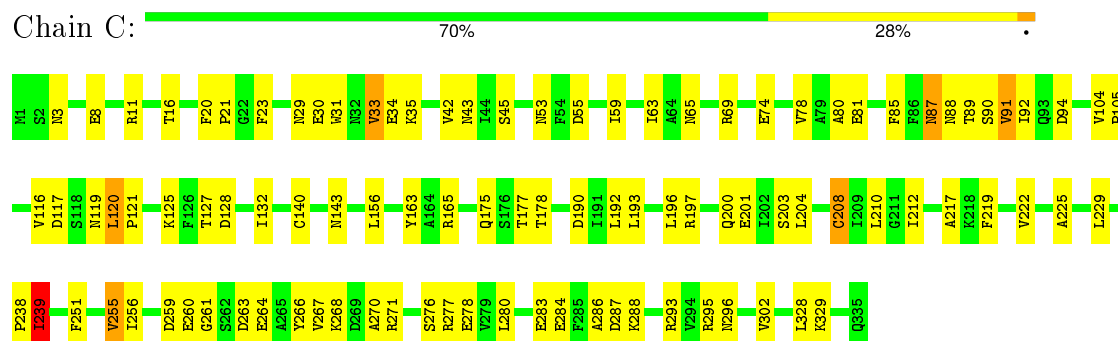




• Molecule 2: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC2



• Molecule 3: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1

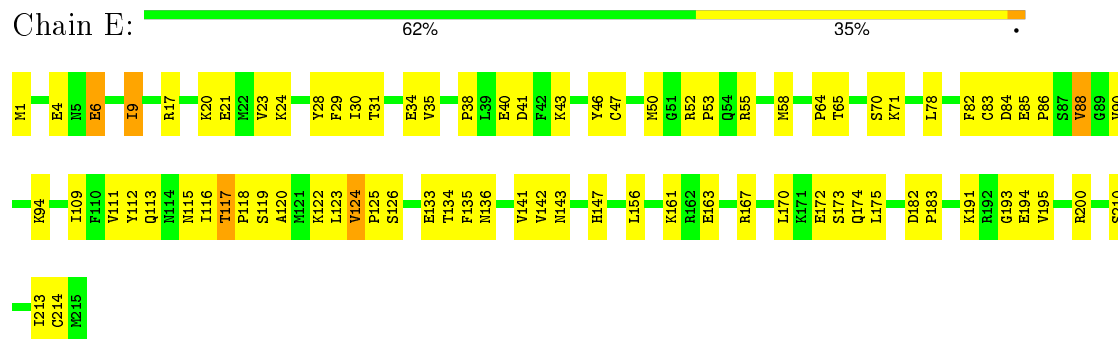


• Molecule 4: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC9

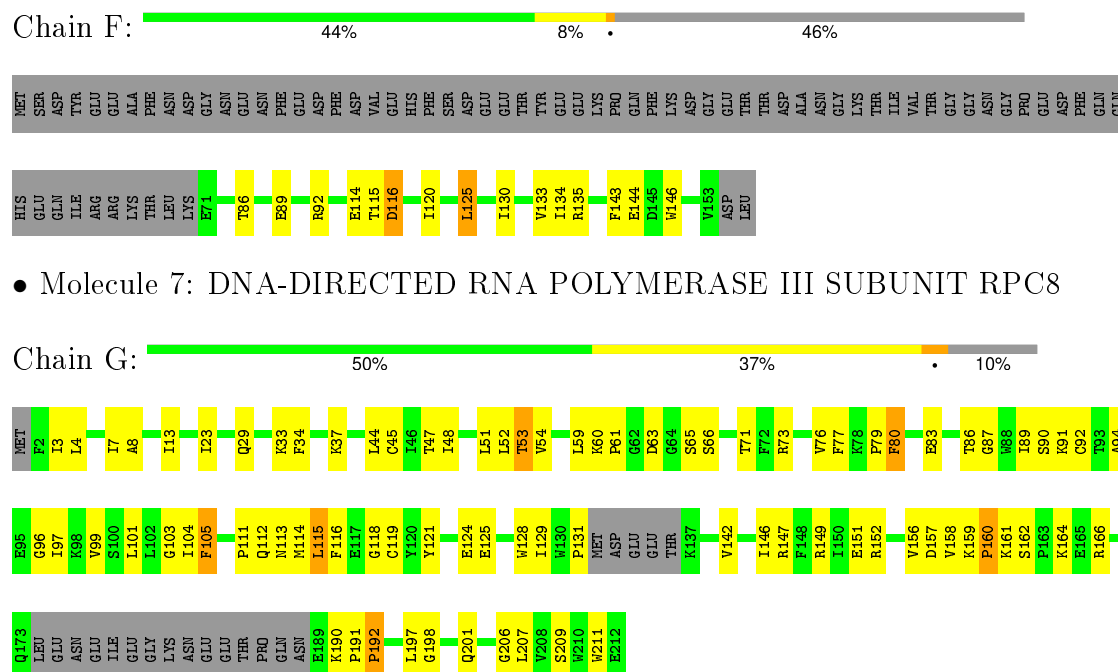




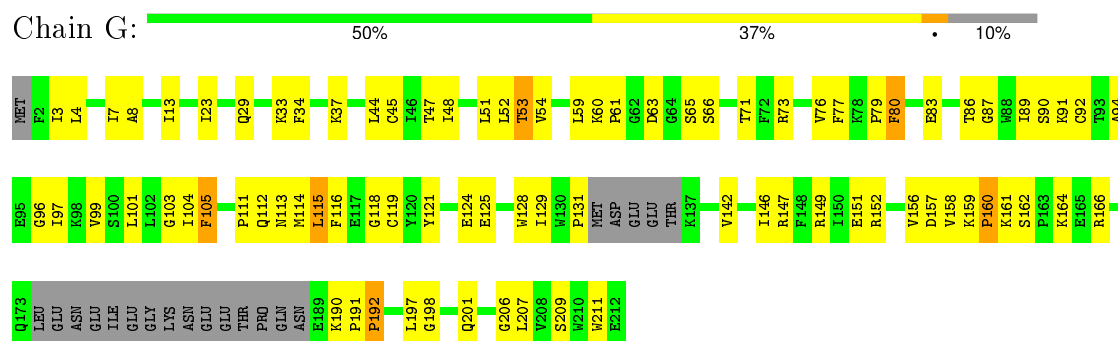
- Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



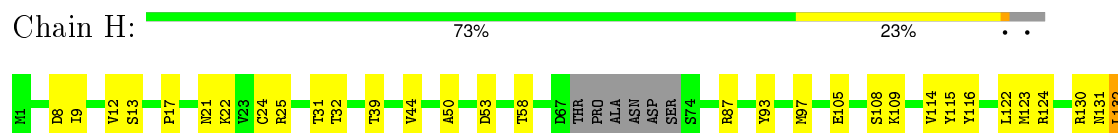
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2



- Molecule 7: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC8



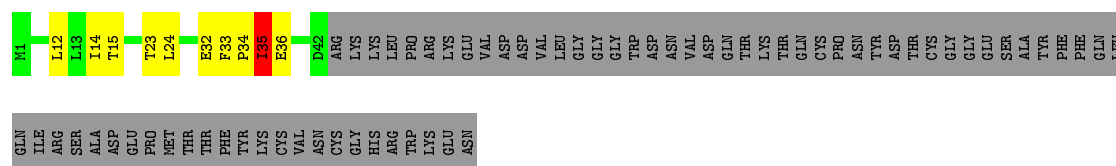
- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3





• Molecule 9: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC10

Chain I: 29% 8% 62%



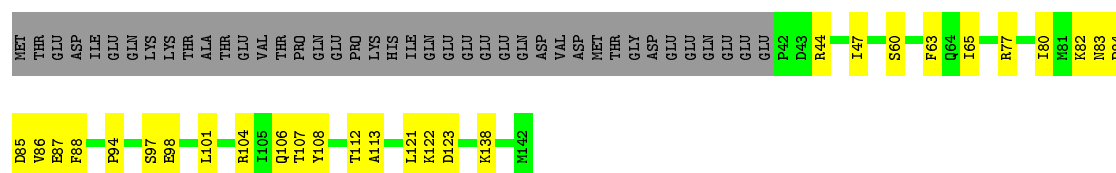
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J: 73% 21%



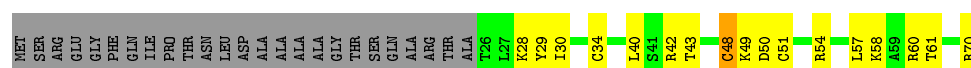
• Molecule 11: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2

Chain K: 51% 20% 29%



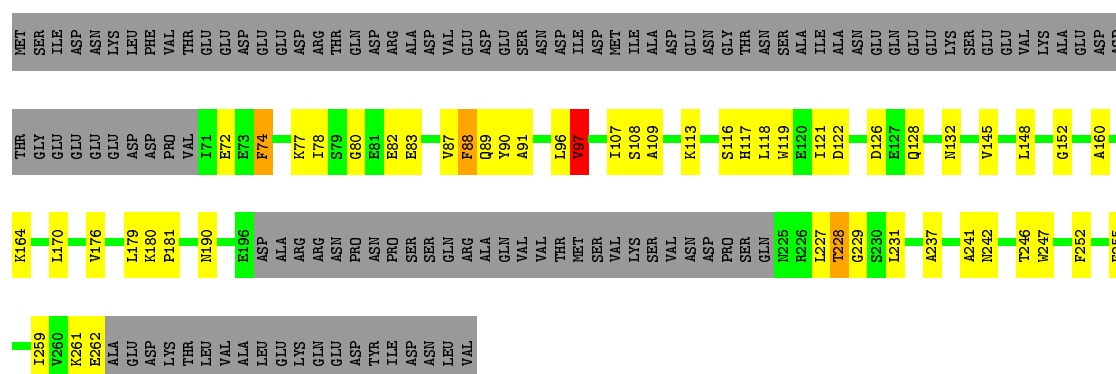
• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L: 40% 23% 36%

