Full wwPDB EM Validation Report (i)

Aug 6, 2026 – 10:08 PM JST

PDB ID	:	8WAN / pdb_00008wan
EMDB ID	:	EMD-37398
Title	:	Structure of transcribing complex 4 (TC4), the initially transcribing complex with Pol II positioned 4nt downstream of TSS.
Authors	:	Chen, X.; Liu, W.; Wang, Q.; Wang, X.; Ren, Y.; Qu, X.; Li, W.; Xu, Y.
Deposited on	:	2023-09-07
Resolution	:	6.07 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 (i) 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 (i)) were used in the production of this report:

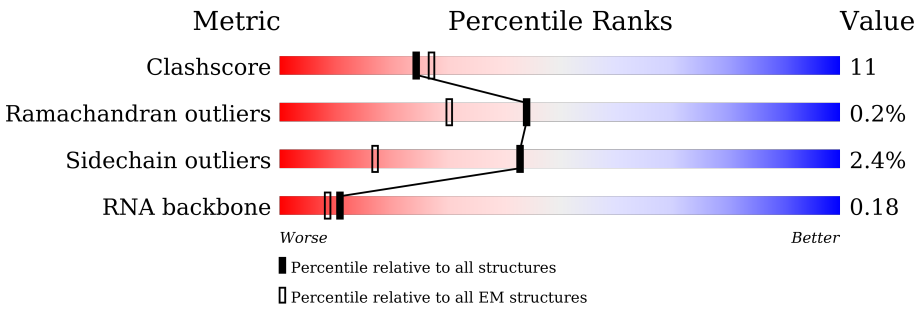
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

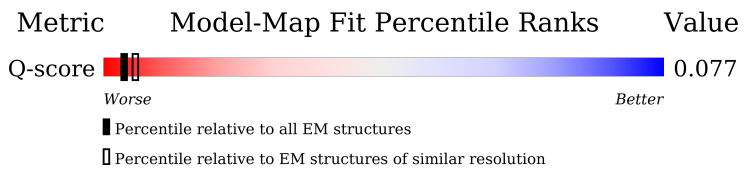
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.07 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	490 (5.57 - 6.56)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	309	32% 38% 16% • 45%
2	1	548	10% 40% 8% 52%
3	2	395	5% 66% 17% 17%

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Mol	Chain	Length	Quality of chain
4	3	308	65% 19% 15%
5	4	462	66% 18% 15%
6	5	71	24% 54% 18% 24%
7	6	782	15% 65% 12% 23%
8	7	760	7% 72% 22% 6%
9	N	8	25% 25% 50%
10	Z	4	50% 25% 25%
11	A	1872	27% 24% 5% 70%
12	B	1199	12% 69% 11% 20%
13	D	1085	8% 12% 85%
13	d	1085	15% 13% 85%
14	E	800	21% 54% 12% 32%
14	e	800	63% 56% 10% 33%
15	F	677	40% 44% 15% 39%
15	f	677	31% 48% 10% 40%
16	G	349	41% 36% 59%
17	H	310	15% 51% 15% 33%
18	I	264	18% 39% 6% 55%
18	i	264	46% 42% 54%
19	J	218	5% 32% 8% 59%
19	j	218	43% 36% 7% 56%
20	L	161	38% 32% 12% 53%
20	l	161	66% 59% 7% 34%
21	O	109	75% 16% 9%
22	P	339	46% 7% 47%

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Mol	Chain	Length	Quality of chain
23	Q	376	27% 70%
24	R	316	74% 14% 11%
25	S	517	24% 9% 66%
26	T	249	73% 15% 11%
27	U	439	23% 19% 58%
28	V	291	23% 33% 43%
29	X	99	31% 32% 36%
30	Y	99	28% 45% 26%
31	c	929	13% 12% 86%
32	k	211	46% 42% 54%
33	m	124	70% 48% 17% 5% 30%
34	o	1970	56% 17% 26%
35	p	1174	77% 20%
36	q	275	74% 19% 7%
37	r	142	63% 27% 10%
38	s	210	82% 18%
39	t	127	58% 6% 35%
40	u	172	68% 31%
41	v	150	85% 14%
42	w	125	67% 22% 9%
43	x	67	82% 16%
44	y	117	79% 20%
45	z	58	53% 22% 24%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
49	W0F	p	1201	-	-	X	-

2 Entry composition (i)

There are 49 unique types of molecules in this entry. The entry contains 108600 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 CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	171	1420	882	249	279	10	0	0

- Molecule 2 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	265	2167	1382	378	395	12	0	0

- Molecule 3 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	329	2567	1621	440	479	27	0	0

- Molecule 4 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	263	2066	1323	344	380	19	0	0

- Molecule 5 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	394	3189	2068	552	557	12	0	0

- Molecule 6 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	54	428	277	67	82	2	0	0

- Molecule 7 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	605	4890	3127	848	885	30	0	0

- Molecule 8 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	7	714	5751	3683	999	1040	29	0	0

- Molecule 9 is a protein called Alpha-amanitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	N	8	64	39	10	14	1	0	0

- Molecule 10 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	Z	4	95	39	14	36	6	0	0

- Molecule 11 is a protein called Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	A	559	4580	2924	795	834	27	0	0

- Molecule 12 is a protein called Transcription initiation factor TFIID subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	B	963	7796	5011	1315	1412	58	0	0

- Molecule 13 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	D	164	1366	851	256	255	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	d	158	1307	814	238	252	3	0	0

- Molecule 14 is a protein called Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	E	547	4376	2774	759	822	21	0	0
			Total	C	N	O	S		
14	e	539	4327	2746	748	814	19	0	0

- Molecule 15 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	F	412	3143	1994	548	583	18	0	0
			Total	C	N	O	S		
15	f	403	3081	1954	533	576	18	0	0

- Molecule 16 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	G	144	1171	742	215	210	4	0	0

- Molecule 17 is a protein called Transcription initiation factor TFIID subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	H	209	1633	1034	283	311	5	0	0

- Molecule 18 is a protein called Transcription initiation factor TFIID subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	I	120	959	610	166	177	6	0	0
			Total	C	N	O	S		
18	i	121	967	615	167	178	7	0	0

- Molecule 19 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	J	90	720	466	115	135	4	0	0
19	j	95	759	488	124	143	4	0	0

- Molecule 20 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	L	76	622	388	109	122	3	0	0
20	l	107	876	547	158	166	5	0	0

- Molecule 21 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	O	99	806	510	142	151	3	0	0

- Molecule 22 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	P	179	1422	923	251	241	7	0	0

- Molecule 23 is a protein called Transcription initiation factor IIA beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Q	113	930	585	152	189	4	0	0

- Molecule 24 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	R	282	2167	1353	384	412	18	0	0

- Molecule 25 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	S	176	1461	921	268	268	4	0	0

- Molecule 26 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	T	222	1788	1127	320	338	3	0	0

- Molecule 27 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	U	184	1520	957	272	280	11	0	0

- Molecule 28 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	V	165	1357	865	235	253	4	0	0

- Molecule 29 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
29	X	63	1299	615	243	378	63	0	0

- Molecule 30 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
30	Y	73	1491	708	276	434	73	0	0

- Molecule 31 is a protein called Transcription initiation factor TFIID subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	c	127	1011	638	174	193	6	0	0

- Molecule 32 is a protein called Transcription initiation factor TFIID subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	k	98	785	499	142	139	5	0	0

- Molecule 33 is a protein called Transcription initiation factor TFIID subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	m	87	724	456	131	131	6	0	0

- Molecule 34 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	o	1452	11510	7235	2056	2146	73	0	0

- Molecule 35 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	p	1149	9175	5796	1614	1701	64	0	0

- Molecule 36 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	q	257	2059	1294	351	408	6	0	0

- Molecule 37 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	r	128	1050	656	178	212	4	0	0

- Molecule 38 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	s	209	1720	1089	300	323	8	0	0

- Molecule 39 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	t	82	657	418	113	121	5	0	0

- Molecule 40 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	u	171	1351	875	219	249	8	0	0

- Molecule 41 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	v	148	1186	750	194	237	5	0	0

- Molecule 42 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	w	114	927	571	166	179	11	0	0

- Molecule 43 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	x	67	533	345	90	92	6	0	0

- Molecule 44 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	y	115	920	593	152	173	2	0	0

- Molecule 45 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	z	44	372	231	72	63	6	0	0

- Molecule 46 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
46	0	2	2	2	0
46	2	3	3	3	0
46	3	2	2	2	0

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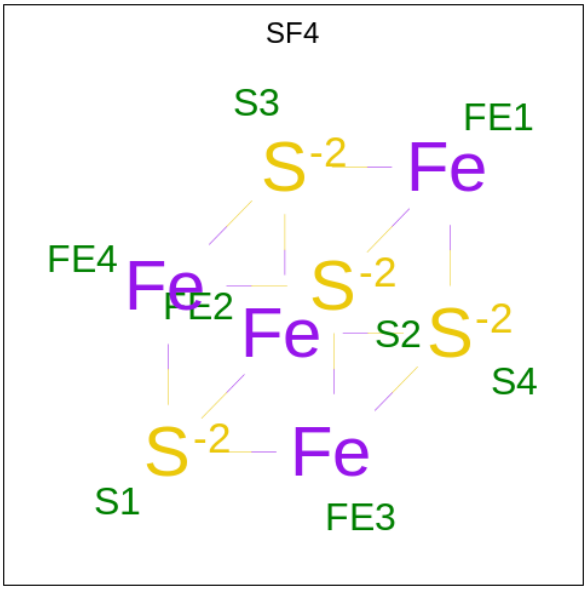
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
46	R	1	1	1	0
46	U	1	1	1	0
46	o	2	2	2	0
46	p	1	1	1	0
46	q	1	1	1	0
46	w	2	2	2	0
46	x	1	1	1	0
46	z	1	1	1	0

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

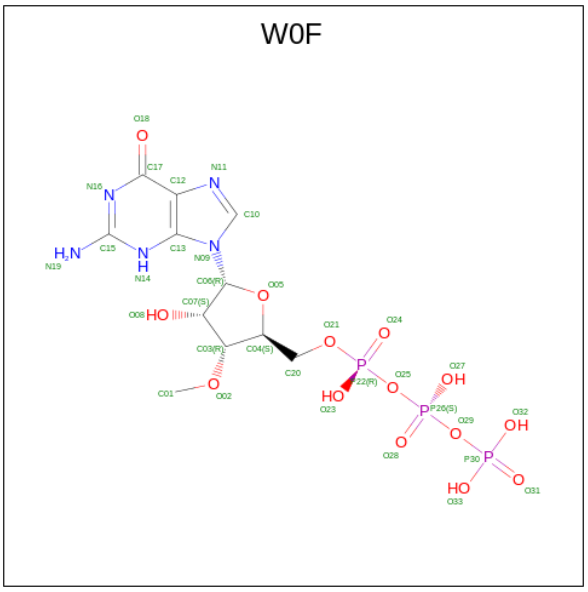


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	7	1	8	4	4	0

- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
48	o	1	1	1	0

- Molecule 49 is [[(2 {S},3 {R},4 {S},5 {R})-5-(2-azanyl-6-oxidanylidene-3 {H}-purin-9-yl)-3-methoxy-4-oxidanyl-oxolan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (CCD ID: W0F) (formula: $C_{11}H_{18}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



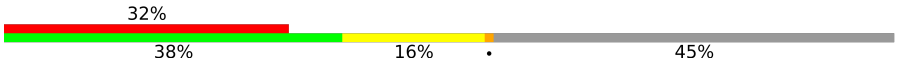
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	p	1	33	11	5	14	3	0

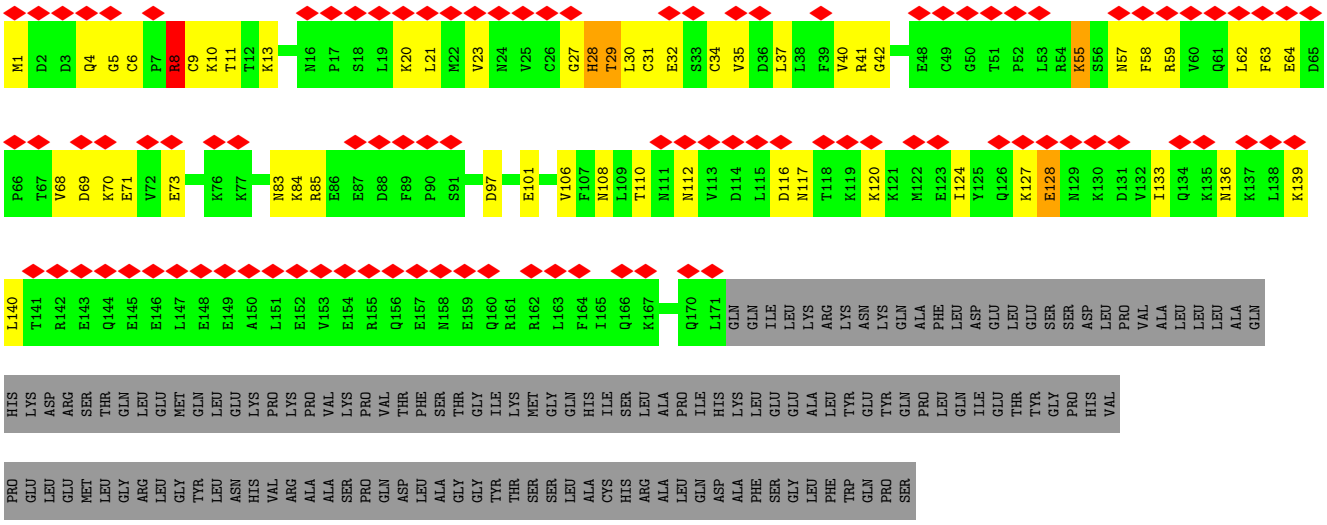
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: CDK-activating kinase assembly factor MAT1

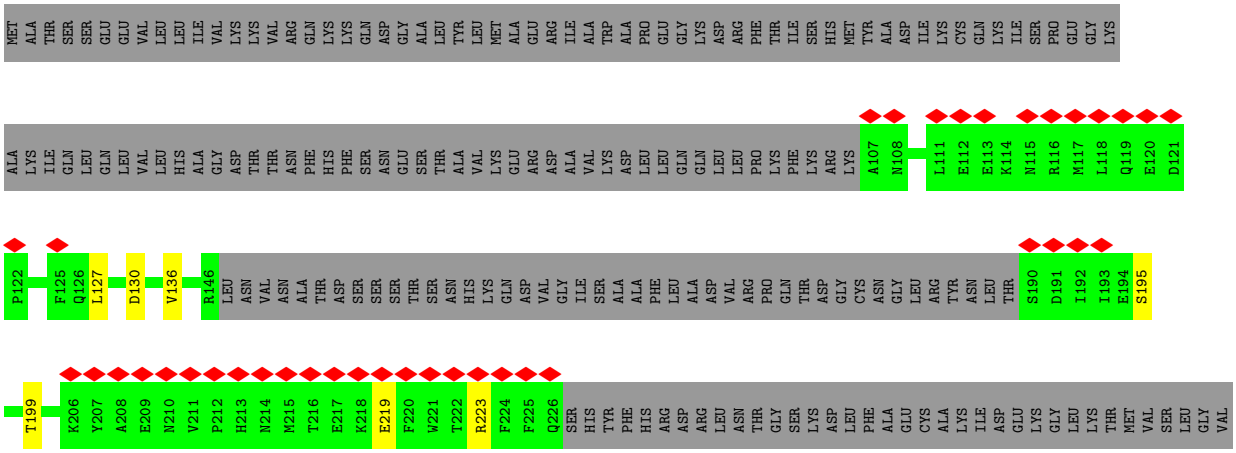
Chain 0:

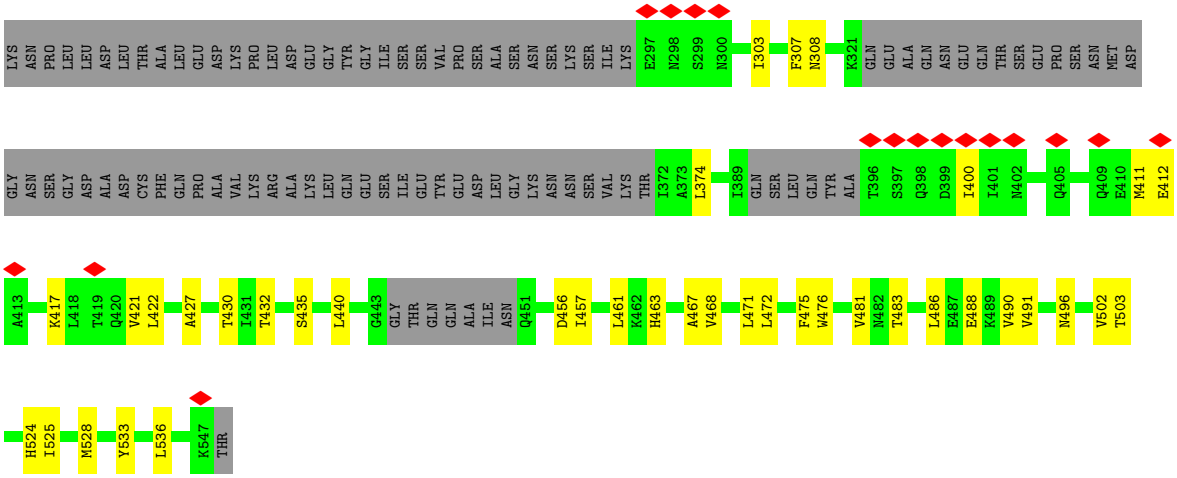




- Molecule 2: General transcription factor IIH subunit 1

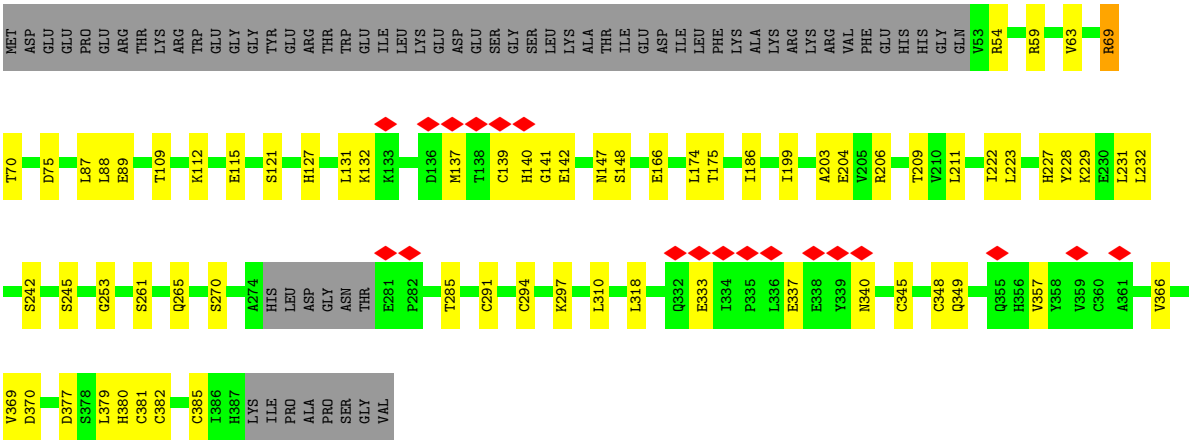
Chain 1:





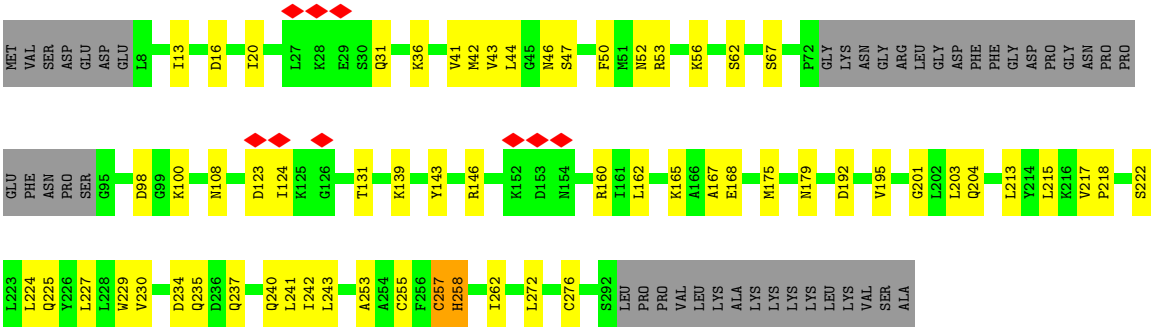
- Molecule 3: General transcription factor IIH subunit 2

Chain 2:



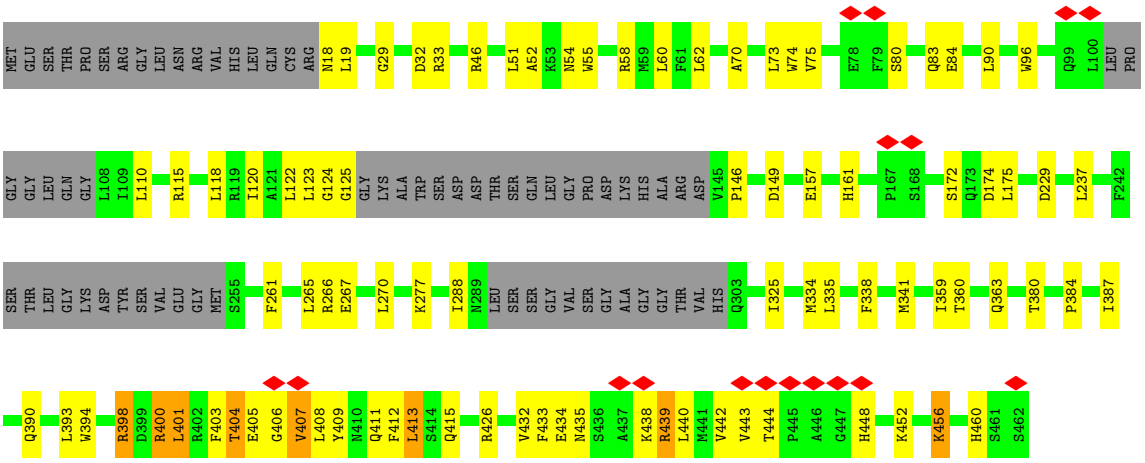
- Molecule 4: General transcription factor IIH subunit 3

Chain 3:



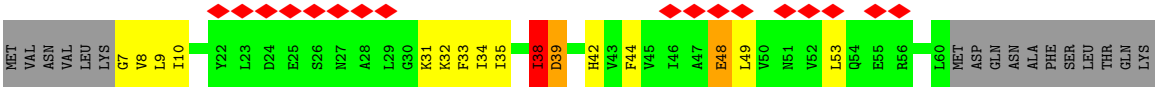
- Molecule 5: General transcription factor IIH subunit 4

Chain 4:



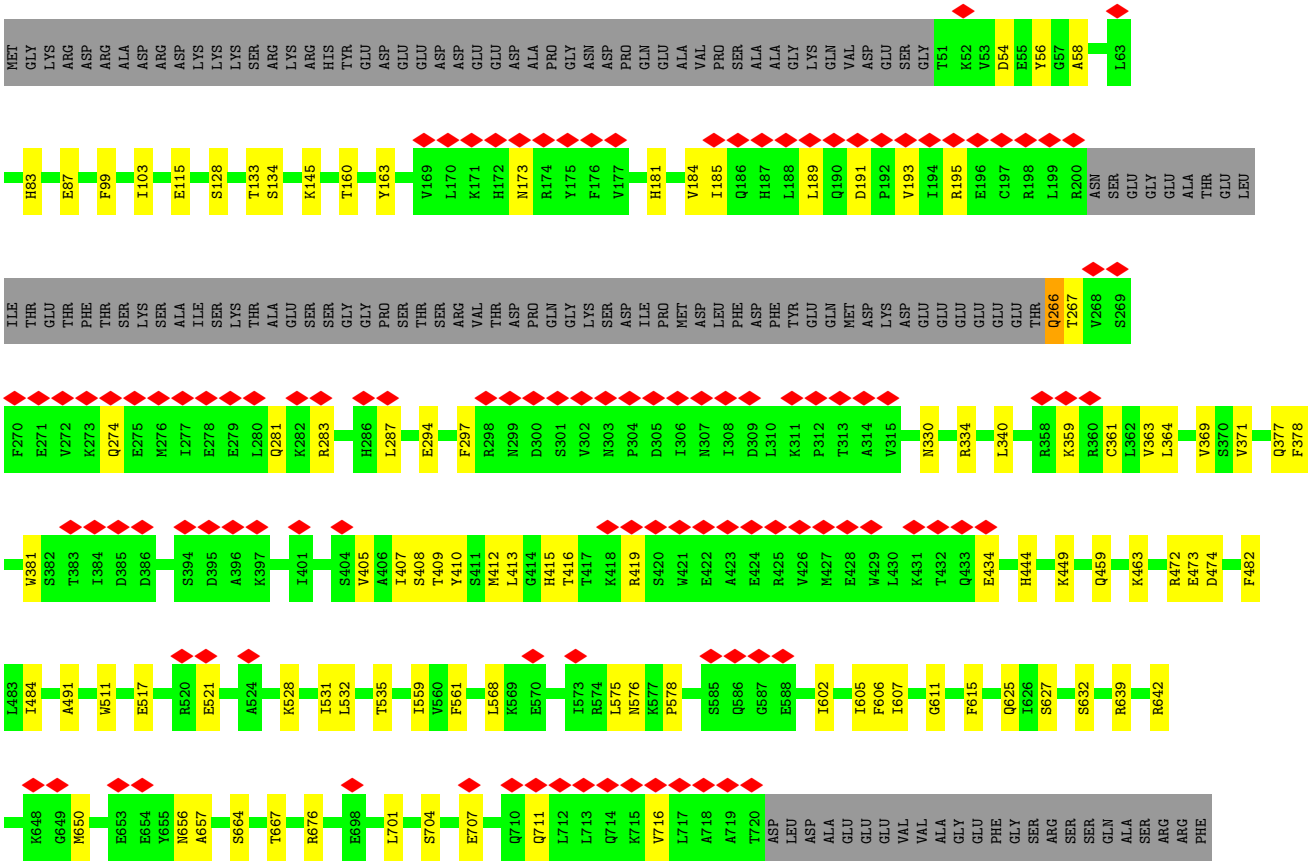
• Molecule 6: General transcription factor IIH subunit 5

Chain 5:



• Molecule 7: General transcription and DNA repair factor IIH helicase subunit XPB

Chain 6:



GLY THR MET SER SER MET SER GLY ALA ASP ASP THR VAL TYR MET GLU TYR HIS SER SER ARG SER LYS ALA PRO SER LYS HIS VAL HIS PRO LEU PHE LYS ARG PHE ARG LYS

- Molecule 8: General transcription and DNA repair factor IIH helicase subunit XPD

Chain 7:

M1 K2 L3 L9 F12 P13 Y14 I17 F22 L28 L32 S44 G45 T46 G47 K48 T49 V50 S51 L52 L55 I56 Q60 R61 A62 Y63 P64 L65 E66 V67 L70 I71 Y72 V77 I80 E81 I84 G99 E100 K101 L102 L107 A108 L109 S110

S111 N114 L115 H118 V121 F126 G127 K128 K133 C134 H135 S136 L137 T138 V142 Q145 Y146 Q147 H148 D149 T150 S151 E167 V168 N176 L177 P191 A195 I199 V206 Y207 Y211 L225 A226 R227 V231 V232 F233 D234 N238 I239 D240 N241

V242 C243 S246 V249 T252 T255 Q260 G261 N262 L263 E264 T265 L266 Q267 K268 L271 R272 E275 T276 D277 E278 Q279 R280 E284 Y285 R286 R287 L288 V289 E290 G291 LEU ARG GLU ALA SER ALA ALA ARG GLU THR ASP ALA HIS LEU A306 V309 L310 I323 R324

F329 F332 L333 R334 R335 E338 W342 R343 L344 R345 V346 Q347 H348 V349 V350 Q351 P354 P355 L361 R364 V365 C366 I367 L372 R373 E377 R378 L382 L383 H384 T385 I388 D393 F394 F403 A404 T405 T409 I416 P420 F421 D422 D423 R424

T425 P426 T427 I428 A429 N430 P431 I432 L433 H434 C437 M438 A443 V454 T460 L461 S462 P463 L464 P475 M478 V488 E512 D513 I514 A515 V516 V531 P532 D533 E554 I557 I561 Q562 R563 T571 Q572 D573 E576 E589 N590 G591 R592 A600

V604 S605 E606 G607 I608 D609 H613 A617 V618 Y627 T628 Q629 I632 L637 E648 F651 H659 A660 A661 Q662 C663 V664 G665 R666 R669 L676 M677 V678 F679 T709 V710 D711 Q715 R722 Q726 P727 F728 HIS ARG GLU ASP GLN LEU GLY LEU

SER LEU LEU SER LEU GLU GLN LEU LEU GLU SER GLU GLU THR LEU LYS ARG ILE GLU GLN ILE ALA GLN GLN LEU

- Molecule 9: Alpha-amanitin

Chain N:

I1 W2 G3 C6 N7 P8

- Molecule 10: RNA

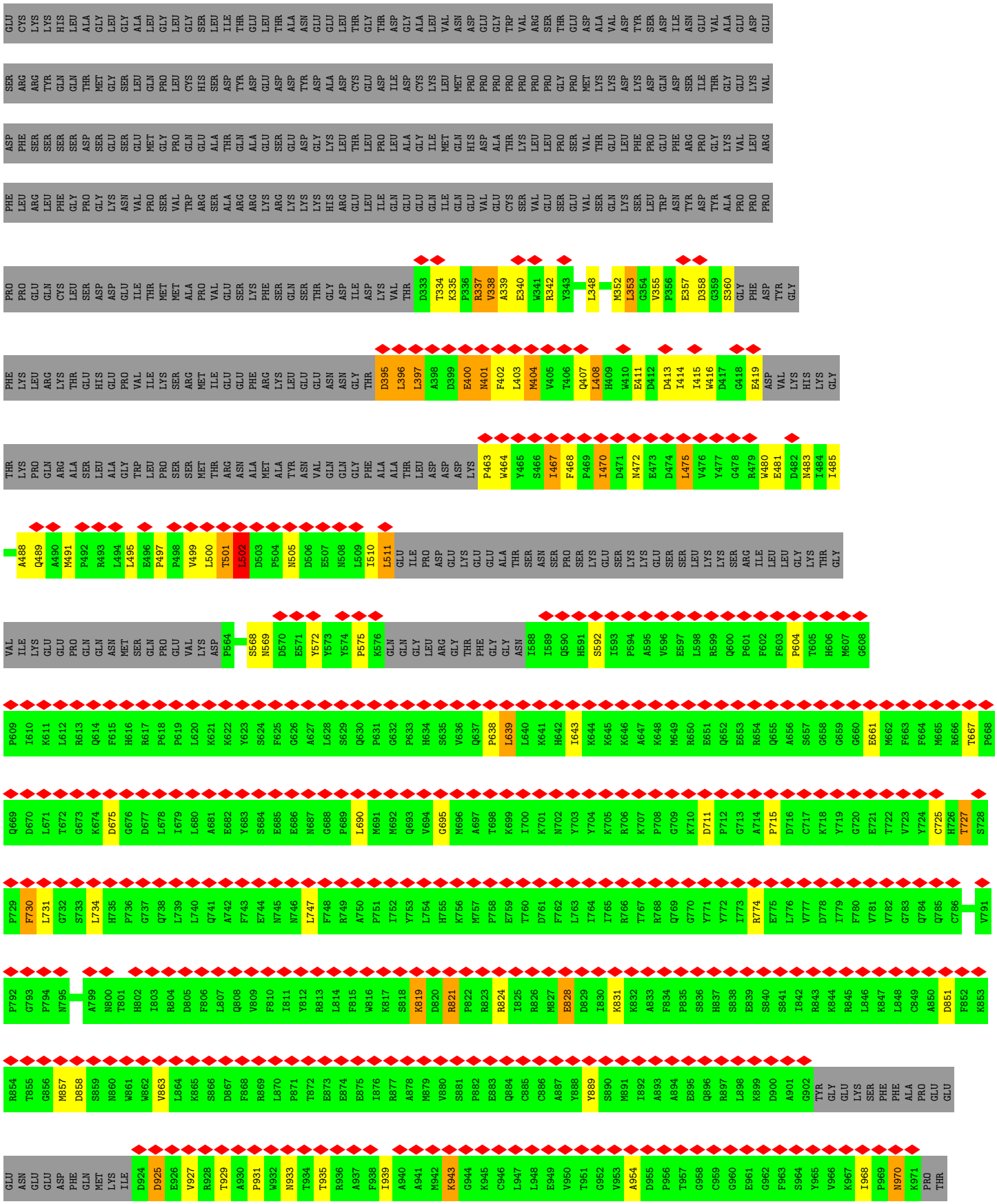
Chain Z:

ATP1 G4

- Molecule 11: Transcription initiation factor TFIID subunit 1

Chain A:

MET GLY PRO GLY CYS ASP LEU LEU LEU ARG THR ALA ALA THR ILE THR ALA ALA ALA ILE MET SER ASP THR ASP SER ASP GLU ASP SER ALA GLY GLY GLY PRO PHE SER LEU ALA GLY PHE LEU PHE GLY ASN ILE ASN GLY ALA ALA GLY GLN LEU GLU GLY GLU SER VAL LEU ASP ASP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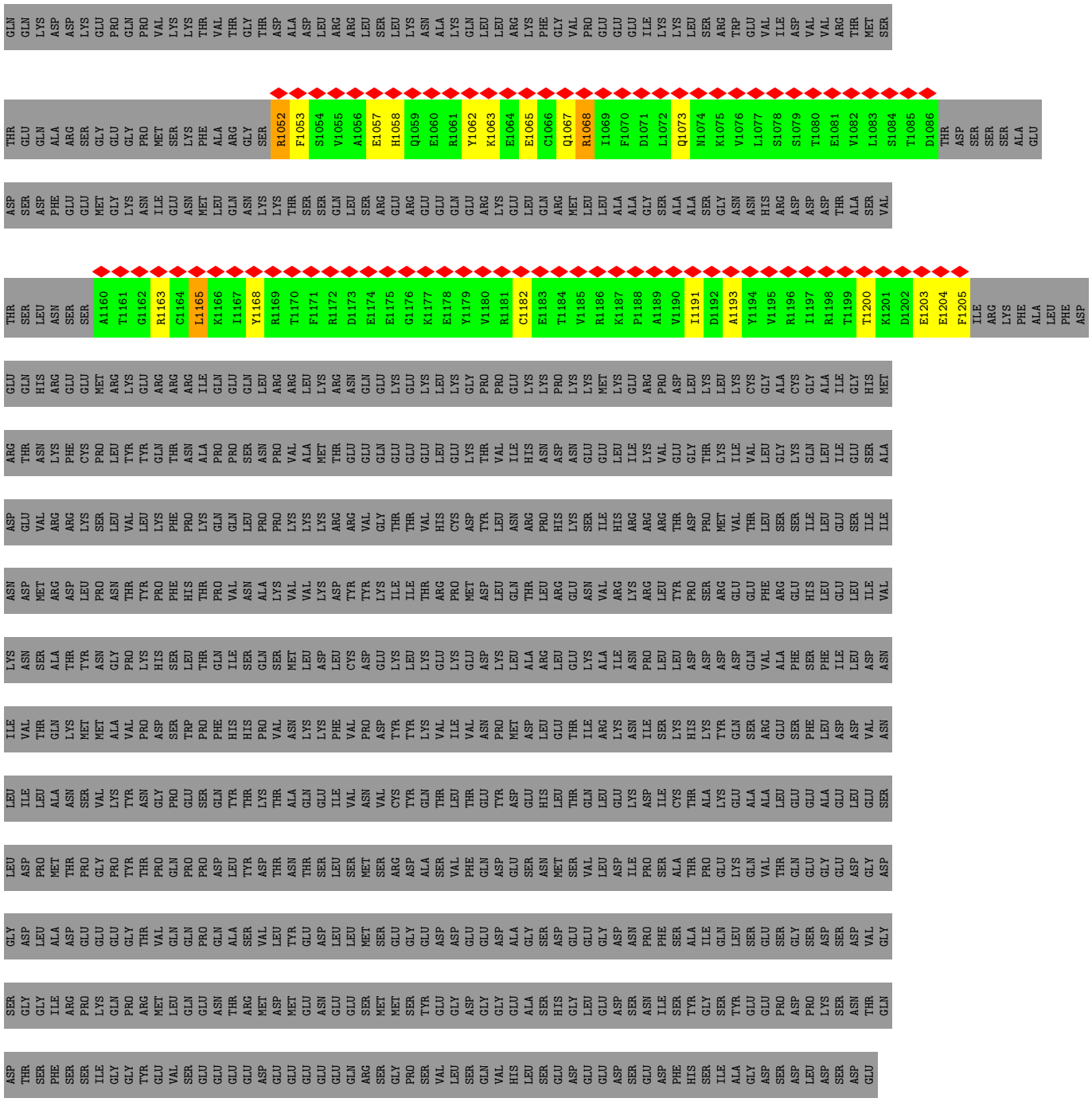
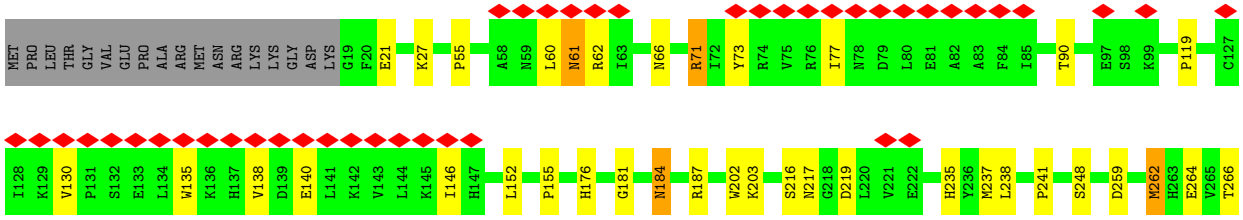
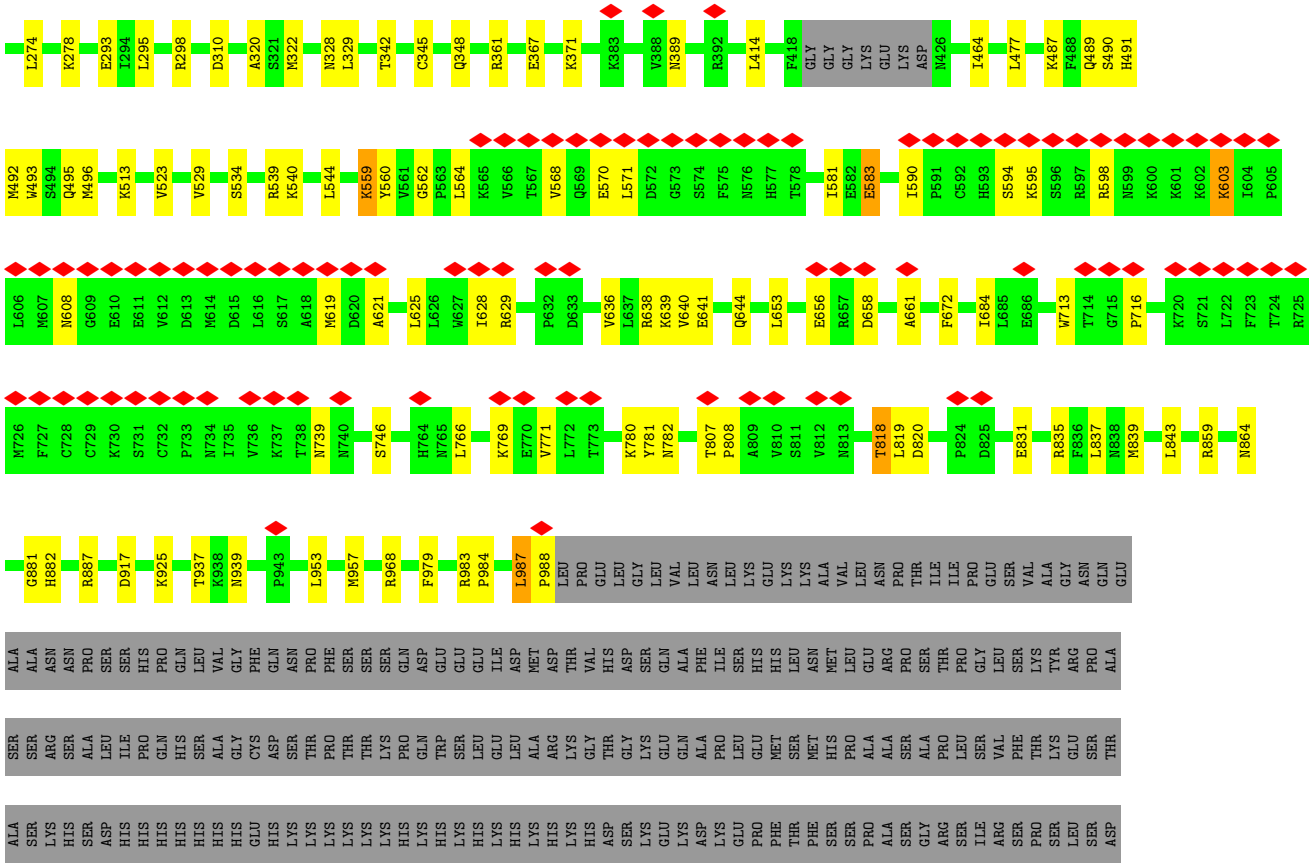
SER ARG ARG TYR GLN GLN THR MET GLY SER GLU GLN PRO LEU CYS HIS SER ASP TYR ASP GLU ASP ASP TYR ASP ALA ASP CYS GLU ASP ILE ASP CYS LYS LEU VAL MET PRO PRO PRO PRO PRO PRO PRO GLY PRO MET LYS LYS ASP LYS ASP GLN ASP SER ILE THR GLY GLU LYS VAL
ASP PHE SER SER SER SER ASP SER GLU SER GLU MET GLY PRO GLN GLU ALA THR GLN ALA GLU SER GLU ASP GLY LYS LEU THR LEU PRO LEU ALA GLY ILE MET GLN HIS ASP ALA THR LYS LEU LEU PRO SER VAL THR GLU LEU PHE PRO GLU PHE ARG PRO GLY LYS VAL LEU ARG
PHE LEU ARG LEU PHE GLY PRO GLY LYS ASN VAL PRO SER VAL TRP ARG SER ALA ARG ARG LYS ARG LYS LYS LYS HIS ARG GLU LEU ILE GLN GLU GLU GLN ILE GLN GLU VAL GLU CYS SER VAL GLU SER GLU VAL SER GLN LYS SER LEU TRP ASN TYR ASP TYR ALA PRO PRO PRO
PRO PRO GLU GLN CYS LEU SER ASP ASP GLU ILE THR MET MET ALA PRO VAL GLU SER LYS PHE SER GLN SER THR GLY ASP ILE ASP LYS VAL THR D333 T334 K335 P336 R337 V338 A339 E340 W341 R342 Y343 L348 M352 L353 G354 V355 P356 E357 D358 G359 S360 GLY PHE ASP TYR GLY
PHE LYS LEU ARG LYS THR GLU HIS GLU PRO VAL ILE LYS SER ARG MET ILE GLU GLU PHE ARG LYS LEU GLU GLU ASN ASN GLY THR D395 L396 L397 A398 D399 E400 N401 F402 L403 M404 V405 T406 Q407 L408 H409 W410 E411 D412 D413 I414 I415 W416 D417 G418 E419 ASP VAL LYS HIS LYS GLY
THR LYS PRO GLN ARG ALA SER LEU ALA GLY TRP LEU PRO SER SER MET THR ARG ASN ALA MET ALA TYR ASN VAL GLN GLN GLY THR ALA ALA THR LEU ASP ASP ASP LYS P463 W464 Y465 S466 I467 F468 P469 I470 D471 N472 E473 D474 L475 V476 Y477 G478 R479 W480 E481 D482 N483 I484 I485
A488 Q489 A490 M491 P492 R493 L494 L495 E496 P497 P498 V499 L500 T501 L502 D503 P504 N505 D506 E507 N508 L509 I510 L511 GLU ILE PRO ASP GLU LYS GLU GLU ALA THR SER ASN SER PRO SER LYS GLU SER LYS LYS GLU SER SER LEU LYS LYS SER ARG ILE LEU LEU GLY LYS THR GLY
VAL ILE LYS GLU GLU PRO GLN GLN ASN MET SER GLN PRO GLU VAL LYS ASP P564 S568 N569 D570 E571 Y572 Y573 Y574 P575 K576 GLN GLN GLY LEU ARG GLY THR PHE GLY GLY ASN I588 I589 Q590 H591 S592 I593 P594 A595 V596 E597 L598 R599 Q600 P601 F602 F603 P604 T605 H606 M607 G608
P609 I610 K611 L612 R613 Q614 F615 H616 R617 P618 P619 L620 K621 K622 Y623 S624 F625 G626 A627 L628 S629 Q630 P631 G632 P633 H634 S635 V636 Q637 P638 L639 L640 K641 H642 I643 K644 K645 K646 A647 K648 M649 R650 E651 Q652 E653 R654 Q655 A656 S657 G658 G659 G660 E661 M662 F663 F664 M665 R666 T667 P668
Q669 D670 L671 T672 G673 K674 D675 G676 D677 L678 I679 L680 A681 E682 Y683 S684 E685 E686 N687 G688 P689 L690 M691 M692 Q693 V694 G695 M696 A697 T698 K699 I700 K701 N702 Y703 Y704 K705 R706 K707 P708 G709 K710 D711 P712 G713 A714 P715 D716 C717 K718 Y719 G720 E721 T722 V723 Y724 C725 H726 T727 S728
P729 F730 L731 G732 S733 L734 H735 P736 G737 Q738 L739 L740 Q741 A742 F743 E744 N745 N746 L747 F748 R749 A750 P751 I752 Y753 L754 H755 K756 M757 F758 E759 T760 D761 F762 L763 I764 I765 R766 T767 R768 Q769 G770 Y771 Y772 T773 R774 E775 L776 V777 D778 I779 F780 V781 V782 G783 Q784 Q785 C786 V791
P792 G793 P794 N795 A799 N800 T801 H802 I803 R804 D805 F806 L807 Q808 V809 F810 I811 Y812 R813 L814 F815 W816 K817 S818 K819 D820 R821 P822 R823 R824 I825 R826 M827 E828 D829 I830 K831 K832 A833 F834 P835 S836 H837 S838 E839 S840 S841 I842 R843 K844 R845 L846 K847 L848 C849 A850 D851 F852 K853
R854 T855 G856 M857 D858 S859 N860 W861 W862 V863 L864 K865 S866 D867 F868 R869 L870 P871 T872 E873 E874 E875 I876 R877 A878 M879 V880 S881 P882 E883 Q884 C885 C886 A887 Y888 Y889 S890 M891 I892 A893 A894 E895 Q896 R897 L898 K899 D900 A901 G902 TYR GLY GLU LYS SER PHE PHE ALA PRO GLU GLU
GLU ASN GLU GLU ASP PHE GLN MET LYS ILE D924 D925 E926 V927 R928 T929 A930 P931 W932 N933 T934 T935 R936 A937 F938 I939 A940 A941 M942 K943 G944 K945 C946 L947 L948 E949 V950 T951 G952 V953 A954 D955 P956 T957 G958 C959 G960 E961 G962 F963 S964 Y965 V966 K967 I968 P969 N970 K971 PRO THR

