



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 21, 2017 – 10:51 PM EDT

PDB ID : 5M5W  
EMDB ID: : EMD-3446  
Title : RNA Polymerase I open complex  
Authors : Tafur, L.; Sadian, Y.; Hoffmann, N.A.; Jakobi, A.J.; Wetzels, R.; Hagen, W.J.H.; Sachse, C.; Muller, C.W.  
Deposited on : unknown  
Resolution : 3.80 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

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>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

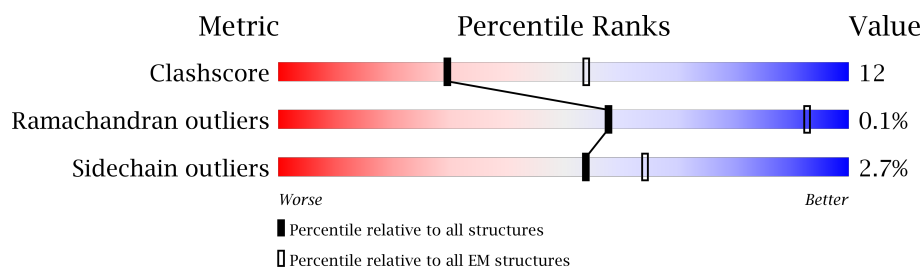
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	1664	65% 24% 10%
2	B	1203	67% 30% ..
3	C	335	72% 19% 9%
4	D	137	30% 12% 57%
5	E	215	73% 24% .
6	F	155	45% 20% 35%
7	G	326	44% 18% 37%
8	H	146	66% 23% 8%
9	I	125	70% 20% 9%

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Mol	Chain	Length	Quality of chain
10	J	70	<div><div></div><div>63%34%..</div></div>
11	K	142	<div><div></div><div>54%15%•30%</div></div>
12	L	70	<div><div></div><div>49%13%39%</div></div>
13	M	415	<div><div></div><div>15%10%74%</div></div>
14	N	233	<div><div></div><div>48%13%•37%</div></div>
15	S	70	<div><div></div><div>9%17%74%</div></div>
16	T	70	<div><div></div><div>23%13%64%</div></div>

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 34780 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 I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1493	Total	C	N	O	S	0	0
			11760	7424	2048	2226	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1183	Total	C	N	O	S	0	0
			9389	5936	1642	1760	51		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	304	Total	C	N	O	S	0	0
			2418	1536	414	460	8		

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	59	Total	C	N	O	0	0
			467	293	80	94		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1751	1111	309	320	11		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	100	Total	C	N	O	S	0	0
			823	522	144	154	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	205	Total	C	N	O	S	0	0
			1624	1040	280	299	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	134	Total	C	N	O	S	0	0
			1075	677	182	212	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	114	Total	C	N	O	S	0	0
			869	541	146	173	9		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	100	Total	C	N	O	S	0	0
			785	491	129	160	5		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	43	Total	C	N	O	S	0	0
			344	211	69	60	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	107	Total	C	N	O		0	0
			850	540	141	169			

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	146	Total	C	N	O	S	0	0
			1164	743	188	229	4		

- Molecule 15 is a DNA chain called Non-template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	18	Total	C	N	O	P	0	0
			376	178	77	103	18		

- Molecule 16 is a DNA chain called Template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	25	Total	C	N	O	P	0	0
			509	244	86	154	25		

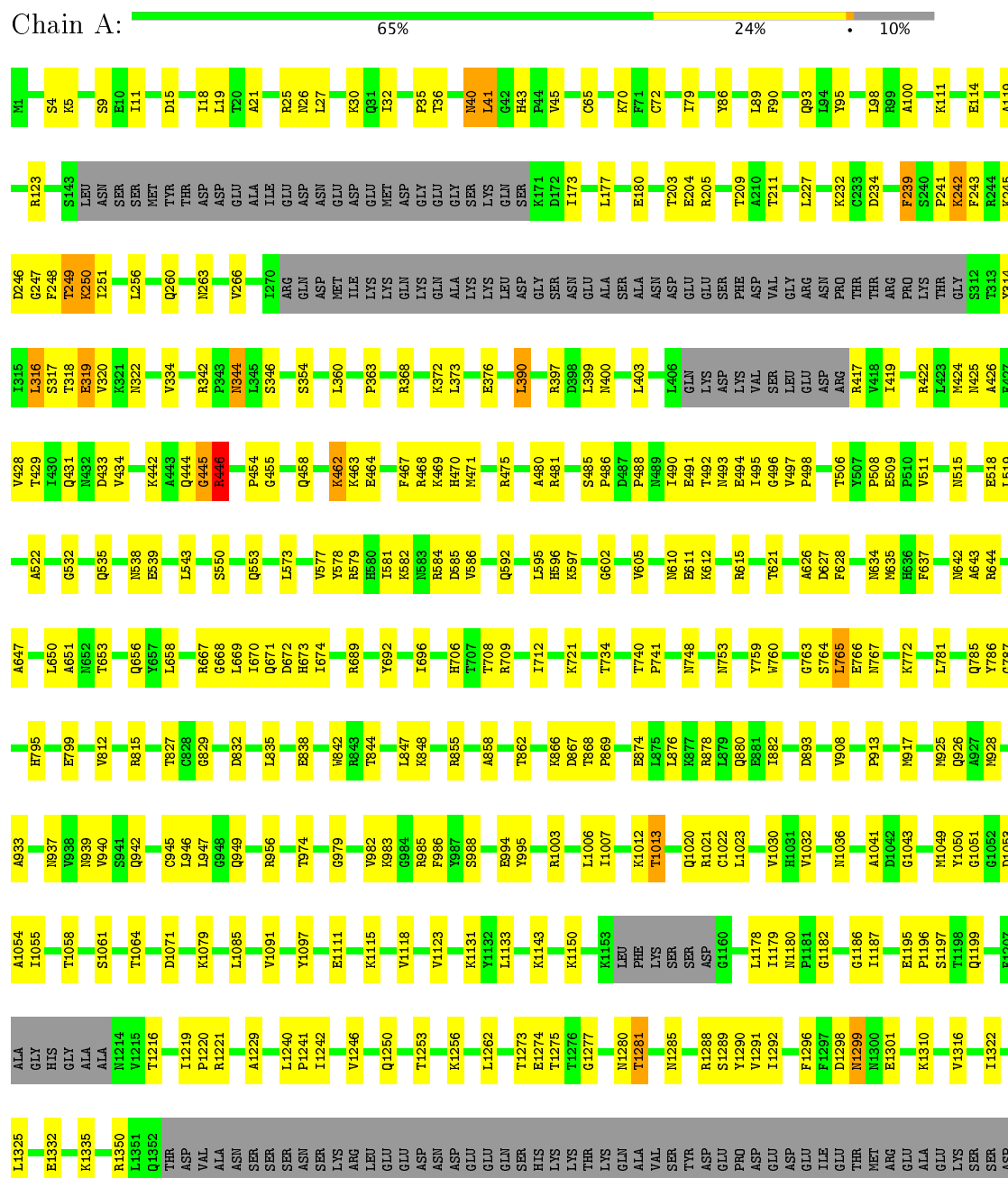
- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

### 3 Residue-property plots

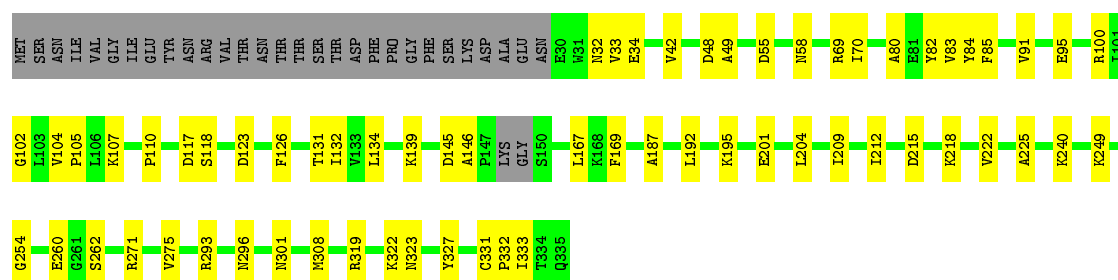
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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 I subunit RPA190



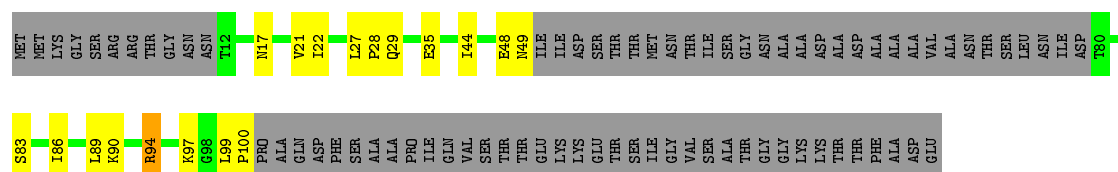






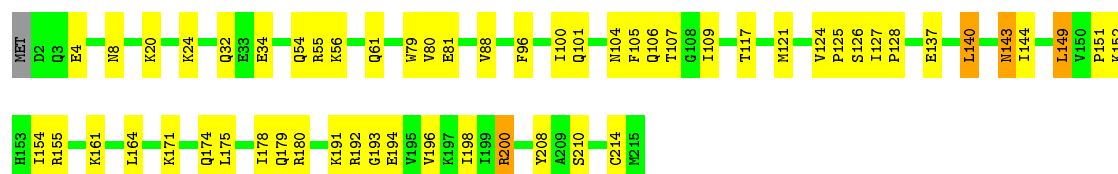
- Molecule 4: DNA-directed RNA polymerase I subunit RPA14

Chain D: 30% 12% 57%



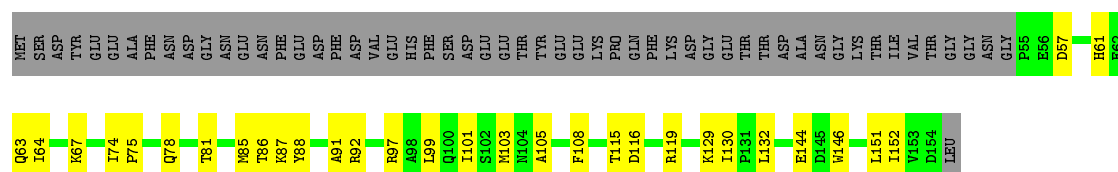
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 73% 24%



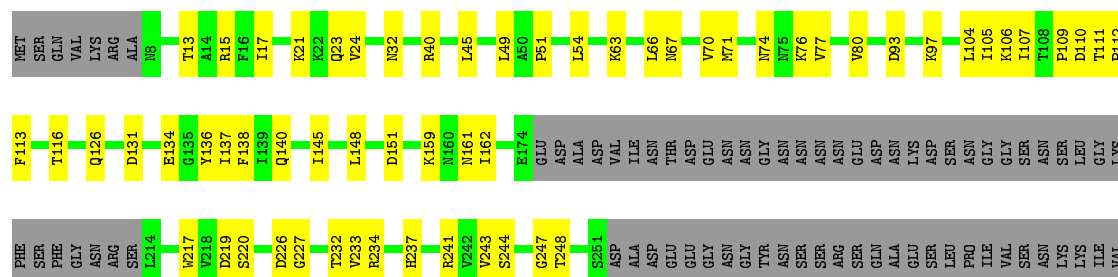
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 45% 20% 35%



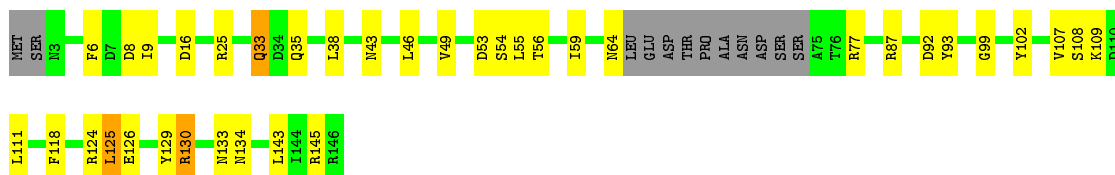
- Molecule 7: DNA-directed RNA polymerase I subunit RPA43