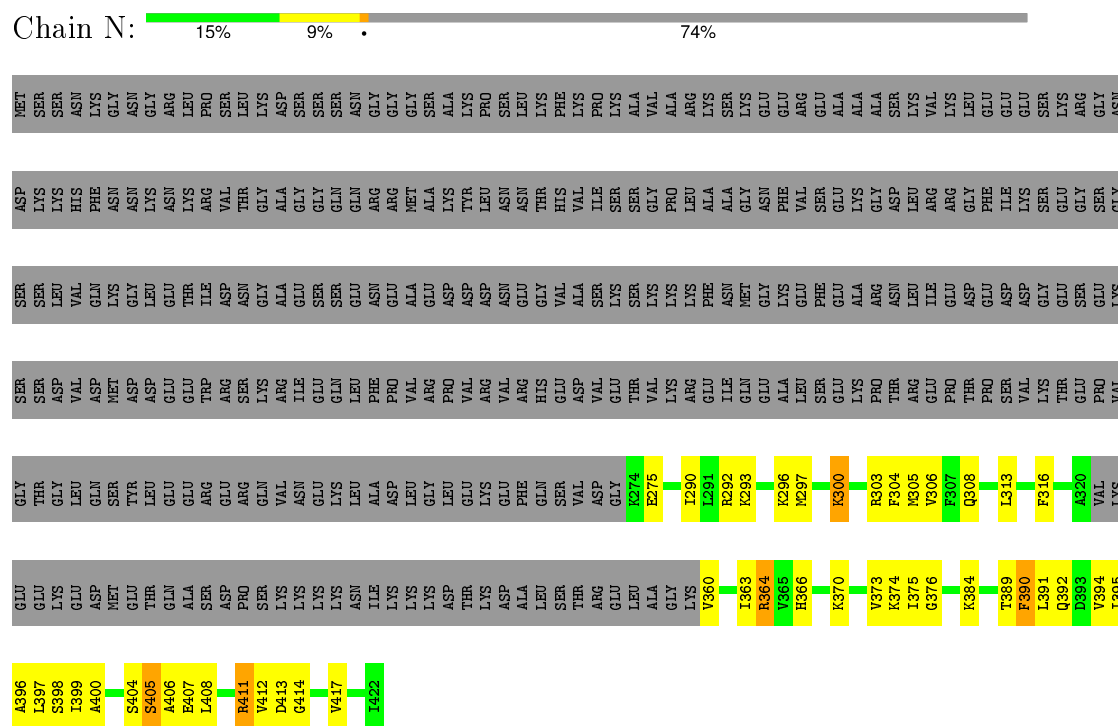


• Molecule 13: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC5

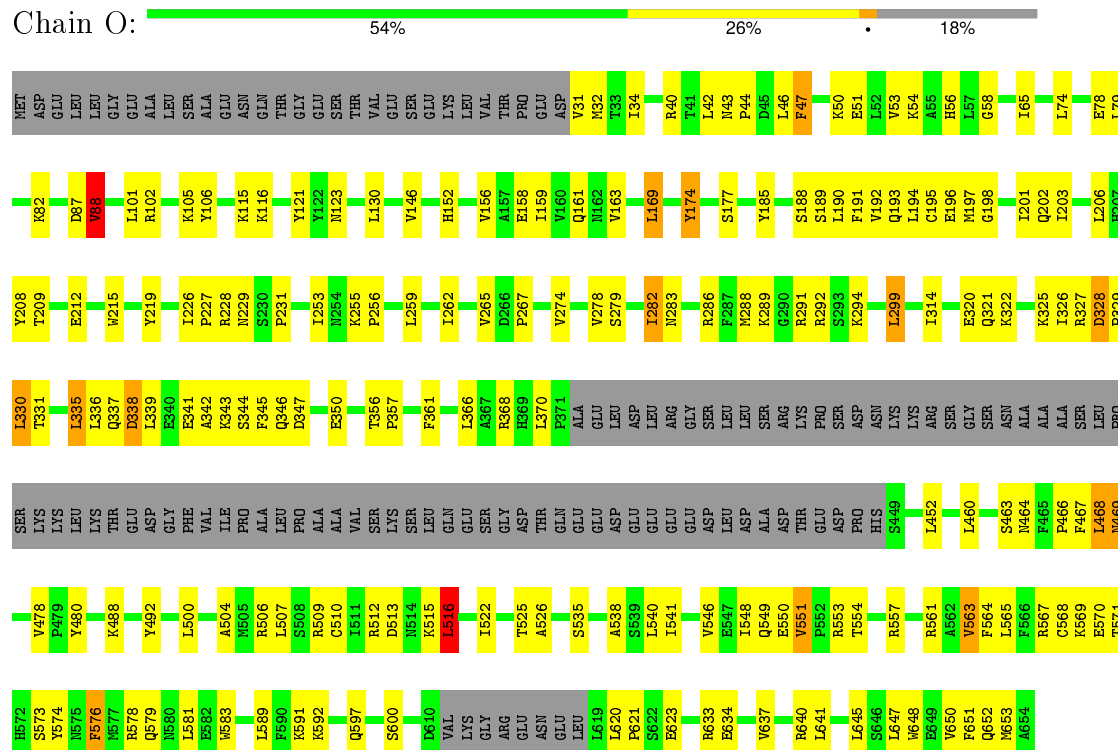
Chain M: 40% 17% 42%



• Molecule 14: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC4



• Molecule 15: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC3



• Molecule 16: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC6





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	4200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4K X 4K)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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  >2	RMSZ	# Z  >2
1	A	0.22	0/11328	0.47	0/15303
10	J	0.21	0/558	0.45	0/750
11	K	0.22	0/803	0.43	0/1083
12	L	0.24	0/360	0.49	0/478
13	M	0.23	0/1369	0.46	0/1851
14	N	0.26	0/855	0.56	0/1149
15	O	0.23	0/4394	0.50	1/5928 (0.0%)
16	P	0.28	0/750	0.53	0/1017
17	Q	0.27	0/219	0.44	0/294
18	R	0.47	0/526	0.89	0/809
19	S	0.51	0/346	0.94	0/532
2	B	0.22	0/8943	0.45	0/12068
20	T	0.13	0/218	0.69	0/338
3	C	0.23	0/2711	0.46	1/3676 (0.0%)
4	D	0.23	0/991	0.51	0/1328
5	E	0.23	0/1795	0.45	0/2416
6	F	0.21	0/683	0.42	0/923
7	G	0.23	0/1583	0.49	0/2146
8	H	0.21	0/1138	0.45	0/1540
9	I	0.30	0/328	0.48	0/445
All	All	0.23	0/39898	0.49	2/54074 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
11	K	0	1
14	N	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
All	All	0	8

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	120	LEU	CA-CB-CG	5.32	127.52	115.30
15	O	516	LEU	CA-CB-CG	5.19	127.24	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	38	ASP	Peptide
1	A	599	LYS	Peptide
1	A	601	TYR	Peptide
2	B	319	ILE	Peptide
2	B	839	GLY	Peptide
11	K	44	ARG	Peptide
14	N	300	LYS	Peptide
14	N	405	SER	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11130	0	11258	310	0
2	B	8788	0	8902	246	0
3	C	2655	0	2628	73	0
4	D	977	0	983	35	0
5	E	1759	0	1788	53	0
6	F	671	0	692	12	0
7	G	1544	0	1540	66	0
8	H	1120	0	1089	24	0
9	I	321	0	304	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	549	0	560	13	0
11	K	792	0	790	22	0
12	L	358	0	381	21	0
13	M	1338	0	1307	41	0
14	N	845	0	891	36	0
15	O	4329	0	4497	168	0
16	P	738	0	719	41	0
17	Q	390	0	269	5	0
18	R	470	0	260	12	0
19	S	309	0	171	6	0
20	T	195	0	100	2	0
21	A	2	0	0	0	0
21	B	1	0	0	0	0
21	I	1	0	0	0	0
21	J	1	0	0	0	0
21	L	1	0	0	0	0
All	All	39284	0	39129	1053	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 14.