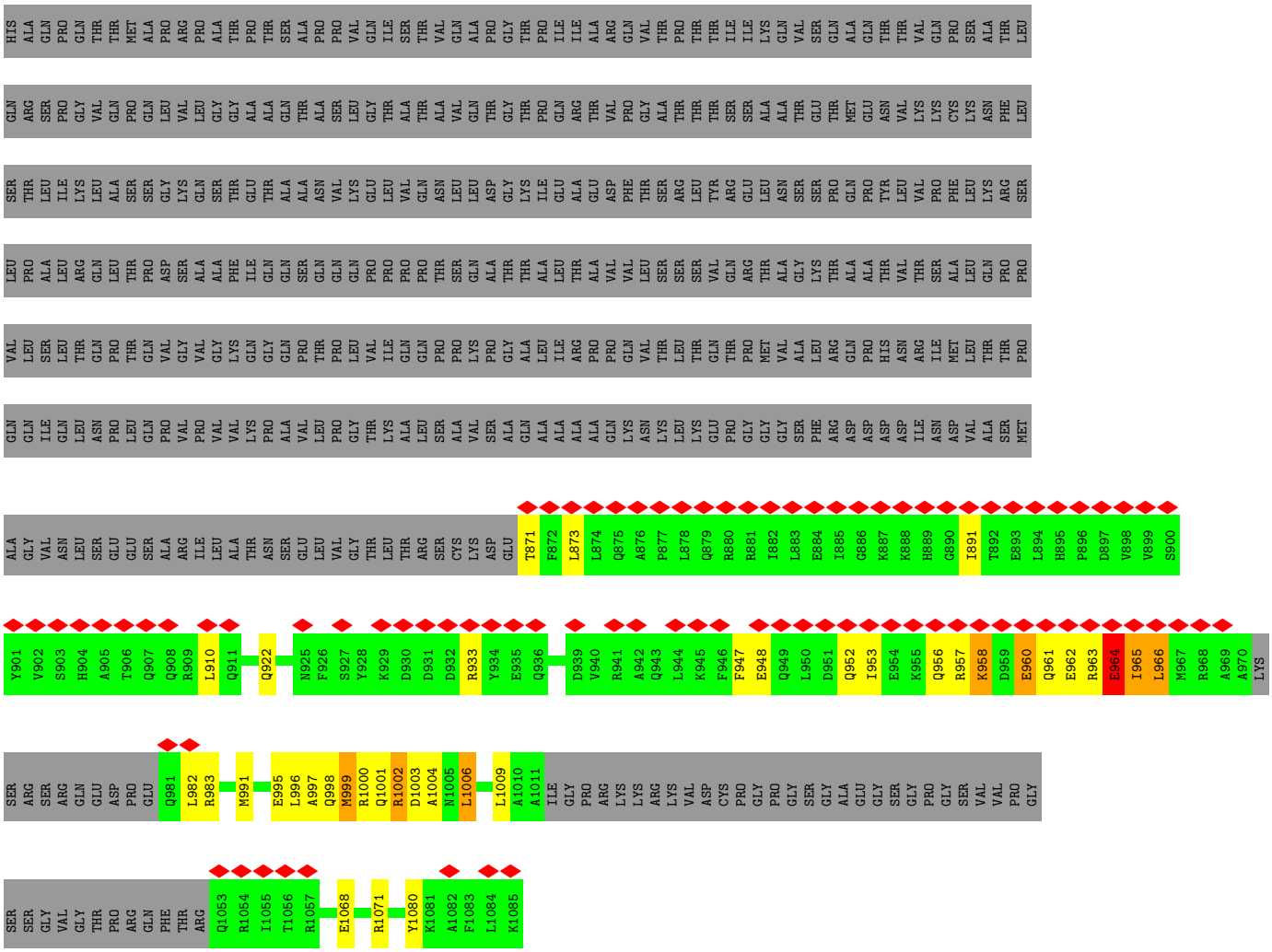


• Molecule 12: Transcription initiation factor TFIID subunit 2

Chain B:

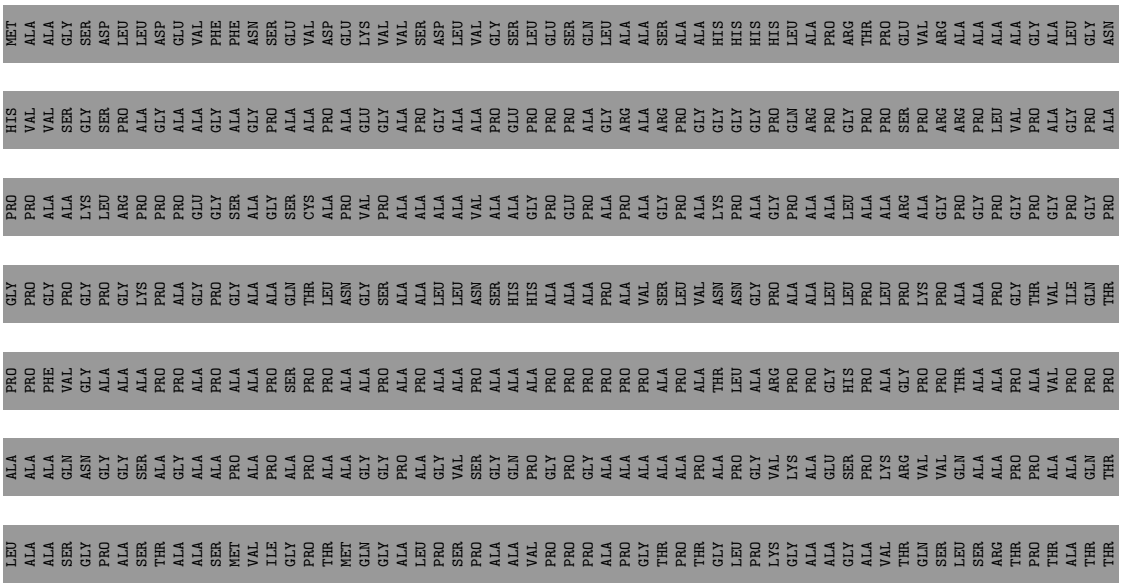



L274 K278 E293 I294 L295 R298 D310 A320 S321 N322 N328 L329 T342 C345 Q348 R361 E367 K371 K383 V388 N389 R392 L414 F418 GLY GLY GLY LYS GLU LYS ASP N426 I464 L477 K487 F488 Q489 S490 H491
M492 W493 S494 Q495 M496 K513 V523 V529 S534 R539 K540 L544 K559 Y560 V561 G562 P563 L564 K565 V566 T567 V568 Q569 E570 L571 D572 G573 S574 F575 N576 H577 T578 I581 E582 E583 I590 P591 C592 H593 S594 K595 S596 R597 R598 N599 K600 K601 K602 K603 I604 P605
L606 M607 N608 G609 E610 E611 V612 D613 M614 D615 L616 S617 A618 M619 D620 A621 L625 L626 W627 I628 R629 P632 D633 V636 L637 R638 K639 V640 E641 Q644 L653 E656 R657 D658 A661 F672 I684 L685 E686 W713 T714 G715 P716 K720 S721 L722 F723 T724 R725
M726 F727 C728 C729 K730 S731 C732 P733 N734 I735 V736 K737 T738 N739 N740 S746 H764 N765 L766 K769 E770 V771 L772 T773 K780 Y781 N782 T807 P808 A809 V810 S811 V812 N813 T818 L819 D820 P824 D825 E831 R835 F836 L837 N838 M839 L843 R859 N864
G881 H882 R887 D917 K925 T937 K938 N939 P943 L953 M957 R968 F979 R983 P984 L987 P988 LEU PRO GLU LEU GLY LEU VAL LEU ASN LEU LYS GLU LYS LYS ALA VAL LEU ASN PRO THR ILE ILE PRO GLU SER VAL ALA GLY ASN GLN GLU
ALA ALA ASN ASN PRO SER SER HIS PRO GLN LEU VAL GLY PHE GLN ASN PRO PHE SER SER SER GLN ASP GLU GLU GLU ILE ASP MET ASP THR VAL HIS ASP SER GLN ALA PHE ILE SER HIS HIS LEU ASN MET LEU GLU ARG PRO SER THR PRO GLY LEU SER LYS TYR ARG PRO ALA
SER SER ARG SER ALA LEU ILE PRO GLN HIS SER ALA GLY CYS ASP SER THR PRO THR THR LYS PRO GLN TRP SER LEU GLU LEU ALA ARG LYS GLY THR GLY LYS SER GLU GLN ALA PRO LEU GLU MET SER MET HIS PRO ALA ALA SER ALA PRO LEU SER VAL PHE THR LYS GLU SER THR
ALA SER LYS HIS SER ASP HIS HIS HIS HIS HIS HIS GLU HIS LYS LYS LYS LYS LYS LYS HIS LYS HIS LYS HIS LYS HIS LYS HIS LYS HIS ASP SER LYS GLU LYS ASP LYS GLU PRO PHE THR PHE SER SER PRO ALA SER GLY ARG SER ILE ARG SER PRO SER LEU SER ASP
• Molecule 13: Transcription initiation factor TFIID subunit 4
Chain D:
8%
12%
85%
MET ALA ALA GLY SER ASP LEU LEU ASP GLU VAL PHE PHE ASN SER GLU VAL ASP GLU LYS VAL VAL SER ASP LEU VAL GLY SER LEU GLU SER GLN LEU ALA ALA SER ALA ALA HIS HIS HIS HIS LEU ALA PRO ARG THR PRO GLU VAL ARG ALA ALA ALA GLY ALA LEU GLY ASN
HIS VAL VAL SER GLY SER PRO ALA GLY ALA ALA GLY ALA GLY PRO ALA ALA PRO ALA ALA ALA PRO GLY ALA ALA ALA PRO GLU PRO PRO PRO ALA GLY ARG ALA ARG PRO GLY GLY GLY GLY PRO GLN ARG PRO GLY PRO PRO SER PRO ARG ARG PRO LEU VAL PRO ALA GLY PRO ALA
PRO PRO ALA ALA LYS LEU ARG PRO PRO PRO GLU GLU GLY SER ALA GLY SER CYS ALA PRO VAL PRO ALA ALA ALA ALA VAL ALA ALA GLY PRO GLU PRO ALA PRO ALA ALA GLY PRO ALA LYS PRO ALA GLY PRO ALA ALA ALA LEU LEU ALA ALA ARG PRO GLY PRO GLY PRO GLY PRO GLY PRO
GLY PRO GLY PRO GLY GLY PRO ALA GLY PRO GLY ALA ALA ALA GLN THR LEU ASN GLY SER ALA ALA LEU LEU ASN SER HIS HIS ALA ALA ALA PRO ALA VAL SER LEU VAL ASN ASN GLY GLY PRO ALA ALA LEU LEU PRO LEU PRO LYS PRO GLY THR VAL ILE GLN THR
PRO PRO PHE VAL GLY ALA ALA ALA PRO PRO ALA ALA PRO ALA ALA PRO SER PRO ALA ALA ALA ALA ALA ALA PRO PRO PRO PRO PRO ALA ALA ALA PRO ALA THR LEU ALA ARG PRO PRO GLY HIS PRO ALA GLY PRO PRO THR ALA ALA PRO ALA VAL PRO PRO
ALA ALA ALA GLN ASN GLY GLY SER ALA GLY ALA ALA ALA PRO ALA ALA PRO ALA ALA ALA GLY VAL SER PRO GLY GLN PRO GLY PRO GLY ALA ALA PRO ALA ALA GLY VAL LYS ALA GLU SER PRO LYS ARG VAL VAL GLN ALA ALA ALA PRO PRO ALA ALA GLN THR
LEU ALA ALA SER GLY PRO ALA SER THR ALA GLY ALA ALA SER MET VAL ILE GLY PRO THR MET GLN GLY GLY ALA LEU PRO SER PRO ALA ALA VAL PRO GLY PRO PRO PRO ALA PRO GLY GLY THR PRO THR GLY LEU PRO LYS GLY ALA ALA GLY VAL THR GLN SER LEU SER ARG THR PRO THR ALA ALA THR THR
SER GLY ILE ARG ALA THR LEU THR PRO THR VAL LEU ALA PRO ARG LEU PRO GLN PRO PRO GLN ASN PRO THR ASN ILE GLN ASN PHE GLN LEU PRO PRO GLY MET VAL LEU VAL ARG SER GLU ASN GLY GLN LEU LEU MET ILE PRO GLN GLN ALA LEU ALA GLN MET GLN ALA ALA GLN ALA



- Molecule 13: Transcription initiation factor TFIID subunit 4

Chain d: 15% 13% 85%



SER GLY ILE ARG ALA THR LEU THR PRO THR VAL LEU ALA PRO ARG LEU PRO GLN PRO PRO GLN ASN PRO THR ASN ILE GLN ASN PHE GLN LEU PRO PRO GLY GLN MET VAL LEU VAL ARG SER GLU ASN GLY GLN LEU LEU MET ILE PRO GLN GLN ALA LEU ALA GLN MET GLN ALA GLN ALA
HIS ALA GLN PRO GLN THR THR MET ALA PRO ARG PRO ALA THR PRO THR SER ALA PRO PRO VAL GLN ILE SER THR VAL GLN ALA PRO GLY THR PRO ILE ILE ARG GLN VAL THR PRO THR THR THR ILE ILE LYS GLN VAL SER GLN ALA GLN THR THR VAL GLN PRO SER ALA THR LEU
GLN ARG SER PRO GLY VAL GLN PRO GLN LEU VAL LEU GLY GLY ALA ALA GLN THR ALA SER SER LEU GLY THR ALA THR ALA VAL GLN THR GLY THR PRO GLN ARG THR VAL PRO GLY ALA THR THR THR SER SER ALA ALA THR GLU THR MET GLU ASN VAL LYS LYS CYS LYS ASN PHE LEU
SER THR LEU ILE LYS LEU ALA SER SER GLY LYS GLN SER THR GLU THR ALA ALA ASN VAL LYS GLU LEU VAL GLN SER LEU LEU ASP GLY LYS ILE GLU ALA GLU ASP PHE THR SER ARG LEU TYR ARG GLU LEU ASN SER SER PRO GLN PRO TYR LEU VAL PRO PHE LEU LYS ARG SER
LEU PRO ALA LEU ARG GLN LEU THR PRO ASP SER ALA ALA PHE ILE GLN GLN SER GLN GLN GLN PRO PRO PRO PRO THR SER GLN GLN ALA THR THR ALA ALA VAL LEU SER SER SER VAL GLN ARG THR ALA GLY LYS THR ALA ALA THR VAL THR SER ALA LEU GLN PRO PRO
VAL LEU SER LEU THR GLN VAL GLY VAL GLY LYS GLN GLY GLN PRO THR PRO LEU VAL ILE GLN GLN PRO LYS PRO GLY ALA LEU ILE ARG PRO PRO GLN VAL THR LEU THR GLN THR PRO MET VAL ALA LEU ARG GLN PRO HIS ASN ARG ILE MET LEU THR THR PRO
GLN GLN ILE GLN LEU ASN PRO LEU GLN PRO VAL VAL LYS PRO ALA VAL LEU PRO GLY THR LYS ALA LEU SER ALA VAL SER ALA GLN ALA ALA ALA GLN LYS ASN LYS LEU LYS GLU PRO GLY GLY GLY SER PHE ARG ASP ASP ASP ILE ASN ASP VAL ALA SER MET

ALA GLY V843 N844 L845 S846 E847 E848 S849 A850 R851 I852 L853 A854 T855 N856 S857 E858 L859 V860 G861 T862 L863 T864 R865 S866 C867 K868 D869 E870 T871 F872 L873 L874 Q875 A876 P877 L878 Q879 R880 R881 I882 L883 E884 I885 G886 K887 K888 H889 G890 I891 T892 E893 L894 H895 P896 D897 V898 V899 S900

Y901 V902 S903 H904 A905 T906 Q907 Q908 R909 L910 Q911 N912 L913 V914 E915 K916 I917 S918 E919 T920 A921 Q922 Q923 K924 N925 F926 S927 Y928 K929 D930 D931 D932 R933 Y934 E935 Q936 A937 S938 D939 V940 R941 A942 Q943 L944 K945 F946 F947 E948 Q949 L950 D951 Q952 I953 E954 K955 Q956 R957 K958 D959 E960

Q961 E962 R963 E964 I965 L966 M967 R968 ALA ALA LYS SER ARG SER ARG GLN GLU ASP PRO GLU GLN GLN LEU ARG LEU LYS GLN LYS ALA LYS GLU MET GLN GLN GLN GLU LEU ALA GLN MET ARG GLN ARG ASP ALA ASN LEU THR ALA LEU ALA ALA ILE GLY PRO ARG LYS LYS ARG LYS VAL

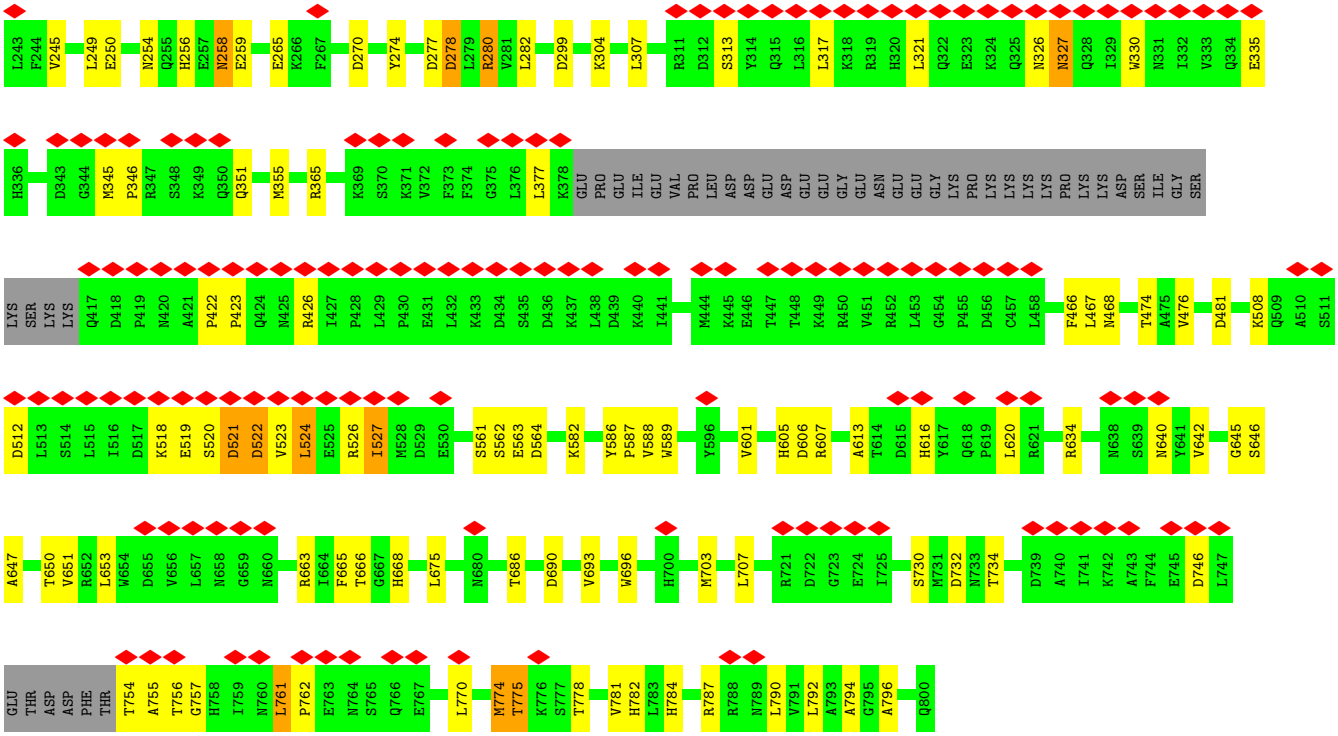
ASP CYS PRO GLY PRO GLY SER GLY ALA GLU GLY SER GLY PRO GLY SER VAL VAL PRO GLY SER SER GLY VAL GLY THR PRO ARG GLN PHE THR ARG GLN R1054 I1055 T1056 R1057 V1058 N1059 L1060 R1061 D1062 L1063 I1064 F1065 C1066 L1067 E1068 N1069 E1070 R1071 E1072 T1073 S1074 H1075 S1076 L1077 L1078 L1079 Y1080

K1081 A1082 F1083 L1084 K1085

- Molecule 14: Transcription initiation factor TFIID subunit 5

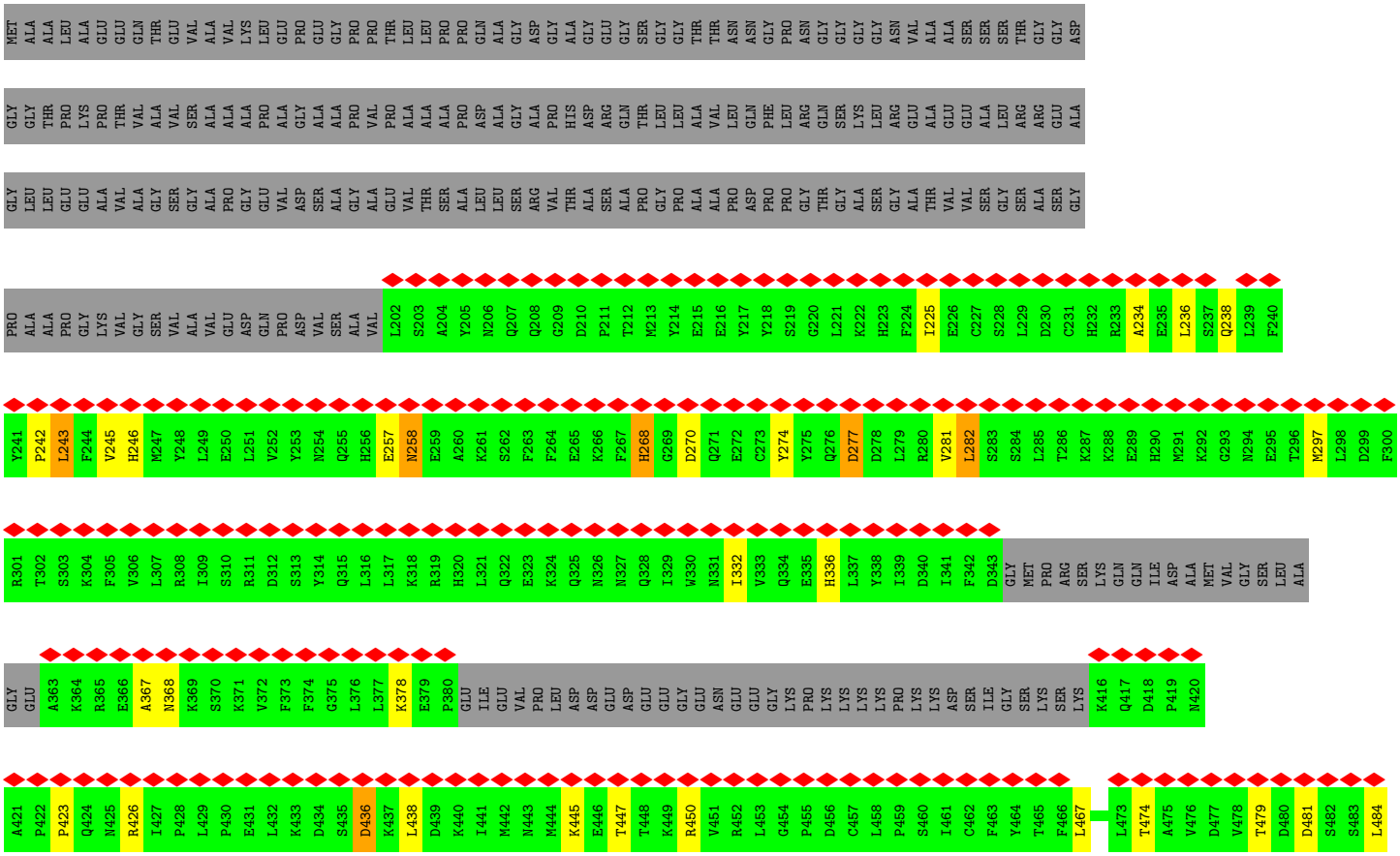
Chain E: 21% 54% 12% • 32%

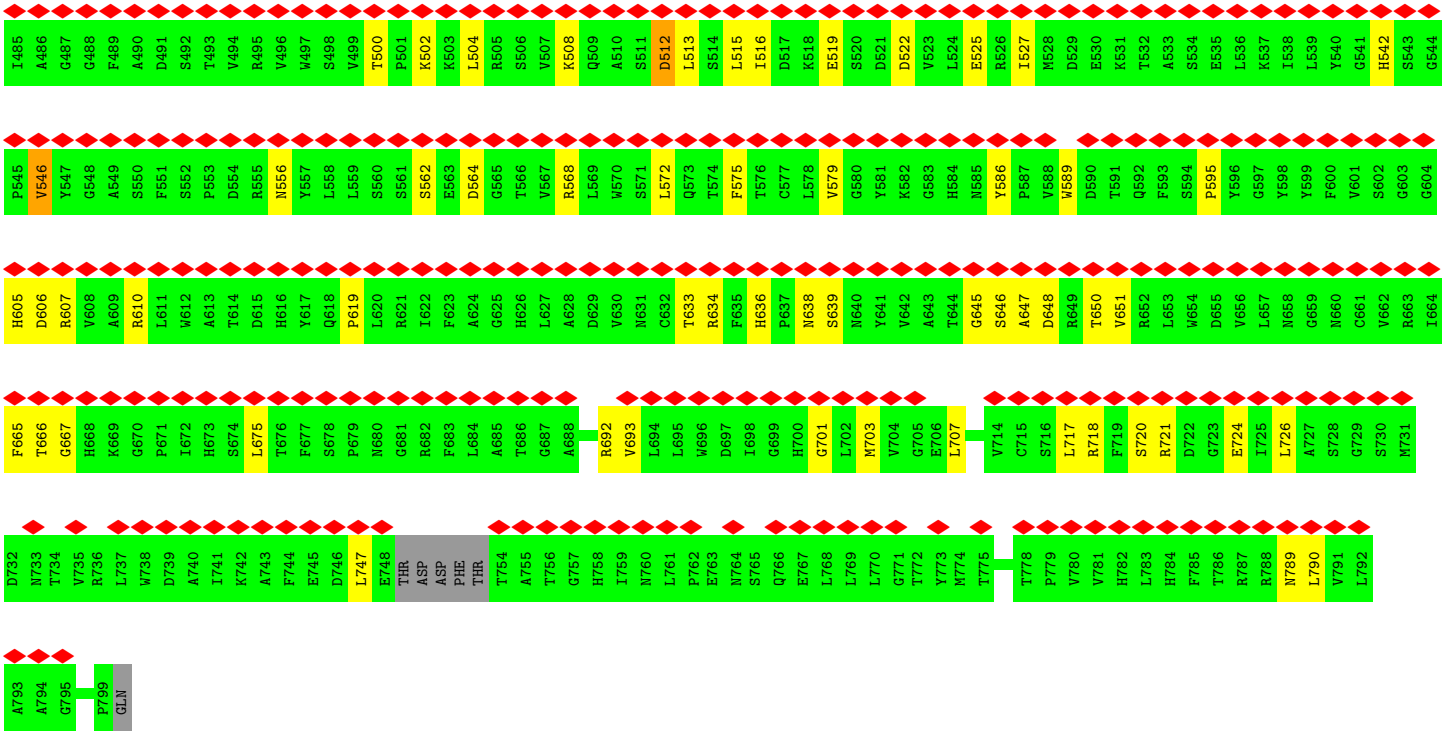
MET ALA ALA LEU ALA GLU GLU GLN THR GLU VAL ALA VAL LYS LEU GLU PRO GLU GLY PRO PRO THR LEU LEU PRO PRO GLN ALA GLY ASP GLY ALA GLY GLU GLY SER GLY GLY THR THR ASN ASN GLY PRO ASN GLY GLY GLY GLY GLY ASN VAL ALA ALA SER SER SER THR GLY GLY ASP
GLY GLY THR PRO LYS PRO THR VAL ALA VAL SER ALA ALA ALA PRO ALA GLY ALA PRO ASP ALA GLY ALA PRO HIS ASP ARG GLN THR LEU LEU ALA VAL LEU GLN PHE LEU ARG GLN SER LYS LEU ARG GLU ALA GLU GLU ALA LEU ARG ARG GLU ALA
GLY LEU LEU GLU GLU ALA VAL ALA GLY SER GLY ALA PRO GLY GLU VAL ASP SER ALA GLY ALA VAL THR SER ALA LEU LEU SER ARG VAL THR ALA SER ALA PRO GLY PRO PRO ALA ALA PRO ASP PRO PRO GLY THR GLY ALA SER GLY ALA THR VAL VAL SER GLY ALA SER GLY
PRO ALA ALA PRO GLY LYS VAL GLY SER VAL ALA VAL GLU ASP GLN PRO ASP VAL SER ALA VAL LEU SER ALA TYR ASN GLN GLN GLY D210 P211 T212 M213 Y214 E215 E216 Y217 Y218 S219 G220 L221 K222 H223 F224 I225 E226 C227 S228 L229 D230 C231 H232 R233 A234 E235 L236 L239 F240



- Molecule 14: Transcription initiation factor TFIID subunit 5

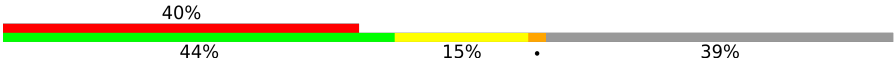
Chain e:

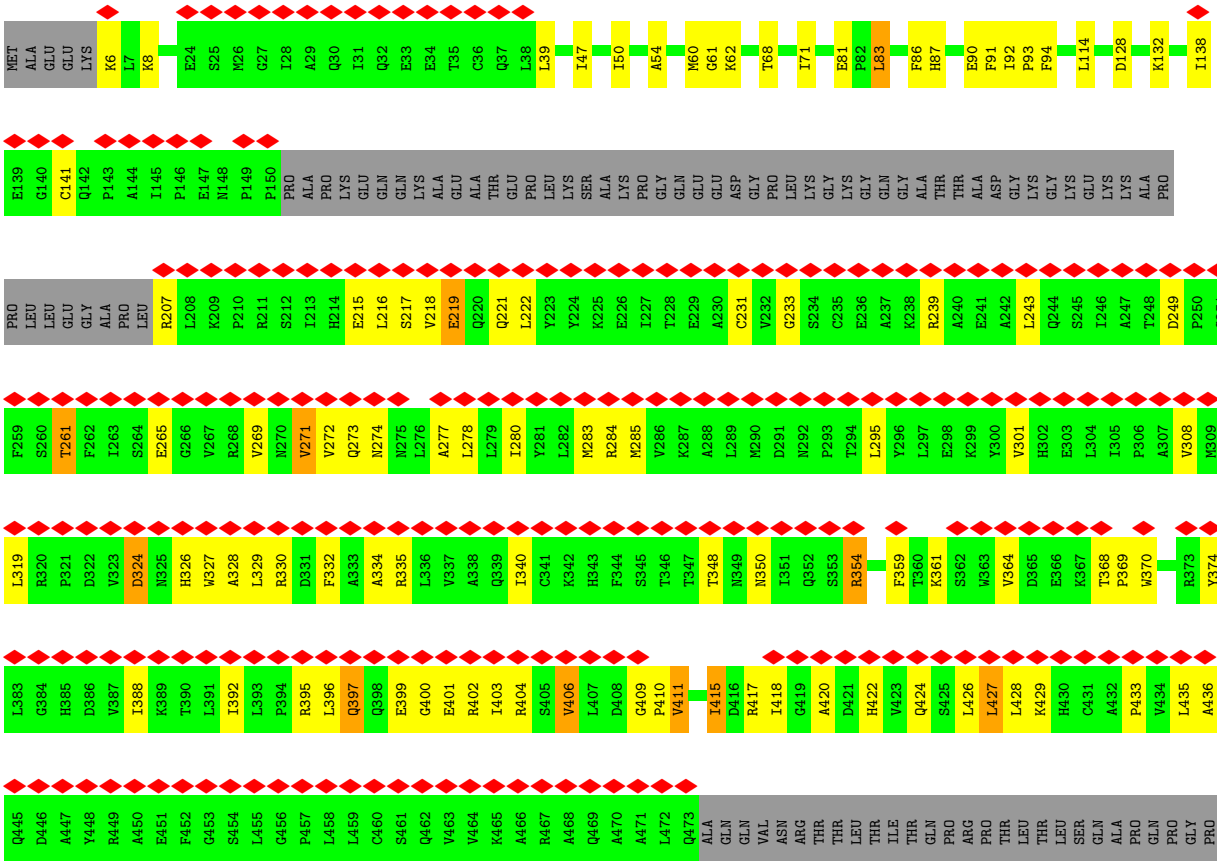




- Molecule 15: Transcription initiation factor TFIID subunit 6

Chain F:





GLY LEU LEU LYS VAL PRO GLY SER ILE ALA LEU PRO VAL GLN THR LEU VAL SER ALA ARG ALA ALA ALA PRO PRO GLN PRO SER PRO PRO PRO PRO THR LYS PHE ILE VAL MET SER SER SER SER SER SER ALA PRO SER THR GLN GLN VAL LEU SER LEU SER THR SER ALA PRO GLY SER GLY

SER THR THR THR SER PRO VAL THR THR THR VAL PRO SER VAL GLN PRO ILE VAL LYS LEU VAL SER THR ALA THR THR ALA PRO PRO SER THR ALA PRO SER GLY PRO GLY SER VAL GLN LYS TYR ILE VAL VAL SER LEU PRO PRO THR GLY GLU GLY LYS GLY GLY PRO THR SER HIS

PRO SER PRO VAL PRO PRO PRO ALA SER SER PRO SER PRO LEU SER GLY SER ALA LEU CYS GLY GLY GLY LYS GLN GLU ALA GLY ASP SER PRO PRO PRO ALA PRO GLY THR PRO LYS ALA ASN GLY SER GLN PRO ASN SER GLY SER PRO GLN PRO ALA PRO

- Molecule 15: Transcription initiation factor TFIID subunit 6

Chain f: 31% 48% 10% • 40%

MET ALA GLU GLU LYS LYS LEU LYS L9 S10 N11 T12 V13 L14 P15 S16 E17 S18 M19 K20 V21 V22 A23 E24 S25 M26 G27 I28 A29 Q30 I31 Q32 E33 E34 T35 C36 Q37 L38 L39 T40 D41 E42 V43 S44 Y45 R46 I47 K48 E49 I50 A51 Q52 L55 M58 H59 M60 G61 K62

R63 Q64 K65 L66 T67 T68 S69 D70 I71 D72 Y73 A74 L75 K76 L77 K78 N79 V80 E81 P82 L83 Y84 G85 F86 H87 A88 Q89 E90 F91 I92 P93 F94 R95 F96 A97 S98 G99 G100 G101 R102 E103 L104 Y105 F106 Y107 E108 E109 K110 E111 V112 D113 L114 S115 D116 I117 I118 N119 T120 P121 L122

P123 R124 V125 P126 L127 L131 K132 A133 H134 W135 L136 S137 I138 E139 G140 C141 Q142 P143 P149 P150 P151 ALA PRO LYS GLU GLN GLN LYS ALA GLU ALA THR GLU PRO LEU LYS SER ALA LYS PRO GLY GLN GLU GLU ASP GLY PRO LEU LYS GLY LYS GLY GLN GLY ALA THR THR ALA

ASP GLY LYS GLY LYS GLU LYS LYS ALA PRO PRO LEU LEU GLU GLU GLY ALA PRO LEU ARG LEU LYS PRO ARG SER ILE H214 E215 L216 S217 Y218 E219 Q220 Y223 E226 K238 R239 Y253 Q254 N255 L256 P257 R258 T261 V271 Y272 Q273 I280 M283 R284 Y296 L297

E298 K299 Y300 V301 H302 T310 L317 C318 L319 R320 P321 D322 V323 D324 N325 H326 W327 A328 L329 R330 T346 T347 T348 N349 N350 I351 Q352 S353 R354 I355 T356 K357 T358 F359 T360 K361 S362 W363 V364 D365 E366 K367 T368 T371 V387 I388 K389 T390 L391 P394 R395 L396 Q397 Q398

E399 G400 E401 R402 I403 R404 S405 V406 L407 D408 G409 P410 V411 L412 S413 N414 I415 D416 R417 I418 D421 L428 A432 R439 P440 P441 P442 D443 N444 Q445 D446 A447 Y448 R449 A450 E451 F452 G453 S454 L455 G456 P457 L458 L459 C460 S461 Q462 V463 V464 R467 A468 Q469 A470 A471 L472

Q473 ALA GLN GLN VAL ASN ARG THR THR LEU THR ILE THR GLN PRO ARG PRO THR LEU THR LEU SER GLN ALA PRO GLN PRO GLY PRO ARG THR PRO GLY LEU LEU LYS VAL PRO GLY SER ILE ALA LEU PRO VAL GLN THR LEU VAL SER ALA ARG ALA ALA ALA PRO PRO GLN PRO SER

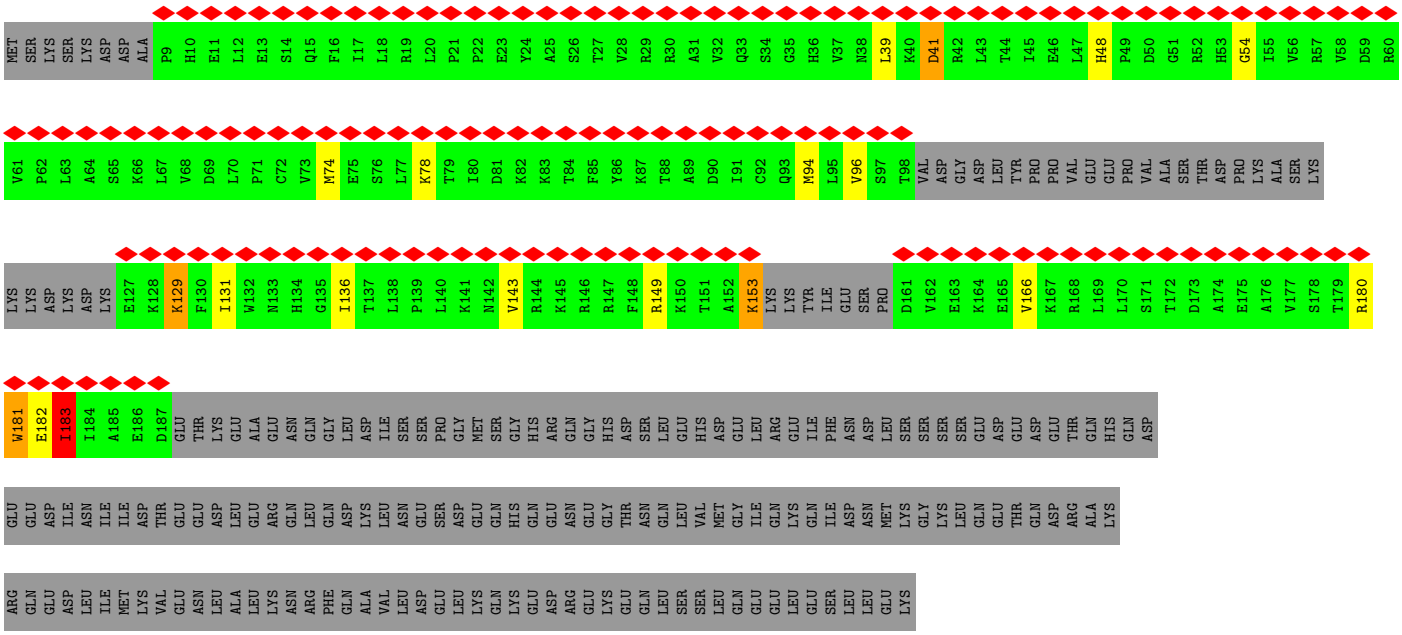
PRO PRO PRO THR LYS PHE ILE VAL MET SER SER SER SER ALA PRO SER THR GLN GLN VAL LEU SER SER LEU SER THR SER ALA PRO GLY SER GLY SER THR THR THR SER PRO VAL THR THR THR VAL PRO SER VAL GLN PRO ILE VAL LYS LEU VAL SER THR ALA THR THR ALA PRO

PRO SER THR ALA PRO SER GLY PRO GLY SER VAL GLN LYS TYR ILE VAL VAL SER LEU PRO PRO THR GLY GLU GLY LYS GLY GLY PRO THR SER HIS PRO SER PRO VAL PRO PRO PRO ALA SER SER PRO SER PRO LEU SER GLY SER ALA LEU CYS GLY GLY LYS GLN GLU ALA GLY ASP

SER PRO PRO PRO ALA PRO GLY THR PRO LYS ALA ASN GLY SER GLN PRO ASN SER GLY SER PRO GLN PRO ALA PRO

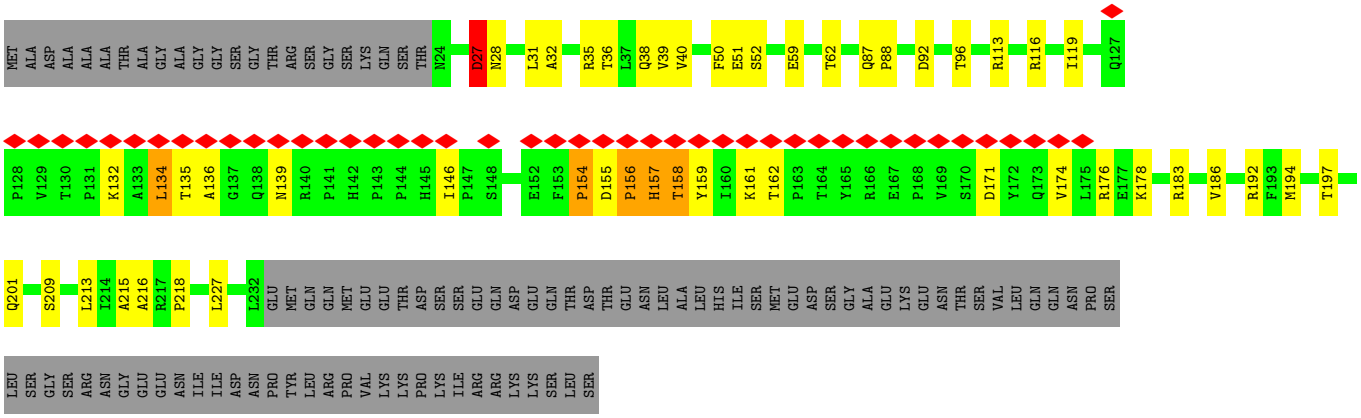
- Molecule 16: Transcription initiation factor TFIID subunit 7

Chain G: 41% 36% • • 59%



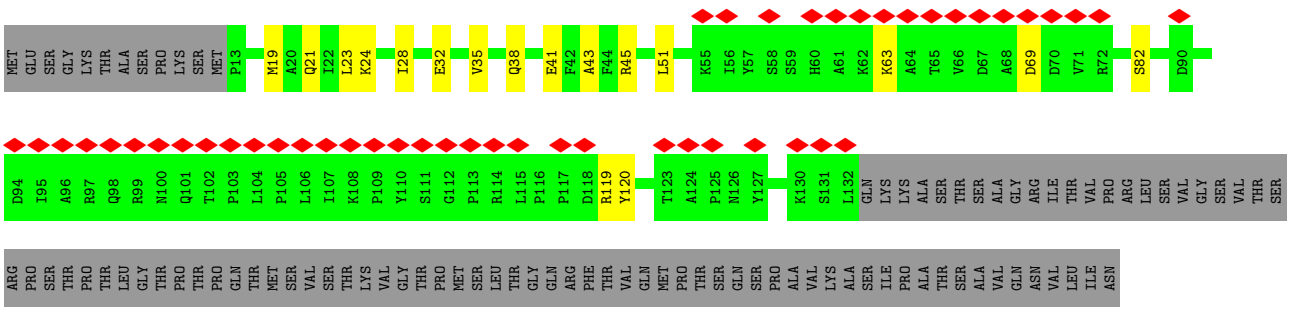
• Molecule 17: Transcription initiation factor TFIID subunit 8

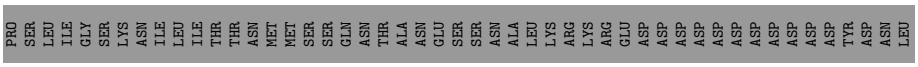
Chain H:



• Molecule 18: Transcription initiation factor TFIID subunit 9

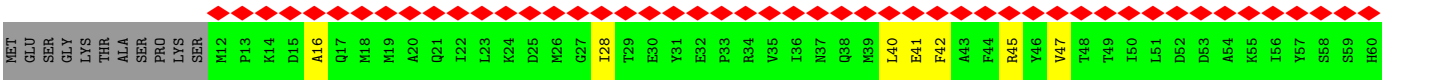
Chain I:

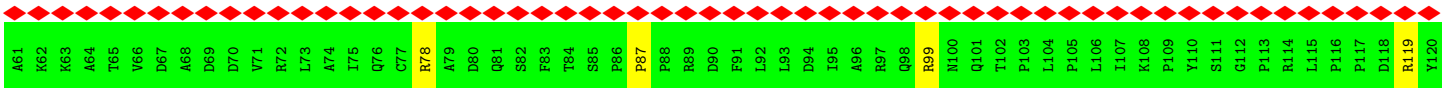


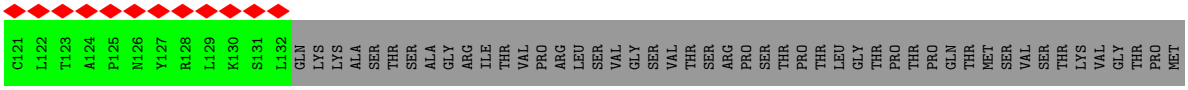


• Molecule 18: Transcription initiation factor TFIID subunit 9

Chain i:

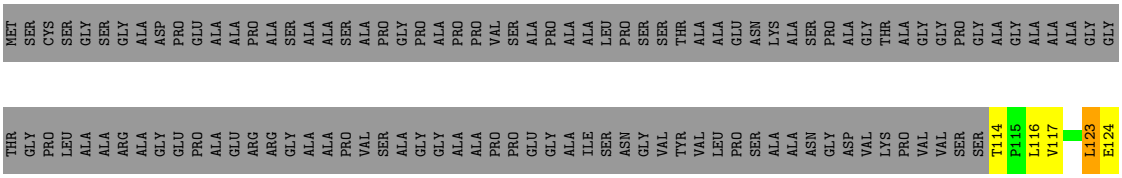


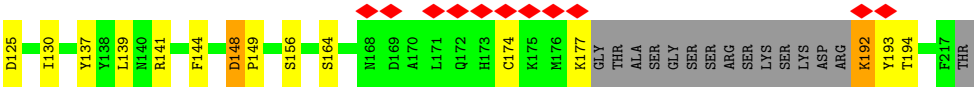




• Molecule 19: Transcription initiation factor TFIID subunit 10

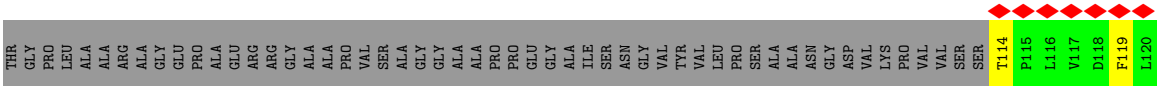
Chain J:

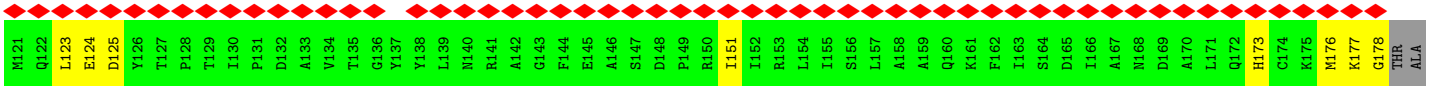


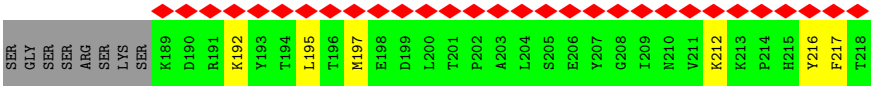


• Molecule 19: Transcription initiation factor TFIID subunit 10

Chain j:

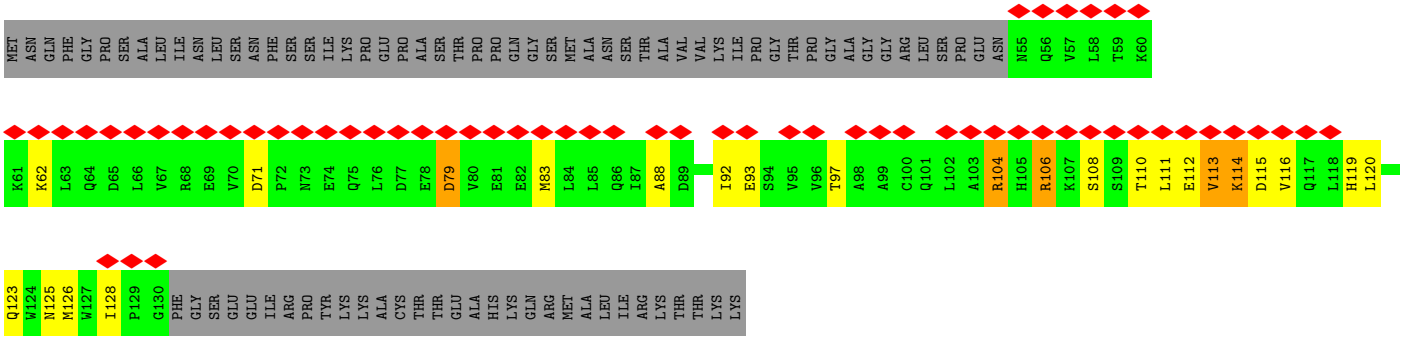






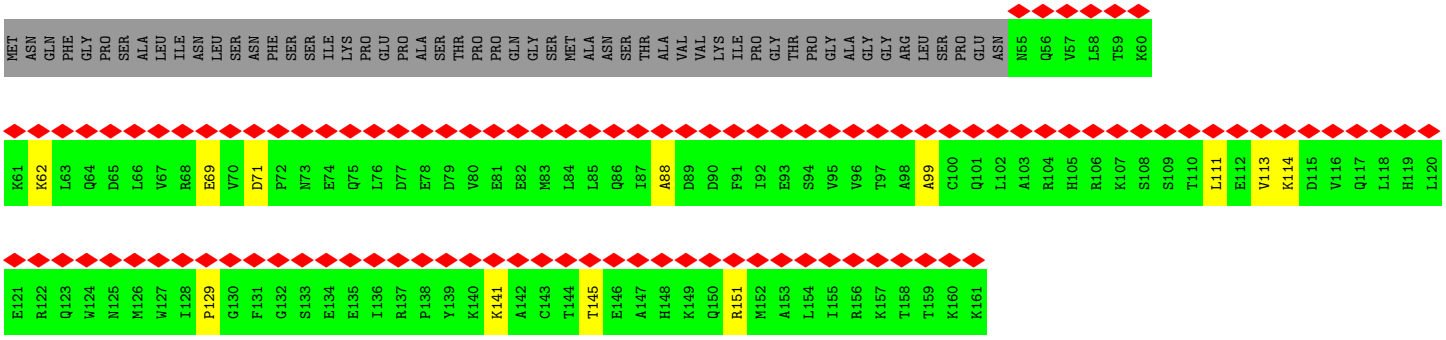
• Molecule 20: Transcription initiation factor TFIID subunit 12

Chain L:



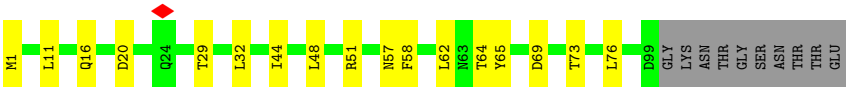
• Molecule 20: Transcription initiation factor TFIID subunit 12

Chain l:



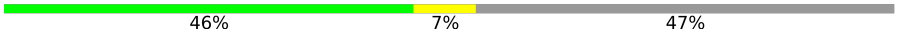
• Molecule 21: Transcription initiation factor IIA subunit 2

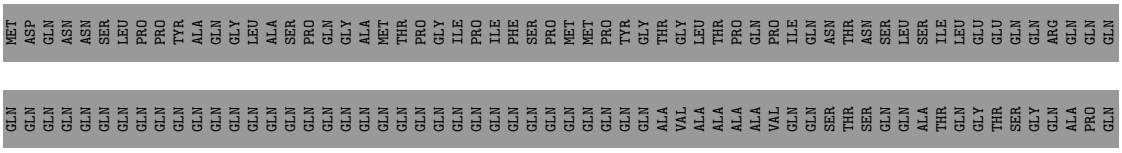
Chain O:

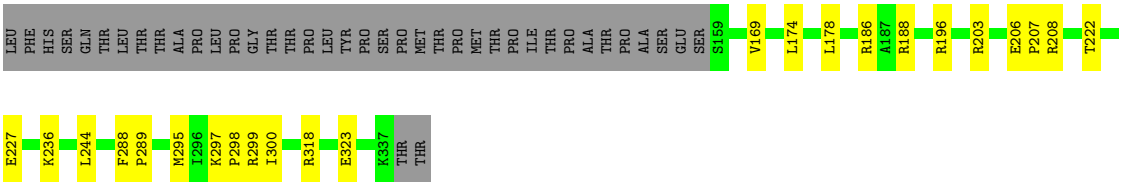


• Molecule 22: TATA-box-binding protein

Chain P:

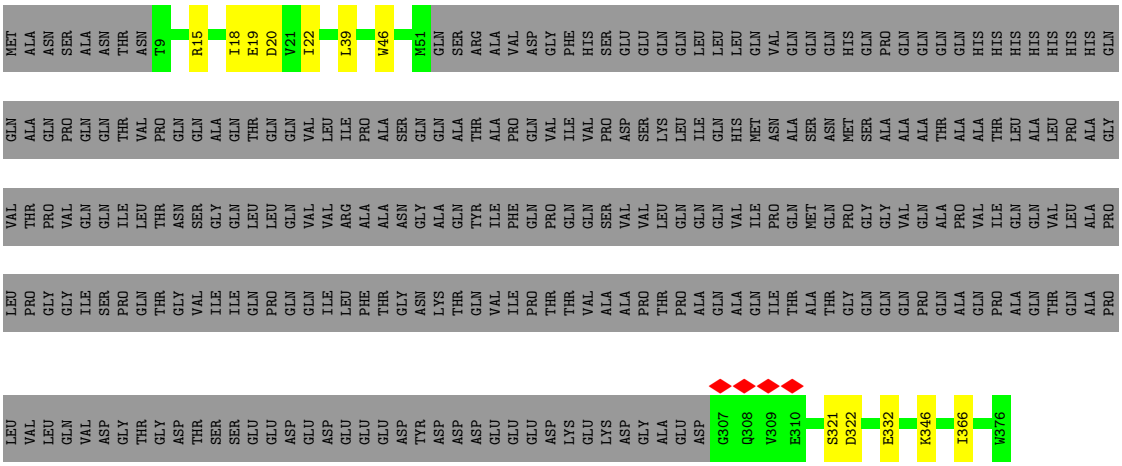






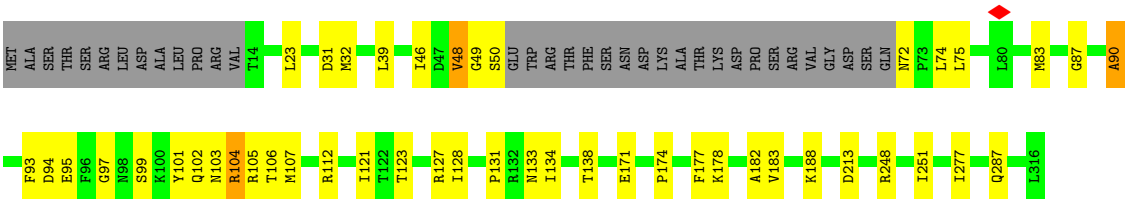
• Molecule 23: Transcription initiation factor IIA beta chain

Chain Q:



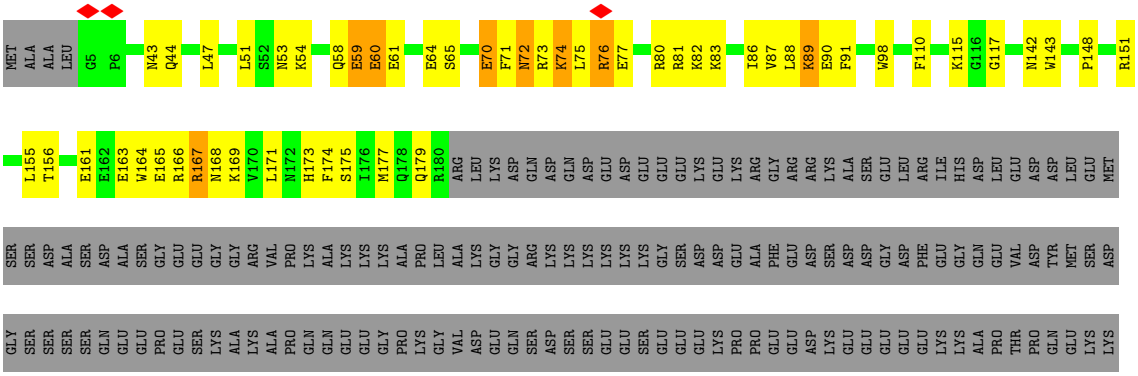
• Molecule 24: Transcription initiation factor IIB

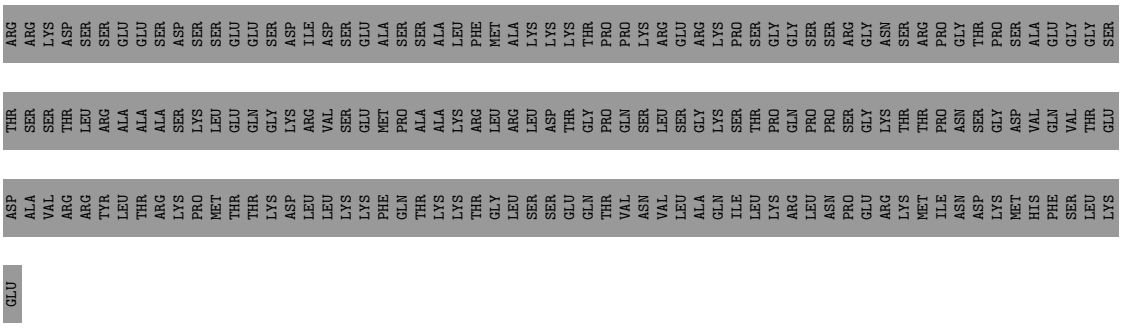
Chain R:



• Molecule 25: General transcription factor IIF subunit 1

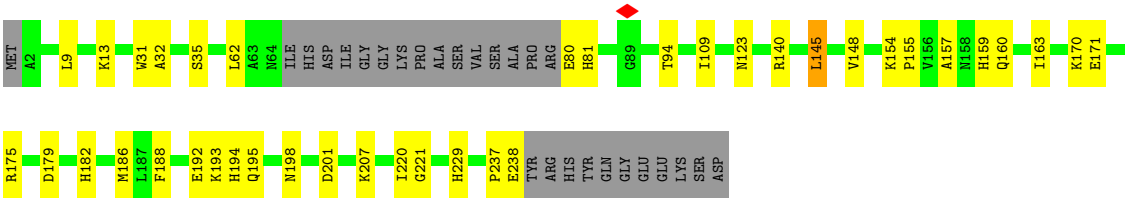
Chain S:





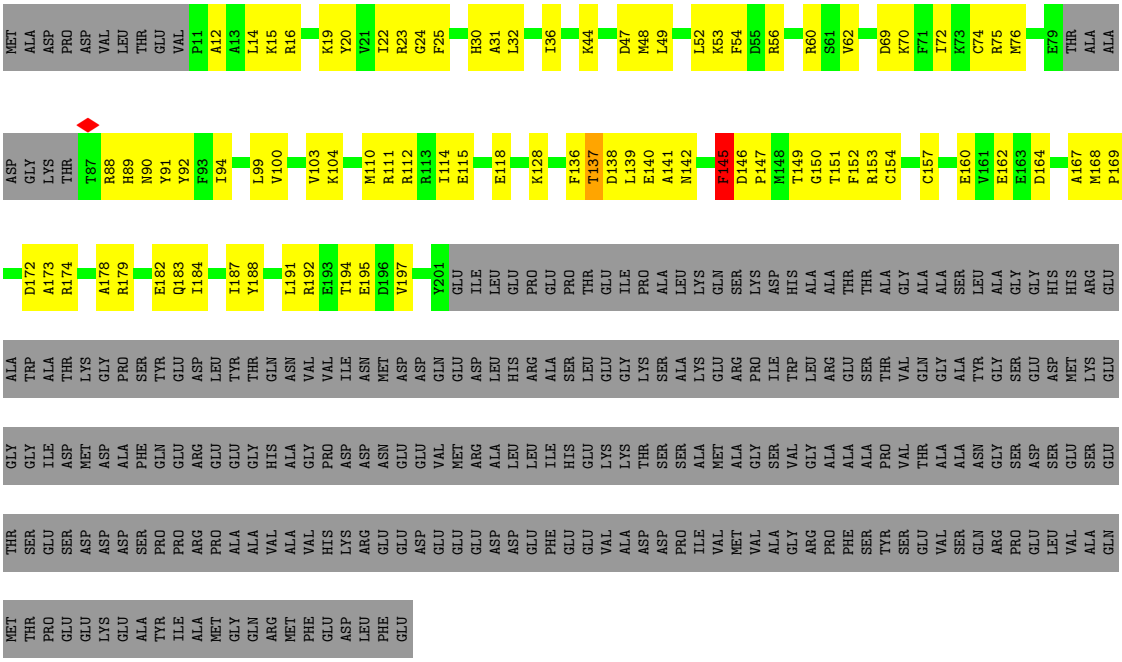
• Molecule 26: General transcription factor IIF subunit 2

Chain T:



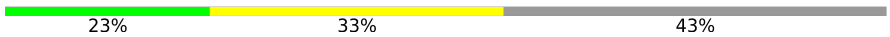
• Molecule 27: General transcription factor IIE subunit 1

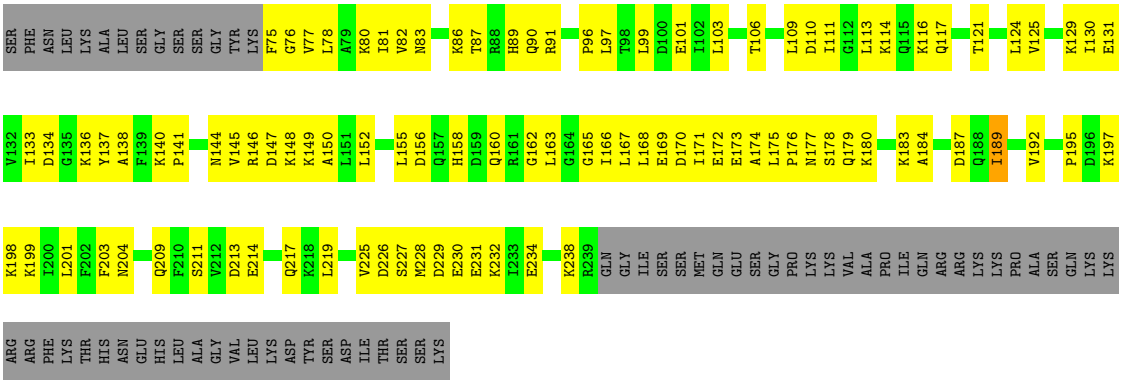
Chain U:



• Molecule 28: Transcription initiation factor IIE subunit beta

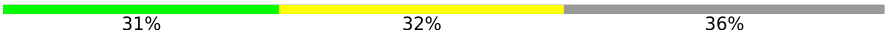
Chain V:

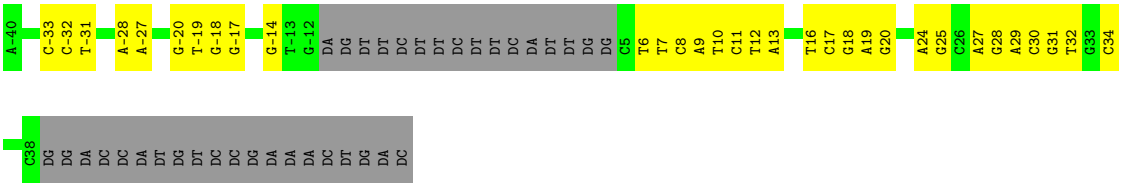




- Molecule 29: non-template DNA

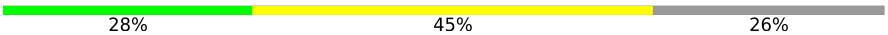
Chain X:

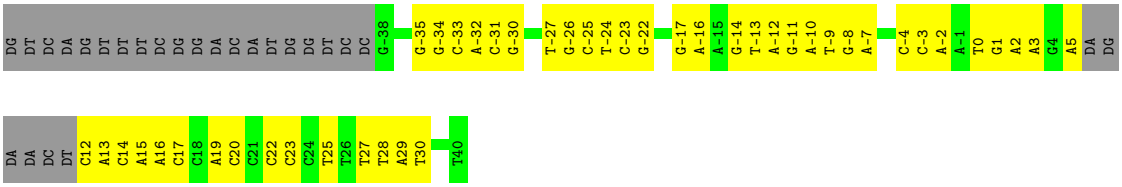




- Molecule 30: template DNA

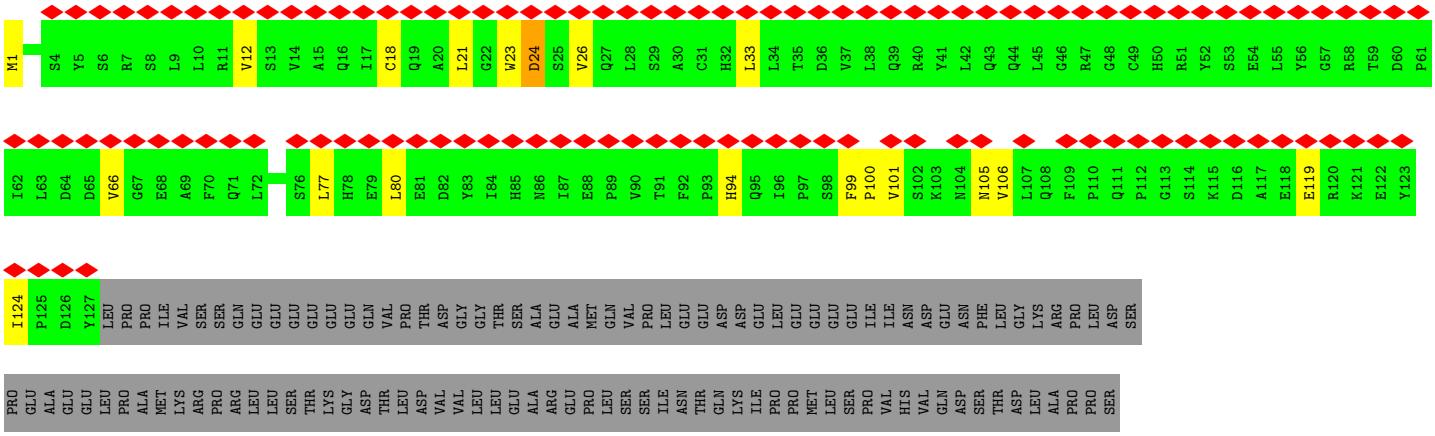
Chain Y:





- Molecule 31: Transcription initiation factor TFIID subunit 3

Chain c:



PRO GLU PRO PRO MET LEU ALA PRO VAL ALA LYS SER GLN MET PRO THR ALA LYS PRO LEU GLU THR LYS SER PHE THR PRO LYS THR LYS THR LYS THR SER SER PRO GLY GLN LYS THR LYS SER PRO LYS THR ALA GLN SER PRO ALA MET VAL GLY SER PRO ILE ARG SER PRO LYS

THR VAL SER LYS GLU LYS LYS SER PRO GLY ARG SER LYS SER PRO LYS SER PRO LYS VAL THR THR HIS ILE PRO GLN THR PRO VAL ARG PRO GLU THR PRO ASN ARG THR PRO SER ALA THR LEU SER GLU LYS ILE SER LYS GLU THR ILE GLN VAL LYS GLN ILE GLN

THR PRO PRO ASP ALA GLY LYS LEU ASN SER GLN GLU ASN GLN PRO LYS LYS ALA VAL VAL ALA ASP LYS THR ILE GLU ALA SER ILE ASP ALA VAL ILE ALA ARG PRO GLU ALA CYS ALA GLU ARG GLU PRO ASP PRO PHE GLU PHE SER SER GLY SER GLU SER GLY GLY ASP ILE PHE THR SER PRO

LYS ARG ILE SER GLY PRO GLU CYS THR THR PRO LYS ALA SER THR SER ALA ASN ASN PHE THR LYS SER GLY SER THR PRO LEU PRO LEU SER LYS THR LYS SER SER SER ASN SER TRP THR MET ASP ALA SER ILE ASP GLU VAL VAL ARG LYS ALA LYS LEU GLY THR SER PRO

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LEU LYS ASP GLY LEU VAL ARG LYS GLU LYS GLU LYS HIS LYS ASP LYS LYS LYS LYS ARG GLU LYS GLY LYS LYS ASP LYS ASP LYS LYS ARG GLU LYS LYS ASP LYS GLY ARG GLU ASP LYS MET LYS ALA PRO ALA PRO PRO LEU VAL LEU PRO PRO LYS GLU LEU ALA LEU

PRO LEU PHE SER PRO ALA THR ALA SER ARG VAL PRO ALA MET LEU PRO SER LEU LEU PRO VAL LEU PRO GLU LYS LEU PHE GLU GLU LYS GLU LYS VAL LYS GLU LYS GLU LYS LYS LYS ASP LYS LYS GLU LYS LYS LYS LYS LYS GLU GLU GLU LYS GLU LYS GLU GLU ARG

GLU LYS GLU LYS ARG GLU ARG GLU LYS ARG ARG GLU LYS GLU LYS HIS LYS HIS GLU LYS ILE LYS VAL GLU PRO VAL ALA LEU ALA PRO SER PRO VAL ILE PRO ARG LEU THR LEU ARG VAL GLY ALA GLY GLN ASP LYS ILE VAL ILE SER LYS VAL VAL PRO ALA PRO GLU ALA

LYS PRO ALA PRO SER GLN ASN ARG PRO LYS THR PRO PRO PRO ALA PRO ALA PRO ALA PRO GLY PRO MET LEU VAL SER PRO ALA PRO VAL PRO LEU PRO LEU LEU ALA GLN ALA ALA ALA GLY PRO ALA LEU LEU PRO SER PRO GLY PRO ALA ALA SER GLY ALA SER ALA LYS ALA PRO

VAL ARG SER VAL VAL THR GLU THR VAL SER THR TYR VAL ILE ARG ASP GLU TRP GLY ASN GLN ILE TRP ILE CYS PRO GLY CYS ASN LYS PRO ASP ASP GLY SER PRO MET ILE GLY CYS ASP ASP CYS ASP ASP TRP TRP HIS TRP PRO CYS VAL GLY ILE MET THR ALA PRO PRO GLU

GLU MET GLN TRP PHE CYS PRO LYS CYS ALA ASN LYS LYS LYS ASP LYS LYS HIS LYS LYS ARG LYS HIS ARG ALA HIS

- Molecule 32: Transcription initiation factor TFIID subunit 11

Chain k:

MET ASP ASP ALA HIS GLU SER PRO SER ASP LYS GLY GLY GLU THR GLY GLU SER ASP GLU THR ALA VAL PRO GLY ASP PRO GLY ALA THR ASP THR ASP GLY ILE PRO GLU GLU THR ASP GLY ASP ALA ASP VAL ASP LEU LYS GLU ALA ALA ALA GLU GLU GLY GLU LEU GLU SER

GLN ASP VAL SER ASP LEU THR THR VAL GLU ARG GLU ASP SER SER LEU LEU ASN PRO ALA ALA LYS LYS LEU LYS ILE ASP THR LYS GLU LYS LYS GLU LYS LYS GLN LYS VAL ASP GLU ASP GLU ILE GLN LYS MET GLN ILE LEU VAL SER SER PHE S114 E115 E116 Q117 L118 N119 R120

Y121 E122 M123 Y124 R125 R126 S127 A128 F129 P130 K131 A132 A133 I134 K135 R136 L137 I138 Q139 S140 I141 T142 G143 T144 S145 V146 S147 Q148 N149 V150 V151 I152 A153 M154 S155 G156 I157 S158 K159 V160 F161 V162 G163 E164 V165 V166 E167 E168 A169 L170 D171 V172 C173 E174 K175 W176 G177 E178 M179 P180

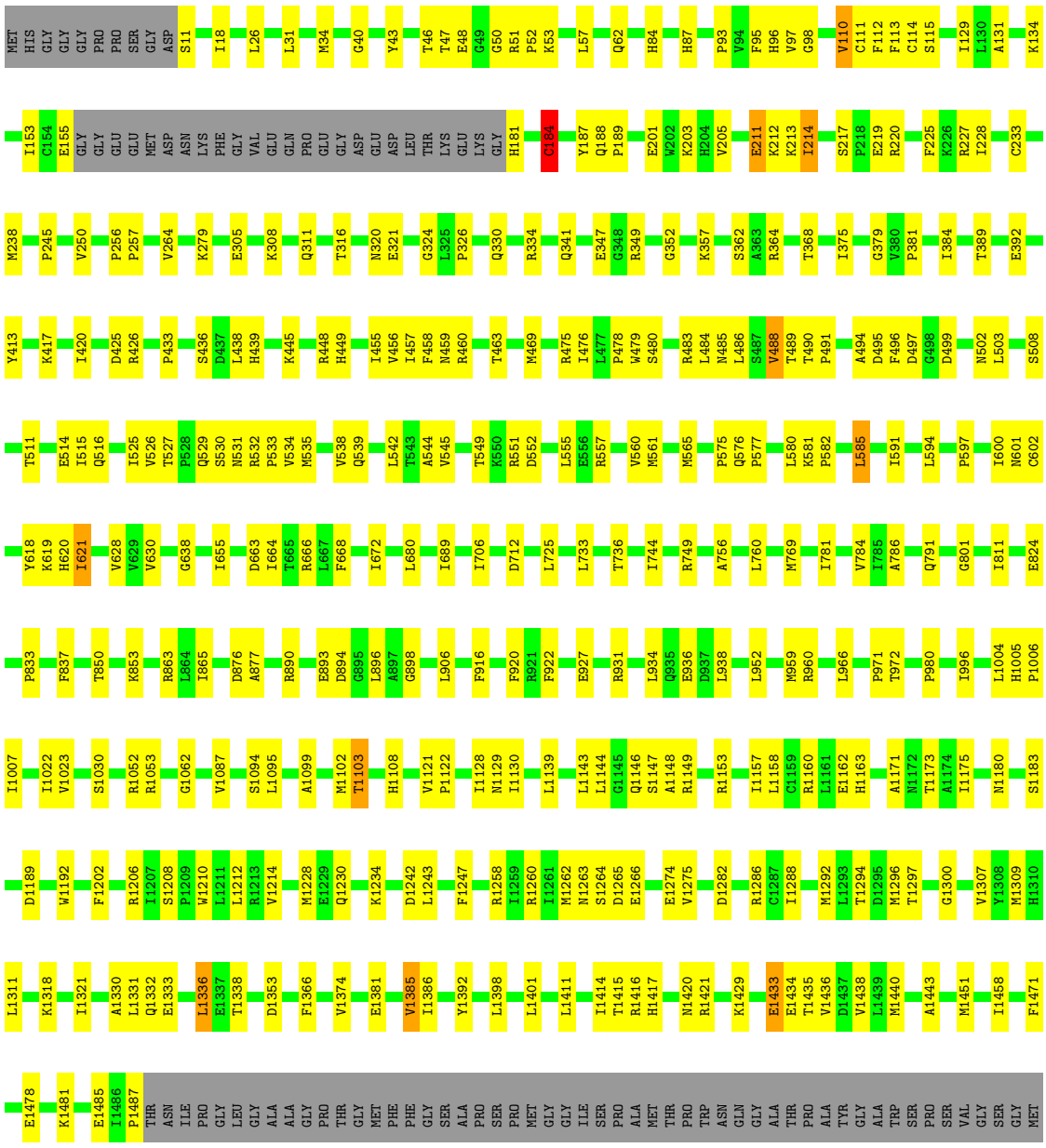
P181 L182 Q183 P184 K185 H186 M187 R188 E189 A190 V191 R192 R193 L194 K195 S196 K197 G198 Q199 I200 P201 N202 S203 K204 H205 K206 K207 I208 I209 F210 F211

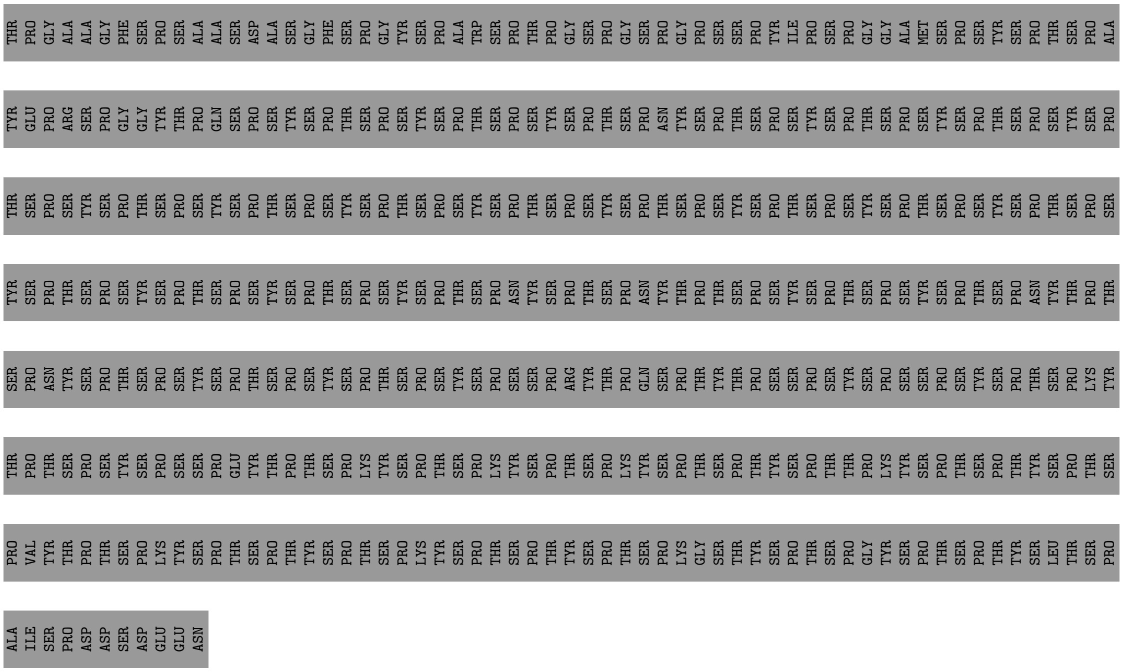
- Molecule 33: Transcription initiation factor TFIID subunit 13

Chain m:

- Molecule 34: DNA-directed RNA polymerase subunit

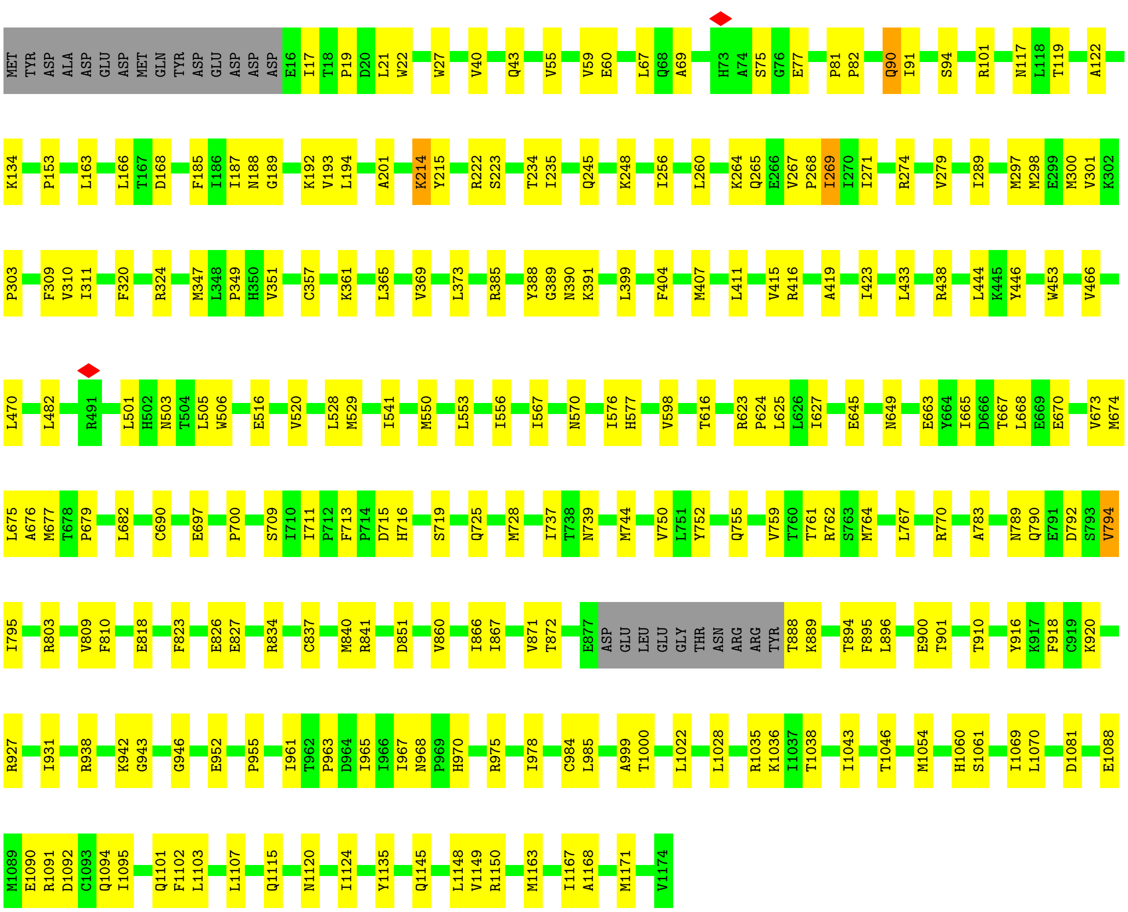
Chain o: 56% 17% • 26%





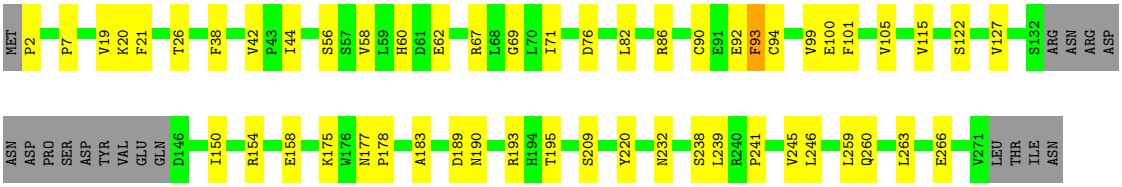
- Molecule 35: DNA-directed RNA polymerase subunit beta

Chain p:



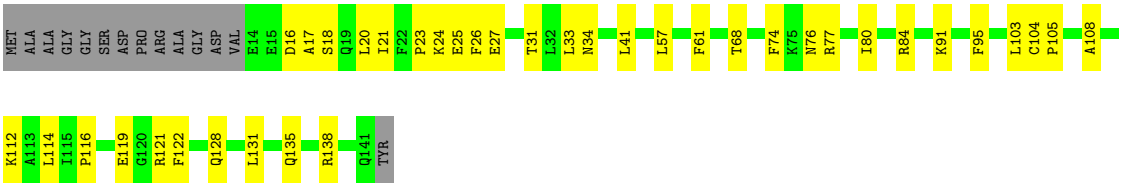
- Molecule 36: DNA-directed RNA polymerase II subunit RPB3

Chain q:



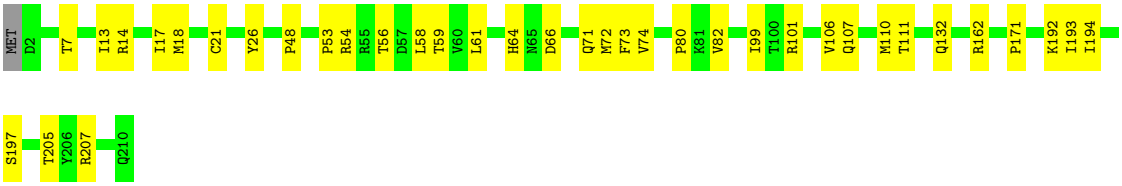
- Molecule 37: DNA-directed RNA polymerase II subunit RPB4

Chain r:



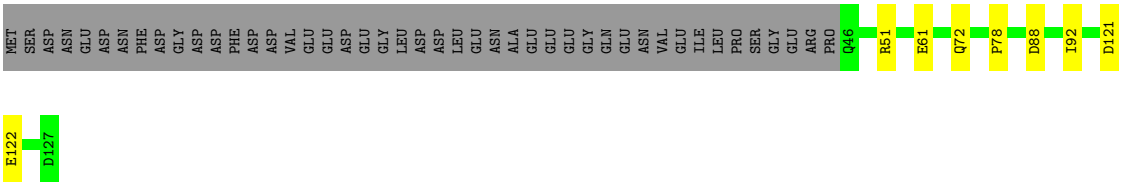
- Molecule 38: DNA-directed RNA polymerase II subunit E

Chain s:



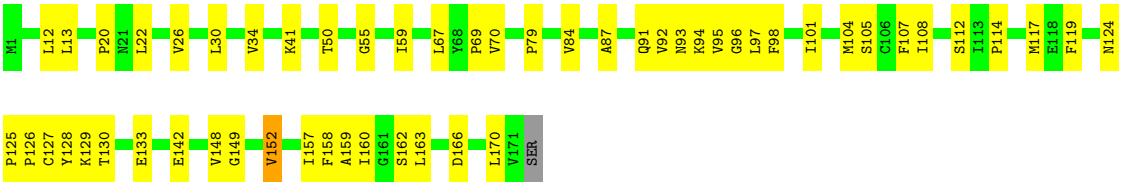
- Molecule 39: DNA-directed RNA polymerase II subunit F

Chain t:



- Molecule 40: DNA-directed RNA polymerase II subunit RPB7

Chain u:

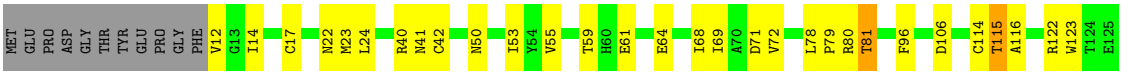


• Molecule 41: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain v:

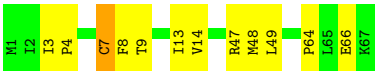
• Molecule 42: DNA-directed RNA polymerase II subunit RPB9

Chain w:



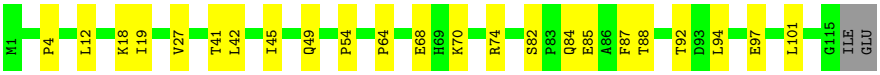
• Molecule 43: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain x:



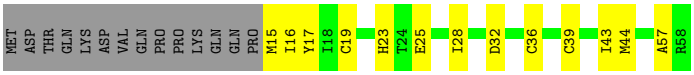
• Molecule 44: DNA-directed RNA polymerase II subunit RPB11-a

Chain y:



• Molecule 45: RPB12

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5141	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.238	Depositor
Minimum map value	-1.677	Depositor
Average map value	0.037	Depositor
Map value standard deviation	0.178	Depositor
Recommended contour level	0.42	Depositor
Map size (Å)	426.88, 426.88, 426.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.334, 1.334, 1.334	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: MG, SF4, G2L, ZN, TRX, HYP, ATP, CSX, ILX, W0F

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	0	0.41	0/1437	0.71	3/1926 (0.2%)
2	1	0.20	0/2210	0.34	0/2975
3	2	0.18	0/2624	0.33	1/3555 (0.0%)
4	3	0.24	0/2103	0.36	0/2846
5	4	0.31	0/3262	0.45	1/4418 (0.0%)
6	5	0.40	0/433	0.79	1/585 (0.2%)
7	6	0.19	0/4994	0.33	0/6745
8	7	0.17	0/5875	0.30	0/7955
9	N	0.41	0/22	0.98	0/26
10	Z	0.35	0/43	0.52	0/64
11	A	0.63	0/4698	0.95	5/6345 (0.1%)
12	B	0.46	1/7993 (0.0%)	0.69	6/10836 (0.1%)
13	D	0.55	0/1379	0.88	3/1843 (0.2%)
13	d	0.47	0/1321	0.71	0/1772
14	E	0.45	1/4482 (0.0%)	0.72	4/6069 (0.1%)
14	e	0.55	1/4433 (0.0%)	0.77	0/6004
15	F	0.63	1/3201 (0.0%)	1.00	7/4347 (0.2%)
15	f	0.47	0/3140	0.80	6/4268 (0.1%)
16	G	0.68	0/1190	0.95	1/1601 (0.1%)
17	H	0.63	3/1673 (0.2%)	0.86	5/2285 (0.2%)
18	I	0.20	0/981	0.41	0/1332
18	i	0.22	0/989	0.40	0/1343
19	J	0.83	0/736	1.15	2/998 (0.2%)
19	j	0.74	0/775	0.96	0/1049
20	L	0.69	0/630	1.14	1/852 (0.1%)
20	l	0.59	0/888	0.88	0/1194
21	O	0.26	0/816	0.36	0/1105
22	P	0.12	0/1448	0.24	0/1948
23	Q	0.19	0/945	0.35	0/1274
24	R	0.19	0/2199	0.38	0/2967
25	S	0.15	0/1496	0.38	0/2013
26	T	0.14	0/1817	0.28	0/2445

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
27	U	0.35	0/1545	0.69	1/2075 (0.0%)
28	V	0.24	0/1380	0.58	0/1854
29	X	0.28	0/1457	0.58	0/2246
30	Y	0.30	0/1671	0.53	0/2572
31	c	0.48	0/1035	0.67	0/1406
32	k	0.28	0/799	0.53	1/1070 (0.1%)
33	m	0.85	0/733	1.18	1/977 (0.1%)
34	o	0.27	0/11723	0.38	0/15830
35	p	0.28	0/9358	0.35	0/12633
36	q	0.30	0/2102	0.37	0/2857
37	r	0.11	0/1064	0.22	0/1428
38	s	0.23	0/1751	0.32	0/2366
39	t	0.26	0/667	0.30	0/901
40	u	0.16	0/1382	0.30	0/1874
41	v	0.25	0/1207	0.32	0/1628
42	w	0.19	0/948	0.30	0/1284
43	x	0.30	0/542	0.35	0/730
44	y	0.29	0/939	0.35	0/1271
45	z	0.22	0/377	0.34	0/500
All	All	0.38	7/110913 (0.0%)	0.59	49/150487 (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
24	R	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	28	ASN	C-O	-7.51	1.15	1.24
17	H	27	ASP	C-O	-7.07	1.15	1.24
17	H	31	LEU	C-O	-6.26	1.16	1.24
12	B	61	ASN	C-O	-6.20	1.18	1.24
14	E	524	LEU	C-O	5.77	1.30	1.24
14	e	445	LYS	C-O	5.63	1.30	1.24
15	F	395	ARG	C-O	5.62	1.31	1.24

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	55	LYS	CB-CA-C	-11.45	95.01	111.85
12	B	491	HIS	N-CA-C	-9.43	101.00	111.28
15	f	149	PRO	O-C-N	9.01	125.45	121.31
14	E	756	THR	N-CA-C	-8.38	103.19	113.50
17	H	32	ALA	N-CA-C	-8.26	102.23	111.07
17	H	27	ASP	N-CA-C	-7.98	102.66	111.36
14	E	762	PRO	N-CA-C	7.38	124.24	114.27
15	F	271	VAL	N-CA-C	-7.36	105.83	112.90
11	A	715	PRO	N-CA-C	-7.09	100.11	111.03
12	B	495	GLN	N-CA-C	-7.06	104.66	113.28
6	5	38	ILE	N-CA-CB	-6.94	102.44	110.55
32	k	180	PRO	N-CA-C	6.79	118.99	110.70
1	0	8	ARG	N-CA-CB	-6.74	99.10	110.49
11	A	396	LEU	N-CA-C	-6.73	104.81	113.16
15	f	326	HIS	N-CA-C	-6.67	104.25	112.38
15	f	319	LEU	N-CA-C	-6.59	103.92	112.68
11	A	467	ILE	N-CA-C	-6.43	103.99	111.00
3	2	70	THR	N-CA-C	-6.33	104.48	111.82
13	D	999	MET	N-CA-C	-6.26	104.37	111.07
11	A	1205	PHE	CA-CB-CG	-6.23	107.57	113.80
5	4	439	ARG	CB-CA-C	6.21	122.77	110.42
13	D	964	GLU	N-CA-C	-6.18	97.64	110.80
17	H	27	ASP	CA-C-O	-6.08	113.98	120.42
19	J	148	ASP	CA-C-N	6.06	125.78	119.05
19	J	148	ASP	C-N-CA	6.06	125.78	119.05
15	f	255	MET	N-CA-C	-5.89	104.95	114.09
12	B	181	GLY	CA-C-O	-5.76	118.16	122.37
15	F	316	GLN	CB-CA-C	5.75	120.17	110.79
27	U	145	PHE	CA-CB-CG	5.74	119.54	113.80
12	B	583	GLU	CB-CA-C	-5.73	101.29	110.79
15	F	310	THR	CB-CA-C	5.72	120.29	110.79
1	0	8	ARG	CB-CG-CD	-5.69	98.21	111.30
15	F	330	ARG	N-CA-C	-5.68	105.08	111.28
15	f	150	PRO	N-CA-C	5.59	117.52	110.70
15	F	324	ASP	N-CA-C	-5.58	105.29	111.71
13	D	1002	ARG	CB-CA-C	5.57	122.06	110.32
12	B	264	GLU	N-CA-C	-5.54	106.19	113.17
33	m	71	LYS	CB-CA-C	5.44	119.81	110.79
14	E	270	ASP	CB-CA-C	5.41	119.12	110.09
16	G	183	ILE	N-CA-C	-5.40	102.56	109.30
15	f	329	LEU	N-CA-C	-5.37	106.43	112.87
15	F	272	VAL	N-CA-C	-5.35	105.17	110.62
12	B	491	HIS	CB-CA-C	5.29	119.57	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	L	106	ARG	N-CA-C	-5.25	106.90	113.15
17	H	134	LEU	CB-CA-C	-5.16	110.60	116.54
11	A	1067	GLN	CB-CA-C	5.15	119.33	110.79
15	F	438	LEU	N-CA-C	5.05	118.53	111.30
17	H	51	GLU	CB-CA-C	-5.03	100.50	109.71
14	E	770	LEU	N-CA-C	-5.00	105.50	112.45

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	R	106	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1420	0	1420	124	0
2	1	2167	0	2175	39	0
3	2	2567	0	2539	95	0
4	3	2066	0	2097	103	0
5	4	3189	0	3243	140	0
6	5	428	0	434	43	0
7	6	4890	0	4949	94	0
8	7	5751	0	5794	146	0
9	N	64	0	51	9	0
10	Z	95	0	40	4	0
11	A	4580	0	4502	100	0
12	B	7796	0	7751	116	0
13	D	1366	0	1390	75	0
13	d	1307	0	1318	14	0
14	E	4376	0	4256	74	0
14	e	4327	0	4197	60	0
15	F	3143	0	3093	101	0
15	f	3081	0	3012	71	0
16	G	1171	0	1222	16	0
17	H	1633	0	1621	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	I	959	0	969	13	0
18	i	967	0	977	10	0
19	J	720	0	719	13	0
19	j	759	0	759	14	0
20	L	622	0	620	19	0
20	l	876	0	893	10	0
21	O	806	0	818	18	0
22	P	1422	0	1514	18	0
23	Q	930	0	888	12	0
24	R	2167	0	2193	35	0
25	S	1461	0	1429	44	0
26	T	1788	0	1819	54	0
27	U	1520	0	1520	212	0
28	V	1357	0	1381	89	0
29	X	1299	0	709	40	0
30	Y	1491	0	819	47	0
31	c	1011	0	975	18	0
32	k	785	0	818	8	0
33	m	724	0	744	23	0
34	o	11510	0	11615	243	0
35	p	9175	0	9196	178	0
36	q	2059	0	2007	39	0
37	r	1050	0	1033	23	0
38	s	1720	0	1737	21	0
39	t	657	0	684	6	0
40	u	1351	0	1358	132	0
41	v	1186	0	1147	15	0
42	w	927	0	860	28	0
43	x	533	0	553	10	0
44	y	920	0	942	18	0
45	z	372	0	378	10	0
46	0	2	0	0	0	0
46	2	3	0	0	0	0
46	3	2	0	0	0	0
46	R	1	0	0	0	0
46	U	1	0	0	0	0
46	o	2	0	0	0	0
46	p	1	0	0	0	0
46	q	1	0	0	0	0
46	w	2	0	0	0	0
46	x	1	0	0	0	0
46	z	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	7	8	0	0	0	0
48	o	1	0	0	0	0
49	p	33	0	0	9	0
All	All	108600	0	107178	2295	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 11.

