wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:17 PM BST

PDB ID	:	5FJ9
EMDB ID:	:	EMD-3179
Title	:	Cryo-EM structure of yeast apo RNA polymerase III at 4.6 A
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	:	4.60 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
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

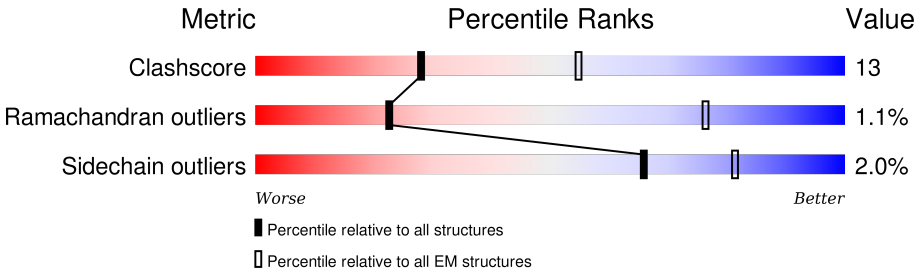
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 4.60 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

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

Mol	Chain	Length	Quality of chain
1	A	1460	71% 25% • •
2	B	1149	70% 26% • •
3	C	335	75% 24% •
4	D	161	46% 27% • 26%
5	E	215	67% 32% •
6	F	155	46% 6% • 46%
7	G	212	48% 40% • 10%
8	H	146	69% 27% •
9	I	110	65% 18% • 16%

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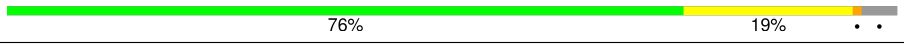
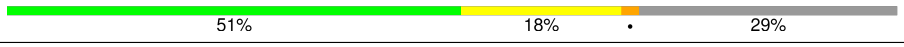
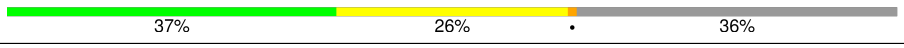
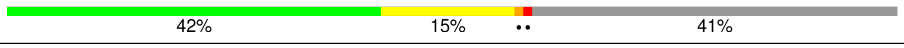
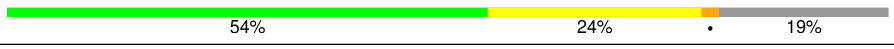
Mol	Chain	Length	Quality of chain
10	J	70	
11	K	142	
12	L	70	
13	M	282	
14	N	422	
15	O	654	
16	P	317	
17	Q	104	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 38680 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
			Total	C	N	O	S		
1	A	1412	11071	6979	1954	2079	59	0	0

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

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

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

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

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

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

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

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

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

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	92	Total	C	N	O	S	0	0
			728	455	117	145	11		

- 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	165	Total	C	N	O	S	0	0
			1347	862	229	255	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	105	Total	C	N	O	S	0	0
			802	508	144	147	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	528	Total	C	N	O	S	0	0
			4247	2705	725	798	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	98	Total	C	N	O	S	0	0
			820	533	126	157	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	70	Total	C	N	O	0	0
			446	282	80	84		

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

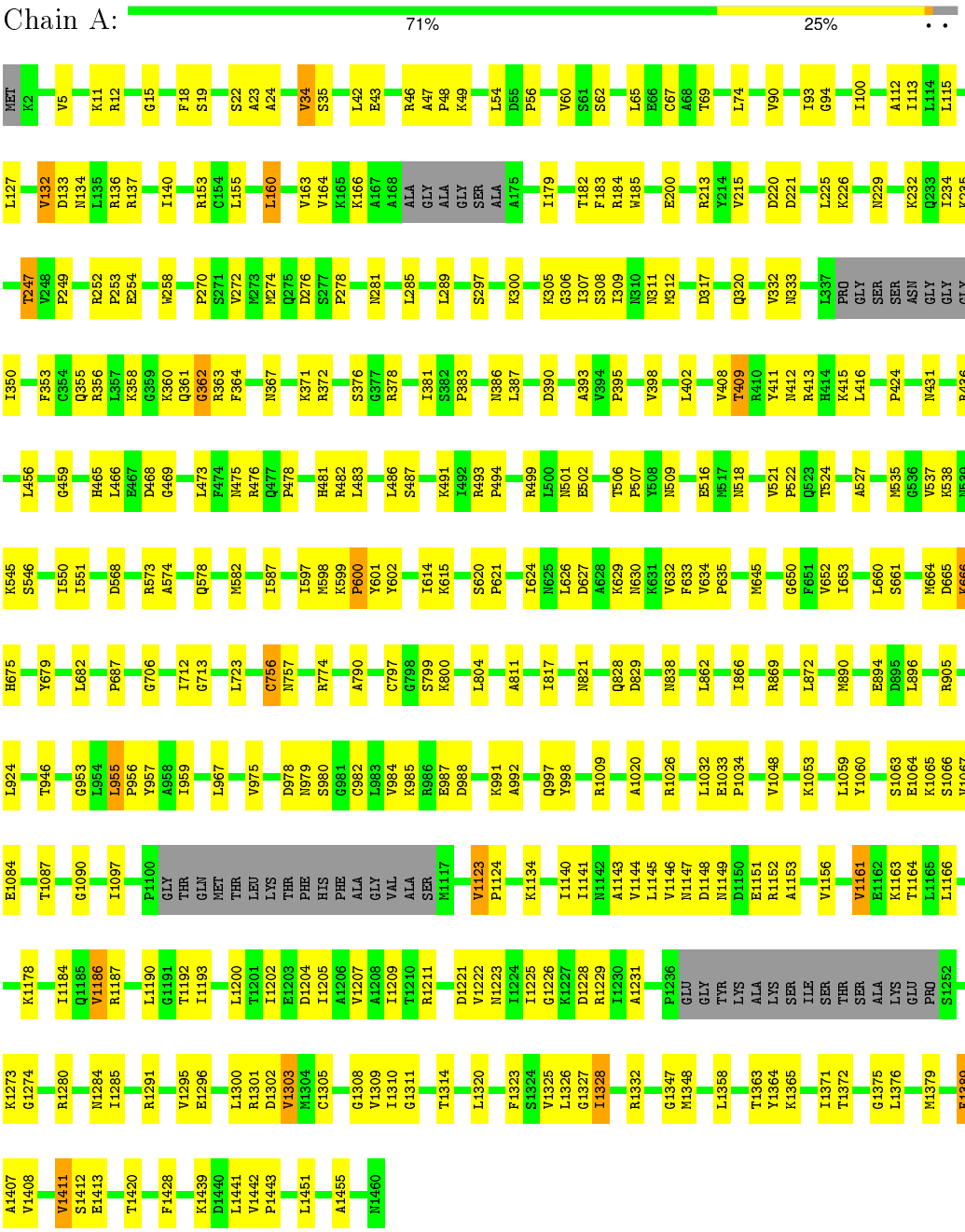
Mol	Chain	Residues	Atoms		AltConf
18	B	1	Total	Zn	0
			1	1	
18	A	2	Total	Zn	0
			2	2	
18	L	1	Total	Zn	0
			1	1	
18	J	1	Total	Zn	0
			1	1	
18	I	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

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.

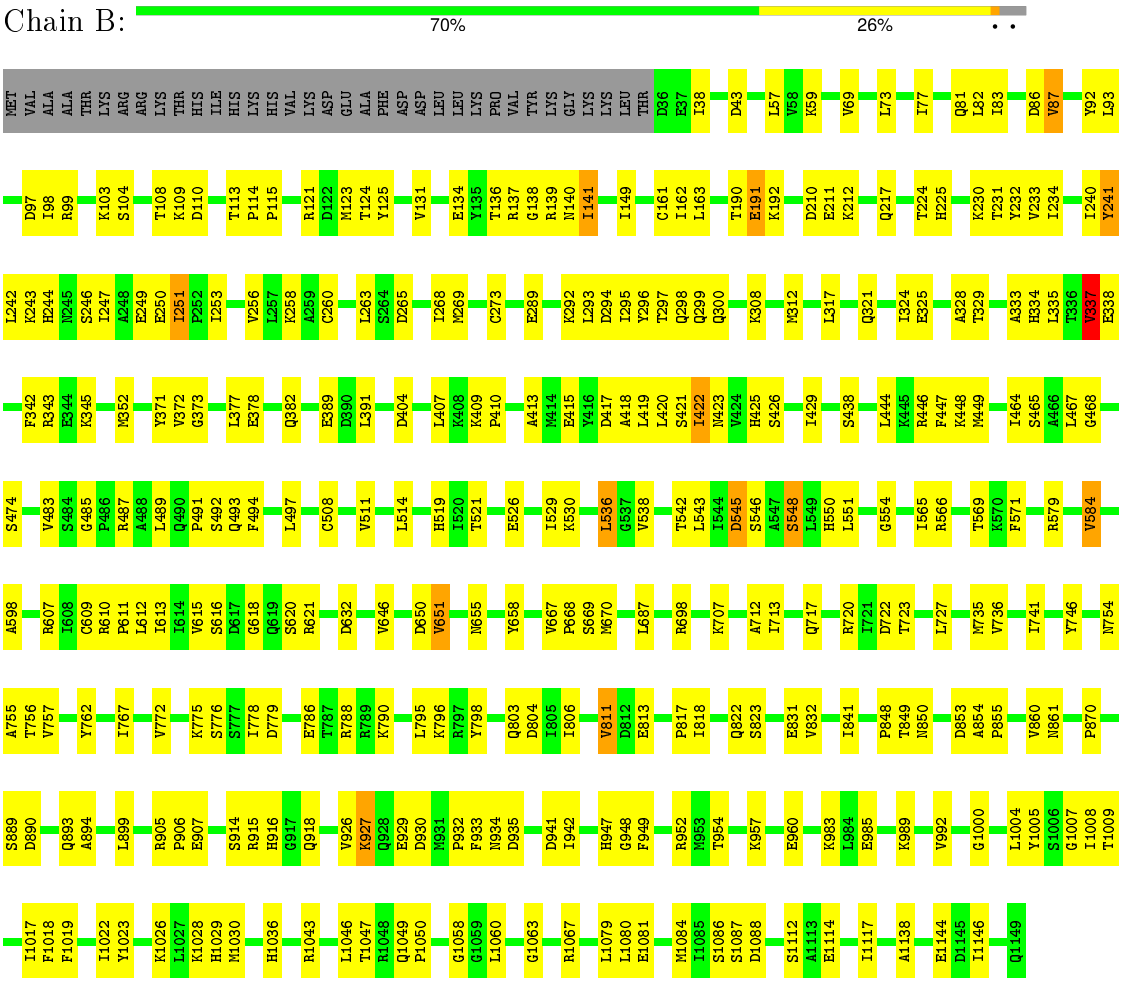
- Molecule 1: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC1

Chain A:



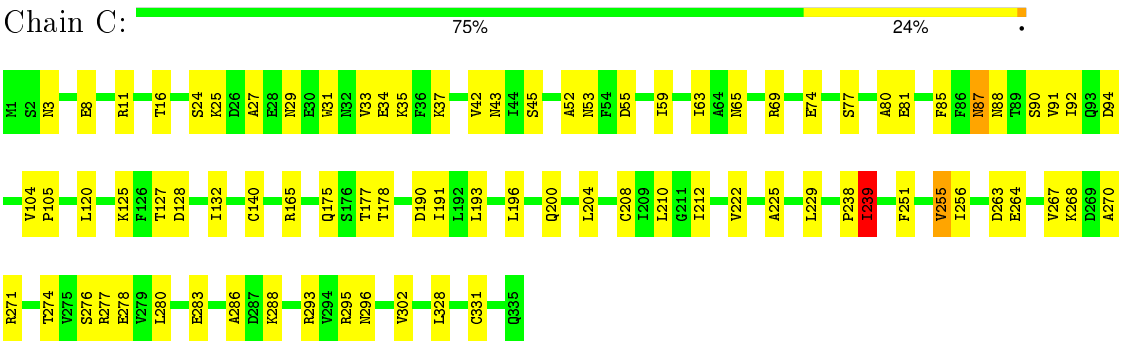
• Molecule 2: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC2

Chain B:



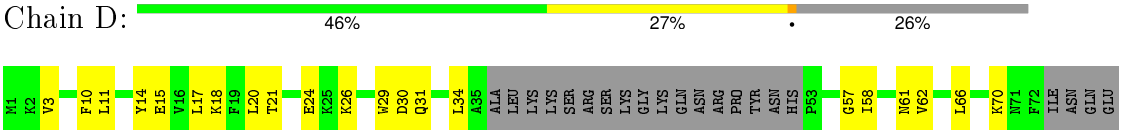
• Molecule 3: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1

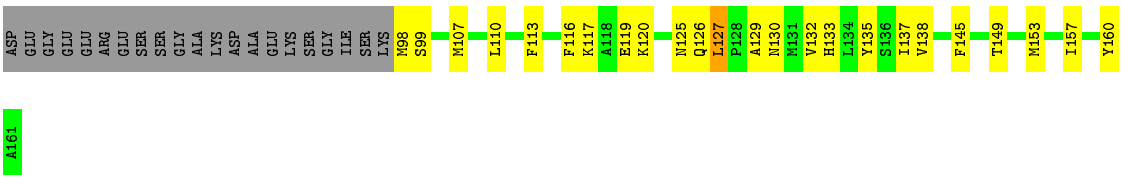
Chain C:



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

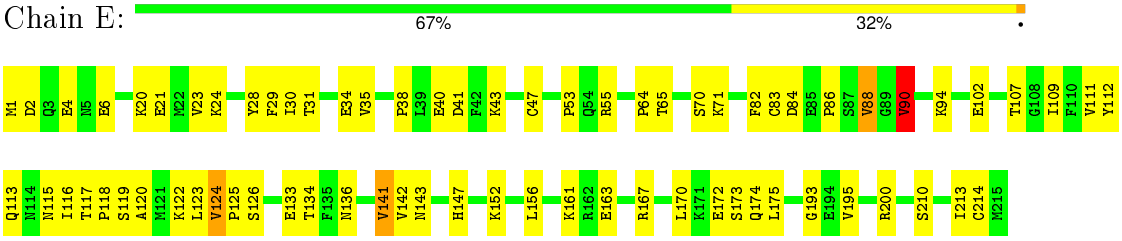
Chain D:





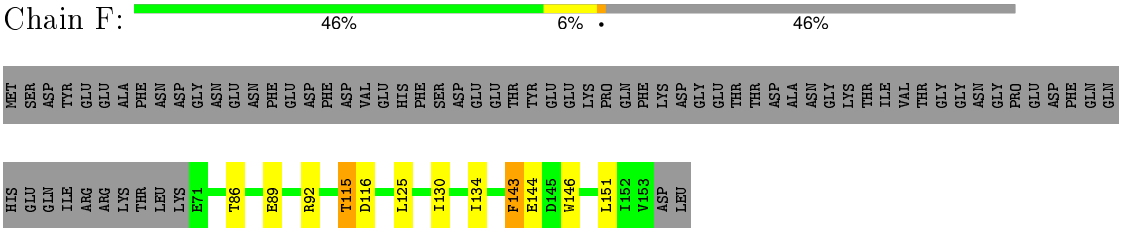
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain E:



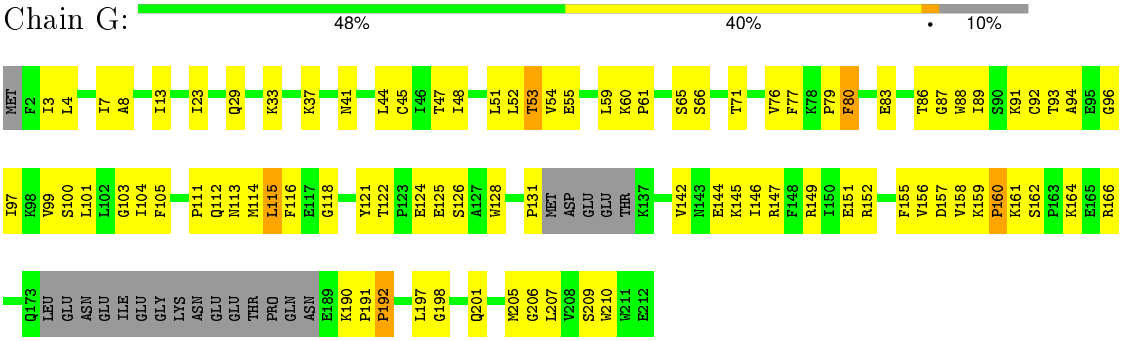
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F:



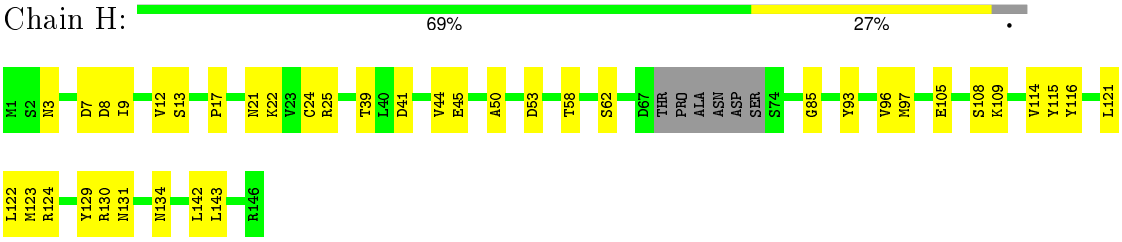
• Molecule 7: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC8

Chain G:



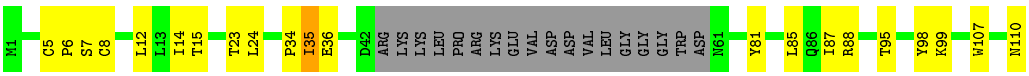
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H:



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

Chain I:

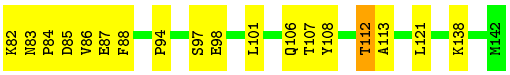


• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J:

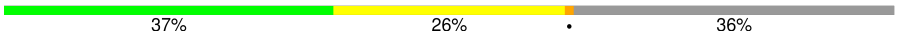
• Molecule 11: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2

Chain K:



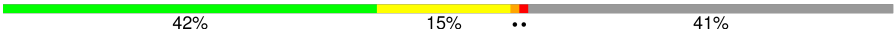
• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L:



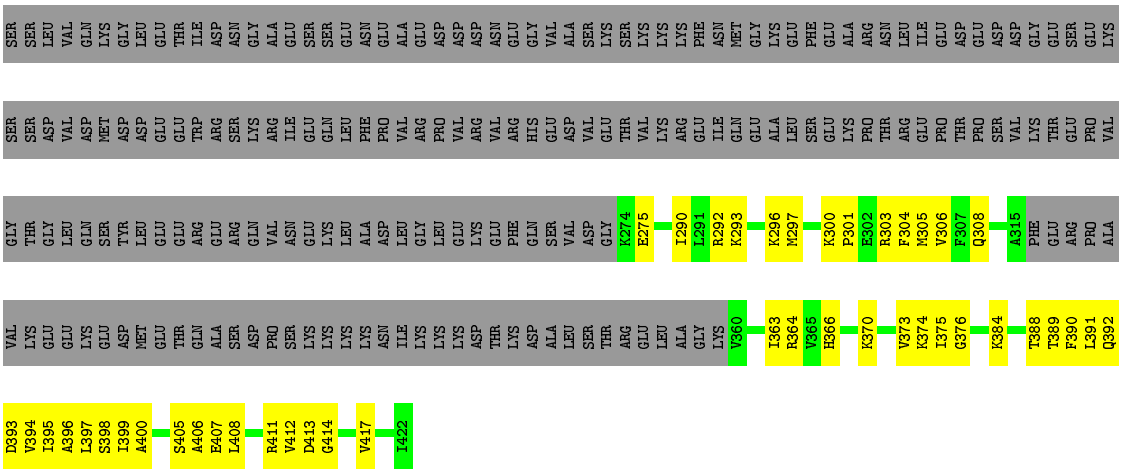
• Molecule 13: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC5

Chain M:



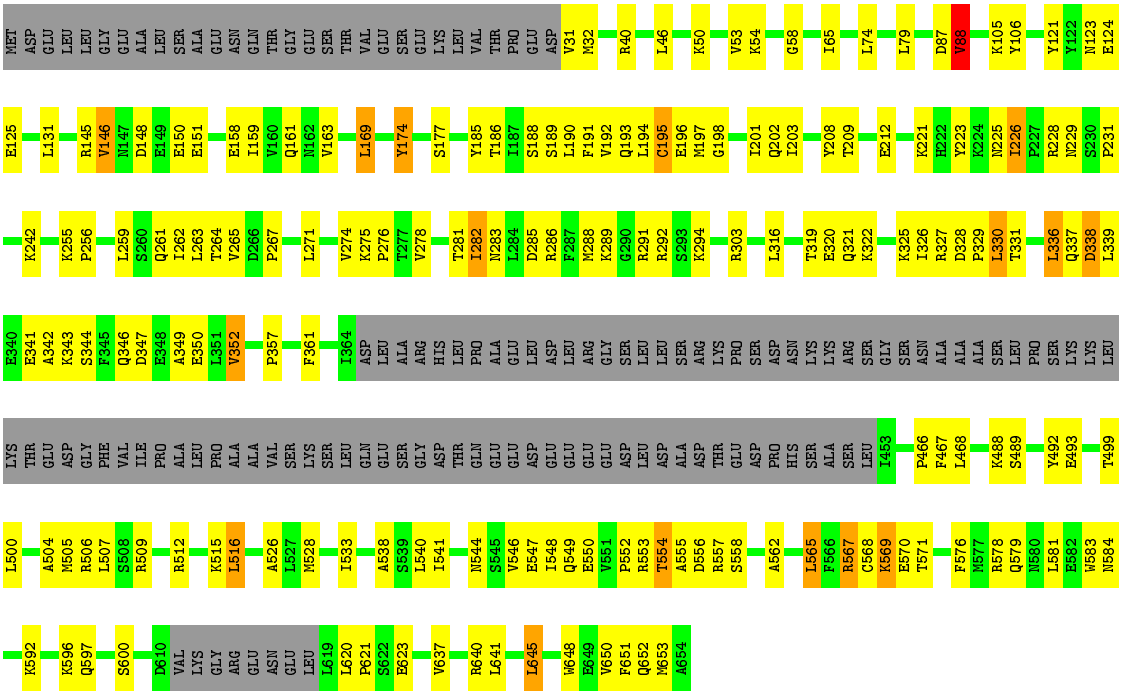
• Molecule 14: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC4

Chain N:



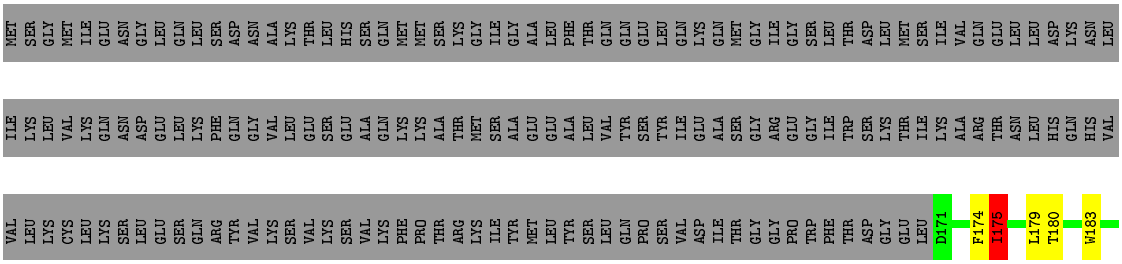
• Molecule 15: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC3

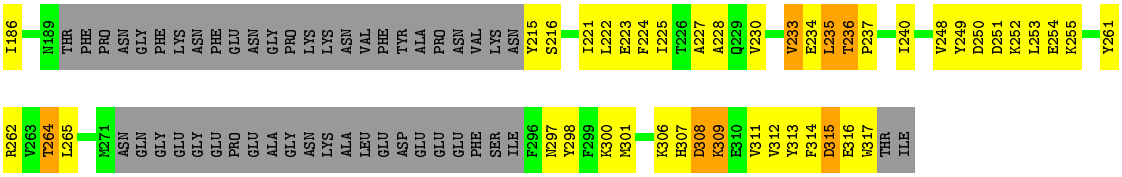
Chain O:



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

Chain P:





- Molecule 17: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC7

Chain Q:

4 Experimental information (i)

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 ($e^-/Å^2$)	42	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	0/11267	0.46	0/15220
10	J	0.21	0/558	0.44	0/750
11	K	0.22	0/803	0.45	0/1083
12	L	0.22	0/360	0.48	0/478
13	M	0.23	0/1378	0.46	0/1863
14	N	0.23	0/810	0.52	0/1088
15	O	0.23	0/4310	0.50	0/5813
16	P	0.29	0/837	0.55	0/1134
17	Q	0.24	0/278	0.49	0/377
2	B	0.22	0/8943	0.45	0/12068
3	C	0.23	0/2711	0.45	0/3676
4	D	0.23	0/991	0.52	0/1328
5	E	0.22	0/1795	0.44	0/2416
6	F	0.21	0/683	0.42	0/923
7	G	0.23	0/1583	0.50	0/2146
8	H	0.21	0/1138	0.44	0/1540
9	I	0.22	0/745	0.42	0/1007
All	All	0.22	0/39190	0.47	0/52910

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11071	0	11200	272	0
2	B	8788	0	8902	221	0
3	C	2655	0	2628	55	0
4	D	977	0	983	33	0
5	E	1759	0	1788	48	0
6	F	671	0	692	9	0
7	G	1544	0	1540	62	0
8	H	1120	0	1089	28	0
9	I	728	0	672	18	0
10	J	549	0	560	8	0
11	K	792	0	790	23	0
12	L	358	0	381	18	0
13	M	1347	0	1315	39	0
14	N	802	0	851	40	0
15	O	4247	0	4413	156	0
16	P	820	0	795	51	0
17	Q	446	0	324	10	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	I	1	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
All	All	38680	0	38923	974	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 13.