All (1053) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1163:LYS:HZ1	1:A:1280:ARG:HA	1.36	0.91
1:A:829:ASP:OD2	1:A:838:ASN:ND2	2.03	0.91
1:A:615:LYS:NZ	1:A:620:SER:O	2.05	0.88
4:D:126:GLN:HG3	4:D:127:LEU:HG	1.56	0.88
3:C:16:THR:O	3:C:295:ARG:NH1	2.07	0.87
2:B:192:LYS:NZ	2:B:438:SER:O	2.08	0.85
2:B:373:GLY:HA2	2:B:607:ARG:HH22	1.42	0.85
1:A:360:LYS:NZ	18:R:16:DG:OP1	2.10	0.84
15:O:488:LYS:NZ	15:O:650:VAL:O	2.10	0.83
1:A:232:LYS:NZ	16:P:316:GLU:OE1	2.11	0.83
16:P:248:VAL:O	16:P:255:LYS:NZ	2.13	0.82
1:A:43:GLU:HB2	1:A:48:PRO:HD2	1.62	0.81
1:A:476:ARG:NH1	1:A:509:ASN:O	2.13	0.81
1:A:413:ARG:NH1	1:A:456:LEU:O	2.15	0.80
15:O:460:LEU:HD11	15:O:468:LEU:HD23	1.62	0.80
2:B:1026:LYS:NZ	2:B:1030:MET:SD	2.55	0.79
5:E:124:VAL:HG13	5:E:125:PRO:HD3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:LYS:HG3	1:A:1392:THR:HG21	1.65	0.78
5:E:85:GLU:HG3	5:E:86:PRO:HD3	1.65	0.77
7:G:207:LEU:HD23	7:G:209:SER:H	1.50	0.76
1:A:69:THR:HA	7:G:164:LYS:HZ3	1.48	0.76
12:L:48:CYS:SG	12:L:51:CYS:HB2	2.18	0.76
7:G:146:ILE:HG23	7:G:206:GLY:HA2	1.68	0.75
2:B:294:ASP:HB3	2:B:300:GLN:HG3	1.67	0.75
2:B:121:ARG:HH12	12:L:54:ARG:HH21	1.33	0.74
14:N:363:ILE:HG12	14:N:373:VAL:HG13	1.68	0.74
13:M:87:VAL:HA	14:N:396:ALA:HA	1.70	0.74
1:A:550:ILE:HG23	1:A:551:ILE:HG23	1.70	0.73
7:G:115:LEU:HD23	7:G:116:PHE:H	1.52	0.73
1:A:996:ASP:OD2	1:A:1002:ARG:NH2	2.22	0.73
4:D:110:LEU:HB3	4:D:120:LYS:HZ1	1.54	0.73
4:D:119:GLU:HG3	4:D:138:VAL:HB	1.71	0.72
2:B:796:LYS:NZ	2:B:798:TYR:OH	2.23	0.72
11:K:65:ILE:HB	11:K:101:LEU:HB3	1.72	0.72
7:G:89:ILE:HA	7:G:99:VAL:HA	1.72	0.71
1:A:132:VAL:HG11	1:A:137:ARG:NH1	2.06	0.71
2:B:139:ARG:HE	2:B:141:ILE:HD11	1.53	0.71
2:B:258:LYS:HB3	2:B:297:THR:HA	1.70	0.71
1:A:49:LYS:HD2	1:A:54:LEU:HB3	1.72	0.70
13:M:113:LYS:HD3	13:M:241:ALA:HB2	1.73	0.70
10:J:12:LYS:HE3	10:J:43:ARG:NH2	2.07	0.70
15:O:322:LYS:HB3	15:O:361:PHE:HE1	1.57	0.70
7:G:96:GLY:HA3	7:G:111:PRO:HA	1.73	0.70
4:D:110:LEU:HB3	4:D:120:LYS:NZ	2.06	0.69
4:D:126:GLN:NE2	7:G:86:THR:OG1	2.22	0.69
2:B:121:ARG:NH1	12:L:54:ARG:HH21	1.89	0.69
1:A:69:THR:HG22	7:G:164:LYS:HZ3	1.57	0.69
2:B:234:ILE:HB	2:B:240:ILE:HG22	1.72	0.69
11:K:47:ILE:HG12	11:K:65:ILE:HG12	1.74	0.69
1:A:153:ARG:HA	1:A:160:LEU:HD22	1.75	0.68
1:A:482:ARG:HH12	1:A:924:LEU:HD11	1.59	0.68
2:B:755:ALA:HA	10:J:48:ARG:HH12	1.58	0.68
11:K:88:PHE:HB3	11:K:106:GLN:HB3	1.75	0.68
4:D:127:LEU:HB2	4:D:133:HIS:HB3	1.75	0.68
1:A:436:ARG:HD3	1:A:459:GLY:HA3	1.75	0.68
2:B:121:ARG:HH12	12:L:54:ARG:NH2	1.92	0.68
1:A:272:VAL:HG23	1:A:281:ASN:HB3	1.76	0.68
1:A:1020:ALA:HB2	1:A:1032:LEU:HD11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:419:LEU:O	2:B:423:ASN:ND2	2.25	0.68
2:B:778:ILE:HD11	2:B:906:PRO:HG2	1.76	0.68
13:M:247:TRP:HD1	14:N:406:ALA:HB1	1.58	0.67
8:H:24:CYS:SG	8:H:25:ARG:N	2.67	0.67
15:O:488:LYS:HZ1	15:O:651:PHE:HA	1.59	0.67
16:P:223:GLU:O	16:P:227:ALA:N	2.23	0.67
15:O:516:LEU:HB2	15:O:565:LEU:HD23	1.75	0.67
15:O:549:GLN:HG3	15:O:565:LEU:HB2	1.76	0.67
5:E:161:LYS:NZ	5:E:193:GLY:O	2.27	0.67
13:M:148:LEU:HG	13:M:181:PRO:HB3	1.77	0.67
13:M:247:TRP:HE1	14:N:408:LEU:HB2	1.59	0.67
1:A:1431:VAL:HG21	6:F:135:ARG:NH1	2.10	0.67
1:A:995:VAL:HG23	1:A:996:ASP:H	1.60	0.66
15:O:488:LYS:NZ	15:O:651:PHE:HA	2.10	0.66
2:B:755:ALA:HA	10:J:48:ARG:NH1	2.10	0.66
15:O:327:ARG:NH1	15:O:330:LEU:HD22	2.10	0.66
1:A:1162:GLU:HB2	1:A:1163:LYS:HD3	1.76	0.66
17:Q:43:ILE:HG23	17:Q:44:ASN:H	1.61	0.65
15:O:507:LEU:HD13	15:O:540:LEU:HD22	1.78	0.65
2:B:698:ARG:HH21	2:B:952:ARG:HG2	1.61	0.65
1:A:1045:ASP:HB2	1:A:1053:LYS:HE2	1.78	0.65
19:S:6:DA:H2"	19:S:7:DA:OP2	1.96	0.65
3:C:270:ALA:HB3	3:C:271:ARG:HH11	1.61	0.65
2:B:543:LEU:HD21	13:M:176:VAL:HG21	1.79	0.65
1:A:121:ARG:NH2	15:O:212:GLU:OE1	2.29	0.65
9:I:14:ILE:HD13	9:I:24:LEU:HB3	1.78	0.65
7:G:161:LYS:HE3	7:G:166:ARG:HA	1.78	0.65
15:O:185:TYR:HA	15:O:188:SER:HB2	1.78	0.65
1:A:378:ARG:HE	1:A:516:GLU:HB3	1.61	0.65
7:G:104:ILE:HG23	7:G:105:PHE:H	1.62	0.65
1:A:179:ILE:HD12	15:O:557:ARG:HE	1.62	0.65
2:B:1067:ARG:NH1	2:B:1079:LEU:HD22	2.12	0.64
2:B:914:SER:OG	2:B:957:LYS:NZ	2.20	0.64
1:A:310:ASN:HD21	15:O:561:ARG:H	1.44	0.64
1:A:200:GLU:HB3	15:O:516:LEU:HD21	1.79	0.64
2:B:389:GLU:OE2	2:B:446:ARG:NH2	2.30	0.64
2:B:265:ASP:O	2:B:268:ILE:N	2.27	0.64
8:H:58:THR:HB	8:H:143:LEU:HB3	1.78	0.64
1:A:360:LYS:HB2	1:A:365:ARG:HH21	1.63	0.64
1:A:905:ARG:HH22	5:E:170:LEU:HD21	1.63	0.64
1:A:3:GLU:OE2	7:G:37:LYS:HE3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:ILE:HD12	2:B:256:VAL:HB	1.79	0.64
3:C:270:ALA:HB3	3:C:271:ARG:NH1	2.13	0.64
8:H:132:LEU:HD12	8:H:133:ASN:H	1.62	0.64
2:B:247:ILE:HG21	2:B:251:ILE:HD11	1.79	0.63
1:A:645:MET:HE3	8:H:124:ARG:HD2	1.80	0.63
1:A:1164:THR:HB	1:A:1271:VAL:HA	1.80	0.63
15:O:633:ARG:NH2	16:P:308:ASP:O	2.31	0.63
1:A:1372:THR:O	1:A:1376:LEU:N	2.31	0.63
2:B:373:GLY:HA2	2:B:607:ARG:NH2	2.11	0.63
1:A:160:LEU:HD21	15:O:339:LEU:HG	1.79	0.63
16:P:218:THR:HB	16:P:221:ILE:HB	1.81	0.63
4:D:130:ASN:O	4:D:133:HIS:ND1	2.32	0.63
20:T:9:A:H5'	20:T:10:C:OP2	1.98	0.63
1:A:220:ASP:OD1	1:A:220:ASP:N	2.32	0.63
15:O:106:TYR:HB3	15:O:208:TYR:HE2	1.63	0.62
3:C:222:VAL:HG11	3:C:225:ALA:HB2	1.81	0.62
1:A:1084:GLU:HB2	6:F:86:THR:HG23	1.82	0.62
1:A:956:PRO:HG2	1:A:957:TYR:HD1	1.65	0.62
2:B:483:VAL:HG12	2:B:485:GLY:H	1.63	0.62
10:J:17:LYS:HB3	10:J:39:LEU:HD21	1.81	0.62
1:A:252:ARG:O	1:A:254:GLU:N	2.32	0.62
5:E:90:VAL:HG12	5:E:94:LYS:HG2	1.82	0.62
16:P:174:PHE:O	16:P:175:ILE:HG12	2.00	0.62
1:A:1161:VAL:HG11	1:A:1303:VAL:HG23	1.82	0.62
1:A:38:ASP:HB3	1:A:39:LEU:HD12	1.82	0.62
2:B:426:SER:O	2:B:427:ASN:ND2	2.33	0.61
2:B:81:GLN:HG2	2:B:82:LEU:HG	1.83	0.61
3:C:29:ASN:HB2	3:C:35:LYS:NZ	2.15	0.61
16:P:179:LEU:O	16:P:183:TRP:NE1	2.33	0.61
9:I:32:GLU:HG2	13:M:132:ASN:HB2	1.82	0.61
3:C:81:GLU:OE2	12:L:70:ARG:NH2	2.33	0.61
2:B:230:LYS:HB2	2:B:333:ALA:HB1	1.82	0.61
1:A:347:VAL:HB	1:A:350:ILE:HD11	1.82	0.61
2:B:698:ARG:HE	2:B:952:ARG:HB3	1.65	0.61
5:E:112:TYR:HB2	5:E:136:ASN:HA	1.82	0.61
1:A:378:ARG:NH1	18:R:18:DC:H4'	2.15	0.61
8:H:97:MET:HB2	8:H:142:LEU:HB3	1.82	0.61
13:M:77:LYS:HE3	13:M:262:GLU:HB3	1.83	0.61
1:A:476:ARG:HG2	1:A:478:PRO:HD2	1.83	0.61
14:N:305:MET:HG2	14:N:414:GLY:H	1.65	0.61
4:D:11:LEU:HD22	7:G:4:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:775:LYS:HA	2:B:778:ILE:HG22	1.82	0.61
1:A:486:LEU:HD23	1:A:537:VAL:HG22	1.83	0.61
15:O:578:ARG:HG2	15:O:648:TRP:HZ3	1.66	0.61
15:O:341:GLU:HG2	15:O:344:SER:HB2	1.81	0.61
3:C:31:TRP:H	11:K:82:LYS:HE2	1.66	0.61
16:P:252:LYS:NZ	16:P:253:LEU:HB2	2.16	0.61
15:O:198:GLY:HA3	15:O:286:ARG:HG2	1.83	0.60
1:A:573:ARG:HH21	11:K:87:GLU:HB3	1.65	0.60
1:A:393:ALA:HA	1:A:491:LYS:HB2	1.83	0.60
15:O:105:LYS:HB3	15:O:121:TYR:HB2	1.83	0.60
14:N:398:SER:HB3	14:N:407:GLU:HB3	1.83	0.60
9:I:35:ILE:HD12	9:I:36:GLU:H	1.66	0.60
12:L:29:TYR:HE2	12:L:40:LEU:HB2	1.65	0.60
12:L:42:ARG:HG3	12:L:43:THR:HG23	1.84	0.60
1:A:15:GLY:H	1:A:1408:VAL:HG12	1.66	0.60
2:B:493:GLN:HG3	2:B:497:LEU:HB2	1.84	0.60
1:A:712:ILE:HG23	1:A:790:ALA:HB3	1.82	0.60
6:F:92:ARG:HH12	7:G:61:PRO:HB3	1.67	0.60
15:O:31:VAL:HG12	15:O:32:MET:HG3	1.83	0.60
2:B:1112:SER:HB2	2:B:1114:GLU:HG2	1.82	0.60
7:G:101:LEU:HD22	7:G:104:ILE:HG22	1.84	0.60
15:O:538:ALA:HA	15:O:541:ILE:HG22	1.84	0.60
5:E:117:THR:HG23	5:E:119:SER:H	1.66	0.60
1:A:1169:VAL:HG13	1:A:1192:THR:HB	1.83	0.60
15:O:190:LEU:HG	15:O:193:GLN:HB3	1.82	0.60
4:D:127:LEU:HD11	4:D:137:ILE:HD13	1.84	0.59
1:A:15:GLY:HA2	1:A:1407:ALA:HA	1.84	0.59
1:A:712:ILE:HD12	2:B:949:PHE:HD2	1.66	0.59
2:B:832:VAL:HG12	12:L:60:ARG:HG3	1.84	0.59
9:I:12:LEU:HB3	9:I:24:LEU:HD13	1.84	0.59
16:P:221:ILE:HA	16:P:224:PHE:HB2	1.84	0.59
1:A:1420:THR:HG22	2:B:1080:LEU:HD21	1.84	0.59
15:O:286:ARG:NH1	15:O:320:GLU:O	2.35	0.59
1:A:1144:VAL:HG23	1:A:1310:ILE:HG23	1.84	0.59
15:O:469:ASN:H	15:O:478:VAL:HG22	1.67	0.59
2:B:137:ARG:HH11	2:B:139:ARG:HB2	1.67	0.59
4:D:129:ALA:HB2	4:D:157:ILE:HG23	1.85	0.59
1:A:1141:ILE:N	1:A:1295:VAL:O	2.31	0.59
1:A:221:ASP:H	15:O:550:GLU:HG3	1.67	0.59
16:P:223:GLU:HB3	16:P:240:ILE:HD13	1.85	0.59
15:O:328:ASP:OD1	15:O:328:ASP:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:TYR:OH	1:A:1379:MET:SD	2.61	0.59
1:A:828:GLN:HB3	2:B:655:ASN:HD21	1.68	0.59
2:B:1007:GLY:O	3:C:69:ARG:NH1	2.35	0.59
13:M:108:SER:OG	13:M:109:ALA:N	2.36	0.59
2:B:299:GLN:HG3	2:B:300:GLN:H	1.68	0.59
4:D:24:GLU:OE2	4:D:30:ASP:HB2	2.03	0.59
2:B:948:GLY:HA2	2:B:952:ARG:NH1	2.17	0.58
1:A:538:LYS:HB3	1:A:687:PRO:HB2	1.85	0.58
1:A:329:SER:HB3	1:A:355:GLN:HE22	1.68	0.58
1:A:666:LYS:HA	1:A:670:GLY:HA3	1.83	0.58
3:C:165:ARG:NH2	3:C:190:ASP:OD1	2.37	0.58
2:B:297:THR:HG23	2:B:298:GLN:HG2	1.84	0.58
7:G:156:VAL:HG11	7:G:190:LYS:HZ3	1.68	0.58
1:A:360:LYS:HA	1:A:365:ARG:HE	1.69	0.58
2:B:775:LYS:HB3	2:B:927:LYS:HA	1.83	0.58
1:A:1257:PHE:HB2	9:I:14:ILE:HB	1.85	0.58
5:E:21:GLU:HB3	5:E:35:VAL:HG21	1.86	0.58
18:R:18:DC:H2"	18:R:19:DT:H5'	1.85	0.58
15:O:633:ARG:HE	16:P:307:HIS:HB2	1.66	0.58
15:O:158:GLU:OE1	15:O:161:GLN:NE2	2.37	0.58
8:H:87:ARG:HB2	8:H:87:ARG:HH11	1.69	0.58
7:G:112:GLN:HG2	7:G:115:LEU:HD13	1.86	0.57
15:O:163:VAL:HG22	15:O:169:LEU:HD22	1.85	0.57
2:B:616:SER:HB2	2:B:621:ARG:HH21	1.68	0.57
1:A:541:LEU:HG	1:A:551:ILE:HD11	1.84	0.57
2:B:860:VAL:HG13	2:B:861:ASN:H	1.69	0.57
15:O:347:ASP:HA	15:O:350:GLU:HB2	1.86	0.57
15:O:620:LEU:HD12	15:O:621:PRO:HD2	1.86	0.57
1:A:225:LEU:O	1:A:229:ASN:ND2	2.37	0.57
1:A:1163:LYS:HZ1	1:A:1280:ARG:CA	2.14	0.57
2:B:832:VAL:HB	12:L:60:ARG:HA	1.86	0.57
2:B:1008:ILE:HG13	2:B:1009:THR:H	1.69	0.57
5:E:83:CYS:SG	5:E:84:ASP:N	2.78	0.57
12:L:50:ASP:OD1	12:L:51:CYS:N	2.36	0.57
1:A:235:LYS:HZ2	15:O:44:PRO:HD2	1.68	0.57
1:A:574:ALA:O	11:K:77:ARG:NH2	2.38	0.57
1:A:991:LYS:HG3	1:A:993:GLU:HG2	1.87	0.57
11:K:107:THR:OG1	11:K:108:TYR:N	2.36	0.57
2:B:57:LEU:HD22	2:B:467:LEU:HD11	1.86	0.57
12:L:49:LYS:N	12:L:51:CYS:SG	2.78	0.57
5:E:200:ARG:NH1	5:E:210:SER:OG	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:THR:HG22	7:G:164:LYS:NZ	2.20	0.57
3:C:140:CYS:HB2	3:C:196:LEU:HD13	1.86	0.57
1:A:402:LEU:HD23	1:A:466:LEU:HD22	1.87	0.57
12:L:28:LYS:HG3	12:L:29:TYR:HD2	1.69	0.57
15:O:159:ILE:HD12	15:O:174:TYR:HE1	1.68	0.57
15:O:288:MET:SD	15:O:291:ARG:NH1	2.78	0.57
1:A:213:ARG:NH1	1:A:213:ARG:O	2.38	0.57
1:A:42:LEU:H	1:A:42:LEU:HD12	1.70	0.57
15:O:540:LEU:HD21	15:O:546:VAL:HG11	1.85	0.56
15:O:228:ARG:HH12	15:O:231:PRO:HD3	1.69	0.56
1:A:22:SER:O	1:A:24:ALA:N	2.36	0.56
6:F:125:LEU:HA	6:F:130:ILE:HD11	1.86	0.56
13:M:113:LYS:NZ	13:M:237:ALA:HB1	2.20	0.56
2:B:161:CYS:SG	2:B:162:ILE:N	2.78	0.56
7:G:157:ASP:OD1	7:G:157:ASP:N	2.37	0.56
2:B:926:VAL:HG11	2:B:930:ASP:HB2	1.87	0.56
15:O:338:ASP:OD1	15:O:339:LEU:N	2.39	0.56
7:G:91:LYS:HG2	7:G:92:CYS:H	1.71	0.56
14:N:392:GLN:HB3	14:N:394:VAL:HG23	1.87	0.56
2:B:87:VAL:HG11	2:B:407:LEU:HB3	1.87	0.56
1:A:112:ALA:HA	1:A:234:ILE:HD11	1.88	0.56
15:O:640:ARG:NH1	17:Q:42:PRO:O	2.36	0.56
15:O:292:ARG:HE	15:O:326:ILE:HD11	1.71	0.56
1:A:39:LEU:O	1:A:41:ASP:N	2.38	0.56
7:G:114:MET:O	7:G:201:GLN:HB3	2.06	0.56
2:B:1004:LEU:HD12	2:B:1017:ILE:HD12	1.88	0.56
2:B:1036:HIS:CE1	2:B:1058:GLY:HA3	2.41	0.56
1:A:799:SER:OG	1:A:800:LYS:N	2.38	0.56
1:A:62:SER:HB3	1:A:65:LEU:HG	1.88	0.56
2:B:554:GLY:H	2:B:598:ALA:HA	1.70	0.56
1:A:473:LEU:HA	1:A:487:SER:HA	1.88	0.56
2:B:934:ASN:OD1	2:B:935:ASP:N	2.38	0.56
1:A:1332:ARG:HB2	1:A:1363:THR:HG21	1.88	0.56
1:A:34:VAL:HG23	1:A:35:SER:H	1.71	0.56
2:B:521:THR:OG1	2:B:609:CYS:SG	2.64	0.55
10:J:12:LYS:HE3	10:J:43:ARG:HH22	1.71	0.55
2:B:242:LEU:HD11	2:B:253:ILE:HD13	1.87	0.55
1:A:1373:ARG:HD3	1:A:1390:GLU:OE2	2.06	0.55
15:O:509:ARG:HG2	16:P:249:TYR:HB2	1.88	0.55
1:A:412:ASN:HB3	1:A:416:LEU:HD13	1.86	0.55
11:K:65:ILE:HD12	11:K:101:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:480:SER:HB3	2:B:483:VAL:HB	1.88	0.55
15:O:343:LYS:O	15:O:347:ASP:N	2.34	0.55
15:O:338:ASP:HB3	15:O:342:ALA:N	2.22	0.55
