



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:13 AM UTC

PDB ID : 8JCH / pdb_00008jch
EMDB ID : EMD-36162
Title : Cryo-EM structure of yeast Rat1-bound Pol II pre-termination transcription complex 1 (Pol II Rat1-PTTC1)
Authors : Zeng, Y.; Zhang, Y.
Deposited on : 2023-05-11
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

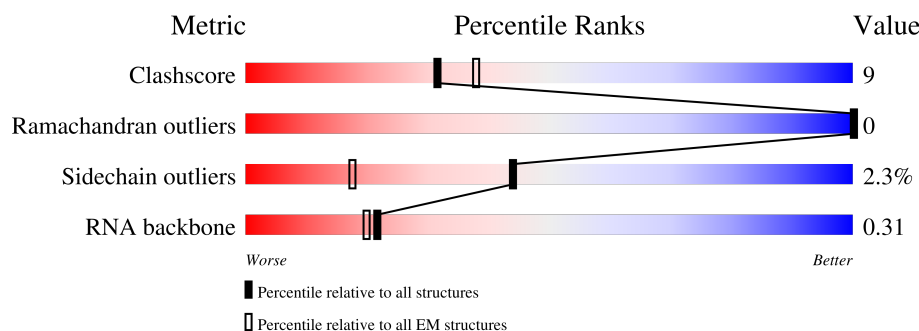
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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.



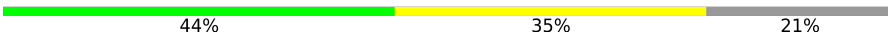
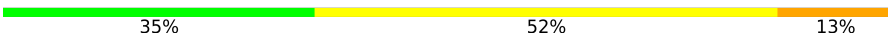
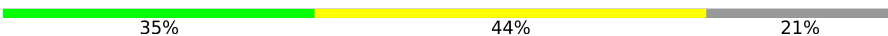
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

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

Mol	Chain	Length	Quality of chain
1	A	1733	65% 16% 18%
2	B	1259	76% 16% 8%
3	C	318	73% 12% 15%
4	D	221	54% 27% 19%
5	E	215	82% 18%
6	F	155	43% 11% 46%
7	G	171	69% 30% .

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Mol	Chain	Length	Quality of chain
8	H	146	 77% 21% •
9	I	122	 68% 25% • 6%
10	J	70	 74% 20% 6%
11	K	120	 72% 20% 8%
12	L	70	 54% 11% 34%
13	M	1019	 51% 19% • 29%
14	N	48	 44% 35% 21%
15	O	387	 71% 19% • 10%
16	P	23	 35% 52% 13%
17	T	48	 35% 44% 21%
18	W	1063	 6% • 93%

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 42732 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1419	Total	C	N	O	S	0	0
			11132	7019	1949	2106	58		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1157	Total	C	N	O	S	0	0
			9193	5819	1604	1714	56		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1225	GLU	-	expression tag	UNP P08518
B	1226	ASN	-	expression tag	UNP P08518
B	1227	LEU	-	expression tag	UNP P08518
B	1228	TYR	-	expression tag	UNP P08518
B	1229	PHE	-	expression tag	UNP P08518
B	1230	GLN	-	expression tag	UNP P08518
B	1231	GLY	-	expression tag	UNP P08518
B	1232	HIS	-	expression tag	UNP P08518
B	1233	HIS	-	expression tag	UNP P08518
B	1234	HIS	-	expression tag	UNP P08518
B	1235	HIS	-	expression tag	UNP P08518
B	1236	HIS	-	expression tag	UNP P08518
B	1237	HIS	-	expression tag	UNP P08518
B	1238	ASP	-	expression tag	UNP P08518
B	1239	TYR	-	expression tag	UNP P08518
B	1240	LYS	-	expression tag	UNP P08518
B	1241	ASP	-	expression tag	UNP P08518
B	1242	HIS	-	expression tag	UNP P08518
B	1243	ASP	-	expression tag	UNP P08518
B	1244	GLY	-	expression tag	UNP P08518
B	1245	ASP	-	expression tag	UNP P08518

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1246	TYR	-	expression tag	UNP P08518
B	1247	LYS	-	expression tag	UNP P08518
B	1248	ASP	-	expression tag	UNP P08518
B	1249	HIS	-	expression tag	UNP P08518
B	1250	ASP	-	expression tag	UNP P08518
B	1251	ILE	-	expression tag	UNP P08518
B	1252	ASP	-	expression tag	UNP P08518
B	1253	TYR	-	expression tag	UNP P08518
B	1254	LYS	-	expression tag	UNP P08518
B	1255	ASP	-	expression tag	UNP P08518
B	1256	ASP	-	expression tag	UNP P08518
B	1257	ASP	-	expression tag	UNP P08518
B	1258	ASP	-	expression tag	UNP P08518
B	1259	LYS	-	expression tag	UNP P08518

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	270	Total	C	N	O	S	0	0
			2125	1336	353	422	14		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	180	Total	C	N	O	S	0	0
			1455	899	262	292	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1704	1080	305	310	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			670	428	113	126	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	144	Total	C	N	O	S	0	0
			1104	695	184	221	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	115	Total	C	N	O	S	0	0
			871	542	147	171	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			540	345	94	95	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	111	Total	C	N	O	S	0	0
			895	575	152	166	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			364	224	72	64	4		

- Molecule 13 is a protein called 5'-3' exoribonuclease 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	721	Total	C	N	O	S	0	0
			5834	3756	994	1059	25		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-12	MET	-	initiating methionine	UNP Q02792
M	-11	GLY	-	expression tag	UNP Q02792
M	-10	SER	-	expression tag	UNP Q02792
M	-9	SER	-	expression tag	UNP Q02792
M	-8	HIS	-	expression tag	UNP Q02792
M	-7	HIS	-	expression tag	UNP Q02792
M	-6	HIS	-	expression tag	UNP Q02792
M	-5	HIS	-	expression tag	UNP Q02792
M	-4	HIS	-	expression tag	UNP Q02792
M	-3	HIS	-	expression tag	UNP Q02792
M	-2	SER	-	expression tag	UNP Q02792
M	-1	GLN	-	expression tag	UNP Q02792
M	0	ASP	-	expression tag	UNP Q02792

- Molecule 14 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	38	Total	C	N	O	P	0	0
			787	375	141	233	38		

- Molecule 15 is a protein called Decapping nuclease RAI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	350	Total	C	N	O	S	0	0
			2880	1841	487	544	8		

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	23	Total	C	N	O	P	0	0
			493	220	90	160	23		

- Molecule 17 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	38	Total	C	N	O	P	0	0
			769	367	137	227	38		

- Molecule 18 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	W	71	Total	C	N	O	0	0
			565	349	111	105		

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

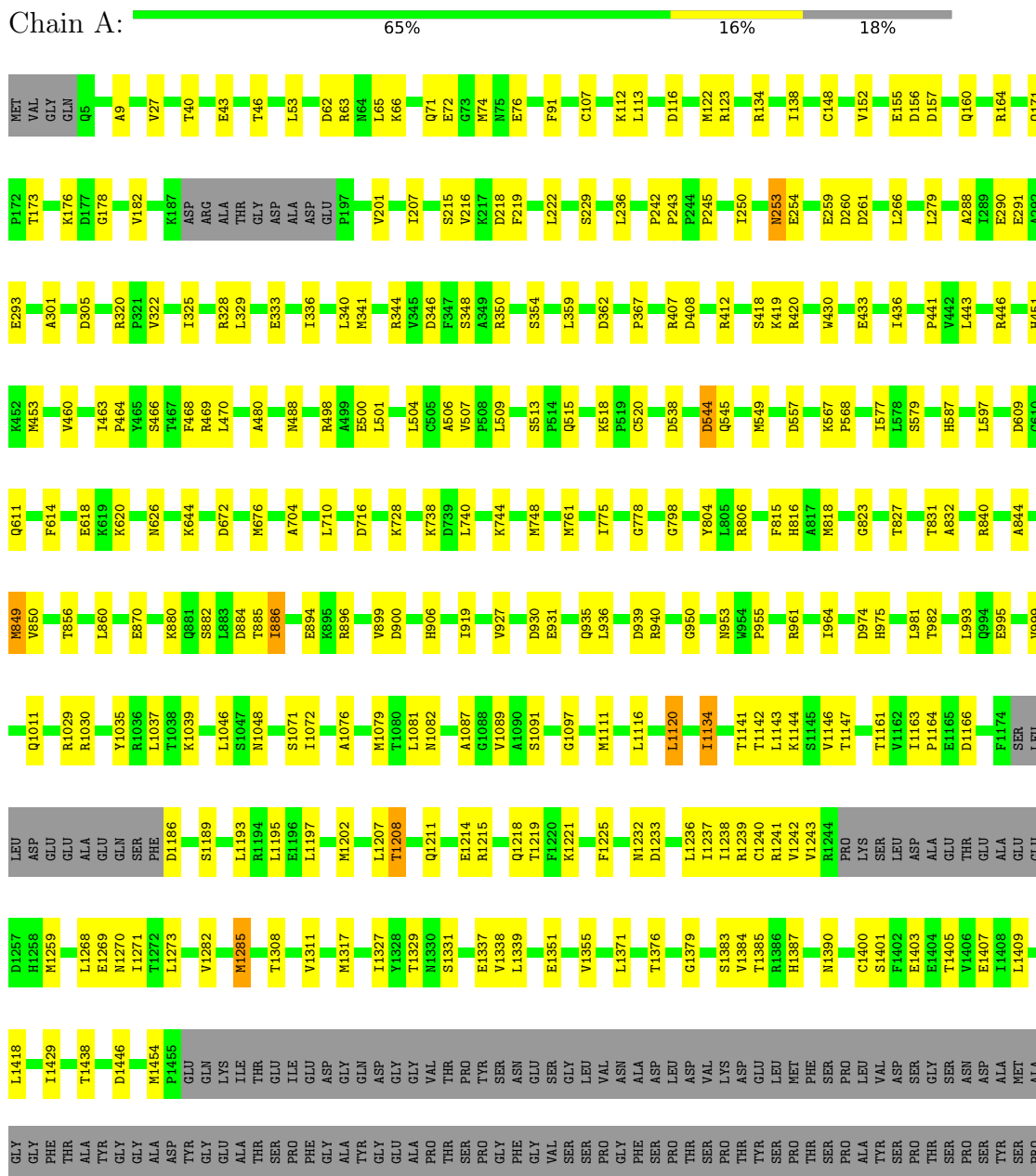
- Molecule 20 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

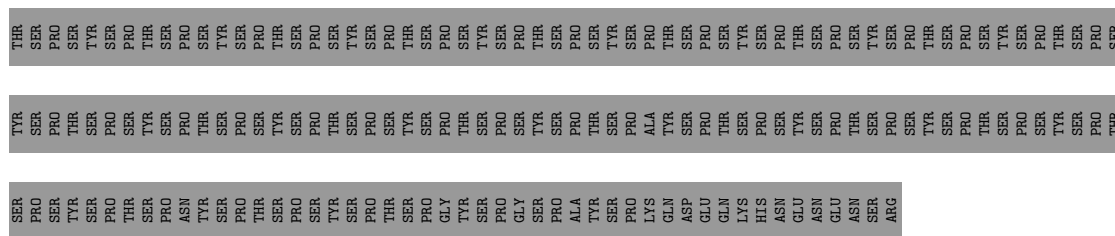
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total 1	Mg 1	0
20	M	1	Total 1	Mg 1	0
20	O	1	Total 1	Mg 1	0