All (974) 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)
15:O:516:LEU:CD2	15:O:567:ARG:HE	1.08	1.58
15:O:516:LEU:HD23	15:O:567:ARG:NE	1.20	1.41
15:O:516:LEU:HD23	15:O:567:ARG:CD	1.60	1.30
1:A:597:ILE:HB	1:A:600:PRO:HG3	1.15	1.15
15:O:516:LEU:HD22	15:O:567:ARG:HE	1.08	1.08
1:A:598:MET:C	1:A:600:PRO:HD3	1.78	1.04
1:A:597:ILE:CB	1:A:600:PRO:HG3	1.87	1.02
15:O:516:LEU:HB3	15:O:567:ARG:HG3	1.42	1.01
15:O:569:LYS:HA	15:O:569:LYS:HE3	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:251:PHE:HB3	3:C:255:VAL:HG11	1.51	0.92
2:B:548:SER:HB3	2:B:550:HIS:CE1	2.04	0.92
1:A:229:ASN:HB3	15:O:544:ASN:HD21	1.37	0.90
1:A:597:ILE:HB	1:A:600:PRO:CG	2.02	0.86
1:A:43:GLU:HB2	1:A:48:PRO:HD2	1.55	0.86
4:D:126:GLN:HG3	4:D:127:LEU:HG	1.57	0.86
15:O:549:GLN:HG3	15:O:565:LEU:HB2	1.58	0.85
1:A:226:LYS:HE2	15:O:548:ILE:HG13	1.56	0.85
15:O:547:GLU:HG3	15:O:569:LYS:HD3	1.59	0.84
15:O:512:ARG:HG2	15:O:568:CYS:SG	2.17	0.84
15:O:569:LYS:HA	15:O:569:LYS:CE	2.07	0.83
15:O:516:LEU:HD23	15:O:567:ARG:CG	2.08	0.83
15:O:547:GLU:CG	15:O:569:LYS:HD3	2.10	0.80
13:M:113:LYS:HD3	13:M:241:ALA:HB2	1.63	0.79
2:B:294:ASP:HB3	2:B:300:GLN:HG3	1.64	0.79
5:E:124:VAL:HG13	5:E:125:PRO:HD3	1.64	0.79
15:O:493:GLU:OE2	15:O:512:ARG:NH1	2.16	0.78
1:A:598:MET:C	1:A:600:PRO:CD	2.53	0.77
15:O:516:LEU:CB	15:O:567:ARG:HG3	2.13	0.77
1:A:599:LYS:N	1:A:600:PRO:CD	2.46	0.77
1:A:229:ASN:CB	15:O:544:ASN:HD21	1.97	0.76
1:A:829:ASP:OD2	1:A:838:ASN:ND2	2.20	0.75
1:A:550:ILE:HG23	1:A:551:ILE:HG23	1.69	0.74
1:A:756:CYS:SG	1:A:757:ASN:N	2.59	0.73
15:O:570:GLU:HG3	15:O:571:THR:HG23	1.70	0.73
1:A:49:LYS:HD2	1:A:54:LEU:HB3	1.69	0.73
3:C:120:LEU:HD23	3:C:125:LYS:HG2	1.72	0.72
15:O:538:ALA:HA	15:O:541:ILE:HG22	1.72	0.72
11:K:65:ILE:HB	11:K:101:LEU:HB3	1.72	0.72
16:P:236:THR:HG22	16:P:237:PRO:HD2	1.69	0.72
1:A:597:ILE:CG2	1:A:600:PRO:HG3	2.19	0.72
7:G:146:ILE:HG23	7:G:206:GLY:HA2	1.70	0.72
14:N:363:ILE:HG12	14:N:373:VAL:HG13	1.72	0.72
15:O:552:PRO:HB3	15:O:557:ARG:H	1.55	0.71
1:A:215:VAL:HG21	15:O:554:THR:H	1.53	0.71
16:P:216:SER:HB3	16:P:222:LEU:HD11	1.71	0.71
7:G:207:LEU:HD23	7:G:209:SER:H	1.55	0.71
15:O:190:LEU:HG	15:O:193:GLN:HB3	1.71	0.70
2:B:822:GLN:HG3	2:B:823:SER:H	1.55	0.70
15:O:124:GLU:HG3	15:O:125:GLU:N	2.06	0.70
13:M:87:VAL:HA	14:N:396:ALA:HA	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:48:CYS:SG	12:L:51:CYS:HB2	2.17	0.70
15:O:499:THR:HA	17:Q:41:LEU:HD21	1.72	0.70
15:O:555:ALA:HB1	15:O:558:SER:HB2	1.73	0.70
2:B:234:ILE:HB	2:B:240:ILE:HG22	1.74	0.70
4:D:127:LEU:HB2	4:D:133:HIS:HB3	1.73	0.69
13:M:148:LEU:HG	13:M:181:PRO:HB3	1.74	0.69
1:A:436:ARG:HD3	1:A:459:GLY:HA3	1.75	0.69
15:O:507:LEU:HD13	15:O:540:LEU:HD22	1.75	0.69
1:A:332:VAL:HG13	1:A:333:ASN:H	1.57	0.69
9:I:81:TYR:HB2	9:I:99:LYS:HB3	1.74	0.69
7:G:96:GLY:HA3	7:G:111:PRO:HA	1.73	0.69
2:B:265:ASP:O	2:B:268:ILE:N	2.25	0.68
1:A:1020:ALA:HB2	1:A:1032:LEU:HD11	1.75	0.68
2:B:548:SER:CB	2:B:550:HIS:CE1	2.76	0.68
1:A:600:PRO:O	1:A:601:TYR:HB2	1.92	0.68
3:C:16:THR:O	3:C:295:ARG:NH1	2.26	0.68
1:A:160:LEU:HD21	15:O:339:LEU:HG	1.76	0.68
1:A:153:ARG:HA	1:A:160:LEU:HD22	1.76	0.68
4:D:126:GLN:NE2	7:G:86:THR:OG1	2.24	0.68
1:A:476:ARG:HG2	1:A:478:PRO:HD2	1.76	0.68
16:P:308:ASP:OD1	16:P:309:LYS:HG3	1.94	0.67
8:H:24:CYS:SG	8:H:25:ARG:N	2.67	0.67
1:A:615:LYS:NZ	1:A:620:SER:O	2.26	0.67
16:P:248:VAL:HG23	16:P:255:LYS:HE2	1.76	0.67
1:A:1178:LYS:HE2	9:I:36:GLU:HB3	1.76	0.67
11:K:88:PHE:HB3	11:K:106:GLN:HB3	1.74	0.67
1:A:221:ASP:HB3	15:O:550:GLU:HG3	1.76	0.67
11:K:47:ILE:HG12	11:K:65:ILE:HG12	1.76	0.66
15:O:123:ASN:O	15:O:124:GLU:HG2	1.95	0.66
16:P:223:GLU:O	16:P:227:ALA:N	2.22	0.66
2:B:778:ILE:HD11	2:B:906:PRO:HG2	1.78	0.66
8:H:58:THR:HB	8:H:143:LEU:HB3	1.79	0.65
15:O:541:ILE:HD11	15:O:548:ILE:HG12	1.78	0.65
10:J:17:LYS:HB3	10:J:39:LEU:HD21	1.78	0.65
1:A:69:THR:HA	7:G:164:LYS:HZ3	1.60	0.65
1:A:226:LYS:HD3	15:O:547:GLU:OE1	1.96	0.65
2:B:247:ILE:HG21	2:B:251:ILE:HD11	1.79	0.65
2:B:419:LEU:O	2:B:423:ASN:ND2	2.23	0.65
15:O:341:GLU:HG2	15:O:344:SER:HB2	1.77	0.65
4:D:130:ASN:O	4:D:133:HIS:ND1	2.30	0.65
2:B:59:LYS:HE2	2:B:519:HIS:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1112:SER:HB2	2:B:1114:GLU:HG2	1.79	0.65
1:A:215:VAL:HG11	15:O:554:THR:HA	1.78	0.64
7:G:161:LYS:HE3	7:G:166:ARG:HA	1.79	0.64
16:P:308:ASP:O	16:P:309:LYS:HB2	1.98	0.64
4:D:119:GLU:HG3	4:D:138:VAL:HB	1.80	0.64
9:I:12:LEU:HB3	9:I:24:LEU:HD13	1.79	0.64
3:C:222:VAL:HG11	3:C:225:ALA:HB2	1.78	0.64
16:P:233:VAL:HG12	16:P:234:GLU:H	1.62	0.64
1:A:599:LYS:H	1:A:602:TYR:HE1	1.43	0.64
12:L:31:CYS:HB3	12:L:34:CYS:HB2	1.80	0.64
15:O:150:GLU:HG3	15:O:151:GLU:HG2	1.80	0.64
2:B:258:LYS:HB3	2:B:297:THR:HA	1.80	0.64
16:P:221:ILE:HA	16:P:224:PHE:HB2	1.80	0.63
1:A:645:MET:HE3	8:H:124:ARG:HD2	1.81	0.63
7:G:115:LEU:HD23	7:G:116:PHE:H	1.62	0.63
2:B:543:LEU:HD21	13:M:176:VAL:HG21	1.81	0.63
1:A:956:PRO:HG2	1:A:957:TYR:HD1	1.64	0.63
7:G:104:ILE:HG23	7:G:105:PHE:H	1.63	0.63
15:O:185:TYR:HA	15:O:188:SER:HB2	1.78	0.63
16:P:307:HIS:O	16:P:308:ASP:HB3	1.98	0.63
2:B:81:GLN:HG2	2:B:82:LEU:HG	1.80	0.63
2:B:192:LYS:NZ	2:B:438:SER:O	2.31	0.63
15:O:516:LEU:HD23	15:O:567:ARG:HG3	1.81	0.62
2:B:137:ARG:HH11	2:B:139:ARG:HB2	1.63	0.62
1:A:573:ARG:HH21	11:K:87:GLU:HB3	1.63	0.62
1:A:1161:VAL:HG11	1:A:1303:VAL:HG23	1.82	0.62
2:B:775:LYS:HA	2:B:778:ILE:HG22	1.81	0.62
6:F:92:ARG:HH12	7:G:61:PRO:HB3	1.64	0.62
2:B:253:ILE:HD12	2:B:256:VAL:HB	1.82	0.62
1:A:67:CYS:SG	1:A:69:THR:OG1	2.57	0.62
15:O:488:LYS:NZ	15:O:650:VAL:O	2.33	0.62
12:L:29:TYR:HE2	12:L:40:LEU:HB2	1.65	0.62
3:C:80:ALA:HA	3:C:208:CYS:HA	1.82	0.62
1:A:1420:THR:HG22	2:B:1080:LEU:HD21	1.82	0.62
1:A:1169:VAL:HG13	1:A:1192:THR:HB	1.82	0.61
1:A:413:ARG:NH1	1:A:456:LEU:O	2.34	0.61
1:A:112:ALA:HA	1:A:234:ILE:HD11	1.81	0.61
1:A:213:ARG:NH1	1:A:213:ARG:O	2.32	0.61
7:G:87:GLY:O	7:G:146:ILE:N	2.30	0.61
2:B:139:ARG:HE	2:B:141:ILE:HD11	1.64	0.61
1:A:393:ALA:HA	1:A:491:LYS:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:ILE:HD12	2:B:949:PHE:HD2	1.65	0.61
12:L:42:ARG:HG3	12:L:43:THR:HG23	1.83	0.61
1:A:1372:THR:O	1:A:1376:LEU:N	2.34	0.61
2:B:757:VAL:HG23	2:B:942:ILE:HB	1.82	0.61
1:A:1257:PHE:HB2	9:I:14:ILE:HB	1.82	0.61
5:E:112:TYR:HB2	5:E:136:ASN:HA	1.82	0.61
1:A:252:ARG:O	1:A:254:GLU:N	2.33	0.61
15:O:106:TYR:HB3	15:O:208:TYR:HE2	1.65	0.61
15:O:198:GLY:HA3	15:O:286:ARG:HG2	1.83	0.60
15:O:547:GLU:HG2	15:O:569:LYS:HD3	1.84	0.60
16:P:311:VAL:O	16:P:312:VAL:HG12	2.01	0.60
2:B:1007:GLY:O	3:C:69:ARG:NH1	2.34	0.60
15:O:584:ASN:OD1	16:P:312:VAL:HG23	2.00	0.60
1:A:599:LYS:N	1:A:600:PRO:HD2	2.17	0.60
15:O:286:ARG:NH1	15:O:320:GLU:O	2.35	0.60
7:G:89:ILE:HA	7:G:99:VAL:HA	1.82	0.60
1:A:62:SER:HB3	1:A:65:LEU:HG	1.84	0.60
4:D:127:LEU:HD11	4:D:137:ILE:HD13	1.83	0.60
16:P:313:TYR:HB2	17:Q:39:ILE:HD11	1.84	0.60
1:A:1048:VAL:HG11	1:A:1053:LYS:HB2	1.83	0.60
1:A:121:ARG:NH2	15:O:212:GLU:OE1	2.35	0.60
5:E:88:VAL:HG23	5:E:117:THR:HG22	1.83	0.60
13:M:91:ALA:HA	14:N:391:LEU:HD21	1.83	0.60
1:A:1144:VAL:HG23	1:A:1310:ILE:HG23	1.84	0.60
1:A:1164:THR:HB	1:A:1271:VAL:HA	1.83	0.60
15:O:31:VAL:HG12	15:O:32:MET:HG3	1.82	0.60
2:B:775:LYS:HB3	2:B:927:LYS:HA	1.83	0.59
1:A:15:GLY:HA2	1:A:1407:ALA:HA	1.83	0.59
15:O:357:PRO:HA	15:O:361:PHE:CD2	2.36	0.59
16:P:179:LEU:O	16:P:183:TRP:NE1	2.34	0.59
3:C:31:TRP:H	11:K:82:LYS:HE2	1.67	0.59
14:N:305:MET:HG2	14:N:414:GLY:H	1.66	0.59
8:H:97:MET:HB2	8:H:142:LEU:HB3	1.82	0.59
1:A:486:LEU:HD23	1:A:537:VAL:HG22	1.83	0.59
1:A:1084:GLU:HB2	6:F:86:THR:HG23	1.83	0.59
4:D:129:ALA:HB2	4:D:157:ILE:HG23	1.84	0.59
1:A:15:GLY:H	1:A:1408:VAL:HG12	1.66	0.59
7:G:157:ASP:OD1	7:G:157:ASP:N	2.36	0.59
14:N:363:ILE:HG23	14:N:373:VAL:HG22	1.84	0.59
9:I:87:ILE:HG23	9:I:88:ARG:HG3	1.83	0.59
7:G:101:LEU:HD22	7:G:104:ILE:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:108:SER:OG	13:M:109:ALA:N	2.36	0.58
2:B:137:ARG:HD2	2:B:415:GLU:HB2	1.85	0.58
1:A:402:LEU:HD23	1:A:466:LEU:HD22	1.85	0.58
15:O:286:ARG:NH2	15:O:321:GLN:O	2.36	0.58
2:B:616:SER:HB2	2:B:621:ARG:HH21	1.68	0.58
1:A:360:LYS:HD2	1:A:1389:PHE:O	2.04	0.58
15:O:288:MET:SD	15:O:291:ARG:NH1	2.77	0.58
1:A:828:GLN:HB3	2:B:655:ASN:HD21	1.68	0.58
3:C:33:VAL:O	3:C:34:GLU:HG3	2.03	0.58
11:K:45:GLU:O	11:K:46:LYS:HD2	2.04	0.58
15:O:547:GLU:HG2	15:O:569:LYS:CD	2.33	0.58
3:C:165:ARG:NH2	3:C:190:ASP:OD1	2.35	0.58
2:B:926:VAL:HG11	2:B:930:ASP:HB2	1.86	0.58
15:O:357:PRO:HA	15:O:361:PHE:HD2	1.68	0.58
1:A:358:LYS:HG2	1:A:1392:THR:HG21	1.86	0.58
2:B:832:VAL:HG12	12:L:60:ARG:HG3	1.86	0.58
1:A:538:LYS:HB3	1:A:687:PRO:HB2	1.86	0.58
15:O:105:LYS:N	15:O:123:ASN:HB2	2.18	0.57
11:K:107:THR:OG1	11:K:108:TYR:N	2.36	0.57
15:O:163:VAL:HG22	15:O:169:LEU:HD22	1.85	0.57
16:P:174:PHE:O	16:P:175:ILE:HG12	2.04	0.57
1:A:225:LEU:O	1:A:229:ASN:ND2	2.37	0.57
15:O:191:PHE:HD2	15:O:274:VAL:HG21	1.69	0.57
13:M:247:TRP:HE1	14:N:408:LEU:HB2	1.69	0.57
2:B:1004:LEU:HD12	2:B:1017:ILE:HD12	1.86	0.57
2:B:554:GLY:H	2:B:598:ALA:HA	1.68	0.57
2:B:87:VAL:HG11	2:B:407:LEU:HB3	1.86	0.57
1:A:1059:LEU:HD21	8:H:105:GLU:HA	1.86	0.57
15:O:105:LYS:HB3	15:O:121:TYR:HB2	1.84	0.57
2:B:343:ARG:HH22	2:B:546:SER:HB3	1.69	0.57
1:A:412:ASN:HB3	1:A:416:LEU:HD13	1.86	0.57
15:O:124:GLU:HG3	15:O:125:GLU:H	1.67	0.57
15:O:338:ASP:OD1	15:O:339:LEU:N	2.38	0.57
13:M:77:LYS:HE3	13:M:262:GLU:HB3	1.85	0.57
13:M:183:PHE:HB2	13:M:186:ILE:HG13	1.87	0.57
5:E:21:GLU:HB3	5:E:35:VAL:HG21	1.85	0.57
1:A:270:PRO:HD3	2:B:1046:LEU:HD13	1.87	0.57
9:I:5:CYS:HB2	9:I:12:LEU:HD21	1.85	0.57
2:B:389:GLU:OE2	2:B:446:ARG:NH2	2.37	0.57
1:A:232:LYS:NZ	16:P:316:GLU:OE1	2.37	0.57
12:L:48:CYS:CB	12:L:51:CYS:HB2	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:314:PHE:C	16:P:316:GLU:H	2.08	0.57
5:E:90:VAL:HG12	5:E:94:LYS:HG2	1.86	0.57
12:L:49:LYS:N	12:L:51:CYS:SG	2.78	0.57
1:A:317:ASP:OD1	1:A:320:GLN:NE2	2.38	0.57
2:B:373:GLY:HA2	2:B:607:ARG:HH22	1.70	0.57
15:O:158:GLU:OE1	15:O:161:GLN:NE2	2.38	0.57
2:B:536:LEU:HD22	2:B:571:PHE:HD1	1.70	0.56
11:K:80:ILE:HG22	11:K:86:VAL:HG11	1.87	0.56
7:G:118:GLY:HA3	7:G:131:PRO:HD3	1.86	0.56
15:O:540:LEU:HD21	15:O:546:VAL:HG11	1.86	0.56
16:P:186:ILE:HG23	16:P:253:LEU:HD21	1.87	0.56
7:G:112:GLN:HG2	7:G:115:LEU:HD13	1.86	0.56
2:B:698:ARG:HE	2:B:952:ARG:HB3	1.69	0.56
1:A:574:ALA:O	11:K:77:ARG:NH2	2.38	0.56
2:B:493:GLN:HG3	2:B:497:LEU:HB2	1.88	0.56
7:G:91:LYS:HG2	7:G:92:CYS:H	1.70	0.56
4:D:17:LEU:HB2	4:D:66:LEU:HD23	1.87	0.56
12:L:28:LYS:HG3	12:L:29:TYR:HD2	1.70	0.56
2:B:325:GLU:O	2:B:329:THR:N	2.34	0.56
15:O:221:LYS:O	15:O:225:ASN:ND2	2.39	0.56
2:B:57:LEU:HD22	2:B:467:LEU:HD11	1.86	0.56
15:O:347:ASP:HA	15:O:350:GLU:HB2	1.88	0.56
1:A:276:ASP:OD1	1:A:276:ASP:N	2.39	0.56
5:E:83:CYS:SG	5:E:84:ASP:N	2.77	0.56
1:A:712:ILE:HG23	1:A:790:ALA:HB3	1.87	0.56
1:A:272:VAL:HG23	1:A:281:ASN:HB3	1.86	0.56
1:A:799:SER:OG	1:A:800:LYS:N	2.39	0.56
3:C:140:CYS:HB2	3:C:196:LEU:HD13	1.87	0.56
1:A:1332:ARG:HB2	1:A:1363:THR:HG21	1.88	0.56
1:A:1364:TYR:OH	1:A:1379:MET:SD	2.62	0.56
11:K:65:ILE:HD12	11:K:101:LEU:HD23	1.86	0.56
1:A:252:ARG:HB3	1:A:253:PRO:HD2	1.87	0.56