Chain G: 44% 18% 37%



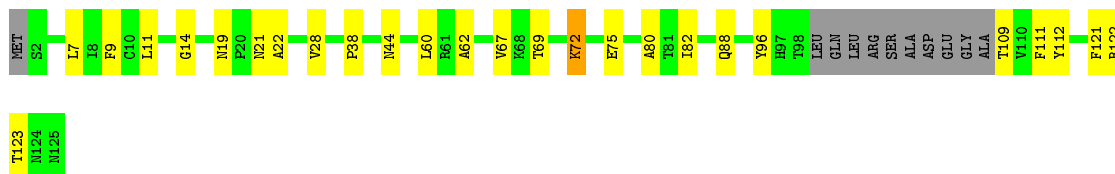
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:  66% 23% • 8%



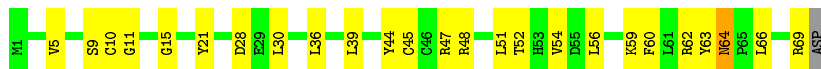
- Molecule 9: DNA-directed RNA polymerase I subunit RPA12

Chain I:  70% 20% 9%



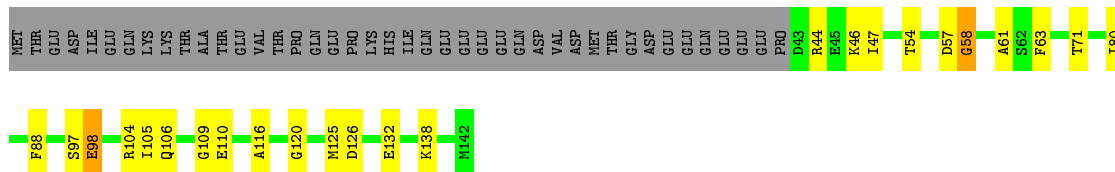
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  63% 34% ..



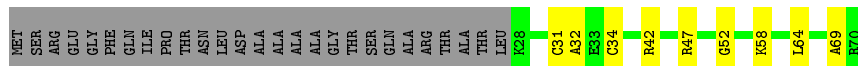
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:  54% 15% 30%



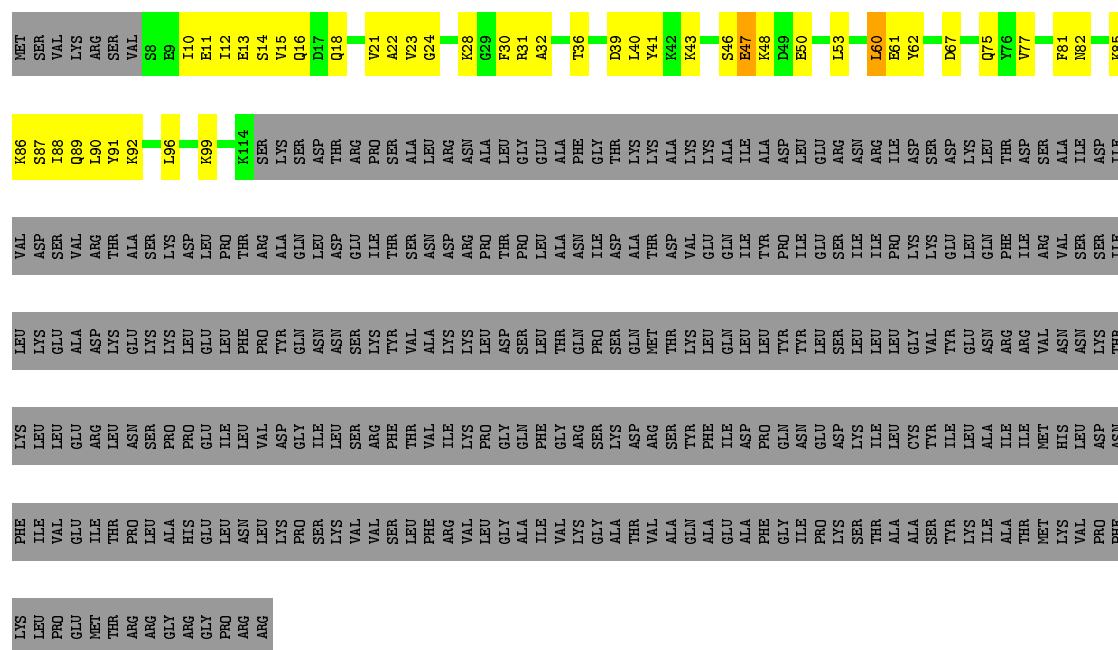
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:  49% 13% 39%

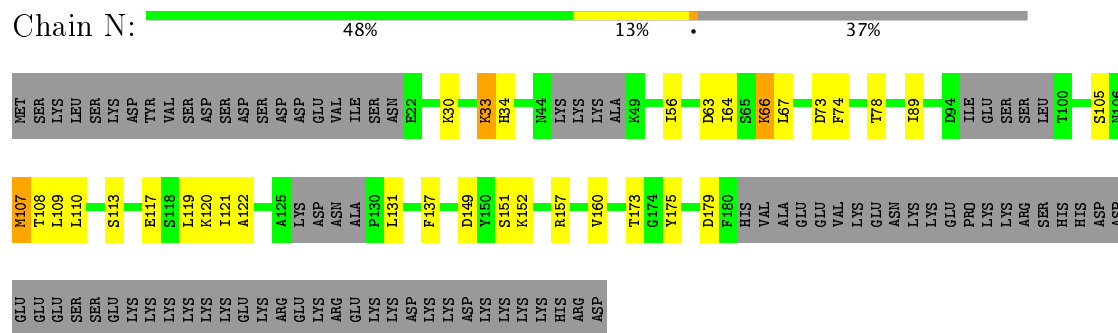


- Molecule 13: DNA-directed RNA polymerase I subunit RPA49

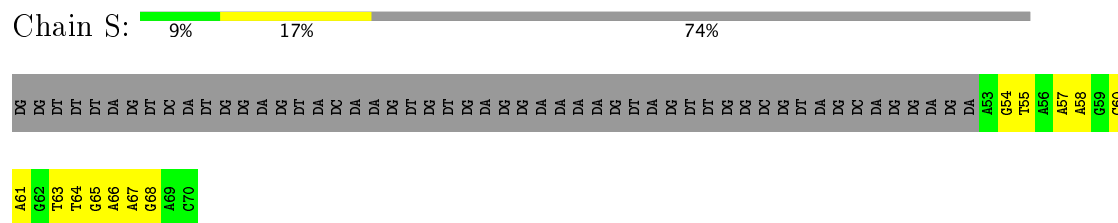
Chain M:  15% 10% 74%



- Molecule 14: DNA-directed RNA polymerase I subunit RPA34



- Molecule 15: Non-template strand



- Molecule 16: Template strand



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	98430	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (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	0.25	1/11976 (0.0%)	0.43	3/16180 (0.0%)
10	J	0.22	0/578	0.40	0/775
11	K	0.50	3/795 (0.4%)	0.81	5/1072 (0.5%)
12	L	0.22	0/346	0.45	0/457
13	M	0.24	0/866	0.46	0/1162
14	N	0.24	0/1186	0.44	0/1596
15	S	0.47	0/424	0.81	0/653
16	T	0.48	0/568	0.94	0/874
2	B	0.24	0/9596	0.46	4/12971 (0.0%)
3	C	0.24	0/2469	0.41	0/3347
4	D	0.23	0/473	0.44	0/641
5	E	0.24	0/1787	0.41	0/2406
6	F	0.22	0/838	0.38	0/1129
7	G	0.24	0/1662	0.44	0/2260
8	H	0.24	0/1093	0.48	0/1480
9	I	0.24	0/881	0.47	0/1187
All	All	0.26	4/35538 (0.0%)	0.47	12/48190 (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
11	K	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	57	ASP	N-CA	10.18	1.66	1.46
1	A	250	LYS	CA-C	-5.97	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	57	ASP	CA-CB	5.24	1.65	1.53
11	K	58	GLY	CA-C	-5.23	1.43	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	57	ASP	N-CA-C	-14.03	73.12	111.00
11	K	57	ASP	CB-CA-C	-11.85	86.70	110.40
2	B	1064	LYS	N-CA-C	-11.72	79.37	111.00
1	A	444	GLN	C-N-CA	-8.56	104.32	122.30
2	B	359	LEU	CA-CB-CG	8.24	134.25	115.30
11	K	57	ASP	N-CA-CB	-8.18	95.88	110.60
2	B	1064	LYS	CB-CA-C	-7.29	95.81	110.40
11	K	58	GLY	N-CA-C	-5.86	98.46	113.10
11	K	58	GLY	CA-C-O	-5.51	110.69	120.60
1	A	250	LYS	N-CA-CB	-5.33	101.00	110.60
1	A	446	ARG	N-CA-C	5.31	125.34	111.00
2	B	1154	ASP	CB-CG-OD2	5.18	122.96	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	K	58	GLY	Mainchain

## 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	11760	0	11838	303	0
2	B	9389	0	9269	280	0
3	C	2418	0	2401	47	0
4	D	467	0	468	13	0
5	E	1751	0	1776	37	0
6	F	823	0	841	23	0
7	G	1624	0	1625	52	0
8	H	1075	0	1045	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	869	0	862	22	0
10	J	569	0	585	20	0
11	K	785	0	782	18	0
12	L	344	0	363	9	0
13	M	850	0	850	34	0
14	N	1164	0	1160	27	0
15	S	376	0	202	6	0
16	T	509	0	285	11	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
All	All	34780	0	34352	795	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 12.