3 Residue-property plots

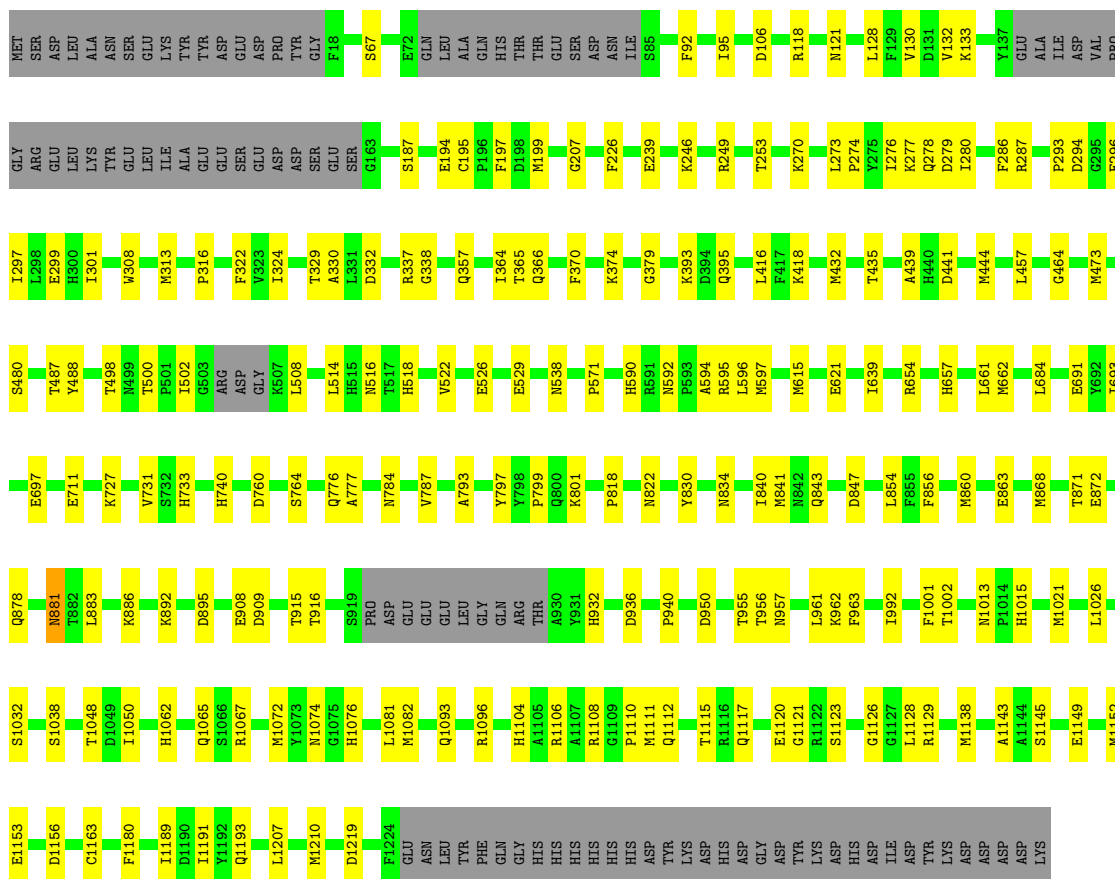
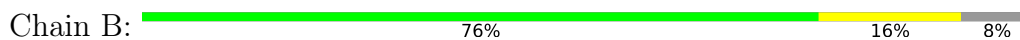
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 II subunit RPB1

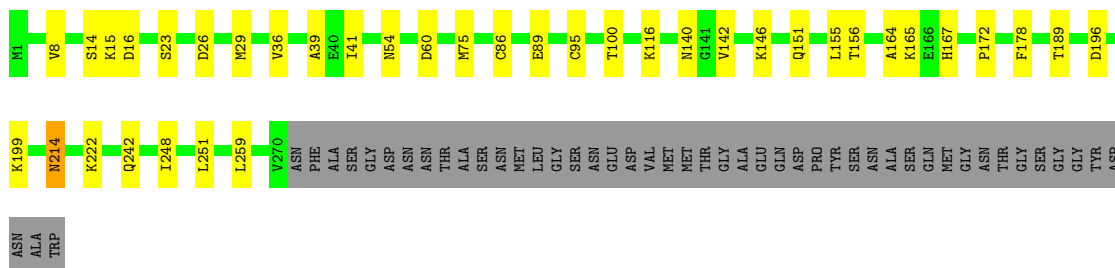




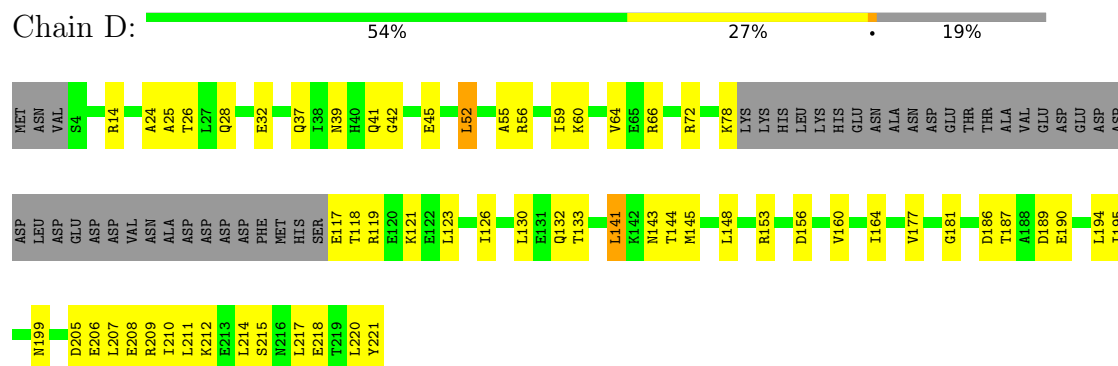
- Molecule 2: DNA-directed RNA polymerase II subunit RPB2



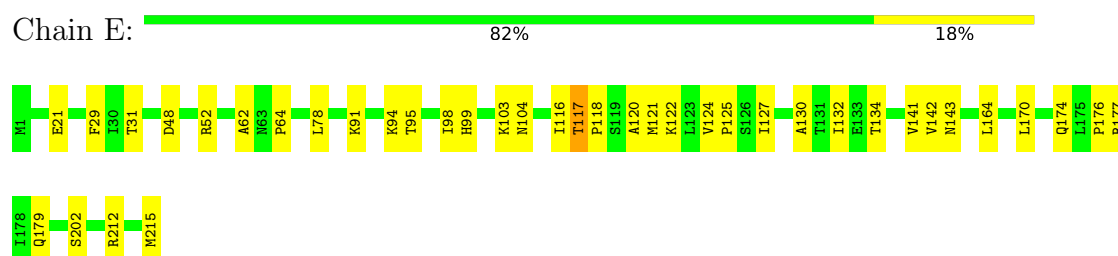
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



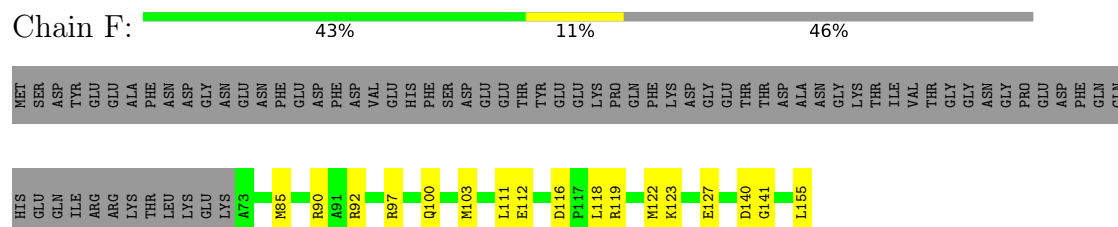
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



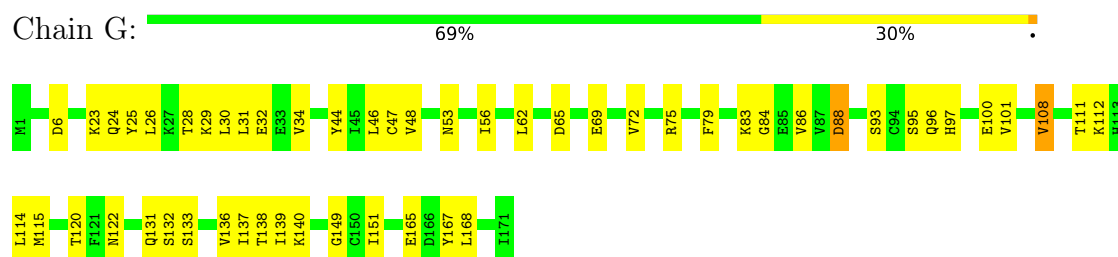
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



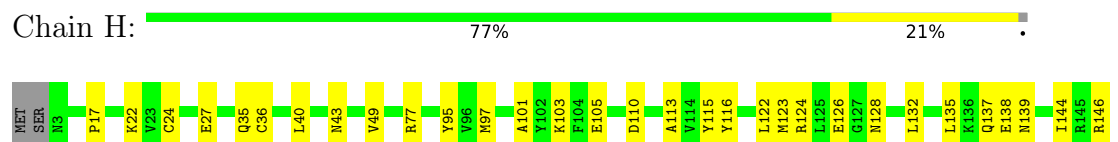
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

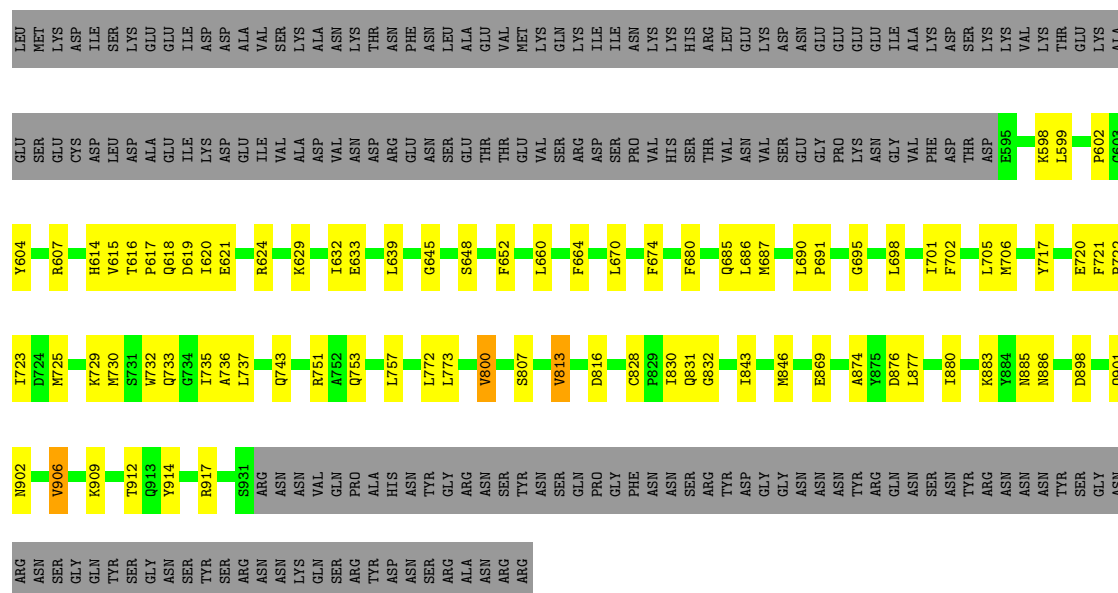


- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

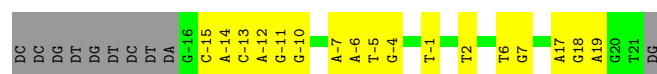


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

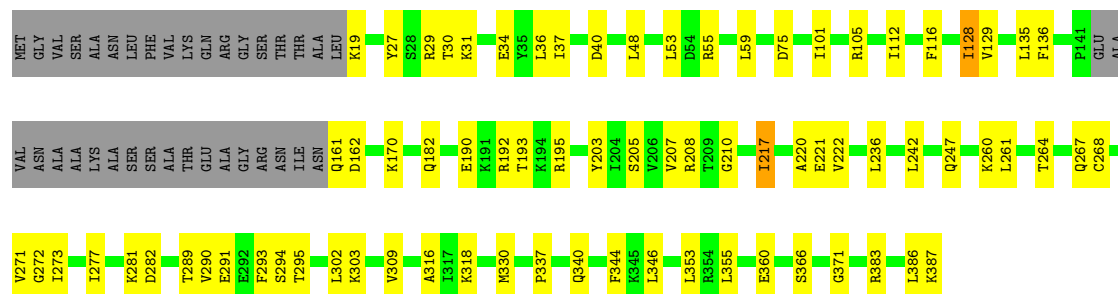




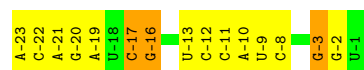
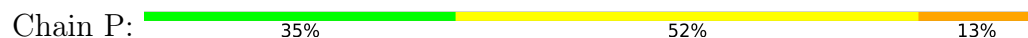
- Molecule 14: DNA (38-MER)