2:B:161:CYS:SG	2:B:162:ILE:N	2.79	0.56
7:G:45:CYS:HA	7:G:76:VAL:HA	1.87	0.56
7:G:3:ILE:HG13	7:G:76:VAL:HG23	1.87	0.56
2:B:244:HIS:HD1	2:B:246:SER:HG	1.53	0.56
12:L:50:ASP:OD1	12:L:51:CYS:N	2.39	0.55
15:O:316:LEU:HA	15:O:319:THR:HG22	1.89	0.55
15:O:505:MET:HB3	16:P:250:ASP:OD2	2.07	0.55
2:B:618:GLY:HA2	2:B:668:PRO:HB3	1.88	0.55
16:P:314:PHE:O	16:P:316:GLU:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:228:ARG:HH12	15:O:231:PRO:HD3	1.72	0.55
16:P:312:VAL:O	16:P:312:VAL:HG13	2.05	0.55
1:A:476:ARG:NH1	1:A:509:ASN:O	2.39	0.55
9:I:14:ILE:HD13	9:I:24:LEU:HB3	1.87	0.55
1:A:1084:GLU:O	1:A:1087:THR:OG1	2.25	0.55
2:B:233:VAL:HG11	2:B:243:LYS:HE3	1.89	0.55
7:G:207:LEU:HD22	7:G:210:TRP:CD1	2.41	0.55
6:F:125:LEU:HA	6:F:130:ILE:HD11	1.88	0.55
13:M:123:ILE:O	13:M:146:GLN:N	2.36	0.55
2:B:1036:HIS:CE1	2:B:1058:GLY:HA3	2.41	0.55
7:G:13:ILE:HG13	7:G:66:SER:HB3	1.88	0.55
16:P:223:GLU:HG2	16:P:240:ILE:HA	1.87	0.55
15:O:185:TYR:O	15:O:189:SER:N	2.39	0.55
2:B:519:HIS:O	2:B:609:CYS:N	2.38	0.55
5:E:38:PRO:HB2	5:E:40:GLU:HG2	1.87	0.55
14:N:366:HIS:HB3	14:N:370:LYS:HB2	1.89	0.55
16:P:235:LEU:HD12	16:P:236:THR:H	1.72	0.55
5:E:117:THR:HG23	5:E:119:SER:H	1.72	0.55
2:B:483:VAL:HG12	2:B:485:GLY:H	1.71	0.55
15:O:328:ASP:OD1	15:O:328:ASP:N	2.40	0.55
1:A:541:LEU:HG	1:A:551:ILE:HD11	1.89	0.54
1:A:155:LEU:HG	15:O:336:LEU:HD23	1.89	0.54
5:E:156:LEU:HD11	5:E:195:VAL:HB	1.89	0.54
16:P:223:GLU:HB3	16:P:240:ILE:HD13	1.89	0.54
2:B:115:PRO:HG3	2:B:163:LEU:HD11	1.89	0.54
13:M:88:PHE:HD2	14:N:397:LEU:HD13	1.72	0.54
2:B:242:LEU:HD11	2:B:253:ILE:HD13	1.88	0.54
16:P:251:ASP:OD1	16:P:252:LYS:N	2.36	0.54
2:B:860:VAL:HG13	2:B:861:ASN:H	1.71	0.54
1:A:1141:ILE:N	1:A:1295:VAL:O	2.34	0.54
13:M:83:GLU:HB2	14:N:400:ALA:HB2	1.90	0.54
5:E:31:THR:HG22	5:E:34:GLU:HG2	1.89	0.54
4:D:11:LEU:HD22	7:G:4:LEU:HD13	1.88	0.54
7:G:113:ASN:OD1	7:G:113:ASN:N	2.40	0.54
14:N:397:LEU:HD11	14:N:408:LEU:HD12	1.90	0.54
2:B:343:ARG:NH2	2:B:546:SER:HB3	2.23	0.54
15:O:578:ARG:HG2	15:O:648:TRP:HZ3	1.73	0.54
2:B:521:THR:OG1	2:B:609:CYS:SG	2.66	0.54
5:E:109:ILE:HG22	5:E:133:GLU:HB3	1.90	0.54
15:O:652:GLN:HG3	15:O:653:MET:HG3	1.90	0.54
5:E:141:VAL:HG23	5:E:142:VAL:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:ILE:O	2:B:296:TYR:CG	2.60	0.54
12:L:30:ILE:N	12:L:57:LEU:O	2.41	0.54
15:O:516:LEU:CD2	15:O:567:ARG:CD	2.55	0.54
16:P:252:LYS:HD3	16:P:253:LEU:H	1.72	0.54
2:B:137:ARG:HG2	2:B:138:GLY:H	1.73	0.54
5:E:20:LYS:HB3	5:E:35:VAL:HG23	1.90	0.54
1:A:22:SER:O	1:A:24:ALA:N	2.37	0.54
4:D:125:ASN:OD1	4:D:126:GLN:N	2.40	0.53
2:B:914:SER:HB3	2:B:918:GLN:HB2	1.89	0.53
3:C:270:ALA:HB3	3:C:271:ARG:HH11	1.73	0.53
14:N:398:SER:HB3	14:N:407:GLU:HB3	1.90	0.53
15:O:337:GLN:O	15:O:338:ASP:HB2	2.09	0.53
1:A:247:THR:HG23	1:A:249:PRO:HD3	1.90	0.53
5:E:28:TYR:HA	5:E:64:PRO:HA	1.90	0.53
2:B:712:ALA:O	2:B:717:GLN:NE2	2.42	0.53
3:C:229:LEU:O	3:C:293:ARG:NH2	2.39	0.53
3:C:8:GLU:HB3	3:C:11:ARG:HG2	1.89	0.53
7:G:89:ILE:HG23	7:G:142:VAL:HA	1.91	0.53
2:B:727:LEU:HD11	2:B:788:ARG:HE	1.73	0.53
1:A:1223:ASN:HB3	1:A:1231:ALA:HB3	1.91	0.53
1:A:100:ILE:HG13	1:A:166:LYS:HD3	1.89	0.53
1:A:473:LEU:HA	1:A:487:SER:HA	1.90	0.53
7:G:114:MET:O	7:G:201:GLN:HB3	2.08	0.53
1:A:1311:GLY:O	5:E:147:HIS:NE2	2.41	0.53
15:O:50:LYS:HA	15:O:53:VAL:HG12	1.91	0.53
1:A:1325:VAL:HG23	1:A:1326:LEU:H	1.74	0.53
16:P:254:GLU:HB2	16:P:262:ARG:HB2	1.91	0.53
14:N:290:ILE:HG13	14:N:293:LYS:HE2	1.90	0.53
15:O:292:ARG:HE	15:O:326:ILE:HD11	1.73	0.53
1:A:372:ARG:HG2	2:B:1049:GLN:HG2	1.90	0.53
7:G:190:LYS:C	7:G:192:PRO:HD3	2.28	0.53
7:G:44:LEU:O	7:G:77:PHE:N	2.42	0.53
3:C:81:GLU:OE2	12:L:70:ARG:NH2	2.42	0.53
13:M:122:ASP:HB3	13:M:145:VAL:HG21	1.90	0.53
2:B:934:ASN:OD1	2:B:935:ASP:N	2.41	0.53
5:E:123:LEU:HD11	5:E:126:SER:HB3	1.91	0.53
2:B:832:VAL:HB	12:L:60:ARG:HA	1.89	0.53
3:C:45:SER:HB2	3:C:53:ASN:HB3	1.91	0.53
1:A:1443:PRO:HG3	7:G:52:LEU:HD11	1.90	0.53
1:A:200:GLU:HA	15:O:515:LYS:HE3	1.90	0.53
2:B:1026:LYS:NZ	2:B:1030:MET:SD	2.69	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:526:GLU:O	2:B:529:ILE:HG22	2.09	0.53
10:J:30:LEU:HD22	10:J:31:ASP:H	1.73	0.53
1:A:200:GLU:HG2	15:O:515:LYS:HD2	1.90	0.52
16:P:255:LYS:HE3	16:P:261:TYR:CE1	2.43	0.52
15:O:150:GLU:HG3	15:O:151:GLU:H	1.72	0.52
8:H:114:VAL:HG21	8:H:130:ARG:HH11	1.74	0.52
3:C:94:ASP:N	3:C:94:ASP:OD1	2.41	0.52
9:I:34:PRO:O	9:I:35:ILE:HB	2.09	0.52
1:A:535:MET:O	1:A:540:ASN:ND2	2.42	0.52
2:B:289:GLU:HA	2:B:292:LYS:HG2	1.91	0.52
15:O:338:ASP:HB3	15:O:342:ALA:N	2.25	0.52
1:A:378:ARG:HE	1:A:516:GLU:HB3	1.75	0.52
5:E:161:LYS:NZ	5:E:193:GLY:O	2.37	0.52
4:D:15:GLU:HA	4:D:18:LYS:HB3	1.90	0.52
15:O:343:LYS:HA	15:O:346:GLN:HB3	1.91	0.52
2:B:417:ASP:HA	2:B:420:LEU:HG	1.90	0.52
15:O:620:LEU:HD12	15:O:621:PRO:HD2	1.91	0.52
1:A:1207:VAL:O	1:A:1211:ARG:HG2	2.09	0.52
2:B:249:GLU:O	2:B:308:LYS:NZ	2.42	0.52
8:H:39:THR:N	8:H:124:ARG:O	2.41	0.52
1:A:362:GLY:O	1:A:363:ARG:HB2	2.10	0.52
1:A:5:VAL:HG22	7:G:37:LYS:HB3	1.92	0.52
1:A:652:VAL:HG21	1:A:668:VAL:HG11	1.91	0.52
16:P:228:ALA:HA	16:P:233:VAL:HG13	1.92	0.52
2:B:299:GLN:HG3	13:M:186:ILE:HG22	1.90	0.52
4:D:57:GLY:O	4:D:61:ASN:ND2	2.43	0.52
9:I:15:THR:HG23	9:I:23:THR:HG23	1.92	0.52
1:A:1408:VAL:HG23	1:A:1413:GLU:HG3	1.92	0.52
1:A:665:ASP:OD1	1:A:797:CYS:HB3	2.10	0.52
1:A:1221:ASP:OD1	1:A:1222:VAL:N	2.43	0.52
11:K:46:LYS:O	11:K:47:ILE:C	2.48	0.52
11:K:47:ILE:HG23	11:K:63:PHE:HB3	1.92	0.52
2:B:667:VAL:O	2:B:669:SER:N	2.41	0.52
1:A:182:THR:HG22	1:A:185:TRP:HE1	1.74	0.52
7:G:121:TYR:HB2	7:G:128:TRP:CZ3	2.45	0.52
3:C:239:ILE:HG22	3:C:288:LYS:HE2	1.92	0.52
1:A:1140:ILE:HG22	1:A:1296:GLU:HG3	1.92	0.52
1:A:127:LEU:HD11	1:A:140:ILE:HG21	1.91	0.52
3:C:132:ILE:H	3:C:208:CYS:HB3	1.75	0.51
1:A:1420:THR:HA	2:B:1080:LEU:HD11	1.92	0.51
12:L:29:TYR:CE2	12:L:40:LEU:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:988:ASP:HA	1:A:991:LYS:HB3	1.91	0.51
13:M:80:GLY:HA3	13:M:261:LYS:HE2	1.90	0.51
2:B:372:VAL:O	2:B:607:ARG:NH1	2.41	0.51
4:D:20:LEU:HD12	4:D:62:VAL:HG11	1.91	0.51
1:A:305:LYS:HG3	1:A:306:GLY:H	1.75	0.51
9:I:23:THR:OG1	9:I:24:LEU:N	2.44	0.51
5:E:88:VAL:HB	5:E:120:ALA:HB2	1.91	0.51
2:B:796:LYS:NZ	2:B:798:TYR:OH	2.44	0.51
1:A:614:ILE:HD13	1:A:624:ILE:HD12	1.93	0.51
13:M:89:GLN:HB3	14:N:394:VAL:HG22	1.93	0.51
7:G:104:ILE:HG13	7:G:105:PHE:CD2	2.45	0.51
2:B:723:THR:HA	2:B:790:LYS:HG2	1.92	0.51
5:E:112:TYR:HE2	5:E:134:THR:HB	1.75	0.51
1:A:244:ILE:HG21	1:A:253:PRO:HD3	1.91	0.51
11:K:85:ASP:O	11:K:107:THR:OG1	2.20	0.51
1:A:1323:PHE:HA	1:A:1327:GLY:HA2	1.93	0.51
10:J:7:CYS:SG	10:J:11:GLY:N	2.77	0.51
1:A:11:LYS:HG3	2:B:1117:ILE:HD13	1.92	0.51
1:A:252:ARG:HH12	15:O:46:LEU:HD22	1.74	0.51
1:A:896:LEU:HB3	1:A:1090:GLY:HA3	1.92	0.51
8:H:8:ASP:OD1	8:H:9:ILE:N	2.43	0.51
2:B:333:ALA:HB1	2:B:345:LYS:HD3	1.91	0.51
1:A:578:GLN:O	1:A:582:MET:N	2.43	0.51
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.91	0.51
16:P:309:LYS:HD3	17:Q:43:ILE:HD11	1.93	0.51
1:A:1143:ALA:HA	1:A:1314:THR:HG22	1.92	0.51
1:A:376:SER:HB2	2:B:1060:LEU:HD12	1.93	0.51
15:O:192:VAL:HG12	15:O:274:VAL:H	1.76	0.51
5:E:88:VAL:HG21	5:E:117:THR:H	1.74	0.51
2:B:337:VAL:HG23	2:B:338:GLU:H	1.75	0.51
1:A:12:ARG:HG3	2:B:1146:ILE:HG12	1.92	0.51
1:A:1347:GLY:O	1:A:1348:MET:HG2	2.12	0.51
5:E:200:ARG:NH1	5:E:210:SER:OG	2.44	0.51
2:B:140:ASN:O	2:B:140:ASN:ND2	2.44	0.51
2:B:338:GLU:H	2:B:345:LYS:HZ3	1.58	0.50
7:G:124:GLU:O	7:G:125:GLU:HB3	2.12	0.50
4:D:3:VAL:HG13	7:G:7:ILE:HG22	1.92	0.50
1:A:482:ARG:HH12	1:A:924:LEU:HD11	1.75	0.50
15:O:190:LEU:HD23	15:O:194:LEU:HG	1.92	0.50
2:B:698:ARG:HH21	2:B:952:ARG:HG2	1.76	0.50
1:A:905:ARG:HH22	5:E:170:LEU:HD21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:195:CYS:SG	15:O:196:GLU:N	2.84	0.50
1:A:984:VAL:HG21	1:A:988:ASP:HB3	1.94	0.50
6:F:115:THR:HG22	6:F:116:ASP:H	1.76	0.50
15:O:547:GLU:HG2	15:O:569:LYS:HG2	1.94	0.50
1:A:235:LYS:HD2	1:A:252:ARG:HH11	1.76	0.50
15:O:343:LYS:O	15:O:347:ASP:N	2.33	0.50
2:B:211:GLU:HG3	2:B:212:LYS:HD2	1.94	0.50
2:B:98:ILE:HG13	2:B:131:VAL:HG12	1.94	0.50
17:Q:48:THR:O	17:Q:51:GLU:N	2.44	0.50
2:B:756:THR:HG23	2:B:941:ASP:H	1.76	0.50
1:A:524:THR:HG23	1:A:527:ALA:H	1.76	0.50
2:B:404:ASP:HA	2:B:407:LEU:HB2	1.92	0.50
1:A:1372:THR:HG23	1:A:1375:GLY:H	1.77	0.50
2:B:210:ASP:OD1	2:B:211:GLU:N	2.45	0.50
1:A:997:GLN:O	1:A:998:TYR:HB2	2.12	0.50
15:O:265:VAL:HG12	15:O:267:PRO:HD3	1.94	0.50
15:O:488:LYS:HZ1	15:O:651:PHE:HA	1.76	0.50
1:A:372:ARG:HD3	2:B:1087:SER:HB3	1.93	0.50
1:A:723:LEU:HD21	1:A:811:ALA:HA	1.94	0.50
15:O:54:LYS:HA	15:O:58:GLY:HA2	1.94	0.50
15:O:500:LEU:HD23	15:O:504:ALA:HB2	1.94	0.49
2:B:615:VAL:HG12	2:B:620:SER:HA	1.94	0.49
5:E:115:ASN:OD1	5:E:116:ILE:N	2.45	0.49
2:B:487:ARG:HH21	2:B:508:CYS:HB3	1.76	0.49
2:B:121:ARG:HH12	12:L:54:ARG:HH21	1.58	0.49
14:N:389:THR:OG1	14:N:390:PHE:N	2.40	0.49
15:O:303:ARG:HD2	15:O:467:PHE:HE2	1.77	0.49
13:M:95:ARG:NH1	14:N:393:ASP:OD1	2.45	0.49
1:A:653:ILE:HG23	1:A:660:LEU:HB2	1.92	0.49
2:B:297:THR:HG23	2:B:298:GLN:HG2	1.94	0.49
12:L:29:TYR:HA	12:L:58:LYS:HA	1.93	0.49
8:H:105:GLU:HG2	8:H:115:TYR:HE1	1.77	0.49
2:B:422:ILE:HA	2:B:425:HIS:HB3	1.94	0.49
7:G:23:ILE:HG22	7:G:51:LEU:HD23	1.95	0.49
1:A:1273:LYS:HG2	1:A:1274:GLY:H	1.78	0.49
15:O:592:LYS:HG3	15:O:637:VAL:HG11	1.93	0.49
2:B:296:TYR:HB2	2:B:300:GLN:OE1	2.13	0.49
7:G:89:ILE:HD12	7:G:97:ILE:HB	1.94	0.49
2:B:312:MET:HB3	2:B:317:LEU:HG	1.93	0.49
2:B:391:LEU:HD23	2:B:429:ILE:HA	1.93	0.49
4:D:61:ASN:HB3	7:G:103:GLY:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:90:TYR:HB3	13:M:179:LEU:HB3	1.93	0.49
2:B:989:LYS:HA	2:B:992:VAL:HG12	1.93	0.49
1:A:46:ARG:HG3	1:A:48:PRO:HG3	1.94	0.49
1:A:598:MET:O	1:A:600:PRO:HD3	2.11	0.49
1:A:387:LEU:HD21	1:A:393:ALA:HB2	1.94	0.49
1:A:393:ALA:HB3	1:A:499:ARG:HG3	1.95	0.49
2:B:934:ASN:HA	2:B:1005:TYR:CD2	2.48	0.49
5:E:213:ILE:HG12	5:E:214:CYS:H	1.77	0.49
13:M:142:GLY:O	13:M:143:VAL:HG12	2.12	0.49
1:A:629:LYS:HB3	1:A:633:PHE:HE2	1.76	0.49
15:O:145:ARG:O	15:O:146:VAL:HB	2.13	0.49
2:B:804:ASP:HB3	2:B:848:PRO:HD3	1.93	0.49
3:C:24:SER:HB2	3:C:27:ALA:HB2	1.93	0.49
2:B:831:GLU:N	2:B:831:GLU:OE1	2.43	0.49
1:A:862:LEU:HD21	2:B:491:PRO:HA	1.95	0.49
3:C:191:ILE:HG23	10:J:15:GLY:HA3	1.93	0.49
1:A:1205:ILE:O	1:A:1209:ILE:N	2.42	0.49
13:M:96:LEU:O	13:M:97:VAL:HG12	2.13	0.49
1:A:408:VAL:HG23	1:A:412:ASN:HB2	1.95	0.49
14:N:392:GLN:HB3	14:N:394:VAL:HG23	1.93	0.49
14:N:304:PHE:O	14:N:413:ASP:N	2.31	0.49
15:O:188:SER:HA	15:O:191:PHE:HB2	1.94	0.48
2:B:543:LEU:HG	13:M:176:VAL:HG11	1.95	0.48
14:N:292:ARG:O	14:N:296:LYS:N	2.44	0.48
15:O:620:LEU:HD23	15:O:623:GLU:HB2	1.95	0.48
2:B:97:ASP:OD2	2:B:99:ARG:NH1	2.41	0.48
2:B:371:TYR:HB2	2:B:492:SER:OG	2.13	0.48
15:O:556:ASP:O	15:O:557:ARG:HG2	2.13	0.48
2:B:536:LEU:HD22	2:B:571:PHE:CD1	2.48	0.48
1:A:1064:GLU:HB3	1:A:1065:LYS:H	1.42	0.48
2:B:1022:ILE:HG22	2:B:1023:TYR:H	1.76	0.48
6:F:134:ILE:N	6:F:146:TRP:O	2.46	0.48
2:B:853:ASP:HB2	2:B:855:PRO:HD3	1.95	0.48
14:N:389:THR:O	14:N:390:PHE:HB3	2.12	0.48
1:A:1284:ASN:OD1	1:A:1285:ILE:N	2.45	0.48