All (795) 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)
2:B:1140:LYS:HE2	7:G:17:ILE:CD1	1.46	1.44
1:A:248:PHE:CE1	1:A:442:LYS:NZ	2.04	1.26
2:B:1140:LYS:CE	7:G:17:ILE:HD11	1.75	1.15
1:A:248:PHE:CD1	1:A:442:LYS:NZ	2.17	1.10
10:J:10:CYS:HB3	10:J:45:CYS:SG	1.94	1.07
2:B:1140:LYS:HE2	7:G:17:ILE:HD11	1.09	1.05
1:A:764:SER:O	1:A:766:GLU:N	1.93	0.99
1:A:248:PHE:CE1	1:A:442:LYS:CE	2.46	0.99
2:B:1107:CYS:HB3	2:B:1131:CYS:SG	2.03	0.98
2:B:1104:CYS:HB3	2:B:1107:CYS:SG	2.09	0.92
1:A:248:PHE:CE1	1:A:442:LYS:HE3	2.06	0.87
2:B:1140:LYS:HE2	7:G:17:ILE:HD13	1.55	0.87
2:B:1140:LYS:CE	7:G:17:ILE:CD1	2.39	0.87
2:B:1140:LYS:CD	7:G:17:ILE:HD11	2.04	0.87
1:A:173:ILE:HD12	1:A:173:ILE:O	1.79	0.83
2:B:358:VAL:HG22	2:B:359:LEU:HD12	1.58	0.82
2:B:1063:ARG:HA	2:B:1067:GLY:H	1.44	0.81
2:B:186:GLU:HB3	2:B:189:GLU:HB2	1.62	0.81
3:C:58:ASN:HA	3:C:296:ASN:HB3	1.65	0.78
1:A:1459:LYS:HE2	1:A:1473:LYS:HG2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:TRP:HB2	1:A:764:SER:OG	1.82	0.76
2:B:480:GLN:HE22	2:B:508:PHE:H	1.33	0.76
2:B:675:ALA:HB3	2:B:689:VAL:HG12	1.67	0.76
1:A:248:PHE:CZ	1:A:442:LYS:HE3	2.19	0.75
1:A:670:ILE:HG13	1:A:671:GLN:HG3	1.66	0.75
2:B:654:ARG:HD2	2:B:691:PHE:HB3	1.69	0.74
7:G:136:TYR:HB3	7:G:148:LEU:HB2	1.71	0.73
14:N:78:THR:HG21	14:N:89:ILE:HG13	1.71	0.73
2:B:803:MET:HB3	2:B:907:ILE:HB	1.72	0.72
1:A:763:GLY:O	1:A:765:LEU:HD22	1.90	0.72
13:M:16:GLN:HE21	13:M:18:GLN:H	1.37	0.71
1:A:1456:PHE:HB3	1:A:1474:LEU:HG	1.71	0.71
2:B:790:ASN:HB2	2:B:946:ASP:HA	1.74	0.70
16:T:20:DT:H2''	16:T:21:DG:H5'	1.74	0.69
6:F:74:ILE:HB	6:F:144:GLU:HB3	1.74	0.69
14:N:56:ILE:HG12	14:N:137:PHE:HB2	1.75	0.69
2:B:292:ILE:HA	2:B:379:ARG:HD3	1.75	0.69
1:A:462:LYS:HD2	1:A:463:LYS:HG2	1.73	0.69
1:A:764:SER:C	1:A:766:GLU:H	1.95	0.69
14:N:66:LYS:HZ3	14:N:67:LEU:HD23	1.58	0.68
1:A:1240:LEU:HD23	1:A:1519:LEU:HD23	1.75	0.68
1:A:1482:LYS:NZ	2:B:307:GLU:OE1	2.25	0.68
2:B:494:TYR:HD1	2:B:700:LEU:HD22	1.59	0.68
13:M:46:SER:O	13:M:47:GLU:C	2.31	0.68
3:C:301:ASN:HD22	14:N:173:THR:HG22	1.59	0.68
2:B:320:LEU:HB3	2:B:326:VAL:HG12	1.77	0.67
2:B:766:PRO:HG3	10:J:54:VAL:HG11	1.76	0.67
2:B:741:LEU:HB2	2:B:804:TYR:HB2	1.77	0.67
3:C:70:ILE:HD13	11:K:71:THR:HG21	1.77	0.66
1:A:986:PHE:HB3	2:B:960:ILE:HD13	1.77	0.66
2:B:731:VAL:HG11	10:J:59:LYS:HE2	1.76	0.66
5:E:200:ARG:HE	5:E:208:TYR:HD2	1.43	0.66
1:A:249:THR:HG22	1:A:431:GLN:HG2	1.77	0.66
13:M:22:ALA:HB2	13:M:40:LEU:HD21	1.76	0.66
1:A:1003:ARG:HD2	2:B:520:LEU:HB2	1.78	0.65
2:B:216:ALA:HB1	2:B:384:LEU:HD13	1.79	0.65
2:B:726:MET:SD	2:B:1035:ARG:NH1	2.69	0.65
8:H:130:ARG:H	8:H:130:ARG:HD2	1.60	0.65
1:A:316:LEU:HD13	1:A:317:SER:H	1.61	0.65
1:A:490:ILE:HG23	1:A:494:GLU:HG3	1.77	0.65
2:B:285:ASP:OD2	2:B:314:LYS:NZ	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:921:HIS:NE2	2:B:965:GLU:OE1	2.29	0.65
2:B:781:TYR:HB2	2:B:788:ILE:HD11	1.78	0.65
3:C:271:ARG:NH1	14:N:175:TYR:OH	2.30	0.65
2:B:617:THR:HG22	2:B:619:GLY:H	1.60	0.64
2:B:588:ILE:HA	2:B:642:LEU:HB2	1.79	0.64
2:B:633:THR:O	2:B:634:ARG:NH2	2.31	0.64
2:B:554:GLN:OE1	2:B:646:HIS:NE2	2.30	0.64
8:H:56:THR:HB	8:H:145:ARG:HB2	1.79	0.64
2:B:240:ARG:NH2	2:B:356:ARG:O	2.30	0.64
1:A:1660:VAL:HG21	7:G:105:ILE:HD13	1.79	0.64
2:B:240:ARG:HD3	2:B:244:THR:HG23	1.78	0.64
7:G:161:ASN:ND2	7:G:247:GLY:O	2.29	0.64
11:K:104:ARG:HH21	11:K:106:GLN:HE21	1.45	0.64
2:B:492:ASN:HD22	2:B:725:THR:HG22	1.63	0.64
1:A:469:LYS:HA	2:B:1070:ARG:HH11	1.62	0.64
2:B:237:ARG:NH1	2:B:401:GLU:OE1	2.30	0.64
7:G:136:TYR:O	7:G:148:LEU:N	2.24	0.64
5:E:151:PRO:HB3	5:E:200:ARG:HB3	1.80	0.63
13:M:46:SER:O	13:M:48:LYS:N	2.31	0.63
16:T:7:DA:H2"	16:T:8:DA:H5"	1.79	0.63
1:A:1550:LEU:HD21	1:A:1594:THR:HB	1.79	0.63
2:B:752:VAL:O	2:B:920:ARG:NH1	2.28	0.63
13:M:16:GLN:NE2	13:M:18:GLN:OE1	2.32	0.63
2:B:28:PRO:HB2	2:B:178:TYR:HA	1.81	0.63
2:B:1104:CYS:CB	2:B:1107:CYS:SG	2.79	0.63
2:B:826:GLY:HA3	12:L:42:ARG:HH22	1.63	0.63
3:C:83:VAL:HG23	12:L:69:ALA:HB2	1.81	0.63
2:B:236:ILE:HD11	2:B:377:MET:HG2	1.81	0.62
2:B:547:HIS:HE1	2:B:702:ASN:HD22	1.47	0.62
1:A:15:ASP:HB3	1:A:1631:ARG:HD2	1.81	0.62
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.82	0.62
1:A:1635:ASP:O	1:A:1648:ASN:ND2	2.32	0.62
13:M:32:ALA:HB1	14:N:121:ILE:HG21	1.80	0.62
1:A:1350:ARG:NH2	2:B:267:ASN:OD1	2.33	0.62
2:B:906:ARG:NH1	3:C:95:GLU:OE1	2.33	0.62
2:B:394:PRO:O	2:B:400:GLN:NE2	2.33	0.62
2:B:292:ILE:HG22	2:B:293:ILE:H	1.65	0.61
1:A:913:PRO:HB3	1:A:926:GLN:HE22	1.65	0.61
2:B:718:GLN:HE21	2:B:922:GLY:H	1.48	0.61
8:H:16:ASP:HB3	8:H:25:ARG:HB3	1.82	0.61
1:A:445:GLY:O	1:A:446:ARG:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ARG:HE	1:A:446:ARG:N	1.98	0.61
2:B:184:LYS:HE3	2:B:735:HIS:HD2	1.66	0.61
6:F:63:GLN:HG3	6:F:67:LYS:HE3	1.81	0.61
7:G:161:ASN:HD21	7:G:248:THR:HA	1.66	0.61
2:B:52:LEU:HA	2:B:60:LEU:HD23	1.82	0.61
1:A:15:ASP:OD2	2:B:1197:ARG:NH2	2.34	0.61
2:B:379:ARG:NH2	2:B:383:SER:OG	2.33	0.61
1:A:995:TYR:OH	2:B:715:ASN:ND2	2.34	0.61
1:A:1050:TYR:HB3	1:A:1054:ALA:HA	1.82	0.61
1:A:611:GLU:HG2	1:A:612:LYS:H	1.66	0.61
2:B:50:ASN:OD1	2:B:168:ASN:ND2	2.31	0.61
14:N:63:ASP:O	14:N:66:LYS:NZ	2.31	0.61
1:A:939:ASN:ND2	2:B:955:PRO:O	2.31	0.60
1:A:11:ILE:HG12	2:B:1200:VAL:HG22	1.83	0.60
2:B:17:ARG:HG3	2:B:20:GLU:HB3	1.83	0.60
2:B:119:ARG:NH1	12:L:52:GLY:O	2.34	0.60
2:B:986:PHE:HE1	14:N:160:VAL:HG21	1.65	0.60
2:B:1140:LYS:HD3	7:G:13:THR:HG21	1.84	0.60
13:M:77:VAL:HG12	13:M:92:LYS:HA	1.81	0.60
1:A:1187:ILE:HD11	2:B:1077:ASP:HB2	1.84	0.60
1:A:1316:VAL:HG11	1:A:1498:ILE:HA	1.84	0.60
1:A:1593:GLY:HA3	5:E:179:GLN:HE21	1.66	0.60
3:C:222:VAL:HG11	3:C:225:ALA:HB2	1.82	0.60
9:I:72:LYS:HE3	9:I:75:GLU:HG2	1.84	0.60
5:E:4:GLU:OE1	5:E:8:ASN:ND2	2.35	0.59
1:A:462:LYS:HE2	1:A:469:LYS:HB2	1.85	0.59
2:B:718:GLN:OE1	2:B:1034:GLN:NE2	2.34	0.59
1:A:692:TYR:OH	1:A:734:THR:OG1	2.18	0.59
2:B:84:GLU:HG3	2:B:86:SER:H	1.67	0.59
14:N:113:SER:OG	14:N:117:GLU:OE2	2.19	0.59
1:A:1256:LYS:O	1:A:1499:ARG:NH2	2.35	0.59
1:A:1655:ASP:OD2	7:G:106:LYS:NZ	2.35	0.59
2:B:193:TYR:HA	2:B:202:LEU:HD23	1.84	0.59
3:C:218:LYS:NZ	12:L:69:ALA:O	2.32	0.59
1:A:1131:LYS:NZ	6:F:81:THR:O	2.34	0.59
11:K:80:ILE:HG12	11:K:120:GLY:HA3	1.84	0.59
1:A:1573:TYR:HA	9:I:122:ARG:HH21	1.68	0.59
2:B:982:THR:HG23	2:B:985:ILE:HD13	1.85	0.59
6:F:146:TRP:HB3	6:F:151:LEU:HD21	1.85	0.59
7:G:24:VAL:HG11	7:G:126:GLN:HE22	1.68	0.59
2:B:218:ILE:HD11	2:B:384:LEU:HD21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:23:VAL:HG12	14:N:107:MET:HB2	1.84	0.59
1:A:1574:ALA:HB3	9:I:122:ARG:HG2	1.85	0.59
3:C:100:ARG:NH2	3:C:192:LEU:O	2.36	0.58
12:L:31:CYS:CB	12:L:34:CYS:SG	2.91	0.58
1:A:1656:VAL:HB	6:F:92:ARG:HE	1.69	0.58
1:A:519:LEU:HD21	1:A:577:VAL:HB	1.83	0.58
2:B:292:ILE:HG13	2:B:306:LEU:HD22	1.85	0.58
2:B:845:LEU:HD21	2:B:887:LEU:HD21	1.85	0.58
1:A:203:THR:HG22	1:A:204:GLU:H	1.68	0.58
14:N:63:ASP:HB2	14:N:66:LYS:HD2	1.85	0.58
8:H:124:ARG:NH1	8:H:126:GLU:OE2	2.37	0.58
8:H:64:ASN:O	8:H:87:ARG:NH1	2.36	0.58
1:A:1253:THR:HA	1:A:1256:LYS:HD3	1.84	0.58
5:E:178:ILE:HG22	5:E:214:CYS:HA	1.84	0.58
9:I:112:TYR:HB2	9:I:121:PHE:HB2	1.84	0.58
2:B:286:ARG:HH22	9:I:9:PHE:HB3	1.69	0.58
15:S:63:DT:H2''	15:S:64:DT:H3'	1.86	0.58
1:A:40:ASN:HD22	1:A:41:LEU:H	1.52	0.58
1:A:399:LEU:HD21	1:A:422:ARG:HG3	1.86	0.58
1:A:1180:ASN:HD21	6:F:87:LYS:HG2	1.69	0.58
2:B:656:LEU:HB2	2:B:657:PRO:HD3	1.85	0.58
1:A:1290:TYR:HB2	1:A:1474:LEU:HB2	1.86	0.58
2:B:246:GLN:HE22	2:B:357:ILE:HG22	1.69	0.58
2:B:207:ILE:HD11	2:B:400:GLN:HB3	1.86	0.58
1:A:1566:ILE:HA	1:A:1569:VAL:HG22	1.85	0.57
1:A:1021:ARG:NH2	16:T:19:DA:OP1	2.37	0.57
2:B:209:GLN:O	2:B:237:ARG:NH1	2.37	0.57
2:B:221:SER:OG	2:B:225:ARG:NH1	2.37	0.57
2:B:636:GLN:NE2	2:B:671:TYR:OH	2.37	0.57
3:C:80:ALA:HB3	3:C:102:GLY:HA2	1.84	0.57
1:A:1457:ILE:HG12	1:A:1460:TYR:HB2	1.85	0.57
1:A:245:LYS:HG2	1:A:247:GLY:H	1.69	0.57
2:B:773:VAL:N	2:B:1029:GLY:O	2.32	0.57
2:B:219:ARG:HG2	2:B:221:SER:H	1.69	0.57
2:B:573:ALA:HB2	2:B:594:GLY:HA2	1.87	0.57
1:A:1274:GLU:OE2	1:A:1288:ARG:NH1	2.37	0.57
2:B:182:GLN:O	10:J:69:ARG:NH1	2.38	0.57
1:A:462:LYS:HD3	1:A:469:LYS:HE2	1.86	0.57
5:E:24:LYS:NZ	5:E:32:GLN:OE1	2.38	0.57
13:M:43:LYS:HG3	13:M:50:GLU:HB3	1.86	0.57
1:A:316:LEU:HD12	1:A:318:THR:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:ARG:O	2:B:21:ARG:NH2	2.38	0.57
1:A:173:ILE:C	1:A:173:ILE:HD12	2.25	0.56
3:C:107:LYS:HG3	3:C:187:ALA:HA	1.87	0.56
7:G:63:LYS:HA	7:G:67:ASN:HD22	1.70	0.56
1:A:1482:LYS:HD3	2:B:311:ARG:HH12	1.71	0.56
3:C:327:TYR:HE2	11:K:46:LYS:HG3	1.69	0.56
7:G:74:ASN:HB3	7:G:77:VAL:HG12	1.87	0.56
1:A:709:ARG:NH1	1:A:740:THR:O	2.37	0.56
13:M:46:SER:O	13:M:48:LYS:O	2.23	0.56
2:B:1116:SER:OG	2:B:1127:CYS:SG	2.64	0.56
1:A:1111:GLU:HG2	1:A:1115:LYS:HB2	1.88	0.56
2:B:237:ARG:HA	2:B:247:THR:HA	1.87	0.56
5:E:88:VAL:O	5:E:117:THR:OG1	2.24	0.56
7:G:159:LYS:HA	7:G:162:ILE:HD12	1.88	0.56
9:I:11:LEU:HD13	13:M:31:ARG:HH12	1.70	0.56
1:A:674:ILE:HD11	1:A:933:ALA:HB2	1.87	0.56
4:D:44:ILE:HD13	4:D:89:LEU:HD22	1.88	0.56
1:A:1051:GLY:HA3	1:A:1580:ARG:HD2	1.87	0.56
1:A:592:GLN:HE22	1:A:634:ASN:HD21	1.54	0.56
2:B:60:LEU:HD11	2:B:243:GLN:HE21	1.71	0.56
2:B:743:ARG:NH2	2:B:804:TYR:OH	2.39	0.56
2:B:935:ASP:HB3	3:C:69:ARG:HH22	1.71	0.56
2:B:96:SER:HB3	2:B:144:SER:HB2	1.86	0.55
5:E:106:GLN:OE1	5:E:107:THR:OG1	2.24	0.55
5:E:80:VAL:HA	5:E:109:ILE:HG23	1.88	0.55
2:B:976:GLY:HA2	10:J:51:LEU:HD11	1.88	0.55
13:M:36:THR:O	14:N:120:LYS:NZ	2.38	0.55
1:A:1647:ASN:OD1	1:A:1648:ASN:N	2.38	0.55
2:B:33:SER:HA	2:B:177:PRO:HG3	1.88	0.55
2:B:196:VAL:HG12	2:B:197:ASN:H	1.71	0.55
1:A:647:ALA:HA	1:A:651:ALA:HB3	1.89	0.55
1:A:1350:ARG:HH22	2:B:266:LYS:HD2	1.72	0.55
1:A:464:GLU:OE2	1:A:1617:THR:N	2.39	0.55
1:A:475:ARG:HD3	2:B:1070:ARG:HB2	1.89	0.55
1:A:481:ARG:HB3	2:B:1045:GLN:HB2	1.89	0.55
5:E:161:LYS:NZ	5:E:193:GLY:O	2.40	0.55
14:N:122:ALA:HB3	14:N:131:LEU:HD23	1.88	0.55
13:M:75:GLN:HE22	14:N:64:ILE:HD11	1.71	0.55
2:B:1076:ARG:HG2	2:B:1088:LEU:HD11	1.89	0.55
2:B:897:GLU:OE1	2:B:899:GLN:NE2	2.39	0.55
4:D:94:ARG:NH2	7:G:151:ASP:OD2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:97:ARG:HG2	6:F:130:ILE:HD12	1.89	0.54
1:A:1332:GLU:HA	1:A:1335:LYS:HB2	1.88	0.54
1:A:994:GLU:OE1	1:A:994:GLU:N	2.40	0.54
2:B:269:TYR:HE2	2:B:337:VAL:HG21	1.72	0.54
2:B:631:PRO:HB3	2:B:638:PRO:HG3	1.90	0.54
6:F:99:LEU:HB3	7:G:112:PRO:HG3	1.88	0.54
2:B:501:ARG:HD2	2:B:545:PHE:HB2	1.89	0.54
2:B:1016:GLY:O	3:C:69:ARG:NH1	2.39	0.54
9:I:11:LEU:HD13	13:M:31:ARG:HH22	1.73	0.54
1:A:35:PRO:HB3	1:A:390:LEU:HB3	1.89	0.54
3:C:301:ASN:ND2	14:N:173:THR:O	2.40	0.54
1:A:9:SER:OG	2:B:1201:GLU:O	2.25	0.54
1:A:584:ARG:NH1	6:F:115:THR:O	2.40	0.54
1:A:27:LEU:HD23	2:B:1130:ARG:HB2	1.89	0.54
2:B:654:ARG:NH2	2:B:659:ASP:OD2	2.41	0.54
4:D:28:PRO:HD2	7:G:23:GLN:HG2	1.89	0.54
5:E:124:VAL:HG23	5:E:125:PRO:HD3	1.90	0.53
1:A:1273:THR:HB	1:A:1291:VAL:HG23	1.89	0.53
1:A:1559:ARG:NH1	1:A:1583:ASP:OD1	2.42	0.53
2:B:127:ARG:NH2	2:B:193:TYR:OH	2.41	0.53
1:A:1240:LEU:HB3	1:A:1519:LEU:HB3	1.90	0.53
1:A:446:ARG:HE	1:A:446:ARG:H	1.56	0.53
1:A:1310:LYS:HZ2	1:A:1467:GLY:HA3	1.72	0.53
1:A:1504:ILE:HA	1:A:1523:GLY:HA3	1.89	0.53
2:B:883:GLU:HG2	2:B:884:GLU:HG2	1.88	0.53
2:B:73:ILE:HD11	2:B:95:LEU:HD22	1.90	0.53
3:C:32:ASN:ND2	3:C:34:GLU:OE2	2.41	0.53
7:G:237:HIS:HB2	7:G:244:SER:HB3	1.90	0.53
2:B:211:ARG:HE	2:B:239:VAL:HG11	1.73	0.53
2:B:362:LEU:HB2	2:B:370:LYS:HD3	1.89	0.53
3:C:212:ILE:HD12	3:C:215:ASP:H	1.74	0.53
13:M:15:VAL:HA	13:M:90:LEU:HD21	1.90	0.53
1:A:1484:LEU:H	1:A:1484:LEU:HD23	1.73	0.53
1:A:1569:VAL:O	1:A:1572:ARG:NE	2.41	0.53
3:C:275:VAL:HG21	3:C:293:ARG:HH21	1.74	0.53
1:A:342:ARG:HE	1:A:1631:ARG:H	1.57	0.53
1:A:360:LEU:HD21	1:A:434:VAL:HG23	1.91	0.53
2:B:398:GLN:HB2	2:B:667:PHE:HD1	1.73	0.53
3:C:134:LEU:HD12	3:C:167:LEU:HB3	1.90	0.53
2:B:809:VAL:HG13	2:B:901:VAL:HG13	1.91	0.53
2:B:71:LYS:HE3	2:B:425:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.91	0.52
13:M:81:PHE:HE1	13:M:86:LYS:HA	1.74	0.52