All (2295) 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)
27:U:152:PHE:CE1	40:u:95:VAL:HB	1.24	1.66
27:U:139:LEU:HB2	40:u:160:ILE:CG1	1.22	1.59
1:0:41:ARG:CG	27:U:169:PRO:HG2	1.34	1.54
27:U:139:LEU:CB	40:u:160:ILE:HG12	1.42	1.49
6:5:33:PHE:CE1	6:5:49:LEU:HD12	1.44	1.49
27:U:139:LEU:CA	40:u:160:ILE:HG12	1.47	1.43
3:2:174:LEU:HD11	3:2:203:ALA:CB	1.51	1.39
4:3:50:PHE:CZ	5:4:118:LEU:HD11	1.57	1.39
6:5:31:LYS:HB3	12:B:540:LYS:NZ	1.31	1.39
1:0:41:ARG:HG3	27:U:169:PRO:CG	1.56	1.36
27:U:141:ALA:CB	40:u:107:PHE:CD1	2.07	1.36
4:3:237:GLN:NE2	5:4:51:LEU:HD22	1.39	1.35
27:U:139:LEU:CB	40:u:160:ILE:CG1	1.96	1.32
13:D:960:GLU:CG	13:D:983:ARG:HG2	1.59	1.30
27:U:139:LEU:HB2	40:u:160:ILE:CD1	1.64	1.28
1:0:85:ARG:HH22	1:0:139:LYS:C	1.40	1.28
27:U:142:ASN:ND2	40:u:105:SER:HB2	1.46	1.27
4:3:237:GLN:CD	5:4:51:LEU:CD2	2.08	1.27
27:U:138:ASP:OD1	40:u:160:ILE:HD13	1.16	1.27
6:5:31:LYS:CB	12:B:540:LYS:HZ3	1.47	1.26
1:0:85:ARG:NH1	1:0:140:LEU:HG	1.51	1.25
27:U:152:PHE:CE1	40:u:95:VAL:CB	2.20	1.23
1:0:42:GLY:N	27:U:168:MET:HE1	1.54	1.22
6:5:31:LYS:CB	12:B:540:LYS:NZ	2.01	1.22
7:6:528:LYS:CG	7:6:531:ILE:CD1	2.17	1.21
3:2:175:THR:HG23	8:7:592:ARG:CD	1.72	1.20
7:6:528:LYS:HG2	7:6:531:ILE:HD13	1.21	1.19
27:U:139:LEU:CD2	40:u:158:PHE:HD1	1.53	1.19
4:3:50:PHE:CZ	5:4:118:LEU:CD1	2.25	1.18
27:U:138:ASP:CG	40:u:160:ILE:HG21	1.69	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:21:LEU:HD22	1:0:69:ASP:OD2	1.43	1.15
3:2:174:LEU:CD1	3:2:203:ALA:CB	2.24	1.15
3:2:174:LEU:CD1	3:2:203:ALA:HB2	1.75	1.14
4:3:237:GLN:NE2	5:4:51:LEU:CD2	2.11	1.14
13:D:960:GLU:CG	13:D:983:ARG:CG	2.25	1.14
1:0:85:ARG:HH22	1:0:140:LEU:N	1.46	1.13
7:6:528:LYS:HG2	7:6:531:ILE:CD1	1.76	1.13
4:3:50:PHE:HZ	5:4:118:LEU:CD1	1.58	1.13
13:D:960:GLU:HG3	13:D:983:ARG:HG2	1.29	1.12
4:3:229:TRP:CZ3	5:4:58:ARG:NH1	2.18	1.12
27:U:152:PHE:CD1	40:u:95:VAL:HB	1.84	1.12
3:2:175:THR:HG23	8:7:592:ARG:HD2	1.17	1.12
1:0:85:ARG:NH2	1:0:139:LYS:C	2.07	1.11
3:2:175:THR:CG2	8:7:592:ARG:HD2	1.81	1.11
4:3:237:GLN:CD	5:4:51:LEU:HD22	1.70	1.10
6:5:33:PHE:CE1	6:5:49:LEU:CD1	2.34	1.10
27:U:141:ALA:CB	40:u:107:PHE:CE1	2.34	1.09
27:U:152:PHE:CZ	40:u:95:VAL:HB	1.86	1.09
11:A:1200:THR:O	11:A:1204:GLU:HG2	1.52	1.09
27:U:141:ALA:CB	40:u:107:PHE:CG	2.36	1.09
27:U:139:LEU:HD21	40:u:158:PHE:C	1.76	1.09
1:0:37:LEU:HD11	27:U:173:ALA:HA	1.34	1.09
4:3:237:GLN:CD	5:4:51:LEU:HD23	1.75	1.07
1:0:83:ASN:OD1	1:0:140:LEU:HD11	1.54	1.07
27:U:138:ASP:O	40:u:107:PHE:CD2	2.07	1.07
27:U:139:LEU:HD12	40:u:160:ILE:HG13	1.36	1.07
13:D:960:GLU:HG2	13:D:983:ARG:HG2	1.29	1.06
27:U:141:ALA:HB3	40:u:107:PHE:CD1	1.89	1.06
1:0:5:GLY:HA3	1:0:10:LYS:HB2	1.37	1.06
27:U:139:LEU:HB2	40:u:160:ILE:HG13	1.31	1.04
27:U:139:LEU:HA	40:u:160:ILE:HG12	1.38	1.04
1:0:84:LYS:HA	1:0:136:ASN:ND2	1.73	1.04
27:U:139:LEU:HD11	40:u:159:ALA:HA	1.39	1.04
3:2:174:LEU:HD21	3:2:203:ALA:HB1	1.36	1.04
13:D:1006:LEU:HD13	21:O:69:ASP:OD2	1.56	1.03
6:5:33:PHE:HE1	6:5:49:LEU:CD1	1.66	1.03
3:2:175:THR:CG2	8:7:592:ARG:NE	2.21	1.02
3:2:175:THR:CG2	8:7:592:ARG:CD	2.35	1.02
27:U:139:LEU:CD2	40:u:158:PHE:CD1	2.43	1.02
27:U:141:ALA:HB1	40:u:107:PHE:CE1	1.95	1.01
11:A:339:ALA:HB3	11:A:355:VAL:HG21	1.42	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:238:GLU:HB3	28:V:130:ILE:HG12	1.42	1.00
27:U:141:ALA:HB3	40:u:107:PHE:CG	1.96	0.99
19:J:192:LYS:N	19:J:192:LYS:HE3	1.77	0.99
7:6:528:LYS:HG3	7:6:531:ILE:CD1	1.92	0.98
1:0:10:LYS:NZ	27:U:178:ALA:HB1	1.77	0.98
11:A:725:CYS:SG	11:A:725:CYS:O	2.22	0.98
1:0:37:LEU:HD13	27:U:173:ALA:HB2	1.45	0.98
3:2:174:LEU:CD2	3:2:203:ALA:HB1	1.93	0.97
1:0:8:ARG:CZ	27:U:173:ALA:HB2	1.94	0.97
27:U:145:PHE:CD1	27:U:149:THR:OG1	2.17	0.97
10:Z:4:G2L:N1	30:Y:-3:DC:N3	2.12	0.97
27:U:138:ASP:OD1	40:u:160:ILE:CD1	2.12	0.97
13:D:960:GLU:HG2	13:D:983:ARG:CG	1.92	0.96
3:2:174:LEU:HD21	3:2:203:ALA:CB	1.95	0.95
27:U:139:LEU:CD1	40:u:160:ILE:HG13	1.95	0.95
1:0:41:ARG:CG	27:U:169:PRO:CG	2.27	0.95
11:A:467:ILE:H	15:F:221:GLN:NE2	1.64	0.95
3:2:175:THR:HG23	8:7:592:ARG:NE	1.82	0.94
3:2:174:LEU:CG	3:2:203:ALA:CB	2.44	0.94
27:U:139:LEU:HB2	40:u:160:ILE:HD11	1.50	0.94
27:U:142:ASN:HD22	40:u:105:SER:HB2	1.13	0.94
1:0:37:LEU:HD13	27:U:173:ALA:CB	1.97	0.93
8:7:726:GLN:HG3	8:7:727:PRO:HD2	1.51	0.93
27:U:139:LEU:HG	40:u:159:ALA:C	1.92	0.93
1:0:41:ARG:CD	27:U:169:PRO:HG2	1.99	0.93
27:U:139:LEU:HD21	40:u:158:PHE:O	1.69	0.93
27:U:141:ALA:HB2	40:u:107:PHE:CD2	2.03	0.93
27:U:141:ALA:HB2	40:u:107:PHE:CD1	2.02	0.92
27:U:139:LEU:HD22	40:u:158:PHE:HD1	1.35	0.92
1:0:21:LEU:CD2	1:0:69:ASP:OD2	2.18	0.91
4:3:229:TRP:CE3	5:4:58:ARG:NE	2.39	0.91
13:D:960:GLU:HG3	13:D:983:ARG:CG	1.97	0.91
16:G:153:LYS:HD3	16:G:153:LYS:H	1.36	0.91
1:0:85:ARG:HH12	1:0:140:LEU:HG	1.34	0.91
25:S:65:SER:HA	25:S:81:ARG:HH12	1.32	0.91
5:4:442:VAL:HG21	6:5:44:PHE:HZ	1.35	0.91
27:U:141:ALA:HB2	40:u:107:PHE:CG	2.02	0.91
27:U:141:ALA:HB1	40:u:107:PHE:CD1	2.00	0.91
27:U:140:GLU:OE2	40:u:158:PHE:HE1	1.53	0.90
8:7:726:GLN:CG	8:7:727:PRO:HD2	2.01	0.90
1:0:27:GLY:HA3	1:0:70:LYS:HD3	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:141:ALA:HB2	40:u:107:PHE:CE1	2.06	0.90
4:3:108:ASN:OD1	5:4:123:LEU:HD13	1.69	0.90
14:E:365:ARG:HD3	14:E:757:GLY:HA3	1.54	0.90
3:2:174:LEU:HD11	3:2:203:ALA:HB2	0.93	0.90
1:0:8:ARG:HH22	1:0:37:LEU:HB3	1.34	0.89
13:D:963:ARG:C	13:D:965:ILE:H	1.72	0.89
27:U:141:ALA:HB2	40:u:107:PHE:CE2	2.07	0.89
4:3:50:PHE:CG	5:4:122:LEU:HD12	2.07	0.89
4:3:229:TRP:CE3	5:4:58:ARG:CZ	2.55	0.89
13:D:1006:LEU:HD13	21:O:69:ASP:CG	1.97	0.89
4:3:237:GLN:HE21	5:4:51:LEU:HD22	1.38	0.89
7:6:528:LYS:CG	7:6:531:ILE:HD11	2.00	0.89
7:6:528:LYS:CE	7:6:531:ILE:HD11	2.04	0.88
4:3:229:TRP:CZ3	5:4:58:ARG:CZ	2.57	0.88
7:6:528:LYS:HG3	7:6:531:ILE:HD11	1.53	0.88
27:U:141:ALA:HB2	40:u:107:PHE:CZ	2.09	0.88
3:2:174:LEU:O	8:7:591:GLY:HA3	1.74	0.88
13:D:1006:LEU:CD1	21:O:69:ASP:OD2	2.21	0.88
27:U:53:LYS:HD2	28:V:166:ILE:HD11	1.56	0.88
27:U:152:PHE:CD1	40:u:95:VAL:CB	2.51	0.88
27:U:145:PHE:CE1	27:U:149:THR:OG1	2.27	0.88
5:4:438:LYS:HE2	12:B:621:ALA:CB	2.04	0.87
26:T:238:GLU:HB3	28:V:130:ILE:CG1	2.03	0.87
5:4:442:VAL:HG21	6:5:44:PHE:CZ	2.09	0.87
1:0:83:ASN:CG	1:0:140:LEU:CD1	2.47	0.87
11:A:475:LEU:HD11	15:f:351:ILE:HD11	1.57	0.87
27:U:140:GLU:OE2	40:u:158:PHE:CE1	2.27	0.87
6:5:35:ILE:O	12:B:539:ARG:HD3	1.75	0.86
7:6:528:LYS:HE3	7:6:531:ILE:HD11	1.57	0.86
34:o:497:ASP:OD2	49:p:1201:W0F:O33	1.94	0.86
7:6:528:LYS:CG	7:6:531:ILE:HD13	1.90	0.86
3:2:174:LEU:HD11	3:2:203:ALA:HB3	1.57	0.86
11:A:511:LEU:H	11:A:511:LEU:HD22	1.37	0.86
26:T:238:GLU:CB	28:V:130:ILE:HG12	2.05	0.86
29:X:7:DT:H4'	29:X:8:DC:H5'	1.57	0.86
13:D:963:ARG:C	13:D:965:ILE:N	2.25	0.85
35:p:975:ARG:NH2	49:p:1201:W0F:O32	2.08	0.85
13:D:1006:LEU:HD11	21:O:69:ASP:HB3	1.58	0.85
1:0:37:LEU:CD1	27:U:173:ALA:HA	2.06	0.84
4:3:100:LYS:HG2	5:4:124:GLY:O	1.76	0.84
7:6:528:LYS:CE	7:6:531:ILE:CD1	2.55	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:55:LYS:HB2	40:u:166:ASP:OD2	1.78	0.84
6:5:31:LYS:CB	12:B:540:LYS:HZ1	1.88	0.84
14:e:508:LYS:HB3	14:e:512:ASP:HB2	1.59	0.84
3:2:174:LEU:CG	3:2:203:ALA:HB1	2.07	0.83
4:3:50:PHE:CE2	5:4:118:LEU:HD11	2.12	0.83
5:4:448:HIS:O	5:4:452:LYS:HG2	1.78	0.83
27:U:56:ARG:O	27:U:60:ARG:HG3	1.78	0.83
27:U:138:ASP:O	40:u:107:PHE:HD2	1.61	0.83
3:2:175:THR:CG2	8:7:592:ARG:HE	1.92	0.83
2:1:503:THR:HG1	2:1:533:TYR:HH	1.19	0.83
27:U:142:ASN:ND2	40:u:105:SER:CB	2.39	0.83
5:4:432:VAL:HG12	6:5:9:LEU:HD22	1.61	0.82
9:N:3:GLY:HA3	34:o:749:ARG:NH1	1.94	0.82
11:A:1065:GLU:OE1	11:A:1065:GLU:HA	1.78	0.82
1:0:83:ASN:ND2	1:0:140:LEU:CD1	2.43	0.82
6:5:31:LYS:HB3	12:B:540:LYS:HZ3	0.80	0.82
11:A:821:ARG:CZ	11:A:821:ARG:HA	2.10	0.82
9:N:1:ILX:HG23	34:o:791:GLN:HE22	1.43	0.81
1:0:85:ARG:NH2	1:0:140:LEU:N	2.26	0.81
7:6:266:GLN:N	7:6:266:GLN:HE21	1.79	0.81
15:f:447:ALA:HA	15:f:456:GLY:HA3	1.61	0.81
13:D:960:GLU:HB3	13:D:983:ARG:HG3	1.63	0.81
15:F:324:ASP:HA	15:F:327:TRP:HB3	1.63	0.81
1:0:8:ARG:HD2	27:U:173:ALA:H	1.44	0.81
33:m:77:ARG:HH11	33:m:77:ARG:HG2	1.45	0.81
5:4:438:LYS:CE	12:B:621:ALA:H	1.94	0.80
27:U:139:LEU:CG	40:u:160:ILE:HG13	2.11	0.80
27:U:139:LEU:HD23	40:u:158:PHE:HD1	1.45	0.80
13:D:1006:LEU:CD1	21:O:69:ASP:CG	2.55	0.80
14:E:327:ASN:HD22	14:E:327:ASN:H	1.30	0.80
34:o:1242:ASP:HA	34:o:1262:MET:HB2	1.63	0.80
4:3:16:ASP:HA	4:3:62:SER:OG	1.82	0.80
1:0:8:ARG:NE	1:0:9:CYS:SG	2.54	0.80
26:T:188:PHE:CD2	28:V:80:LYS:HB2	2.16	0.80
27:U:138:ASP:OD1	40:u:160:ILE:HG21	1.81	0.80
5:4:334:MET:SD	7:6:56:TYR:CD2	2.76	0.79
27:U:56:ARG:NH1	27:U:60:ARG:NH1	2.30	0.79
2:1:430:THR:OG1	4:3:222:SER:OG	2.00	0.79
27:U:139:LEU:CD1	40:u:159:ALA:HA	2.12	0.79
1:0:83:ASN:OD1	1:0:140:LEU:CD1	2.31	0.79
22:P:188:ARG:NH2	23:Q:321:SER:OG	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:33:PHE:CZ	6:5:49:LEU:HD12	2.17	0.79
1:0:83:ASN:CG	1:0:140:LEU:HD11	2.07	0.79
3:2:174:LEU:CD2	3:2:203:ALA:CB	2.57	0.79
14:E:774:MET:HE2	14:E:774:MET:H	1.46	0.79
15:F:273:GLN:NE2	15:F:273:GLN:H	1.81	0.79
34:o:111:CYS:SG	34:o:188:GLN:NE2	2.56	0.79
27:U:151:THR:HG23	27:U:153:ARG:HD3	1.65	0.78
27:U:139:LEU:HD22	40:u:158:PHE:CD1	2.16	0.78
14:e:747:LEU:HD23	14:e:747:LEU:H	1.47	0.78
4:3:237:GLN:CG	5:4:51:LEU:CD2	2.60	0.78
15:F:274:ASN:ND2	15:F:316:GLN:HA	1.99	0.78
33:m:31:LEU:HD23	33:m:31:LEU:H	1.47	0.78
5:4:393:LEU:HD21	7:6:511:TRP:CZ3	2.19	0.78
27:U:139:LEU:CA	40:u:160:ILE:CG1	2.42	0.78
9:N:8:HYP:HD23	34:o:1108:HIS:CE1	2.17	0.78
4:3:56:LYS:NZ	4:3:143:TYR:OH	2.16	0.78
3:2:69:ARG:HG2	3:2:140:HIS:HA	1.66	0.77
5:4:456:LYS:O	5:4:460:HIS:CD2	2.37	0.77
30:Y:28:DT:H2'	30:Y:29:DA:C8	2.20	0.77
1:0:37:LEU:CD1	27:U:173:ALA:CB	2.63	0.77
3:2:223:LEU:HD12	8:7:726:GLN:HB2	1.67	0.77
26:T:192:GLU:HG3	28:V:75:PHE:HB3	1.67	0.76
1:0:37:LEU:HD11	27:U:173:ALA:CA	2.14	0.76
7:6:449:LYS:HD3	29:X:31:DG:OP1	1.84	0.76
1:0:85:ARG:HH22	1:0:140:LEU:CA	1.98	0.76
3:2:69:ARG:HD3	3:2:140:HIS:CD2	2.20	0.76
13:D:963:ARG:C	13:D:982:LEU:HD11	2.10	0.76
36:q:190:ASN:ND2	36:q:195:THR:O	2.19	0.76
4:3:46:ASN:OD1	5:4:123:LEU:HD22	1.85	0.76
5:4:432:VAL:CG1	6:5:9:LEU:HD22	2.15	0.76
1:0:41:ARG:HG2	27:U:168:MET:HE3	1.68	0.76
4:3:240:GLN:NE2	5:4:51:LEU:HD21	2.01	0.75
34:o:1307:VAL:HG13	34:o:1338:THR:HG22	1.68	0.75
15:F:429:LYS:O	15:F:433:PRO:HD2	1.85	0.75
40:u:142:GLU:HB2	40:u:170:LEU:HD22	1.68	0.75
11:A:467:ILE:H	15:F:221:GLN:HE21	1.33	0.75
27:U:152:PHE:CD2	40:u:95:VAL:HG11	2.21	0.75
1:0:42:GLY:H	27:U:168:MET:HE1	1.50	0.75
1:0:41:ARG:HB2	27:U:168:MET:SD	2.26	0.74
1:0:84:LYS:CA	1:0:136:ASN:ND2	2.48	0.74
8:7:711:ASP:OD1	8:7:715:GLN:NE2	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:33:PHE:HE1	6:5:49:LEU:HD12	0.84	0.74
27:U:141:ALA:HB1	40:u:98:PHE:HE1	1.52	0.74
1:0:8:ARG:NH2	1:0:34:CYS:SG	2.61	0.74
27:U:48:MET:HE2	27:U:52:LEU:HB2	1.69	0.74
34:o:585:LEU:HD22	41:v:47:ILE:HD11	1.69	0.74
4:3:47:SER:HA	5:4:122:LEU:HD11	1.68	0.74
11:A:970:ASN:OD1	11:A:970:ASN:N	2.21	0.74
27:U:138:ASP:O	40:u:107:PHE:CE2	2.41	0.74
5:4:438:LYS:HE2	12:B:621:ALA:HB3	1.70	0.74
36:q:90:CYS:SG	36:q:94:CYS:HB3	2.28	0.74
11:A:639:LEU:HD11	11:A:774:ARG:HG2	1.70	0.73
6:5:31:LYS:HB3	12:B:540:LYS:CE	2.17	0.73
15:F:359:PHE:HB3	15:F:380:LEU:HG	1.68	0.73
1:0:41:ARG:C	27:U:168:MET:HE1	2.13	0.73
35:p:69:ALA:HB3	35:p:81:PRO:HB3	1.68	0.73
11:A:488:ALA:HB1	15:f:271:VAL:HG23	1.70	0.73
27:U:152:PHE:CD1	40:u:95:VAL:CG2	2.71	0.73
35:p:269:ILE:HD11	35:p:369:VAL:HG21	1.68	0.73
7:6:371:VAL:HG23	7:6:407:ILE:HG22	1.69	0.73
37:r:25:GLU:HG3	40:u:41:LYS:HE2	1.71	0.73
6:5:31:LYS:CG	12:B:540:LYS:HZ3	2.01	0.73
8:7:231:VAL:HG13	8:7:454:VAL:HG23	1.70	0.73
40:u:92:VAL:HB	40:u:126:PRO:HB2	1.70	0.73
4:3:237:GLN:OE1	5:4:54:ASN:OD1	2.07	0.72
6:5:34:ILE:O	12:B:539:ARG:NH2	2.22	0.72
4:3:50:PHE:CD2	5:4:122:LEU:HD12	2.24	0.72
15:F:418:ILE:H	15:F:418:ILE:HD12	1.54	0.72
23:Q:346:LYS:NZ	30:Y:29:DA:OP1	2.23	0.72
27:U:147:PRO:HA	40:u:91:GLN:CD	2.14	0.72
34:o:46:THR:HG22	34:o:57:LEU:HB2	1.71	0.72
26:T:188:PHE:HE2	28:V:80:LYS:HG3	1.55	0.72
1:0:23:VAL:HG21	1:0:73:GLU:HG3	1.71	0.72
36:q:2:PRO:HB3	44:y:54:PRO:HD2	1.70	0.72
25:S:64:GLU:O	25:S:81:ARG:NH2	2.20	0.72
28:V:131:GLU:HG3	28:V:140:LYS:HA	1.72	0.72
1:0:10:LYS:HZ2	27:U:178:ALA:HB1	1.55	0.72
5:4:120:ILE:HG23	5:4:125:GLY:HA2	1.72	0.72
27:U:152:PHE:CZ	40:u:95:VAL:CB	2.62	0.72
11:A:353:LEU:HD21	15:f:272:VAL:HG21	1.72	0.71
1:0:85:ARG:NH2	1:0:139:LYS:O	2.23	0.71
4:3:237:GLN:CG	5:4:51:LEU:HD22	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:160:ARG:NH2	4:3:234:ASP:OD1	2.23	0.71
2:1:195:SER:O	2:1:199:THR:OG1	2.05	0.71
5:4:29:GLY:O	5:4:33:ARG:NE	2.23	0.71
14:e:274:TYR:HB3	14:e:367:ALA:HB2	1.72	0.71
5:4:404:THR:HG22	6:5:9:LEU:H	1.56	0.71
1:0:42:GLY:N	27:U:168:MET:CE	2.44	0.71
4:3:272:LEU:O	4:3:272:LEU:HD23	1.90	0.71
6:5:31:LYS:HB2	12:B:540:LYS:NZ	2.06	0.71
24:R:72:ASN:HB2	24:R:75:LEU:HG	1.72	0.70
27:U:139:LEU:CB	40:u:160:ILE:HG13	1.94	0.70
1:0:8:ARG:HH22	1:0:37:LEU:CB	2.04	0.70
12:B:241:PRO:HG2	12:B:496:MET:HE1	1.72	0.70
27:U:23:ARG:HD2	27:U:31:ALA:HB1	1.73	0.70
4:3:67:SER:O	4:3:139:LYS:NZ	2.24	0.70
4:3:237:GLN:HG3	5:4:51:LEU:CD2	2.21	0.70
13:D:960:GLU:HG2	13:D:983:ARG:CD	2.22	0.70
1:0:120:LYS:O	1:0:124:ILE:HD12	1.91	0.70
28:V:197:LYS:HG3	28:V:198:LYS:HG3	1.71	0.70
13:D:961:GLN:HG3	13:D:983:ARG:HH12	1.56	0.70
14:E:258:ASN:H	14:E:258:ASN:ND2	1.89	0.70
7:6:528:LYS:HE2	7:6:531:ILE:CD1	2.22	0.70
30:Y:1:DG:H2"	30:Y:2:DA:H5'	1.72	0.70
27:U:75:ARG:H	27:U:91:TYR:HB2	1.55	0.70
29:X:18:DG:H2"	29:X:19:DA:C8	2.26	0.70
28:V:234:GLU:OE1	28:V:238:LYS:NZ	2.25	0.70
35:p:761:THR:H	35:p:764:MET:HE3	1.54	0.70
34:o:922:PHE:H	34:o:1052:ARG:HD2	1.57	0.70
11:A:339:ALA:CB	11:A:355:VAL:HG21	2.21	0.69
3:2:206:ARG:HB3	8:7:589:GLU:O	1.91	0.69
35:p:910:THR:HG22	45:z:43:ILE:HA	1.75	0.69
34:o:877:ALA:HB3	34:o:890:ARG:HH11	1.55	0.69
7:6:191:ASP:O	7:6:195:ARG:NH1	2.25	0.69
27:U:36:ILE:HD11	28:V:163:LEU:HD22	1.74	0.69
35:p:975:ARG:NE	49:p:1201:W0F:O32	2.25	0.69
16:G:129:LYS:O	16:G:129:LYS:NZ	2.23	0.69
34:o:689:ILE:HD12	35:p:985:LEU:HD22	1.73	0.69
15:f:447:ALA:CA	15:f:456:GLY:HA3	2.23	0.69
7:6:611:GLY:O	7:6:642:ARG:NH2	2.25	0.69
8:7:252:THR:HG22	8:7:432:ILE:HG22	1.74	0.69
2:1:468:VAL:HG21	2:1:525:ILE:HD11	1.74	0.69
5:4:438:LYS:HE3	12:B:621:ALA:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:24:GLY:HA2	28:V:209:GLN:HG2	1.75	0.69
7:6:56:TYR:C	7:6:58:ALA:H	2.01	0.69
4:3:242:ILE:HD11	5:4:75:VAL:C	2.17	0.69
9:N:1:ILX:HG23	34:o:791:GLN:NE2	2.08	0.69
12:B:490:SER:HA	12:B:493:TRP:HB2	1.75	0.68
35:p:407:MET:HE1	35:p:444:LEU:HG	1.74	0.68
8:7:637:LEU:HD11	8:7:648:GLU:HA	1.74	0.68
15:F:274:ASN:HB2	15:F:317:LEU:H	1.58	0.68
27:U:152:PHE:CE2	40:u:95:VAL:CG1	2.77	0.68
30:Y:-17:DG:H1'	30:Y:-16:DA:H5'	1.75	0.68
13:D:991:MET:HE2	26:T:193:LYS:HA	1.76	0.68
27:U:56:ARG:HH11	27:U:60:ARG:NH1	1.89	0.68
27:U:138:ASP:OD2	40:u:160:ILE:HG21	1.91	0.68
3:2:75:ASP:OD2	8:7:722:ARG:NH2	2.26	0.68
32:k:191:VAL:HG13	32:k:200:ILE:HD13	1.74	0.68
3:2:69:ARG:HD2	8:7:563:ARG:HH21	1.58	0.68
11:A:568:SER:HB2	12:B:389:ASN:HB2	1.75	0.68
13:D:998:GLN:NE2	26:T:186:MET:HA	2.08	0.68
15:F:83:LEU:CD1	15:F:83:LEU:H	2.06	0.68
14:e:645:GLY:H	14:e:675:LEU:HD11	1.58	0.68
8:7:72:TYR:OH	8:7:234:ASP:OD2	2.12	0.68
8:7:382:LEU:O	8:7:385:THR:OG1	2.11	0.68
13:D:1002:ARG:HB2	26:T:182:HIS:CD2	2.29	0.68
24:R:103:ASN:HB3	30:Y:12:DC:H5'	1.76	0.68
34:o:560:VAL:HG22	34:o:591:ILE:HD11	1.75	0.67
34:o:784:VAL:HG22	35:p:978:ILE:HD11	1.76	0.67
34:o:1148:ALA:HB1	34:o:1333:GLU:HB2	1.75	0.67
14:E:426:ARG:HH11	14:E:640:ASN:HD22	1.42	0.67
6:5:38:ILE:HG21	6:5:42:HIS:HB2	1.76	0.67
1:0:37:LEU:CD1	27:U:173:ALA:CA	2.72	0.67
3:2:88:LEU:CD2	3:2:131:LEU:HD21	2.24	0.67
3:2:175:THR:HG23	8:7:592:ARG:HE	1.56	0.67
11:A:396:LEU:HD21	15:f:394:PRO:HB2	1.77	0.67
17:H:40:VAL:HG11	19:J:130:ILE:HG12	1.77	0.67
27:U:48:MET:HA	27:U:48:MET:HE3	1.75	0.67
27:U:139:LEU:CG	40:u:160:ILE:CG1	2.67	0.67
35:p:827:GLU:HG2	35:p:871:VAL:HG22	1.75	0.67
1:0:10:LYS:NZ	27:U:178:ALA:CB	2.57	0.67
1:0:85:ARG:NH1	1:0:140:LEU:CG	2.45	0.67
3:2:174:LEU:CD1	3:2:203:ALA:HB3	2.17	0.67
4:3:46:ASN:OD1	5:4:123:LEU:CD2	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:365:ARG:HD3	14:E:757:GLY:CA	2.24	0.67
30:Y:-25:DC:H2"	30:Y:-24:DT:H72	1.76	0.67
20:L:79:ASP:OD1	20:L:79:ASP:N	2.25	0.67
27:U:20:TYR:O	27:U:23:ARG:NH2	2.27	0.67
27:U:136:PHE:O	27:U:137:THR:OG1	2.13	0.67
34:o:760:LEU:HD11	34:o:781:ILE:HG21	1.77	0.67
36:q:259:LEU:HD22	44:y:19:ILE:HD11	1.76	0.67
30:Y:-4:DC:O2	49:p:1201:W0F:N19	2.28	0.67
25:S:76:ARG:HH21	25:S:80:ARG:HD3	1.60	0.67
29:X:29:DA:H2"	29:X:30:DC:C5	2.30	0.67
15:f:239:ARG:HD3	15:f:284:ARG:HH11	1.60	0.67
3:2:75:ASP:OD1	8:7:722:ARG:NH2	2.28	0.67
5:4:60:LEU:HD13	5:4:118:LEU:HD23	1.76	0.66
5:4:409:TYR:HB2	5:4:412:PHE:CZ	2.30	0.66
22:P:206:GLU:OE1	22:P:236:LYS:NZ	2.28	0.66
24:R:102:GLN:HE21	34:o:305:GLU:HG2	1.60	0.66
28:V:227:SER:HB3	28:V:230:GLU:HB2	1.77	0.66
2:1:432:THR:O	2:1:435:SER:OG	2.10	0.66
4:3:43:VAL:HG11	4:3:224:LEU:HD21	1.78	0.66
8:7:60:GLN:OE1	8:7:61:ARG:NH1	2.29	0.66
28:V:141:PRO:HB2	28:V:144:ASN:HB3	1.76	0.66
34:o:877:ALA:HB3	34:o:890:ARG:NH1	2.11	0.66
4:3:237:GLN:OE1	5:4:51:LEU:HD23	1.94	0.66
36:q:67:ARG:NH2	43:x:3:ILE:O	2.28	0.66
13:D:1006:LEU:HD11	21:O:69:ASP:CB	2.25	0.66
33:m:79:GLY:HA2	20:l:141:LYS:HE2	1.76	0.66
4:3:229:TRP:CE3	5:4:58:ARG:HD2	2.31	0.66
5:4:438:LYS:HE3	12:B:621:ALA:N	2.10	0.66
24:R:23:LEU:HD12	24:R:32:MET:HE2	1.78	0.66
34:o:1286:ARG:HH21	42:w:53:ILE:HG22	1.60	0.66
37:r:77:ARG:HA	37:r:80:ILE:HD12	1.78	0.66
38:s:192:LYS:HE3	38:s:194:ILE:HD11	1.78	0.66
1:0:106:VAL:O	1:0:110:THR:HG23	1.95	0.66
21:O:51:ARG:NH2	23:Q:20:ASP:OD2	2.28	0.66
27:U:152:PHE:CD1	40:u:95:VAL:HG21	2.31	0.66
34:o:733:LEU:HB3	42:w:106:ASP:HB2	1.78	0.66
11:A:821:ARG:HA	11:A:821:ARG:NH1	2.11	0.66
4:3:229:TRP:CE3	5:4:58:ARG:CD	2.78	0.66
27:U:141:ALA:HB1	40:u:98:PHE:CE1	2.31	0.66
19:j:123:LEU:C	19:j:125:ASP:H	2.03	0.66
3:2:137:MET:SD	3:2:139:CYS:N	2.67	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:u:92:VAL:HG13	40:u:128:TYR:CE2	2.31	0.65
3:2:175:THR:HG22	8:7:592:ARG:CD	2.27	0.65
8:7:238:ASN:ND2	8:7:662:GLN:OE1	2.29	0.65
13:D:960:GLU:CB	13:D:983:ARG:HG3	2.26	0.65
3:2:174:LEU:O	8:7:591:GLY:CA	2.43	0.65
13:D:1006:LEU:CD1	21:O:69:ASP:CB	2.74	0.65
1:0:8:ARG:NE	27:U:173:ALA:HB2	2.10	0.65
26:T:237:PRO:HB3	28:V:83:ASN:HD21	1.60	0.65
7:6:701:LEU:O	7:6:704:SER:OG	2.14	0.65
27:U:72:ILE:HG22	27:U:94:ILE:HA	1.78	0.65
29:X:8:DC:H42	30:Y:-8:DG:H1	1.43	0.65
4:3:229:TRP:HZ3	5:4:58:ARG:HH11	1.44	0.65
5:4:172:SER:OG	5:4:174:ASP:OD1	2.15	0.65
3:2:174:LEU:HG	3:2:203:ALA:CB	2.27	0.65
4:3:98:ASP:O	5:4:125:GLY:HA3	1.96	0.65
28:V:144:ASN:HA	28:V:173:GLU:HB2	1.78	0.65
33:m:77:ARG:HH11	33:m:77:ARG:CG	2.10	0.65
35:p:975:ARG:HH21	49:p:1201:W0F:P30	2.20	0.65
6:5:38:ILE:CG2	6:5:42:HIS:HB2	2.27	0.64
30:Y:2:DA:H1'	30:Y:3:DA:H5'	1.78	0.64
34:o:1146:GLN:HG2	34:o:1149:ARG:HH12	1.62	0.64
1:0:41:ARG:HG3	27:U:169:PRO:HG2	0.68	0.64
15:F:83:LEU:HD12	15:F:83:LEU:N	2.12	0.64
27:U:139:LEU:HD12	40:u:149:GLY:O	1.98	0.64
15:f:320:ARG:NH1	15:f:320:ARG:HB3	2.12	0.64
4:3:168:GLU:N	4:3:168:GLU:OE1	2.31	0.64
35:p:222:ARG:HB3	35:p:234:THR:HG22	1.79	0.64
35:p:625:LEU:HD13	35:p:675:LEU:HD21	1.77	0.64
35:p:866:ILE:HG22	35:p:867:ILE:HG13	1.79	0.64
37:r:103:LEU:HD13	37:r:114:LEU:HD13	1.77	0.64
11:A:1168:TYR:HB2	16:G:180:ARG:HB3	1.78	0.64
27:U:111:ARG:HD3	27:U:188:TYR:OH	1.97	0.64
34:o:1158:LEU:HD11	34:o:1309:MET:HB2	1.80	0.64
7:6:287:LEU:HD23	7:6:287:LEU:O	1.98	0.64
7:6:330:ASN:OD1	7:6:334:ARG:NH2	2.31	0.64
27:U:145:PHE:HD1	27:U:149:THR:OG1	1.76	0.64
34:o:890:ARG:HE	34:o:1023:VAL:HG22	1.62	0.64
4:3:229:TRP:HE3	5:4:58:ARG:NE	1.91	0.64
5:4:335:LEU:O	7:6:58:ALA:HA	1.98	0.64
6:5:31:LYS:HB2	12:B:540:LYS:HZ1	1.59	0.64
19:j:123:LEU:O	19:j:125:ASP:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:377:ASP:O	3:2:380:HIS:NE2	2.30	0.64
14:E:522:ASP:HB2	14:E:526:ARG:HG2	1.80	0.64
7:6:517:GLU:O	7:6:521:GLU:OE1	2.16	0.64
8:7:513:ASP:OD1	8:7:516:VAL:N	2.29	0.64
27:U:76:MET:HE3	27:U:88:ARG:HD2	1.80	0.64
5:4:55:TRP:CZ2	5:4:83:GLN:NE2	2.66	0.63
1:0:41:ARG:CB	27:U:169:PRO:HG2	2.24	0.63
13:D:960:GLU:CB	13:D:983:ARG:CG	2.75	0.63
27:U:139:LEU:N	40:u:160:ILE:HG12	2.12	0.63
28:V:158:HIS:O	28:V:162:GLY:N	2.29	0.63
7:6:266:GLN:HG2	7:6:267:THR:HG23	1.81	0.63
27:U:152:PHE:CG	40:u:95:VAL:HG11	2.34	0.63
34:o:98:GLY:HA3	34:o:1440:MET:HE2	1.79	0.63
35:p:193:VAL:HG21	35:p:470:LEU:HD13	1.79	0.63
35:p:365:LEU:O	35:p:369:VAL:HG23	1.98	0.63
37:r:114:LEU:HD22	40:u:84:VAL:HG11	1.81	0.63
8:7:726:GLN:HG2	8:7:727:PRO:HD2	1.80	0.63
3:2:175:THR:HG21	8:7:592:ARG:HE	1.63	0.63
3:2:242:SER:O	3:2:245:SER:OG	2.17	0.63
3:2:75:ASP:CG	8:7:722:ARG:NH2	2.57	0.63
3:2:109:THR:OG1	3:2:148:SER:OG	2.05	0.63
3:2:175:THR:HG21	8:7:592:ARG:NE	2.13	0.63
4:3:16:ASP:OD1	4:3:131:THR:OG1	2.16	0.63
13:D:966:LEU:O	13:D:966:LEU:HD22	1.99	0.63
14:e:277:ASP:OD1	14:e:277:ASP:N	2.32	0.63
1:0:27:GLY:CA	1:0:70:LYS:HD3	2.26	0.63
28:V:78:LEU:HD21	28:V:124:LEU:HD22	1.79	0.63
7:6:528:LYS:HG2	7:6:528:LYS:O	1.97	0.63
27:U:138:ASP:CG	40:u:160:ILE:CG2	2.61	0.63
34:o:1208:SER:HA	34:o:1266:GLU:HG3	1.80	0.63
35:p:22:TRP:CE2	35:p:679:PRO:HG3	2.34	0.63
4:3:240:GLN:HE21	5:4:51:LEU:HD21	1.61	0.63
13:D:1002:ARG:HE	26:T:182:HIS:CD2	2.17	0.63
17:H:50:PHE:HD1	19:J:193:TYR:O	1.82	0.63
26:T:188:PHE:CE2	28:V:80:LYS:HG3	2.33	0.63
27:U:152:PHE:CE2	40:u:95:VAL:HG12	2.34	0.63
3:2:87:LEU:HD22	3:2:232:LEU:HD12	1.81	0.62
12:B:361:ARG:HD2	12:B:367:GLU:HB2	1.80	0.62
35:p:851:ASP:HB3	45:z:15:MET:HE1	1.81	0.62
35:p:896:LEU:HD21	35:p:900:GLU:HB3	1.80	0.62
1:0:71:GLU:OE2	8:7:335:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:229:TRP:HE3	5:4:58:ARG:CD	2.12	0.62
1:0:83:ASN:ND2	1:0:140:LEU:HD12	2.14	0.62
12:B:583:GLU:CD	12:B:583:GLU:H	2.06	0.62
15:F:92:ILE:HG13	15:F:93:PRO:HD3	1.81	0.62
3:2:112:LYS:O	3:2:147:ASN:ND2	2.32	0.62
11:A:342:ARG:HG2	11:A:342:ARG:O	1.99	0.62
22:P:208:ARG:NH2	23:Q:346:LYS:O	2.32	0.62
35:p:267:VAL:HG13	35:p:320:PHE:HE2	1.64	0.62
37:r:23:PRO:HG2	37:r:26:PHE:HB2	1.80	0.62
7:6:128:SER:OG	7:6:163:TYR:OH	2.17	0.62
27:U:139:LEU:CB	40:u:160:ILE:CD1	2.54	0.62
34:o:890:ARG:HH21	34:o:1023:VAL:HG13	1.65	0.62
3:2:223:LEU:HD13	8:7:726:GLN:OE1	1.99	0.62
25:S:70:GLU:HA	25:S:74:LYS:HB2	1.81	0.62
27:U:100:VAL:O	27:U:104:LYS:HG2	1.99	0.62
8:7:343:ARG:O	8:7:346:VAL:HG12	1.99	0.62
13:D:960:GLU:CG	13:D:983:ARG:HG3	2.25	0.62
15:F:335:ARG:NE	15:F:382:GLU:OE1	2.33	0.62
34:o:863:ARG:HH21	34:o:1415:THR:HG22	1.64	0.62
1:0:41:ARG:HG3	27:U:169:PRO:CD	2.27	0.62
9:N:3:GLY:HA3	34:o:749:ARG:HH12	1.61	0.62
30:Y:-8:DG:H1'	30:Y:-7:DA:C8	2.34	0.62
35:p:553:LEU:HA	35:p:556:ILE:HD12	1.82	0.62
8:7:2:LYS:HB3	8:7:9:LEU:HD11	1.81	0.62
7:6:371:VAL:HG23	7:6:407:ILE:CG2	2.30	0.62
27:U:152:PHE:CZ	40:u:95:VAL:CG1	2.83	0.62
34:o:203:LYS:HG2	34:o:212:LYS:HE3	1.82	0.62
35:p:404:PHE:HA	35:p:407:MET:HE2	1.82	0.61
13:d:884:GLU:HA	13:d:887:LYS:HE3	1.82	0.61
34:o:458:PHE:HE2	34:o:484:LEU:HD23	1.65	0.61
34:o:769:MET:HE1	35:p:970:HIS:HA	1.82	0.61
36:q:183:ALA:HB3	36:q:232:ASN:HB3	1.83	0.61
13:D:956:GLN:HA	13:D:956:GLN:NE2	2.15	0.61
3:2:379:LEU:HD22	3:2:381:CYS:O	1.99	0.61
6:5:32:LYS:HD3	12:B:540:LYS:HA	1.80	0.61
8:7:609:ASP:OD1	8:7:669:ARG:NH2	2.34	0.61
3:2:206:ARG:HG2	8:7:589:GLU:HA	1.82	0.61
7:6:473:GLU:OE1	7:6:473:GLU:N	2.33	0.61
15:F:114:LEU:HB2	17:H:52:SER:H	1.66	0.61
4:3:53:ARG:HG2	5:4:46:ARG:NH2	2.15	0.61
5:4:401:LEU:HD13	6:5:10:ILE:HD13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:203:LYS:HD3	12:B:237:MET:HE3	1.83	0.61
14:E:613:ALA:HB2	14:E:620:LEU:HD11	1.81	0.61
27:U:147:PRO:HA	40:u:91:GLN:NE2	2.15	0.61
34:o:581:LYS:HG2	34:o:582:PRO:HA	1.81	0.61
38:s:171:PRO:HB2	38:s:207:ARG:HD3	1.82	0.61
5:4:265:LEU:CD1	5:4:270:LEU:HD12	2.31	0.61
7:6:189:LEU:O	7:6:195:ARG:NH1	2.33	0.61
8:7:461:LEU:HD23	8:7:464:LEU:CD2	2.31	0.61
41:v:37:MET:HE3	41:v:127:GLY:HA3	1.83	0.61
31:c:18:CYS:O	31:c:23:TRP:HB2	2.00	0.60
34:o:433:PRO:HG2	34:o:438:LEU:HD21	1.83	0.60
1:0:10:LYS:HZ3	27:U:178:ALA:HB1	1.66	0.60
13:D:996:LEU:O	13:D:1000:ARG:HG3	2.01	0.60
25:S:58:GLN:C	25:S:60:GLU:H	2.08	0.60
28:V:121:THR:O	28:V:125:VAL:HG23	2.01	0.60
28:V:171:ILE:HD13	28:V:177:ASN:HB3	1.83	0.60
33:m:75:ILE:HD11	19:j:176:MET:HE1	1.82	0.60
40:u:93:ASN:O	40:u:128:TYR:OH	2.11	0.60
41:v:96:VAL:HG22	41:v:116:VAL:HG22	1.83	0.60
7:6:528:LYS:HZ3	29:X:34:DC:H5”	1.66	0.60
17:H:192:ARG:NH1	17:H:209:SER:O	2.34	0.60
3:2:357:VAL:HG13	3:2:366:VAL:HG23	1.83	0.60
5:4:18:ASN:OD1	5:4:19:LEU:N	2.35	0.60
8:7:628:THR:O	8:7:628:THR:HG22	2.02	0.60
27:U:25:PHE:O	28:V:217:GLN:NE2	2.33	0.60
12:B:27:LYS:HE3	12:B:490:SER:HB3	1.84	0.60
14:E:754:THR:O	14:E:755:ALA:HB3	2.01	0.60
31:c:99:PHE:HB2	31:c:100:PRO:HD3	1.83	0.60
40:u:152:VAL:HB	40:u:157:ILE:HG12	1.83	0.60
14:e:257:GLU:H	14:e:257:GLU:CD	2.10	0.60
17:H:194:MET:HE1	15:f:226:GLU:HG3	1.83	0.60
28:V:77:VAL:O	28:V:81:ILE:HG12	2.02	0.60
35:p:153:PRO:HB3	35:p:187:ILE:HD11	1.83	0.60
1:0:55:LYS:HB2	40:u:166:ASP:CG	2.25	0.60
33:m:31:LEU:HD23	33:m:31:LEU:N	2.16	0.60
35:p:834:ARG:HA	35:p:840:MET:HG3	1.84	0.60
1:0:55:LYS:HE2	40:u:166:ASP:OD2	2.02	0.60
2:1:422:LEU:HD22	4:3:225:GLN:HE22	1.66	0.60
3:2:175:THR:HG22	8:7:592:ARG:HD2	1.80	0.60
15:F:90:GLU:H	15:F:90:GLU:CD	2.08	0.60
27:U:139:LEU:CB	40:u:160:ILE:HD11	2.25	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:o:479:TRP:HB2	34:o:483:ARG:HH21	1.66	0.60
30:Y:12:DC:H2"	30:Y:13:DA:C8	2.37	0.60
5:4:172:SER:OG	5:4:267:GLU:OE2	2.13	0.59
37:r:16:ASP:H	37:r:21:ILE:HB	1.67	0.59
3:2:174:LEU:HG	3:2:203:ALA:HB1	1.83	0.59
5:4:438:LYS:HE2	12:B:621:ALA:HB2	1.82	0.59
7:6:707:GLU:O	7:6:711:GLN:OE1	2.20	0.59
28:V:174:ALA:HB1	28:V:180:LYS:HZ1	1.67	0.59
38:s:82:VAL:HG23	38:s:106:VAL:HG13	1.84	0.59
11:A:475:LEU:HD13	15:f:349:ASN:OD1	2.02	0.59
27:U:150:GLY:HA2	40:u:93:ASN:OD1	2.01	0.59
34:o:347:GLU:HA	34:o:352:GLY:HA3	1.85	0.59
4:3:242:ILE:HD13	5:4:74:TRP:C	2.27	0.59
34:o:706:ILE:HD13	34:o:824:GLU:HG3	1.84	0.59
1:0:83:ASN:HD21	1:0:140:LEU:HD13	1.66	0.59
33:m:88:PHE:C	33:m:88:PHE:CD1	2.81	0.59
14:e:562:SER:OG	14:e:564:ASP:OD1	2.21	0.59
8:7:462:SER:OG	8:7:463:PRO:HD2	2.02	0.59
34:o:420:ILE:HG12	34:o:426:ARG:HG3	1.84	0.59
34:o:1262:MET:HE2	34:o:1264:SER:HB3	1.84	0.59
35:p:1120:ASN:HB2	35:p:1145:GLN:HB3	1.84	0.59
2:1:130:ASP:OD2	2:1:463:HIS:NE2	2.33	0.59
7:6:528:LYS:HE2	7:6:531:ILE:HD13	1.83	0.59
11:A:1193:ALA:HB3	16:G:166:VAL:HG21	1.83	0.59
40:u:108:ILE:HG21	40:u:163:LEU:HG	1.84	0.59
3:2:88:LEU:HD22	3:2:131:LEU:HD21	1.83	0.59