2:B:464:ILE:O	2:B:468:GLY:N	2.46	0.48
3:C:331:CYS:SG	11:K:46:LYS:HB2	2.53	0.48
16:P:248:VAL:O	16:P:255:LYS:NZ	2.33	0.48
15:O:488:LYS:NZ	15:O:651:PHE:HA	2.28	0.48
2:B:569:THR:OG1	14:N:275:GLU:OE2	2.29	0.48
1:A:372:ARG:HB3	2:B:1050:PRO:HD2	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:170:LEU:HB3	5:E:174:GLN:NE2	2.29	0.48
1:A:444:LEU:HD11	1:A:449:ARG:H	1.78	0.48
1:A:1451:LEU:HG	4:D:107:MET:HB3	1.96	0.48
1:A:60:VAL:HG23	1:A:74:LEU:HD23	1.96	0.48
14:N:308:GLN:HB2	14:N:417:VAL:HG12	1.94	0.48
1:A:62:SER:H	1:A:65:LEU:HD12	1.79	0.48
2:B:776:SER:HA	2:B:779:ASP:HB3	1.94	0.48
16:P:313:TYR:CB	17:Q:39:ILE:HD11	2.43	0.48
7:G:147:ARG:NH2	7:G:205:MET:SD	2.87	0.48
1:A:311:ASN:OD1	1:A:312:MET:N	2.41	0.48
5:E:86:PRO:HA	5:E:113:GLN:HB3	1.96	0.48
15:O:641:LEU:O	15:O:645:LEU:HB2	2.13	0.48
1:A:1225:ILE:HG23	1:A:1226:GLY:H	1.78	0.48
3:C:256:ILE:HG22	3:C:267:VAL:HA	1.96	0.48
17:Q:41:LEU:HB3	17:Q:42:PRO:HD2	1.96	0.48
1:A:220:ASP:HA	15:O:550:GLU:HB3	1.95	0.48
16:P:215:TYR:CZ	16:P:262:ARG:HD3	2.49	0.48
1:A:980:SER:HB3	5:E:163:GLU:HG2	1.96	0.48
1:A:90:VAL:HG13	1:A:258:TRP:HB2	1.94	0.48
1:A:113:ILE:HG12	1:A:115:LEU:H	1.79	0.48
15:O:553:ARG:HB2	15:O:562:ALA:HA	1.96	0.48
4:D:110:LEU:HB3	4:D:120:LYS:NZ	2.28	0.47
1:A:953:GLY:HA2	1:A:1063:SER:HB2	1.95	0.47
1:A:1187:ARG:HG2	1:A:1229:ARG:HG3	1.95	0.47
1:A:132:VAL:HG21	1:A:137:ARG:HH22	1.79	0.47
2:B:823:SER:OG	12:L:63:ARG:NH1	2.42	0.47
14:N:293:LYS:HA	14:N:296:LYS:HB2	1.97	0.47
4:D:116:PHE:O	4:D:120:LYS:HB2	2.14	0.47
2:B:1008:ILE:HG13	2:B:1009:THR:H	1.78	0.47
13:M:72:GLU:O	14:N:364:ARG:HG2	2.14	0.47
15:O:493:GLU:OE1	16:P:249:TYR:OH	2.28	0.47
15:O:570:GLU:O	15:O:571:THR:OG1	2.29	0.47
1:A:1145:LEU:HD21	1:A:1153:ALA:HB1	1.96	0.47
15:O:291:ARG:HA	15:O:294:LYS:HD3	1.95	0.47
2:B:811:VAL:HG12	2:B:813:GLU:H	1.78	0.47
2:B:550:HIS:NE2	2:B:551:LEU:HD23	2.29	0.47
1:A:221:ASP:OD1	15:O:550:GLU:HB2	2.13	0.47
1:A:113:ILE:HD13	1:A:120:LYS:HE2	1.97	0.47
2:B:217:GLN:HG2	2:B:232:TYR:CD1	2.49	0.47
3:C:74:GLU:HA	3:C:212:ILE:HD11	1.95	0.47
13:M:107:ILE:HD12	13:M:124:PRO:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1020:ALA:HA	1:A:1032:LEU:HD21	1.96	0.47
5:E:173:SER:OG	5:E:174:GLN:N	2.46	0.47
1:A:395:PRO:HG2	1:A:398:VAL:HG22	1.96	0.47
2:B:775:LYS:HE3	2:B:927:LYS:HA	1.96	0.47
15:O:322:LYS:HB3	15:O:361:PHE:CE1	2.50	0.47
16:P:314:PHE:CG	16:P:315:ASP:N	2.82	0.47
16:P:315:ASP:O	16:P:317:TRP:HD1	1.97	0.47
2:B:121:ARG:NH1	2:B:123:MET:SD	2.88	0.47
2:B:854:ALA:N	2:B:855:PRO:HD3	2.29	0.47
1:A:34:VAL:HG23	1:A:35:SER:H	1.79	0.47
2:B:1000:GLY:HA3	2:B:1018:PHE:HD1	1.80	0.47
1:A:706:GLY:HA2	2:B:762:TYR:HA	1.97	0.47
2:B:727:LEU:HB2	2:B:786:GLU:HB2	1.97	0.47
8:H:130:ARG:O	8:H:134:ASN:ND2	2.39	0.47
3:C:43:ASN:HB2	3:C:55:ASP:HB3	1.95	0.47
1:A:1202:ILE:HD12	1:A:1228:ASP:HA	1.97	0.47
13:M:78:ILE:HG22	13:M:170:LEU:HD22	1.96	0.47
2:B:613:ILE:HG12	2:B:646:VAL:HG12	1.96	0.47
1:A:666:LYS:O	1:A:667:SER:HB3	2.15	0.47
1:A:598:MET:CA	1:A:600:PRO:HD3	2.43	0.47
15:O:541:ILE:HG13	15:O:546:VAL:HG23	1.97	0.47
12:L:28:LYS:HG3	12:L:29:TYR:CD2	2.48	0.47
15:O:259:LEU:HD21	15:O:261:GLN:HB2	1.97	0.47
15:O:40:ARG:O	16:P:317:TRP:NE1	2.47	0.47
1:A:1190:LEU:HA	1:A:1193:ILE:HD12	1.97	0.47
2:B:741:ILE:HB	2:B:746:TYR:HB3	1.97	0.47
5:E:143:ASN:N	5:E:143:ASN:OD1	2.47	0.47
2:B:849:THR:HG23	2:B:850:ASN:H	1.79	0.47
1:A:220:ASP:OD1	1:A:220:ASP:N	2.48	0.47
1:A:1134:LYS:HA	1:A:1320:LEU:HD23	1.96	0.47
2:B:108:THR:OG1	2:B:109:LYS:N	2.47	0.47
1:A:890:MET:O	1:A:894:GLU:N	2.48	0.47
1:A:133:ASP:OD1	1:A:134:ASN:N	2.48	0.47
16:P:253:LEU:HB3	16:P:261:TYR:HB3	1.96	0.46
1:A:383:PRO:HB3	1:A:502:GLU:HG2	1.97	0.46
2:B:83:ILE:HG13	2:B:93:LEU:HB3	1.96	0.46
5:E:70:SER:OG	5:E:71:LYS:N	2.47	0.46
7:G:151:GLU:HB3	7:G:198:GLY:HA2	1.97	0.46
15:O:255:LYS:HB3	15:O:256:PRO:HD3	1.96	0.46
15:O:174:TYR:O	15:O:177:SER:OG	2.26	0.46
15:O:516:LEU:O	15:O:565:LEU:HD23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:255:LYS:N	16:P:255:LYS:HD2	2.30	0.46
16:P:221:ILE:O	16:P:225:ILE:N	2.39	0.46
14:N:290:ILE:HD13	14:N:384:LYS:HE3	1.97	0.46
2:B:465:SER:OG	2:B:707:LYS:O	2.34	0.46
4:D:98:MET:SD	4:D:160:TYR:OH	2.71	0.46
15:O:282:ILE:HG22	15:O:283:ASN:H	1.80	0.46
15:O:203:ILE:HG13	15:O:203:ILE:O	2.13	0.46
7:G:88:TRP:HB3	7:G:145:LYS:HA	1.97	0.46
1:A:1145:LEU:HD23	1:A:1146:VAL:HG23	1.97	0.46
2:B:1047:THR:HG22	2:B:1049:GLN:HG3	1.97	0.46
2:B:269:MET:O	2:B:273:CYS:HB3	2.15	0.46
14:N:375:ILE:HG22	14:N:376:GLY:H	1.80	0.46
1:A:664:MET:HB2	1:A:669:LEU:HD13	1.97	0.46
15:O:516:LEU:CD2	15:O:567:ARG:HG3	2.44	0.46
2:B:1080:LEU:O	2:B:1084:MET:HB3	2.16	0.46
1:A:913:GLN:NE2	1:A:915:THR:O	2.49	0.46
7:G:80:PHE:CE2	7:G:83:GLU:HB2	2.50	0.46
7:G:156:VAL:HG11	7:G:190:LYS:HZ1	1.79	0.46
2:B:687:LEU:O	2:B:915:ARG:NH2	2.48	0.46
15:O:87:ASP:O	15:O:88:VAL:HG12	2.16	0.46
11:K:112:THR:HG22	11:K:113:ALA:H	1.81	0.46
2:B:806:ILE:HG13	2:B:806:ILE:H	1.60	0.46
7:G:144:GLU:OE2	7:G:207:LEU:HG	2.16	0.46
7:G:88:TRP:O	7:G:100:SER:N	2.30	0.46
13:M:255:PHE:O	13:M:259:ILE:HG12	2.16	0.46
1:A:1441:LEU:HD21	7:G:54:VAL:HG12	1.97	0.46
1:A:1391:LYS:HD2	1:A:1391:LYS:HA	1.70	0.46
15:O:512:ARG:CG	15:O:568:CYS:SG	2.97	0.46
5:E:117:THR:OG1	5:E:118:PRO:HD2	2.15	0.46
16:P:314:PHE:C	16:P:316:GLU:N	2.69	0.46
2:B:77:ILE:HD13	2:B:98:ILE:HB	1.98	0.46
2:B:992:VAL:HG23	3:C:278:GLU:HG2	1.98	0.46
13:M:131:TYR:OH	13:M:143:VAL:HG23	2.16	0.46
2:B:103:LYS:HG2	2:B:104:SER:H	1.79	0.46
5:E:55:ARG:HD2	5:E:82:PHE:HE2	1.81	0.46
2:B:736:VAL:HG21	2:B:960:GLU:HG3	1.97	0.46
3:C:3:ASN:HD21	3:C:296:ASN:HB2	1.80	0.46
15:O:516:LEU:CG	15:O:567:ARG:HG3	2.45	0.46
1:A:47:ALA:N	1:A:48:PRO:HD3	2.31	0.46
4:D:130:ASN:HB3	4:D:133:HIS:CE1	2.51	0.46
1:A:1145:LEU:HG	1:A:1309:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:95:ARG:HD2	13:M:101:PRO:HB2	1.97	0.46
1:A:415:LYS:HD3	6:F:115:THR:HG21	1.97	0.46
1:A:308:SER:OG	1:A:309:ILE:N	2.49	0.46
3:C:175:GLN:O	3:C:178:THR:HG23	2.16	0.46
1:A:597:ILE:HG22	1:A:598:MET:H	1.81	0.46
16:P:306:LYS:HB3	16:P:307:HIS:CD2	2.50	0.46
7:G:162:SER:O	7:G:166:ARG:N	2.42	0.46
2:B:244:HIS:ND1	2:B:246:SER:OG	2.43	0.46
9:I:95:THR:HA	9:I:110:ASN:HA	1.97	0.46
1:A:869:ARG:HH21	2:B:489:LEU:HD12	1.80	0.46
2:B:69:VAL:HA	2:B:73:LEU:HD23	1.97	0.46
3:C:193:LEU:HD12	3:C:193:LEU:H	1.80	0.45
14:N:395:ILE:HG12	14:N:408:LEU:HG	1.99	0.45
7:G:97:ILE:HG22	7:G:128:TRP:NE1	2.31	0.45
3:C:34:GLU:HA	3:C:37:LYS:HB3	1.98	0.45
15:O:466:PRO:HG2	15:O:467:PHE:HD2	1.81	0.45
4:D:10:PHE:HD2	4:D:117:LYS:HE3	1.80	0.45
5:E:29:PHE:HB2	5:E:65:THR:HB	1.98	0.45
1:A:1033:GLU:HG2	1:A:1034:PRO:HD2	1.98	0.45
2:B:916:HIS:CD2	2:B:957:LYS:HB2	2.52	0.45
3:C:29:ASN:ND2	3:C:35:LYS:HE2	2.32	0.45
2:B:1081:GLU:OE2	2:B:1086:SER:OG	2.34	0.45
16:P:264:THR:HG23	16:P:265:LEU:H	1.81	0.45
2:B:804:ASP:N	2:B:804:ASP:OD1	2.50	0.45
2:B:92:TYR:CZ	2:B:136:THR:HG21	2.50	0.45
9:I:98:TYR:HB2	9:I:107:TRP:HE3	1.81	0.45
1:A:542:LEU:HD21	1:A:679:TYR:HE1	1.81	0.45
11:K:97:SER:OG	11:K:98:GLU:N	2.50	0.45
1:A:712:ILE:HG22	1:A:713:GLY:H	1.81	0.45
2:B:933:PHE:O	2:B:934:ASN:ND2	2.50	0.45
1:A:444:LEU:HD21	1:A:449:ARG:HG2	1.97	0.45
1:A:308:SER:N	1:A:311:ASN:HD21	2.15	0.45
15:O:201:ILE:HG22	15:O:202:GLN:H	1.81	0.45
16:P:300:LYS:O	16:P:301:MET:HB2	2.16	0.45
2:B:241:TYR:HB3	2:B:250:GLU:HB3	1.97	0.45
8:H:21:ASN:OD1	8:H:22:LYS:N	2.40	0.45
16:P:253:LEU:O	16:P:255:LYS:NZ	2.43	0.45
1:A:1365:LYS:HE3	1:A:1379:MET:HB2	1.98	0.45
16:P:312:VAL:HG11	17:Q:41:LEU:HB2	1.98	0.45
2:B:325:GLU:HA	2:B:328:ALA:HB3	1.99	0.45
3:C:229:LEU:HB3	3:C:293:ARG:CZ	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ASN:ND2	11:K:94:PRO:O	2.50	0.45
1:A:541:LEU:HD22	1:A:682:LEU:HD22	1.99	0.45
8:H:7:ASP:OD1	8:H:58:THR:OG1	2.34	0.45
2:B:139:ARG:HB3	2:B:141:ILE:HD11	1.99	0.45
2:B:343:ARG:HE	2:B:542:THR:HA	1.82	0.45
3:C:280:LEU:HA	3:C:286:ALA:HB2	1.98	0.45
3:C:283:GLU:O	3:C:286:ALA:N	2.50	0.45
2:B:409:LYS:HA	2:B:410:PRO:HD3	1.85	0.45
1:A:545:LYS:HG3	1:A:546:SER:H	1.82	0.45
5:E:47:CYS:HA	5:E:53:PRO:HA	1.97	0.45
1:A:163:VAL:HG22	1:A:164:VAL:H	1.81	0.45
6:F:143:PHE:O	6:F:144:GLU:HB2	2.17	0.45
14:N:300:LYS:N	14:N:301:PRO:HD2	2.32	0.45
15:O:509:ARG:HA	15:O:512:ARG:HB2	1.99	0.45
15:O:191:PHE:O	15:O:194:LEU:HB2	2.17	0.45
13:M:88:PHE:HE2	14:N:397:LEU:HD22	1.81	0.45
2:B:240:ILE:HG13	2:B:253:ILE:HG21	1.98	0.45
1:A:360:LYS:HE3	1:A:361:GLN:HG3	1.99	0.45
4:D:31:GLN:HA	4:D:34:LEU:HD12	1.98	0.45
9:I:35:ILE:HA	9:I:35:ILE:HD12	1.87	0.44
1:A:235:LYS:HD3	1:A:235:LYS:HA	1.77	0.44
13:M:122:ASP:HB3	13:M:145:VAL:CG2	2.47	0.44
4:D:20:LEU:HD21	7:G:47:THR:HG21	1.98	0.44
2:B:230:LYS:HD2	2:B:334:HIS:HB3	1.99	0.44
2:B:889:SER:OG	2:B:893:GLN:HG2	2.17	0.44
2:B:260:CYS:O	2:B:342:PHE:HB3	2.17	0.44
3:C:328:LEU:HG	11:K:121:LEU:HD21	1.99	0.44
15:O:489:SER:O	15:O:493:GLU:HG2	2.17	0.44
5:E:40:GLU:HG3	5:E:41:ASP:H	1.82	0.44
15:O:581:LEU:HD13	15:O:648:TRP:CE2	2.52	0.44
2:B:1043:ARG:HG2	2:B:1050:PRO:HD3	1.98	0.44
3:C:25:LYS:HE2	8:H:85:GLY:HA2	2.00	0.44
1:A:979:ASN:O	5:E:167:ARG:NH2	2.50	0.44
1:A:1151:GLU:HG3	1:A:1152:ARG:H	1.82	0.44
2:B:795:LEU:HB2	2:B:894:ALA:HB3	1.99	0.44
1:A:183:PHE:CD2	1:A:184:ARG:HG3	2.52	0.44
1:A:475:ASN:HB3	1:A:518:ASN:HB2	1.99	0.44
1:A:1026:ARG:NH1	8:H:129:TYR:OH	2.50	0.44
2:B:932:PRO:HB3	2:B:1004:LEU:HB3	2.00	0.44
5:E:172:GLU:HG2	5:E:173:SER:H	1.82	0.44
2:B:803:GLN:HG2	2:B:804:ASP:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1123:VAL:HG13	1:A:1124:PRO:HD3	1.98	0.44
1:A:200:GLU:HB3	15:O:516:LEU:HD21	2.00	0.44
13:M:108:SER:O	13:M:122:ASP:HB2	2.17	0.44
10:J:12:LYS:HE3	10:J:43:ARG:NH2	2.32	0.44
7:G:122:THR:OG1	7:G:126:SER:O	2.34	0.44
2:B:983:LYS:HG3	2:B:985:GLU:H	1.83	0.44
3:C:92:ILE:H	3:C:92:ILE:HG13	1.56	0.44
2:B:423:ASN:O	2:B:426:SER:OG	2.31	0.44
15:O:289:LYS:HD3	15:O:325:LYS:HB3	1.99	0.44
5:E:195:VAL:HG22	5:E:213:ILE:HG13	1.99	0.44
1:A:93:ILE:HG23	1:A:94:GLY:H	1.83	0.44
7:G:159:LYS:N	7:G:160:PRO:HD3	2.32	0.44
2:B:1067:ARG:NH1	2:B:1079:LEU:HD22	2.33	0.44
1:A:817:ILE:HG13	1:A:821:ASN:O	2.18	0.44
2:B:38:ILE:HD11	2:B:43:ASP:HB3	2.00	0.44
15:O:516:LEU:HD22	15:O:567:ARG:NE	1.91	0.44
15:O:150:GLU:HG3	15:O:151:GLU:N	2.32	0.44
15:O:163:VAL:HA	15:O:169:LEU:HD13	1.98	0.44
15:O:528:MET:HG3	16:P:175:ILE:HG13	2.00	0.44
7:G:52:LEU:O	7:G:53:THR:HG22	2.17	0.44
1:A:862:LEU:HD22	2:B:494:PHE:HB2	1.98	0.44
1:A:1455:ALA:HB2	4:D:120:LYS:HZ3	1.82	0.44
1:A:627:ASP:OD1	1:A:627:ASP:N	2.51	0.44
1:A:1323:PHE:HD1	1:A:1328:ILE:H	1.65	0.44
15:O:506:ARG:HH12	15:O:526:ALA:HB1	1.81	0.44
1:A:653:ILE:HG12	1:A:660:LEU:HD22	1.99	0.44
2:B:1067:ARG:HH22	2:B:1079:LEU:HB3	1.83	0.44
5:E:24:LYS:HB2	5:E:30:ILE:HD11	1.98	0.44
1:A:297:SER:HA	1:A:300:LYS:HB3	2.00	0.44
1:A:626:LEU:HD21	1:A:675:HIS:HB2	2.00	0.44
2:B:224:THR:OG1	2:B:225:HIS:N	2.50	0.44
14:N:366:HIS:N	14:N:370:LYS:O	2.51	0.44
3:C:270:ALA:HB3	3:C:271:ARG:NH1	2.32	0.44
2:B:717:GLN:OE1	2:B:727:LEU:HD22	2.16	0.44
14:N:296:LYS:HD3	14:N:296:LYS:HA	1.78	0.44
2:B:1008:ILE:O	3:C:65:ASN:ND2	2.51	0.44
3:C:85:PHE:CE1	3:C:204:LEU:HD22	2.53	0.44
1:A:367:ASN:O	1:A:371:LYS:HB2	2.18	0.44
1:A:179:ILE:HG12	1:A:221:ASP:HB3	2.00	0.43