15:O:549:GLN:HE21	15:O:565:LEU:HD22	1.72	0.55
15:O:191:PHE:HD2	15:O:274:VAL:HG21	1.71	0.55
13:M:89:GLN:HB3	14:N:394:VAL:HG22	1.89	0.55
1:A:1443:PRO:HG3	7:G:52:LEU:HD11	1.89	0.55
5:E:141:VAL:HG23	5:E:142:VAL:H	1.71	0.55
7:G:87:GLY:O	7:G:146:ILE:N	2.30	0.55
1:A:317:ASP:OD1	1:A:320:GLN:NE2	2.39	0.55
7:G:13:ILE:HG13	7:G:66:SER:HB3	1.87	0.55
3:C:80:ALA:HA	3:C:208:CYS:HA	1.87	0.55
5:E:88:VAL:HG21	5:E:117:THR:H	1.72	0.55
1:A:165:LYS:NZ	19:S:13:DT:OP2	2.40	0.55
5:E:28:TYR:HA	5:E:64:PRO:HA	1.89	0.55
7:G:3:ILE:HG13	7:G:76:VAL:HG23	1.88	0.55
14:N:297:MET:SD	14:N:303:ARG:NH1	2.80	0.55
4:D:17:LEU:O	4:D:21:THR:OG1	2.21	0.55
2:B:59:LYS:HE2	2:B:519:HIS:HA	1.87	0.55
3:C:8:GLU:HB3	3:C:11:ARG:HG2	1.89	0.55
13:M:227:LEU:HD11	13:M:231:LEU:HD22	1.88	0.55
4:D:125:ASN:OD1	4:D:126:GLN:N	2.40	0.54
1:A:69:THR:HA	7:G:164:LYS:NZ	2.19	0.54
2:B:569:THR:OG1	14:N:275:GLU:OE2	2.24	0.54
5:E:38:PRO:HB2	5:E:40:GLU:HG2	1.89	0.54
1:A:11:LYS:HG3	2:B:1117:ILE:HD13	1.90	0.54
1:A:481:HIS:HB3	1:A:1099:GLU:OE2	2.07	0.54
1:A:252:ARG:HB3	1:A:253:PRO:HD2	1.88	0.54
5:E:88:VAL:HG23	5:E:117:THR:HG22	1.90	0.54
4:D:15:GLU:HA	4:D:18:LYS:HB3	1.89	0.54
15:O:652:GLN:HG3	15:O:653:MET:HG3	1.90	0.54
15:O:185:TYR:O	15:O:189:SER:N	2.40	0.54
15:O:286:ARG:NH2	15:O:321:GLN:O	2.41	0.54
4:D:17:LEU:HB2	4:D:66:LEU:HD23	1.89	0.54
1:A:100:ILE:HG13	1:A:166:LYS:HD3	1.88	0.54
1:A:413:ARG:NH1	1:A:456:LEU:HB3	2.23	0.54
3:C:197:ARG:NH1	10:J:61:LEU:HD13	2.23	0.54
2:B:727:LEU:HD11	2:B:788:ARG:HE	1.72	0.54
15:O:466:PRO:HG2	15:O:467:PHE:CD2	2.43	0.54
2:B:263:LEU:HD12	2:B:297:THR:HG22	1.89	0.54
16:P:247:LEU:HB3	16:P:252:LYS:HD3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:343:LYS:HA	15:O:346:GLN:HB3	1.89	0.54
7:G:45:CYS:HA	7:G:76:VAL:HA	1.88	0.54
5:E:31:THR:HG22	5:E:34:GLU:HG2	1.88	0.54
2:B:1022:ILE:HG22	2:B:1023:TYR:H	1.73	0.54
5:E:20:LYS:HB3	5:E:35:VAL:HG23	1.90	0.54
2:B:337:VAL:HG23	2:B:338:GLU:H	1.73	0.54
2:B:757:VAL:HG23	2:B:942:ILE:HB	1.90	0.54
2:B:1038:ARG:HH11	2:B:1057:ASP:CG	2.11	0.53
5:E:156:LEU:HD11	5:E:195:VAL:HB	1.89	0.53
2:B:115:PRO:HG3	2:B:163:LEU:HD11	1.88	0.53
15:O:102:ARG:O	15:O:123:ASN:ND2	2.37	0.53
16:P:248:VAL:HG23	16:P:255:LYS:HE2	1.90	0.53
9:I:33:PHE:CD1	9:I:34:PRO:HD2	2.44	0.53
1:A:1099:GLU:HA	1:A:1100:PRO:C	2.28	0.53
11:K:80:ILE:HG22	11:K:86:VAL:HG11	1.89	0.53
3:C:33:VAL:O	3:C:34:GLU:HG3	2.08	0.53
7:G:190:LYS:C	7:G:192:PRO:HD3	2.28	0.53
2:B:914:SER:HB3	2:B:918:GLN:HB2	1.90	0.53
4:D:20:LEU:HD12	4:D:62:VAL:HG11	1.90	0.53
13:M:117:HIS:HB2	13:M:119:TRP:CD1	2.44	0.53
7:G:89:ILE:HD12	7:G:97:ILE:HB	1.91	0.53
3:C:163:TYR:HD2	3:C:165:ARG:NH1	2.07	0.53
14:N:366:HIS:HB3	14:N:370:LYS:HB2	1.91	0.53
10:J:30:LEU:HD22	10:J:31:ASP:H	1.73	0.53
15:O:322:LYS:HB3	15:O:361:PHE:CE1	2.42	0.53
12:L:30:ILE:N	12:L:57:LEU:O	2.42	0.53
2:B:1061:ARG:HG2	18:R:17:DC:H5"	1.90	0.53
1:A:1059:LEU:HD21	8:H:105:GLU:HA	1.91	0.53
1:A:235:LYS:HD2	1:A:252:ARG:HH11	1.74	0.53
15:O:541:ILE:HD11	15:O:548:ILE:HG12	1.91	0.53
5:E:112:TYR:HE2	5:E:134:THR:HB	1.74	0.53
1:A:1420:THR:HA	2:B:1080:LEU:HD11	1.91	0.53
2:B:618:GLY:HA2	2:B:668:PRO:HB3	1.90	0.53
13:M:80:GLY:HA3	13:M:261:LYS:HE2	1.90	0.53
8:H:50:ALA:N	8:H:53:ASP:OD2	2.42	0.53
6:F:115:THR:HG22	6:F:116:ASP:H	1.73	0.53
15:O:464:ASN:O	15:O:467:PHE:N	2.43	0.52
5:E:88:VAL:HB	5:E:120:ALA:HB2	1.91	0.52
14:N:308:GLN:HB2	14:N:417:VAL:HG12	1.90	0.52
1:A:1223:ASN:HB3	1:A:1231:ALA:HB3	1.91	0.52
2:B:536:LEU:HD22	2:B:571:PHE:CD1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:256:ILE:HG22	3:C:267:VAL:HA	1.90	0.52
1:A:200:GLU:HG2	15:O:515:LYS:HD2	1.90	0.52
8:H:114:VAL:HG21	8:H:130:ARG:HH11	1.74	0.52
2:B:667:VAL:O	2:B:669:SER:N	2.41	0.52
15:O:551:VAL:HG23	15:O:563:VAL:HG23	1.92	0.52
11:K:47:ILE:HG23	11:K:63:PHE:HB3	1.92	0.52
7:G:113:ASN:OD1	7:G:113:ASN:N	2.39	0.52
1:A:244:ILE:HG21	1:A:253:PRO:HD3	1.90	0.52
2:B:332:ILE:HG13	2:B:333:ALA:H	1.74	0.52
14:N:290:ILE:HG13	14:N:293:LYS:HE2	1.90	0.52
1:A:1207:VAL:O	1:A:1211:ARG:HG2	2.08	0.52
1:A:1311:GLY:O	5:E:147:HIS:NE2	2.42	0.52
1:A:247:THR:HG23	1:A:249:PRO:HD3	1.92	0.52
14:N:304:PHE:O	14:N:413:ASP:N	2.35	0.52
2:B:299:GLN:OE1	13:M:190:ASN:ND2	2.43	0.52
2:B:1067:ARG:HH12	2:B:1079:LEU:HD22	1.75	0.52
1:A:1384:LEU:HD12	1:A:1413:GLU:OE2	2.10	0.52
3:C:229:LEU:O	3:C:293:ARG:NH2	2.38	0.52
15:O:467:PHE:HE1	15:O:468:LEU:HD22	1.74	0.52
14:N:363:ILE:HG23	14:N:373:VAL:HG22	1.92	0.52
11:K:85:ASP:O	11:K:107:THR:OG1	2.19	0.52
16:P:254:GLU:HB2	16:P:262:ARG:HB2	1.92	0.52
15:O:337:GLN:O	15:O:338:ASP:HB2	2.09	0.52
1:A:1145:LEU:HD23	1:A:1146:VAL:HG23	1.92	0.52
2:B:536:LEU:HD22	2:B:571:PHE:HD1	1.75	0.52
13:M:96:LEU:O	13:M:97:VAL:HG12	2.09	0.52
1:A:535:MET:O	1:A:540:ASN:ND2	2.42	0.52
1:A:652:VAL:HG21	1:A:668:VAL:HG21	1.91	0.52
2:B:712:ALA:O	2:B:717:GLN:NE2	2.43	0.52
1:A:614:ILE:HD13	1:A:624:ILE:HD12	1.92	0.52
15:O:40:ARG:O	16:P:317:TRP:NE1	2.43	0.52
11:K:112:THR:HG22	11:K:113:ALA:H	1.75	0.52
5:E:109:ILE:HG22	5:E:133:GLU:HB3	1.92	0.52
1:A:304:ASP:O	15:O:535:SER:OG	2.15	0.51
1:A:182:THR:HG22	1:A:185:TRP:HE1	1.75	0.51
4:D:57:GLY:O	4:D:61:ASN:ND2	2.43	0.51
2:B:137:ARG:NH2	2:B:413:ALA:O	2.36	0.51
1:A:221:ASP:N	15:O:550:GLU:HG3	2.25	0.51
18:R:8:DG:N2	19:S:11:DC:O2	2.42	0.51
5:E:50:MET:HG2	5:E:52:ARG:NH1	2.25	0.51
2:B:526:GLU:O	2:B:529:ILE:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:289:LYS:HD3	15:O:325:LYS:HB3	1.92	0.51
1:A:1221:ASP:OD1	1:A:1222:VAL:N	2.43	0.51
2:B:296:TYR:O	2:B:300:GLN:NE2	2.35	0.51
7:G:89:ILE:HG12	7:G:90:SER:N	2.24	0.51
1:A:653:ILE:HG23	1:A:660:LEU:HB2	1.91	0.51
1:A:578:GLN:O	1:A:582:MET:N	2.43	0.51
15:O:188:SER:HA	15:O:191:PHE:HB2	1.92	0.51
3:C:120:LEU:HD13	3:C:125:LYS:HA	1.92	0.51
16:P:311:VAL:O	16:P:313:TYR:N	2.44	0.51
2:B:59:LYS:HZ2	2:B:60:GLN:NE2	2.09	0.51
1:A:383:PRO:HB3	1:A:502:GLU:HG2	1.92	0.51
1:A:1323:PHE:HA	1:A:1327:GLY:HA2	1.93	0.51
1:A:305:LYS:HG3	1:A:306:GLY:H	1.76	0.51
1:A:12:ARG:HG3	2:B:1146:ILE:HG12	1.92	0.51
1:A:155:LEU:HG	15:O:336:LEU:HD23	1.92	0.51
2:B:137:ARG:HG2	2:B:138:GLY:H	1.75	0.51
13:M:78:ILE:HG22	13:M:170:LEU:HD22	1.93	0.51
1:A:363:ARG:NH1	2:B:1131:GLU:OE2	2.43	0.51
8:H:21:ASN:OD1	8:H:22:LYS:N	2.42	0.51
2:B:853:ASP:HB2	2:B:855:PRO:HD3	1.93	0.51
1:A:200:GLU:HA	15:O:515:LYS:HE3	1.92	0.51
1:A:127:LEU:HD11	1:A:140:ILE:HG21	1.93	0.51
4:D:3:VAL:HG13	7:G:7:ILE:HG22	1.93	0.51
3:C:94:ASP:N	3:C:94:ASP:OD1	2.42	0.51
13:M:117:HIS:CE1	13:M:152:GLY:HA3	2.45	0.51
3:C:201:GLU:OE2	3:C:203:SER:HB2	2.10	0.51
1:A:629:LYS:HB3	1:A:633:PHE:HE2	1.76	0.51
15:O:265:VAL:HG12	15:O:267:PRO:HD3	1.93	0.51
1:A:60:VAL:HG23	1:A:74:LEU:HD23	1.93	0.51
2:B:59:LYS:NZ	2:B:520:ILE:HG13	2.25	0.51
2:B:44:LYS:NZ	2:B:663:GLU:HB2	2.26	0.51
9:I:15:THR:HG23	9:I:23:THR:HG23	1.92	0.50
12:L:29:TYR:HA	12:L:58:LYS:HA	1.93	0.50
5:E:20:LYS:O	5:E:23:VAL:HG12	2.11	0.50
14:N:303:ARG:HD3	14:N:411:ARG:HD3	1.93	0.50
2:B:262:ILE:HD11	13:M:180:LYS:NZ	2.26	0.50
2:B:140:ASN:O	2:B:140:ASN:ND2	2.45	0.50
3:C:255:VAL:HG22	3:C:256:ILE:H	1.76	0.50
2:B:723:THR:HA	2:B:790:LYS:HG2	1.94	0.50
2:B:989:LYS:HA	2:B:992:VAL:HG12	1.92	0.50
2:B:390:ASP:OD2	2:B:444:LEU:HG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:VAL:HG22	7:G:37:LYS:HB3	1.93	0.50
15:O:201:ILE:HG22	15:O:202:GLN:H	1.76	0.50
2:B:103:LYS:NZ	2:B:146:ASP:HB2	2.25	0.50
16:P:223:GLU:HG2	16:P:240:ILE:HA	1.94	0.50
1:A:90:VAL:HG13	1:A:258:TRP:HB2	1.93	0.50
2:B:823:SER:OG	2:B:831:GLU:OE2	2.26	0.50
1:A:1048:VAL:HG11	1:A:1053:LYS:HB2	1.93	0.50
7:G:124:GLU:O	7:G:125:GLU:HB3	2.12	0.50
2:B:83:ILE:HG13	2:B:93:LEU:HB3	1.93	0.50
5:E:123:LEU:HD11	5:E:126:SER:HB3	1.93	0.50
15:O:299:LEU:HD22	15:O:467:PHE:HE2	1.76	0.50
12:L:28:LYS:HG3	12:L:29:TYR:CD2	2.47	0.50
12:L:48:CYS:CB	12:L:51:CYS:HB2	2.38	0.50
5:E:173:SER:OG	5:E:174:GLN:N	2.44	0.50
1:A:226:LYS:HE2	15:O:548:ILE:HG13	1.93	0.50
16:P:219:GLN:HB3	16:P:259:ASP:CG	2.32	0.50
5:E:170:LEU:HB3	5:E:174:GLN:NE2	2.27	0.50
1:A:524:THR:HG23	1:A:527:ALA:H	1.76	0.50
1:A:1273:LYS:HG2	1:A:1274:GLY:H	1.76	0.50
2:B:487:ARG:HH21	2:B:508:CYS:HB3	1.77	0.50
15:O:314:ILE:HG21	15:O:370:LEU:HD21	1.94	0.50
1:A:67:CYS:SG	1:A:69:THR:OG1	2.68	0.50
1:A:310:ASN:ND2	15:O:561:ARG:HD3	2.27	0.50
15:O:463:SER:HB3	16:P:262:ARG:HH12	1.77	0.50
1:A:1205:ILE:O	1:A:1209:ILE:N	2.44	0.50
7:G:44:LEU:O	7:G:77:PHE:N	2.44	0.49
2:B:1067:ARG:HH22	2:B:1079:LEU:HB3	1.77	0.49
12:L:29:TYR:CE2	12:L:40:LEU:HB2	2.45	0.49
2:B:831:GLU:OE1	2:B:831:GLU:N	2.38	0.49
1:A:1143:ALA:HA	1:A:1314:THR:HG22	1.93	0.49
1:A:723:LEU:HD21	1:A:811:ALA:HA	1.93	0.49
13:M:72:GLU:O	14:N:364:ARG:HG2	2.12	0.49
2:B:258:LYS:O	2:B:297:THR:OG1	2.16	0.49
1:A:896:LEU:HB3	1:A:1090:GLY:HA3	1.94	0.49
1:A:842:PRO:O	1:A:843:GLN:HB3	2.13	0.49
2:B:113:THR:OG1	2:B:117:GLU:OE1	2.24	0.49
2:B:247:ILE:HG12	2:B:251:ILE:HD11	1.94	0.49
5:E:213:ILE:HG12	5:E:214:CYS:H	1.77	0.49
3:C:90:SER:HB2	3:C:200:GLN:HB3	1.94	0.49
5:E:115:ASN:OD1	5:E:116:ILE:N	2.45	0.49
6:F:134:ILE:N	6:F:146:TRP:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1372:THR:HG23	1:A:1375:GLY:H	1.77	0.49
1:A:984:VAL:HG21	1:A:988:ASP:HB3	1.94	0.49
3:C:45:SER:HB2	3:C:53:ASN:HB3	1.92	0.49
7:G:121:TYR:HB2	7:G:128:TRP:CZ3	2.47	0.49
15:O:574:TYR:HB3	15:O:578:ARG:HH12	1.77	0.49
1:A:127:LEU:HD22	1:A:240:GLU:OE2	2.12	0.49
2:B:404:ASP:HA	2:B:407:LEU:HB2	1.93	0.49
15:O:327:ARG:HH12	15:O:330:LEU:HD22	1.78	0.49
15:O:195:CYS:SG	15:O:196:GLU:N	2.86	0.49
16:P:215:TYR:CZ	16:P:262:ARG:HD3	2.48	0.49
15:O:500:LEU:HD23	15:O:504:ALA:HB2	1.93	0.49
1:A:356:ARG:NH2	2:B:1046:LEU:HD21	2.28	0.49
14:N:292:ARG:O	14:N:296:LYS:N	2.46	0.49
15:O:50:LYS:HA	15:O:53:VAL:HG12	1.93	0.49
2:B:211:GLU:HG3	2:B:212:LYS:HD2	1.93	0.49
2:B:417:ASP:O	2:B:421:SER:HB2	2.12	0.49
2:B:615:VAL:HG12	2:B:620:SER:HA	1.94	0.49
2:B:217:GLN:HG2	2:B:232:TYR:CD1	2.48	0.49
3:C:280:LEU:HA	3:C:286:ALA:HB2	1.95	0.49
3:C:239:ILE:HG22	3:C:288:LYS:HE2	1.95	0.49
1:A:204:VAL:HG12	1:A:212:GLU:OE2	2.13	0.49
1:A:1163:LYS:NZ	1:A:1280:ARG:HA	2.19	0.48
3:C:29:ASN:HB2	3:C:35:LYS:HZ1	1.76	0.48
1:A:303:LEU:HG	15:O:538:ALA:HB1	1.95	0.48
2:B:210:ASP:OD1	2:B:211:GLU:N	2.45	0.48
1:A:599:LYS:HG3	1:A:600:PRO:HD3	1.94	0.48
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.93	0.48
2:B:756:THR:HG23	2:B:941:ASP:H	1.78	0.48
2:B:849:THR:HG23	2:B:850:ASN:H	1.78	0.48
15:O:581:LEU:HD13	15:O:648:TRP:CD2	2.48	0.48
16:P:247:LEU:CB	16:P:252:LYS:HD3	2.44	0.48
2:B:934:ASN:HA	2:B:1005:TYR:CD2	2.48	0.48
7:G:162:SER:O	7:G:166:ARG:N	2.41	0.48
15:O:291:ARG:HA	15:O:294:LYS:HD3	1.94	0.48
1:A:481:HIS:CD2	1:A:483:LEU:HB2	2.49	0.48
2:B:625:ILE:HD12	2:B:628:ARG:HE	1.79	0.48
8:H:39:THR:N	8:H:124:ARG:O	2.41	0.48
16:P:221:ILE:O	16:P:225:ILE:N	2.43	0.48
1:A:955:LEU:HD13	1:A:959:ILE:HG12	1.94	0.48
8:H:105:GLU:HG2	8:H:115:TYR:HE1	1.79	0.48
4:D:61:ASN:HB3	7:G:103:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:329:LYS:NZ	11:K:122:LYS:HB2	2.29	0.48
1:A:742:ILE:HD11	1:A:840:LYS:HE2	1.96	0.48
8:H:8:ASP:OD1	8:H:9:ILE:N	2.43	0.48
1:A:232:LYS:NZ	16:P:316:GLU:HB3	2.28	0.48
16:P:252:LYS:HZ2	16:P:253:LEU:HB2	1.78	0.48
15:O:215:TRP:O	15:O:219:TYR:HB2	2.14	0.48
1:A:862:LEU:HD21	2:B:491:PRO:HA	1.95	0.48
2:B:720:ARG:NH2	2:B:722:ASP:OD2	2.37	0.48
1:A:1187:ARG:HG2	1:A:1229:ARG:HG3	1.95	0.48
15:O:583:TRP:HE1	16:P:315:ASP:HB3	1.79	0.48
1:A:1347:GLY:O	1:A:1348:MET:HG2	2.13	0.48
9:I:23:THR:OG1	9:I:24:LEU:N	2.47	0.48
9:I:33:PHE:CG	9:I:34:PRO:HD2	2.49	0.48
15:O:159:ILE:HD12	15:O:174:TYR:CE1	2.48	0.48
1:A:980:SER:HB3	5:E:163:GLU:HG2	1.95	0.48
18:R:3:DG:N2	19:S:16:DC:N3	2.62	0.48
2:B:464:ILE:O	2:B:468:GLY:N	2.45	0.48
1:A:1225:ILE:HG23	1:A:1226:GLY:H	1.79	0.48
2:B:775:LYS:HE3	2:B:927:LYS:HA	1.94	0.48
2:B:86:ASP:O	2:B:87:VAL:HG23	2.14	0.48
2:B:727:LEU:HB2	2:B:786:GLU:HB2	1.95	0.48
3:C:255:VAL:HG13	3:C:256:ILE:H	1.79	0.48
7:G:23:ILE:HG22	7:G:51:LEU:HD23	1.96	0.48
15:O:564:PHE:C	15:O:565:LEU:HD12	2.34	0.48
3:C:197:ARG:HH11	10:J:61:LEU:HD13	1.78	0.48
1:A:599:LYS:H	1:A:602:TYR:HE1	1.61	0.48