1:A:1118:VAL:HG11	5:E:154:ILE:HG12	1.90	0.52
2:B:1099:THR:OG1	2:B:1178:ILE:O	2.24	0.52
13:M:21:VAL:N	13:M:91:TYR:OH	2.32	0.52
2:B:307:GLU:HG2	9:I:7:LEU:HG	1.92	0.52
2:B:916:LYS:HZ3	2:B:916:LYS:HB3	1.72	0.52
8:H:33:GLN:HE22	8:H:35:GLN:HB3	1.74	0.52
8:H:93:TYR:CG	8:H:143:LEU:HB3	2.45	0.52
1:A:32:ILE:HB	1:A:79:ILE:HG22	1.91	0.52
1:A:637:PHE:O	2:B:1091:ARG:NH1	2.42	0.52
2:B:1010:ASN:HB3	2:B:1025:ASP:HB2	1.91	0.52
2:B:280:LEU:HD13	2:B:354:LEU:HD23	1.91	0.52
2:B:731:VAL:HG23	10:J:63:TYR:HE2	1.74	0.52
1:A:480:ALA:O	1:A:635:MET:N	2.43	0.52
1:A:829:GLY:N	1:A:832:ASP:OD2	2.41	0.52
2:B:1065:ARG:O	2:B:1066:HIS:HB2	2.10	0.52
1:A:373:LEU:HD12	1:A:376:GLU:H	1.74	0.52
2:B:106:LYS:HG2	2:B:107:PRO:HD2	1.92	0.52
2:B:913:ILE:HD12	2:B:929:ARG:HA	1.91	0.52
1:A:956:ARG:HH11	1:A:979:GLY:HA3	1.74	0.52
2:B:898:LEU:H	2:B:898:LEU:HD23	1.74	0.52
2:B:586:VAL:HG22	2:B:640:LEU:HD13	1.91	0.52
6:F:103:MET:HB2	7:G:51:PRO:HG2	1.91	0.52
3:C:331:CYS:SG	11:K:44:ARG:NH1	2.83	0.52
1:A:669:LEU:HB3	1:A:673:HIS:HB2	1.91	0.52
2:B:501:ARG:HG3	2:B:544:HIS:HB3	1.91	0.52
1:A:498:PRO:HB3	1:A:612:LYS:HA	1.91	0.52
1:A:753:ASN:N	1:A:767:ASN:O	2.43	0.52
2:B:215:MET:HB2	2:B:235:GLN:O	2.10	0.52
2:B:711:GLN:HG2	2:B:713:PRO:HD2	1.92	0.52
1:A:318:THR:O	1:A:320:VAL:N	2.43	0.51
3:C:82:TYR:HD2	3:C:126:PHE:HZ	1.56	0.51
7:G:70:VAL:HG12	7:G:71:MET:HG2	1.92	0.51
11:K:105:ILE:HD11	11:K:116:ALA:HB3	1.93	0.51
1:A:488:PRO:HD2	2:B:781:TYR:CD1	2.45	0.51
1:A:672:ASP:HA	2:B:952:HIS:HE1	1.74	0.51
2:B:203:ILE:HG22	2:B:485:THR:HG22	1.91	0.51
5:E:101:GLN:HE21	5:E:127:ILE:HG13	1.75	0.51
7:G:232:THR:N	7:G:248:THR:O	2.43	0.51
7:G:51:PRO:HA	7:G:54:LEU:HD23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:92:ASP:OD2	8:H:145:ARG:NH2	2.44	0.51
1:A:509:GLU:OE2	1:A:515:ASN:ND2	2.43	0.51
2:B:379:ARG:HG2	2:B:579:ALA:HB1	1.92	0.51
2:B:614:GLU:OE1	2:B:616:LYS:NZ	2.35	0.51
3:C:85:PHE:HE1	3:C:204:LEU:HD22	1.74	0.51
2:B:1093:LEU:HD13	2:B:1179:PRO:HG3	1.93	0.51
2:B:985:ILE:O	14:N:157:ARG:NH2	2.42	0.51
13:M:41:TYR:HE1	14:N:30:LYS:H	1.57	0.51
1:A:550:SER:HB2	1:A:553:GLN:HE22	1.74	0.51
1:A:1041:ALA:HB1	1:A:1648:ASN:HD21	1.75	0.51
2:B:167:SER:H	2:B:170:CYS:HB3	1.76	0.51
1:A:855:ARG:NH1	1:A:867:ASP:O	2.43	0.51
1:A:1617:THR:HG22	1:A:1620:GLN:HB2	1.92	0.51
2:B:782:ASP:OD1	2:B:782:ASP:N	2.44	0.51
6:F:81:THR:OG1	6:F:146:TRP:NE1	2.44	0.51
1:A:1007:ILE:HD11	2:B:518:ARG:HB3	1.92	0.50
1:A:1049:MET:HB3	5:E:208:TYR:HE1	1.75	0.50
3:C:48:ASP:OD1	3:C:49:ALA:N	2.42	0.50
1:A:245:LYS:HA	1:A:251:ILE:HG22	1.92	0.50
1:A:248:PHE:HE1	1:A:442:LYS:NZ	1.92	0.50
1:A:835:LEU:HA	1:A:917:MET:H	1.76	0.50
1:A:1296:PHE:N	1:A:1468:LYS:O	2.35	0.50
1:A:426:ALA:HA	1:A:429:THR:HG22	1.93	0.50
1:A:595:LEU:HB3	1:A:1020:GLN:HE22	1.76	0.50
3:C:33:VAL:HG21	11:K:126:ASP:HB3	1.93	0.50
13:M:13:GLU:OE2	13:M:87:SER:OG	2.28	0.50
1:A:1478:ALA:HB1	9:I:21:ASN:HB2	1.93	0.50
1:A:40:ASN:ND2	1:A:41:LEU:H	2.10	0.50
5:E:143:ASN:HD22	5:E:144:ILE:N	2.09	0.50
2:B:1140:LYS:HD3	7:G:17:ILE:HD11	1.90	0.50
1:A:855:ARG:HD2	1:A:869:PRO:HA	1.92	0.50
2:B:132:SER:HB2	2:B:134:ARG:HH11	1.76	0.50
2:B:831:GLU:OE1	2:B:868:LYS:NZ	2.43	0.50
6:F:57:ASP:O	6:F:61:HIS:ND1	2.35	0.50
1:A:1450:ILE:HG23	1:A:1457:ILE:HG21	1.93	0.50
7:G:140:GLN:OE1	7:G:217:TRP:NE1	2.45	0.50
15:S:65:DG:H2"	15:S:66:DA:C8	2.46	0.50
1:A:1216:THR:HG23	1:A:1221:ARG:HD3	1.94	0.50
1:A:643:ALA:HB1	2:B:1087:LEU:HD23	1.93	0.50
2:B:398:GLN:HG3	2:B:399:HIS:ND1	2.27	0.50
15:S:60:DC:H2"	15:S:61:DA:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:GLY:O	2:B:305:ARG:NH2	2.44	0.49
9:I:28:VAL:HG12	9:I:38:PRO:HD3	1.93	0.49
2:B:184:LYS:HE3	2:B:735:HIS:CD2	2.47	0.49
3:C:260:GLU:HG2	3:C:262:SER:H	1.77	0.49
10:J:5:VAL:HG22	10:J:15:GLY:HA3	1.93	0.49
8:H:6:PHE:HB3	8:H:59:ILE:HB	1.93	0.49
12:L:31:CYS:HB3	12:L:34:CYS:SG	2.52	0.49
1:A:538:ASN:OD1	1:A:539:GLU:N	2.45	0.49
1:A:1003:ARG:HH21	2:B:530:PRO:HA	1.78	0.49
1:A:1240:LEU:HG	1:A:1536:ILE:HG21	1.95	0.49
1:A:781:LEU:HA	1:A:785:GLN:HG3	1.94	0.49
5:E:55:ARG:NH1	5:E:137:GLU:OE2	2.45	0.49
7:G:232:THR:O	7:G:248:THR:N	2.43	0.49
8:H:129:TYR:H	8:H:130:ARG:HH11	1.59	0.49
8:H:99:GLY:HA3	8:H:118:PHE:HD1	1.77	0.49
2:B:404:LEU:HD11	2:B:551:ILE:HG21	1.95	0.49
2:B:518:ARG:NH1	2:B:537:SER:O	2.44	0.49
1:A:602:GLY:N	1:A:651:ALA:O	2.46	0.49
1:A:653:THR:OG1	1:A:667:ARG:NH1	2.45	0.49
2:B:1158:ILE:HD11	2:B:1166:LYS:HB3	1.93	0.49
10:J:64:ASN:HD22	10:J:66:LEU:H	1.61	0.49
1:A:1032:VAL:HG23	1:A:1182:GLY:H	1.77	0.49
3:C:131:THR:HB	3:C:209:ILE:HG22	1.95	0.49
3:C:105:PRO:HG2	3:C:187:ALA:HB3	1.93	0.49
1:A:748:ASN:HB2	1:A:1071:ASP:HB3	1.95	0.49
2:B:721:MET:HG2	2:B:1036:LEU:HD21	1.94	0.49
2:B:367:SER:HA	2:B:370:LYS:HB3	1.95	0.49
2:B:609:ARG:HH12	2:B:664:VAL:HG12	1.77	0.49
2:B:1140:LYS:HD3	7:G:13:THR:CG2	2.43	0.49
15:S:57:DA:H2"	15:S:58:DA:C8	2.47	0.49
1:A:496:GLY:HA3	1:A:615:ARG:HB2	1.94	0.49
2:B:218:ILE:HD13	2:B:391:PRO:HB3	1.94	0.49
3:C:332:PRO:O	11:K:44:ARG:NH1	2.43	0.49
1:A:1085:LEU:HD22	6:F:152:ILE:HD13	1.94	0.49
1:A:1064:THR:HG23	1:A:1143:LYS:HD3	1.94	0.48
1:A:111:LYS:HG3	1:A:234:ASP:HB3	1.94	0.48
1:A:1506:ARG:HB3	1:A:1522:GLU:HB2	1.95	0.48
1:A:4:SER:HB2	1:A:573:LEU:HD13	1.94	0.48
1:A:668:GLY:HA3	1:A:787:GLY:HA2	1.95	0.48
1:A:1006:LEU:HD11	2:B:713:PRO:HB3	1.95	0.48
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ASN:HA	1:A:266:VAL:HG22	1.94	0.48
1:A:248:PHE:HE1	1:A:442:LYS:HZ1	1.52	0.48
9:I:111:PHE:HB3	9:I:122:ARG:HH11	1.77	0.48
1:A:1572:ARG:HD3	1:A:1573:TYR:HD1	1.78	0.48
1:A:1655:ASP:OD1	1:A:1656:VAL:N	2.46	0.48
1:A:446:ARG:NE	1:A:446:ARG:N	2.60	0.48
2:B:12:ARG:HG2	2:B:13:THR:HG22	1.93	0.48
2:B:790:ASN:HD22	2:B:791:LYS:N	2.12	0.48
6:F:101:ILE:HA	6:F:105:ALA:HB3	1.95	0.48
1:A:89:LEU:HB3	1:A:1623:THR:HG22	1.94	0.48
1:A:90:PHE:HB3	1:A:93:GLN:HE21	1.78	0.48
2:B:261:ARG:HH21	2:B:270:LEU:HD21	1.78	0.48
4:D:48:GLU:OE2	4:D:90:LYS:NZ	2.46	0.48
3:C:91:VAL:HG11	10:J:60:PHE:HB3	1.94	0.48
1:A:1635:ASP:OD1	1:A:1635:ASP:N	2.47	0.48
7:G:137:ILE:HG12	7:G:145:ILE:HD11	1.94	0.48
2:B:225:ARG:HH21	2:B:261:ARG:HH12	1.60	0.48
7:G:226:ASP:OD1	7:G:227:GLY:N	2.44	0.48
7:G:49:LEU:HD12	7:G:105:ILE:HG21	1.93	0.48
7:G:219:ASP:OD1	7:G:220:SER:N	2.45	0.48
1:A:1003:ARG:HH12	2:B:533:THR:HG21	1.79	0.48
3:C:145:ASP:OD1	3:C:146:ALA:N	2.43	0.48
1:A:1242:ILE:HB	1:A:1517:ARG:HH12	1.78	0.48
1:A:1606:SER:HB3	1:A:1612:LYS:HD3	1.96	0.48
1:A:239:PHE:HD2	1:A:260:GLN:HA	1.79	0.48
1:A:419:ILE:HD12	1:A:422:ARG:HE	1.79	0.48
2:B:277:LEU:HD22	2:B:288:ILE:HG13	1.95	0.48
2:B:963:PHE:O	2:B:1027:TYR:OH	2.32	0.48
1:A:1197:SER:HB2	1:A:1219:ILE:HD13	1.96	0.47
1:A:1229:ALA:HB1	1:A:1595:TYR:CE2	2.49	0.47
2:B:853:GLU:HA	2:B:879:PRO:HB3	1.96	0.47
7:G:136:TYR:HD2	7:G:148:LEU:HD13	1.78	0.47
1:A:246:ASP:HB3	1:A:249:THR:O	2.14	0.47
2:B:1107:CYS:HB2	2:B:1130:ARG:HH11	1.79	0.47
7:G:66:LEU:HD23	7:G:66:LEU:H	1.78	0.47
8:H:8:ASP:OD1	8:H:9:ILE:N	2.42	0.47
9:I:109:THR:OG1	9:I:123:THR:O	2.32	0.47
1:A:1055:ILE:HD11	1:A:1580:ARG:HH12	1.78	0.47
1:A:522:ALA:HA	1:A:532:GLY:HA2	1.97	0.47
2:B:280:LEU:O	2:B:323:ARG:NH2	2.48	0.47
7:G:145:ILE:HD12	7:G:217:TRP:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1298:ASP:OD1	1:A:1299:ASN:N	2.46	0.47
1:A:763:GLY:C	1:A:765:LEU:H	2.17	0.47
7:G:162:ILE:HD13	7:G:217:TRP:CH2	2.49	0.47
14:N:149:ASP:OD2	14:N:151:SER:OG	2.31	0.47
1:A:19:LEU:HD22	2:B:1195:ARG:HB2	1.97	0.47
2:B:650:LEU:HD23	2:B:663:ILE:HG21	1.95	0.47
5:E:126:SER:C	5:E:128:PRO:HD3	2.35	0.47
6:F:85:MET:HB2	6:F:151:LEU:HB3	1.97	0.47
12:L:31:CYS:SG	12:L:32:ALA:N	2.87	0.47
13:M:53:LEU:HD23	13:M:96:LEU:HD13	1.96	0.47
1:A:760:TRP:CB	1:A:764:SER:OG	2.58	0.47
1:A:893:ASP:OD2	1:A:956:ARG:N	2.47	0.47
5:E:198:ILE:HB	5:E:210:SER:O	2.15	0.47
13:M:14:SER:OG	13:M:89:GLN:OE1	2.33	0.47
13:M:28:LYS:HG2	14:N:105:SER:HB2	1.95	0.47
2:B:317:TYR:HE1	2:B:320:LEU:HB2	1.79	0.47
2:B:340:ALA:HB1	2:B:344:GLN:HE21	1.78	0.47
2:B:265:ARG:HD3	2:B:473:GLN:HG3	1.97	0.47
2:B:990:ASP:OD1	2:B:990:ASP:N	2.47	0.47
6:F:108:PHE:HB2	6:F:129:LYS:HB3	1.97	0.47
9:I:21:ASN:OD1	9:I:22:ALA:N	2.48	0.47
9:I:62:ALA:HB1	9:I:69:THR:HG21	1.97	0.47
1:A:1277:GLY:HA3	9:I:44:ASN:HA	1.95	0.47
2:B:863:ASP:OD2	2:B:865:THR:OG1	2.22	0.47
2:B:973:ALA:O	10:J:47:ARG:HD2	2.15	0.47
5:E:20:LYS:NZ	5:E:34:GLU:HB3	2.30	0.47
2:B:285:ASP:HA	2:B:288:ILE:HD13	1.97	0.47
2:B:662:ASP:OD1	2:B:663:ILE:N	2.41	0.47
5:E:127:ILE:N	5:E:128:PRO:HD3	2.30	0.47
1:A:610:ASN:ND2	11:K:97:SER:OG	2.45	0.47
2:B:776:ILE:HG12	2:B:1026:ILE:HD12	1.97	0.46
5:E:152:LYS:HG3	5:E:154:ILE:HD11	1.96	0.46
8:H:133:ASN:OD1	8:H:134:ASN:N	2.47	0.46
13:M:60:LEU:HD13	13:M:61:GLU:N	2.30	0.46
5:E:155:ARG:HA	5:E:196:VAL:HG12	1.96	0.46
9:I:88:GLN:N	9:I:88:GLN:OE1	2.47	0.46
2:B:1195:ARG:HH12	2:B:1197:ARG:HH11	1.63	0.46
2:B:467:THR:OG1	2:B:469:ASN:OD1	2.34	0.46
3:C:84:TYR:HB3	12:L:64:LEU:HD11	1.97	0.46
1:A:1196:PRO:HB3	1:A:1575:ILE:HD13	1.96	0.46
13:M:24:GLY:O	14:N:108:THR:N	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:TYR:CZ	1:A:245:LYS:HB2	2.50	0.46
2:B:1042:ASP:HB2	2:B:1043:LYS:HE2	1.96	0.46
2:B:1080:ILE:HG23	2:B:1088:LEU:HD13	1.98	0.46
2:B:1189:LEU:HB3	2:B:1194:ILE:HG23	1.98	0.46
2:B:532:HIS:HE1	2:B:700:LEU:HD12	1.79	0.46
1:A:1549:VAL:HG21	1:A:1561:THR:HG21	1.98	0.46
1:A:209:THR:HG23	1:A:211:THR:H	1.81	0.46
1:A:579:ARG:HH12	1:A:584:ARG:HH21	1.63	0.46
1:A:610:ASN:HD22	2:B:929:ARG:HH22	1.63	0.46
8:H:53:ASP:OD1	8:H:54:SER:N	2.48	0.46
1:A:696:ILE:HG22	1:A:712:ILE:HD11	1.97	0.46
2:B:358:VAL:O	2:B:370:LYS:NZ	2.48	0.46
7:G:111:THR:HG23	7:G:113:PHE:H	1.80	0.46
11:K:54:THR:HA	11:K:61:ALA:HA	1.98	0.46
1:A:585:ASP:OD1	1:A:586:VAL:N	2.42	0.46
1:A:610:ASN:OD1	1:A:611:GLU:N	2.48	0.46
1:A:795:HIS:CE1	1:A:1061:SER:HB2	2.51	0.46
2:B:738:ASP:HB2	2:B:741:LEU:HD11	1.97	0.46
1:A:772:LYS:HE3	8:H:102:TYR:HA	1.97	0.46
1:A:1195:GLU:O	1:A:1199:GLN:N	2.42	0.45
1:A:429:THR:O	1:A:433:ASP:HB2	2.15	0.45
1:A:535:GLN:HE21	1:A:543:LEU:HG	1.81	0.45
2:B:766:PRO:HD2	10:J:56:LEU:HD11	1.98	0.45
3:C:319:ARG:NH2	11:K:132:GLU:OE2	2.49	0.45
7:G:93:ASP:HB3	7:G:104:LEU:HD21	1.98	0.45
8:H:49:VAL:HG11	8:H:55:LEU:HD21	1.97	0.45
1:A:908:VAL:HG11	9:I:82:ILE:HG13	1.98	0.45
1:A:799:GLU:O	1:A:1079:LYS:NZ	2.47	0.45
1:A:1275:THR:HG23	1:A:1289:SER:HB2	1.98	0.45
1:A:1322:ILE:HA	1:A:1325:LEU:HD12	1.98	0.45
1:A:65:CYS:SG	1:A:72:CYS:HB2	2.57	0.45
1:A:763:GLY:C	1:A:765:LEU:N	2.69	0.45
2:B:1099:THR:HG21	2:B:1180:PHE:HB2	1.98	0.45
2:B:1189:LEU:HD12	2:B:1196:LEU:HD11	1.97	0.45
2:B:145:VAL:HG13	2:B:149:GLU:HG2	1.97	0.45
5:E:54:GLN:HG3	5:E:56:LYS:HG2	1.97	0.45
6:F:92:ARG:HH22	7:G:109:PRO:HB3	1.80	0.45
7:G:110:ASP:OD1	7:G:111:THR:N	2.46	0.45
1:A:248:PHE:HE1	1:A:442:LYS:CE	2.17	0.45
2:B:357:ILE:HG13	2:B:358:VAL:N	2.31	0.45
5:E:149:LEU:H	5:E:149:LEU:HD23	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:43:ASN:HD21	8:H:46:LEU:HD23	1.81	0.45
1:A:1545:ASP:OD1	1:A:1546:VAL:N	2.49	0.45
1:A:232:LYS:HB2	1:A:239:PHE:HE1	1.82	0.45
1:A:1658:ALA:HA	6:F:132:LEU:HD23	1.99	0.45
1:A:454:PRO:HB3	1:A:458:GLN:HG2	1.97	0.45
1:A:596:HIS:HB3	1:A:1195:GLU:HG2	1.98	0.45
1:A:855:ARG:HA	1:A:974:THR:HG22	1.98	0.45
2:B:920:ARG:HD3	2:B:1032:TYR:HD2	1.81	0.45
1:A:458:GLN:CD	1:A:458:GLN:H	2.19	0.45
1:A:581:ILE:HD11	1:A:605:VAL:HG21	1.99	0.45
4:D:22:ILE:HG23	7:G:76:LYS:HG3	1.98	0.45
4:D:27:LEU:H	4:D:27:LEU:HD23	1.81	0.45
13:M:10:ILE:HD13	13:M:88:ILE:HD11	1.99	0.45
1:A:518:GLU:OE2	1:A:582:LYS:NZ	2.43	0.45
2:B:211:ARG:NH2	2:B:243:GLN:OE1	2.36	0.45
10:J:10:CYS:SG	10:J:11:GLY:N	2.90	0.45
6:F:86:THR:HG23	6:F:88:TYR:H	1.82	0.45
2:B:885:VAL:HG23	12:L:58:LYS:HB3	1.99	0.45
13:M:39:ASP:O	13:M:53:LEU:HA	2.17	0.45
1:A:481:ARG:HA	1:A:634:ASN:HA	1.98	0.44
2:B:1094:ASN:HA	2:B:1098:TYR:HB2	1.98	0.44
2:B:750:PRO:HB2	2:B:753:LYS:HB3	2.00	0.44
2:B:1202:PRO:HG2	4:D:21:VAL:HG21	1.98	0.44
1:A:1262:LEU:HA	1:A:1497:ILE:HA	1.98	0.44
1:A:1585:ILE:O	1:A:1589:MET:HG2	2.17	0.44
1:A:242:LYS:HD2	1:A:242:LYS:H	1.83	0.44
2:B:164:MET:HB2	2:B:194:PHE:HE1	1.81	0.44
2:B:286:ARG:HD2	9:I:14:GLY:HA3	1.98	0.44