15:O:242:LYS:NZ	15:O:341:GLU:OE2	2.45	0.43
2:B:929:GLU:HB3	3:C:69:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:60:ARG:HG2	12:L:61:THR:H	1.83	0.43
2:B:325:GLU:O	2:B:329:THR:OG1	2.26	0.43
7:G:149:ARG:O	7:G:198:GLY:HA3	2.18	0.43
1:A:1411:VAL:HG13	1:A:1412:SER:H	1.83	0.43
2:B:87:VAL:HG12	2:B:407:LEU:HD22	2.00	0.43
7:G:47:THR:OG1	7:G:48:ILE:N	2.50	0.43
4:D:70:LYS:HG3	4:D:98:MET:SD	2.59	0.43
1:A:481:HIS:CD2	1:A:483:LEU:HB2	2.52	0.43
1:A:1300:LEU:O	1:A:1303:VAL:HG12	2.17	0.43
1:A:985:LYS:O	1:A:987:GLU:N	2.51	0.43
1:A:661:SER:HB2	8:H:122:LEU:HD11	2.01	0.43
1:A:431:ASN:OD1	1:A:465:HIS:NE2	2.51	0.43
1:A:126:GLU:OE2	1:A:136:ARG:NH2	2.38	0.43
1:A:1059:LEU:HD22	1:A:1060:TYR:CE1	2.53	0.43
1:A:862:LEU:O	1:A:866:ILE:HG12	2.19	0.43
3:C:29:ASN:HB2	3:C:35:LYS:NZ	2.33	0.43
1:A:19:SER:O	2:B:1138:ALA:N	2.52	0.43
1:A:774:ARG:HH22	1:A:804:LEU:HD11	1.84	0.43
1:A:634:VAL:HA	1:A:635:PRO:HD3	1.82	0.43
2:B:190:THR:OG1	2:B:191:GLU:N	2.52	0.43
5:E:2:ASP:O	5:E:6:GLU:HG2	2.18	0.43
8:H:12:VAL:HG12	8:H:13:SER:H	1.82	0.43
2:B:538:VAL:HG12	2:B:565:ILE:HD12	1.99	0.43
15:O:533:ILE:HD13	15:O:533:ILE:HA	1.93	0.43
2:B:757:VAL:O	2:B:1019:PHE:HB2	2.19	0.43
2:B:86:ASP:O	2:B:87:VAL:HG23	2.18	0.43
2:B:373:GLY:HA2	2:B:607:ARG:NH2	2.34	0.43
1:A:988:ASP:O	1:A:992:ALA:N	2.42	0.43
2:B:722:ASP:OD1	2:B:723:THR:N	2.47	0.43
1:A:424:PRO:HG3	1:A:444:LEU:O	2.18	0.43
1:A:42:LEU:HD12	1:A:42:LEU:H	1.84	0.43
2:B:225:HIS:HA	2:B:446:ARG:HH11	1.83	0.43
1:A:272:VAL:HB	1:A:274:MET:HG2	2.01	0.43
15:O:581:LEU:HD13	15:O:648:TRP:CD2	2.53	0.43
3:C:59:ILE:HB	3:C:63:ILE:HD11	2.00	0.43
15:O:327:ARG:NH1	15:O:330:LEU:HD22	2.33	0.43
2:B:110:ASP:N	2:B:110:ASP:OD1	2.52	0.43
9:I:85:LEU:HD23	9:I:85:LEU:HA	1.87	0.43
2:B:1088:ASP:OD1	2:B:1088:ASP:N	2.51	0.43
1:A:49:LYS:HG3	1:A:56:PRO:HD3	2.01	0.43
14:N:373:VAL:HG12	14:N:374:LYS:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:THR:OG1	2:B:125:TYR:N	2.51	0.43
15:O:74:LEU:HD21	15:O:79:LEU:HG	2.01	0.43
7:G:152:ARG:HB3	7:G:197:LEU:HG	2.00	0.43
17:Q:59:ILE:HG22	17:Q:63:LYS:HE3	2.00	0.43
1:A:353:PHE:O	1:A:356:ARG:HG2	2.19	0.43
2:B:905:ARG:O	2:B:907:GLU:N	2.51	0.43
8:H:44:VAL:HG13	8:H:45:GLU:H	1.84	0.43
3:C:255:VAL:O	3:C:268:LYS:HB2	2.19	0.43
13:M:247:TRP:HA	14:N:406:ALA:HB3	2.01	0.43
5:E:20:LYS:O	5:E:23:VAL:HG12	2.19	0.43
15:O:53:VAL:HG21	15:O:65:ILE:HD12	2.00	0.43
1:A:1097:ILE:HD13	1:A:1358:LEU:HD22	2.01	0.43
2:B:444:LEU:O	2:B:448:LYS:HA	2.19	0.43
2:B:650:ASP:OD1	2:B:651:VAL:N	2.47	0.43
13:M:135:LYS:HE3	13:M:140:TRP:CH2	2.54	0.43
1:A:955:LEU:HA	1:A:956:PRO:HD2	1.89	0.42
1:A:182:THR:HG22	1:A:185:TRP:NE1	2.35	0.42
7:G:7:ILE:O	7:G:71:THR:OG1	2.27	0.42
5:E:173:SER:C	5:E:175:LEU:H	2.23	0.42
14:N:399:ILE:HA	14:N:405:SER:HG	1.83	0.42
15:O:492:TYR:HE1	15:O:576:PHE:HE1	1.66	0.42
4:D:113:PHE:CE2	4:D:153:MET:HG2	2.54	0.42
1:A:493:ARG:HB3	1:A:494:PRO:HD2	2.01	0.42
1:A:1302:ASP:OD1	1:A:1303:VAL:N	2.52	0.42
1:A:387:LEU:O	1:A:501:ASN:ND2	2.53	0.42
2:B:417:ASP:O	2:B:421:SER:HB2	2.19	0.42
2:B:720:ARG:NH2	2:B:722:ASP:OD2	2.41	0.42
15:O:500:LEU:HA	15:O:500:LEU:HD12	1.87	0.42
5:E:43:LYS:O	5:E:47:CYS:HB2	2.18	0.42
15:O:597:GLN:HA	15:O:600:SER:HB2	2.00	0.42
2:B:1028:LYS:HG2	2:B:1029:HIS:H	1.83	0.42
2:B:137:ARG:NH2	2:B:413:ALA:O	2.38	0.42
15:O:197:MET:HG3	15:O:198:GLY:H	1.84	0.42
7:G:94:ALA:HB2	7:G:121:TYR:CD2	2.54	0.42
1:A:1145:LEU:O	1:A:1310:ILE:HG22	2.20	0.42
1:A:1308:GLY:HA2	9:I:88:ARG:HA	2.00	0.42
15:O:159:ILE:O	15:O:163:VAL:HG23	2.19	0.42
2:B:418:ALA:O	2:B:422:ILE:HG12	2.19	0.42
1:A:350:ILE:HD12	1:A:350:ILE:HA	1.91	0.42
2:B:113:THR:HA	2:B:114:PRO:HD3	1.88	0.42
2:B:551:LEU:HD22	14:N:388:THR:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:96:VAL:HG12	8:H:143:LEU:HA	2.02	0.42
3:C:263:ASP:OD1	3:C:264:GLU:N	2.51	0.42
2:B:378:GLU:OE2	2:B:382:GLN:HB2	2.20	0.42
16:P:237:PRO:O	16:P:240:ILE:HB	2.19	0.42
7:G:104:ILE:HG23	7:G:105:PHE:N	2.32	0.42
1:A:468:ASP:OD1	1:A:469:GLY:N	2.53	0.42
15:O:275:LYS:HA	15:O:276:PRO:HD3	1.90	0.42
1:A:238:ASP:OD1	1:A:238:ASP:N	2.53	0.42
15:O:338:ASP:O	15:O:342:ALA:HB2	2.20	0.42
2:B:263:LEU:HD12	2:B:297:THR:HG22	2.00	0.42
7:G:115:LEU:HD23	7:G:116:PHE:N	2.33	0.42
2:B:292:LYS:HG3	2:B:293:LEU:H	1.85	0.42
15:O:201:ILE:O	15:O:281:THR:N	2.48	0.42
15:O:576:PHE:O	15:O:579:GLN:HG2	2.19	0.42
1:A:1148:ASP:OD1	1:A:1291:ARG:NH1	2.50	0.42
8:H:3:ASN:ND2	8:H:62:SER:OG	2.38	0.42
2:B:529:ILE:HG23	2:B:530:LYS:N	2.35	0.42
13:M:95:ARG:NH2	14:N:392:GLN:O	2.38	0.42
2:B:474:SER:HA	2:B:511:VAL:HG12	2.02	0.42
1:A:1166:LEU:O	1:A:1170:ALA:HB2	2.20	0.42
2:B:735:MET:HB2	2:B:754:ASN:HD21	1.85	0.42
1:A:1080:LYS:HA	1:A:1080:LYS:HD3	1.94	0.42
7:G:55:GLU:N	7:G:55:GLU:OE1	2.53	0.42
4:D:17:LEU:O	4:D:21:THR:OG1	2.20	0.42
1:A:978:ASP:N	1:A:982:CYS:O	2.48	0.42
7:G:29:GLN:O	7:G:33:LYS:HG2	2.20	0.42
1:A:1173:VAL:HG22	1:A:1186:VAL:HG12	2.01	0.42
7:G:59:LEU:HD13	7:G:65:SER:O	2.19	0.42
1:A:1428:PHE:CZ	6:F:89:GLU:HA	2.55	0.42
2:B:131:VAL:HG21	2:B:149:ILE:HG23	2.01	0.42
16:P:297:ASN:O	16:P:298:TYR:HB3	2.19	0.42
1:A:959:ILE:HG23	1:A:1067:VAL:HG21	2.01	0.42
2:B:755:ALA:HA	10:J:48:ARG:NH1	2.35	0.42
7:G:41:ASN:HA	7:G:155:PHE:CE2	2.54	0.42
4:D:145:PHE:HB2	4:D:149:THR:OG1	2.19	0.42
15:O:262:ILE:HG12	15:O:278:VAL:HG21	2.02	0.42
1:A:1200:LEU:HB2	1:A:1204:ASP:HB2	2.02	0.42
4:D:26:LYS:HE2	4:D:26:LYS:HB2	1.95	0.42
1:A:364:PHE:CD1	1:A:364:PHE:C	2.94	0.42
15:O:325:LYS:HD2	15:O:325:LYS:HA	1.77	0.42
2:B:545:ASP:CG	14:N:391:LEU:HD22	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:SER:O	3:C:210:LEU:HD12	2.20	0.42
2:B:447:PHE:HB3	2:B:449:MET:HG2	2.01	0.42
8:H:50:ALA:N	8:H:53:ASP:OD2	2.53	0.42
4:D:24:GLU:OE2	4:D:30:ASP:HB2	2.20	0.42
1:A:409:THR:O	1:A:411:TYR:N	2.53	0.42
16:P:309:LYS:HD3	17:Q:43:ILE:CD1	2.49	0.41
13:M:77:LYS:HE2	13:M:77:LYS:HB3	1.79	0.41
2:B:915:ARG:HD2	2:B:1023:TYR:HD2	1.85	0.41
3:C:105:PRO:HG3	10:J:6:ARG:HH21	1.85	0.41
11:K:46:LYS:O	11:K:47:ILE:O	2.39	0.41
15:O:193:GLN:NE2	15:O:196:GLU:OE1	2.53	0.41
14:N:395:ILE:HD12	14:N:396:ALA:H	1.84	0.41
3:C:87:ASN:O	3:C:88:ASN:HB2	2.20	0.41
3:C:90:SER:HB2	3:C:200:GLN:HB3	2.01	0.41
2:B:321:GLN:O	2:B:324:ILE:HG22	2.20	0.41
4:D:132:VAL:O	4:D:135:TYR:HB3	2.20	0.41
15:O:640:ARG:NH2	17:Q:43:ILE:HG13	2.35	0.41
8:H:93:TYR:CD2	8:H:143:LEU:HG	2.56	0.41
2:B:1036:HIS:NE2	2:B:1058:GLY:HA3	2.35	0.41
1:A:1442:VAL:HA	1:A:1443:PRO:HD3	1.77	0.41
1:A:984:VAL:HG22	1:A:985:LYS:H	1.86	0.41
2:B:217:GLN:NE2	2:B:352:MET:HG2	2.34	0.41
3:C:104:VAL:HA	3:C:105:PRO:HD3	1.89	0.41
11:K:59:THR:HB	11:K:60:SER:H	1.67	0.41
8:H:131:ASN:N	8:H:131:ASN:OD1	2.52	0.41
9:I:6:PRO:O	9:I:7:SER:OG	2.26	0.41
13:M:88:PHE:CD2	14:N:397:LEU:HD13	2.53	0.41
5:E:82:PHE:CE1	5:E:111:VAL:HB	2.55	0.41
15:O:349:ALA:O	15:O:352:VAL:HG12	2.20	0.41
5:E:152:LYS:HB2	5:E:152:LYS:HE2	1.96	0.41
1:A:967:LEU:HD11	1:A:1009:ARG:HD3	2.03	0.41
15:O:467:PHE:C	15:O:468:LEU:HG	2.40	0.41
1:A:1301:ARG:O	1:A:1305:CYS:N	2.45	0.41
3:C:42:VAL:HG13	11:K:138:LYS:HD3	2.03	0.41
8:H:108:SER:OG	8:H:109:LYS:N	2.53	0.41
13:M:121:ILE:HA	13:M:121:ILE:HD13	1.91	0.41
4:D:58:ILE:HG13	4:D:58:ILE:H	1.74	0.41
1:A:1153:ALA:HA	1:A:1156:VAL:HB	2.02	0.41
13:M:123:ILE:C	13:M:145:VAL:HG23	2.40	0.41
15:O:583:TRP:HE1	16:P:315:ASP:HB3	1.84	0.41
1:A:1184:ILE:O	1:A:1231:ALA:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:14:TYR:OH	4:D:99:SER:O	2.35	0.41
15:O:105:LYS:HD2	15:O:209:THR:N	2.36	0.41
5:E:112:TYR:CE2	5:E:134:THR:HB	2.55	0.41
1:A:1365:LYS:HE2	1:A:1365:LYS:HB2	1.97	0.41
1:A:372:ARG:CD	2:B:1087:SER:HB3	2.51	0.41
1:A:18:PHE:HA	2:B:1138:ALA:O	2.20	0.41
3:C:276:SER:O	3:C:277:ARG:HG2	2.20	0.41
9:I:35:ILE:HG13	9:I:36:GLU:H	1.86	0.41
15:O:286:ARG:HA	15:O:289:LYS:HB2	2.02	0.41
1:A:22:SER:C	1:A:24:ALA:H	2.21	0.41
10:J:42:LYS:HG3	10:J:43:ARG:H	1.86	0.41
2:B:1063:GLY:O	2:B:1067:ARG:N	2.54	0.41
2:B:565:ILE:HG12	2:B:566:ARG:N	2.36	0.41
9:I:7:SER:OG	9:I:8:CYS:N	2.53	0.41
8:H:41:ASP:HB2	8:H:121:LEU:HB3	2.03	0.41
5:E:1:MET:HB3	5:E:4:GLU:HG2	2.02	0.41
11:K:83:ASN:HA	11:K:84:PRO:HD3	1.89	0.41
1:A:1083:LEU:HD23	1:A:1083:LEU:HA	1.90	0.41
14:N:297:MET:SD	14:N:303:ARG:NH1	2.94	0.41
3:C:52:ALA:HB3	3:C:302:VAL:HG12	2.02	0.41
3:C:256:ILE:HA	3:C:268:LYS:H	1.86	0.41
15:O:195:CYS:HB2	15:O:263:LEU:HG	2.03	0.41
8:H:17:PRO:HB3	8:H:24:CYS:HB2	2.03	0.41
7:G:60:LYS:HA	7:G:61:PRO:HD3	1.89	0.41
2:B:948:GLY:HA2	2:B:952:ARG:NH1	2.36	0.41
2:B:841:ILE:HG21	2:B:870:PRO:HB2	2.03	0.41
1:A:946:THR:HG21	1:A:1066:SER:HA	2.03	0.41
15:O:226:ILE:HG23	15:O:229:ASN:H	1.86	0.41
1:A:285:LEU:HD23	1:A:285:LEU:HA	1.91	0.41
13:M:126:ASP:HB3	13:M:128:GLN:HG2	2.03	0.41
2:B:548:SER:HA	2:B:550:HIS:ND1	2.36	0.40
11:K:65:ILE:O	11:K:101:LEU:N	2.54	0.40
2:B:247:ILE:HD11	2:B:308:LYS:HZ1	1.86	0.40
2:B:934:ASN:HB3	2:B:1004:LEU:HA	2.01	0.40
2:B:811:VAL:HA	2:B:817:PRO:HB3	2.03	0.40
1:A:1147:ASN:ND2	1:A:1149:ASN:OD1	2.54	0.40
3:C:127:THR:HG22	3:C:128:ASP:H	1.85	0.40
15:O:329:PRO:O	15:O:331:THR:N	2.44	0.40
2:B:610:ARG:HA	2:B:611:PRO:HD3	1.77	0.40
1:A:630:ASN:ND2	1:A:650:GLY:O	2.53	0.40
1:A:597:ILE:HG22	1:A:598:MET:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:58:THR:O	8:H:143:LEU:N	2.48	0.40
3:C:238:PRO:O	3:C:239:ILE:HG13	2.21	0.40
7:G:8:ALA:HA	7:G:71:THR:HA	2.02	0.40
15:O:596:LYS:O	15:O:600:SER:N	2.54	0.40
13:M:160:ALA:HA	14:N:306:VAL:HA	2.04	0.40
1:A:1439:LYS:HA	1:A:1439:LYS:HE2	2.03	0.40
15:O:148:ASP:N	15:O:148:ASP:OD1	2.46	0.40
2:B:579:ARG:HG3	2:B:584:VAL:O	2.21	0.40
1:A:620:SER:HA	1:A:621:PRO:HD3	1.87	0.40
1:A:1428:PHE:CE2	6:F:92:ARG:HD2	2.57	0.40
1:A:12:ARG:NH2	2:B:1144:GLU:OE2	2.55	0.40
16:P:221:ILE:HA	16:P:221:ILE:HD13	1.98	0.40
5:E:170:LEU:HB3	5:E:174:GLN:HE21	1.86	0.40
1:A:1163:LYS:HZ3	1:A:1280:ARG:HA	1.87	0.40
2:B:658:TYR:CE2	2:B:670:MET:HG2	2.57	0.40
2:B:890:ASP:N	2:B:890:ASP:OD1	2.54	0.40
2:B:497:LEU:HD23	2:B:514:LEU:HD23	2.03	0.40
1:A:800:LYS:HG3	2:B:947:HIS:O	2.21	0.40
2:B:93:LEU:HD12	2:B:134:GLU:O	2.20	0.40
1:A:568:ASP:OD1	8:H:22:LYS:HG2	2.21	0.40
1:A:506:THR:OG1	1:A:507:PRO:HD3	2.22	0.40
1:A:521:VAL:HA	1:A:522:PRO:HD3	1.91	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	1402/1460 (96%)	1157 (82%)	233 (17%)	12 (1%)	21	67
2	B	1112/1149 (97%)	948 (85%)	155 (14%)	9 (1%)	24	69
3	C	333/335 (99%)	282 (85%)	47 (14%)	4 (1%)	16	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	113/161 (70%)	80 (71%)	33 (29%)	0	100 100
5	E	213/215 (99%)	172 (81%)	38 (18%)	3 (1%)	14 59
6	F	81/155 (52%)	73 (90%)	8 (10%)	0	100 100
7	G	185/212 (87%)	154 (83%)	25 (14%)	6 (3%)	5 43
8	H	136/146 (93%)	116 (85%)	20 (15%)	0	100 100
9	I	88/110 (80%)	77 (88%)	10 (11%)	1 (1%)	17 64
10	J	65/70 (93%)	53 (82%)	11 (17%)	1 (2%)	13 58
11	K	99/142 (70%)	83 (84%)	15 (15%)	1 (1%)	19 65
12	L	43/70 (61%)	33 (77%)	10 (23%)	0	100 100
13	M	161/282 (57%)	135 (84%)	22 (14%)	4 (2%)	7 48
14	N	101/422 (24%)	78 (77%)	22 (22%)	1 (1%)	19 65
15	O	522/654 (80%)	428 (82%)	88 (17%)	6 (1%)	17 64
16	P	92/317 (29%)	60 (65%)	26 (28%)	6 (6%)	1 25
17	Q	33/104 (32%)	29 (88%)	4 (12%)	0	100 100
All	All	4779/6004 (80%)	3958 (83%)	767 (16%)	54 (1%)	23 64