1:A:1325:VAL:HG23	1:A:1326:LEU:H	1.79	0.48
1:A:1140:ILE:HG22	1:A:1296:GLU:HG3	1.95	0.48
2:B:371:TYR:HB2	2:B:492:SER:OG	2.13	0.48
15:O:299:LEU:HD22	15:O:467:PHE:CE2	2.49	0.47
15:O:467:PHE:HD1	15:O:468:LEU:HB2	1.79	0.47
15:O:203:ILE:HG13	15:O:203:ILE:O	2.14	0.47
16:P:264:THR:HG23	16:P:265:LEU:H	1.78	0.47
2:B:776:SER:HA	2:B:779:ASP:HB3	1.95	0.47
17:Q:48:THR:HG22	17:Q:51:GLU:H	1.79	0.47
1:A:1441:LEU:HD21	7:G:54:VAL:HG12	1.96	0.47
15:O:553:ARG:NH1	15:O:554:THR:HB	2.29	0.47
10:J:16:ASP:OD1	10:J:16:ASP:N	2.47	0.47
1:A:1020:ALA:HA	1:A:1032:LEU:HD21	1.96	0.47
3:C:284:GLU:CD	3:C:288:LYS:HZ1	2.18	0.47
10:J:7:CYS:SG	10:J:11:GLY:N	2.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:ILE:HA	2:B:425:HIS:HB3	1.96	0.47
2:B:811:VAL:HG12	2:B:813:GLU:H	1.79	0.47
3:C:3:ASN:HD21	3:C:296:ASN:HB2	1.79	0.47
7:G:104:ILE:HG13	7:G:105:PHE:CD2	2.48	0.47
15:O:328:ASP:OD1	15:O:329:PRO:HD3	2.13	0.47
2:B:519:HIS:O	2:B:609:CYS:N	2.45	0.47
1:A:1411:VAL:HG13	1:A:1412:SER:H	1.78	0.47
3:C:105:PRO:HG3	10:J:6:ARG:HH21	1.79	0.47
3:C:43:ASN:HB2	3:C:55:ASP:HB3	1.96	0.47
1:A:766:ILE:HG21	1:A:822:ARG:NH1	2.30	0.47
15:O:255:LYS:HB3	15:O:256:PRO:HD3	1.97	0.47
1:A:1134:LYS:HA	1:A:1320:LEU:HD23	1.95	0.47
14:N:375:ILE:HG22	14:N:376:GLY:H	1.80	0.47
15:O:54:LYS:HA	15:O:58:GLY:HA2	1.96	0.47
5:E:117:THR:OG1	5:E:118:PRO:HD2	2.15	0.47
5:E:86:PRO:HA	5:E:113:GLN:HB3	1.97	0.47
2:B:698:ARG:NH2	2:B:952:ARG:HG2	2.28	0.47
1:A:387:LEU:HD21	1:A:393:ALA:HB2	1.95	0.47
1:A:1408:VAL:HG23	1:A:1413:GLU:HG3	1.95	0.47
8:H:87:ARG:HB2	8:H:87:ARG:NH1	2.29	0.47
1:A:408:VAL:HG23	1:A:412:ASN:HB2	1.96	0.47
2:B:992:VAL:HG23	3:C:278:GLU:HG2	1.97	0.47
1:A:1284:ASN:OD1	1:A:1285:ILE:N	2.47	0.47
2:B:331:VAL:HG23	2:B:335:LEU:HD22	1.97	0.47
1:A:1095:GLN:NE2	2:B:1068:ASP:OD2	2.44	0.47
1:A:444:LEU:HD21	1:A:449:ARG:HG2	1.96	0.47
5:E:70:SER:OG	5:E:71:LYS:N	2.47	0.47
1:A:1064:GLU:HB3	1:A:1065:LYS:H	1.43	0.47
1:A:308:SER:N	1:A:311:ASN:HD21	2.12	0.47
7:G:151:GLU:HB3	7:G:198:GLY:HA2	1.97	0.47
1:A:674:LYS:NZ	1:A:928:GLY:HA2	2.29	0.47
7:G:118:GLY:HA3	7:G:131:PRO:HD3	1.96	0.47
2:B:225:HIS:HA	2:B:446:ARG:HH11	1.80	0.47
9:I:34:PRO:O	9:I:35:ILE:HG13	2.15	0.47
1:A:21:LEU:HD22	1:A:25:ASP:OD2	2.14	0.47
14:N:316:PHE:HE1	14:N:360:VAL:HA	1.80	0.47
7:G:80:PHE:CE2	7:G:83:GLU:HB2	2.50	0.47
1:A:1390:GLU:OE2	18:R:13:DT:H4'	2.15	0.47
15:O:506:ARG:HH12	15:O:526:ALA:HB1	1.79	0.47
5:E:55:ARG:HD2	5:E:82:PHE:HE2	1.80	0.47
2:B:741:ILE:HB	2:B:746:TYR:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ASN:N	1:A:333:ASN:OD1	2.48	0.47
1:A:235:LYS:HZ1	15:O:44:PRO:HG2	1.80	0.46
15:O:325:LYS:HD3	15:O:480:TYR:CD1	2.50	0.46
2:B:204:ARG:NH1	2:B:204:ARG:HB2	2.30	0.46
5:E:143:ASN:N	5:E:143:ASN:OD1	2.48	0.46
1:A:311:ASN:OD1	1:A:312:MET:N	2.43	0.46
1:A:890:MET:O	1:A:894:GLU:N	2.48	0.46
2:B:613:ILE:HG12	2:B:646:VAL:HG12	1.97	0.46
1:A:395:PRO:HG2	1:A:398:VAL:HG22	1.97	0.46
2:B:299:GLN:HB2	13:M:190:ASN:HD22	1.81	0.46
1:A:183:PHE:CD2	1:A:184:ARG:HG3	2.51	0.46
14:N:296:LYS:HD3	14:N:296:LYS:HA	1.76	0.46
2:B:108:THR:OG1	2:B:109:LYS:N	2.47	0.46
5:E:1:MET:HB3	5:E:4:GLU:HG2	1.97	0.46
4:D:98:MET:SD	4:D:160:TYR:OH	2.72	0.46
3:C:30:GLU:HG3	11:K:84:PRO:HD3	1.96	0.46
15:O:51:GLU:OE2	15:O:589:LEU:HB3	2.15	0.46
1:A:133:ASP:OD1	1:A:134:ASN:N	2.48	0.46
15:O:467:PHE:CD1	15:O:468:LEU:HB2	2.50	0.46
15:O:549:GLN:HB2	15:O:565:LEU:O	2.14	0.46
2:B:543:LEU:HG	13:M:176:VAL:HG11	1.97	0.46
2:B:262:ILE:HD11	13:M:180:LYS:HZ3	1.80	0.46
1:A:14:LYS:NZ	2:B:1144:GLU:OE1	2.41	0.46
2:B:269:MET:O	2:B:273:CYS:HB3	2.14	0.46
4:D:130:ASN:HB3	4:D:133:HIS:CE1	2.51	0.46
4:D:135:TYR:HA	4:D:141:CYS:SG	2.55	0.46
1:A:1425:THR:C	6:F:92:ARG:HH21	2.19	0.46
2:B:854:ALA:N	2:B:855:PRO:HD3	2.31	0.46
3:C:127:THR:HG22	3:C:128:ASP:H	1.81	0.46
6:F:143:PHE:O	6:F:144:GLU:HB2	2.16	0.46
1:A:386:ASN:ND2	11:K:94:PRO:O	2.48	0.46
16:P:257:THR:OG1	16:P:258:HIS:N	2.48	0.46
16:P:255:LYS:HE3	16:P:261:TYR:CE1	2.50	0.46
1:A:1033:GLU:HG2	1:A:1034:PRO:HD2	1.96	0.46
2:B:378:GLU:OE2	2:B:382:GLN:HB2	2.15	0.46
1:A:69:THR:CG2	7:G:164:LYS:HZ3	2.28	0.46
2:B:916:HIS:CD2	2:B:957:LYS:HB2	2.51	0.46
1:A:444:LEU:HD11	1:A:449:ARG:H	1.81	0.46
2:B:98:ILE:HG13	2:B:131:VAL:HG12	1.97	0.46
19:S:14:DG:H2"	19:S:15:DA:C8	2.50	0.46
1:A:179:ILE:HD12	15:O:557:ARG:NE	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:192:VAL:HG12	15:O:274:VAL:H	1.80	0.46
5:E:6:GLU:HA	5:E:9:ILE:HG12	1.98	0.46
2:B:121:ARG:CZ	12:L:54:ARG:HH21	2.29	0.46
3:C:251:PHE:CD2	3:C:255:VAL:HG21	2.51	0.46
2:B:831:GLU:OE2	2:B:834:MET:HB3	2.17	0.46
1:A:978:ASP:N	1:A:982:CYS:O	2.45	0.46
1:A:1153:ALA:HA	1:A:1156:VAL:HB	1.96	0.46
3:C:74:GLU:HA	3:C:212:ILE:HD11	1.97	0.46
13:M:255:PHE:O	13:M:259:ILE:HG12	2.15	0.46
4:D:10:PHE:HD2	4:D:117:LYS:HE3	1.81	0.46
3:C:175:GLN:O	3:C:178:THR:HG23	2.16	0.46
1:A:869:ARG:HH21	2:B:489:LEU:HD12	1.81	0.46
15:O:282:ILE:HG22	15:O:283:ASN:H	1.80	0.46
3:C:81:GLU:OE2	3:C:219:PHE:HZ	1.98	0.45
13:M:122:ASP:HB3	13:M:145:VAL:HG21	1.98	0.45
1:A:1059:LEU:HD22	1:A:1060:TYR:CE1	2.51	0.45
16:P:216:SER:HB3	16:P:222:LEU:HD11	1.97	0.45
2:B:572:VAL:HG12	2:B:576:ARG:HH12	1.80	0.45
1:A:1451:LEU:HG	4:D:107:MET:HB3	1.98	0.45
1:A:542:LEU:HD21	1:A:679:TYR:HE1	1.80	0.45
2:B:1088:ASP:OD1	2:B:1088:ASP:N	2.49	0.45
13:M:126:ASP:HB3	13:M:128:GLN:HG2	1.97	0.45
15:O:620:LEU:HD23	15:O:623:GLU:HB2	1.98	0.45
2:B:312:MET:HB3	2:B:317:LEU:HG	1.98	0.45
2:B:92:TYR:CZ	2:B:136:THR:HG21	2.51	0.45
2:B:795:LEU:HB2	2:B:894:ALA:HB3	1.99	0.45
5:E:29:PHE:HB2	5:E:65:THR:HB	1.97	0.45
2:B:239:LYS:NZ	2:B:241:TYR:CZ	2.81	0.45
15:O:515:LYS:O	15:O:516:LEU:HD12	2.16	0.45
3:C:229:LEU:HB3	3:C:293:ARG:CZ	2.47	0.45
4:D:110:LEU:O	4:D:120:LYS:NZ	2.50	0.45
1:A:132:VAL:HG11	1:A:137:ARG:HH11	1.81	0.45
15:O:191:PHE:O	15:O:194:LEU:HB2	2.17	0.45
2:B:625:ILE:HD11	2:B:628:ARG:HH21	1.81	0.45
3:C:116:VAL:HG22	3:C:117:ASP:H	1.81	0.45
1:A:51:ASN:O	1:A:55:ASP:HB2	2.15	0.45
4:D:109:LYS:HB3	4:D:109:LYS:NZ	2.32	0.45
3:C:255:VAL:HG13	3:C:256:ILE:N	2.32	0.45
15:O:492:TYR:HH	15:O:573:SER:HG	1.63	0.45
1:A:163:VAL:HG22	1:A:164:VAL:H	1.81	0.45
5:E:172:GLU:HG2	5:E:173:SER:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:52:LEU:O	7:G:53:THR:HG22	2.17	0.45
15:O:289:LYS:NZ	15:O:325:LYS:HG2	2.32	0.45
1:A:1391:LYS:NZ	18:R:12:DT:H4'	2.32	0.45
15:O:87:ASP:O	15:O:88:VAL:HG12	2.16	0.45
4:D:116:PHE:O	4:D:120:LYS:HB2	2.16	0.45
1:A:235:LYS:HD3	1:A:235:LYS:HA	1.83	0.45
1:A:1151:GLU:HG3	1:A:1152:ARG:H	1.81	0.45
1:A:372:ARG:HG3	2:B:1060:LEU:O	2.17	0.45
2:B:1000:GLY:HA3	2:B:1018:PHE:HD1	1.81	0.45
1:A:11:LYS:NZ	2:B:1145:ASP:HB3	2.32	0.45
1:A:1323:PHE:HD1	1:A:1328:ILE:H	1.63	0.45
2:B:93:LEU:HD12	2:B:134:GLU:O	2.17	0.45
1:A:742:ILE:HG12	1:A:840:LYS:HB3	1.99	0.45
7:G:119:CYS:HA	7:G:129:ILE:O	2.17	0.45
7:G:159:LYS:N	7:G:160:PRO:HD3	2.32	0.45
1:A:1173:VAL:HG22	1:A:1186:VAL:HG12	1.98	0.45
2:B:804:ASP:N	2:B:804:ASP:OD1	2.49	0.45
1:A:310:ASN:HD21	15:O:561:ARG:N	2.10	0.45
1:A:62:SER:H	1:A:65:LEU:HD12	1.82	0.45
4:D:20:LEU:HD21	7:G:47:THR:HG21	1.99	0.45
2:B:889:SER:OG	2:B:893:GLN:HG2	2.17	0.45
2:B:465:SER:OG	2:B:707:LYS:O	2.33	0.45
15:O:569:LYS:HA	15:O:569:LYS:HD3	1.81	0.45
16:P:245:GLU:HA	16:P:248:VAL:HB	1.99	0.45
13:M:121:ILE:O	13:M:148:LEU:N	2.44	0.45
15:O:550:GLU:O	15:O:550:GLU:HG2	2.17	0.45
3:C:222:VAL:HG13	3:C:302:VAL:HG23	1.99	0.45
3:C:256:ILE:HA	3:C:268:LYS:H	1.81	0.45
2:B:103:LYS:HG2	2:B:104:SER:H	1.82	0.45
2:B:77:ILE:HD13	2:B:98:ILE:HB	1.98	0.45
1:A:332:VAL:C	1:A:334:PRO:HD3	2.37	0.45
1:A:913:GLN:NE2	1:A:915:THR:O	2.50	0.45
1:A:997:GLN:HB2	1:A:998:TYR:HD1	1.82	0.44
1:A:1300:LEU:O	1:A:1303:VAL:HG12	2.16	0.44
2:B:217:GLN:NE2	2:B:352:MET:HG2	2.32	0.44
2:B:983:LYS:HG3	2:B:985:GLU:H	1.82	0.44
1:A:1190:LEU:HA	1:A:1193:ILE:HD12	1.99	0.44
7:G:97:ILE:HG22	7:G:128:TRP:NE1	2.32	0.44
1:A:179:ILE:HA	1:A:221:ASP:HA	1.99	0.44
15:O:163:VAL:HA	15:O:169:LEU:HD13	1.99	0.44
3:C:255:VAL:HG22	3:C:256:ILE:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:553:ARG:HH11	15:O:554:THR:HB	1.83	0.44
5:E:47:CYS:HA	5:E:53:PRO:HA	1.98	0.44
2:B:447:PHE:HB3	2:B:449:MET:HG2	1.98	0.44
2:B:289:GLU:HA	2:B:292:LYS:HG2	1.98	0.44
1:A:706:GLY:HA2	2:B:762:TYR:HA	1.99	0.44
1:A:409:THR:O	1:A:411:TYR:N	2.51	0.44
2:B:240:ILE:HG13	2:B:253:ILE:HG21	2.00	0.44
15:O:549:GLN:CD	15:O:567:ARG:HE	2.20	0.44
16:P:252:LYS:HG2	16:P:253:LEU:HG	1.99	0.44
15:O:174:TYR:O	15:O:177:SER:OG	2.28	0.44
2:B:425:HIS:O	2:B:428:ASN:ND2	2.50	0.44
1:A:1163:LYS:HB3	1:A:1164:THR:H	1.41	0.44
15:O:253:ILE:HD13	15:O:330:LEU:HD21	1.99	0.44
7:G:104:ILE:HG23	7:G:105:PHE:N	2.32	0.44
12:L:60:ARG:HG2	12:L:61:THR:H	1.82	0.44
16:P:315:ASP:O	16:P:317:TRP:HD1	1.99	0.44
3:C:85:PHE:CE1	3:C:204:LEU:HD22	2.53	0.44
1:A:378:ARG:HH12	18:R:18:DC:H4'	1.81	0.44
7:G:44:LEU:HD23	7:G:104:ILE:HD11	1.99	0.44
1:A:39:LEU:C	1:A:41:ASP:H	2.21	0.44
2:B:241:TYR:CD2	2:B:250:GLU:HB2	2.53	0.44
1:A:321:LEU:HD22	1:A:336:MET:HG3	2.00	0.44
2:B:97:ASP:OD2	2:B:99:ARG:NH1	2.39	0.44
1:A:365:ARG:HH11	1:A:887:ARG:NH2	2.15	0.44
1:A:22:SER:C	1:A:24:ALA:H	2.21	0.44
2:B:241:TYR:CG	2:B:250:GLU:HB2	2.52	0.44
2:B:804:ASP:HB3	2:B:848:PRO:HD3	1.98	0.44
2:B:842:TYR:HE1	2:B:873:TYR:HB2	1.82	0.44
1:A:630:ASN:ND2	1:A:650:GLY:O	2.51	0.44
1:A:817:ILE:HG13	1:A:821:ASN:O	2.18	0.44
15:O:634:GLU:O	15:O:637:VAL:HG12	2.17	0.44
13:M:88:PHE:HD2	14:N:397:LEU:HD13	1.82	0.44
1:A:627:ASP:OD1	1:A:627:ASP:N	2.51	0.44
2:B:932:PRO:HB3	2:B:1004:LEU:HB3	1.99	0.44
2:B:717:GLN:OE1	2:B:727:LEU:HD22	2.17	0.44
3:C:284:GLU:HA	3:C:287:ASP:OD2	2.18	0.44
15:O:576:PHE:O	15:O:579:GLN:HG2	2.18	0.44
2:B:550:HIS:NE2	2:B:551:LEU:HD23	2.33	0.44
2:B:69:VAL:HA	2:B:73:LEU:HD23	1.99	0.44
14:N:399:ILE:HD13	14:N:406:ALA:H	1.83	0.44
2:B:1008:ILE:O	3:C:65:ASN:ND2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:THR:HG22	1:A:185:TRP:NE1	2.33	0.44
2:B:39:ASN:OD1	2:B:40:THR:N	2.47	0.44
2:B:190:THR:OG1	2:B:191:GLU:N	2.51	0.44
15:O:549:GLN:CG	15:O:565:LEU:HB2	2.46	0.44
2:B:444:LEU:O	2:B:448:LYS:HA	2.18	0.44
3:C:283:GLU:O	3:C:286:ALA:N	2.51	0.44
2:B:803:GLN:HG2	2:B:804:ASP:H	1.82	0.44
17:Q:50:LYS:O	17:Q:53:SER:OG	2.27	0.44
7:G:60:LYS:NZ	7:G:63:ASP:HB2	2.32	0.44
1:A:1202:ILE:HD12	1:A:1228:ASP:HA	1.98	0.44
14:N:373:VAL:HG12	14:N:374:LYS:H	1.83	0.43
1:A:541:LEU:HD22	1:A:682:LEU:HD22	1.98	0.43
1:A:252:ARG:HH12	15:O:46:LEU:HD22	1.83	0.43
2:B:418:ALA:O	2:B:422:ILE:HG12	2.18	0.43
1:A:93:ILE:HG23	1:A:94:GLY:H	1.83	0.43
15:O:74:LEU:HD21	15:O:79:LEU:HG	2.00	0.43
1:A:431:ASN:OD1	1:A:465:HIS:NE2	2.51	0.43
3:C:92:ILE:H	3:C:92:ILE:HG13	1.59	0.43
15:O:641:LEU:O	15:O:645:LEU:HB2	2.17	0.43
2:B:1028:LYS:HG2	2:B:1029:HIS:H	1.83	0.43
18:R:15:DC:H2"	18:R:16:DG:OP2	2.18	0.43
1:A:46:ARG:HG3	1:A:48:PRO:HD3	1.99	0.43
15:O:197:MET:HG3	15:O:198:GLY:H	1.83	0.43
16:P:254:GLU:HG3	16:P:264:THR:HG22	2.01	0.43
1:A:862:LEU:HD22	2:B:494:PHE:HB2	1.99	0.43
15:O:115:LYS:HB3	15:O:116:LYS:H	1.58	0.43
1:A:985:LYS:O	1:A:987:GLU:N	2.51	0.43
8:H:12:VAL:HG12	8:H:13:SER:H	1.82	0.43
2:B:938:ILE:H	2:B:938:ILE:HG13	1.63	0.43
15:O:159:ILE:O	15:O:163:VAL:HG23	2.18	0.43
2:B:934:ASN:HB3	2:B:1004:LEU:HA	2.01	0.43
3:C:33:VAL:HG12	3:C:34:GLU:H	1.84	0.43
14:N:366:HIS:N	14:N:370:LYS:O	2.51	0.43
1:A:988:ASP:O	1:A:992:ALA:N	2.46	0.43
1:A:424:PRO:HG3	1:A:444:LEU:O	2.18	0.43
3:C:177:THR:HG23	3:C:178:THR:H	1.83	0.43
5:E:24:LYS:HB2	5:E:30:ILE:HD11	2.00	0.43
1:A:113:ILE:HG12	1:A:115:LEU:H	1.82	0.43
13:M:228:THR:HG22	13:M:229:GLY:H	1.82	0.43
1:A:387:LEU:O	1:A:501:ASN:ND2	2.51	0.43
3:C:132:ILE:O	3:C:208:CYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:3:DG:H2"	18:R:4:DT:OP2	2.18	0.43
4:D:70:LYS:HG3	4:D:98:MET:SD	2.59	0.43
1:A:143:LYS:HA	1:A:146:ASP:OD2	2.18	0.43
1:A:979:ASN:O	5:E:167:ARG:NH2	2.51	0.43
3:C:328:LEU:HG	11:K:121:LEU:HD21	2.01	0.43
11:K:97:SER:OG	11:K:98:GLU:N	2.52	0.43
1:A:995:VAL:O	1:A:996:ASP:HB3	2.19	0.43
2:B:698:ARG:HH21	2:B:952:ARG:CG	2.29	0.43
2:B:929:GLU:HB3	3:C:69:ARG:HG2	2.00	0.43