5:4:401:LEU:HG	6:5:53:LEU:HD23	1.85	0.59
7:6:266:GLN:N	7:6:266:GLN:NE2	2.49	0.59
27:U:15:LYS:NZ	27:U:94:ILE:O	2.31	0.59
15:f:349:ASN:HB3	15:f:351:ILE:HG13	1.84	0.59
6:5:48:GLU:HG3	6:5:49:LEU:HG	1.84	0.59
7:6:528:LYS:NZ	29:X:34:DC:H5"	2.17	0.59
8:7:372:LEU:HD11	8:7:404:ALA:HB1	1.84	0.59
15:F:312:ILE:HG13	15:F:334:ALA:CB	2.33	0.59
34:o:1004:LEU:HD13	34:o:1062:GLY:HA2	1.85	0.59
36:q:42:VAL:HB	36:q:178:PRO:HG3	1.84	0.59
41:v:124:ARG:HD3	41:v:126:GLN:HG3	1.84	0.59
4:3:195:VAL:HG12	4:3:203:LEU:HD23	1.85	0.58
8:7:405:THR:O	8:7:409:THR:OG1	2.16	0.58
34:o:577:PRO:HG2	34:o:580:LEU:HD23	1.85	0.58
15:f:330:ARG:HH22	15:f:371:THR:HB	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:84:LYS:HA	1:0:136:ASN:CG	2.29	0.58
2:1:417:LYS:HA	2:1:421:VAL:HG23	1.84	0.58
8:7:262:ASN:O	8:7:266:LEU:HD23	2.03	0.58
8:7:571:THR:OG1	8:7:576:GLU:OE1	2.08	0.58
11:A:470:ILE:O	11:A:470:ILE:HG22	2.02	0.58
26:T:238:GLU:CG	28:V:130:ILE:HG12	2.32	0.58
43:x:3:ILE:HD12	43:x:4:PRO:HD2	1.85	0.58
1:0:35:VAL:HG13	1:0:58:PHE:CE2	2.39	0.58
4:3:98:ASP:HB2	4:3:100:LYS:HE3	1.84	0.58
7:6:449:LYS:HB3	29:X:31:DG:OP1	2.03	0.58
8:7:664:VAL:HG22	8:7:677:MET:HG2	1.83	0.58
2:1:422:LEU:HD22	4:3:225:GLN:NE2	2.19	0.58
3:2:69:ARG:CD	8:7:563:ARG:HH21	2.15	0.58
5:4:404:THR:H	6:5:8:VAL:HG13	1.68	0.58
17:H:171:ASP:HB3	17:H:174:VAL:HG12	1.85	0.58
5:4:438:LYS:CE	12:B:621:ALA:N	2.65	0.58
27:U:137:THR:HB	27:U:140:GLU:OE1	2.04	0.58
29:X:7:DT:H1'	29:X:8:DC:C6	2.39	0.58
34:o:555:LEU:HD13	34:o:591:ILE:HD12	1.86	0.58
34:o:1030:SER:HB3	38:s:162:ARG:HE	1.68	0.58
2:1:471:LEU:HD12	2:1:472:LEU:HD22	1.84	0.58
15:F:207:ARG:HD2	15:F:207:ARG:N	2.18	0.58
31:c:12:VAL:HG23	15:f:118:ILE:HA	1.86	0.58
35:p:975:ARG:CZ	49:p:1201:W0F:O32	2.51	0.58
11:A:929:THR:HG22	11:A:954:ALA:HA	1.86	0.58
27:U:36:ILE:HG21	27:U:48:MET:HE1	1.84	0.58
35:p:755:GLN:HE22	43:x:48:MET:HE2	1.69	0.58
35:p:826:GLU:H	35:p:872:THR:HG22	1.67	0.58
27:U:70:LYS:HE2	28:V:226:ASP:HA	1.86	0.58
30:Y:-3:DC:H2'	30:Y:-2:DA:C8	2.39	0.58
34:o:1210:TRP:HZ3	42:w:53:ILE:HG13	1.69	0.58
1:0:8:ARG:O	27:U:178:ALA:HB2	2.04	0.58
3:2:345:CYS:O	3:2:349:GLN:N	2.36	0.58
7:6:56:TYR:C	7:6:58:ALA:N	2.61	0.58
11:A:340:GLU:N	11:A:497:PRO:HG2	2.18	0.58
11:A:1063:LYS:HD3	11:A:1063:LYS:C	2.28	0.58
25:S:73:ARG:CZ	25:S:76:ARG:HD2	2.33	0.58
33:m:67:GLU:HA	33:m:67:GLU:OE1	2.02	0.58
35:p:627:ILE:HD11	35:p:663:GLU:HB2	1.84	0.58
14:e:513:LEU:HD21	14:e:527:ILE:HG23	1.86	0.58
4:3:241:LEU:HD23	4:3:243:LEU:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:S:71:PHE:CE2	26:T:194:HIS:HB3	2.39	0.58
27:U:145:PHE:HB2	27:U:153:ARG:HG2	1.85	0.58
28:V:163:LEU:HG	28:V:201:LEU:HD21	1.85	0.58
30:Y:19:DA:H2"	30:Y:20:DC:H5'	1.85	0.58
31:c:21:LEU:HD12	31:c:21:LEU:C	2.29	0.58
4:3:52:ASN:OD1	4:3:53:ARG:N	2.37	0.57
14:E:522:ASP:O	14:E:524:LEU:N	2.37	0.57
14:e:484:LEU:HD21	14:e:504:LEU:HD21	1.85	0.57
1:0:1:MET:SD	8:7:345:ARG:HD3	2.44	0.57
7:6:528:LYS:CG	7:6:531:ILE:HD12	2.29	0.57
22:P:299:ARG:NH2	29:X:-27:DA:OP1	2.37	0.57
21:O:29:THR:HG23	21:O:32:LEU:H	1.70	0.57
13:d:967:MET:HA	13:d:967:MET:HE2	1.85	0.57
11:A:334:THR:HA	11:A:489:GLN:O	2.04	0.57
14:E:586:TYR:HB3	14:E:605:HIS:HB3	1.85	0.57
29:X:29:DA:H2"	29:X:30:DC:C6	2.39	0.57
30:Y:28:DT:H2'	30:Y:29:DA:N7	2.18	0.57
38:s:73:PHE:HD2	38:s:99:ILE:HD13	1.69	0.57
1:0:8:ARG:NH2	1:0:37:LEU:HB3	2.12	0.57
4:3:215:LEU:HD22	4:3:230:VAL:HG21	1.87	0.57
28:V:148:LYS:HG3	28:V:149:LYS:HE2	1.86	0.57
35:p:309:PHE:HE2	42:w:40:ARG:HB2	1.69	0.57
8:7:252:THR:HG1	8:7:255:THR:HG1	1.51	0.57
15:F:81:GLU:HB3	15:F:83:LEU:HD13	1.85	0.57
15:F:315:ARG:CZ	15:F:369:PRO:HB3	2.35	0.57
38:s:21:CYS:SG	38:s:26:TYR:HB2	2.44	0.57
38:s:48:PRO:HA	38:s:53:PRO:HG2	1.85	0.57
42:w:69:ILE:HG22	42:w:71:ASP:H	1.68	0.57
8:7:240:ASP:OD1	8:7:241:ASN:N	2.37	0.57
10:Z:4:G2L:H2'	49:p:1201:W0F:C10	2.34	0.57
12:B:629:ARG:NH1	12:B:658:ASP:OD2	2.37	0.57
22:P:297:LYS:NZ	22:P:323:GLU:OE2	2.38	0.57
36:q:260:GLN:HE22	44:y:92:THR:HG22	1.69	0.57
15:f:219:GLU:OE1	15:f:219:GLU:N	2.25	0.57
1:0:41:ARG:CD	27:U:169:PRO:CG	2.74	0.57
1:0:84:LYS:CB	1:0:136:ASN:ND2	2.68	0.57
7:6:625:GLN:OE1	7:6:639:ARG:NH1	2.36	0.57
1:0:1:MET:SD	8:7:345:ARG:CD	2.93	0.57
22:P:186:ARG:NH1	22:P:244:LEU:O	2.38	0.57
27:U:160:GLU:OE2	27:U:162:GLU:N	2.38	0.57
12:B:837:LEU:HD22	17:H:213:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:e:257:GLU:CD	14:e:257:GLU:N	2.63	0.57
1:0:41:ARG:CB	27:U:169:PRO:CG	2.81	0.56
12:B:769:LYS:O	12:B:769:LYS:HG3	2.03	0.56
13:D:960:GLU:HB3	13:D:983:ARG:CG	2.35	0.56
25:S:73:ARG:NH1	25:S:76:ARG:HD2	2.20	0.56
28:V:148:LYS:HB3	28:V:183:LYS:HE3	1.87	0.56
34:o:756:ALA:HB2	34:o:786:ALA:HB2	1.87	0.56
35:p:55:VAL:HG12	35:p:91:ILE:HD13	1.87	0.56
15:f:320:ARG:CB	15:f:320:ARG:HH11	2.17	0.56
15:F:335:ARG:HH21	15:F:378:ALA:HB1	1.69	0.56
21:O:62:LEU:HA	21:O:76:LEU:HD23	1.86	0.56
24:R:134:ILE:HG12	24:R:171:GLU:HG3	1.86	0.56
28:V:192:VAL:HG21	28:V:203:PHE:HB3	1.85	0.56
35:p:82:PRO:HB3	35:p:134:LYS:HG2	1.87	0.56
3:2:223:LEU:CD1	8:7:726:GLN:OE1	2.53	0.56
7:6:281:GLN:NE2	7:6:482:PHE:O	2.37	0.56
8:7:664:VAL:HG21	8:7:679:PHE:CE1	2.40	0.56
14:E:345:MET:HE3	14:E:346:PRO:HD2	1.88	0.56
27:U:152:PHE:CD2	40:u:95:VAL:CG1	2.88	0.56
35:p:761:THR:HG23	35:p:1000:THR:HA	1.87	0.56
1:0:8:ARG:CD	27:U:173:ALA:H	2.13	0.56
4:3:108:ASN:HD21	5:4:123:LEU:HD22	1.71	0.56
7:6:54:ASP:HB2	7:6:58:ALA:HB3	1.87	0.56
11:A:851:ASP:OD1	11:A:851:ASP:N	2.38	0.56
12:B:259:ASP:HB3	12:B:262:MET:O	2.06	0.56
26:T:194:HIS:CG	26:T:195:GLN:H	2.23	0.56
3:2:261:SER:OG	3:2:265:GLN:O	2.22	0.56
11:A:401:ASN:H	11:A:401:ASN:HD22	1.53	0.56
13:d:910:LEU:HD11	20:l:88:ALA:HB2	1.86	0.56
14:e:527:ILE:HG22	14:e:527:ILE:O	2.05	0.56
5:4:433:PHE:CE2	6:5:38:ILE:HG23	2.41	0.56
20:L:113:VAL:O	20:L:114:LYS:C	2.49	0.56
25:S:72:ASN:HB3	26:T:201:ASP:OD2	2.06	0.56
28:V:86:LYS:NZ	28:V:140:LYS:HD2	2.21	0.56
34:o:1230:GLN:HG2	34:o:1234:LYS:HE3	1.87	0.56
12:B:560:TYR:CD2	12:B:581:ILE:HD11	2.40	0.56
13:D:956:GLN:HA	13:D:956:GLN:HE21	1.69	0.56
35:p:570:ASN:ND2	35:p:616:THR:OG1	2.37	0.56
38:s:26:TYR:HA	38:s:64:HIS:HA	1.87	0.56
13:d:917:ILE:HD11	13:d:1063:LEU:HD13	1.87	0.56
15:f:223:TYR:HD2	15:f:255:MET:HE1	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:27:LYS:CE	12:B:490:SER:HB3	2.35	0.56
34:o:131:ALA:HA	34:o:134:LYS:HE2	1.88	0.56
14:e:636:HIS:HD2	14:e:638:ASN:H	1.53	0.56
1:0:85:ARG:NH2	1:0:140:LEU:CA	2.69	0.56
4:3:242:ILE:C	4:3:243:LEU:HD12	2.31	0.56
5:4:393:LEU:HD21	7:6:511:TRP:CH2	2.41	0.56
8:7:606:GLU:O	8:7:666:ARG:NH2	2.39	0.56
11:A:402:PHE:HA	11:A:407:GLN:NE2	2.20	0.56
15:F:265:GLU:OE2	15:F:265:GLU:HA	2.06	0.56
20:L:119:HIS:NE2	20:L:123:GLN:OE1	2.38	0.56
34:o:1147:SER:HA	34:o:1153:ARG:HB2	1.87	0.56
34:o:1366:PHE:HB2	34:o:1374:VAL:HG21	1.87	0.56
15:f:280:ILE:O	15:f:284:ARG:HG3	2.05	0.56
12:B:61:ASN:O	12:B:130:VAL:HG23	2.06	0.56
14:E:468:ASN:ND2	15:F:128:ASP:O	2.39	0.56
35:p:265:GLN:OE1	35:p:324:ARG:NH1	2.38	0.56
2:1:456:ASP:OD1	2:1:457:ILE:HD12	2.06	0.55
4:3:44:LEU:HD21	4:3:162:LEU:HD13	1.89	0.55
34:o:11:SER:N	35:p:1135:TYR:HH	2.03	0.55
34:o:1128:ILE:HG23	34:o:1414:ILE:HB	1.86	0.55
26:T:94:THR:HG22	26:T:109:ILE:HG22	1.88	0.55
34:o:321:GLU:HG3	34:o:341:GLN:HE21	1.72	0.55
34:o:1487:PRO:HG2	39:t:78:PRO:HA	1.88	0.55
3:2:59:ARG:NH2	3:2:166:GLU:OE1	2.38	0.55
7:6:444:HIS:O	7:6:472:ARG:NH1	2.39	0.55
8:7:309:VAL:HG12	8:7:309:VAL:O	2.07	0.55
24:R:39:LEU:HD11	34:o:425:ASP:HB3	1.87	0.55
28:V:155:LEU:HD21	28:V:204:ASN:H	1.71	0.55
1:0:20:LYS:HE3	1:0:62:LEU:HD13	1.87	0.55
5:4:407:VAL:N	5:4:443:VAL:O	2.37	0.55
7:6:361:CYS:SG	7:6:405:VAL:HG13	2.46	0.55
15:F:312:ILE:HG13	15:F:334:ALA:HB3	1.88	0.55
15:F:406:VAL:HG11	15:F:420:ALA:HB2	1.88	0.55
25:S:168:ASN:HA	35:p:248:LYS:HD2	1.88	0.55
28:V:149:LYS:HA	28:V:152:LEU:HD12	1.87	0.55
28:V:170:ASP:OD1	28:V:171:ILE:N	2.40	0.55
36:q:56:SER:HB2	36:q:158:GLU:H	1.71	0.55
15:f:253:TYR:O	15:f:254:GLN:HB3	2.06	0.55
20:l:99:ALA:HB1	20:l:111:LEU:HD11	1.87	0.55
7:6:528:LYS:CE	7:6:531:ILE:HD13	2.35	0.55
7:6:664:SER:O	7:6:667:THR:OG1	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:964:GLU:HA	13:D:982:LEU:HG	1.87	0.55
24:R:105:ARG:NH1	30:Y:13:DA:N7	2.53	0.55
27:U:30:HIS:CD2	27:U:62:VAL:HG13	2.42	0.55
27:U:56:ARG:NH1	27:U:60:ARG:HH11	2.02	0.55
34:o:381:PRO:HB3	34:o:480:SER:HA	1.87	0.55
38:s:13:ILE:HD11	38:s:132:GLN:HG3	1.89	0.55
11:A:511:LEU:HD22	11:A:511:LEU:N	2.11	0.55
15:F:83:LEU:CD1	15:F:83:LEU:N	2.67	0.55
25:S:167:ARG:HH11	25:S:168:ASN:H	1.53	0.55
30:Y:16:DA:H2"	30:Y:17:DC:OP2	2.04	0.55
3:2:174:LEU:C	8:7:591:GLY:O	2.49	0.55
7:6:83:HIS:ND1	7:6:115:GLU:OE2	2.39	0.55
8:7:114:ASN:C	8:7:114:ASN:HD22	2.15	0.55
14:E:474:THR:HG22	15:F:61:GLY:HA2	1.88	0.55
15:F:86:PHE:CD1	15:F:86:PHE:N	2.75	0.55
36:q:19:VAL:HG23	36:q:241:PRO:HB2	1.89	0.55
13:d:960:GLU:HG2	13:d:963:ARG:HH21	1.71	0.55
1:0:8:ARG:CZ	1:0:34:CYS:SG	2.94	0.55
11:A:1200:THR:C	11:A:1204:GLU:HG2	2.30	0.55
15:F:71:ILE:HD11	18:I:35:VAL:HG13	1.89	0.55
27:U:14:LEU:HD11	27:U:194:THR:HG23	1.87	0.55
28:V:234:GLU:HB3	28:V:238:LYS:HZ3	1.72	0.55
11:A:1052:ARG:HD2	11:A:1052:ARG:O	2.07	0.55
14:E:561:SER:HB2	14:E:588:VAL:HB	1.88	0.55
28:V:213:ASP:O	28:V:217:GLN:N	2.39	0.55
34:o:26:LEU:HD13	34:o:31:LEU:HD21	1.89	0.55
44:y:88:THR:O	44:y:92:THR:HG23	2.05	0.55
5:4:393:LEU:CD2	7:6:511:TRP:CH2	2.90	0.54
7:6:528:LYS:CD	7:6:531:ILE:CD1	2.85	0.54
11:A:463:PRO:HD3	15:F:222:LEU:HB2	1.89	0.54
13:D:963:ARG:O	13:D:982:LEU:HD11	2.07	0.54
15:F:87:HIS:HB2	18:I:45:ARG:HE	1.71	0.54
15:F:433:PRO:HA	15:F:436:ALA:HB3	1.90	0.54
24:R:90:ALA:HB3	34:o:324:GLY:HA2	1.88	0.54
34:o:628:VAL:HA	34:o:638:GLY:HA3	1.88	0.54
35:p:43:GLN:NE2	35:p:482:LEU:O	2.40	0.54
8:7:17:ILE:HD11	8:7:22:PHE:CZ	2.42	0.54
11:A:355:VAL:O	11:A:355:VAL:HG23	2.07	0.54
21:O:16:GLN:NE2	21:O:20:ASP:OD2	2.40	0.54
22:P:206:GLU:HB3	22:P:207:PRO:HD3	1.89	0.54
34:o:26:LEU:HG	35:p:1168:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:p:794:VAL:HG22	35:p:967:ILE:HG22	1.89	0.54
1:0:42:GLY:CA	27:U:168:MET:HE1	2.33	0.54
4:3:229:TRP:CZ3	5:4:58:ARG:HD2	2.42	0.54
27:U:32:LEU:O	27:U:36:ILE:HG12	2.08	0.54
29:X:8:DC:H2"	29:X:9:DA:C8	2.42	0.54
34:o:769:MET:HE3	35:p:970:HIS:CD2	2.42	0.54
35:p:709:SER:HB2	35:p:767:LEU:HD11	1.89	0.54
1:0:8:ARG:NH2	1:0:37:LEU:HD22	2.21	0.54
7:6:87:GLU:OE2	7:6:145:LYS:NZ	2.40	0.54
8:7:365:VAL:HG22	8:7:365:VAL:O	2.08	0.54
28:V:147:ASP:HB3	28:V:150:ALA:H	1.71	0.54
28:V:170:ASP:HA	28:V:173:GLU:HG2	1.89	0.54
29:X:8:DC:H2"	29:X:9:DA:H8	1.72	0.54
35:p:67:LEU:HD21	35:p:416:ARG:HG3	1.90	0.54
4:3:108:ASN:OD1	5:4:123:LEU:CD1	2.51	0.54
5:4:80:SER:O	5:4:84:GLU:OE1	2.25	0.54
7:6:632:SER:OG	7:6:676:ARG:NH2	2.41	0.54
8:7:80:ILE:HD11	8:7:206:VAL:HB	1.90	0.54
11:A:489:GLN:NE2	11:A:489:GLN:H	2.05	0.54
14:E:524:LEU:O	14:E:527:ILE:HG12	2.07	0.54
15:F:418:ILE:HD12	15:F:418:ILE:N	2.20	0.54
40:u:55:GLY:HA3	40:u:69:PRO:HG2	1.89	0.54
1:0:85:ARG:NH2	1:0:140:LEU:HA	2.22	0.54
2:1:486:LEU:O	2:1:490:VAL:HG23	2.06	0.54
3:2:69:ARG:HB2	8:7:563:ARG:HH22	1.72	0.54
26:T:188:PHE:HB3	28:V:76:GLY:O	2.06	0.54
30:Y:5:DA:H2"	35:p:446:TYR:CD2	2.42	0.54
13:d:911:GLN:NE2	20:l:69:GLU:OE2	2.41	0.54
14:e:368:ASN:ND2	14:e:701:GLY:HA3	2.23	0.54
15:f:390:THR:HG23	15:f:391:LEU:HD22	1.89	0.54
8:7:437:CYS:SG	8:7:438:MET:N	2.81	0.54
12:B:544:LEU:HD23	12:B:590:ILE:HD11	1.88	0.54
15:F:403:ILE:O	15:F:406:VAL:HG22	2.08	0.54
23:Q:15:ARG:HA	23:Q:18:ILE:HD12	1.89	0.54
28:V:89:HIS:NE2	28:V:138:ALA:O	2.38	0.54
34:o:663:ASP:OD1	34:o:666:ARG:NH1	2.40	0.54
34:o:1189:ASP:HA	34:o:1192:TRP:CE2	2.42	0.54
3:2:69:ARG:HB2	8:7:563:ARG:NH2	2.23	0.54
28:V:156:ASP:O	28:V:160:GLN:HG2	2.08	0.54
34:o:460:ARG:HD2	34:o:494:ALA:HB2	1.90	0.54
35:p:1088:GLU:O	35:p:1091:ARG:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:q:38:PHE:HE1	36:q:245:VAL:HA	1.72	0.54
15:f:352:GLN:O	15:f:356:THR:OG1	2.25	0.54
4:3:242:ILE:CD1	5:4:75:VAL:C	2.81	0.54
12:B:248:SER:OG	12:B:322:MET:SD	2.65	0.54
12:B:628:ILE:O	12:B:644:GLN:NE2	2.41	0.54
25:S:115:LYS:NZ	25:S:117:GLY:O	2.37	0.54
27:U:76:MET:HG2	27:U:88:ARG:HB3	1.89	0.54
34:o:459:ASN:HD22	34:o:469:MET:HE3	1.73	0.54
44:y:12:LEU:HD11	44:y:18:LYS:HE2	1.88	0.54
19:j:123:LEU:C	19:j:125:ASP:N	2.66	0.54
1:0:85:ARG:HH12	1:0:140:LEU:N	2.06	0.54
5:4:408:LEU:HD21	5:4:440:LEU:HD22	1.89	0.54
12:B:571:LEU:HD21	12:B:619:MET:HE1	1.89	0.54
12:B:808:PRO:HA	12:B:864:ASN:HB3	1.90	0.54
13:D:963:ARG:C	13:D:982:LEU:CD1	2.79	0.54
13:D:998:GLN:HG3	13:D:1002:ARG:NH1	2.22	0.54
4:3:195:VAL:CG1	4:3:203:LEU:HD23	2.38	0.53
5:4:265:LEU:HD12	5:4:270:LEU:HD12	1.90	0.53
7:6:377:GLN:OE1	7:6:381:TRP:NE1	2.40	0.53
33:m:110:LEU:N	33:m:110:LEU:HD23	2.23	0.53
38:s:106:VAL:HG21	38:s:110:MET:HG3	1.89	0.53
16:G:149:ARG:O	16:G:149:ARG:HG3	2.08	0.53
34:o:375:ILE:HG21	34:o:535:MET:HE1	1.91	0.53
38:s:17:ILE:HD13	38:s:74:VAL:HG11	1.90	0.53
42:w:59:THR:HB	42:w:61:GLU:HG3	1.90	0.53
8:7:420:PRO:HA	8:7:431:PRO:HB3	1.89	0.53
12:B:345:CYS:HA	12:B:348:GLN:HE21	1.73	0.53
13:D:922:GLN:NE2	20:L:71:ASP:OD2	2.41	0.53
14:E:563:GLU:HG2	14:E:587:PRO:HG3	1.90	0.53
14:E:653:LEU:HB2	14:E:663:ARG:HB2	1.90	0.53
24:R:87:GLY:HA3	34:o:326:PRO:HA	1.90	0.53
31:c:33:LEU:HD13	19:j:197:MET:HE1	1.91	0.53
34:o:1436:VAL:O	34:o:1440:MET:HG2	2.08	0.53
35:p:715:ASP:OD1	35:p:715:ASP:N	2.41	0.53
1:0:85:ARG:HH22	1:0:140:LEU:HA	1.72	0.53
3:2:87:LEU:HD11	3:2:229:LYS:HG2	1.91	0.53
3:2:337:GLU:O	3:2:340:ASN:ND2	2.38	0.53
8:7:44:SER:OG	8:7:46:THR:O	2.16	0.53
13:D:998:GLN:HG3	13:D:1002:ARG:HH12	1.74	0.53
14:E:645:GLY:H	14:E:675:LEU:HD11	1.73	0.53
34:o:1258:ARG:HH22	34:o:1260:ARG:HH21	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:e:610:ARG:HD3	14:e:619:PRO:HG3	1.89	0.53
3:2:88:LEU:HD23	3:2:131:LEU:HD21	1.91	0.53
6:5:32:LYS:HB3	12:B:540:LYS:HG3	1.90	0.53
7:6:568:LEU:HD11	7:6:606:PHE:HB3	1.90	0.53
8:7:133:LYS:O	8:7:137:LEU:HD23	2.07	0.53
8:7:289:VAL:HG22	8:7:324:ARG:NH1	2.23	0.53
12:B:937:THR:HG23	12:B:939:ASN:H	1.74	0.53
1:0:8:ARG:HB2	27:U:172:ASP:OD2	2.09	0.53
8:7:488:VAL:HG23	8:7:488:VAL:O	2.09	0.53
11:A:395:ASP:OD1	11:A:395:ASP:N	2.41	0.53
30:Y:29:DA:H2'	30:Y:30:DT:C6	2.43	0.53
35:p:75:SER:O	35:p:77:GLU:HG2	2.09	0.53
49:p:1201:W0F:C01	49:p:1201:W0F:C20	2.85	0.53
14:e:423:PRO:HG2	14:e:426:ARG:HB2	1.91	0.53
14:e:646:SER:OG	14:e:647:ALA:N	2.41	0.53
6:5:38:ILE:HG22	6:5:39:ASP:N	2.24	0.53
13:D:910:LEU:HD11	20:L:88:ALA:HB2	1.91	0.53
15:F:335:ARG:HD2	15:F:382:GLU:HB2	1.90	0.53
7:6:528:LYS:CD	7:6:531:ILE:HD11	2.39	0.53
27:U:139:LEU:CD1	40:u:149:GLY:O	2.57	0.53
35:p:223:SER:HB2	35:p:349:PRO:HD2	1.90	0.53
15:f:283:MET:HG3	15:f:329:LEU:HD11	1.91	0.53
2:1:127:LEU:HD12	2:1:467:ALA:HA	1.91	0.53
4:3:44:LEU:HD22	4:3:227:LEU:HB3	1.91	0.53
6:5:31:LYS:HB3	12:B:540:LYS:HZ1	1.44	0.53
7:6:528:LYS:HG3	7:6:531:ILE:HD12	1.88	0.53
34:o:189:PRO:HA	34:o:205:VAL:HG21	1.90	0.53
34:o:495:ASP:OD1	34:o:495:ASP:N	2.42	0.53
8:7:28:LEU:HD22	8:7:55:LEU:HD23	1.91	0.53
11:A:675:ASP:OD1	16:G:78:LYS:NZ	2.37	0.53
12:B:66:ASN:HD21	12:B:119:PRO:HB3	1.73	0.53
29:X:6:DT:H2"	29:X:7:DT:H2'	1.90	0.53
34:o:110:VAL:HG13	34:o:115:SER:HA	1.91	0.53
34:o:602:CYS:HB2	34:o:655:ILE:HD12	1.91	0.53
35:p:841:ARG:HD2	35:p:895:PHE:CZ	2.44	0.53
40:u:148:VAL:N	40:u:160:ILE:O	2.42	0.53
3:2:174:LEU:HD21	3:2:203:ALA:HB2	1.89	0.52
4:3:50:PHE:HZ	5:4:118:LEU:HD13	1.61	0.52
4:3:108:ASN:CG	5:4:123:LEU:HD13	2.34	0.52
5:4:32:ASP:OD1	5:4:33:ARG:N	2.42	0.52
14:E:304:LYS:NZ	14:E:335:GLU:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:G:181:TRP:CE3	16:G:181:TRP:O	2.63	0.52
27:U:183:GLN:NE2	28:V:211:SER:O	2.43	0.52
34:o:863:ARG:NH2	34:o:1415:THR:HG22	2.24	0.52
35:p:789:ASN:HB3	35:p:795:ILE:HG13	1.91	0.52
13:D:960:GLU:HG2	13:D:983:ARG:HD3	1.92	0.52
14:E:562:SER:OG	14:E:564:ASP:OD1	2.28	0.52
26:T:188:PHE:HB3	28:V:76:GLY:C	2.35	0.52
27:U:146:ASP:HB2	27:U:147:PRO:HD2	1.90	0.52
34:o:938:LEU:HD22	34:o:1005:HIS:HD1	1.74	0.52
8:7:393:ASP:OD1	8:7:394:PHE:N	2.42	0.52
13:D:873:LEU:HD21	20:L:92:ILE:HD11	1.91	0.52
13:D:998:GLN:HB2	13:D:1002:ARG:HH22	1.73	0.52
30:Y:-11:DG:H1'	30:Y:-10:DA:H5'	1.91	0.52
1:0:83:ASN:CG	1:0:140:LEU:HD12	2.34	0.52
5:4:438:LYS:HE2	12:B:621:ALA:H	1.74	0.52
12:B:202:TRP:HB2	12:B:238:LEU:HB3	1.92	0.52
26:T:238:GLU:HB3	28:V:130:ILE:CD1	2.40	0.52
26:T:238:GLU:OE1	28:V:82:VAL:HG11	2.09	0.52
34:o:1173:THR:HG22	34:o:1214:VAL:HG22	1.91	0.52
42:w:12:VAL:HG23	42:w:50:ASN:HD21	1.73	0.52
15:f:447:ALA:O	15:f:453:GLY:HA2	2.09	0.52
15:F:39:LEU:HD11	18:I:51:LEU:HD21	1.92	0.52
27:U:184:ILE:HG23	27:U:187:ILE:HB	1.91	0.52
34:o:1143:LEU:HD21	34:o:1336:LEU:HD11	1.91	0.52
7:6:340:LEU:HD23	7:6:491:ALA:HB2	1.92	0.52
27:U:139:LEU:CG	40:u:159:ALA:C	2.76	0.52
34:o:375:ILE:HD13	34:o:485:ASN:HD22	1.75	0.52
35:p:860:VAL:HG12	35:p:896:LEU:HD22	1.92	0.52
5:4:413:LEU:HB2	12:B:672:PHE:HE1	1.74	0.52
15:F:273:GLN:H	15:F:273:GLN:CD	2.17	0.52
28:V:117:GLN:O	28:V:121:THR:OG1	2.18	0.52
34:o:392:GLU:HB2	34:o:448:ARG:NH1	2.24	0.52
40:u:97:LEU:HD23	40:u:108:ILE:HD13	1.92	0.52
14:e:595:PRO:HD2	14:e:639:SER:HB3	1.91	0.52
7:6:181:HIS:O	7:6:184:VAL:HG12	2.10	0.52
12:B:529:VAL:HG11	12:B:560:TYR:HB2	1.91	0.52
14:E:601:VAL:HG21	14:E:642:VAL:HG11	1.92	0.52
15:F:257:PRO:O	15:F:261:THR:OG1	2.26	0.52
24:R:177:PHE:HB3	24:R:188:LYS:HG3	1.92	0.52
28:V:175:LEU:HB2	28:V:180:LYS:HE2	1.91	0.52
14:e:607:ARG:NH1	18:i:87:PRO:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:318:CYS:SG	15:f:326:HIS:HB3	2.49	0.52
12:B:66:ASN:OD1	12:B:187:ARG:NH1	2.43	0.52
14:E:278:ASP:OD1	14:E:278:ASP:N	2.43	0.52
15:F:219:GLU:HG2	17:H:156:PRO:C	2.35	0.52
34:o:330:GLN:HE21	34:o:334:ARG:HE	1.57	0.52
36:q:38:PHE:CE1	36:q:245:VAL:HA	2.45	0.52
2:1:136:VAL:HG11	2:1:502:VAL:HG12	1.92	0.52
8:7:115:LEU:HD13	8:7:191:PRO:HB2	1.92	0.52
11:A:339:ALA:HA	11:A:497:PRO:HG3	1.92	0.52
14:E:522:ASP:OD1	14:E:522:ASP:N	2.42	0.52
19:J:114:THR:HB	19:J:117:VAL:HB	1.92	0.52
19:J:137:TYR:OH	19:J:141:ARG:NH2	2.43	0.52
27:U:48:MET:O	27:U:52:LEU:N	2.42	0.52
30:Y:19:DA:H8	30:Y:19:DA:OP2	1.93	0.52
34:o:1005:HIS:HD2	34:o:1007:ILE:HG22	1.75	0.52
3:2:54:ARG:NH2	3:2:245:SER:O	2.42	0.51
13:D:960:GLU:HB3	13:D:983:ARG:HH11	1.74	0.51
14:E:781:VAL:HG13	15:F:62:LYS:HD3	1.90	0.51
27:U:110:MET:O	27:U:114:ILE:HG12	2.10	0.51
29:X:9:DA:H4'	34:o:1417:HIS:CG	2.45	0.51
34:o:455:ILE:HD13	34:o:516:GLN:HB2	1.91	0.51
34:o:1386:ILE:HD12	34:o:1398:LEU:HD21	1.91	0.51
36:q:154:ARG:HD3	43:x:64:PRO:HD3	1.92	0.51
14:e:747:LEU:HG	14:e:747:LEU:O	2.09	0.51
14:E:423:PRO:HG2	14:E:426:ARG:HB2	1.92	0.51
15:F:243:LEU:HD21	15:F:284:ARG:HB3	1.92	0.51
27:U:128:LYS:O	27:U:162:GLU:HB3	2.10	0.51
27:U:139:LEU:CD1	40:u:159:ALA:CA	2.86	0.51
33:m:28:ARG:HH21	33:m:31:LEU:HD21	1.76	0.51
38:s:59:THR:HB	38:s:73:PHE:HE1	1.75	0.51
1:0:8:ARG:NE	27:U:173:ALA:CB	2.73	0.51
11:A:828:GLU:HA	11:A:831:LYS:HB2	1.92	0.51
28:V:97:LEU:HG	28:V:101:GLU:CD	2.35	0.51
35:p:737:ILE:HG22	35:p:739:ASN:H	1.75	0.51
8:7:126:PHE:CE2	8:7:128:LYS:HB2	2.46	0.51
8:7:709:THR:HG22	8:7:710:VAL:N	2.25	0.51
12:B:656:GLU:HG2	12:B:661:ALA:HB3	1.92	0.51
22:P:295:MET:HG2	22:P:298:PRO:HD2	1.91	0.51
24:R:50:SER:C	35:p:1069:ILE:HG13	2.36	0.51
27:U:139:LEU:CD2	40:u:158:PHE:O	2.53	0.51
15:f:320:ARG:NH1	15:f:320:ARG:CB	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:41:ARG:C	27:U:168:MET:CE	2.81	0.51
2:1:471:LEU:HD13	2:1:475:PHE:HE2	1.75	0.51
11:A:338:VAL:HG12	11:A:497:PRO:HD3	1.91	0.51
16:G:181:TRP:CD2	16:G:181:TRP:C	2.87	0.51
21:O:57:ASN:OD1	21:O:58:PHE:N	2.44	0.51
26:T:160:GLN:O	26:T:163:ILE:HG12	2.11	0.51
34:o:894:ASP:O	34:o:1022:ILE:HD13	2.10	0.51
3:2:204:GLU:OE1	3:2:209:THR:OG1	2.28	0.51
4:3:165:LYS:NZ	4:3:167:ALA:O	2.37	0.51
5:4:266:ARG:HE	5:4:277:LYS:HZ2	1.56	0.51
7:6:363:VAL:HG21	7:6:378:PHE:HE2	1.75	0.51
7:6:463:LYS:O	7:6:484:ILE:HG23	2.10	0.51
12:B:90:THR:O	12:B:968:ARG:NH2	2.43	0.51
12:B:489:GLN:OE1	12:B:489:GLN:N	2.34	0.51
12:B:780:LYS:O	17:H:183:ARG:NH1	2.44	0.51
17:H:52:SER:O	19:J:194:THR:HA	2.10	0.51
31:c:21:LEU:HD12	31:c:21:LEU:O	2.11	0.51
14:e:650:THR:HG22	14:e:666:THR:HG22	1.93	0.51
12:B:983:ARG:HH11	12:B:983:ARG:HG3	1.76	0.51
14:E:746:ASP:OD1	14:E:746:ASP:N	2.42	0.51
34:o:597:PRO:HD2	34:o:600:ILE:HD12	1.91	0.51
34:o:1228:MET:HE3	34:o:1247:PHE:HB2	1.91	0.51
34:o:1429:LYS:HB2	34:o:1438:VAL:HG11	1.92	0.51
8:7:3:LEU:O	8:7:9:LEU:HD12	2.11	0.51
9:N:8:HYP:HD23	34:o:1108:HIS:HE1	1.74	0.51
11:A:1163:ARG:HB3	16:G:183:ILE:HG22	1.92	0.51
12:B:739:ASN:ND2	12:B:782:ASN:OD1	2.44	0.51
27:U:74:CYS:HA	27:U:91:TYR:O	2.11	0.51
31:c:1:MET:HG3	15:f:126:PRO:HB3	1.93	0.51
8:7:726:GLN:CG	8:7:727:PRO:CD	2.84	0.51
24:R:128:ILE:HG23	24:R:183:VAL:HG11	1.93	0.51
25:S:73:ARG:CZ	26:T:229:HIS:HB2	2.41	0.51
27:U:164:ASP:HB2	27:U:167:ALA:HA	1.93	0.51
30:Y:-31:DC:H2"	30:Y:-30:DG:C8	2.46	0.51
34:o:43:TYR:HB3	34:o:53:LYS:HE3	1.93	0.51
34:o:927:GLU:O	34:o:931:ARG:HG2	2.10	0.51
38:s:14:ARG:O	38:s:18:MET:HG2	2.10	0.51
4:3:100:LYS:HG2	5:4:124:GLY:C	2.35	0.50
5:4:409:TYR:HB2	5:4:412:PHE:HZ	1.74	0.50
8:7:45:GLY:O	8:7:48:LYS:NZ	2.44	0.50
8:7:637:LEU:HD13	8:7:651:PHE:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:R:248:ARG:NH2	24:R:287:GLN:OE1	2.44	0.50
27:U:139:LEU:HD11	40:u:158:PHE:O	2.11	0.50
28:V:179:GLN:O	28:V:183:LYS:HB2	2.10	0.50
28:V:227:SER:O	28:V:231:GLU:HG2	2.11	0.50
34:o:217:SER:HB3	34:o:220:ARG:HG3	1.93	0.50
34:o:1158:LEU:HD23	34:o:1336:LEU:HD13	1.93	0.50
34:o:1381:GLU:O	34:o:1385:VAL:HG13	2.11	0.50
34:o:1443:ALA:HB2	35:p:1167:ILE:HG23	1.93	0.50
15:f:24:GLU:HG2	20:l:145:THR:HG21	1.93	0.50
7:6:274:GLN:OE1	7:6:459:GLN:NE2	2.44	0.50
8:7:284:GLU:HA	8:7:287:ARG:HG2	1.94	0.50
8:7:377:GLU:OE1	8:7:377:GLU:N	2.44	0.50
14:E:256:HIS:HB3	14:E:259:GLU:HG2	1.93	0.50
20:L:126:MET:HE3	20:L:128:ILE:HD11	1.93	0.50
24:R:127:ARG:HD2	24:R:183:VAL:HB	1.93	0.50
34:o:544:ALA:HB2	34:o:680:LEU:HD13	1.93	0.50
35:p:75:SER:OG	35:p:77:GLU:OE2	2.26	0.50
35:p:309:PHE:CE2	42:w:40:ARG:HB2	2.46	0.50
14:e:500:THR:HG22	14:e:502:LYS:H	1.76	0.50
3:2:121:SER:OG	3:2:127:HIS:NE2	2.39	0.50
11:A:510:ILE:HB	11:A:511:LEU:HD13	1.93	0.50
12:B:274:LEU:HG	12:B:278:LYS:HE2	1.93	0.50
30:Y:-9:DT:H2"	30:Y:-8:DG:C8	2.46	0.50
34:o:1481:LYS:HG2	40:u:20:PRO:HA	1.94	0.50
5:4:390:GLN:HE21	5:4:394:TRP:NE1	2.09	0.50
12:B:983:ARG:HG3	12:B:983:ARG:NH1	2.26	0.50
22:P:169:VAL:HG21	29:X:-27:DA:C2	2.47	0.50
31:c:77:LEU:HD23	31:c:77:LEU:O	2.11	0.50
34:o:1440:MET:SD	35:p:1167:ILE:HD11	2.52	0.50
14:e:527:ILE:O	14:e:527:ILE:CG2	2.59	0.50
1:0:8:ARG:HD3	1:0:34:CYS:SG	2.52	0.50
2:1:412:GLU:OE1	2:1:412:GLU:N	2.44	0.50
4:3:108:ASN:ND2	5:4:123:LEU:HD22	2.26	0.50
25:S:142:ASN:OD1	25:S:143:TRP:N	2.44	0.50
34:o:1294:THR:HG21	35:p:245:GLN:NE2	2.26	0.50
40:u:94:LYS:HA	40:u:119:PHE:HB3	1.94	0.50
41:v:113:SER:HB3	41:v:126:GLN:HG2	1.93	0.50
2:1:471:LEU:HD13	2:1:475:PHE:CE2	2.47	0.50
2:1:524:HIS:ND1	3:2:270:SER:OG	2.39	0.50
7:6:369:VAL:HG11	7:6:615:PHE:HA	1.93	0.50
15:F:316:GLN:NE2	15:F:319:LEU:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:93:GLU:O	20:L:97:THR:HG23	2.11	0.50
34:o:201:GLU:HG3	34:o:213:LYS:HG3	1.94	0.50
34:o:463:THR:HG21	35:p:1090:GLU:HG3	1.92	0.50
34:o:565:MET:HE1	44:y:74:ARG:HB2	1.94	0.50
35:p:297:MET:O	35:p:301:VAL:HG23	2.11	0.50
41:v:65:TYR:HD1	41:v:84:ARG:HG2	1.76	0.50
13:d:1080:TYR:OH	14:e:606:ASP:OD2	2.26	0.50
13:D:998:GLN:NE2	26:T:186:MET:SD	2.85	0.50
17:H:113:ARG:O	17:H:116:ARG:NH1	2.44	0.50
35:p:201:ALA:N	35:p:390:ASN:O	2.44	0.50
44:y:49:GLN:HB2	44:y:94:LEU:HD21	1.93	0.50
8:7:118:HIS:HB3	8:7:121:VAL:HG22	1.94	0.50
12:B:882:HIS:HE1	17:H:216:ALA:HB1	1.77	0.50
1:0:27:GLY:HA3	1:0:70:LYS:CD	2.34	0.50
7:6:578:PRO:HG3	7:6:602:ILE:HD11	1.94	0.50
15:F:71:ILE:HD12	18:I:38:GLN:HE21	1.76	0.50
21:O:73:THR:O	21:O:73:THR:HG22	2.12	0.50
27:U:145:PHE:HB2	27:U:153:ARG:CG	2.41	0.50
33:m:69:THR:HG22	33:m:73:MET:HE2	1.94	0.50
34:o:18:ILE:HG12	35:p:1171:MET:HB2	1.94	0.50
37:r:33:LEU:HG	37:r:84:ARG:NH2	2.26	0.50
3:2:285:THR:O	3:2:297:LYS:NZ	2.45	0.49
12:B:152:LEU:HD23	12:B:155:PRO:HB3	1.94	0.49
12:B:820:ASP:OD1	12:B:820:ASP:N	2.37	0.49
14:E:327:ASN:H	14:E:327:ASN:ND2	2.05	0.49
22:P:297:LYS:HB3	22:P:298:PRO:HD3	1.94	0.49
25:S:73:ARG:NH1	26:T:229:HIS:HB2	2.27	0.49
28:V:87:THR:O	28:V:91:ARG:HG2	2.11	0.49
28:V:113:LEU:HA	28:V:116:LYS:HE2	1.94	0.49
34:o:508:SER:HB3	34:o:511:THR:HG22	1.92	0.49
14:e:586:TYR:HB3	14:e:605:HIS:HB3	1.94	0.49
5:4:438:LYS:CE	12:B:621:ALA:HB2	2.42	0.49
7:6:650:MET:SD	7:6:656:ASN:ND2	2.82	0.49
22:P:203:ARG:NH1	30:Y:27:DT:OP1	2.45	0.49
29:X:-18:DG:H2”	29:X:-17:DG:H8	1.76	0.49
34:o:349:ARG:HH21	35:p:1070:LEU:HD21	1.77	0.49
34:o:575:PRO:HG3	34:o:594:LEU:HD11	1.94	0.49
35:p:256:ILE:HD11	35:p:373:LEU:HD21	1.93	0.49
35:p:665:ILE:HD13	35:p:673:VAL:HG21	1.93	0.49
35:p:984:CYS:SG	35:p:1046:THR:OG1	2.58	0.49
42:w:14:ILE:HG21	42:w:23:MET:HE2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:69:ARG:CG	3:2:141:GLY:H	2.23	0.49
5:4:406:GLY:HA2	5:4:444:THR:HA	1.94	0.49
8:7:284:GLU:HG2	8:7:385:THR:HG21	1.94	0.49
13:D:965:ILE:C	13:D:965:ILE:HD13	2.37	0.49
14:E:232:HIS:HD1	14:E:313:SER:HG	1.57	0.49
19:J:139:LEU:HB3	19:J:144:PHE:HB3	1.93	0.49
27:U:30:HIS:CE1	27:U:62:VAL:HG22	2.47	0.49
34:o:51:ARG:HB2	34:o:52:PRO:HD3	1.94	0.49
34:o:486:LEU:HD13	35:p:790:GLN:CD	2.38	0.49
36:q:101:PHE:CE2	36:q:122:SER:HB3	2.47	0.49
2:1:374:LEU:HD12	2:1:374:LEU:O	2.13	0.49
11:A:821:ARG:HA	11:A:821:ARG:NE	2.25	0.49
14:E:481:ASP:HB3	14:E:787:ARG:HH22	1.77	0.49
35:p:289:ILE:HD11	35:p:301:VAL:HG21	1.94	0.49
41:v:65:TYR:HE1	41:v:84:ARG:HH11	1.60	0.49
15:f:97:ALA:HB2	15:f:106:PHE:HE1	1.77	0.49
3:2:87:LEU:HD11	3:2:229:LYS:CG	2.43	0.49
7:6:449:LYS:HB3	29:X:31:DG:P	2.52	0.49
15:F:312:ILE:HG22	15:F:313:VAL:HG13	1.95	0.49
11:A:927:VAL:O	11:A:933:ASN:ND2	2.45	0.49
12:B:818:THR:OG1	12:B:819:LEU:N	2.44	0.49
27:U:139:LEU:HD11	40:u:159:ALA:CA	2.26	0.49
30:Y:-31:DC:H2"	30:Y:-30:DG:H8	1.77	0.49
35:p:792:ASP:O	35:p:943:GLY:HA3	2.12	0.49
4:3:237:GLN:HG3	5:4:51:LEU:HD21	1.94	0.49
5:4:405:GLU:O	5:4:444:THR:HG22	2.11	0.49
14:E:693:VAL:HB	14:E:707:LEU:HB2	1.94	0.49
16:G:48:HIS:HD2	16:G:54:GLY:HA2	1.78	0.49
16:G:94:MET:HE3	16:G:96:VAL:HG22	1.94	0.49
27:U:99:LEU:O	27:U:103:VAL:HG23	2.13	0.49
34:o:1243:LEU:HD21	34:o:1288:ILE:HD13	1.95	0.49
3:2:63:VAL:HG11	3:2:88:LEU:HD11	1.95	0.49
27:U:139:LEU:HD23	40:u:158:PHE:CD1	2.30	0.49
32:k:191:VAL:HG13	32:k:200:ILE:CD1	2.42	0.49
34:o:1416:ARG:O	34:o:1420:ASN:HB2	2.13	0.49
35:p:1115:GLN:HG2	35:p:1150:ARG:HG2	1.94	0.49
1:0:4:GLN:OE1	1:0:10:LYS:HD3	2.13	0.49
5:4:338:PHE:N	5:4:341:MET:O	2.44	0.49
8:7:134:CYS:O	8:7:138:THR:HG22	2.12	0.49