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	587	ILE
1	A	632	VAL
1	A	1371	ILE
9	I	35	ILE
11	K	47	ILE
13	M	97	VAL
13	M	107	ILE
13	M	143	VAL
15	O	88	VAL
15	O	146	VAL
16	P	175	ILE
16	P	230	VAL
1	A	362	GLY
2	B	87	VAL
3	C	239	ILE
16	P	233	VAL
1	A	307	ILE
1	A	975	VAL

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Mol	Chain	Res	Type
2	B	811	VAL
2	B	927	LYS
3	C	255	VAL
14	N	411	ARG
16	P	308	ASP
16	P	315	ASP
1	A	23	ALA
1	A	1328	ILE
2	B	632	ASP
2	B	651	VAL
2	B	713	ILE
2	B	767	ILE
3	C	87	ASN
3	C	91	VAL
15	O	338	ASP
16	P	309	LYS
1	A	1389	PHE
7	G	79	PRO
7	G	80	PHE
7	G	191	PRO
10	J	65	PRO
15	O	330	LEU
15	O	554	THR
1	A	666	LYS
5	E	122	LYS
15	O	285	ASP
5	E	88	VAL
1	A	278	PRO
7	G	158	VAL
13	M	114	PRO
1	A	600	PRO
2	B	584	VAL
5	E	90	VAL
7	G	192	PRO
2	B	337	VAL
7	G	160	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	1225/1257 (98%)	1208 (99%)	17 (1%)	74	89
2	B	975/1006 (97%)	958 (98%)	17 (2%)	68	88
3	C	296/296 (100%)	293 (99%)	3 (1%)	82	92
4	D	110/145 (76%)	108 (98%)	2 (2%)	66	87
5	E	197/197 (100%)	192 (98%)	5 (2%)	55	82
6	F	73/137 (53%)	70 (96%)	3 (4%)	37	72
7	G	170/190 (90%)	167 (98%)	3 (2%)	66	87
8	H	123/128 (96%)	123 (100%)	0	100	100
9	I	83/98 (85%)	83 (100%)	0	100	100
10	J	62/65 (95%)	60 (97%)	2 (3%)	46	77
11	K	91/130 (70%)	88 (97%)	3 (3%)	45	77
12	L	40/57 (70%)	39 (98%)	1 (2%)	55	82
13	M	143/249 (57%)	140 (98%)	3 (2%)	61	85
14	N	88/360 (24%)	87 (99%)	1 (1%)	80	91
15	O	486/593 (82%)	468 (96%)	18 (4%)	41	75
16	P	94/285 (33%)	89 (95%)	5 (5%)	28	67
17	Q	31/56 (55%)	30 (97%)	1 (3%)	46	77
All	All	4287/5249 (82%)	4203 (98%)	84 (2%)	66	86