- Molecule 15: Decapping nuclease RAI1

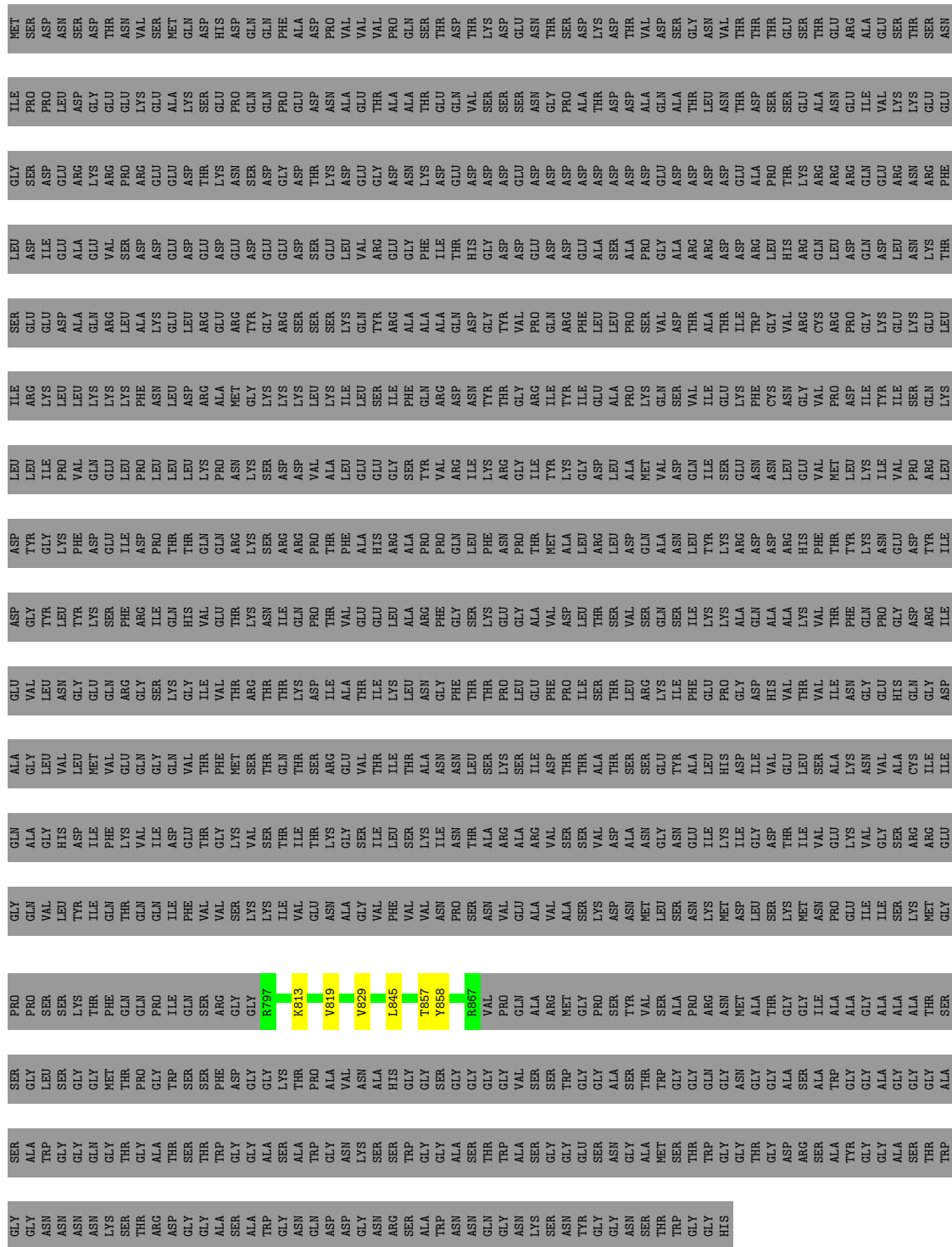


- Molecule 16: RNA



- Molecule 17: DNA (38-MER)





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	416223	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.09	0/11334	0.26	0/15335
2	B	0.09	0/9376	0.25	0/12647
3	C	0.08	0/2163	0.20	0/2930
4	D	0.11	0/1466	0.32	0/1963
5	E	0.12	0/1739	0.31	0/2347
6	F	0.10	0/682	0.27	0/922
7	G	0.14	0/1368	0.38	0/1844
8	H	0.10	0/1123	0.27	0/1529
9	I	0.12	0/889	0.35	0/1207
10	J	0.14	0/549	0.37	0/738
11	K	0.07	0/913	0.21	0/1232
12	L	0.15	0/366	0.39	0/485
13	M	0.21	0/5991	0.37	0/8129
14	N	0.16	0/882	0.34	0/1362
15	O	0.09	0/2941	0.26	0/3963
16	P	0.19	0/551	0.36	0/857
17	T	0.19	0/860	0.37	0/1322
18	W	0.05	0/571	0.17	0/762
All	All	0.12	0/43764	0.29	0/59574

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 [i](#)

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11132	0	11172	192	0
2	B	9193	0	9182	132	0
3	C	2125	0	2090	26	0
4	D	1455	0	1477	43	0
5	E	1704	0	1687	23	0
6	F	670	0	688	12	0
7	G	1340	0	1357	34	0
8	H	1104	0	1047	20	0
9	I	871	0	777	21	0
10	J	540	0	553	11	0
11	K	895	0	903	18	0
12	L	364	0	386	6	0
13	M	5834	0	5727	145	0
14	N	787	0	432	15	0
15	O	2880	0	2849	49	0
16	P	493	0	248	16	0
17	T	769	0	428	18	0
18	W	565	0	580	3	0
19	A	2	0	0	0	0
19	B	1	0	0	0	0
19	C	1	0	0	0	0
19	I	2	0	0	0	0
19	J	1	0	0	0	0
19	L	1	0	0	0	0
20	A	1	0	0	0	0
20	M	1	0	0	0	0
20	O	1	0	0	0	0
All	All	42732	0	41583	729	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 9.