1:A:666:LYS:HG2	1:A:797:CYS:O	2.19	0.43
2:B:87:VAL:HG12	2:B:407:LEU:HD22	1.99	0.43
1:A:862:LEU:O	1:A:866:ILE:HG12	2.19	0.43
3:C:59:ILE:HB	3:C:63:ILE:HD11	2.01	0.43
15:O:226:ILE:HG23	15:O:229:ASN:H	1.83	0.43
15:O:262:ILE:HG12	15:O:278:VAL:HG21	2.00	0.43
7:G:89:ILE:HG23	7:G:142:VAL:HA	2.00	0.43
15:O:356:THR:HB	15:O:357:PRO:HD3	2.01	0.43
1:A:310:ASN:HD22	15:O:561:ARG:HD3	1.83	0.43
7:G:7:ILE:O	7:G:71:THR:OG1	2.27	0.43
15:O:597:GLN:HA	15:O:600:SER:HB2	2.01	0.43
13:M:90:TYR:HB3	13:M:179:LEU:HB3	2.01	0.43
1:A:379:THR:HG22	1:A:380:VAL:H	1.84	0.43
1:A:757:ASN:N	1:A:757:ASN:OD1	2.52	0.43
15:O:516:LEU:HB3	15:O:567:ARG:HD3	1.99	0.43
1:A:378:ARG:HH21	1:A:516:GLU:HB2	1.83	0.43
5:E:173:SER:C	5:E:175:LEU:H	2.22	0.43
1:A:1426:GLY:HA2	6:F:92:ARG:NH2	2.34	0.43
7:G:47:THR:OG1	7:G:48:ILE:N	2.51	0.43
11:K:83:ASN:HA	11:K:84:PRO:HD3	1.87	0.43
5:E:43:LYS:O	5:E:47:CYS:HB2	2.19	0.43
1:A:661:SER:HB2	8:H:122:LEU:HD11	1.99	0.43
1:A:1439:LYS:HA	1:A:1439:LYS:HE2	2.00	0.43
1:A:1365:LYS:HE3	1:A:1379:MET:HB2	1.99	0.43
1:A:1442:VAL:HA	1:A:1443:PRO:HD3	1.76	0.43
5:E:40:GLU:HG3	5:E:41:ASP:H	1.82	0.43
15:O:370:LEU:HD13	15:O:370:LEU:HA	1.91	0.43
7:G:147:ARG:NH2	7:G:211:TRP:HH2	2.17	0.43
2:B:327:ILE:O	2:B:330:THR:OG1	2.35	0.43
17:Q:59:ILE:HG22	17:Q:63:LYS:HE3	2.01	0.43
1:A:493:ARG:HB3	1:A:494:PRO:HD2	2.01	0.43
1:A:1038:GLU:HB3	1:A:1042:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:C	1:A:41:ASP:N	2.72	0.43
14:N:290:ILE:HD13	14:N:384:LYS:HE3	2.00	0.43
15:O:53:VAL:HA	15:O:56:HIS:HB3	2.00	0.43
1:A:376:SER:HB2	2:B:1060:LEU:HD12	2.01	0.43
16:P:235:LEU:C	16:P:236:THR:HG1	2.22	0.43
2:B:736:VAL:HG21	2:B:960:GLU:HG3	2.01	0.43
2:B:676:GLU:HA	2:B:677:PRO:HD2	1.91	0.43
16:P:255:LYS:N	16:P:255:LYS:HD2	2.34	0.43
1:A:220:ASP:HA	15:O:550:GLU:OE2	2.19	0.43
8:H:132:LEU:HD12	8:H:133:ASN:N	2.32	0.43
1:A:1084:GLU:O	1:A:1087:THR:OG1	2.34	0.43
2:B:687:LEU:O	2:B:915:ARG:NH2	2.52	0.43
3:C:104:VAL:HA	3:C:105:PRO:HD3	1.90	0.43
2:B:795:LEU:HD23	2:B:845:LYS:HZ2	1.84	0.43
13:M:109:ALA:HB3	13:M:122:ASP:HB2	2.01	0.42
2:B:401:LEU:HA	2:B:404:ASP:OD2	2.19	0.42
2:B:933:PHE:O	2:B:934:ASN:ND2	2.52	0.42
15:O:510:CYS:HA	15:O:513:ASP:OD2	2.19	0.42
1:A:635:PRO:HA	1:A:636:PRO:HD3	1.88	0.42
1:A:545:LYS:HG3	1:A:546:SER:H	1.83	0.42
1:A:1174:GLN:HB3	1:A:1185:GLN:HB3	2.01	0.42
1:A:196:ILE:O	1:A:200:GLU:HG3	2.20	0.42
1:A:393:ALA:HB3	1:A:499:ARG:HG3	2.00	0.42
2:B:88:ASP:CG	2:B:89:PRO:HD2	2.39	0.42
14:N:395:ILE:HD12	14:N:396:ALA:H	1.84	0.42
1:A:165:LYS:HZ2	1:A:184:ARG:HH22	1.67	0.42
1:A:185:TRP:HE3	1:A:194:LYS:HE2	1.85	0.42
1:A:308:SER:OG	1:A:309:ILE:N	2.52	0.42
1:A:774:ARG:HH22	1:A:804:LEU:HD11	1.83	0.42
2:B:610:ARG:HA	2:B:611:PRO:HD3	1.77	0.42
2:B:260:CYS:O	2:B:342:PHE:HB3	2.19	0.42
2:B:905:ARG:O	2:B:907:GLU:N	2.50	0.42
2:B:38:ILE:HD11	2:B:43:ASP:OD2	2.19	0.42
15:O:467:PHE:CE1	15:O:468:LEU:HD22	2.53	0.42
15:O:192:VAL:HG12	15:O:274:VAL:HG13	2.02	0.42
8:H:58:THR:O	8:H:143:LEU:N	2.48	0.42
1:A:1302:ASP:OD1	1:A:1303:VAL:N	2.53	0.42
2:B:364:LYS:HG3	2:B:365:MET:H	1.84	0.42
1:A:667:SER:HA	1:A:671:ASP:O	2.19	0.42
13:M:91:ALA:HA	14:N:391:LEU:HD21	2.01	0.42
2:B:372:VAL:O	2:B:607:ARG:NH1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:113:LYS:HG3	13:M:116:SER:O	2.19	0.42
15:O:105:LYS:HD2	15:O:209:THR:N	2.35	0.42
1:A:712:ILE:HG22	1:A:713:GLY:H	1.84	0.42
1:A:270:PRO:HD3	2:B:1046:LEU:HD13	2.01	0.42
2:B:675:ILE:HG13	2:B:676:GLU:H	1.84	0.42
3:C:192:LEU:HD11	10:J:19:GLU:HG2	2.01	0.42
4:D:113:PHE:CE2	4:D:153:MET:HG2	2.55	0.42
1:A:1166:LEU:O	1:A:1170:ALA:HB2	2.20	0.42
1:A:468:ASP:OD1	1:A:469:GLY:N	2.52	0.42
3:C:20:PHE:CE2	3:C:23:PHE:HB3	2.54	0.42
13:M:164:LYS:NZ	14:N:300:LYS:HG2	2.35	0.42
19:S:6:DA:C8	19:S:6:DA:OP2	2.73	0.42
15:O:156:VAL:HA	15:O:159:ILE:HG12	2.02	0.42
5:E:195:VAL:HG22	5:E:213:ILE:HG13	2.01	0.42
14:N:293:LYS:HA	14:N:296:LYS:HB2	2.02	0.42
15:O:78:GLU:HG2	15:O:82:LYS:HZ1	1.84	0.42
7:G:29:GLN:O	7:G:33:LYS:HG2	2.20	0.42
1:A:952:LYS:HB3	1:A:953:GLY:H	1.53	0.42
2:B:110:ASP:N	2:B:110:ASP:OD1	2.53	0.42
10:J:42:LYS:HG3	10:J:43:ARG:H	1.85	0.42
1:A:235:LYS:HZ2	15:O:44:PRO:CD	2.31	0.42
5:E:82:PHE:CE1	5:E:111:VAL:HB	2.55	0.42
15:O:512:ARG:HH22	15:O:568:CYS:HA	1.84	0.42
2:B:911:LYS:HD3	2:B:919:LYS:NZ	2.35	0.42
2:B:806:ILE:HG13	2:B:806:ILE:H	1.62	0.42
2:B:121:ARG:NH2	12:L:54:ARG:HH21	2.17	0.42
5:E:112:TYR:N	5:E:135:PHE:O	2.45	0.42
15:O:203:ILE:HG12	15:O:279:SER:HB2	2.02	0.42
3:C:120:LEU:HA	3:C:121:PRO:HD2	1.88	0.42
5:E:182:ASP:HA	5:E:183:PRO:HD2	1.85	0.42
2:B:321:GLN:O	2:B:324:ILE:HG22	2.19	0.42
2:B:474:SER:HA	2:B:511:VAL:HG12	2.01	0.42
3:C:260:GLU:HG2	3:C:261:GLY:H	1.84	0.42
3:C:259:ASP:HB2	3:C:266:TYR:HE1	1.85	0.42
7:G:59:LEU:HD13	7:G:65:SER:O	2.19	0.42
1:A:967:LEU:HD11	1:A:1009:ARG:HD3	2.02	0.42
1:A:360:LYS:HD2	1:A:360:LYS:HA	1.83	0.42
15:O:46:LEU:HB3	15:O:47:PHE:H	1.64	0.42
7:G:149:ARG:O	7:G:198:GLY:HA3	2.19	0.42
1:A:1148:ASP:OD1	1:A:1291:ARG:NH1	2.52	0.42
2:B:502:THR:HA	2:B:503:PRO:HD3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:89:ILE:HG12	7:G:90:SER:H	1.85	0.42
7:G:4:LEU:HD23	7:G:73:ARG:HH21	1.85	0.42
7:G:8:ALA:HA	7:G:71:THR:HA	2.01	0.42
2:B:779:ASP:OD2	3:C:217:ALA:N	2.32	0.42
15:O:570:GLU:HG2	15:O:571:THR:N	2.35	0.42
2:B:586:GLU:HG3	2:B:648:TYR:HD2	1.85	0.42
4:D:138:VAL:HG13	4:D:141:CYS:HB2	2.01	0.41
1:A:955:LEU:HA	1:A:956:PRO:HD2	1.89	0.41
15:O:53:VAL:HG21	15:O:65:ILE:HD12	2.01	0.41
1:A:95:TYR:O	1:A:99:THR:N	2.52	0.41
1:A:643:ASN:HB2	1:A:651:PHE:CE2	2.55	0.41
8:H:131:ASN:N	8:H:131:ASN:OD1	2.53	0.41
2:B:529:ILE:HG23	2:B:530:LYS:N	2.35	0.41
3:C:263:ASP:OD1	3:C:264:GLU:N	2.52	0.41
2:B:319:ILE:HA	2:B:319:ILE:HD12	1.92	0.41
8:H:93:TYR:CD2	8:H:143:LEU:HG	2.55	0.41
15:O:193:GLN:NE2	15:O:196:GLU:OE1	2.53	0.41
16:P:314:PHE:CG	16:P:315:ASP:N	2.86	0.41
2:B:800:ASN:ND2	2:B:853:ASP:O	2.51	0.41
5:E:191:LYS:HB2	5:E:194:GLU:OE2	2.20	0.41
3:C:87:ASN:O	3:C:88:ASN:HB2	2.20	0.41
6:F:114:GLU:OE2	6:F:120:ILE:HG22	2.20	0.41
2:B:477:PHE:HB3	2:B:478:GLU:H	1.47	0.41
15:O:591:LYS:HB2	16:P:308:ASP:OD2	2.21	0.41
15:O:43:ASN:HB3	15:O:47:PHE:HB2	2.03	0.41
9:I:35:ILE:CD1	9:I:36:GLU:H	2.32	0.41
2:B:1080:LEU:O	2:B:1084:MET:HB3	2.20	0.41
15:O:169:LEU:O	15:O:279:SER:HB3	2.21	0.41
2:B:915:ARG:HD2	2:B:1023:TYR:HD2	1.85	0.41
15:O:335:LEU:HD12	15:O:336:LEU:O	2.20	0.41
1:A:1065:LYS:HA	1:A:1068:ARG:HB2	2.02	0.41
3:C:91:VAL:HB	3:C:92:ILE:H	1.63	0.41
2:B:124:THR:OG1	2:B:125:TYR:N	2.53	0.41
13:M:82:GLU:O	13:M:83:GLU:HG2	2.20	0.41
13:M:83:GLU:HB2	14:N:400:ALA:HB2	2.01	0.41
1:A:571:TYR:O	1:A:604:TRP:N	2.49	0.41
1:A:220:ASP:HA	15:O:550:GLU:CG	2.50	0.41
2:B:134:GLU:HG2	2:B:144:HIS:ND1	2.35	0.41
15:O:592:LYS:HG3	15:O:637:VAL:HG11	2.03	0.41
1:A:326:TYR:CD2	1:A:327:ILE:HG23	2.56	0.41
11:K:60:SER:HB3	11:K:104:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:152:ARG:HB3	7:G:197:LEU:HG	2.02	0.41
2:B:145:LYS:HD2	2:B:419:LEU:HD21	2.02	0.41
1:A:827:PHE:HB3	2:B:655:ASN:OD1	2.20	0.41
2:B:757:VAL:O	2:B:1019:PHE:HB2	2.19	0.41
3:C:238:PRO:O	3:C:239:ILE:HG13	2.20	0.41
3:C:42:VAL:HG13	11:K:138:LYS:HD3	2.03	0.41
15:O:468:LEU:HA	15:O:468:LEU:HD12	1.85	0.41
1:A:995:VAL:HB	1:A:997:GLN:H	1.86	0.41
1:A:1172:TYR:HE1	1:A:1174:GLN:HB2	1.85	0.41
13:M:246:THR:O	14:N:405:SER:HB2	2.21	0.41
1:A:792:LEU:O	1:A:796:THR:OG1	2.26	0.41
1:A:371:LYS:HB3	1:A:371:LYS:HE3	1.95	0.41
1:A:132:VAL:HG13	1:A:136:ARG:HB2	2.01	0.41
15:O:208:TYR:O	15:O:209:THR:OG1	2.37	0.41
2:B:576:ARG:HG2	2:B:580:ARG:HD3	2.03	0.41
5:E:46:TYR:CZ	5:E:58:MET:HA	2.56	0.41
1:A:1026:ARG:NH2	1:A:1052:VAL:HG13	2.36	0.41
15:O:101:LEU:HD21	15:O:130:LEU:HD11	2.03	0.41
8:H:108:SER:OG	8:H:109:LYS:N	2.53	0.41
2:B:796:LYS:HZ3	2:B:798:TYR:HE1	1.65	0.41
7:G:94:ALA:HB2	7:G:121:TYR:CD2	2.56	0.41
1:A:132:VAL:HG11	1:A:137:ARG:HH12	1.80	0.41
2:B:139:ARG:HB3	2:B:141:ILE:HD11	2.02	0.41
13:M:113:LYS:HE3	13:M:118:LEU:HD23	2.02	0.41
15:O:357:PRO:HA	15:O:361:PHE:CD2	2.55	0.41
15:O:516:LEU:O	15:O:565:LEU:HD23	2.21	0.41
2:B:265:ASP:O	2:B:267:GLU:N	2.54	0.41
15:O:591:LYS:HE2	16:P:308:ASP:OD2	2.20	0.41
16:P:252:LYS:HE3	16:P:252:LYS:HB3	1.94	0.41
5:E:17:ARG:HD3	5:E:35:VAL:HG22	2.03	0.41
4:D:13:ASP:OD2	4:D:66:LEU:HG	2.21	0.41
13:M:74:PHE:CE2	14:N:364:ARG:NH1	2.89	0.41
1:A:14:LYS:HZ3	2:B:1144:GLU:HB3	1.86	0.41
14:N:404:SER:OG	14:N:405:SER:N	2.54	0.41
1:A:1428:PHE:CZ	6:F:89:GLU:HA	2.56	0.41
20:T:12:A:H2'	20:T:13:G:O4'	2.21	0.41
15:O:331:THR:HG1	15:O:345:PHE:HZ	1.65	0.41
2:B:890:ASP:N	2:B:890:ASP:OD1	2.54	0.41
14:N:389:THR:O	14:N:390:PHE:CD2	2.74	0.41
1:A:297:SER:HA	1:A:300:LYS:HB3	2.02	0.41
2:B:841:ILE:HG12	2:B:841:ILE:H	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:115:LEU:HD23	7:G:116:PHE:HD1	1.85	0.41
7:G:34:PHE:O	7:G:37:LYS:HD3	2.21	0.41
3:C:21:PRO:HD2	11:K:82:LYS:HA	2.02	0.41
1:A:1145:LEU:O	1:A:1310:ILE:HG22	2.21	0.41
2:B:934:ASN:ND2	2:B:1004:LEU:HD22	2.36	0.41
1:A:115:LEU:HG	1:A:116:SER:H	1.86	0.41
13:M:160:ALA:HA	14:N:306:VAL:HA	2.03	0.41
15:O:366:LEU:HD23	15:O:452:LEU:HD13	2.03	0.41
2:B:538:VAL:HG12	2:B:565:ILE:HD12	2.02	0.41
15:O:647:LEU:O	15:O:650:VAL:HG12	2.21	0.40
8:H:17:PRO:HB3	8:H:24:CYS:HB2	2.03	0.40
2:B:224:THR:OG1	2:B:225:HIS:N	2.50	0.40
13:M:122:ASP:HB3	13:M:145:VAL:CG2	2.51	0.40
1:A:653:ILE:HG12	1:A:660:LEU:HD22	2.03	0.40
1:A:382:SER:HA	1:A:383:PRO:HD3	1.83	0.40
2:B:180:ASP:HA	2:B:181:PRO:HD3	1.89	0.40
2:B:735:MET:HB2	2:B:754:ASN:HD21	1.85	0.40
1:A:1021:ASN:HA	1:A:1024:LYS:HG2	2.03	0.40
1:A:96:PHE:CZ	1:A:166:LYS:HD2	2.56	0.40
2:B:757:VAL:HG12	2:B:1020:GLY:O	2.21	0.40
15:O:492:TYR:OH	15:O:573:SER:OG	2.32	0.40
8:H:31:THR:OG1	8:H:32:THR:N	2.54	0.40
4:D:151:GLU:HA	4:D:154:LEU:HD13	2.03	0.40
3:C:276:SER:O	3:C:277:ARG:HG2	2.21	0.40
1:A:238:ASP:OD1	1:A:238:ASP:N	2.53	0.40
1:A:620:SER:HA	1:A:621:PRO:HD3	1.85	0.40
15:O:550:GLU:OE1	15:O:550:GLU:N	2.54	0.40
1:A:905:ARG:NH2	5:E:170:LEU:HD21	2.32	0.40
3:C:31:TRP:CE2	11:K:123:ASP:HB3	2.57	0.40
1:A:1184:ILE:O	1:A:1231:ALA:HA	2.21	0.40
18:R:2:DA:H2''	18:R:3:DG:H5'	2.03	0.40
1:A:1083:LEU:HD23	1:A:1083:LEU:HA	1.91	0.40
4:D:31:GLN:HA	4:D:34:LEU:HD12	2.02	0.40
1:A:252:ARG:HH22	15:O:46:LEU:CD2	2.34	0.40
1:A:1391:LYS:HD2	1:A:1391:LYS:HA	1.58	0.40
15:O:568:CYS:HB3	15:O:569:LYS:H	1.48	0.40
1:A:953:GLY:HA2	1:A:1063:SER:HB2	2.02	0.40
3:C:143:ASN:HB3	3:C:156:LEU:O	2.22	0.40
1:A:284:ASP:O	1:A:288:LYS:HG2	2.22	0.40
2:B:257:LEU:HD12	2:B:257:LEU:HA	1.95	0.40
15:O:522:ILE:HD13	15:O:522:ILE:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:34:ILE:HD12	15:O:34:ILE:HA	1.98	0.40
2:B:121:ARG:NH1	12:L:54:ARG:NH2	2.57	0.40
15:O:581:LEU:HD13	15:O:648:TRP:CE2	2.57	0.40
6:F:115:THR:HG22	6:F:116:ASP:N	2.35	0.40
2:B:834:MET:HE3	2:B:834:MET:HB2	1.92	0.40
2:B:113:THR:HA	2:B:114:PRO:HD3	1.88	0.40
2:B:565:ILE:HG12	2:B:566:ARG:N	2.36	0.40
1:A:946:THR:HG21	1:A:1066:SER:HA	2.04	0.40
16:P:180:THR:HG23	16:P:181:ILE:H	1.86	0.40
2:B:688:ILE:H	2:B:688:ILE:HD12	1.87	0.40
4:D:58:ILE:HG13	4:D:58:ILE:H	1.74	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	A	1414/1460 (97%)	1166 (82%)	234 (16%)	14 (1%)	19	64
2	B	1112/1149 (97%)	943 (85%)	160 (14%)	9 (1%)	24	68
3	C	333/335 (99%)	284 (85%)	44 (13%)	5 (2%)	13	57
4	D	113/161 (70%)	83 (74%)	30 (26%)	0	100	100
5	E	213/215 (99%)	172 (81%)	39 (18%)	2 (1%)	21	65
6	F	81/155 (52%)	73 (90%)	8 (10%)	0	100	100
7	G	185/212 (87%)	155 (84%)	24 (13%)	6 (3%)	5	43
8	H	136/146 (93%)	115 (85%)	21 (15%)	0	100	100
9	I	40/110 (36%)	33 (82%)	6 (15%)	1 (2%)	7	48
10	J	65/70 (93%)	53 (82%)	11 (17%)	1 (2%)	13	57
11	K	99/142 (70%)	84 (85%)	15 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	43/70 (61%)	34 (79%)	9 (21%)	0	100	100
13	M	160/282 (57%)	138 (86%)	20 (12%)	2 (1%)	15	59
14	N	106/422 (25%)	82 (77%)	23 (22%)	1 (1%)	21	65
15	O	533/654 (82%)	437 (82%)	89 (17%)	7 (1%)	15	59
16	P	83/317 (26%)	54 (65%)	24 (29%)	5 (6%)	2	27
17	Q	26/104 (25%)	23 (88%)	2 (8%)	1 (4%)	4	38
All	All	4742/6004 (79%)	3929 (83%)	759 (16%)	54 (1%)	23	63