11:A:468:PHE:CE1	15:F:216:LEU:HD12	2.47	0.49
14:E:589:TRP:CE3	15:F:60:MET:HG3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:F:273:GLN:CD	15:F:273:GLN:N	2.70	0.49
22:P:227:GLU:OE1	22:P:318:ARG:NH2	2.44	0.49
25:S:174:PHE:HD1	42:w:40:ARG:HA	1.78	0.49
29:X:-19:DT:C2	29:X:-18:DG:N7	2.80	0.49
34:o:392:GLU:HB2	34:o:448:ARG:HH11	1.77	0.49
35:p:516:GLU:HA	35:p:520:VAL:HG22	1.95	0.49
3:2:69:ARG:HD2	8:7:563:ARG:NH2	2.28	0.49
8:7:136:SER:O	8:7:142:VAL:HG21	2.13	0.49
8:7:243:CYS:SG	8:7:443:ALA:HB3	2.53	0.49
34:o:1321:ILE:HD12	34:o:1331:LEU:HD12	1.95	0.49
35:p:320:PHE:HE1	35:p:324:ARG:HE	1.61	0.49
14:e:651:VAL:HG13	14:e:665:PHE:HB2	1.95	0.49
14:e:720:SER:OG	14:e:721:ARG:N	2.46	0.49
2:1:440:LEU:HD11	4:3:218:PRO:CD	2.43	0.48
3:2:69:ARG:HG2	3:2:141:GLY:H	1.78	0.48
3:2:348:CYS:O	4:3:146:ARG:NH2	2.45	0.48
30:Y:15:DA:H5"	30:Y:15:DA:H8	1.77	0.48
40:u:93:ASN:N	40:u:128:TYR:OH	2.42	0.48
14:e:525:GLU:OE1	14:e:525:GLU:N	2.41	0.48
14:e:633:THR:O	14:e:634:ARG:NH2	2.45	0.48
4:3:13:ILE:HD13	4:3:41:VAL:HG13	1.94	0.48
5:4:174:ASP:OD1	5:4:175:LEU:N	2.45	0.48
11:A:337:ARG:HH11	11:A:338:VAL:H	1.60	0.48
14:E:256:HIS:HB3	14:E:259:GLU:CG	2.43	0.48
14:E:651:VAL:HB	14:E:665:PHE:HB2	1.95	0.48
20:L:113:VAL:O	20:L:116:VAL:N	2.46	0.48
34:o:48:GLU:HB2	34:o:53:LYS:HD2	1.95	0.48
34:o:115:SER:OG	34:o:227:ARG:HB2	2.12	0.48
34:o:833:PRO:HB2	35:p:677:MET:HE2	1.96	0.48
37:r:108:ALA:HB2	37:r:128:GLN:HB2	1.95	0.48
37:r:112:LYS:HB3	37:r:119:GLU:HG2	1.95	0.48
2:1:456:ASP:OD1	2:1:456:ASP:N	2.47	0.48
7:6:575:LEU:O	7:6:576:ASN:OD1	2.31	0.48
8:7:81:GLU:O	8:7:84:ILE:HG22	2.13	0.48
11:A:569:ASN:HB3	11:A:572:TYR:HD2	1.78	0.48
12:B:329:LEU:HB3	12:B:342:THR:HG23	1.96	0.48
12:B:560:TYR:HD2	12:B:581:ILE:HD11	1.78	0.48
12:B:598:ARG:HH11	12:B:619:MET:HE3	1.77	0.48
13:D:1068:GLU:OE2	14:E:582:LYS:NZ	2.45	0.48
14:E:467:LEU:HD11	15:F:132:LYS:HD3	1.94	0.48
15:F:409:GLY:O	15:F:417:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:110:ASP:OD1	28:V:114:LYS:HD3	2.12	0.48
30:Y:-33:DC:H2"	30:Y:-32:DA:C8	2.49	0.48
40:u:92:VAL:HG12	40:u:119:PHE:CD1	2.48	0.48
43:x:66:GLU:HA	45:z:23:HIS:HB3	1.94	0.48
7:6:363:VAL:HG21	7:6:378:PHE:CE2	2.47	0.48
7:6:449:LYS:HD3	29:X:31:DG:P	2.53	0.48
12:B:559:LYS:HZ3	12:B:559:LYS:HB2	1.78	0.48
14:E:299:ASP:OD2	14:E:607:ARG:NH2	2.38	0.48
20:L:106:ARG:O	20:L:106:ARG:HG2	2.14	0.48
23:Q:18:ILE:HD11	23:Q:46:TRP:CZ3	2.48	0.48
27:U:150:GLY:C	40:u:93:ASN:OD1	2.57	0.48
28:V:176:PRO:O	28:V:178:SER:N	2.46	0.48
35:p:567:ILE:HD11	35:p:577:HIS:HB2	1.94	0.48
35:p:809:VAL:HG21	36:q:60:HIS:CE1	2.48	0.48
40:u:13:LEU:HD11	40:u:26:VAL:HG22	1.96	0.48
43:x:7:CYS:HB2	43:x:48:MET:HG3	1.94	0.48
8:7:115:LEU:HD12	8:7:115:LEU:O	2.13	0.48
12:B:953:LEU:HD12	12:B:979:PHE:HE2	1.79	0.48
17:H:197:THR:HB	15:f:238:LYS:HG2	1.95	0.48
27:U:30:HIS:NE2	27:U:62:VAL:HA	2.28	0.48
34:o:62:GLN:HG3	34:o:84:HIS:O	2.13	0.48
34:o:668:PHE:CZ	34:o:672:ILE:HD11	2.49	0.48
34:o:1143:LEU:HB2	34:o:1148:ALA:HB2	1.95	0.48
35:p:810:PHE:CB	35:p:927:ARG:HE	2.27	0.48
1:0:8:ARG:NH2	1:0:34:CYS:HA	2.29	0.48
2:1:481:VAL:HG23	2:1:483:THR:HG23	1.94	0.48
12:B:570:GLU:HA	12:B:625:LEU:HA	1.95	0.48
26:T:80:GLU:OE1	26:T:81:HIS:N	2.45	0.48
27:U:139:LEU:HD21	40:u:158:PHE:CD1	2.43	0.48
31:c:119:GLU:HG3	14:e:790:LEU:HD11	1.96	0.48
34:o:1292:MET:O	34:o:1296:MET:HB2	2.12	0.48
35:p:764:MET:HE1	35:p:938:ARG:NH1	2.29	0.48
1:0:8:ARG:CD	1:0:34:CYS:SG	3.01	0.48
3:2:175:THR:HG23	8:7:592:ARG:HA	1.96	0.48
8:7:52:LEU:HD21	8:7:232:VAL:HG11	1.96	0.48
8:7:310:LEU:HG	8:7:409:THR:HG21	1.95	0.48
11:A:338:VAL:HG13	11:A:360:SER:HB2	1.96	0.48
12:B:636:VAL:HG23	12:B:638:ARG:HB3	1.96	0.48
14:E:703:MET:HE2	14:E:761:LEU:HD21	1.95	0.48
17:H:39:VAL:HG12	17:H:119:ILE:HG12	1.96	0.48
25:S:169:LYS:HD2	25:S:173:HIS:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:44:LYS:HG3	27:U:89:HIS:CD2	2.48	0.48
27:U:141:ALA:O	40:u:98:PHE:CZ	2.66	0.48
35:p:298:MET:HB3	42:w:14:ILE:HD12	1.95	0.48
35:p:713:PHE:HB3	35:p:716:HIS:HD2	1.78	0.48
15:f:257:PRO:O	15:f:261:THR:OG1	2.31	0.48
1:0:63:PHE:HB2	1:0:69:ASP:OD1	2.13	0.48
2:1:427:ALA:HB1	5:4:62:LEU:CD1	2.44	0.48
34:o:456:VAL:HG21	34:o:503:LEU:HD11	1.96	0.48
35:p:117:ASN:HA	35:p:189:GLY:HA3	1.94	0.48
14:e:693:VAL:HB	14:e:707:LEU:HB2	1.94	0.48
5:4:438:LYS:CE	12:B:621:ALA:CB	2.86	0.48
25:S:71:PHE:CZ	26:T:194:HIS:HB3	2.49	0.48
27:U:114:ILE:O	27:U:174:ARG:NH2	2.47	0.48
34:o:784:VAL:HG13	35:p:978:ILE:HD11	1.96	0.48
35:p:168:ASP:N	35:p:168:ASP:OD1	2.47	0.48
35:p:271:ILE:HG21	35:p:320:PHE:CD2	2.49	0.48
35:p:918:PHE:HE2	35:p:920:LYS:HE3	1.77	0.48
3:2:253:GLY:N	3:2:310:LEU:HD21	2.29	0.48
5:4:433:PHE:CE2	6:5:38:ILE:CG2	2.97	0.48
11:A:638:PRO:HB3	16:G:39:LEU:HD23	1.95	0.48
15:F:415:ILE:O	15:F:415:ILE:HG12	2.14	0.48
24:R:131:PRO:HG3	35:p:101:ARG:HG3	1.95	0.48
28:V:234:GLU:HB3	28:V:238:LYS:NZ	2.28	0.48
5:4:398:ARG:HA	5:4:398:ARG:HE	1.79	0.47
11:A:824:ARG:HB3	11:A:863:VAL:HG12	1.95	0.47
14:E:634:ARG:HG3	14:E:675:LEU:HB2	1.95	0.47
18:I:63:LYS:NZ	18:I:69:ASP:OD1	2.47	0.47
22:P:174:LEU:HD12	22:P:178:LEU:HD11	1.94	0.47
25:S:54:LYS:HG2	25:S:59:GLU:OE1	2.13	0.47
26:T:238:GLU:OE1	28:V:130:ILE:HG13	2.14	0.47
27:U:76:MET:HB2	27:U:90:ASN:OD1	2.14	0.47
29:X:-20:DG:C8	29:X:-19:DT:H72	2.49	0.47
34:o:557:ARG:O	34:o:561:MET:HG2	2.14	0.47
34:o:1153:ARG:O	34:o:1157:ILE:HG12	2.14	0.47
34:o:1374:VAL:HG11	34:o:1411:LEU:HD21	1.95	0.47
35:p:674:MET:HE2	35:p:690:CYS:SG	2.54	0.47
35:p:1094:GLN:HB2	35:p:1103:LEU:HD13	1.96	0.47
36:q:99:VAL:HG21	36:q:127:VAL:HG21	1.96	0.47
40:u:114:PRO:HD3	40:u:163:LEU:HB2	1.96	0.47
13:d:922:GLN:NE2	20:l:71:ASP:OD2	2.47	0.47
14:e:724:GLU:OE1	14:e:789:ASN:ND2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:254:GLN:O	15:f:258:ARG:NH2	2.47	0.47
11:A:639:LEU:O	11:A:643:ILE:HG13	2.13	0.47
12:B:135:TRP:HA	12:B:138:VAL:HG12	1.95	0.47
13:D:998:GLN:HG2	13:D:999:MET:N	2.29	0.47
27:U:56:ARG:HD3	27:U:60:ARG:CZ	2.44	0.47
33:m:67:GLU:O	33:m:71:LYS:HG2	2.14	0.47
35:p:794:VAL:HG13	35:p:965:ILE:HG23	1.96	0.47
36:q:76:ASP:HA	36:q:239:LEU:HD23	1.97	0.47
36:q:263:LEU:HD22	44:y:87:PHE:HD2	1.78	0.47
41:v:17:PRO:HG3	41:v:29:HIS:NE2	2.29	0.47
44:y:41:THR:O	44:y:45:ILE:HG13	2.14	0.47
2:1:422:LEU:HD13	4:3:225:GLN:NE2	2.29	0.47
2:1:488:GLU:O	2:1:491:VAL:HG22	2.13	0.47
5:4:261:PHE:O	5:4:265:LEU:HD23	2.14	0.47
7:6:605:ILE:HD12	7:6:607:ILE:HD11	1.96	0.47
11:A:485:ILE:HB	15:f:310:THR:HG23	1.94	0.47
11:A:501:THR:O	11:A:502:LEU:C	2.57	0.47
15:F:90:GLU:CD	15:F:90:GLU:N	2.72	0.47
32:k:173:CYS:SG	32:k:179:MET:O	2.72	0.47
14:e:474:THR:OG1	14:e:546:VAL:O	2.28	0.47
15:f:39:LEU:HD22	18:i:47:VAL:HG13	1.95	0.47
1:0:41:ARG:HD2	27:U:169:PRO:CG	2.44	0.47
11:A:475:LEU:O	15:f:354:ARG:NH2	2.47	0.47
14:E:774:MET:HE2	14:E:774:MET:N	2.22	0.47
25:S:65:SER:HA	25:S:81:ARG:NH1	2.14	0.47
29:X:-20:DG:H2"	29:X:-19:DT:OP2	2.15	0.47
29:X:19:DA:H5"	38:s:111:THR:HB	1.96	0.47
34:o:525:ILE:HG12	34:o:535:MET:HE2	1.96	0.47
35:p:645:GLU:O	35:p:649:ASN:HB2	2.14	0.47
35:p:728:MET:SD	35:p:942:LYS:HB3	2.54	0.47
37:r:105:PRO:HG2	37:r:131:LEU:HD22	1.97	0.47
42:w:22:ASN:ND2	42:w:41:ASN:HD22	2.13	0.47
3:2:87:LEU:HD13	3:2:228:TYR:HD2	1.80	0.47
4:3:235:GLN:O	4:3:235:GLN:NE2	2.47	0.47
5:4:360:THR:HG22	5:4:363:GLN:OE1	2.13	0.47
7:6:297:PHE:O	7:6:359:LYS:NZ	2.38	0.47
11:A:730:PHE:CD1	11:A:730:PHE:N	2.82	0.47
14:E:696:TRP:HA	14:E:703:MET:HA	1.96	0.47
15:F:317:LEU:N	15:F:317:LEU:HD23	2.30	0.47
24:R:123:THR:O	24:R:127:ARG:HG3	2.14	0.47
26:T:179:ASP:OD1	26:T:179:ASP:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:14:LEU:HD13	27:U:197:VAL:HG22	1.96	0.47
27:U:69:ASP:OD1	27:U:69:ASP:N	2.39	0.47
28:V:103:LEU:HA	28:V:106:THR:HG22	1.96	0.47
29:X:9:DA:H4'	34:o:1417:HIS:CD2	2.49	0.47
34:o:1294:THR:HG21	35:p:245:GLN:HE22	1.79	0.47
14:e:589:TRP:HB3	15:f:60:MET:HE3	1.96	0.47
11:A:575:PRO:HD3	12:B:608:ASN:HD22	1.79	0.47
13:D:1003:ASP:HA	13:D:1006:LEU:HD23	1.96	0.47
14:E:732:ASP:OD1	14:E:734:THR:OG1	2.31	0.47
27:U:140:GLU:OE1	27:U:140:GLU:N	2.48	0.47
29:X:-33:DC:C2	29:X:-32:DC:C5	3.02	0.47
15:f:330:ARG:NH1	15:f:371:THR:O	2.48	0.47
10:Z:4:G2L:O2'	34:o:460:ARG:NH2	2.48	0.47
13:D:991:MET:HE1	26:T:192:GLU:HG2	1.95	0.47
15:F:317:LEU:N	15:F:317:LEU:CD2	2.77	0.47
17:H:35:ARG:HD3	17:H:35:ARG:HA	1.59	0.47
20:L:104:ARG:HH21	20:L:104:ARG:HA	1.80	0.47
28:V:225:VAL:HG13	28:V:226:ASP:OD2	2.15	0.47
30:Y:22:DC:H2"	30:Y:23:DC:C6	2.49	0.47
33:m:56:ILE:HG23	20:l:129:PRO:HB2	1.97	0.47
34:o:621:ILE:HG23	41:v:115:TYR:HD2	1.79	0.47
35:p:783:ALA:O	35:p:789:ASN:ND2	2.48	0.47
36:q:92:GLU:HG3	36:q:93:PHE:H	1.80	0.47
37:r:104:CYS:SG	37:r:138:ARG:HD2	2.55	0.47
39:t:51:ARG:NH1	39:t:122:GLU:OE1	2.46	0.47
14:e:556:ASN:HA	14:e:572:LEU:HB2	1.96	0.47
3:2:291:CYS:SG	3:2:294:CYS:N	2.82	0.47
5:4:404:THR:O	6:5:8:VAL:HG22	2.15	0.47
15:F:424:GLN:O	15:F:428:LEU:HG	2.15	0.47
18:I:119:ARG:NH1	18:I:120:TYR:OH	2.48	0.47
23:Q:321:SER:OG	23:Q:322:ASP:N	2.48	0.47
24:R:182:ALA:HB2	26:T:155:PRO:HA	1.97	0.47
27:U:49:LEU:O	27:U:53:LYS:HA	2.15	0.47
27:U:150:GLY:O	40:u:93:ASN:OD1	2.33	0.47
34:o:413:TYR:O	34:o:449:HIS:HD2	1.98	0.47
34:o:478:PRO:O	44:y:4:PRO:HD3	2.15	0.47
34:o:488:VAL:O	34:o:491:PRO:HD2	2.15	0.47
34:o:1160:ARG:O	34:o:1300:GLY:HA2	2.14	0.47
13:d:916:LYS:NZ	13:d:1070:GLU:OE2	2.42	0.47
4:3:20:ILE:H	4:3:20:ILE:HD12	1.79	0.47
11:A:1165:LEU:HB2	11:A:1191:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:71:ARG:HD3	12:B:73:TYR:CE1	2.50	0.47
15:F:411:VAL:HG13	15:F:411:VAL:O	2.15	0.47
28:V:99:LEU:HD23	28:V:114:LYS:HZ2	1.80	0.47
34:o:811:ILE:HG21	42:w:79:PRO:HB3	1.97	0.47
34:o:920:PHE:CD1	34:o:959:MET:HE1	2.50	0.47
35:p:752:TYR:HE1	35:p:809:VAL:HG23	1.79	0.47
40:u:124:ASN:HB2	40:u:125:PRO:HD3	1.97	0.47
12:B:564:LEU:HB2	12:B:581:ILE:HD13	1.97	0.47
25:S:43:ASN:OD1	25:S:44:GLN:N	2.48	0.47
27:U:36:ILE:HG21	27:U:48:MET:CE	2.45	0.47
27:U:152:PHE:CZ	40:u:96:GLY:N	2.83	0.47
31:c:26:VAL:HG23	19:j:195:LEU:HB3	1.96	0.47
37:r:57:LEU:HD13	37:r:61:PHE:CE2	2.50	0.47
15:f:326:HIS:O	15:f:330:ARG:HG2	2.15	0.47
1:0:8:ARG:CZ	1:0:9:CYS:SG	3.02	0.46
1:0:28:HIS:HB3	1:0:30:LEU:HG	1.96	0.46
4:3:44:LEU:HD21	4:3:162:LEU:CD1	2.45	0.46
12:B:217:ASN:ND2	12:B:320:ALA:O	2.35	0.46
12:B:781:TYR:O	17:H:176:ARG:NH2	2.47	0.46
26:T:238:GLU:CD	28:V:130:ILE:HG12	2.40	0.46
27:U:179:ARG:HA	27:U:182:GLU:HG2	1.96	0.46
35:p:17:ILE:O	35:p:19:PRO:HD3	2.15	0.46
35:p:759:VAL:HG12	35:p:999:ALA:HB2	1.97	0.46
37:r:34:ASN:O	37:r:68:THR:OG1	2.33	0.46
37:r:131:LEU:O	37:r:135:GLN:HG2	2.15	0.46
44:y:84:GLN:O	44:y:88:THR:HG23	2.15	0.46
4:3:50:PHE:CZ	5:4:118:LEU:HD12	2.38	0.46
8:7:617:ALA:HB2	8:7:676:LEU:HD21	1.97	0.46
11:A:397:LEU:HD21	15:f:361:LYS:HB3	1.97	0.46
13:D:963:ARG:O	13:D:966:LEU:N	2.48	0.46
13:D:965:ILE:HD13	13:D:965:ILE:O	2.15	0.46
14:E:321:LEU:HB3	14:E:330:TRP:HB2	1.97	0.46
15:F:418:ILE:H	15:F:418:ILE:CD1	2.26	0.46
26:T:188:PHE:CE2	28:V:80:LYS:HB2	2.49	0.46
30:Y:27:DT:C6	30:Y:28:DT:H72	2.50	0.46
34:o:733:LEU:HA	34:o:736:THR:HG22	1.98	0.46
35:p:955:PRO:O	35:p:963:PRO:HD2	2.15	0.46
37:r:74:PHE:HB2	37:r:80:ILE:HG12	1.97	0.46
15:f:102:ARG:HD3	20:l:151:ARG:HG3	1.95	0.46
15:f:326:HIS:ND1	15:f:326:HIS:N	2.64	0.46
15:f:328:ALA:C	15:f:330:ARG:N	2.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:229:TRP:CH2	5:4:58:ARG:NH1	2.79	0.46
11:A:470:ILE:O	15:f:299:LYS:NZ	2.48	0.46
15:F:47:ILE:HD13	18:I:19:MET:HE1	1.96	0.46
15:F:83:LEU:H	15:F:83:LEU:HD12	1.71	0.46
15:F:215:GLU:O	15:F:254:GLN:NE2	2.39	0.46
30:Y:-35:DG:H2"	30:Y:-34:DG:C8	2.50	0.46
34:o:733:LEU:CB	42:w:106:ASP:HB2	2.45	0.46
44:y:82:SER:HB3	44:y:85:GLU:HG3	1.96	0.46
13:d:1061:ARG:NH1	18:i:119:ARG:O	2.48	0.46
14:e:747:LEU:H	14:e:747:LEU:CD2	2.22	0.46
4:3:13:ILE:HG21	4:3:41:VAL:HG13	1.97	0.46
16:G:41:ASP:OD1	16:G:41:ASP:N	2.48	0.46
34:o:379:GLY:HA2	34:o:475:ARG:O	2.16	0.46
35:p:40:VAL:HG11	35:p:482:LEU:HD13	1.98	0.46
15:f:58:MET:HE3	15:f:64:GLN:HA	1.98	0.46
2:1:427:ALA:HB1	5:4:62:LEU:HD11	1.98	0.46
3:2:382:CYS:HB3	3:2:385:CYS:HB3	1.96	0.46
6:5:32:LYS:HB2	12:B:540:LYS:O	2.16	0.46
7:6:294:GLU:OE2	7:6:334:ARG:NH1	2.49	0.46
14:E:277:ASP:O	14:E:280:ARG:HG2	2.16	0.46
18:I:38:GLN:HA	18:I:41:GLU:HB2	1.98	0.46
20:L:106:ARG:NH1	20:L:115:ASP:OD2	2.48	0.46
24:R:50:SER:O	34:o:264:VAL:HA	2.16	0.46
25:S:73:ARG:HD2	25:S:73:ARG:HA	1.65	0.46
27:U:139:LEU:HD12	40:u:160:ILE:N	2.31	0.46
31:c:80:LEU:HB3	19:j:119:PHE:CZ	2.50	0.46
34:o:384:ILE:HG12	35:p:1061:SER:HB3	1.98	0.46
34:o:526:VAL:HA	34:o:533:PRO:HA	1.98	0.46
34:o:865:ILE:HG21	35:p:1092:ASP:CG	2.40	0.46
42:w:17:CYS:HB2	42:w:24:LEU:HD21	1.98	0.46
42:w:64:GLU:O	42:w:68:ILE:HG12	2.16	0.46
1:0:8:ARG:CD	27:U:172:ASP:HB2	2.45	0.46
4:3:53:ARG:HD2	5:4:46:ARG:HH12	1.80	0.46
8:7:28:LEU:O	8:7:32:LEU:HD23	2.16	0.46
24:R:31:ASP:OD1	24:R:31:ASP:N	2.48	0.46
26:T:31:TRP:HD1	26:T:62:LEU:HD21	1.80	0.46
27:U:112:ARG:O	27:U:115:GLU:HG2	2.16	0.46
34:o:712:ASP:HB3	34:o:744:ILE:HD13	1.96	0.46
34:o:1471:PHE:CZ	39:t:61:GLU:HA	2.51	0.46
44:y:45:ILE:HG22	44:y:94:LEU:HD22	1.98	0.46
14:e:717:LEU:HD22	14:e:726:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:357:VAL:CG1	3:2:366:VAL:HG23	2.45	0.46
11:A:404:MET:O	11:A:408:LEU:HB2	2.16	0.46
26:T:170:LYS:HE3	26:T:170:LYS:HB3	1.71	0.46
27:U:150:GLY:CA	40:u:93:ASN:OD1	2.64	0.46
14:e:234:ALA:HB2	14:e:648:ASP:HB2	1.96	0.46
14:e:238:GLN:O	14:e:242:PRO:HD2	2.16	0.46
1:0:8:ARG:HH21	1:0:37:LEU:HD22	1.80	0.46
1:0:31:CYS:SG	1:0:34:CYS:HB2	2.55	0.46
1:0:128:GLU:HB3	1:0:133:ILE:HG12	1.98	0.46
4:3:31:GLN:OE1	4:3:36:LYS:NZ	2.42	0.46
7:6:656:ASN:OD1	7:6:657:ALA:N	2.49	0.46
8:7:77:VAL:HA	8:7:80:ILE:HG22	1.97	0.46
14:E:646:SER:OG	14:E:647:ALA:N	2.49	0.46
21:O:64:THR:HG22	21:O:65:TYR:N	2.31	0.46
28:V:176:PRO:C	28:V:178:SER:H	2.23	0.46
29:X:-14:DG:O6	30:Y:13:DA:N6	2.49	0.46
34:o:459:ASN:HD21	35:p:1090:GLU:HG3	1.81	0.46
34:o:1206:ARG:H	34:o:1263:ASN:HB3	1.81	0.46
34:o:1311:LEU:HD11	34:o:1332:GLN:HB3	1.98	0.46
36:q:20:LYS:HE2	36:q:232:ASN:ND2	2.31	0.46
14:e:519:GLU:O	14:e:519:GLU:HG3	2.16	0.46
1:0:37:LEU:O	1:0:40:VAL:HG12	2.16	0.46
11:A:467:ILE:N	15:F:221:GLN:NE2	2.48	0.46
12:B:559:LYS:HB2	12:B:559:LYS:NZ	2.31	0.46
26:T:194:HIS:CG	26:T:195:GLN:N	2.82	0.46
28:V:168:LEU:O	28:V:172:GLU:HG2	2.16	0.46
42:w:114:CYS:HB2	42:w:123:TRP:HZ3	1.80	0.46
15:F:141:CYS:SG	17:H:158:THR:HB	2.56	0.46
27:U:54:PHE:CE1	28:V:195:PRO:HG3	2.51	0.46
35:p:667:THR:HA	35:p:670:GLU:HB2	1.97	0.46
15:f:327:TRP:O	15:f:330:ARG:HB2	2.15	0.46
4:3:98:ASP:CB	4:3:100:LYS:HE3	2.47	0.45
7:6:185:ILE:HG22	7:6:189:LEU:HD13	1.97	0.45
8:7:361:LEU:O	8:7:365:VAL:HG12	2.16	0.45
19:J:123:LEU:HD12	19:J:123:LEU:HA	1.73	0.45
26:T:220:ILE:HG13	26:T:221:GLY:H	1.80	0.45
29:X:-32:DC:H6	29:X:-32:DC:H5'	1.81	0.45
34:o:931:ARG:NH1	34:o:936:GLU:HG3	2.31	0.45
34:o:971:PRO:O	34:o:972:THR:OG1	2.29	0.45
40:u:30:LEU:HD22	40:u:70:VAL:HG11	1.97	0.45
40:u:112:SER:HB3	40:u:162:SER:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:w:72:VAL:HG12	42:w:78:LEU:HD11	1.99	0.45
42:w:81:THR:HG23	42:w:96:PHE:CE1	2.51	0.45
5:4:435:ASN:HB3	5:4:440:LEU:HB2	1.97	0.45
8:7:137:LEU:O	8:7:142:VAL:HG11	2.15	0.45
8:7:329:PHE:O	8:7:333:LEU:HD23	2.17	0.45
12:B:184:ASN:ND2	12:B:184:ASN:N	2.63	0.45
12:B:568:VAL:HG22	12:B:628:ILE:HG23	1.98	0.45
15:F:426:LEU:C	15:F:426:LEU:HD23	2.41	0.45
33:m:84:GLU:H	33:m:84:GLU:HG3	1.42	0.45
34:o:95:PHE:HB2	34:o:311:GLN:HE22	1.80	0.45
34:o:420:ILE:HB	34:o:445:LYS:HB2	1.99	0.45
14:e:718:ARG:HD3	14:e:718:ARG:HA	1.76	0.45
1:0:5:GLY:HA3	1:0:10:LYS:CB	2.25	0.45
5:4:334:MET:SD	7:6:56:TYR:CE2	3.09	0.45
13:D:871:THR:HG21	13:D:910:LEU:HD12	1.98	0.45
14:E:245:VAL:HG13	14:E:282:LEU:HD11	1.97	0.45
17:H:87:GLN:HA	17:H:88:PRO:HD3	1.82	0.45
26:T:140:ARG:HH21	35:p:90:GLN:HG2	1.81	0.45
35:p:789:ASN:O	35:p:968:ASN:HB2	2.15	0.45
44:y:64:PRO:HG3	44:y:70:LYS:HE2	1.97	0.45
14:e:243:LEU:HD13	14:e:243:LEU:HA	1.73	0.45
2:1:472:LEU:HD12	2:1:476:TRP:CD1	2.52	0.45
8:7:109:LEU:HD12	8:7:207:TYR:CD2	2.51	0.45
14:E:730:SER:OG	14:E:732:ASP:OD1	2.33	0.45
17:H:27:ASP:OD1	17:H:27:ASP:N	2.48	0.45
23:Q:22:ILE:HG22	23:Q:39:LEU:HD11	1.98	0.45
28:V:97:LEU:O	28:V:137:TYR:HE1	2.00	0.45
30:Y:15:DA:H2'	30:Y:16:DA:C8	2.50	0.45
34:o:1434:GLU:C	34:o:1435:THR:HG1	2.21	0.45
35:p:1035:ARG:NH1	35:p:1036:LYS:O	2.49	0.45
36:q:105:VAL:HG11	36:q:115:VAL:HG22	1.97	0.45
38:s:64:HIS:HD2	38:s:66:ASP:H	1.64	0.45
14:e:281:VAL:HG11	14:e:297:MET:HB3	1.98	0.45
1:0:21:LEU:HD21	1:0:29:THR:HG23	1.98	0.45
1:0:37:LEU:HD11	27:U:118:GLU:OE2	2.17	0.45
1:0:55:LYS:C	1:0:57:ASN:H	2.24	0.45
2:1:308:ASN:ND2	8:7:576:GLU:OE2	2.49	0.45
2:1:457:ILE:HG22	2:1:461:LEU:HD13	1.98	0.45
17:H:186:VAL:HG21	15:f:220:GLN:HB3	1.97	0.45
34:o:1180:ASN:O	34:o:1183:SER:OG	2.29	0.45
34:o:1485:GLU:HG2	40:u:20:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:z:17:TYR:HB3	45:z:44:MET:HB3	1.98	0.45
14:e:258:ASN:OD1	14:e:258:ASN:N	2.38	0.45
11:A:401:ASN:HD22	11:A:401:ASN:N	2.14	0.45
11:A:690:LEU:HD22	11:A:747:LEU:HD22	1.99	0.45
11:A:857:MET:HE3	11:A:858:ASP:H	1.81	0.45
15:F:68:THR:OG1	18:I:32:GLU:OE1	2.35	0.45
15:F:217:SER:HB3	17:H:157:HIS:HB2	1.99	0.45
25:S:47:LEU:HD11	25:S:98:TRP:HB3	1.99	0.45
34:o:381:PRO:HB3	34:o:479:TRP:O	2.16	0.45
34:o:459:ASN:OD1	34:o:460:ARG:N	2.50	0.45
34:o:530:SER:O	34:o:532:ARG:HG3	2.16	0.45
34:o:538:VAL:HG22	34:o:539:GLN:HG2	1.99	0.45
35:p:260:LEU:HD22	35:p:347:MET:SD	2.57	0.45
15:f:219:GLU:H	15:f:219:GLU:CD	2.21	0.45
4:3:201:GLY:O	4:3:204:GLN:HG2	2.17	0.45
5:4:411:GLN:HE22	12:B:534:SER:HB2	1.82	0.45
11:A:475:LEU:HD23	11:A:480:TRP:HE1	1.82	0.45
27:U:76:MET:CG	27:U:88:ARG:HB3	2.46	0.45
27:U:179:ARG:HH21	27:U:183:GLN:HG3	1.81	0.45
29:X:27:DA:H2"	29:X:28:DG:C8	2.52	0.45
34:o:490:THR:OG1	34:o:491:PRO:HD3	2.17	0.45
34:o:906:LEU:HD13	34:o:966:LEU:HD22	1.99	0.45
34:o:1282:ASP:N	34:o:1282:ASP:OD1	2.50	0.45
34:o:1416:ARG:HB3	34:o:1433:GLU:OE1	2.17	0.45
36:q:175:LYS:NZ	45:z:57:ALA:HB3	2.32	0.45
15:f:83:LEU:HD22	18:i:41:GLU:HG2	1.99	0.45
5:4:406:GLY:O	6:5:7:GLY:N	2.49	0.45
11:A:1182:CYS:O	11:A:1182:CYS:SG	2.75	0.45
13:D:960:GLU:CB	13:D:983:ARG:HH11	2.29	0.45
14:E:690:ASP:N	14:E:690:ASP:OD1	2.44	0.45
27:U:112:ARG:HA	27:U:115:GLU:OE2	2.16	0.45
34:o:279:LYS:HE2	34:o:316:THR:HB	1.99	0.45
34:o:916:PHE:HE2	34:o:960:ARG:HG2	1.82	0.45
14:e:436:ASP:N	14:e:436:ASP:OD1	2.49	0.45
15:f:317:LEU:HD12	15:f:329:LEU:HD23	1.98	0.45
3:2:174:LEU:O	8:7:591:GLY:C	2.60	0.45
3:2:199:ILE:CG2	3:2:222:ILE:HD11	2.47	0.45
3:2:242:SER:N	3:2:245:SER:OG	2.50	0.45
13:D:966:LEU:HD22	13:D:966:LEU:C	2.42	0.45
23:Q:332:GLU:OE1	23:Q:332:GLU:N	2.49	0.45
28:V:86:LYS:HZ2	28:V:140:LYS:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y:16:DA:H1'	30:Y:17:DC:O5'	2.17	0.45
33:m:47:GLN:HG2	13:d:860:VAL:HA	1.98	0.45
34:o:436:SER:HA	34:o:439:HIS:HD2	1.80	0.45
34:o:920:PHE:CE1	34:o:1053:ARG:HD2	2.51	0.45
37:r:20:LEU:HD12	37:r:121:ARG:HH22	1.81	0.45
39:t:121:ASP:OD1	39:t:121:ASP:N	2.50	0.45
13:d:1084:LEU:HB3	18:i:99:ARG:HH21	1.81	0.45
14:e:245:VAL:HG12	14:e:282:LEU:HD11	1.99	0.45
1:0:6:CYS:O	1:0:10:LYS:HE3	2.17	0.45
5:4:325:ILE:H	5:4:325:ILE:HD12	1.82	0.45
7:6:133:THR:HB	7:6:160:THR:HG21	1.99	0.45
8:7:373:ARG:O	8:7:405:THR:OG1	2.24	0.45
8:7:460:THR:HB	8:7:661:ALA:HB1	1.98	0.45
13:D:947:PHE:HE1	14:E:527:ILE:HD12	1.82	0.45
25:S:72:ASN:ND2	26:T:198:ASN:H	2.15	0.45
25:S:173:HIS:HB2	42:w:40:ARG:HD3	1.98	0.45
28:V:130:ILE:HD12	28:V:140:LYS:HG3	1.99	0.45
34:o:457:ILE:HG13	34:o:515:ILE:HD13	1.99	0.45
34:o:1139:LEU:HB3	34:o:1338:THR:OG1	2.17	0.45
34:o:1478:GLU:HA	34:o:1481:LYS:HE2	1.99	0.45
35:p:1090:GLU:N	35:p:1090:GLU:OE1	2.50	0.45
43:x:47:ARG:CZ	43:x:48:MET:HE3	2.47	0.45
1:0:1:MET:SD	8:7:345:ARG:HD2	2.57	0.44
8:7:285:TYR:O	8:7:289:VAL:HG23	2.17	0.44
14:E:250:GLU:O	14:E:254:ASN:ND2	2.51	0.44
14:E:784:HIS:HB3	14:E:792:LEU:HB2	1.99	0.44
21:O:65:TYR:OH	22:P:203:ARG:NE	2.50	0.44
25:S:70:GLU:CA	25:S:74:LYS:HB2	2.46	0.44
27:U:12:ALA:O	27:U:16:ARG:HG2	2.18	0.44
27:U:145:PHE:HB3	27:U:153:ARG:H	1.82	0.44
29:X:16:DT:H4'	29:X:17:DC:H5'	1.99	0.44
30:Y:-4:DC:H2'	30:Y:-3:DC:C6	2.53	0.44
34:o:801:GLY:HA3	35:p:503:ASN:HB2	1.99	0.44
34:o:1417:HIS:O	34:o:1421:ARG:HG2	2.17	0.44
35:p:1060:HIS:HE1	35:p:1081:ASP:HA	1.81	0.44
3:2:175:THR:HA	8:7:591:GLY:C	2.42	0.44
4:3:42:MET:SD	4:3:108:ASN:ND2	2.86	0.44
7:6:528:LYS:CD	7:6:531:ILE:HD13	2.47	0.44
8:7:475:PRO:HG3	8:7:478:MET:HE2	1.99	0.44
11:A:1053:PHE:HB2	11:A:1057:GLU:HB2	1.99	0.44
24:R:107:MET:O	24:R:112:ARG:NH2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:96:PRO:HB3	28:V:136:LYS:HD2	1.98	0.44
34:o:93:PRO:HD2	34:o:219:GLU:HG2	2.00	0.44
35:p:357:CYS:SG	35:p:361:LYS:NZ	2.90	0.44
35:p:713:PHE:HB3	35:p:716:HIS:CD2	2.52	0.44
35:p:744:MET:HE3	35:p:744:MET:HB3	1.83	0.44
36:q:44:ILE:HD13	36:q:238:SER:HB2	1.99	0.44
36:q:71:ILE:HD11	36:q:150:ILE:HG12	1.99	0.44
40:u:92:VAL:HG11	40:u:127:CYS:N	2.31	0.44
40:u:96:GLY:O	40:u:128:TYR:OH	2.36	0.44
1:0:8:ARG:CG	27:U:172:ASP:HB2	2.47	0.44
4:3:16:ASP:HA	4:3:62:SER:HG	1.78	0.44
4:3:123:ASP:OD1	4:3:124:ILE:N	2.45	0.44
4:3:242:ILE:CD1	5:4:75:VAL:N	2.80	0.44
8:7:434:HIS:CB	8:7:632:ILE:HD11	2.47	0.44
8:7:613:HIS:ND1	8:7:613:HIS:O	2.50	0.44
11:A:1063:LYS:HD3	11:A:1063:LYS:O	2.16	0.44
12:B:925:LYS:HD3	12:B:925:LYS:HA	1.78	0.44
14:E:650:THR:HG22	14:E:666:THR:HG22	1.99	0.44
15:F:328:ALA:O	15:F:332:PHE:N	2.50	0.44
16:G:129:LYS:HA	16:G:129:LYS:HD2	1.77	0.44
24:R:102:GLN:HE21	34:o:305:GLU:CG	2.28	0.44
25:S:73:ARG:NE	25:S:76:ARG:HH11	2.15	0.44
33:m:57:LEU:HA	33:m:57:LEU:HD23	1.73	0.44
34:o:153:ILE:HG12	34:o:187:TYR:CD1	2.52	0.44
35:p:1115:GLN:HB3	35:p:1148:LEU:HD11	1.99	0.44
19:j:176:MET:O	19:j:178:GLY:N	2.43	0.44
5:4:52:ALA:HB1	5:4:90:LEU:HD21	1.99	0.44
6:5:35:ILE:C	12:B:539:ARG:HD3	2.42	0.44
7:6:415:HIS:HD2	7:6:419:ARG:HH22	1.65	0.44
8:7:600:ALA:HB1	8:7:659:HIS:HD2	1.82	0.44
14:E:249:LEU:HD21	14:E:282:LEU:HD22	2.00	0.44
15:F:361:LYS:HA	15:F:364:VAL:HG22	1.99	0.44
25:S:175:SER:O	25:S:179:GLN:HG2	2.17	0.44
28:V:129:LYS:HA	28:V:129:LYS:HE3	1.97	0.44
34:o:597:PRO:HB3	34:o:664:ILE:HG22	1.98	0.44
34:o:837:PHE:HB2	35:p:506:TRP:HZ3	1.83	0.44
34:o:850:THR:O	34:o:853:LYS:HG2	2.18	0.44
45:z:43:ILE:O	45:z:44:MET:HE2	2.18	0.44
14:e:525:GLU:N	14:e:525:GLU:CD	2.76	0.44
1:0:97:ASP:O	1:0:101:GLU:OE1	2.36	0.44
4:3:229:TRP:HE3	5:4:58:ARG:HD2	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:726:GLN:HG2	8:7:727:PRO:CD	2.47	0.44
11:A:463:PRO:O	15:F:218:VAL:HG23	2.17	0.44
27:U:152:PHE:CZ	40:u:95:VAL:HG12	2.49	0.44
34:o:459:ASN:HD21	34:o:463:THR:HG21	1.82	0.44
34:o:1144:LEU:HG	34:o:1353:ASP:HA	2.00	0.44
35:p:19:PRO:C	35:p:21:LEU:H	2.25	0.44
35:p:1028:LEU:HD11	35:p:1043:ILE:HD11	1.99	0.44
36:q:193:ARG:HG2	36:q:220:TYR:HD1	1.83	0.44
2:1:400:ILE:H	2:1:400:ILE:HD12	1.82	0.44
4:3:242:ILE:CD1	5:4:74:TRP:C	2.91	0.44
7:6:415:HIS:CE1	30:Y:-27:DT:H5"	2.53	0.44
8:7:107:LEU:HD12	8:7:195:ALA:HB1	1.99	0.44
12:B:839:MET:HE1	12:B:843:LEU:HD13	2.00	0.44
13:D:1001:GLN:O	13:D:1004:ALA:HB3	2.18	0.44
15:F:47:ILE:HD11	18:I:43:ALA:HB2	1.98	0.44
17:H:59:GLU:HA	17:H:62:THR:HG22	1.99	0.44
28:V:111:ILE:O	28:V:114:LYS:N	2.51	0.44
29:X:-19:DT:H1'	29:X:-18:DG:C8	2.52	0.44
30:Y:-23:DC:H2"	30:Y:-22:DG:C8	2.52	0.44
34:o:896:LEU:HD13	34:o:980:PRO:HB3	2.00	0.44
35:p:27:TRP:CD1	35:p:762:ARG:HH21	2.35	0.44
3:2:87:LEU:HD23	3:2:87:LEU:O	2.18	0.44
5:4:157:GLU:O	5:4:161:HIS:ND1	2.51	0.44
5:4:288:ILE:H	5:4:288:ILE:HD12	1.83	0.44
12:B:859:ARG:HA	12:B:859:ARG:HD2	1.80	0.44
27:U:53:LYS:O	28:V:199:LYS:HE2	2.18	0.44
28:V:214:GLU:HA	28:V:217:GLN:HB3	1.99	0.44
34:o:457:ILE:HD12	35:p:1102:PHE:CE2	2.52	0.44
34:o:491:PRO:HG3	34:o:535:MET:HG2	1.99	0.44
34:o:1171:ALA:HA	42:w:59:THR:HG23	1.99	0.44
35:p:927:ARG:HD3	35:p:1054:MET:SD	2.58	0.44
40:u:87:ALA:HB2	40:u:101:ILE:HG12	1.99	0.44
40:u:129:LYS:HD2	40:u:133:GLU:HG2	2.00	0.44
14:e:542:HIS:CE1	14:e:568:ARG:HG3	2.53	0.44
6:5:9:LEU:HD11	6:5:42:HIS:HD2	1.83	0.44
11:A:1165:LEU:HD22	11:A:1165:LEU:HA	1.87	0.44
12:B:653:LEU:HG	12:B:684:ILE:HG13	1.99	0.44
13:D:933:ARG:HD2	19:J:117:VAL:HG11	2.00	0.44
13:D:1080:TYR:OH	14:E:606:ASP:OD2	2.30	0.44
15:F:400:GLY:O	15:F:404:ARG:HG2	2.18	0.44
34:o:96:HIS:HB2	34:o:250:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:p:955:PRO:HB2	35:p:1028:LEU:HD13	2.00	0.44
15:f:447:ALA:CB	15:f:456:GLY:HA3	2.48	0.44
20:l:113:VAL:O	20:l:113:VAL:HG22	2.17	0.44
8:7:332:PHE:CZ	8:7:367:ILE:HG23	2.53	0.44
11:A:400:GLU:HG3	11:A:401:ASN:N	2.32	0.44
12:B:414:LEU:HB2	12:B:523:VAL:HG13	2.00	0.44
13:D:997:ALA:O	13:D:1001:GLN:N	2.48	0.44
13:D:1071:ARG:HH22	18:I:82:SER:HA	1.83	0.44
14:E:564:ASP:OD1	14:E:564:ASP:N	2.51	0.44
15:F:427:LEU:HD12	15:F:427:LEU:HA	1.72	0.44
35:p:163:LEU:HA	35:p:166:LEU:HD12	2.00	0.44
35:p:711:ILE:HG12	35:p:725:GLN:HG2	2.00	0.44
3:2:369:VAL:HG13	3:2:370:ASP:N	2.33	0.43
7:6:99:PHE:CZ	7:6:103:ILE:HD13	2.53	0.43
12:B:492:MET:HE3	12:B:492:MET:HB2	1.85	0.43
14:E:481:ASP:N	14:E:481:ASP:OD1	2.41	0.43
20:L:113:VAL:C	20:L:115:ASP:N	2.75	0.43
21:O:48:LEU:HG	23:Q:366:ILE:HD11	2.00	0.43
31:c:24:ASP:CB	19:j:192:LYS:HD2	2.48	0.43
35:p:803:ARG:HH21	36:q:177:ASN:HD22	1.66	0.43
35:p:818:GLU:HG3	35:p:827:GLU:O	2.18	0.43
18:i:45:ARG:HG3	19:j:212:LYS:HB3	2.00	0.43
1:0:116:ASP:OD1	1:0:117:ASN:N	2.51	0.43
8:7:354:PRO:HB2	8:7:355:PRO:HD3	2.00	0.43
14:E:377:LEU:HD21	14:E:422:PRO:HG2	2.00	0.43
15:F:283:MET:HE1	15:F:308:VAL:HG12	2.00	0.43
17:H:194:MET:HE2	17:H:194:MET:HB2	1.85	0.43
23:Q:18:ILE:HD11	23:Q:46:TRP:CH2	2.54	0.43
24:R:93:PHE:HB2	24:R:97:GLY:HA2	2.00	0.43
28:V:78:LEU:O	28:V:82:VAL:HG23	2.18	0.43
28:V:229:ASP:HA	28:V:232:LYS:HE2	1.99	0.43
33:m:87:VAL:HG13	33:m:97:PHE:HE1	1.83	0.43
34:o:552:ASP:OD1	41:v:22:PHE:HB3	2.17	0.43
1:0:68:VAL:HG11	8:7:338:GLU:HG2	2.00	0.43
11:A:340:GLU:H	11:A:497:PRO:HG2	1.83	0.43
12:B:328:ASN:HA	17:H:227:LEU:HD21	2.00	0.43
12:B:766:LEU:HA	12:B:807:THR:HG21	2.00	0.43
15:F:6:LYS:HE2	15:F:8:LYS:HG3	2.01	0.43
25:S:77:GLU:OE2	25:S:81:ARG:NH2	2.51	0.43
29:X:-18:DG:H2”	29:X:-17:DG:C8	2.52	0.43
32:k:179:MET:HB3	32:k:180:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:o:457:ILE:HD11	34:o:515:ILE:HG12	2.00	0.43
43:x:49:LEU:HD23	43:x:49:LEU:HA	1.79	0.43
14:e:268:HIS:O	14:e:268:HIS:CG	2.70	0.43
3:2:206:ARG:CB	8:7:589:GLU:O	2.63	0.43
18:I:23:LEU:HD22	18:I:28:ILE:HD12	2.00	0.43
35:p:837:CYS:SG	35:p:889:LYS:HD3	2.58	0.43
7:6:184:VAL:HG13	7:6:185:ILE:N	2.33	0.43
8:7:67:VAL:HG23	8:7:67:VAL:O	2.19	0.43
12:B:603:LYS:H	12:B:603:LYS:HG2	1.64	0.43
13:D:998:GLN:CG	13:D:1002:ARG:HH12	2.31	0.43
14:E:466:PHE:HB2	14:E:796:ALA:HA	2.00	0.43