All (729) 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)
13:M:107:ARG:HG2	13:M:652:PHE:HB3	1.58	0.86
13:M:110:MET:HE2	13:M:685:GLN:HG3	1.63	0.81
13:M:615:VAL:HG23	13:M:620:ILE:HG22	1.66	0.77
8:H:35:GLN:N	8:H:35:GLN:OE1	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1111:MET:HE3	2:B:1112:GLN:H	1.52	0.75
13:M:113:GLN:HG3	13:M:116:ARG:HH22	1.53	0.73
5:E:116:ILE:HG12	5:E:121:MET:HE3	1.70	0.73
2:B:1120:GLU:N	2:B:1120:GLU:OE2	2.22	0.73
13:M:732:TRP:CH2	16:P:-21:A:H2'	2.23	0.72
2:B:239:GLU:OE2	2:B:239:GLU:N	2.22	0.72
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.71	0.72
2:B:95:ILE:HD11	2:B:128:LEU:HD12	1.71	0.72
15:O:182:GLN:OE1	15:O:182:GLN:N	2.21	0.71
5:E:29:PHE:HB2	5:E:64:PRO:HG3	1.73	0.71
1:A:1215:ARG:HG2	1:A:1273:LEU:HA	1.73	0.71
14:N:19:DA:N1	17:T:-18:DC:N4	2.40	0.69
1:A:333:GLU:OE2	1:A:333:GLU:N	2.26	0.69
2:B:195:CYS:HB2	2:B:784:ASN:HB2	1.74	0.69
2:B:270:LYS:HB3	2:B:279:ASP:HB3	1.76	0.68
1:A:1195:LEU:HB2	1:A:1238:ILE:HB	1.76	0.68
13:M:874:ALA:HA	13:M:877:LEU:HD12	1.74	0.67
14:N:-5:DT:H4'	14:N:-4:DG:H5'	1.77	0.67
1:A:1076:ALA:HA	1:A:1079:MET:HE2	1.77	0.67
13:M:51:TYR:HB3	13:M:208:ILE:HD12	1.77	0.67
2:B:199:MET:SD	2:B:199:MET:N	2.68	0.67
15:O:105:ARG:HG2	15:O:267:GLN:HE22	1.60	0.66
7:G:44:TYR:HB2	7:G:79:PHE:HB3	1.77	0.66
13:M:869:GLU:HG3	13:M:909:LYS:HE2	1.77	0.66
1:A:1329:THR:HG22	1:A:1331:SER:H	1.60	0.66
1:A:961:ARG:HH11	1:A:961:ARG:HG3	1.61	0.66
5:E:121:MET:HE1	5:E:134:THR:HG21	1.79	0.65
12:L:49:LYS:HE3	12:L:49:LYS:HA	1.78	0.65
1:A:676:MET:HE2	1:A:806:ARG:HH21	1.61	0.65
13:M:12:ARG:NH1	16:P:-17:C:O2	2.30	0.65
13:M:725:MET:SD	13:M:737:LEU:HB2	2.37	0.65
13:M:210:ASN:OD1	13:M:213:ARG:NH2	2.30	0.64
1:A:618:GLU:N	1:A:618:GLU:OE1	2.30	0.64
1:A:975:HIS:O	1:A:975:HIS:ND1	2.30	0.64
2:B:654:ARG:H	2:B:657:HIS:HD2	1.44	0.64
2:B:776:GLN:HE22	16:P:-2:G:H5'	1.62	0.64
1:A:1141:THR:HG22	1:A:1142:THR:H	1.63	0.64
1:A:804:TYR:HH	1:A:816:HIS:HE2	1.43	0.64
1:A:1407:GLU:N	1:A:1407:GLU:OE1	2.29	0.64
13:M:49:ASN:ND2	13:M:51:TYR:OH	2.31	0.64
1:A:544:ASP:N	1:A:544:ASP:OD1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:88:ASP:OD1	7:G:88:ASP:N	2.31	0.64
13:M:706:MET:HA	13:M:706:MET:HE2	1.78	0.64
2:B:277:LYS:H	2:B:277:LYS:HD2	1.64	0.63
1:A:157:ASP:HB2	1:A:160:GLN:HE21	1.64	0.63
14:N:-11:DG:H2'	14:N:-10:DG:C8	2.34	0.62
15:O:192:ARG:HG2	15:O:195:ARG:HD2	1.80	0.62
13:M:729:LYS:HG2	13:M:733:GLN:HB3	1.81	0.62
2:B:908:GLU:N	2:B:908:GLU:OE2	2.31	0.62
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.81	0.62
2:B:278:GLN:HE21	2:B:337:ARG:HD2	1.65	0.62
1:A:62:ASP:OD1	1:A:63:ARG:N	2.32	0.62
2:B:287:ARG:NH1	2:B:324:ILE:O	2.32	0.62
13:M:632:ILE:HD11	13:M:670:LEU:HD23	1.80	0.62
17:T:-1:DT:H2'	17:T:0:DA:H8	1.65	0.62
4:D:164:ILE:HD12	4:D:164:ILE:H	1.65	0.62
14:N:18:DG:O6	14:N:19:DA:N6	2.33	0.62
1:A:123:ARG:HH22	1:A:155:GLU:HG2	1.65	0.61
17:T:7:DG:H2'	17:T:8:DA:C8	2.36	0.61
1:A:1390:ASN:HD21	1:A:1403:GLU:CD	2.09	0.61
2:B:621:GLU:N	2:B:621:GLU:OE1	2.34	0.61
13:M:886:ASN:HD21	16:P:-16:G:H4'	1.65	0.61
1:A:464:PRO:HB2	11:K:4:PRO:HG3	1.83	0.60
7:G:24:GLN:O	7:G:28:THR:HG23	2.02	0.60
8:H:27:GLU:N	8:H:27:GLU:OE2	2.34	0.60
13:M:105:ALA:HB3	13:M:110:MET:SD	2.41	0.60
2:B:529:GLU:CD	2:B:529:GLU:H	2.08	0.60
13:M:732:TRP:HH2	16:P:-21:A:H2'	1.66	0.60
2:B:1048:THR:HG23	2:B:1050:ILE:H	1.65	0.60
2:B:432:MET:HE2	2:B:432:MET:HA	1.84	0.60
8:H:22:LYS:O	8:H:43:ASN:ND2	2.34	0.60
13:M:725:MET:HE3	13:M:737:LEU:HD13	1.83	0.60
17:T:-1:DT:H2'	17:T:0:DA:C8	2.36	0.59
17:T:-18:DC:H6	17:T:-18:DC:H5'	1.66	0.59
15:O:27:TYR:HH	15:O:29:ARG:HH11	1.51	0.59
3:C:151:GLN:HE21	10:J:65:PRO:HB3	1.67	0.59
13:M:617:PRO:O	13:M:620:ILE:HG13	2.02	0.59
1:A:182:VAL:HG12	1:A:201:VAL:HG22	1.85	0.59
1:A:113:LEU:O	1:A:164:ARG:NH2	2.36	0.59
2:B:883:LEU:HD22	2:B:932:HIS:HB3	1.85	0.59
1:A:823:GLY:O	1:A:827:THR:HG23	2.02	0.59
1:A:433:GLU:OE2	2:B:1108:ARG:NH2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:ALA:HB2	17:T:-1:DT:H71	1.84	0.58
3:C:26:ASP:OD2	3:C:26:ASP:N	2.34	0.58
4:D:186:ASP:O	4:D:212:LYS:NZ	2.36	0.58
13:M:330:CYS:HA	13:M:341:LEU:HD23	1.85	0.58
2:B:957:ASN:HD21	2:B:961:LEU:HB2	1.68	0.58
13:M:19:SER:HB3	13:M:291:TRP:HB2	1.84	0.58
13:M:705:LEU:HD13	13:M:753:GLN:HE21	1.68	0.58
15:O:291:GLU:OE1	15:O:293:PHE:N	2.32	0.58
13:M:232:LEU:HA	13:M:252:ARG:HD3	1.85	0.58
8:H:105:GLU:HG2	8:H:113:ALA:HB3	1.85	0.58
1:A:672:ASP:OD1	1:A:672:ASP:N	2.37	0.58
2:B:296:GLU:OE1	9:I:11:ASN:ND2	2.37	0.58
13:M:680:PHE:HZ	13:M:743:GLN:HE22	1.52	0.58
15:O:268:CYS:O	15:O:272:GLY:N	2.35	0.58
13:M:381:LEU:HD22	13:M:664:PHE:HB3	1.85	0.58
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.86	0.58
8:H:116:TYR:HB2	8:H:123:MET:HE2	1.86	0.58
13:M:107:ARG:O	13:M:110:MET:HB2	2.04	0.58
13:M:117:ARG:HH11	13:M:158:ASN:HA	1.69	0.57
13:M:122:ARG:NH1	13:M:721:PHE:O	2.37	0.57
3:C:100:THR:HG22	3:C:156:THR:HG23	1.86	0.57
1:A:1214:GLU:O	1:A:1218:GLN:NE2	2.38	0.57
2:B:286:PHE:HB3	2:B:297:ILE:HD12	1.87	0.57
1:A:219:PHE:HA	1:A:222:LEU:HB2	1.86	0.57
7:G:29:LYS:HA	7:G:29:LYS:HE2	1.87	0.57
1:A:587:HIS:HD2	1:A:609:ASP:H	1.52	0.57
9:I:44:TYR:HE2	9:I:46:HIS:HB2	1.69	0.57
1:A:1161:THR:HG21	1:A:1239:ARG:HH21	1.70	0.57
13:M:147:ASP:OD1	13:M:147:ASP:N	2.36	0.57
1:A:1146:VAL:HG23	1:A:1197:LEU:HD22	1.86	0.57
1:A:1269:GLU:OE1	1:A:1270:ASN:ND2	2.38	0.57
10:J:14:VAL:HG12	10:J:17:LYS:HG3	1.87	0.57
6:F:97:ARG:NH1	6:F:100:GLN:OE1	2.38	0.57
13:M:339:PRO:HG2	13:M:660:LEU:HD22	1.87	0.57
15:O:205:SER:O	15:O:220:ALA:N	2.38	0.57
1:A:1376:THR:O	5:E:212:ARG:NH2	2.38	0.56
2:B:881:ASN:OD1	2:B:881:ASN:N	2.38	0.56
15:O:340:GLN:NE2	15:O:360:GLU:OE2	2.38	0.56
1:A:91:PHE:HZ	1:A:207:ILE:HD12	1.70	0.56
13:M:122:ARG:NH1	13:M:720:GLU:OE2	2.38	0.56
1:A:107:CYS:SG	1:A:171:GLN:NE2	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ARG:NH1	1:A:488:ASN:OD1	2.37	0.56
7:G:100:GLU:OE2	7:G:100:GLU:N	2.38	0.56
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.87	0.56
3:C:165:LYS:HG2	11:K:9:LEU:HD11	1.88	0.56
8:H:110:ASP:OD1	8:H:110:ASP:N	2.36	0.56
13:M:615:VAL:HB	13:M:619:ASP:HB3	1.88	0.56
7:G:111:THR:HB	7:G:114:LEU:HD23	1.86	0.56
4:D:55:ALA:O	4:D:59:ILE:HG22	2.05	0.56
1:A:122:MET:HE2	1:A:122:MET:HA	1.87	0.56
3:C:214:ASN:OD1	3:C:214:ASN:N	2.36	0.56
5:E:121:MET:HE2	5:E:121:MET:HA	1.88	0.56
2:B:518:HIS:HB3	2:B:522:VAL:HG22	1.88	0.55
1:A:579:SER:HB3	1:A:611:GLN:HA	1.88	0.55
1:A:1225:PHE:O	1:A:1241:ARG:N	2.39	0.55
2:B:639:ILE:HD11	2:B:691:GLU:HB3	1.88	0.55
15:O:53:LEU:HD11	15:O:290:VAL:HB	1.88	0.55
11:K:10:PHE:HA	11:K:37:LYS:HB3	1.88	0.55
1:A:336:ILE:HD12	1:A:1405:THR:HG21	1.89	0.55
2:B:955:THR:HG23	2:B:963:PHE:HB3	1.89	0.55
4:D:56:ARG:HG3	4:D:145:MET:HE1	1.89	0.55
12:L:42:ARG:HG3	12:L:42:ARG:HH11	1.71	0.55
1:A:896:ARG:HD3	1:A:1030:ARG:HD3	1.87	0.55
3:C:196:ASP:HB3	3:C:199:LYS:HG3	1.88	0.55
13:M:131:ARG:O	13:M:135:MET:HE3	2.05	0.55
1:A:76:GLU:N	1:A:76:GLU:OE1	2.38	0.55
15:O:337:PRO:HG2	15:O:387:LYS:HB2	1.88	0.55
2:B:1082:MET:HG2	3:C:189:THR:HA	1.89	0.55
13:M:71:GLU:HB2	13:M:75:GLU:HB2	1.87	0.55
14:N:6:DT:H2'	14:N:7:DG:C8	2.42	0.55
1:A:545:GLN:O	1:A:549:MET:HG3	2.07	0.54
5:E:177:ARG:HB3	5:E:215:MET:HG2	1.88	0.54
13:M:332:ASN:HD21	13:M:335:LEU:HB2	1.71	0.54
2:B:370:PHE:HB2	2:B:374:LYS:HE3	1.88	0.54
4:D:132:GLN:NE2	4:D:133:THR:OG1	2.40	0.54
13:M:816:ASP:HB2	13:M:846:MET:HA	1.88	0.54
13:M:730:MET:SD	13:M:730:MET:N	2.81	0.54
9:I:26:LEU:HD12	9:I:35:VAL:HG13	1.90	0.54
9:I:29:CYS:SG	9:I:30:ARG:N	2.80	0.54
13:M:108:ALA:O	13:M:112:GLN:HG2	2.06	0.54
13:M:110:MET:HE1	13:M:685:GLN:HE21	1.72	0.54
4:D:60:LYS:O	4:D:64:VAL:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:29:LYS:HE2	7:G:32:GLU:OE1	2.07	0.54
1:A:43:GLU:O	1:A:46:THR:OG1	2.24	0.54
7:G:56:ILE:HG12	7:G:72:VAL:HG12	1.89	0.54
10:J:32:GLU:N	10:J:32:GLU:OE2	2.41	0.54
13:M:162:PRO:HB3	13:M:198:ALA:HB1	1.90	0.54
1:A:346:ASP:OD1	2:B:1106:ARG:NH1	2.40	0.54
1:A:325:ILE:HA	1:A:328:ARG:HB2	1.88	0.54
1:A:367:PRO:HB3	1:A:466:SER:HA	1.90	0.54
9:I:13:MET:C	9:I:13:MET:HE2	2.32	0.54
1:A:412:ARG:HG3	1:A:412:ARG:HH11	1.72	0.54
13:M:15:PRO:O	13:M:16:LYS:HG3	2.07	0.54
3:C:89:GLU:H	3:C:89:GLU:CD	2.16	0.53
1:A:325:ILE:HB	2:B:1210:MET:HE1	1.91	0.53
3:C:8:VAL:HG21	11:K:105:PHE:HA	1.90	0.53
7:G:83:LYS:HB2	7:G:149:GLY:HA2	1.90	0.53
9:I:102:VAL:HG22	9:I:109:ILE:HG12	1.89	0.53
13:M:47:LEU:HD13	13:M:249:LYS:HE3	1.89	0.53
1:A:418:SER:O	1:A:420:ARG:NE	2.42	0.53
1:A:463:ILE:HD13	1:A:469:ARG:HG3	1.91	0.53
16:P:-10:A:H2'	16:P:-9:U:C6	2.42	0.53
1:A:626:ASN:N	1:A:626:ASN:OD1	2.42	0.53
2:B:594:ALA:HB3	2:B:595:ARG:HE	1.73	0.53
13:M:50:LEU:HD22	13:M:93:PRO:HG3	1.90	0.53
13:M:800:VAL:HG22	13:M:813:VAL:HG22	1.90	0.53
1:A:840:ARG:NH1	1:A:1384:VAL:O	2.41	0.53
2:B:693:ILE:HG23	2:B:697:GLU:HB3	1.91	0.53
2:B:895:ASP:N	2:B:895:ASP:OD1	2.41	0.53
3:C:248:ILE:HG21	11:K:102:LYS:HB2	1.90	0.53
2:B:301:ILE:HD13	2:B:379:GLY:HA2	1.91	0.53
13:M:88:LEU:HD21	13:M:97:LEU:HD22	1.91	0.53
13:M:773:LEU:HB3	13:M:843:ILE:HD11	1.90	0.53
14:N:-7:DA:H2''	14:N:-5:DT:H3	1.74	0.53
13:M:828:CYS:O	13:M:831:GLN:NE2	2.42	0.53
1:A:597:LEU:HD13	8:H:103:LYS:HG2	1.91	0.53
13:M:117:ARG:O	13:M:118:PHE:C	2.52	0.53
15:O:105:ARG:HB2	15:O:220:ALA:HA	1.91	0.53
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.91	0.52
2:B:95:ILE:HG13	2:B:130:VAL:HG12	1.89	0.52
2:B:1002:THR:HG23	2:B:1072:MET:HE3	1.91	0.52
13:M:233:ASP:HB3	13:M:236:LEU:HD23	1.92	0.52
13:M:917:ARG:HD2	15:O:53:LEU:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.92	0.52
8:H:95:TYR:HD2	8:H:144:ILE:HD12	1.74	0.52
5:E:21:GLU:OE1	5:E:143:ASN:ND2	2.42	0.52
3:C:54:ASN:ND2	3:C:60:ASP:OD1	2.43	0.52
6:F:112:GLU:N	6:F:112:GLU:OE2	2.42	0.52
13:M:107:ARG:HA	13:M:110:MET:HG2	1.92	0.52
15:O:208:ARG:HA	15:O:217:ILE:HA	1.91	0.52
13:M:621:GLU:O	13:M:624:ARG:HG2	2.10	0.52
1:A:1400:CYS:HB2	1:A:1405:THR:HG23	1.92	0.52
7:G:120:THR:OG1	7:G:122:ASN:OD1	2.28	0.52
8:H:124:ARG:NH1	8:H:126:GLU:OE2	2.37	0.52
1:A:549:MET:HE2	1:A:577:ILE:HG21	1.91	0.52
7:G:131:GLN:HE21	7:G:136:VAL:HG23	1.73	0.52
8:H:128:ASN:HB2	8:H:132:LEU:HD23	1.91	0.52
2:B:892:LYS:NZ	2:B:909:ASP:OD2	2.39	0.51
7:G:65:ASP:OD2	7:G:65:ASP:N	2.43	0.51
7:G:139:ILE:HG22	7:G:140:LYS:HG3	1.92	0.51
13:M:876:ASP:O	13:M:880:ILE:HG12	2.10	0.51
1:A:9:ALA:O	2:B:1193:GLN:NE2	2.42	0.51
9:I:14:LEU:HB3	9:I:27:PHE:HB3	1.92	0.51
13:M:917:ARG:HG3	15:O:289:THR:HG23	1.93	0.51
15:O:273:ILE:O	15:O:295:THR:OG1	2.28	0.51
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.92	0.51
4:D:118:THR:OG1	4:D:119:ARG:N	2.40	0.51
13:M:687:MET:HE3	13:M:687:MET:O	2.11	0.51
17:T:-12:DA:H2''	17:T:-11:DT:H5''	1.92	0.51
1:A:1143:LEU:HD22	1:A:1143:LEU:H	1.75	0.51
2:B:830:TYR:OH	2:B:1074:ASN:O	2.24	0.51
15:O:30:THR:OG1	15:O:31:LYS:N	2.42	0.51
15:O:190:GLU:O	15:O:193:THR:OG1	2.28	0.51
2:B:435:THR:OG1	2:B:439:ALA:O	2.22	0.51
7:G:112:LYS:HA	7:G:115:MET:HE1	1.92	0.51
14:N:-12:DA:H2''	14:N:-11:DG:N7	2.26	0.51
1:A:618:GLU:HG2	1:A:620:LYS:H	1.75	0.51
1:A:1072:ILE:HD13	1:A:1371:LEU:HD22	1.91	0.51
1:A:744:LYS:O	1:A:748:MET:HG3	2.11	0.51
9:I:73:ARG:HB3	9:I:83:ASN:HD21	1.76	0.51
4:D:37:GLN:N	4:D:45:GLU:O	2.44	0.51
17:T:7:DG:H2'	17:T:8:DA:H8	1.73	0.51
1:A:336:ILE:HA	1:A:340:LEU:HB2	1.91	0.50
1:A:900:ASP:OD1	1:A:900:ASP:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.92	0.50
15:O:383:ARG:HA	15:O:386:LEU:HD12	1.92	0.50
1:A:354:SER:N	1:A:468:PHE:O	2.43	0.50
1:A:567:LYS:HB3	1:A:568:PRO:HD3	1.92	0.50
1:A:806:ARG:NH1	2:B:727:LYS:O	2.43	0.50