2:B:205:MET:SD	2:B:404:LEU:HA	2.57	0.44
6:F:64:ILE:HA	6:F:67:LYS:HZ2	1.82	0.44
8:H:126:GLU:N	8:H:126:GLU:OE1	2.51	0.44
1:A:481:ARG:HH22	16:T:23:DA:H5'	1.82	0.44
2:B:1118:PRO:HD3	2:B:1125:THR:HG21	1.99	0.44
13:M:60:LEU:HD12	13:M:62:TYR:CZ	2.53	0.44
1:A:1030:VAL:HG23	1:A:1186:GLY:HA3	1.98	0.44
1:A:1246:VAL:HA	1:A:1250:GLN:HE21	1.83	0.44
1:A:241:PRO:HB3	1:A:256:LEU:HD13	1.99	0.44
1:A:947:LEU:HB3	1:A:982:VAL:HG21	1.99	0.44
2:B:1133:MET:N	2:B:1133:MET:SD	2.91	0.44
2:B:1140:LYS:HE2	7:G:17:ILE:HD12	1.75	0.44
2:B:167:SER:O	2:B:173:ASN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:107:VAL:HG12	8:H:108:SER:H	1.82	0.44
14:N:73:ASP:OD1	14:N:74:PHE:N	2.50	0.44
1:A:1441:LYS:HB3	1:A:1441:LYS:HE2	1.88	0.44
1:A:316:LEU:HA	1:A:316:LEU:HD22	1.87	0.44
1:A:586:VAL:HG22	1:A:644:ARG:HG3	2.00	0.44
1:A:876:LEU:O	1:A:880:GLN:HG2	2.17	0.44
2:B:353:VAL:O	2:B:357:ILE:HG12	2.18	0.44
2:B:402:VAL:HG21	2:B:545:PHE:HZ	1.83	0.44
2:B:923:GLN:HE21	2:B:959:THR:HG21	1.82	0.44
5:E:164:LEU:HD21	5:E:175:LEU:HD21	2.00	0.44
3:C:254:GLY:N	14:N:179:ASP:OD2	2.50	0.44
1:A:1658:ALA:HB2	7:G:107:ILE:HD11	1.99	0.44
1:A:838:GLU:OE2	1:A:842:TRP:NE1	2.50	0.44
2:B:250:LEU:HD23	2:B:260:PHE:HA	2.00	0.44
2:B:527:PHE:HE2	2:B:666:PRO:HA	1.81	0.44
14:N:33:LYS:HG2	14:N:34:HIS:CD2	2.53	0.44
1:A:1241:PRO:HD2	1:A:1541:ILE:HG22	2.00	0.44
1:A:467:PHE:HA	1:A:471:MET:HB2	1.99	0.44
1:A:1594:THR:HG23	5:E:179:GLN:HG3	1.99	0.44
7:G:51:PRO:HG3	7:G:112:PRO:HB2	2.00	0.44
2:B:117:VAL:HG13	2:B:118:GLU:H	1.82	0.44
1:A:721:LYS:NZ	8:H:93:TYR:O	2.41	0.44
13:M:12:ILE:HD12	13:M:88:ILE:HB	1.99	0.44
2:B:652:PRO:HA	2:B:662:ASP:O	2.18	0.43
7:G:105:ILE:HG13	7:G:116:THR:HG21	2.00	0.43
14:N:110:LEU:HB2	14:N:119:LEU:HD13	2.00	0.43
16:T:21:DG:OP2	16:T:21:DG:H3'	2.17	0.43
1:A:1298:ASP:HB3	1:A:1301:GLU:HB2	2.00	0.43
1:A:621:THR:OG1	1:A:626:ALA:O	2.36	0.43
3:C:42:VAL:O	11:K:138:LYS:HE3	2.18	0.43
7:G:45:LEU:HD23	7:G:45:LEU:H	1.83	0.43
2:B:181:VAL:HG11	10:J:62:ARG:HB3	2.00	0.43
11:K:109:GLY:O	11:K:110:GLU:HG2	2.18	0.43
16:T:20:DT:C2'	16:T:21:DG:H5'	2.44	0.43
1:A:65:CYS:SG	1:A:72:CYS:CB	2.95	0.43
2:B:1064:LYS:C	2:B:1066:HIS:H	2.22	0.43
8:H:38:LEU:HD12	8:H:125:LEU:HB3	1.99	0.43
1:A:344:ASN:HD22	1:A:346:SER:H	1.67	0.43
1:A:708:THR:HG21	1:A:741:PRO:HA	2.00	0.43
2:B:296:ASP:OD1	2:B:297:VAL:N	2.51	0.43
2:B:93:ASN:OD1	2:B:93:ASN:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:LYS:HA	2:B:94:LYS:HE2	2.00	0.43
2:B:104:ILE:HD13	2:B:161:LEU:HD11	2.01	0.43
2:B:562:PRO:HB3	2:B:593:ILE:HD12	2.00	0.43
2:B:586:VAL:HA	2:B:640:LEU:HB2	1.99	0.43
3:C:123:ASP:N	3:C:123:ASP:OD1	2.52	0.43
1:A:1055:ILE:HA	1:A:1178:LEU:HA	2.00	0.43
1:A:1301:GLU:HG2	9:I:60:LEU:HD21	2.00	0.43
1:A:1482:LYS:HD3	2:B:311:ARG:HH22	1.82	0.43
1:A:98:LEU:HD12	1:A:243:PHE:HE2	1.83	0.43
1:A:470:HIS:HB3	2:B:1181:VAL:HG21	1.98	0.43
2:B:328:GLN:N	2:B:328:GLN:OE1	2.45	0.43
5:E:180:ARG:HH21	5:E:192:ARG:HH11	1.67	0.43
1:A:1012:LYS:O	1:A:1013:THR:HG23	2.19	0.43
1:A:1561:THR:O	1:A:1565:GLU:HG3	2.19	0.43
1:A:945:CYS:SG	1:A:946:LEU:N	2.92	0.43
2:B:677:THR:O	2:B:679:GLN:N	2.46	0.43
9:I:111:PHE:CD1	9:I:122:ARG:HD2	2.53	0.43
1:A:100:ALA:HB1	1:A:227:LEU:HB3	1.99	0.43
1:A:658:LEU:HB2	1:A:1058:THR:HG23	1.99	0.43
2:B:1014:TYR:OH	3:C:293:ARG:NH1	2.51	0.43
2:B:241:PRO:O	2:B:243:GLN:NE2	2.49	0.43
2:B:71:LYS:HB3	2:B:425:ILE:HD11	2.00	0.43
2:B:714:ARG:HH22	2:B:957:ARG:HH11	1.67	0.43
4:D:99:LEU:HD21	7:G:136:TYR:HB2	2.00	0.43
8:H:93:TYR:CD2	8:H:145:ARG:HG3	2.54	0.43
10:J:36:LEU:HG	10:J:51:LEU:HD12	2.01	0.43
2:B:720:GLN:O	2:B:724:GLN:HG2	2.18	0.43
2:B:830:ASP:OD1	2:B:830:ASP:N	2.51	0.43
2:B:970:LYS:HD3	2:B:1000:LEU:HD21	2.01	0.43
3:C:117:ASP:OD1	3:C:118:SER:N	2.50	0.43
3:C:132:ILE:HB	3:C:169:PHE:HE1	1.84	0.43
3:C:333:ILE:H	3:C:333:ILE:HG13	1.70	0.43
4:D:83:SER:HA	4:D:86:ILE:HB	2.00	0.43
1:A:1219:ILE:N	1:A:1220:PRO:HD2	2.33	0.43
1:A:759:TYR:CE1	1:A:913:PRO:HG3	2.54	0.43
10:J:28:ASP:HB3	10:J:30:LEU:HG	2.00	0.43
1:A:712:ILE:HG22	11:K:106:GLN:NE2	2.34	0.43
13:M:82:ASN:OD1	13:M:85:LYS:HG2	2.19	0.43
1:A:1280:ASN:O	1:A:1281:THR:HG23	2.18	0.42
5:E:180:ARG:HH22	5:E:191:LYS:HA	1.84	0.42
4:D:29:GLN:HG2	7:G:40:ARG:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1613:MET:HB3	1:A:1618:THR:HG23	2.02	0.42
1:A:403:LEU:HD12	1:A:419:ILE:HG13	2.01	0.42
2:B:372:ARG:HA	2:B:375:LEU:HB3	2.01	0.42
2:B:609:ARG:HG2	2:B:626:ILE:HG21	1.99	0.42
2:B:740:LYS:NZ	2:B:803:MET:SD	2.81	0.42
2:B:841:ASP:OD1	2:B:841:ASP:N	2.52	0.42
1:A:1558:ALA:HA	1:A:1561:THR:HG22	2.01	0.42
1:A:1589:MET:O	1:A:1596:LEU:N	2.52	0.42
1:A:1660:VAL:HA	1:A:1661:PRO:HD3	1.93	0.42
1:A:316:LEU:HD13	1:A:317:SER:N	2.32	0.42
1:A:491:GLU:O	1:A:493:ASN:N	2.52	0.42
1:A:495:ILE:HG23	1:A:497:VAL:HG13	2.00	0.42
1:A:508:PRO:HB3	1:A:578:TYR:CE1	2.54	0.42
1:A:858:ALA:O	1:A:862:THR:OG1	2.29	0.42
2:B:206:LEU:HD11	2:B:480:GLN:HG3	2.01	0.42
2:B:676:VAL:HG12	2:B:693:PRO:HB3	2.01	0.42
2:B:886:ASN:HB2	2:B:902:SER:HB3	2.00	0.42
1:A:1510:PRO:HG3	1:A:1520:VAL:HG23	2.00	0.42
1:A:468:ARG:O	2:B:1070:ARG:NH1	2.52	0.42
2:B:181:VAL:HG13	10:J:63:TYR:CE1	2.55	0.42
4:D:99:LEU:HD12	4:D:100:PRO:HD2	2.00	0.42
16:T:22:DA:H2'	16:T:23:DA:H8	1.84	0.42
1:A:511:VAL:HG12	1:A:519:LEU:HD23	2.01	0.42
2:B:476:LEU:HA	2:B:476:LEU:HD12	1.89	0.42
2:B:840:LEU:HA	2:B:846:PRO:HA	2.01	0.42
1:A:650:LEU:HD13	6:F:91:ALA:HB2	2.01	0.42
2:B:27:ASN:HA	10:J:62:ARG:HH12	1.84	0.42
1:A:1637:PRO:HA	1:A:1640:ARG:HB2	2.01	0.42
1:A:363:PRO:HG2	1:A:368:ARG:HD3	2.01	0.42
1:A:399:LEU:HD11	1:A:422:ARG:HD2	2.02	0.42
1:A:485:SER:HA	1:A:486:PRO:HD3	1.90	0.42
1:A:627:ASP:OD1	1:A:628:PHE:N	2.47	0.42
1:A:874:GLU:OE2	1:A:878:ARG:NE	2.52	0.42
2:B:1063:ARG:C	2:B:1066:HIS:H	2.22	0.42
2:B:207:ILE:HG22	2:B:505:ARG:HA	2.00	0.42
2:B:633:THR:C	2:B:634:ARG:HG3	2.40	0.42
2:B:882:ILE:HG12	2:B:905:TYR:CE1	2.55	0.42
3:C:80:ALA:O	3:C:218:LYS:NZ	2.36	0.42
8:H:93:TYR:CD2	8:H:143:LEU:HB3	2.54	0.42
11:K:88:PHE:O	11:K:106:GLN:N	2.46	0.42
13:M:21:VAL:HG13	14:N:110:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:ASP:OD2	1:A:1580:ARG:NH1	2.52	0.42
1:A:1491:GLU:OE2	1:A:1494:ARG:NH2	2.53	0.42
1:A:812:VAL:HG22	1:A:815:ARG:HH21	1.85	0.42
2:B:772:VAL:HA	2:B:1030:VAL:HG12	2.00	0.42
3:C:110:PRO:HG2	3:C:308:MET:HE1	2.01	0.42
2:B:973:ALA:HB1	10:J:44:TYR:HB2	2.00	0.42
11:K:98:GLU:HG3	11:K:98:GLU:H	1.64	0.42
16:T:18:DC:H2''	16:T:19:DA:H3'	2.02	0.42
4:D:35:GLU:OE1	4:D:35:GLU:N	2.53	0.42
1:A:942:GLN:HG2	1:A:947:LEU:HA	2.02	0.42
2:B:1047:ARG:HD2	2:B:1066:HIS:O	2.20	0.42
3:C:139:LYS:HG3	3:C:201:GLU:HG3	2.02	0.42
1:A:486:PRO:HG3	1:A:628:PHE:CG	2.55	0.42
2:B:214:PRO:HB2	2:B:380:LYS:NZ	2.35	0.42
2:B:705:PRO:HG2	2:B:921:HIS:HE2	1.85	0.42
5:E:191:LYS:N	5:E:194:GLU:OE2	2.47	0.42
1:A:1012:LYS:H	1:A:1012:LYS:HD3	1.84	0.41
1:A:1437:ASN:ND2	1:A:1438:ASN:H	2.17	0.41
2:B:211:ARG:HH12	2:B:646:HIS:HB2	1.85	0.41
2:B:46:ILE:O	2:B:50:ASN:HB2	2.20	0.41
2:B:553:THR:O	2:B:646:HIS:ND1	2.52	0.41
5:E:79:TRP:NE1	5:E:81:GLU:OE2	2.49	0.41
13:M:67:ASP:N	13:M:67:ASP:OD1	2.53	0.41
1:A:319:GLU:O	1:A:322:ASN:N	2.53	0.41
1:A:937:ASN:HA	1:A:940:VAL:HG22	2.02	0.41
1:A:827:THR:HA	2:B:951:PRO:HG3	2.02	0.41
1:A:1292:ILE:HD13	1:A:1474:LEU:HD13	2.02	0.41
1:A:177:LEU:HA	1:A:180:GLU:HG3	2.02	0.41
2:B:478:LEU:HD23	2:B:478:LEU:H	1.84	0.41
2:B:629:VAL:HB	2:B:638:PRO:HA	2.02	0.41
2:B:986:PHE:CD2	2:B:992:PRO:HB3	2.55	0.41
5:E:61:GLN:HB2	5:E:79:TRP:CE3	2.55	0.41
13:M:30:PHE:CE2	13:M:32:ALA:HB2	2.55	0.41
1:A:245:LYS:HG2	1:A:247:GLY:N	2.33	0.41
2:B:74:PHE:CE2	2:B:343:ASP:HB2	2.55	0.41
2:B:588:ILE:HG22	2:B:589:ASP:OD1	2.20	0.41
2:B:654:ARG:HG2	2:B:689:VAL:O	2.19	0.41
6:F:116:ASP:HB3	6:F:119:ARG:HB3	2.01	0.41
15:S:54:DG:H2'	15:S:55:DT:H71	2.02	0.41
1:A:119:ALA:HB2	1:A:334:VAL:HG22	2.02	0.41
1:A:1494:ARG:HD2	1:A:1495:LYS:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1582:LEU:HA	1:A:1585:ILE:HG22	2.02	0.41
1:A:535:GLN:NE2	1:A:543:LEU:HG	2.35	0.41
1:A:844:THR:O	1:A:848:LYS:HG2	2.20	0.41
2:B:140:LYS:HB3	2:B:155:VAL:HG22	2.01	0.41
2:B:752:VAL:HA	2:B:979:GLN:O	2.20	0.41
13:M:11:GLU:HB2	13:M:87:SER:HB3	2.01	0.41
1:A:1091:VAL:HG13	1:A:1133:LEU:HD22	2.03	0.41
1:A:424:MET:O	1:A:428:VAL:HG23	2.21	0.41
1:A:36:THR:HB	1:A:45:VAL:HG21	2.03	0.41
1:A:672:ASP:HA	2:B:952:HIS:CE1	2.55	0.41
1:A:706:HIS:CD2	1:A:815:ARG:HH22	2.38	0.41
1:A:925:MET:HA	1:A:928:MET:HE2	2.02	0.41
2:B:303:THR:O	2:B:307:GLU:HG3	2.21	0.41
15:S:67:DA:H2"	15:S:68:DG:C8	2.55	0.41
1:A:86:TYR:H	1:A:431:GLN:HE22	1.67	0.41
5:E:140:LEU:O	5:E:140:LEU:HD13	2.20	0.41
1:A:111:LYS:HB2	1:A:114:GLU:OE1	2.21	0.41
1:A:26:ASN:ND2	2:B:1130:ARG:O	2.54	0.41
1:A:318:THR:HB	1:A:319:GLU:H	1.68	0.41
2:B:94:LYS:O	2:B:145:VAL:HA	2.21	0.41
2:B:490:LYS:HG3	2:B:729:PRO:HB3	2.01	0.41
2:B:627:GLY:HA2	2:B:668:GLU:OE1	2.20	0.41
2:B:825:PHE:HE2	2:B:899:GLN:HA	1.86	0.41
3:C:100:ARG:O	3:C:104:VAL:HG23	2.21	0.41
4:D:29:GLN:N	4:D:29:GLN:OE1	2.54	0.41
1:A:1043:GLY:C	5:E:174:GLN:HE21	2.24	0.41
5:E:20:LYS:HZ1	5:E:34:GLU:HB3	1.86	0.41
11:K:47:ILE:HD11	11:K:63:PHE:HB3	2.03	0.41
1:A:1575:ILE:H	1:A:1575:ILE:HG13	1.55	0.41
1:A:18:ILE:HG21	1:A:354:SER:HB2	2.02	0.41
1:A:506:THR:HG21	1:A:578:TYR:HB3	2.03	0.41
2:B:1088:LEU:HG	2:B:1092:LEU:HD13	2.03	0.41
2:B:14:ALA:HB3	2:B:980:ASP:HB3	2.03	0.41
14:N:107:MET:SD	14:N:107:MET:N	2.71	0.41
16:T:21:DG:OP2	16:T:22:DA:OP2	2.38	0.41
1:A:597:LYS:NZ	1:A:656:GLN:HE22	2.19	0.41
1:A:880:GLN:HB3	2:B:634:ARG:NH1	2.36	0.41
1:A:985:ARG:HH11	1:A:988:SER:HB3	1.85	0.41
3:C:192:LEU:HD21	3:C:195:LYS:HE3	2.03	0.41
16:T:6:DC:H2"	16:T:7:DA:C8	2.56	0.41
1:A:1556:GLU:HA	1:A:1559:ARG:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:847:LEU:HD12	1:A:983:LYS:HD2	2.03	0.40
2:B:264:TRP:CG	2:B:265:ARG:N	2.88	0.40
2:B:773:VAL:HA	2:B:947:ILE:HG23	2.03	0.40
2:B:709:PHE:CZ	2:B:992:PRO:HG3	2.56	0.40
3:C:322:LYS:HG3	11:K:125:MET:SD	2.61	0.40
7:G:17:ILE:O	7:G:21:LYS:HG2	2.22	0.40
1:A:882:ILE:HD11	9:I:67:VAL:HG11	2.02	0.40
1:A:1032:VAL:HG11	1:A:1179:ILE:HD13	2.02	0.40
1:A:239:PHE:CD2	1:A:260:GLN:HA	2.57	0.40
2:B:213:HIS:HD2	2:B:214:PRO:HD2	1.85	0.40
3:C:55:ASP:OD1	3:C:271:ARG:NH2	2.54	0.40
9:I:80:ALA:HB1	9:I:96:TYR:CE1	2.56	0.40
1:A:1097:TYR:CD2	1:A:1123:VAL:HG12	2.57	0.40
1:A:1502:PRO:O	1:A:1525:ASN:ND2	2.47	0.40
1:A:866:LYS:HD2	1:A:868:THR:HG22	2.03	0.40
2:B:274:VAL:O	2:B:278:LYS:HG2	2.22	0.40
2:B:862:PHE:HD1	2:B:869:THR:HB	1.86	0.40
3:C:212:ILE:H	3:C:212:ILE:HG13	1.78	0.40
13:M:60:LEU:HD12	13:M:62:TYR:CE1	2.56	0.40
14:N:109:LEU:HB3	14:N:131:LEU:HD21	2.03	0.40
16:T:22:DA:H2'	16:T:23:DA:C8	2.56	0.40
1:A:1022:CYS:SG	1:A:1023:LEU:N	2.94	0.40
1:A:1043:GLY:O	5:E:174:GLN:NE2	2.49	0.40
1:A:41:LEU:HG	1:A:43:HIS:HD2	1.87	0.40
1:A:455:GLY:H	1:A:458:GLN:HE21	1.69	0.40
1:A:469:LYS:HG2	1:A:470:HIS:CD2	2.56	0.40
1:A:673:HIS:O	1:A:786:TYR:OH	2.38	0.40
2:B:768:GLY:N	2:B:1032:TYR:OH	2.55	0.40
5:E:81:GLU:HG3	5:E:96:PHE:CE1	2.56	0.40
1:A:1242:ILE:HB	1:A:1517:ARG:NH1	2.37	0.40
1:A:21:ALA:O	1:A:25:ARG:HD2	2.22	0.40
1:A:764:SER:C	1:A:766:GLU:N	2.57	0.40
2:B:1053:ASN:O	2:B:1057:MET:N	2.44	0.40
2:B:827:PHE:CZ	2:B:832:TRP:HB2	2.57	0.40
7:G:131:ASP:O	7:G:233:VAL:HG22	2.21	0.40
7:G:80:VAL:HG22	7:G:243:VAL:HG21	2.02	0.40
10:J:21:TYR:HB2	10:J:39:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	1479/1664 (89%)	1413 (96%)	62 (4%)	4 (0%)	44	81
2	B	1177/1203 (98%)	1118 (95%)	59 (5%)	0	100	100
3	C	300/335 (90%)	292 (97%)	8 (3%)	0	100	100
4	D	55/137 (40%)	55 (100%)	0	0	100	100
5	E	212/215 (99%)	206 (97%)	6 (3%)	0	100	100
6	F	98/155 (63%)	96 (98%)	2 (2%)	0	100	100
7	G	201/326 (62%)	193 (96%)	8 (4%)	0	100	100
8	H	130/146 (89%)	125 (96%)	5 (4%)	0	100	100
9	I	110/125 (88%)	105 (96%)	5 (4%)	0	100	100
10	J	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
11	K	98/142 (69%)	92 (94%)	6 (6%)	0	100	100
12	L	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
13	M	105/415 (25%)	99 (94%)	5 (5%)	1 (1%)	18	61
14	N	138/233 (59%)	129 (94%)	9 (6%)	0	100	100
All	All	4211/5236 (80%)	4026 (96%)	180 (4%)	5 (0%)	58	88