18:I:21:GLN:HE22	18:I:24:LYS:HE2	1.84	0.43
24:R:174:PRO:HD2	24:R:213:ASP:HB3	2.00	0.43
28:V:184:ALA:O	28:V:189:ILE:HG23	2.19	0.43
34:o:1099:ALA:HA	34:o:1102:MET:HG2	2.01	0.43
35:p:385:ARG:O	35:p:391:LYS:HE3	2.18	0.43
35:p:399:LEU:HB3	35:p:453:TRP:NE1	2.33	0.43
35:p:1060:HIS:CE1	35:p:1081:ASP:HA	2.53	0.43
37:r:76:ASN:O	37:r:80:ILE:HG13	2.19	0.43
41:v:37:MET:HE2	41:v:37:MET:HB3	1.80	0.43
15:f:11:ASN:OD1	15:f:48:LYS:NZ	2.51	0.43
18:i:16:ALA:HB2	18:i:40:LEU:HD11	2.00	0.43
7:6:133:THR:HG23	7:6:134:SER:N	2.33	0.43
11:A:639:LEU:O	11:A:639:LEU:CD1	2.67	0.43
13:D:891:ILE:HG21	20:L:111:LEU:HB2	2.01	0.43
13:D:958:LYS:HD2	13:D:958:LYS:HA	1.62	0.43
13:D:963:ARG:O	13:D:965:ILE:N	2.52	0.43
14:E:351:GLN:HG2	14:E:355:MET:HE2	2.01	0.43
14:E:613:ALA:HB3	14:E:616:HIS:HD2	1.83	0.43
15:F:50:ILE:O	15:F:54:ALA:N	2.47	0.43
15:F:370:TRP:CZ3	15:F:420:ALA:HA	2.53	0.43
20:L:83:MET:HE3	20:L:83:MET:HB3	1.61	0.43
29:X:-32:DC:H2'	29:X:-31:DT:H71	1.99	0.43
29:X:12:DT:H1'	29:X:13:DA:C8	2.53	0.43
35:p:81:PRO:HA	35:p:82:PRO:HD3	1.91	0.43
35:p:389:GLY:HA3	35:p:668:LEU:HG	1.99	0.43
35:p:501:LEU:HD12	35:p:505:LEU:HD12	2.00	0.43
38:s:54:ARG:C	38:s:56:THR:H	2.25	0.43
3:2:112:LYS:N	3:2:142:GLU:O	2.41	0.43
5:4:426:ARG:NH2	5:4:434:GLU:OE1	2.52	0.43
8:7:168:VAL:O	8:7:168:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1052:ARG:O	11:A:1052:ARG:CG	2.67	0.43
14:E:518:LYS:C	14:E:520:SER:H	2.26	0.43
15:F:138:ILE:HB	17:H:159:TYR:HB3	2.00	0.43
19:J:124:GLU:O	19:J:125:ASP:HB3	2.17	0.43
19:J:192:LYS:N	19:J:192:LYS:CE	2.66	0.43
34:o:34:MET:SD	35:p:1124:ILE:HG21	2.58	0.43
34:o:952:LEU:HD21	34:o:1006:PRO:HB2	2.00	0.43
34:o:1130:ILE:HD13	34:o:1411:LEU:HD22	2.01	0.43
35:p:528:LEU:HD23	35:p:528:LEU:HA	1.78	0.43
37:r:41:LEU:HD22	37:r:61:PHE:CE1	2.54	0.43
15:f:105:TYR:O	19:j:217:PHE:N	2.51	0.43
2:1:303:ILE:HG22	2:1:307:PHE:CE2	2.54	0.43
7:6:532:LEU:HD23	7:6:532:LEU:O	2.19	0.43
30:Y:-26:DG:H8	30:Y:-26:DG:OP2	2.01	0.43
31:c:101:VAL:HG22	15:f:127:LEU:HA	2.00	0.43
34:o:527:THR:HB	34:o:534:VAL:HG22	2.01	0.43
34:o:893:GLU:OE1	38:s:197:SER:OG	2.29	0.43
40:u:91:GLN:HB3	40:u:98:PHE:HB2	1.99	0.43
43:x:8:PHE:CD2	43:x:48:MET:HE1	2.53	0.43
7:6:193:VAL:HG11	7:6:283:ARG:CD	2.49	0.43
11:A:727:THR:HG23	11:A:727:THR:O	2.19	0.43
19:J:148:ASP:HA	19:J:149:PRO:HD2	1.80	0.43
29:X:-18:DG:C6	29:X:-17:DG:C6	3.07	0.43
31:c:21:LEU:HD11	31:c:23:TRP:CD1	2.54	0.43
31:c:66:VAL:HG21	19:j:151:ILE:HG23	2.01	0.43
31:c:124:ILE:HD11	15:f:133:ALA:HB1	2.00	0.43
34:o:47:THR:HB	34:o:50:GLY:O	2.19	0.43
34:o:211:GLU:H	34:o:211:GLU:HG3	1.48	0.43
35:p:194:LEU:HD23	35:p:194:LEU:HA	1.88	0.43
35:p:1038:THR:HA	36:q:195:THR:HA	2.01	0.43
7:6:532:LEU:CD2	7:6:716:VAL:HG13	2.49	0.43
8:7:109:LEU:HD11	8:7:199:ILE:HD11	2.01	0.43
8:7:249:VAL:HG21	8:7:403:PHE:HB2	2.00	0.43
9:N:6:CSX:HB2	9:N:7:ASN:H	1.43	0.43
10:Z:1:ATP:N1	30:Y:0:DT:O2	2.52	0.43
15:F:402:ARG:O	15:F:406:VAL:HG13	2.19	0.43
16:G:181:TRP:O	16:G:181:TRP:CD2	2.72	0.43
25:S:53:ASN:HB2	25:S:91:PHE:CZ	2.54	0.43
1:0:6:CYS:SG	1:0:8:ARG:HB3	2.59	0.42
1:0:23:VAL:HG12	1:0:59:ARG:HB2	2.01	0.42
2:1:496:ASN:HB3	2:1:536:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:925:ASP:N	11:A:925:ASP:OD1	2.52	0.42
12:B:882:HIS:CE1	17:H:216:ALA:HB1	2.54	0.42
15:F:401:GLU:C	15:F:401:GLU:CD	2.87	0.42
24:R:48:VAL:HG23	35:p:1069:ILE:HG12	2.01	0.42
27:U:16:ARG:HA	27:U:16:ARG:HD2	1.94	0.42
34:o:48:GLU:HB3	34:o:53:LYS:HA	2.01	0.42
34:o:155:GLU:HB2	34:o:181:HIS:CD2	2.55	0.42
37:r:24:LYS:HA	37:r:27:GLU:CD	2.44	0.42
14:e:667:GLY:O	14:e:692:ARG:NH2	2.52	0.42
15:f:55:LEU:HD13	18:i:28:ILE:HG12	2.01	0.42
1:0:64:GLU:OE1	8:7:345:ARG:NH2	2.52	0.42
5:4:70:ALA:HB1	5:4:74:TRP:CZ2	2.54	0.42
5:4:433:PHE:CE2	6:5:38:ILE:HG12	2.54	0.42
7:6:408:SER:HB3	7:6:413:LEU:HD11	2.01	0.42
8:7:111:SER:N	8:7:211:TYR:OH	2.52	0.42
11:A:353:LEU:HD22	15:f:273:GLN:HE22	1.85	0.42
12:B:831:GLU:OE1	12:B:835:ARG:NH2	2.52	0.42
14:E:327:ASN:HD22	14:E:327:ASN:N	2.07	0.42
17:H:38:GLN:HG2	17:H:62:THR:HG21	2.01	0.42
27:U:44:LYS:HB2	27:U:47:ASP:OD1	2.19	0.42
27:U:56:ARG:HH11	27:U:60:ARG:HH11	1.60	0.42
33:m:91:ARG:HG2	33:m:92:LYS:N	2.34	0.42
34:o:876:ASP:O	34:o:890:ARG:NH1	2.52	0.42
36:q:69:GLY:HA3	45:z:57:ALA:HB1	2.01	0.42
42:w:68:ILE:HB	42:w:122:ARG:HD2	2.02	0.42
13:d:871:THR:O	20:l:62:LYS:NZ	2.42	0.42
15:f:223:TYR:CD2	15:f:255:MET:HE1	2.52	0.42
5:4:456:LYS:HA	5:4:456:LYS:HD2	1.50	0.42
8:7:49:THR:HG23	8:7:50:VAL:N	2.34	0.42
11:A:468:PHE:HE1	15:F:221:GLN:HG3	1.85	0.42
11:A:931:PRO:O	11:A:935:THR:OG1	2.25	0.42
15:F:233:GLY:HA2	15:F:239:ARG:HE	1.82	0.42
25:S:76:ARG:NH2	25:S:77:GLU:OE1	2.52	0.42
26:T:159:HIS:O	26:T:163:ILE:HG23	2.19	0.42
27:U:188:TYR:O	27:U:192:ARG:HG2	2.20	0.42
27:U:188:TYR:O	27:U:191:LEU:HG	2.20	0.42
28:V:228:MET:O	28:V:232:LYS:HG3	2.20	0.42
29:X:19:DA:H2"	29:X:20:DG:C8	2.55	0.42
32:k:182:LEU:HD23	32:k:182:LEU:HA	1.85	0.42
34:o:18:ILE:HD11	35:p:1149:VAL:HG11	2.01	0.42
34:o:1175:ILE:HG12	34:o:1212:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:o:1451:MET:HE3	34:o:1451:MET:HB3	1.91	0.42
35:p:541:ILE:HD13	35:p:616:THR:HG21	2.01	0.42
36:q:19:VAL:HG12	36:q:21:PHE:HD1	1.84	0.42
37:r:91:LYS:H	37:r:122:PHE:HZ	1.67	0.42
40:u:22:LEU:O	40:u:26:VAL:HG23	2.19	0.42
40:u:117:MET:HA	40:u:130:THR:HA	2.01	0.42
15:f:317:LEU:HG	15:f:330:ARG:HE	1.83	0.42
4:3:175:MET:HE3	4:3:179:ASN:ND2	2.35	0.42
7:6:409:THR:O	7:6:413:LEU:HD13	2.19	0.42
11:A:357:GLU:HB3	11:A:358:ASP:H	1.60	0.42
17:H:178:LYS:HD3	17:H:178:LYS:HA	1.82	0.42
24:R:133:ASN:OD1	24:R:134:ILE:N	2.52	0.42
27:U:74:CYS:SG	27:U:92:TYR:HA	2.60	0.42
29:X:-28:DA:H2'	29:X:-27:DA:C8	2.54	0.42
34:o:364:ARG:NH1	34:o:502:ASN:OD1	2.52	0.42
34:o:1202:PHE:HB3	34:o:1263:ASN:HD22	1.85	0.42
35:p:1163:MET:HA	35:p:1167:ILE:O	2.19	0.42
45:z:36:CYS:HB3	45:z:39:CYS:SG	2.59	0.42
14:e:447:THR:O	14:e:450:ARG:HB2	2.19	0.42
4:3:53:ARG:HG3	5:4:46:ARG:CZ	2.50	0.42
7:6:535:THR:HG23	7:6:627:SER:HB2	2.02	0.42
8:7:56:ILE:HG21	8:7:70:LEU:HD22	2.01	0.42
14:E:476:VAL:HB	14:E:782:HIS:HB2	2.00	0.42
15:F:397:GLN:H	15:F:397:GLN:HG3	1.60	0.42
22:P:298:PRO:HB2	22:P:300:ILE:HG12	2.00	0.42
24:R:46:ILE:O	24:R:49:GLY:N	2.52	0.42
25:S:166:ARG:O	25:S:169:LYS:HG2	2.18	0.42
25:S:177:MET:HG2	42:w:40:ARG:O	2.18	0.42
34:o:357:LYS:HD2	35:p:1107:LEU:O	2.20	0.42
35:p:214:LYS:HD3	35:p:214:LYS:H	1.85	0.42
42:w:115:THR:HG22	42:w:116:ALA:H	1.84	0.42
14:e:225:ILE:HD12	14:e:236:LEU:HB3	2.02	0.42
15:f:26:MET:HE3	15:f:26:MET:HB3	1.77	0.42
2:1:524:HIS:NE2	2:1:528:MET:SD	2.93	0.42
5:4:442:VAL:HG21	6:5:44:PHE:CE2	2.54	0.42
8:7:661:ALA:HA	8:7:664:VAL:HG12	2.02	0.42
11:A:468:PHE:CE1	15:F:221:GLN:HG3	2.54	0.42
12:B:487:LYS:O	12:B:487:LYS:CG	2.67	0.42
15:F:410:PRO:O	15:F:411:VAL:C	2.63	0.42
28:V:165:GLY:HA2	28:V:169:GLU:OE1	2.18	0.42
29:X:7:DT:C6	29:X:8:DC:C5	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:p:550:MET:HE2	35:p:550:MET:HB3	1.93	0.42
35:p:623:ARG:HH12	35:p:697:GLU:CD	2.28	0.42
36:q:86:ARG:H	36:q:86:ARG:HG2	1.63	0.42
37:r:17:ALA:HB1	37:r:95:PHE:CZ	2.54	0.42
38:s:193:ILE:HB	38:s:205:THR:OG1	2.18	0.42
39:t:72:GLN:HE22	40:u:59:ILE:HD13	1.85	0.42
42:w:106:ASP:OD1	42:w:106:ASP:N	2.51	0.42
14:e:504:LEU:HD22	14:e:575:PHE:HZ	1.84	0.42
15:f:432:ALA:HB1	15:f:462:GLN:CB	2.49	0.42
3:2:174:LEU:CD2	3:2:203:ALA:HB2	2.42	0.42
5:4:380:THR:O	5:4:380:THR:HG23	2.18	0.42
5:4:433:PHE:CD2	6:5:38:ILE:HG12	2.53	0.42
8:7:557:ILE:HG22	8:7:561:ILE:HD12	2.01	0.42
11:A:464:TRP:CD1	11:A:464:TRP:C	2.96	0.42
12:B:562:GLY:O	12:B:581:ILE:HG12	2.19	0.42
13:D:998:GLN:HA	13:D:1001:GLN:HB2	2.01	0.42
15:F:324:ASP:CG	15:F:327:TRP:HD1	2.28	0.42
24:R:127:ARG:NH2	35:p:433:LEU:O	2.52	0.42
26:T:140:ARG:HD3	35:p:60:GLU:OE2	2.20	0.42
32:k:130:PRO:HD3	33:m:35:GLU:HG2	2.01	0.42
34:o:214:ILE:H	34:o:214:ILE:HG13	1.44	0.42
34:o:320:ASN:HB3	34:o:341:GLN:NE2	2.35	0.42
35:p:59:VAL:HG21	35:p:91:ILE:HD12	2.00	0.42
1:0:85:ARG:NH2	1:0:139:LYS:HB3	2.34	0.42
5:4:261:PHE:CZ	5:4:265:LEU:HD21	2.54	0.42
5:4:415:GLN:HB2	5:4:439:ARG:HH21	1.85	0.42
7:6:559:ILE:HG22	7:6:561:PHE:CE1	2.55	0.42
11:A:968:ILE:HD12	11:A:968:ILE:HA	1.94	0.42
12:B:216:SER:OG	12:B:217:ASN:N	2.52	0.42
12:B:594:SER:OG	12:B:595:LYS:N	2.52	0.42
13:D:1002:ARG:HB2	26:T:182:HIS:HD2	1.78	0.42
20:L:62:LYS:HD2	20:L:62:LYS:HA	1.87	0.42
26:T:32:ALA:HA	26:T:35:SER:HB2	2.01	0.42
28:V:145:VAL:C	28:V:146:ARG:HD2	2.45	0.42
32:k:179:MET:HB3	32:k:180:PRO:CD	2.50	0.42
34:o:114:CYS:SG	34:o:184:CYS:HB3	2.58	0.42
34:o:514:GLU:CD	35:p:1101:GLN:HB2	2.45	0.42
1:0:8:ARG:HG3	27:U:173:ALA:N	2.34	0.42
2:1:374:LEU:HD12	2:1:374:LEU:C	2.45	0.42
7:6:412:MET:HA	7:6:415:HIS:CD2	2.55	0.42
8:7:462:SER:OG	8:7:463:PRO:CD	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:790:LEU:HD13	17:H:146:ILE:HG12	2.00	0.42
20:L:120:LEU:HD23	20:L:128:ILE:HG12	2.01	0.42
20:L:120:LEU:O	20:L:125:ASN:N	2.52	0.42
22:P:288:PHE:CD1	22:P:289:PRO:HD2	2.54	0.42
25:S:164:TRP:HZ2	35:p:268:PRO:HG2	1.85	0.42
26:T:154:LYS:HE3	26:T:154:LYS:HB2	1.94	0.42
26:T:175:ARG:HD2	26:T:207:LYS:HA	2.01	0.42
27:U:139:LEU:N	40:u:160:ILE:CD1	2.83	0.42
27:U:154:CYS:HB3	27:U:157:CYS:O	2.20	0.42
29:X:24:DA:H2"	29:X:25:DG:N7	2.34	0.42
34:o:475:ARG:HH21	44:y:68:GLU:CD	2.28	0.42
38:s:61:LEU:HB2	38:s:73:PHE:CE2	2.55	0.42
14:e:332:ILE:HA	14:e:336:HIS:HD2	1.84	0.42
15:f:104:LEU:HD22	19:j:216:TYR:HB2	2.02	0.42
2:1:503:THR:OG1	2:1:533:TYR:OH	2.01	0.42
8:7:114:ASN:C	8:7:114:ASN:ND2	2.78	0.42
8:7:272:ARG:HA	8:7:275:GLU:HG2	2.02	0.42
11:A:472:ASN:ND2	15:f:299:LYS:O	2.53	0.42
15:F:329:LEU:HA	15:F:332:PHE:HB3	2.01	0.42
25:S:51:LEU:O	25:S:54:LYS:HG3	2.19	0.42
27:U:76:MET:HG3	27:U:89:HIS:C	2.45	0.42
28:V:231:GLU:OE1	28:V:231:GLU:HA	2.18	0.42
30:Y:-14:DG:H2"	30:Y:-13:DT:H71	2.02	0.42
30:Y:-12:DA:H2"	30:Y:-11:DG:OP2	2.20	0.42
31:c:94:HIS:CD2	15:f:122:LEU:HD22	2.55	0.42
34:o:529:GLN:HG3	34:o:1094:SER:HB3	2.02	0.42
34:o:1189:ASP:HA	34:o:1192:TRP:CZ2	2.55	0.42
34:o:1262:MET:HB3	34:o:1265:ASP:CB	2.50	0.42
35:p:677:MET:CE	35:p:700:PRO:HB3	2.50	0.42
35:p:867:ILE:HB	35:p:894:THR:OG1	2.20	0.42
1:0:85:ARG:NH1	1:0:140:LEU:N	2.68	0.41
4:3:42:MET:HE3	4:3:108:ASN:HA	2.02	0.41
4:3:253:ALA:O	4:3:262:ILE:N	2.42	0.41
8:7:354:PRO:HA	8:7:416:ILE:HD12	2.02	0.41
13:D:998:GLN:HB2	13:D:1002:ARG:NH2	2.35	0.41
15:F:231:CYS:HB3	15:F:285:MET:HE2	2.02	0.41
15:F:233:GLY:CA	15:F:239:ARG:HE	2.33	0.41
17:H:154:PRO:HB2	17:H:155:ASP:H	1.46	0.41
21:O:11:LEU:HD23	21:O:44:ILE:HD12	2.02	0.41
25:S:58:GLN:C	25:S:60:GLU:N	2.74	0.41
27:U:14:LEU:HD12	27:U:194:THR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y:-3:DC:H2'	30:Y:-2:DA:H8	1.84	0.41
34:o:486:LEU:HD23	34:o:496:PHE:HE2	1.84	0.41
34:o:531:ASN:HD21	34:o:1392:TYR:HE2	1.67	0.41
34:o:1163:HIS:CE1	34:o:1297:THR:HG23	2.55	0.41
35:p:818:GLU:O	35:p:916:TYR:HB3	2.20	0.41
35:p:942:LYS:CE	49:p:1201:W0F:O31	2.67	0.41
38:s:80:PRO:HA	38:s:107:GLN:HB2	2.02	0.41
40:u:30:LEU:O	40:u:34:VAL:HG22	2.19	0.41
41:v:88:PHE:CG	41:v:144:LEU:HB3	2.55	0.41
14:e:703:MET:HE2	14:e:703:MET:HB3	1.83	0.41
15:f:428:LEU:HD13	15:f:458:LEU:CB	2.49	0.41
3:2:174:LEU:HD23	8:7:533:ASP:OD2	2.20	0.41
4:3:257:CYS:HB2	4:3:258:HIS:CD2	2.54	0.41
5:4:403:PHE:HA	6:5:8:VAL:HG13	2.01	0.41
8:7:323:ILE:O	8:7:378:ARG:NH1	2.53	0.41
11:A:639:LEU:O	11:A:639:LEU:HD13	2.20	0.41
12:B:176:HIS:HE1	12:B:310:ASP:H	1.68	0.41
12:B:496:MET:HE3	12:B:496:MET:HB2	1.83	0.41
12:B:713:TRP:NE1	12:B:716:PRO:O	2.50	0.41
15:F:249:ASP:HB3	15:F:252:LEU:HB2	2.03	0.41
27:U:44:LYS:HA	27:U:44:LYS:HD3	1.86	0.41
28:V:109:LEU:HD23	28:V:109:LEU:H	1.84	0.41
28:V:229:ASP:HA	28:V:232:LYS:HG3	2.02	0.41
34:o:497:ASP:HB3	35:p:792:ASP:HB2	2.02	0.41
34:o:1095:LEU:HD13	34:o:1401:LEU:HD22	2.02	0.41
34:o:1180:ASN:HB2	34:o:1183:SER:HB3	2.02	0.41
1:0:8:ARG:CZ	1:0:37:LEU:HD13	2.50	0.41
1:0:85:ARG:CZ	1:0:140:LEU:HG	2.38	0.41
4:3:175:MET:HE3	4:3:179:ASN:CG	2.45	0.41
11:A:464:TRP:CD1	11:A:464:TRP:O	2.73	0.41
11:A:819:LYS:HE2	11:A:819:LYS:HB2	1.94	0.41
13:D:963:ARG:HA	13:D:966:LEU:H	1.85	0.41
24:R:121:ILE:HD13	24:R:138:THR:HG22	2.02	0.41
24:R:178:LYS:HE3	26:T:157:ALA:HB2	2.01	0.41
25:S:169:LYS:HE3	35:p:310:VAL:CG2	2.50	0.41
25:S:177:MET:HE2	42:w:41:ASN:HA	2.02	0.41
26:T:123:ASN:OD1	26:T:123:ASN:N	2.52	0.41
33:m:93:ASP:OD1	33:m:93:ASP:C	2.64	0.41
34:o:233:CYS:SG	34:o:238:MET:HB2	2.60	0.41
35:p:419:ALA:O	35:p:423:ILE:HG12	2.19	0.41
39:t:88:ASP:O	39:t:92:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:98:ASP:O	5:4:125:GLY:CA	2.66	0.41
4:3:192:ASP:OD1	4:3:213:LEU:N	2.45	0.41
5:4:237:LEU:HD21	5:4:261:PHE:HZ	1.86	0.41
7:6:173:ASN:N	7:6:434:GLU:OE2	2.49	0.41
8:7:383:LEU:HD21	8:7:388:ILE:HD11	2.02	0.41
12:B:371:LYS:HA	12:B:371:LYS:HD3	1.87	0.41
13:D:1002:ARG:NE	26:T:182:HIS:CD2	2.86	0.41
15:F:388:ILE:HA	15:F:392:ILE:HG12	2.02	0.41
27:U:172:ASP:O	27:U:173:ALA:C	2.64	0.41
28:V:166:ILE:HG22	28:V:167:LEU:H	1.86	0.41
30:Y:13:DA:C4	30:Y:14:DC:C5	3.09	0.41
33:m:70:HIS:HA	33:m:73:MET:HE3	2.02	0.41
34:o:112:PHE:HB3	34:o:113:PHE:CD1	2.56	0.41
34:o:863:ARG:NH2	34:o:1129:ASN:OD1	2.53	0.41
35:p:185:PHE:HB3	35:p:187:ILE:HD13	2.01	0.41
35:p:676:ALA:HA	35:p:682:LEU:HD22	2.01	0.41
36:q:26:THR:HG23	44:y:97:GLU:OE2	2.20	0.41
45:z:16:ILE:HG22	45:z:25:GLU:HB3	2.01	0.41
15:f:83:LEU:HD11	18:i:42:PHE:HB2	2.03	0.41
15:f:402:ARG:HH22	15:f:403:ILE:HD12	1.85	0.41
1:0:55:LYS:O	1:0:57:ASN:N	2.54	0.41
3:2:89:GLU:OE2	3:2:132:LYS:NZ	2.42	0.41
4:3:255:CYS:HB2	4:3:276:CYS:N	2.36	0.41
5:4:359:ILE:HG22	5:4:360:THR:N	2.35	0.41
5:4:400:ARG:NE	5:4:400:ARG:HA	2.36	0.41
7:6:193:VAL:HG11	7:6:283:ARG:HD3	2.01	0.41
7:6:364:LEU:HD23	7:6:410:TYR:CD1	2.56	0.41
11:A:337:ARG:HD3	11:A:338:VAL:H	1.85	0.41
11:A:463:PRO:HD2	15:F:218:VAL:HG22	2.03	0.41
12:B:984:PRO:HG2	12:B:987:LEU:HD22	2.02	0.41
13:D:962:GLU:C	13:D:965:ILE:HG22	2.45	0.41
25:S:161:GLU:O	25:S:165:GLU:HG2	2.20	0.41
27:U:194:THR:O	27:U:195:GLU:HG3	2.21	0.41
30:Y:5:DA:H2"	35:p:446:TYR:CE2	2.54	0.41
34:o:489:THR:HB	34:o:494:ALA:O	2.21	0.41
34:o:1318:LYS:HE2	34:o:1330:ALA:HB1	2.03	0.41
14:e:481:ASP:OD1	14:e:481:ASP:N	2.52	0.41
14:e:513:LEU:CD2	14:e:527:ILE:HG23	2.48	0.41
5:4:96:TRP:HB3	5:4:110:LEU:HD23	2.02	0.41
5:4:146:PRO:HA	5:4:149:ASP:OD2	2.21	0.41
8:7:618:VAL:HG11	8:7:664:VAL:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:352:MET:HE3	11:A:352:MET:HB3	1.81	0.41
12:B:639:LYS:NZ	12:B:641:GLU:OE2	2.43	0.41
14:E:476:VAL:HG11	14:E:794:ALA:HB3	2.02	0.41
14:E:508:LYS:HB3	14:E:512:ASP:HB2	2.02	0.41
27:U:104:LYS:HE3	27:U:191:LEU:HB2	2.01	0.41
27:U:139:LEU:HG	40:u:159:ALA:CA	2.49	0.41
27:U:172:ASP:OD1	27:U:172:ASP:N	2.51	0.41
34:o:368:THR:HG21	35:p:931:ILE:O	2.21	0.41
35:p:21:LEU:HD12	35:p:21:LEU:HA	1.93	0.41
35:p:300:MET:O	35:p:303:PRO:HD2	2.20	0.41
14:e:378:LYS:HZ3	14:e:378:LYS:HG2	1.61	0.41
1:0:8:ARG:NH1	1:0:9:CYS:SG	2.94	0.41
7:6:128:SER:O	7:6:334:ARG:NH2	2.51	0.41
11:A:413:ASP:O	11:A:414:ILE:C	2.63	0.41
13:D:960:GLU:OE1	13:D:960:GLU:N	2.53	0.41
15:F:396:LEU:HA	15:F:399:GLU:OE1	2.20	0.41
20:L:110:THR:HG23	20:L:112:GLU:HG3	2.02	0.41
26:T:9:LEU:O	26:T:13:LYS:HG2	2.20	0.41
26:T:31:TRP:CD1	26:T:62:LEU:HD21	2.56	0.41
28:V:187:ASP:HB2	28:V:189:ILE:HG22	2.02	0.41
34:o:531:ASN:HB3	34:o:898:GLY:O	2.21	0.41
35:p:269:ILE:HG21	35:p:269:ILE:HD13	1.75	0.41
35:p:794:VAL:O	35:p:946:GLY:N	2.53	0.41
15:f:216:LEU:HD21	15:f:254:GLN:O	2.21	0.41
15:f:320:ARG:HH11	15:f:320:ARG:HB2	1.83	0.41
2:1:422:LEU:HD21	4:3:224:LEU:HB3	2.02	0.41
3:2:186:ILE:HG12	3:2:211:LEU:HD12	2.03	0.41
3:2:333:GLU:O	3:2:333:GLU:HG2	2.21	0.41
4:3:217:VAL:O	4:3:217:VAL:HG23	2.20	0.41
12:B:55:PRO:HB3	12:B:60:LEU:HD22	2.02	0.41
12:B:544:LEU:HD22	12:B:625:LEU:HD22	2.02	0.41
13:D:995:GLU:OE2	26:T:193:LYS:HD2	2.20	0.41
14:E:521:ASP:OD1	14:E:521:ASP:N	2.52	0.41
15:F:258:ARG:HA	15:F:258:ARG:HD2	1.83	0.41
25:S:164:TRP:CD1	35:p:311:ILE:HD11	2.56	0.41
30:Y:5:DA:O5'	35:p:188:ASN:ND2	2.53	0.41
34:o:40:GLY:HA2	34:o:87:HIS:O	2.21	0.41
34:o:618:TYR:HA	34:o:621:ILE:HG13	2.02	0.41
34:o:1162:GLU:O	34:o:1300:GLY:HA3	2.20	0.41
35:p:553:LEU:HA	35:p:553:LEU:HD23	1.88	0.41
36:q:7:PRO:HB3	36:q:26:THR:OG1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:u:79:PRO:HG3	40:u:104:MET:SD	2.61	0.41
19:j:173:HIS:HA	19:j:176:MET:HE3	2.02	0.41
1:0:13:LYS:HD3	1:0:13:LYS:N	2.35	0.41
1:0:55:LYS:CE	40:u:166:ASP:OD2	2.69	0.41
1:0:84:LYS:CB	1:0:136:ASN:HD21	2.33	0.41
3:2:115:GLU:N	3:2:115:GLU:OE1	2.54	0.41
3:2:379:LEU:O	3:2:379:LEU:HD23	2.21	0.41
4:3:229:TRP:CZ3	5:4:58:ARG:CD	3.03	0.41
5:4:229:ASP:OD1	5:4:229:ASP:N	2.54	0.41
7:6:474:ASP:OD1	7:6:474:ASP:N	2.54	0.41
8:7:145:GLN:HG2	8:7:150:THR:HG22	2.03	0.41
8:7:195:ALA:O	8:7:199:ILE:HG12	2.21	0.41
11:A:335:LYS:HE2	11:A:495:LEU:HB2	2.03	0.41
11:A:731:LEU:HD23	11:A:731:LEU:HA	1.92	0.41
12:B:62:ARG:H	12:B:62:ARG:HG2	1.58	0.41
12:B:77:ILE:HG12	12:B:146:ILE:HG23	2.03	0.41
12:B:203:LYS:HZ3	12:B:235:HIS:HB3	1.85	0.41
12:B:295:LEU:HD13	12:B:477:LEU:HD11	2.03	0.41
12:B:887:ARG:NH2	12:B:917:ASP:OD2	2.49	0.41
13:D:998:GLN:HE22	26:T:186:MET:HA	1.82	0.41
14:E:236:LEU:HD21	14:E:317:LEU:HB2	2.03	0.41
14:E:775:THR:CG2	14:E:778:THR:HB	2.51	0.41
15:F:114:LEU:HB2	17:H:52:SER:N	2.35	0.41
15:F:277:ALA:O	15:F:278:LEU:C	2.64	0.41
15:F:312:ILE:HG13	15:F:334:ALA:HB1	2.00	0.41
24:R:46:ILE:HD13	24:R:46:ILE:HA	1.86	0.41
25:S:44:GLN:HE21	25:S:44:GLN:HB3	1.66	0.41
25:S:73:ARG:NH2	26:T:229:HIS:HB2	2.36	0.41
27:U:19:LYS:HA	27:U:22:ILE:HB	2.03	0.41
27:U:110:MET:HE1	28:V:219:LEU:HB3	2.02	0.41
28:V:90:GLN:HE22	28:V:176:PRO:HG3	1.84	0.41
28:V:146:ARG:NE	28:V:173:GLU:O	2.54	0.41
29:X:31:DG:H2"	29:X:32:DT:H71	2.02	0.41
30:Y:-27:DT:H2"	30:Y:-26:DG:C8	2.56	0.41
34:o:129:ILE:HD13	34:o:129:ILE:HA	1.97	0.41
34:o:542:LEU:O	34:o:545:VAL:HG12	2.20	0.41
34:o:1175:ILE:HD12	34:o:1286:ARG:HG2	2.03	0.41
35:p:264:LYS:HE2	35:p:264:LYS:HB3	1.89	0.41
35:p:411:LEU:O	35:p:415:VAL:HG23	2.21	0.41
35:p:556:ILE:HD11	35:p:576:ILE:HG12	2.02	0.41
35:p:1091:ARG:O	35:p:1095:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:q:260:GLN:NE2	44:y:92:THR:HG22	2.35	0.41
40:u:92:VAL:HG13	40:u:128:TYR:CD2	2.55	0.41
45:z:28:ILE:HG23	45:z:32:ASP:HB3	2.03	0.41
13:d:1064:ILE:HD13	13:d:1064:ILE:HA	1.94	0.41
14:e:246:HIS:CD2	14:e:246:HIS:C	2.98	0.41
15:f:254:GLN:O	15:f:254:GLN:HG3	2.21	0.41
4:3:46:ASN:OD1	5:4:123:LEU:HD23	2.20	0.41
8:7:225:LEU:O	8:7:227:ARG:NH1	2.53	0.41
8:7:243:CYS:O	8:7:246:SER:OG	2.37	0.41
12:B:881:GLY:HA3	17:H:218:PRO:HB3	2.02	0.41
14:E:265:GLU:OE1	14:E:265:GLU:HA	2.20	0.41
14:E:668:HIS:NE2	14:E:686:THR:OG1	2.42	0.41
15:F:370:TRP:CH2	15:F:402:ARG:HB3	2.56	0.41
15:F:374:TYR:CE1	15:F:422:HIS:HB3	2.56	0.41
15:F:396:LEU:HA	15:F:399:GLU:CD	2.46	0.41
22:P:169:VAL:HG22	22:P:222:THR:HG22	2.02	0.41
22:P:196:ARG:NH1	30:Y:25:DT:O3'	2.54	0.41
24:R:74:LEU:CD2	35:p:823:PHE:HB2	2.51	0.41
24:R:251:ILE:H	24:R:251:ILE:HD12	1.86	0.41
25:S:110:PHE:CE2	25:S:148:PRO:HB3	2.55	0.41
28:V:189:ILE:HB	28:V:204:ASN:HB2	2.03	0.41
30:Y:-8:DG:H2"	30:Y:-7:DA:OP2	2.21	0.41
32:k:142:THR:OG1	32:k:143:GLY:N	2.55	0.41
34:o:1130:ILE:HD13	34:o:1411:LEU:HB3	2.03	0.41
36:q:7:PRO:HB2	44:y:101:LEU:HD13	2.02	0.41
36:q:44:ILE:HD11	36:q:178:PRO:HB3	2.03	0.41
40:u:104:MET:HE2	40:u:104:MET:HB3	1.98	0.41
41:v:15:ILE:HD11	41:v:51:ASP:HA	2.02	0.41
4:3:237:GLN:HG3	5:4:51:LEU:HD22	1.93	0.40
4:3:242:ILE:HD13	5:4:73:LEU:O	2.21	0.40
5:4:384:PRO:HB2	5:4:387:ILE:HG12	2.03	0.40
8:7:12:PHE:CE2	8:7:14:TYR:HB2	2.56	0.40
11:A:592:SER:OG	11:A:695:GLY:O	2.31	0.40
11:A:604:PRO:O	11:A:889:TYR:OH	2.34	0.40
12:B:464:ILE:HG12	12:B:513:LYS:HE2	2.02	0.40
12:B:987:LEU:HG	12:B:988:PRO:HD2	2.03	0.40
23:Q:19:GLU:O	23:Q:22:ILE:HG12	2.21	0.40
27:U:139:LEU:HD12	40:u:160:ILE:H	1.85	0.40
28:V:166:ILE:HG22	28:V:167:LEU:N	2.36	0.40
33:m:52:GLU:OE1	33:m:52:GLU:N	2.40	0.40
33:m:77:ARG:CZ	33:m:77:ARG:HB3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:o:551:ARG:HG2	41:v:121:LEU:HD23	2.03	0.40
35:p:274:ARG:HG2	35:p:279:VAL:HA	2.03	0.40
35:p:529:MET:HE3	35:p:624:PRO:HG2	2.02	0.40
35:p:961:ILE:HG23	43:x:9:THR:HG21	2.03	0.40
40:u:12:LEU:HD11	40:u:67:LEU:HD12	2.02	0.40
6:5:32:LYS:HE3	12:B:539:ARG:NH2	2.36	0.40
8:7:28:LEU:HD22	8:7:55:LEU:CD2	2.52	0.40
11:A:1068:ARG:HD2	11:A:1068:ARG:C	2.46	0.40
12:B:957:MET:O	12:B:968:ARG:NH1	2.53	0.40
14:E:651:VAL:HG21	14:E:686:THR:HG21	2.01	0.40
15:F:329:LEU:HA	15:F:332:PHE:CB	2.52	0.40
24:R:83:MET:HB2	24:R:104:ARG:HH11	1.86	0.40
27:U:152:PHE:HZ	40:u:96:GLY:N	2.17	0.40
27:U:192:ARG:O	27:U:195:GLU:HB3	2.22	0.40
34:o:225:PHE:HB3	34:o:245:PRO:HB2	2.03	0.40
34:o:576:GLN:HG3	34:o:577:PRO:HD2	2.02	0.40
34:o:725:LEU:HB3	34:o:733:LEU:HD11	2.03	0.40
41:v:37:MET:HE1	41:v:132:LEU:HD21	2.03	0.40
1:0:108:ASN:OD1	1:0:112:ASN:HB3	2.22	0.40
2:1:219:GLU:O	2:1:223:ARG:HG2	2.21	0.40
2:1:303:ILE:HG22	2:1:307:PHE:HE2	1.87	0.40
2:1:411:MET:HG2	2:1:411:MET:O	2.22	0.40
3:2:318:LEU:HD12	4:3:272:LEU:CD2	2.51	0.40
5:4:62:LEU:O	5:4:115:ARG:NH2	2.54	0.40
7:6:340:LEU:CD2	7:6:491:ALA:HB2	2.52	0.40
8:7:101:LYS:C	8:7:102:LEU:HD12	2.46	0.40
8:7:176:ASN:OD1	8:7:177:LEU:N	2.49	0.40
9:N:1:ILX:HA	34:o:791:GLN:NE2	2.36	0.40
11:A:411:GLU:H	11:A:411:GLU:HG3	1.64	0.40
11:A:725:CYS:SG	11:A:734:LEU:HD12	2.61	0.40
12:B:219:ASP:OD1	12:B:219:ASP:N	2.52	0.40
13:D:963:ARG:C	13:D:966:LEU:H	2.29	0.40
15:F:312:ILE:HG22	15:F:313:VAL:CG1	2.50	0.40
17:H:92:ASP:O	17:H:96:THR:OG1	2.32	0.40
24:R:94:ASP:O	24:R:97:GLY:N	2.38	0.40
25:S:89:LYS:HE2	25:S:89:LYS:HB2	1.76	0.40
29:X:10:DT:H2"	29:X:11:DC:C6	2.57	0.40
34:o:389:THR:HG21	34:o:417:LYS:HB2	2.03	0.40
34:o:619:LYS:HG3	34:o:620:HIS:CD2	2.56	0.40
35:p:119:THR:HG23	35:p:187:ILE:HA	2.03	0.40
36:q:189:ASP:OD1	36:q:209:SER:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:w:79:PRO:HG2	42:w:96:PHE:O	2.21	0.40
1:0:1:MET:HG3	8:7:345:ARG:NH1	2.37	0.40
1:0:85:ARG:HH12	1:0:140:LEU:H	1.67	0.40
3:2:227:HIS:CE1	3:2:231:LEU:HD11	2.57	0.40
5:4:448:HIS:CD2	5:4:452:LYS:HE3	2.56	0.40
8:7:72:TYR:HB3	8:7:206:VAL:HG12	2.04	0.40
8:7:604:VAL:O	8:7:608:ILE:HG22	2.22	0.40
11:A:511:LEU:N	11:A:511:LEU:HD13	2.36	0.40
12:B:298:ARG:HH11	12:B:298:ARG:HD3	1.68	0.40
14:E:239:LEU:HB3	14:E:307:LEU:HD21	2.03	0.40
15:F:350:ASN:O	15:F:354:ARG:HB2	2.22	0.40
28:V:133:ILE:HG22	28:V:134:ASP:N	2.36	0.40
31:c:105:ASN:OD1	31:c:105:ASN:N	2.55	0.40
34:o:601:ASN:HA	34:o:630:VAL:O	2.21	0.40
34:o:1121:VAL:N	34:o:1122:PRO:HD2	2.36	0.40
35:p:94:SER:O	35:p:122:ALA:HB1	2.22	0.40
35:p:770:ARG:HE	35:p:770:ARG:HB2	1.70	0.40
36:q:193:ARG:HA	36:q:193:ARG:HD3	1.78	0.40
36:q:246:LEU:HD23	36:q:246:LEU:HA	1.90	0.40
36:q:259:LEU:HA	36:q:259:LEU:HD23	1.81	0.40
37:r:18:SER:HB2	37:r:116:PRO:HD2	2.04	0.40
37:r:31:THR:HG21	37:r:95:PHE:HA	2.03	0.40
38:s:72:MET:HG3	38:s:101:ARG:HD2	2.04	0.40
40:u:91:GLN:HG2	40:u:92:VAL:N	2.36	0.40
42:w:78:LEU:HD23	42:w:78:LEU:HA	1.89	0.40
15:f:149:PRO:HA	15:f:150:PRO:HD3	1.83	0.40
15:f:284:ARG:HH21	15:f:284:ARG:HD2	1.76	0.40
15:f:446:ASP:O	15:f:450:ALA:N	2.54	0.40
1:0:32:GLU:OE1	1:0:32:GLU:N	2.47	0.40
3:2:174:LEU:O	8:7:591:GLY:O	2.40	0.40
8:7:329:PHE:CZ	8:7:333:LEU:HD21	2.57	0.40
8:7:531:VAL:HG12	8:7:532:PRO:O	2.22	0.40
9:N:2:TRX:CE3	34:o:749:ARG:HD2	2.52	0.40
11:A:939:ILE:HG22	11:A:943:LYS:NZ	2.37	0.40
13:D:933:ARG:CZ	19:J:114:THR:HG21	2.51	0.40
13:D:1001:GLN:HG2	21:O:1:MET:HB3	2.04	0.40
15:F:324:ASP:CA	15:F:327:TRP:HB3	2.44	0.40
15:F:433:PRO:C	15:F:435:LEU:N	2.78	0.40
16:G:74:MET:HE1	16:G:136:ILE:HD12	2.03	0.40
17:H:132:LYS:HG3	17:H:134:LEU:H	1.86	0.40
17:H:201:GLN:HG3	17:H:215:ALA:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:R:101:TYR:O	24:R:102:GLN:HG3	2.22	0.40
26:T:145:LEU:HD22	26:T:145:LEU:HA	1.94	0.40
34:o:115:SER:HB3	34:o:228:ILE:HG12	2.03	0.40
34:o:256:PRO:HA	34:o:257:PRO:HD3	1.96	0.40
34:o:362:SER:HA	34:o:503:LEU:O	2.22	0.40
35:p:810:PHE:HB2	35:p:927:ARG:HE	1.86	0.40
14:e:467:LEU:HD23	14:e:467:LEU:HA	1.93	0.40
14:e:479:THR:OG1	14:e:481:ASP:O	2.32	0.40
15:f:217:SER:H	15:f:220:GLN:HE21	1.70	0.40
18:i:78:ARG:HD3	18:i:78:ARG:HA	1.78	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	0	169/309 (55%)	157 (93%)	12 (7%)	0	100	100
2	1	253/548 (46%)	243 (96%)	10 (4%)	0	100	100
3	2	325/395 (82%)	313 (96%)	12 (4%)	0	100	100
4	3	259/308 (84%)	253 (98%)	6 (2%)	0	100	100
5	4	384/462 (83%)	365 (95%)	19 (5%)	0	100	100
6	5	52/71 (73%)	48 (92%)	2 (4%)	2 (4%)	2	19
7	6	601/782 (77%)	574 (96%)	26 (4%)	1 (0%)	43	77
8	7	710/760 (93%)	683 (96%)	27 (4%)	0	100	100
9	N	4/8 (50%)	3 (75%)	1 (25%)	0	100	100
11	A	543/1872 (29%)	519 (96%)	23 (4%)	1 (0%)	43	77
12	B	959/1199 (80%)	911 (95%)	48 (5%)	0	100	100
13	D	158/1085 (15%)	153 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	d	154/1085 (14%)	150 (97%)	4 (3%)	0	100	100
14	E	541/800 (68%)	518 (96%)	22 (4%)	1 (0%)	43	77
14	e	531/800 (66%)	482 (91%)	48 (9%)	1 (0%)	43	77
15	F	408/677 (60%)	391 (96%)	16 (4%)	1 (0%)	43	77
15	f	399/677 (59%)	381 (96%)	18 (4%)	0	100	100
16	G	138/349 (40%)	135 (98%)	3 (2%)	0	100	100
17	H	207/310 (67%)	189 (91%)	13 (6%)	5 (2%)	4	27
18	I	118/264 (45%)	115 (98%)	3 (2%)	0	100	100
18	i	119/264 (45%)	115 (97%)	4 (3%)	0	100	100
19	J	86/218 (39%)	82 (95%)	4 (5%)	0	100	100
19	j	91/218 (42%)	85 (93%)	4 (4%)	2 (2%)	5	29
20	L	74/161 (46%)	72 (97%)	2 (3%)	0	100	100
20	l	105/161 (65%)	100 (95%)	5 (5%)	0	100	100
21	O	97/109 (89%)	95 (98%)	2 (2%)	0	100	100
22	P	177/339 (52%)	175 (99%)	2 (1%)	0	100	100
23	Q	109/376 (29%)	102 (94%)	7 (6%)	0	100	100
24	R	278/316 (88%)	262 (94%)	14 (5%)	2 (1%)	18	56
25	S	174/517 (34%)	162 (93%)	11 (6%)	1 (1%)	21	59
26	T	218/249 (88%)	211 (97%)	7 (3%)	0	100	100
27	U	180/439 (41%)	153 (85%)	26 (14%)	1 (1%)	21	59
28	V	163/291 (56%)	139 (85%)	24 (15%)	0	100	100
31	c	125/929 (14%)	116 (93%)	9 (7%)	0	100	100
32	k	96/211 (46%)	91 (95%)	5 (5%)	0	100	100
33	m	85/124 (68%)	82 (96%)	3 (4%)	0	100	100
34	o	1448/1970 (74%)	1396 (96%)	47 (3%)	5 (0%)	36	72
35	p	1145/1174 (98%)	1105 (96%)	40 (4%)	0	100	100
36	q	253/275 (92%)	246 (97%)	7 (3%)	0	100	100
37	r	126/142 (89%)	126 (100%)	0	0	100	100
38	s	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
39	t	80/127 (63%)	79 (99%)	1 (1%)	0	100	100
40	u	169/172 (98%)	167 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	v	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
42	w	112/125 (90%)	108 (96%)	4 (4%)	0	100	100
43	x	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
44	y	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
45	z	42/58 (72%)	40 (95%)	2 (5%)	0	100	100
All	All	12996/22270 (58%)	12409 (96%)	564 (4%)	23 (0%)	44	77