4:D:220:LEU:HD13	4:D:221:TYR:HD1	1.76	0.50
7:G:95:SER:OG	7:G:96:GLN:N	2.44	0.50
11:K:1:MET:HG3	11:K:3:ALA:H	1.76	0.50
13:M:18:ILE:HG23	13:M:290:LEU:HB2	1.92	0.50
13:M:98:VAL:HG22	13:M:194:ILE:HB	1.92	0.50
16:P:-23:A:H3'	16:P:-22:C:H6	1.76	0.50
1:A:176:LYS:NZ	1:A:178:GLY:O	2.44	0.50
2:B:590:HIS:CD2	2:B:596:LEU:HD22	2.47	0.50
1:A:513:SER:HB3	1:A:520:CYS:HB3	1.93	0.50
1:A:1259:MET:SD	1:A:1259:MET:N	2.79	0.50
11:K:30:ALA:HB2	11:K:76:GLN:HG3	1.92	0.50
13:M:735:ILE:HG22	13:M:736:ALA:N	2.26	0.50
16:P:-9:U:H2'	16:P:-8:C:C6	2.47	0.50
1:A:443:LEU:HD13	1:A:501:LEU:HD11	1.93	0.50
15:O:75:ASP:OD1	15:O:75:ASP:N	2.44	0.50
1:A:259:GLU:HA	1:A:259:GLU:OE2	2.12	0.50
1:A:880:LYS:HA	1:A:955:PRO:HA	1.94	0.50
2:B:595:ARG:H	2:B:595:ARG:NE	2.09	0.50
5:E:118:PRO:HB3	17:T:-13:DG:H4'	1.94	0.50
14:N:17:DA:H2''	14:N:18:DG:C8	2.47	0.50
1:A:557:ASP:N	1:A:557:ASP:OD1	2.38	0.50
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.93	0.50
2:B:464:GLY:HA2	2:B:480:SER:HB3	1.94	0.50
2:B:1156:ASP:OD1	2:B:1156:ASP:N	2.45	0.50
6:F:85:MET:HE2	6:F:90:ARG:HA	1.94	0.50
1:A:65:LEU:HD23	1:A:65:LEU:H	1.77	0.49
1:A:818:MET:HG2	2:B:514:LEU:HB3	1.94	0.49
1:A:1116:LEU:HD21	1:A:1327:ILE:HD11	1.94	0.49
1:A:1438:THR:O	6:F:92:ARG:NH1	2.44	0.49
1:A:348:SER:HB2	2:B:1128:LEU:HD23	1.92	0.49
2:B:654:ARG:H	2:B:657:HIS:CD2	2.28	0.49
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.93	0.49
5:E:94:LYS:O	5:E:98:ILE:HG13	2.13	0.49
9:I:56:ALA:HB2	9:I:89:GLN:HE21	1.78	0.49
13:M:110:MET:CE	13:M:685:GLN:HE21	2.25	0.49
1:A:961:ARG:O	1:A:964:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:181:GLY:HA2	4:D:214:LEU:HD21	1.94	0.49
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.95	0.49
2:B:487:THR:OG1	2:B:777:ALA:O	2.31	0.49
13:M:604:TYR:HA	13:M:607:ARG:HH21	1.78	0.49
13:M:629:LYS:HG3	13:M:670:LEU:HD21	1.95	0.49
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.95	0.49
4:D:208:GLU:O	4:D:212:LYS:HG2	2.13	0.49
13:M:104:VAL:HB	13:M:201:PRO:HB3	1.95	0.49
1:A:419:LYS:HD2	1:A:419:LYS:O	2.13	0.49
1:A:1166:ASP:HB3	1:A:1239:ARG:HH12	1.77	0.49
7:G:131:GLN:NE2	7:G:137:ILE:O	2.35	0.49
13:M:118:PHE:HA	13:M:691:PRO:HB3	1.93	0.49
2:B:277:LYS:NZ	2:B:338:GLY:O	2.45	0.49
8:H:138:GLU:HG2	8:H:139:ASN:HB2	1.94	0.49
10:J:36:LEU:HD22	10:J:47:ARG:HG2	1.95	0.49
13:M:79:ALA:O	13:M:82:GLU:HG3	2.13	0.49
13:M:310:LEU:HD11	13:M:314:PHE:HB2	1.93	0.49
13:M:772:LEU:HD12	13:M:773:LEU:H	1.77	0.49
2:B:324:ILE:HG23	2:B:329:THR:HG23	1.95	0.48
2:B:868:MET:O	2:B:868:MET:HE3	2.13	0.48
2:B:872:GLU:HG2	2:B:916:THR:HB	1.94	0.48
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.95	0.48
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.95	0.48
12:L:51:CYS:SG	12:L:53:HIS:HB2	2.53	0.48
13:M:197:ASP:N	13:M:197:ASP:OD1	2.45	0.48
1:A:518:LYS:HG2	1:A:626:ASN:HB3	1.94	0.48
4:D:66:ARG:NH2	7:G:48:VAL:O	2.45	0.48
13:M:233:ASP:HA	16:P:-22:C:H4'	1.94	0.48
15:O:105:ARG:HD3	15:O:221:GLU:H	1.77	0.48
1:A:72:GLU:N	1:A:72:GLU:OE1	2.46	0.48
1:A:882:SER:OG	1:A:953:ASN:OD1	2.31	0.48
2:B:276:ILE:HG21	2:B:280:ILE:HD11	1.95	0.48
13:M:182:LEU:HD23	13:M:188:TRP:HB3	1.95	0.48
15:O:128:ILE:HG12	15:O:344:PHE:HB2	1.95	0.48
1:A:961:ARG:HG3	1:A:961:ARG:NH1	2.27	0.48
13:M:192:GLN:NE2	13:M:807:SER:OG	2.46	0.48
7:G:165:GLU:HB3	7:G:168:LEU:HD22	1.95	0.48
9:I:13:MET:HE1	9:I:15:TYR:CD2	2.48	0.48
13:M:279:PHE:HA	13:M:282:LYS:HZ2	1.78	0.48
1:A:885:THR:HG22	1:A:940:ARG:HB2	1.95	0.48
2:B:597:MET:HE1	2:B:615:MET:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:9:TRP:HA	13:M:12:ARG:HE	1.78	0.48
13:M:112:GLN:HG3	13:M:333:ASP:O	2.14	0.48
15:O:19:LYS:N	15:O:210:GLY:O	2.46	0.48
13:M:233:ASP:O	13:M:252:ARG:NH1	2.47	0.48
1:A:418:SER:O	1:A:419:LYS:HG3	2.14	0.48
1:A:453:MET:HE3	1:A:513:SER:HB2	1.96	0.48
15:O:366:SER:O	15:O:371:GLY:N	2.46	0.48
2:B:508:LEU:HD11	14:N:2:DT:H5'	1.95	0.48
13:M:125:GLN:HA	13:M:128:ASN:ND2	2.28	0.48
1:A:260:ASP:OD1	1:A:261:ASP:N	2.47	0.47
1:A:407:ARG:HG2	1:A:430:TRP:CE2	2.49	0.47
16:P:-10:A:H2'	16:P:-9:U:H6	1.79	0.47
1:A:242:PRO:HD2	1:A:266:LEU:HD11	1.96	0.47
1:A:1446:ASP:OD1	1:A:1446:ASP:N	2.39	0.47
2:B:1104:HIS:NE2	2:B:1126:GLY:O	2.36	0.47
4:D:144:THR:HG21	7:G:46:LEU:HD22	1.95	0.47
16:P:-20:G:P	16:P:-20:G:H21	2.37	0.47
1:A:738:LYS:HD3	1:A:740:LEU:HD11	1.97	0.47
1:A:1189:SER:HB3	1:A:1241:ARG:HD3	1.96	0.47
13:M:119:ARG:O	13:M:122:ARG:N	2.47	0.47
15:O:346:LEU:HD21	15:O:353:LEU:HD13	1.95	0.47
1:A:587:HIS:CD2	1:A:609:ASP:H	2.33	0.47
1:A:886:ILE:HD11	1:A:950:GLY:HA2	1.96	0.47
1:A:899:VAL:HG22	1:A:1029:ARG:HE	1.80	0.47
2:B:299:GLU:HG2	2:B:571:PRO:HG2	1.96	0.47
4:D:25:ALA:HB2	7:G:84:GLY:HA3	1.96	0.47
9:I:78:CYS:SG	9:I:80:SER:OG	2.67	0.47
13:M:37:ASP:O	13:M:92:ARG:NH1	2.47	0.47
2:B:797:TYR:HE1	2:B:854:LEU:HG	1.79	0.47
13:M:110:MET:HE3	13:M:110:MET:HA	1.97	0.47
18:W:819:VAL:HG12	18:W:829:VAL:HG22	1.96	0.47
1:A:538:ASP:OD1	1:A:538:ASP:N	2.43	0.47
1:A:1379:GLY:HA3	5:E:179:GLN:HG2	1.95	0.47
2:B:249:ARG:NH1	14:N:-1:DT:O4	2.47	0.47
13:M:114:ARG:HH22	13:M:717:TYR:HD1	1.62	0.47
13:M:118:PHE:CD1	13:M:721:PHE:HD2	2.31	0.47
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.35	0.47
4:D:209:ARG:HD3	4:D:210:ILE:HG23	1.96	0.47
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.97	0.47
13:M:315:ASP:OD1	13:M:315:ASP:N	2.46	0.47
2:B:760:ASP:OD1	2:B:760:ASP:N	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:801:LYS:O	2:B:822:ASN:ND2	2.48	0.47
7:G:101:VAL:HB	7:G:108:VAL:HG13	1.97	0.47
2:B:364:ILE:HG22	2:B:365:THR:HG22	1.97	0.47
2:B:1112:GLN:HB2	2:B:1117:GLN:O	2.15	0.47
5:E:48:ASP:OD1	5:E:52:ARG:N	2.48	0.47
5:E:176:PRO:HB2	5:E:212:ARG:HG2	1.96	0.47
17:T:14:DT:H2''	17:T:15:DG:H5''	1.97	0.47
1:A:116:ASP:OD1	1:A:116:ASP:N	2.48	0.47
1:A:999:VAL:HG12	1:A:1011:GLN:HG2	1.95	0.47
1:A:1385:THR:HG23	1:A:1387:HIS:H	1.80	0.47
2:B:441:ASP:OD1	2:B:441:ASP:N	2.47	0.47
2:B:1111:MET:HE3	2:B:1112:GLN:N	2.26	0.47
4:D:194:LEU:HD22	7:G:86:VAL:HG11	1.96	0.47
7:G:30:LEU:O	7:G:34:VAL:HG22	2.15	0.47
8:H:137:GLN:HG2	8:H:138:GLU:H	1.79	0.47
16:P:-3:G:H2'	16:P:-2:G:C8	2.50	0.47
18:W:857:THR:OG1	18:W:858:TYR:N	2.48	0.47
1:A:500:GLU:O	1:A:504:LEU:HB2	2.14	0.46
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.96	0.46
3:C:14:SER:OG	3:C:15:LYS:N	2.48	0.46
9:I:61:ASP:O	9:I:64:SER:OG	2.33	0.46
13:M:125:GLN:HA	13:M:128:ASN:HD21	1.80	0.46
14:N:-6:DA:H1'	14:N:-5:DT:H2'	1.97	0.46
15:O:207:VAL:HG21	15:O:236:LEU:HD21	1.97	0.46
1:A:250:ILE:HG23	16:P:-10:A:H1'	1.97	0.46
3:C:142:VAL:HG13	10:J:15:GLY:HA3	1.95	0.46
5:E:91:LYS:O	5:E:95:THR:HG23	2.15	0.46
1:A:1087:ALA:HB1	1:A:1091:SER:HA	1.97	0.46
2:B:322:PHE:CZ	9:I:30:ARG:HG3	2.50	0.46
3:C:86:CYS:SG	3:C:95:CYS:HB3	2.55	0.46
1:A:336:ILE:HG23	1:A:340:LEU:HD12	1.97	0.46
1:A:935:GLN:NE2	1:A:939:ASP:OD2	2.46	0.46
1:A:1166:ASP:OD1	1:A:1166:ASP:N	2.49	0.46
3:C:36:VAL:HG21	3:C:251:LEU:HD13	1.98	0.46
4:D:186:ASP:OD1	7:G:167:TYR:OH	2.25	0.46
6:F:155:LEU:HD23	6:F:155:LEU:H	1.80	0.46
13:M:107:ARG:O	13:M:107:ARG:HG3	2.16	0.46
15:O:203:TYR:HB3	15:O:222:VAL:HB	1.98	0.46
1:A:340:LEU:HD13	1:A:1429:ILE:HG12	1.96	0.46
1:A:1143:LEU:O	1:A:1147:THR:N	2.42	0.46
8:H:49:VAL:HA	8:H:146:ARG:HH22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:96:SER:OG	9:I:97:MET:N	2.49	0.46
13:M:313:THR:OG1	15:O:55:ARG:NH1	2.49	0.46
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.80	0.46
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.96	0.46
5:E:29:PHE:HB3	5:E:62:ALA:HB3	1.97	0.46
6:F:103:MET:O	6:F:103:MET:HG3	2.15	0.46
1:A:1454:MET:HA	1:A:1454:MET:HE2	1.97	0.46
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.97	0.46
4:D:207:LEU:O	4:D:210:ILE:HD12	2.16	0.46
1:A:156:ASP:OD1	1:A:156:ASP:N	2.38	0.46
2:B:1128:LEU:HD22	2:B:1128:LEU:H	1.81	0.46
1:A:1120:LEU:HD11	1:A:1134:ILE:HG21	1.98	0.46
4:D:32:GLU:O	4:D:37:GLN:NE2	2.34	0.46
4:D:39:ASN:OD1	4:D:42:GLY:N	2.29	0.46
4:D:195:ILE:HD12	4:D:195:ILE:O	2.16	0.46
5:E:170:LEU:HD22	5:E:174:GLN:HB3	1.98	0.46
13:M:912:THR:HG22	13:M:914:TYR:H	1.81	0.46
15:O:116:PHE:HE2	15:O:316:ALA:HB2	1.81	0.46
15:O:247:GLN:N	15:O:281:LYS:O	2.49	0.46
2:B:915:THR:HG22	2:B:936:ASP:HA	1.97	0.46
1:A:134:ARG:O	1:A:138:ILE:HG12	2.15	0.45
2:B:818:PRO:HG3	10:J:54:VAL:HG21	1.98	0.45
8:H:35:GLN:HE21	8:H:128:ASN:ND2	2.14	0.45
13:M:126:ILE:O	13:M:129:GLU:HG3	2.15	0.45
15:O:267:GLN:O	15:O:271:VAL:HG12	2.16	0.45
1:A:1082:ASN:HB3	1:A:1097:GLY:HA3	1.98	0.45
1:A:1193:LEU:O	1:A:1240:CYS:N	2.45	0.45
5:E:141:VAL:HG12	5:E:142:VAL:HG23	1.99	0.45
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.75	0.45
8:H:77:ARG:HB3	8:H:77:ARG:CZ	2.46	0.45
9:I:33:SER:OG	9:I:34:TYR:N	2.48	0.45
1:A:290:GLU:O	1:A:293:GLU:HG3	2.16	0.45
4:D:199:ASN:OD1	4:D:199:ASN:N	2.49	0.45
10:J:42:LYS:HB3	10:J:42:LYS:HE3	1.84	0.45
1:A:362:ASP:OD1	1:A:362:ASP:N	2.39	0.45
1:A:927:VAL:HA	1:A:930:ASP:OD2	2.15	0.45
8:H:17:PRO:HB3	8:H:24:CYS:HA	1.99	0.45
10:J:50:ILE:HD12	10:J:50:ILE:C	2.41	0.45
2:B:776:GLN:HB3	2:B:1096:ARG:HG2	1.97	0.45
7:G:62:LEU:HD21	7:G:69:GLU:HG3	1.98	0.45
13:M:18:ILE:HG13	13:M:290:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-15:DC:H2'	14:N:-14:DA:C8	2.51	0.45
1:A:614:PHE:HB3	8:H:122:LEU:HD21	1.99	0.45
1:A:1189:SER:HB2	1:A:1243:VAL:HG22	1.98	0.45
3:C:86:CYS:O	18:W:813:LYS:NZ	2.50	0.45
4:D:52:LEU:HD13	4:D:148:LEU:HD23	1.99	0.45
13:M:249:LYS:HB3	13:M:293:HIS:ND1	2.32	0.45
15:O:101:ILE:HG12	15:O:135:LEU:HB2	1.98	0.45
15:O:346:LEU:HD11	15:O:353:LEU:HB3	1.99	0.45
1:A:261:ASP:N	1:A:261:ASP:OD1	2.50	0.45
1:A:408:ASP:N	1:A:408:ASP:OD1	2.48	0.45
2:B:662:MET:HA	2:B:662:MET:HE3	1.99	0.45
4:D:205:ASP:O	4:D:208:GLU:HG3	2.17	0.45
7:G:53:ASN:ND2	7:G:53:ASN:O	2.50	0.45
13:M:687:MET:HB2	13:M:702:PHE:HE2	1.81	0.45
15:O:162:ASP:OD1	15:O:162:ASP:N	2.48	0.45
16:P:-23:A:H3'	16:P:-22:C:C6	2.52	0.45
1:A:229:SER:O	1:A:229:SER:OG	2.35	0.45
2:B:293:PRO:HB2	9:I:11:ASN:HB3	1.99	0.45
13:M:179:ALA:HA	13:M:843:ILE:HD12	1.98	0.45
1:A:66:LYS:HZ1	1:A:71:GLN:HB3	1.82	0.45
2:B:1180:PHE:HB2	2:B:1191:ILE:HG13	1.99	0.45
4:D:153:ARG:HH21	4:D:218:GLU:HG2	1.82	0.45
5:E:117:THR:HG23	5:E:120:ALA:HB2	1.99	0.45
13:M:295:ASN:HD21	13:M:906:VAL:HG12	1.81	0.45
1:A:894:GLU:OE2	1:A:906:HIS:NE2	2.51	0.45
12:L:50:ASP:OD1	12:L:50:ASP:N	2.50	0.45
1:A:288:ALA:O	1:A:291:GLU:HG3	2.16	0.44
1:A:320:ARG:HB2	1:A:320:ARG:NH1	2.32	0.44
1:A:850:VAL:HG22	1:A:856:THR:HG22	1.98	0.44
2:B:843:GLN:NE2	2:B:847:ASP:OD1	2.49	0.44
13:M:772:LEU:HD23	13:M:846:MET:HE2	2.00	0.44
1:A:761:MET:HG3	2:B:1021:MET:HG3	1.99	0.44
1:A:1116:LEU:HB3	1:A:1308:THR:HB	2.00	0.44
13:M:206:HIS:HA	13:M:209:MET:HE3	1.99	0.44
17:T:1:DC:H2'	17:T:2:DC:C6	2.52	0.44
1:A:1163:ILE:HD12	1:A:1164:PRO:HD2	1.99	0.44
1:A:1208:THR:HB	1:A:1211:GLN:HB2	1.99	0.44
4:D:117:GLU:HA	4:D:121:LYS:HB2	1.99	0.44
4:D:206:GLU:O	4:D:210:ILE:HG13	2.18	0.44
5:E:122:LYS:O	5:E:125:PRO:HD2	2.17	0.44
8:H:40:LEU:HD11	8:H:97:MET:HE1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:51:LEU:HA	11:K:51:LEU:HD23	1.80	0.44
13:M:167:MET:HE2	13:M:167:MET:N	2.32	0.44
15:O:59:LEU:HA	15:O:170:LYS:HG2	1.99	0.44
2:B:273:LEU:HD13	2:B:274:PRO:HD2	2.00	0.44
2:B:444:MET:C	2:B:444:MET:HE2	2.42	0.44
2:B:1013:ASN:HD22	2:B:1015:HIS:HB2	1.83	0.44
2:B:1219:ASP:OD1	4:D:14:ARG:NH2	2.50	0.44
11:K:39:ASP:OD1	11:K:39:ASP:N	2.51	0.44
13:M:729:LYS:HG2	13:M:733:GLN:CG	2.47	0.44
1:A:63:ARG:HA	1:A:74:MET:HG3	1.98	0.44
2:B:886:LYS:HE3	2:B:940:PRO:HD3	1.99	0.44
13:M:44:ASN:HD22	13:M:291:TRP:HE1	1.66	0.44