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	765	LEU
1	A	250	LYS
1	A	319	GLU
13	M	47	GLU
1	A	445	GLY

### 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	1313/1465 (90%)	1276 (97%)	37 (3%)	49	76
2	B	1034/1053 (98%)	1008 (98%)	26 (2%)	53	79
3	C	269/296 (91%)	266 (99%)	3 (1%)	78	89
4	D	56/116 (48%)	52 (93%)	4 (7%)	17	55
5	E	196/197 (100%)	189 (96%)	7 (4%)	40	72
6	F	90/137 (66%)	90 (100%)	0	100	100
7	G	183/291 (63%)	176 (96%)	7 (4%)	38	70
8	H	117/128 (91%)	111 (95%)	6 (5%)	28	64
9	I	102/110 (93%)	100 (98%)	2 (2%)	60	83
10	J	64/65 (98%)	61 (95%)	3 (5%)	30	66
11	K	90/130 (69%)	89 (99%)	1 (1%)	78	89
12	L	38/57 (67%)	37 (97%)	1 (3%)	51	78
13	M	97/371 (26%)	95 (98%)	2 (2%)	59	82
14	N	136/220 (62%)	132 (97%)	4 (3%)	48	76
All	All	3785/4636 (82%)	3682 (97%)	103 (3%)	54	77