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	VAL
1	A	132	VAL
1	A	160	LEU
1	A	247	THR
1	A	289	LEU
1	A	355	GLN
1	A	381	ILE
1	A	390	ASP
1	A	409	THR
1	A	756	CYS
1	A	872	LEU
1	A	955	LEU

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Mol	Chain	Res	Type
1	A	1123	VAL
1	A	1161	VAL
1	A	1186	VAL
1	A	1303	VAL
1	A	1411	VAL
2	B	141	ILE
2	B	191	GLU
2	B	231	THR
2	B	241	TYR
2	B	251	ILE
2	B	335	LEU
2	B	337	VAL
2	B	377	LEU
2	B	422	ILE
2	B	536	LEU
2	B	545	ASP
2	B	548	SER
2	B	612	LEU
2	B	772	VAL
2	B	818	ILE
2	B	899	LEU
2	B	954	THR
3	C	177	THR
3	C	239	ILE
3	C	274	THR
4	D	29	TRP
4	D	127	LEU
5	E	90	VAL
5	E	102	GLU
5	E	107	THR
5	E	124	VAL
5	E	141	VAL
6	F	115	THR
6	F	143	PHE
6	F	151	LEU
7	G	53	THR
7	G	93	THR
7	G	115	LEU
10	J	39	LEU
10	J	54	VAL
11	K	57	ASP
11	K	59	THR

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Mol	Chain	Res	Type
11	K	112	THR
12	L	48	CYS
13	M	83	GLU
13	M	97	VAL
13	M	143	VAL
14	N	412	VAL
15	O	88	VAL
15	O	131	LEU
15	O	169	LEU
15	O	174	TYR
15	O	186	THR
15	O	195	CYS
15	O	223	TYR
15	O	226	ILE
15	O	264	THR
15	O	271	LEU
15	O	282	ILE
15	O	336	LEU
15	O	352	VAL
15	O	516	LEU
15	O	565	LEU
15	O	567	ARG
15	O	569	LYS
15	O	645	LEU
16	P	175	ILE
16	P	180	THR
16	P	235	LEU
16	P	236	THR
16	P	264	THR
17	Q	47	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	431	ASN
1	A	518	ASN
1	A	566	HIS
2	B	286	ASN
2	B	299	GLN
2	B	552	ASN
2	B	902	GLN
2	B	936	GLN

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Mol	Chain	Res	Type
4	D	122	GLN
5	E	174	GLN
9	I	110	ASN
13	M	190	ASN
15	O	337	GLN
15	O	544	ASN
15	O	580	ASN
15	O	652	GLN
16	P	219	GLN
16	P	307	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.