13:M:725:MET:CE	13:M:737:LEU:HD13	2.47	0.44
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.81	0.44
1:A:1186:ASP:N	1:A:1186:ASP:OD1	2.51	0.44
2:B:132:VAL:HG23	2:B:133:LYS:H	1.82	0.44
4:D:39:ASN:OD1	4:D:41:GLN:N	2.49	0.44
7:G:25:TYR:O	7:G:29:LYS:HG2	2.18	0.44
13:M:292:LEU:HD23	13:M:292:LEU:HA	1.89	0.44
13:M:648:SER:HB3	13:M:674:PHE:HB3	2.00	0.44
14:N:6:DT:H2'	14:N:7:DG:H8	1.81	0.44
1:A:1111:MET:H	1:A:1111:MET:HG2	1.66	0.44
13:M:259:ASP:OD1	13:M:259:ASP:N	2.49	0.44
15:O:261:LEU:HA	15:O:264:THR:HG22	1.98	0.44
17:T:12:DT:H2''	17:T:13:DG:C8	2.53	0.44
2:B:473:MET:SD	2:B:473:MET:N	2.91	0.44
2:B:691:GLU:OE2	2:B:740:HIS:NE2	2.35	0.44
4:D:186:ASP:OD2	4:D:187:THR:N	2.50	0.44
7:G:132:SER:OG	7:G:133:SER:N	2.50	0.44
17:T:3:DT:H2'	17:T:4:DC:H6	1.83	0.44
1:A:362:ASP:HB3	1:A:507:VAL:HB	2.00	0.43
1:A:870:GLU:OE1	5:E:202:SER:OG	2.30	0.43
1:A:1141:THR:HG22	1:A:1142:THR:N	2.30	0.43
2:B:357:GLN:NE2	2:B:366:GLN:O	2.51	0.43
2:B:526:GLU:HG2	2:B:538:ASN:HB2	2.00	0.43
5:E:124:VAL:HG13	5:E:132:ILE:HB	2.00	0.43
9:I:19:ASP:O	9:I:21:GLU:N	2.51	0.43
2:B:67:SER:HB2	2:B:92:PHE:HB2	1.99	0.43
2:B:197:PHE:O	2:B:488:TYR:OH	2.34	0.43
2:B:308:TRP:CD1	2:B:308:TRP:H	2.36	0.43
2:B:841:MET:HE3	2:B:841:MET:HB2	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:863:GLU:OE1	2:B:962:LYS:HB2	2.17	0.43
6:F:112:GLU:OE2	6:F:123:LYS:NZ	2.51	0.43
11:K:2:ASN:OD1	11:K:2:ASN:N	2.51	0.43
13:M:107:ARG:CG	13:M:652:PHE:HB3	2.39	0.43
15:O:330:MET:C	15:O:330:MET:HE2	2.44	0.43
2:B:444:MET:HE2	2:B:444:MET:O	2.18	0.43
7:G:96:GLN:HE22	7:G:97:HIS:CD2	2.36	0.43
9:I:36:GLU:HG2	9:I:38:ALA:H	1.83	0.43
13:M:213:ARG:NH2	13:M:645:GLY:H	2.15	0.43
13:M:229:ILE:HD13	13:M:248:PHE:CZ	2.54	0.43
13:M:325:PHE:HB2	13:M:639:LEU:HD11	2.00	0.43
14:N:-13:DC:H2"	14:N:-12:DA:C8	2.53	0.43
15:O:36:LEU:HD22	15:O:37:ILE:H	1.83	0.43
1:A:215:SER:OG	1:A:218:ASP:OD1	2.32	0.43
13:M:298:ARG:HG2	13:M:316:LEU:HD21	2.00	0.43
1:A:506:ALA:HB3	1:A:509:LEU:HG	2.01	0.43
1:A:644:LYS:HD2	1:A:644:LYS:HA	1.83	0.43
1:A:1351:GLU:O	1:A:1355:VAL:HG23	2.18	0.43
2:B:313:MET:O	2:B:316:PRO:HD2	2.18	0.43
2:B:1149:GLU:HA	2:B:1153:GLU:HG2	2.00	0.43
11:K:12:LEU:HD12	11:K:12:LEU:HA	1.92	0.43
1:A:515:GLN:HG3	1:A:1071:SER:HB3	2.00	0.43
1:A:1202:MET:HA	1:A:1207:LEU:HG	2.00	0.43
2:B:106:ASP:OD1	2:B:106:ASP:N	2.52	0.43
5:E:103:LYS:C	5:E:104:ASN:OD1	2.61	0.43
13:M:109:LYS:HA	13:M:109:LYS:HD3	1.73	0.43
13:M:701:ILE:HG12	13:M:757:LEU:HD13	2.01	0.43
3:C:29:MET:HE3	3:C:29:MET:HB2	1.84	0.43
1:A:152:VAL:HG23	1:A:164:ARG:HB2	2.01	0.43
4:D:164:ILE:HD12	4:D:164:ILE:N	2.33	0.43
6:F:140:ASP:OD1	6:F:141:GLY:N	2.51	0.43
12:L:29:TYR:C	12:L:30:ILE:HD13	2.44	0.43
13:M:722:PRO:HG2	13:M:737:LEU:HB3	2.01	0.43
1:A:1219:THR:HG21	1:A:1271:ILE:HG23	1.99	0.43
2:B:1106:ARG:NH2	2:B:1110:PRO:O	2.52	0.43
4:D:189:ASP:OD2	4:D:190:GLU:N	2.52	0.43
8:H:101:ALA:HB2	8:H:116:TYR:CZ	2.53	0.43
11:K:26:LYS:HD2	11:K:26:LYS:HA	1.78	0.43
13:M:616:THR:O	13:M:620:ILE:HG23	2.19	0.43
1:A:1144:LYS:HA	1:A:1147:THR:HG22	2.01	0.42
1:A:1403:GLU:CD	1:A:1403:GLU:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:98:ILE:HD12	5:E:99:HIS:N	2.34	0.42
13:M:725:MET:SD	13:M:735:ILE:HB	2.59	0.42
1:A:1259:MET:H	1:A:1259:MET:CE	2.32	0.42
2:B:950:ASP:OD1	2:B:950:ASP:N	2.46	0.42
4:D:130:LEU:HD13	4:D:141:LEU:HD12	2.01	0.42
4:D:215:SER:O	4:D:218:GLU:HG3	2.19	0.42
6:F:119:ARG:HA	6:F:122:MET:HG3	2.01	0.42
11:K:91:CYS:O	11:K:95:ILE:HG12	2.20	0.42
15:O:40:ASP:OD1	15:O:203:TYR:OH	2.29	0.42
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.91	0.42
1:A:1282:VAL:HG22	1:A:1308:THR:HG23	2.00	0.42
2:B:329:THR:HA	2:B:332:ASP:OD2	2.20	0.42
2:B:711:GLU:HB2	2:B:733:HIS:HE1	1.85	0.42
4:D:212:LYS:N	4:D:212:LYS:HE2	2.35	0.42
10:J:62:ARG:HD2	10:J:62:ARG:HA	1.83	0.42
13:M:599:LEU:O	13:M:602:PRO:HD2	2.19	0.42
2:B:860:MET:HB3	2:B:860:MET:HE3	1.75	0.42
9:I:55:THR:OG1	9:I:56:ALA:N	2.52	0.42
13:M:686:LEU:HD11	13:M:690:LEU:HD22	2.01	0.42
1:A:340:LEU:HD23	1:A:340:LEU:HA	1.92	0.42
2:B:246:LYS:HD3	2:B:246:LYS:HA	1.90	0.42
2:B:293:PRO:O	2:B:297:ILE:HG12	2.18	0.42
2:B:955:THR:OG1	2:B:956:THR:N	2.50	0.42
7:G:31:LEU:HD23	7:G:31:LEU:HA	1.81	0.42
13:M:162:PRO:HA	13:M:167:MET:HG3	2.01	0.42
13:M:751:ARG:HA	13:M:751:ARG:HD2	1.86	0.42
1:A:844:ALA:HB2	1:A:1384:VAL:HG13	2.02	0.42
1:A:1035:TYR:O	1:A:1037:LEU:HG	2.20	0.42
4:D:24:ALA:HB3	4:D:28:GLN:HB3	2.01	0.42
7:G:26:LEU:HD12	7:G:56:ILE:HD13	2.02	0.42
8:H:103:LYS:HB3	8:H:115:TYR:HB2	2.02	0.42
13:M:618:GLN:CD	13:M:618:GLN:H	2.27	0.42
14:N:-14:DA:H2''	14:N:-13:DC:H5'	2.00	0.42
2:B:118:ARG:NH2	2:B:194:GLU:OE2	2.53	0.42
2:B:595:ARG:HE	2:B:595:ARG:H	1.65	0.42
3:C:146:LYS:HE3	10:J:57:ILE:HG21	2.02	0.42
15:O:53:LEU:HD21	15:O:290:VAL:HG23	2.01	0.42
1:A:341:MET:HE2	1:A:1401:SER:HB2	2.01	0.42
1:A:931:GLU:OE1	1:A:931:GLU:C	2.63	0.42
1:A:1268:LEU:HD12	1:A:1268:LEU:HA	1.87	0.42
2:B:1074:ASN:ND2	2:B:1076:HIS:HB2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:51:ASN:OD1	9:I:51:ASN:N	2.53	0.42
17:T:-17:DT:H2''	17:T:-16:DA:C8	2.55	0.42
17:T:4:DC:H2'	17:T:5:DT:H6	1.84	0.42
1:A:112:LYS:HE3	1:A:112:LYS:HB3	1.88	0.42
1:A:173:THR:O	1:A:173:THR:OG1	2.36	0.42
1:A:441:PRO:HG2	1:A:498:ARG:HG2	2.00	0.42
13:M:299:GLU:H	13:M:299:GLU:HG3	1.71	0.42
13:M:372:LEU:HD12	13:M:372:LEU:HA	1.94	0.42
17:T:-19:DT:H2'	17:T:-18:DC:C5	2.55	0.42
1:A:253:ASN:O	1:A:254:GLU:HB3	2.20	0.41
1:A:279:LEU:HD11	1:A:288:ALA:HB1	2.01	0.41
1:A:728:LYS:HB2	1:A:728:LYS:HE3	1.75	0.41
13:M:44:ASN:N	13:M:44:ASN:OD1	2.52	0.41
13:M:330:CYS:SG	13:M:351:LEU:HD21	2.60	0.41
1:A:419:LYS:HD2	1:A:419:LYS:C	2.45	0.41
1:A:704:ALA:HB2	1:A:710:LEU:HG	2.01	0.41
1:A:778:GLY:HA3	2:B:516:ASN:HB2	2.01	0.41
1:A:860:LEU:HD23	1:A:860:LEU:HA	1.90	0.41
2:B:1152:MET:HE3	2:B:1152:MET:HB3	1.80	0.41
3:C:89:GLU:OE2	3:C:89:GLU:N	2.30	0.41
6:F:127:GLU:H	6:F:127:GLU:HG2	1.69	0.41
7:G:6:ASP:OD1	7:G:75:ARG:NH1	2.53	0.41
13:M:120:SER:HA	13:M:123:ASP:OD2	2.20	0.41
13:M:124:ALA:O	13:M:127:GLU:HG3	2.19	0.41
1:A:436:ILE:HG22	1:A:460:VAL:HG11	2.02	0.41
2:B:878:GLN:HG3	13:M:401:ARG:HH22	1.85	0.41
3:C:75:MET:HE1	3:C:242:GLN:HG3	2.02	0.41
13:M:729:LYS:HG2	13:M:733:GLN:CB	2.48	0.41
15:O:192:ARG:HA	15:O:195:ARG:HB3	2.02	0.41
16:P:-23:A:C5	16:P:-22:C:C4	3.08	0.41
1:A:1207:LEU:HD23	1:A:1207:LEU:HA	1.95	0.41
15:O:346:LEU:HD13	15:O:355:LEU:HD13	2.02	0.41
1:A:849:MET:O	1:A:856:THR:HA	2.20	0.41
7:G:23:LYS:HE2	7:G:23:LYS:HB3	1.91	0.41
15:O:129:VAL:HB	15:O:136:PHE:HB2	2.02	0.41
15:O:242:LEU:HA	15:O:277:ILE:O	2.20	0.41
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.91	0.41
1:A:919:ILE:H	1:A:919:ILE:HG13	1.69	0.41
1:A:1269:GLU:OE2	1:A:1269:GLU:N	2.52	0.41
2:B:1138:MET:HE3	2:B:1143:ALA:HB3	2.02	0.41
4:D:217:LEU:HD23	4:D:220:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:830:ILE:HG23	13:M:832:GLY:H	1.86	0.41
15:O:318:LYS:HA	15:O:318:LYS:HD2	1.76	0.41
1:A:1317:MET:HG2	1:A:1327:ILE:HG21	2.02	0.41
1:A:1338:VAL:HG23	1:A:1339:LEU:HG	2.01	0.41
2:B:592:ASN:HB3	2:B:595:ARG:CZ	2.50	0.41
13:M:23:GLU:O	13:M:25:GLN:NE2	2.53	0.41
13:M:632:ILE:HG13	13:M:633:GLU:N	2.35	0.41
15:O:34:GLU:OE1	15:O:36:LEU:HB2	2.20	0.41
17:T:-11:DT:H2''	17:T:-10:DA:C8	2.56	0.41
1:A:974:ASP:OD1	1:A:974:ASP:N	2.54	0.41
2:B:1038:SER:HB3	2:B:1062:HIS:CE1	2.55	0.41
3:C:222:LYS:HE2	3:C:222:LYS:HB2	1.90	0.41
9:I:13:MET:HE2	9:I:14:LEU:N	2.36	0.41
13:M:364:THR:OG1	13:M:365:TYR:N	2.54	0.41
13:M:598:LYS:HA	13:M:598:LYS:HD3	1.79	0.41
1:A:74:MET:HB3	1:A:74:MET:HE3	1.81	0.41
1:A:216:VAL:HA	1:A:219:PHE:CE2	2.56	0.41
1:A:301:ALA:O	1:A:305:ASP:N	2.49	0.41
1:A:344:ARG:HA	2:B:1129:ARG:HA	2.03	0.41
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.56	0.41
1:A:1039:LYS:HE3	1:A:1039:LYS:HB2	1.87	0.41
2:B:416:LEU:HD23	2:B:457:LEU:HD23	2.03	0.41
2:B:418:LYS:HE3	2:B:418:LYS:HB2	1.85	0.41
2:B:886:LYS:HB2	2:B:886:LYS:HE2	1.75	0.41
2:B:1121:GLY:O	2:B:1126:GLY:N	2.54	0.41
4:D:143:ASN:OD1	4:D:143:ASN:N	2.51	0.41
5:E:127:ILE:HG22	5:E:130:ALA:HB3	2.03	0.41
11:K:11:LEU:HD23	11:K:11:LEU:HA	1.91	0.41
11:K:37:LYS:HA	11:K:37:LYS:HD3	1.92	0.41
11:K:110:ASN:HD22	11:K:110:ASN:HA	1.68	0.41
13:M:34:LEU:HD13	13:M:35:PRO:HD2	2.03	0.41
13:M:99:MET:HE2	13:M:99:MET:HB3	2.00	0.41
13:M:114:ARG:O	13:M:115:ALA:C	2.63	0.41
13:M:156:ASP:OD2	13:M:158:ASN:ND2	2.54	0.41
13:M:222:ASN:HB3	13:M:225:THR:HG23	2.01	0.41
16:P:-22:C:H2'	16:P:-21:A:C8	2.56	0.41
1:A:236:LEU:HD13	1:A:236:LEU:HA	1.94	0.41
1:A:1089:VAL:HG21	1:A:1285:MET:HE1	2.02	0.41
4:D:156:ASP:O	4:D:160:VAL:HG12	2.20	0.41
7:G:96:GLN:O	7:G:112:LYS:NZ	2.39	0.41
10:J:10:CYS:SG	10:J:11:GLY:N	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:320:ILE:H	13:M:320:ILE:HG12	1.69	0.41
13:M:695:GLY:HA2	13:M:698:LEU:HD12	2.02	0.41
15:O:260:LYS:HA	15:O:260:LYS:HD2	1.87	0.41
1:A:1221:LYS:HE3	1:A:1221:LYS:HB3	1.92	0.40
2:B:133:LYS:HE2	2:B:133:LYS:HA	2.03	0.40
13:M:117:ARG:O	13:M:120:SER:N	2.55	0.40
13:M:232:LEU:H	13:M:232:LEU:HD23	1.86	0.40
13:M:350:ILE:HG21	13:M:391:ILE:HD11	2.03	0.40
13:M:883:LYS:NZ	13:M:885:ASN:HB2	2.36	0.40
15:O:161:GLN:HB2	15:O:162:ASP:H	1.58	0.40
17:T:4:DC:H2'	17:T:5:DT:C6	2.56	0.40
1:A:827:THR:O	1:A:831:THR:HG22	2.22	0.40
2:B:834:ASN:HB3	2:B:840:ILE:HG13	2.03	0.40
3:C:167:HIS:CD2	12:L:70:ARG:HG3	2.56	0.40
15:O:282:ASP:OD1	15:O:282:ASP:N	2.52	0.40
2:B:324:ILE:HG21	2:B:330:ALA:HB2	2.03	0.40
4:D:60:LYS:HB3	4:D:60:LYS:HE2	1.92	0.40
4:D:78:LYS:HG2	15:O:303:LYS:HD3	2.03	0.40
13:M:178:THR:HG21	13:M:773:LEU:HD13	2.03	0.40
13:M:333:ASP:OD1	13:M:333:ASP:N	2.53	0.40
1:A:775:ILE:HG23	1:A:818:MET:HE1	2.02	0.40
2:B:615:MET:H	2:B:615:MET:HG2	1.79	0.40
4:D:211:LEU:HD23	4:D:211:LEU:HA	1.90	0.40
6:F:116:ASP:OD2	6:F:116:ASP:C	2.64	0.40
13:M:104:VAL:O	13:M:202:GLY:N	2.44	0.40
13:M:107:ARG:HA	13:M:110:MET:HB2	2.03	0.40
13:M:898:ASP:HA	13:M:901:GLN:NE2	2.36	0.40
4:D:123:LEU:HA	4:D:126:ILE:HD11	2.03	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	1411/1733 (81%)	1356 (96%)	55 (4%)	0	100	100
2	B	1147/1259 (91%)	1106 (96%)	41 (4%)	0	100	100
3	C	268/318 (84%)	261 (97%)	7 (3%)	0	100	100
4	D	176/221 (80%)	168 (96%)	8 (4%)	0	100	100
5	E	213/215 (99%)	206 (97%)	7 (3%)	0	100	100
6	F	81/155 (52%)	78 (96%)	3 (4%)	0	100	100
7	G	169/171 (99%)	154 (91%)	15 (9%)	0	100	100
8	H	142/146 (97%)	132 (93%)	10 (7%)	0	100	100
9	I	113/122 (93%)	103 (91%)	10 (9%)	0	100	100
10	J	64/70 (91%)	60 (94%)	4 (6%)	0	100	100
11	K	109/120 (91%)	108 (99%)	1 (1%)	0	100	100
12	L	44/70 (63%)	41 (93%)	3 (7%)	0	100	100
13	M	713/1019 (70%)	677 (95%)	36 (5%)	0	100	100
15	O	346/387 (89%)	333 (96%)	13 (4%)	0	100	100
18	W	69/1063 (6%)	64 (93%)	5 (7%)	0	100	100
All	All	5065/7069 (72%)	4847 (96%)	218 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1231/1520 (81%)	1199 (97%)	32 (3%)	40	70
2	B	998/1094 (91%)	978 (98%)	20 (2%)	48	76
3	C	238/274 (87%)	233 (98%)	5 (2%)	47	75
4	D	162/200 (81%)	157 (97%)	5 (3%)	35	65
5	E	181/197 (92%)	177 (98%)	4 (2%)	45	74
6	F	73/137 (53%)	71 (97%)	2 (3%)	39	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	152/152 (100%)	146 (96%)	6 (4%)	28	57
8	H	116/128 (91%)	114 (98%)	2 (2%)	53	79
9	I	95/116 (82%)	93 (98%)	2 (2%)	47	75
10	J	61/65 (94%)	61 (100%)	0	100	100
11	K	96/102 (94%)	95 (99%)	1 (1%)	68	86
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	632/909 (70%)	618 (98%)	14 (2%)	45	74
15	O	320/346 (92%)	313 (98%)	7 (2%)	45	74
18	W	59/876 (7%)	58 (98%)	1 (2%)	53	79
All	All	4454/6173 (72%)	4353 (98%)	101 (2%)	44	73