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	30	LYS
1	A	40	ASN
1	A	41	LEU
1	A	70	LYS
1	A	123	ARG
1	A	205	ARG
1	A	239	PHE
1	A	242	LYS
1	A	249	THR
1	A	314	TYR

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Mol	Chain	Res	Type
1	A	316	LEU
1	A	344	ASN
1	A	372	LYS
1	A	390	LEU
1	A	397	ARG
1	A	400	ASN
1	A	417	ARG
1	A	425	ASN
1	A	446	ARG
1	A	462	LYS
1	A	492	THR
1	A	642	ASN
1	A	689	ARG
1	A	949	GLN
1	A	1013	THR
1	A	1036	ASN
1	A	1150	LYS
1	A	1281	THR
1	A	1285	ASN
1	A	1299	ASN
1	A	1437	ASN
1	A	1484	LEU
1	A	1494	ARG
1	A	1575	ILE
1	A	1591	ARG
1	A	1634	LEU
2	B	17	ARG
2	B	209	GLN
2	B	244	THR
2	B	266	LYS
2	B	305	ARG
2	B	311	ARG
2	B	323	ARG
2	B	359	LEU
2	B	384	LEU
2	B	441	LYS
2	B	478	LEU
2	B	543	ASN
2	B	616	LYS
2	B	634	ARG
2	B	651	ARG
2	B	721	MET