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	587	ILE
1	A	1371	ILE
13	M	97	VAL
13	M	107	ILE
15	O	88	VAL
15	O	146	VAL
16	P	175	ILE
16	P	311	VAL
16	P	312	VAL
1	A	40	PHE
1	A	602	TYR
1	A	632	VAL
2	B	87	VAL
3	C	239	ILE
14	N	411	ARG
15	O	469	ASN
16	P	230	VAL
1	A	39	LEU
1	A	307	ILE
1	A	975	VAL
1	A	995	VAL
2	B	811	VAL
2	B	927	LYS
9	I	35	ILE
1	A	23	ALA
1	A	601	TYR
1	A	1328	ILE
2	B	632	ASP
2	B	651	VAL

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Mol	Chain	Res	Type
2	B	713	ILE
2	B	767	ILE
3	C	91	VAL
3	C	119	ASN
3	C	255	VAL
7	G	191	PRO
15	O	338	ASP
15	O	368	ARG
17	Q	43	ILE
1	A	599	LYS
1	A	1389	PHE
2	B	264	SER
3	C	87	ASN
7	G	79	PRO
7	G	80	PHE
10	J	65	PRO
5	E	122	LYS
15	O	330	LEU
16	P	233	VAL
5	E	88	VAL
7	G	158	VAL
7	G	160	PRO
7	G	192	PRO
2	B	584	VAL
15	O	227	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	A	1231/1257 (98%)	1213 (98%)	18 (2%)	72	89
2	B	975/1006 (97%)	960 (98%)	15 (2%)	72	89
3	C	296/296 (100%)	289 (98%)	7 (2%)	57	82
4	D	110/145 (76%)	107 (97%)	3 (3%)	52	80
5	E	197/197 (100%)	192 (98%)	5 (2%)	55	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	73/137 (53%)	70 (96%)	3 (4%)	37	73
7	G	170/190 (90%)	167 (98%)	3 (2%)	66	87
8	H	123/128 (96%)	121 (98%)	2 (2%)	70	88
9	I	38/98 (39%)	37 (97%)	1 (3%)	54	81
10	J	62/65 (95%)	60 (97%)	2 (3%)	46	78
11	K	91/130 (70%)	91 (100%)	0	100	100
12	L	40/57 (70%)	38 (95%)	2 (5%)	30	68
13	M	142/249 (57%)	136 (96%)	6 (4%)	36	72
14	N	92/360 (26%)	88 (96%)	4 (4%)	35	72
15	O	495/593 (84%)	477 (96%)	18 (4%)	42	76
16	P	86/285 (30%)	85 (99%)	1 (1%)	78	90
17	Q	24/56 (43%)	24 (100%)	0	100	100
All	All	4245/5249 (81%)	4155 (98%)	90 (2%)	64	85