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	40	THR
1	A	148	CYS
1	A	253	ASN
1	A	322	VAL
1	A	329	LEU
1	A	451	HIS
1	A	470	LEU
1	A	544	ASP
1	A	716	ASP
1	A	849	MET
1	A	884	ASP
1	A	886	ILE
1	A	936	LEU
1	A	981	LEU
1	A	982	THR
1	A	995	GLU
1	A	1048	ASN
1	A	1081	LEU
1	A	1120	LEU
1	A	1134	ILE
1	A	1208	THR
1	A	1232	ASN
1	A	1233	ASP
1	A	1236	LEU

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Mol	Chain	Res	Type
1	A	1237	ILE
1	A	1242	VAL
1	A	1285	MET
1	A	1311	VAL
1	A	1337	GLU
1	A	1383	SER
1	A	1418	LEU
2	B	187	SER
2	B	253	THR
2	B	393	LYS
2	B	498	THR
2	B	500	THR
2	B	502	ILE
2	B	731	VAL
2	B	764	SER
2	B	787	VAL
2	B	871	THR
2	B	881	ASN
2	B	1026	LEU
2	B	1032	SER
2	B	1081	LEU
2	B	1093	GLN
2	B	1115	THR
2	B	1123	SER
2	B	1145	SER
2	B	1163	CYS
2	B	1189	ILE
3	C	16	ASP
3	C	23	SER
3	C	155	LEU
3	C	214	ASN
3	C	259	LEU
4	D	26	THR
4	D	52	LEU
4	D	72	ARG
4	D	141	LEU
4	D	177	VAL
5	E	31	THR
5	E	78	LEU
5	E	117	THR
5	E	164	LEU
6	F	111	LEU