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Mol	Chain	Res	Type
2	B	739	ASN
2	B	755	ASN
2	B	790	ASN
2	B	841	ASP
2	B	946	ASP
2	B	1018	THR
2	B	1033	TYR
2	B	1039	MET
2	B	1063	ARG
2	B	1133	MET
3	C	240	LYS
3	C	249	LYS
3	C	323	ASN
4	D	17	ASN
4	D	49	ASN
4	D	94	ARG
4	D	97	LYS
5	E	104	ASN
5	E	121	MET
5	E	140	LEU
5	E	143	ASN
5	E	149	LEU
5	E	171	LYS
5	E	200	ARG
7	G	15	ARG
7	G	32	ASN
7	G	97	LYS
7	G	134	GLU
7	G	138	PHE
7	G	234	ARG
7	G	241	ARG
8	H	33	GLN
8	H	77	ARG
8	H	109	LYS
8	H	111	LEU
8	H	125	LEU
8	H	130	ARG
9	I	19	ASN
9	I	72	LYS
10	J	48	ARG
10	J	52	THR
10	J	64	ASN

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Mol	Chain	Res	Type
11	K	98	GLU
12	L	47	ARG
13	M	60	LEU
13	M	99	LYS
14	N	33	LYS
14	N	66	LYS
14	N	107	MET
14	N	152	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	43	HIS
1	A	344	ASN
1	A	470	HIS
1	A	535	GLN
1	A	553	GLN
1	A	571	HIS
1	A	592	GLN
1	A	642	ASN
1	A	656	GLN
1	A	671	GLN
1	A	673	HIS
1	A	785	GLN
1	A	795	HIS
1	A	926	GLN
1	A	1020	GLN
1	A	1036	ASN
1	A	1062	HIS
1	A	1141	GLN
1	A	1250	GLN
1	A	1285	ASN
1	A	1299	ASN
1	A	1437	ASN
1	A	1453	HIS
1	A	1601	GLN
2	B	128	GLN
2	B	146	ASN
2	B	213	HIS
2	B	368	GLN
2	B	423	ASN

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Mol	Chain	Res	Type
2	B	532	HIS
2	B	636	GLN
2	B	688	HIS
2	B	702	ASN
2	B	710	ASN
2	B	715	ASN
2	B	718	GLN
2	B	735	HIS
2	B	739	ASN
2	B	790	ASN
2	B	823	GLN
2	B	886	ASN
2	B	923	GLN
2	B	1034	GLN
2	B	1157	GLN
3	C	130	ASN
3	C	207	HIS
3	C	301	ASN
4	D	49	ASN
5	E	101	GLN
5	E	104	ASN
5	E	143	ASN
5	E	179	GLN
7	G	67	ASN
7	G	126	GLN
7	G	144	HIS
8	H	43	ASN
8	H	139	ASN
9	I	19	ASN
10	J	64	ASN
11	K	106	GLN
12	L	53	HIS
13	M	16	GLN
14	N	34	HIS
14	N	132	GLN

### 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 7 ligands modelled in this entry, 7 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.