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	160	LEU
1	A	247	THR
1	A	364	PHE
1	A	379	THR
1	A	446	TYR
1	A	506	THR
1	A	712	ILE
1	A	904	VAL
1	A	955	LEU
1	A	1029	LEU
1	A	1053	LYS
1	A	1059	LEU
1	A	1087	THR
1	A	1161	VAL
1	A	1164	THR
1	A	1325	VAL
1	A	1391	LYS
2	B	133	ILE
2	B	296	TYR
2	B	337	VAL

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Mol	Chain	Res	Type
2	B	383	LEU
2	B	427	ASN
2	B	511	VAL
2	B	536	LEU
2	B	545	ASP
2	B	612	LEU
2	B	615	VAL
2	B	723	THR
2	B	818	ILE
2	B	824	LEU
2	B	899	LEU
2	B	954	THR
3	C	33	VAL
3	C	78	VAL
3	C	89	THR
3	C	193	LEU
3	C	208	CYS
3	C	210	LEU
3	C	239	ILE
4	D	29	TRP
4	D	127	LEU
4	D	142	ASP
5	E	6	GLU
5	E	9	ILE
5	E	78	LEU
5	E	117	THR
5	E	124	VAL
6	F	116	ASP
6	F	125	LEU
6	F	133	VAL
7	G	53	THR
7	G	105	PHE
7	G	115	LEU
8	H	44	VAL
8	H	132	LEU
9	I	35	ILE
10	J	13	VAL
10	J	16	ASP
12	L	34	CYS
12	L	48	CYS
13	M	74	PHE
13	M	88	PHE

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Mol	Chain	Res	Type
13	M	97	VAL
13	M	228	THR
13	M	242	ASN
13	M	252	PHE
14	N	313	LEU
14	N	364	ARG
14	N	390	PHE
14	N	412	VAL
15	O	42	LEU
15	O	47	PHE
15	O	88	VAL
15	O	152	HIS
15	O	169	LEU
15	O	174	TYR
15	O	206	LEU
15	O	259	LEU
15	O	282	ILE
15	O	299	LEU
15	O	328	ASP
15	O	335	LEU
15	O	468	LEU
15	O	516	LEU
15	O	525	THR
15	O	551	VAL
15	O	563	VAL
15	O	576	PHE
16	P	250	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	HIS
1	A	310	ASN
1	A	355	GLN
1	A	431	ASN
2	B	60	GLN
2	B	299	GLN
2	B	552	ASN
13	M	117	HIS
13	M	190	ASN
15	O	580	ASN
15	O	652	GLN

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Mol	Chain	Res	Type
16	P	219	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	T	9/9 (100%)	2 (22%)	1 (11%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	T	8	G
20	T	10	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	T	7	A

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.