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Mol	Chain	Res	Type
6	F	118	LEU
7	G	47	CYS
7	G	88	ASP
7	G	93	SER
7	G	108	VAL
7	G	138	THR
7	G	151	ILE
8	H	36	CYS
8	H	135	LEU
9	I	9	ASP
9	I	29	CYS
11	K	70	ARG
13	M	3	VAL
13	M	61	CYS
13	M	96	VAL
13	M	107	ARG
13	M	109	LYS
13	M	110	MET
13	M	111	ASN
13	M	227	HIS
13	M	614	HIS
13	M	723	ILE
13	M	800	VAL
13	M	813	VAL
13	M	902	ASN
13	M	906	VAL
15	O	48	LEU
15	O	112	ILE
15	O	128	ILE
15	O	217	ILE
15	O	294	SER
15	O	302	LEU
15	O	309	VAL
18	W	845	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	HIS
1	A	160	GLN
1	A	445	ASN
1	A	471	ASN

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Mol	Chain	Res	Type
1	A	493	GLN
1	A	576	GLN
1	A	587	HIS
1	A	589	GLN
1	A	650	GLN
1	A	659	HIS
1	A	660	ASN
1	A	723	ASN
1	A	736	ASN
1	A	741	ASN
1	A	745	GLN
1	A	802	ASN
1	A	903	ASN
1	A	1008	GLN
1	A	1110	ASN
1	A	1278	ASN
1	A	1390	ASN
1	A	1432	GLN
2	B	115	GLN
2	B	236	HIS
2	B	300	HIS
2	B	383	ASN
2	B	657	HIS
2	B	716	ASN
2	B	762	ASN
2	B	770	GLN
2	B	776	GLN
2	B	1013	ASN
2	B	1062	HIS
2	B	1074	ASN
2	B	1076	HIS
2	B	1084	GLN
2	B	1117	GLN
2	B	1141	HIS
3	C	73	GLN
3	C	135	GLN
3	C	151	GLN
3	C	195	GLN
4	D	34	GLN
4	D	132	GLN
4	D	137	ASN
4	D	157	GLN

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Mol	Chain	Res	Type
5	E	99	HIS
5	E	179	GLN
7	G	10	ASN
7	G	57	GLN
7	G	71	ASN
7	G	96	GLN
7	G	153	GLN
8	H	33	GLN
8	H	71	ASN
8	H	128	ASN
8	H	134	ASN
9	I	87	GLN
9	I	89	GLN
10	J	23	ASN
10	J	53	HIS
10	J	64	ASN
11	K	40	HIS
11	K	96	ASN
11	K	104	ASN
11	K	110	ASN
13	M	27	GLN
13	M	49	ASN
13	M	112	GLN
13	M	192	GLN
13	M	222	ASN
13	M	287	GLN
13	M	373	ASN
13	M	383	HIS
13	M	396	HIS
13	M	685	GLN
13	M	743	GLN
13	M	753	GLN
13	M	776	ASN
13	M	886	ASN
15	O	42	ASN
15	O	132	ASN
15	O	247	GLN
15	O	267	GLN
15	O	308	GLN
18	W	837	HIS
18	W	863	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	22/23 (95%)	7 (31%)	0

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	-19	A
16	P	-17	C
16	P	-16	G
16	P	-13	U
16	P	-12	C
16	P	-11	C
16	P	-3	G

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36162. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section was not generated.