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	5	48	GLU
14	E	523	VAL
17	H	156	PRO
25	S	87	VAL
34	o	1103	THR
14	e	522	ASP
19	j	124	GLU
11	A	502	LEU
15	F	411	VAL
17	H	154	PRO
19	j	177	LYS
6	5	39	ASP
17	H	136	ALA
17	H	139	ASN
24	R	90	ALA
24	R	99	SER
7	6	416	THR
34	o	1433	GLU
34	o	1274	GLU
17	H	158	THR
27	U	137	THR
34	o	184	CYS
34	o	1275	VAL

5.3.2 Protein sidechains (i)

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	0	164/283 (58%)	158 (96%)	6 (4%)	30	51
2	1	241/484 (50%)	241 (100%)	0	100	100
3	2	295/352 (84%)	294 (100%)	1 (0%)	86	85
4	3	234/272 (86%)	232 (99%)	2 (1%)	70	78
5	4	346/399 (87%)	339 (98%)	7 (2%)	48	66
6	5	48/64 (75%)	47 (98%)	1 (2%)	47	65
7	6	536/688 (78%)	535 (100%)	1 (0%)	87	86
8	7	624/664 (94%)	624 (100%)	0	100	100
9	N	2/2 (100%)	2 (100%)	0	100	100
11	A	496/1665 (30%)	452 (91%)	44 (9%)	9	28
12	B	876/1083 (81%)	862 (98%)	14 (2%)	55	70
13	D	147/815 (18%)	136 (92%)	11 (8%)	12	33
13	d	146/815 (18%)	144 (99%)	2 (1%)	59	72
14	E	480/657 (73%)	467 (97%)	13 (3%)	39	60
14	e	475/657 (72%)	462 (97%)	13 (3%)	39	60
15	F	328/574 (57%)	307 (94%)	21 (6%)	16	37
15	f	322/574 (56%)	312 (97%)	10 (3%)	35	56
16	G	132/322 (41%)	124 (94%)	8 (6%)	17	38
17	H	181/270 (67%)	175 (97%)	6 (3%)	33	55
18	I	106/235 (45%)	106 (100%)	0	100	100
18	i	107/235 (46%)	107 (100%)	0	100	100
19	J	79/154 (51%)	72 (91%)	7 (9%)	9	28
19	j	83/154 (54%)	82 (99%)	1 (1%)	63	75
20	L	71/141 (50%)	66 (93%)	5 (7%)	14	36
20	l	98/141 (70%)	97 (99%)	1 (1%)	68	78
21	O	90/98 (92%)	90 (100%)	0	100	100
22	P	154/293 (53%)	154 (100%)	0	100	100
23	Q	105/324 (32%)	105 (100%)	0	100	100
24	R	238/268 (89%)	234 (98%)	4 (2%)	53	69
25	S	154/448 (34%)	134 (87%)	20 (13%)	4	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	T	196/218 (90%)	193 (98%)	3 (2%)	57	72
27	U	167/373 (45%)	166 (99%)	1 (1%)	78	82
28	V	150/261 (58%)	149 (99%)	1 (1%)	76	81
31	c	113/833 (14%)	111 (98%)	2 (2%)	51	68
32	k	87/182 (48%)	87 (100%)	0	100	100
33	m	80/106 (76%)	71 (89%)	9 (11%)	5	19
34	o	1280/1749 (73%)	1261 (98%)	19 (2%)	57	72
35	p	1004/1027 (98%)	986 (98%)	18 (2%)	51	68
36	q	234/252 (93%)	228 (97%)	6 (3%)	40	61
37	r	118/126 (94%)	118 (100%)	0	100	100
38	s	191/192 (100%)	188 (98%)	3 (2%)	55	70
39	t	71/111 (64%)	71 (100%)	0	100	100
40	u	152/153 (99%)	150 (99%)	2 (1%)	61	74
41	v	129/131 (98%)	128 (99%)	1 (1%)	73	80
42	w	103/112 (92%)	98 (95%)	5 (5%)	22	43
43	x	56/56 (100%)	53 (95%)	3 (5%)	20	41
44	y	104/106 (98%)	102 (98%)	2 (2%)	50	67
45	z	41/55 (74%)	40 (98%)	1 (2%)	43	63
All	All	11634/19174 (61%)	11360 (98%)	274 (2%)	43	63

All (274) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	8	ARG
1	0	11	THR
1	0	28	HIS
1	0	29	THR
1	0	127	LYS
1	0	128	GLU
3	2	69	ARG
4	3	257	CYS
4	3	258	HIS
5	4	398	ARG
5	4	400	ARG
5	4	401	LEU
5	4	404	THR

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Mol	Chain	Res	Type
5	4	407	VAL
5	4	413	LEU
5	4	456	LYS
6	5	38	ILE
7	6	266	GLN
11	A	337	ARG
11	A	338	VAL
11	A	348	LEU
11	A	353	LEU
11	A	395	ASP
11	A	397	LEU
11	A	400	GLU
11	A	401	ASN
11	A	403	LEU
11	A	404	MET
11	A	408	LEU
11	A	415	ILE
11	A	416	TRP
11	A	419	GLU
11	A	470	ILE
11	A	475	LEU
11	A	481	GLU
11	A	483	ASN
11	A	491	MET
11	A	499	VAL
11	A	500	LEU
11	A	501	THR
11	A	502	LEU
11	A	505	ASN
11	A	511	LEU
11	A	639	LEU
11	A	661	GLU
11	A	667	THR
11	A	711	ASP
11	A	727	THR
11	A	730	PHE
11	A	819	LYS
11	A	821	ARG
11	A	828	GLU
11	A	925	ASP
11	A	943	LYS
11	A	970	ASN

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Mol	Chain	Res	Type
11	A	1052	ARG
11	A	1058	HIS
11	A	1062	TYR
11	A	1068	ARG
11	A	1073	GLN
11	A	1165	LEU
11	A	1203	GLU
12	B	21	GLU
12	B	71	ARG
12	B	140	GLU
12	B	184	ASN
12	B	262	MET
12	B	266	THR
12	B	293	GLU
12	B	559	LYS
12	B	603	LYS
12	B	640	VAL
12	B	746	SER
12	B	771	VAL
12	B	818	THR
12	B	987	LEU
13	D	948	GLU
13	D	952	GLN
13	D	953	ILE
13	D	957	ARG
13	D	958	LYS
13	D	960	GLU
13	D	964	GLU
13	D	965	ILE
13	D	966	LEU
13	D	1006	LEU
13	D	1009	LEU
14	E	258	ASN
14	E	274	TYR
14	E	278	ASP
14	E	280	ARG
14	E	326	ASN
14	E	327	ASN
14	E	519	GLU
14	E	521	ASP
14	E	522	ASP
14	E	527	ILE

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Mol	Chain	Res	Type
14	E	761	LEU
14	E	774	MET
14	E	775	THR
15	F	83	LEU
15	F	91	PHE
15	F	94	PHE
15	F	219	GLU
15	F	261	THR
15	F	269	VAL
15	F	271	VAL
15	F	280	ILE
15	F	295	LEU
15	F	301	VAL
15	F	312	ILE
15	F	317	LEU
15	F	326	HIS
15	F	340	ILE
15	F	348	THR
15	F	354	ARG
15	F	368	THR
15	F	397	GLN
15	F	406	VAL
15	F	415	ILE
15	F	427	LEU
16	G	41	ASP
16	G	129	LYS
16	G	131	ILE
16	G	143	VAL
16	G	153	LYS
16	G	181	TRP
16	G	182	GLU
16	G	183	ILE
17	H	27	ASP
17	H	36	THR
17	H	135	THR
17	H	157	HIS
17	H	161	LYS
17	H	162	THR
19	J	116	LEU
19	J	123	LEU
19	J	156	SER
19	J	164	SER

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Mol	Chain	Res	Type
19	J	174	CYS
19	J	177	LYS
19	J	192	LYS
20	L	79	ASP
20	L	104	ARG
20	L	108	SER
20	L	113	VAL
20	L	114	LYS
24	R	48	VAL
24	R	95	GLU
24	R	104	ARG
24	R	277	ILE
25	S	59	GLU
25	S	60	GLU
25	S	61	GLU
25	S	70	GLU
25	S	72	ASN
25	S	74	LYS
25	S	75	LEU
25	S	76	ARG
25	S	82	LYS
25	S	83	LYS
25	S	86	ILE
25	S	88	LEU
25	S	89	LYS
25	S	90	GLU
25	S	151	ARG
25	S	155	LEU
25	S	156	THR
25	S	163	GLU
25	S	167	ARG
25	S	171	LEU
26	T	145	LEU
26	T	148	VAL
26	T	171	GLU
27	U	145	PHE
28	V	189	ILE
31	c	24	ASP
31	c	106	VAL
33	m	31	LEU
33	m	55	ASP
33	m	58	GLU

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Mol	Chain	Res	Type
33	m	77	ARG
33	m	83	VAL
33	m	84	GLU
33	m	90	ILE
33	m	91	ARG
33	m	110	LEU
34	o	97	VAL
34	o	110	VAL
34	o	184	CYS
34	o	211	GLU
34	o	214	ILE
34	o	308	LYS
34	o	476	ILE
34	o	488	VAL
34	o	499	ASP
34	o	549	THR
34	o	585	LEU
34	o	621	ILE
34	o	934	LEU
34	o	996	ILE
34	o	1087	VAL
34	o	1103	THR
34	o	1336	LEU
34	o	1385	VAL
34	o	1458	ILE
35	p	90	GLN
35	p	192	LYS
35	p	214	LYS
35	p	215	TYR
35	p	235	ILE
35	p	269	ILE
35	p	351	VAL
35	p	388	TYR
35	p	438	ARG
35	p	466	VAL
35	p	598	VAL
35	p	719	SER
35	p	750	VAL
35	p	794	VAL
35	p	888	THR
35	p	901	THR
35	p	952	GLU

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Mol	Chain	Res	Type
35	p	1022	LEU
36	q	58	VAL
36	q	62	GLU
36	q	82	LEU
36	q	93	PHE
36	q	100	GLU
36	q	266	GLU
38	s	7	THR
38	s	58	LEU
38	s	71	GLN
40	u	50	THR
40	u	152	VAL
41	v	141	VAL
42	w	42	CYS
42	w	55	VAL
42	w	80	ARG
42	w	81	THR
42	w	115	THR
43	x	7	CYS
43	x	13	ILE
43	x	14	VAL
44	y	27	VAL
44	y	42	LEU
45	z	19	CYS
13	d	950	LEU
13	d	951	ASP
14	e	243	LEU
14	e	258	ASN
14	e	268	HIS
14	e	270	ASP
14	e	277	ASP
14	e	282	LEU
14	e	436	ASP
14	e	438	LEU
14	e	512	ASP
14	e	515	LEU
14	e	516	ILE
14	e	546	VAL
14	e	579	VAL
15	f	215	GLU
15	f	253	TYR
15	f	261	THR

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Mol	Chain	Res	Type
15	f	272	VAL
15	f	322	ASP
15	f	323	VAL
15	f	326	HIS
15	f	356	THR
15	f	366	GLU
15	f	421	ASP
19	j	114	THR
20	l	114	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (214) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	24	ASN
1	0	45	ASN
1	0	136	ASN
2	1	420	GLN
2	1	537	HIS
3	2	140	HIS
3	2	227	HIS
3	2	293	GLN
3	2	317	HIS
4	3	9	ASN
4	3	48	HIS
4	3	240	GLN
5	4	211	GLN
5	4	218	GLN
5	4	352	GLN
5	4	390	GLN
5	4	411	GLN
5	4	424	HIS
5	4	458	GLN
5	4	460	HIS
6	5	42	HIS
7	6	281	GLN
7	6	415	HIS
7	6	498	ASN
7	6	598	HIS
7	6	629	HIS
7	6	709	GLN
8	7	201	HIS
8	7	560	ASN

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Mol	Chain	Res	Type
8	7	645	GLN
11	A	401	ASN
11	A	472	ASN
11	A	489	GLN
11	A	590	GLN
11	A	630	GLN
11	A	702	ASN
11	A	755	HIS
11	A	802	HIS
11	A	896	GLN
11	A	1073	GLN
12	B	30	HIS
12	B	36	ASN
12	B	137	HIS
12	B	176	HIS
12	B	183	GLN
12	B	235	HIS
12	B	348	GLN
12	B	439	HIS
12	B	450	GLN
12	B	509	ASN
12	B	577	HIS
12	B	644	GLN
12	B	652	GLN
12	B	750	GLN
12	B	813	ASN
12	B	864	ASN
12	B	882	HIS
12	B	908	GLN
12	B	912	ASN
12	B	963	HIS
13	D	875	GLN
13	D	908	GLN
13	D	912	ASN
13	D	925	ASN
13	D	936	GLN
13	D	956	GLN
13	D	998	GLN
14	E	254	ASN
14	E	255	GLN
14	E	256	HIS
14	E	258	ASN

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Mol	Chain	Res	Type
14	E	327	ASN
14	E	351	GLN
14	E	616	HIS
14	E	640	ASN
14	E	673	HIS
14	E	733	ASN
14	E	758	HIS
14	E	800	GLN
15	F	37	GLN
15	F	59	HIS
15	F	79	ASN
15	F	89	GLN
15	F	119	ASN
15	F	221	GLN
15	F	270	ASN
15	F	273	GLN
15	F	275	ASN
15	F	326	HIS
15	F	430	HIS
16	G	10	HIS
16	G	48	HIS
16	G	142	ASN
17	H	24	ASN
17	H	142	HIS
17	H	145	HIS
18	I	21	GLN
18	I	38	GLN
18	I	98	GLN
19	J	210	ASN
20	L	117	GLN
21	O	35	GLN
21	O	54	ASN
22	P	229	GLN
22	P	278	GLN
24	R	98	ASN
24	R	103	ASN
24	R	116	ASN
25	S	44	GLN
25	S	72	ASN
25	S	96	GLN
25	S	152	HIS
25	S	178	GLN

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Mol	Chain	Res	Type
26	T	64	ASN
26	T	152	ASN
26	T	182	HIS
26	T	195	GLN
27	U	109	HIS
27	U	142	ASN
27	U	181	ASN
27	U	183	GLN
28	V	83	ASN
28	V	90	GLN
28	V	117	GLN
28	V	157	GLN
31	c	19	GLN
31	c	27	GLN
31	c	50	HIS
32	k	186	HIS
32	k	199	GLN
32	k	202	ASN
32	k	205	HIS
33	m	107	ASN
34	o	143	HIS
34	o	181	HIS
34	o	273	GLN
34	o	412	GLN
34	o	439	HIS
34	o	493	ASN
34	o	504	HIS
34	o	531	ASN
34	o	599	HIS
34	o	620	HIS
34	o	703	GLN
34	o	721	HIS
34	o	735	GLN
34	o	764	ASN
34	o	780	ASN
34	o	783	GLN
34	o	791	GLN
34	o	804	HIS
34	o	839	HIS
34	o	861	GLN
34	o	904	GLN
34	o	1032	GLN

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Mol	Chain	Res	Type
34	o	1105	ASN
34	o	1230	GLN
34	o	1263	ASN
34	o	1384	HIS
34	o	1410	HIS
35	p	72	GLN
35	p	90	GLN
35	p	98	HIS
35	p	145	GLN
35	p	188	ASN
35	p	245	GLN
35	p	319	ASN
35	p	461	GLN
35	p	481	HIS
35	p	525	ASN
35	p	639	HIS
35	p	699	HIS
35	p	725	GLN
35	p	755	GLN
35	p	986	GLN
35	p	1007	ASN
35	p	1025	ASN
35	p	1097	HIS
36	q	217	GLN
36	q	260	GLN
36	q	265	HIS
37	r	38	HIS
37	r	48	ASN
37	r	66	ASN
37	r	76	ASN
37	r	129	GLN
38	s	64	HIS
38	s	71	GLN
38	s	210	GLN
41	v	44	ASN
41	v	131	ASN
42	w	22	ASN
42	w	50	ASN
42	w	118	HIS
44	y	36	ASN
13	d	912	ASN
13	d	943	GLN

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Mol	Chain	Res	Type
14	e	246	HIS
14	e	320	HIS
14	e	336	HIS
14	e	368	ASN
14	e	424	GLN
14	e	640	ASN
15	f	30	GLN
15	f	119	ASN
15	f	134	HIS
15	f	273	GLN
15	f	325	ASN
19	j	172	GLN
19	j	173	HIS
20	l	73	ASN
20	l	86	GLN
20	l	105	HIS
20	l	119	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	Z	2/4 (50%)	1 (50%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	Z	4	G2L

There are no RNA pucker outliers to report.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	ILX	N	1	9	8,9,10	0.62	0	9,11,13	1.33	2 (22%)
9	CSX	N	6	9	3,6,7	1.05	0	1,6,8	2.24	1 (100%)
9	HYP	N	8	9	6,8,9	0.74	0	5,10,12	2.18	2 (40%)
9	TRX	N	2	9	15,16,17	1.00	1 (6%)	19,22,24	1.53	2 (10%)
10	G2L	Z	4	10,48,30	23,26,30	1.21	3 (13%)	32,38,44	2.06	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ILX	N	1	9	-	7/11/12/14	-
9	CSX	N	6	9	-	1/1/5/7	-
9	HYP	N	8	9	-	0/0/11/13	0/1/1/1
9	TRX	N	2	9	-	2/5/6/8	0/2/2/2
10	G2L	Z	4	10,48,30	-	2/9/27/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Z	4	G2L	C5-C4	3.16	1.47	1.38
10	Z	4	G2L	C6-N1	-2.46	1.34	1.38
10	Z	4	G2L	C5-N7	-2.13	1.35	1.39
9	N	2	TRX	CD2-CE2	2.07	1.44	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	Z	4	G2L	C5-C4-N3	-6.12	118.53	128.46
9	N	2	TRX	CA-CB-CG	5.19	123.42	113.51
10	Z	4	G2L	C2-N3-C4	4.88	121.00	112.30
10	Z	4	G2L	N9-C4-N3	4.60	135.19	125.94
9	N	8	HYP	O-C-CA	-3.27	116.21	124.78
10	Z	4	G2L	C6-C5-N7	3.14	136.10	130.25
9	N	8	HYP	CB-CG-CD	3.08	107.05	103.27
9	N	1	ILX	OD1-CD1-CG1	-2.90	104.75	111.07
10	Z	4	G2L	C3'-C2'-C1'	2.71	105.89	99.89
10	Z	4	G2L	C4-C5-N7	-2.59	106.62	110.72
9	N	6	CSX	CA-CB-SG	2.24	118.25	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	Z	4	G2L	O6-C6-C5	-2.09	121.06	126.60
9	N	1	ILX	CB-CA-C	-2.08	110.13	112.94
9	N	2	TRX	CZ3-CH2-CZ2	2.07	122.44	120.17

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	N	1	ILX	C-CA-CB-CG2
9	N	1	ILX	OD1-CD1-CG1-CB
9	N	1	ILX	OD1-CD1-CG1-OG1
9	N	6	CSX	N-CA-CB-SG
10	Z	4	G2L	C3'-C4'-C5'-O5'
9	N	2	TRX	CA-CB-CG-CD2
10	Z	4	G2L	O4'-C4'-C5'-O5'
9	N	2	TRX	CA-CB-CG-CD1
9	N	1	ILX	C-CA-CB-CG1
9	N	1	ILX	CG2-CB-CG1-CD1
9	N	1	ILX	O-C-CA-CB
9	N	1	ILX	N-CA-CB-CG2

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	N	1	ILX	3	0
9	N	6	CSX	1	0
9	N	8	HYP	2	0
9	N	2	TRX	1	0
10	Z	4	G2L	3	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 18 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
47	SF4	7	1000	8	0,12,12	-	-	-		
49	W0F	p	1201	-	31,35,35	2.90	10 (32%)	38,55,55	3.53	16 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	SF4	7	1000	8	-	-	0/6/5/5
49	W0F	p	1201	-	-	3/24/40/40	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	p	1201	W0F	C03-C04	-9.44	1.27	1.52
49	p	1201	W0F	O05-C04	6.83	1.60	1.45
49	p	1201	W0F	O05-C06	-5.85	1.28	1.42
49	p	1201	W0F	C12-C13	5.74	1.47	1.38
49	p	1201	W0F	C13-N09	-3.18	1.33	1.37
49	p	1201	W0F	C07-C03	-2.89	1.46	1.52
49	p	1201	W0F	C20-C04	2.47	1.59	1.51
49	p	1201	W0F	C06-N09	2.28	1.54	1.47
49	p	1201	W0F	C12-N11	-2.19	1.34	1.39
49	p	1201	W0F	P22-O21	2.11	1.67	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	p	1201	W0F	O05-C06-N09	-14.42	75.40	108.36
49	p	1201	W0F	C07-C06-N09	8.15	136.29	113.22
49	p	1201	W0F	O05-C04-C03	-5.66	92.74	104.87
49	p	1201	W0F	O05-C04-C20	4.78	125.10	109.37
49	p	1201	W0F	O05-C06-C07	-4.10	97.71	106.64
49	p	1201	W0F	O21-C20-C04	3.95	122.58	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	p	1201	W0F	O32-P30-O29	3.90	117.73	104.64
49	p	1201	W0F	O33-P30-O31	-3.31	97.72	110.68
49	p	1201	W0F	C06-N09-C10	-3.23	117.49	126.70
49	p	1201	W0F	P26-O25-P22	-3.10	122.19	132.83
49	p	1201	W0F	O08-C07-C06	2.92	119.79	110.02
49	p	1201	W0F	P26-O29-P30	2.74	142.23	132.83
49	p	1201	W0F	O33-P30-O29	2.66	113.56	104.64
49	p	1201	W0F	O21-P22-O24	-2.35	99.88	109.07
49	p	1201	W0F	C13-C12-N11	-2.11	106.48	109.23
49	p	1201	W0F	C10-N09-C13	2.03	108.39	106.71

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
49	p	1201	W0F	C20-O21-P22-O24
49	p	1201	W0F	C20-O21-P22-O25
49	p	1201	W0F	C03-C04-C20-O21

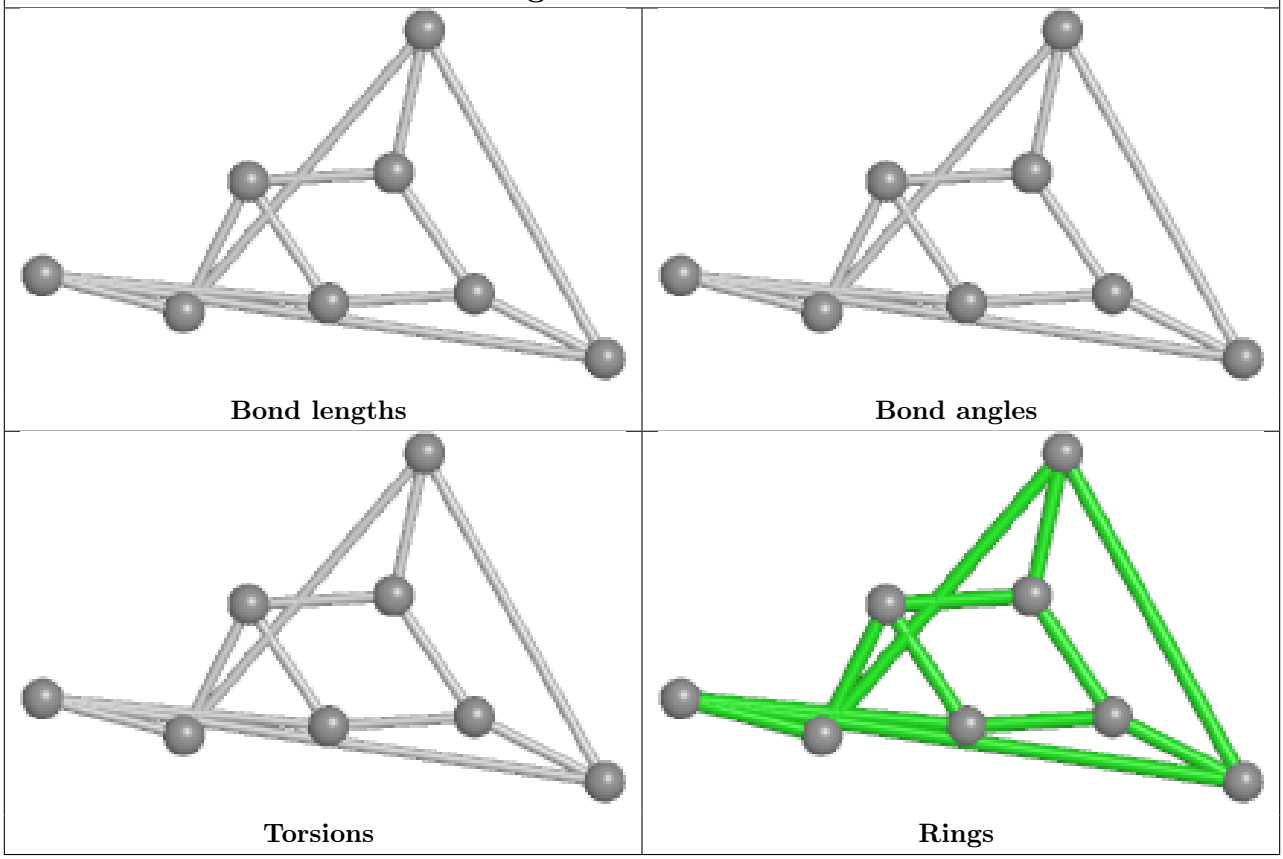
There are no ring outliers.

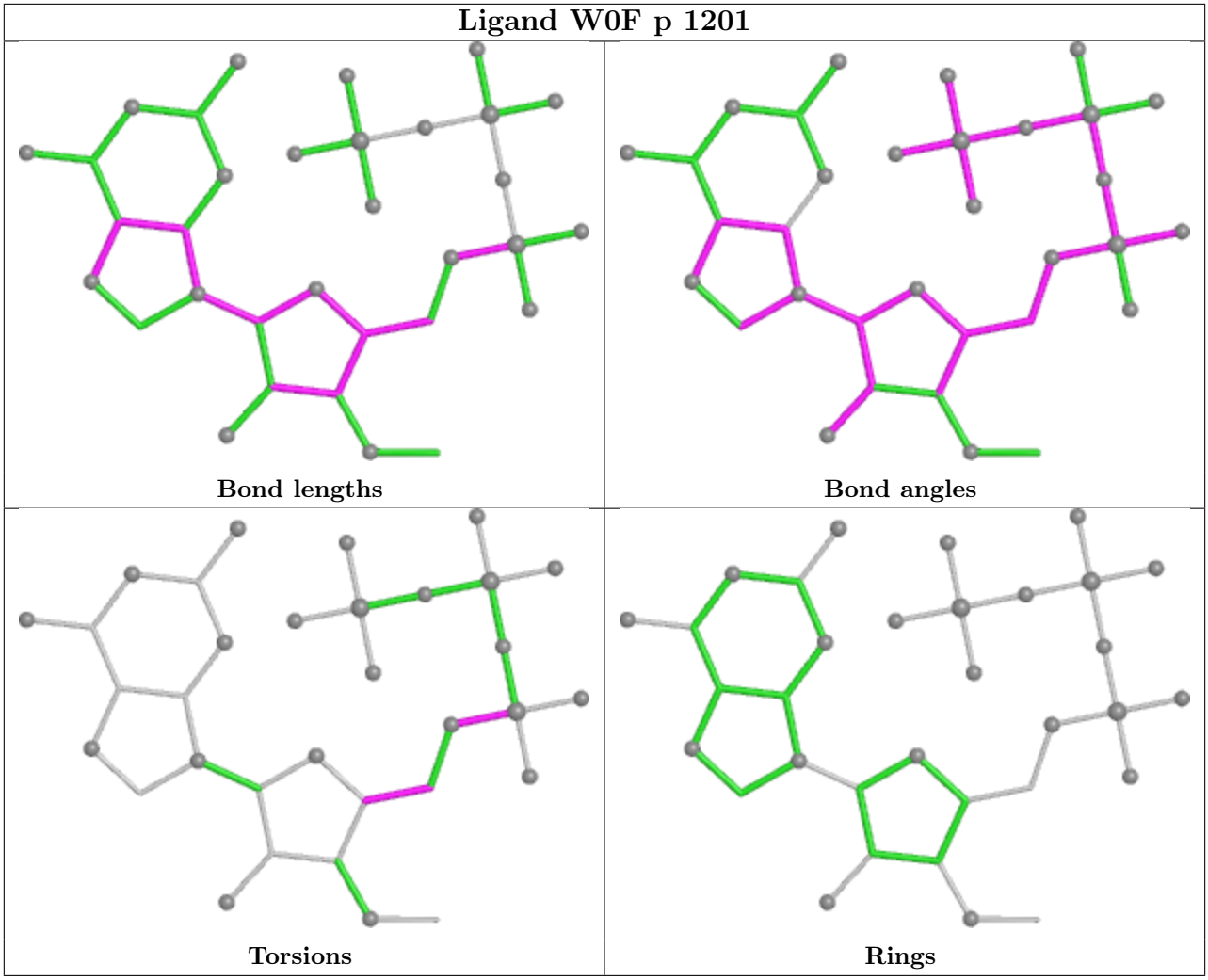
1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	p	1201	W0F	9	0

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

Ligand SF4 7 1000





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

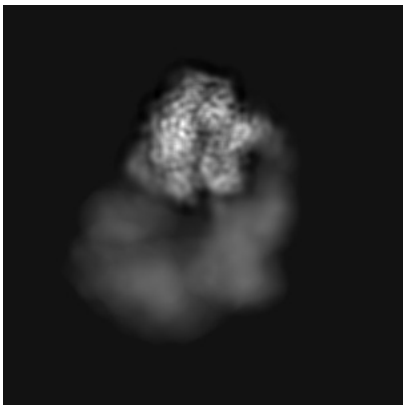
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-37398. 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 (i)

6.1.1 Primary map



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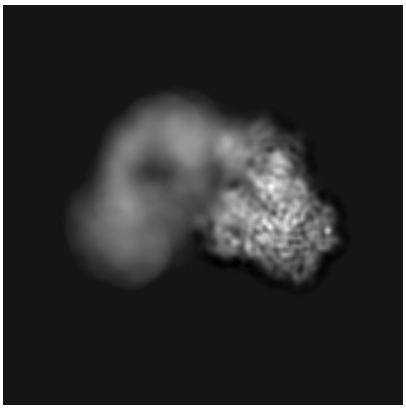
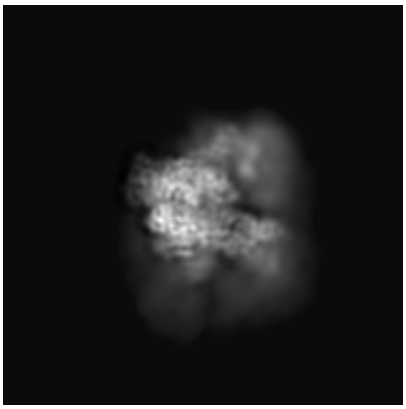
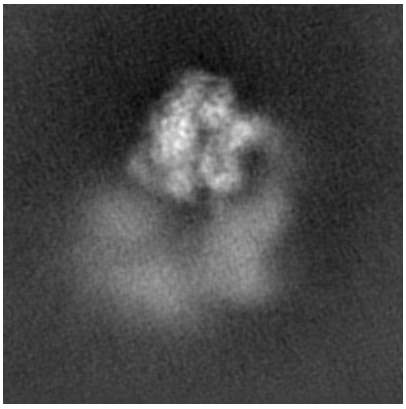


Y



Z

6.1.2 Raw map



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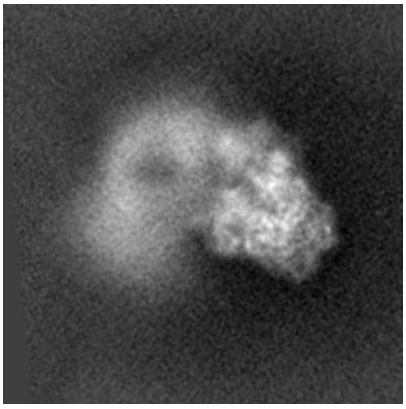
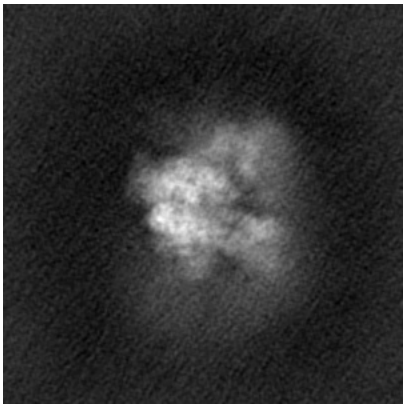


Y

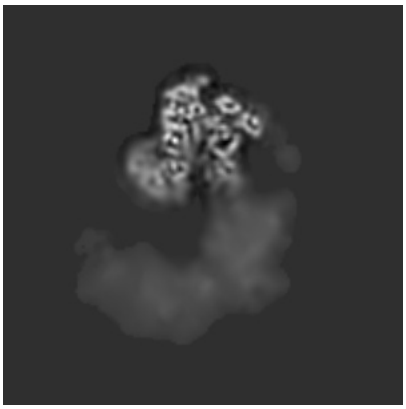


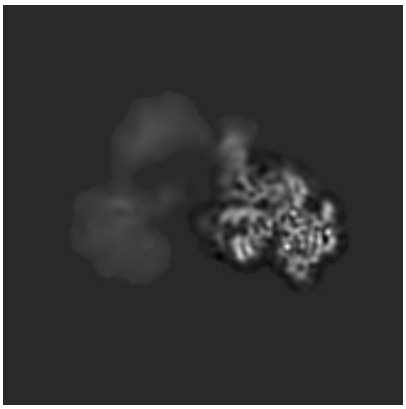
Z

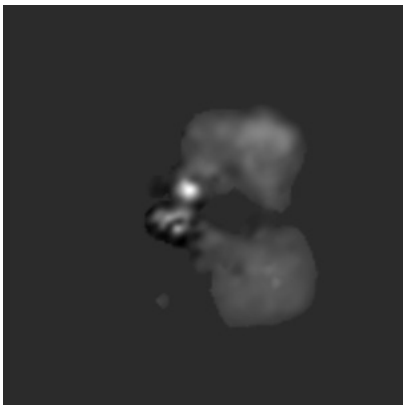
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

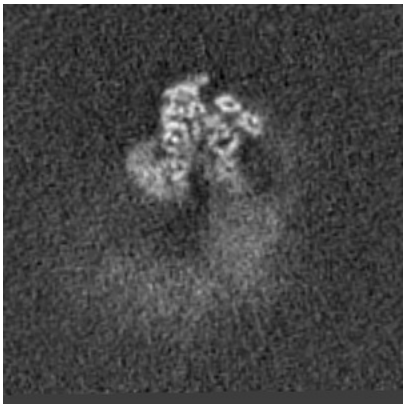
6.2.1 Primary map


X Index: 160


Y Index: 160


Z Index: 160

6.2.2 Raw map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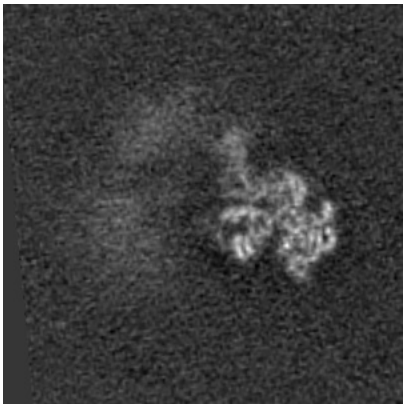
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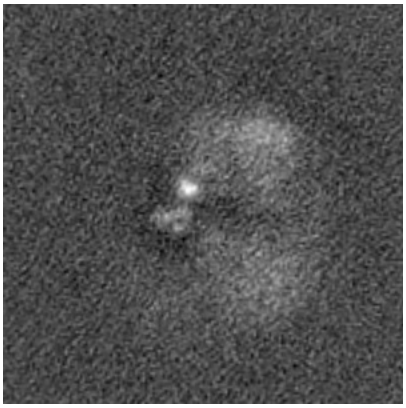
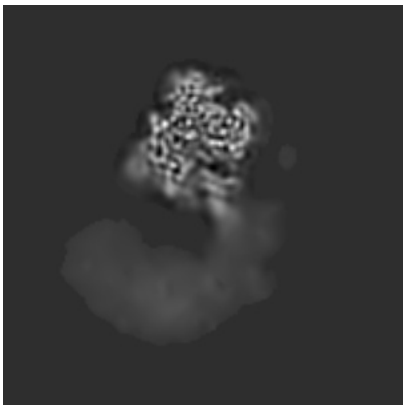
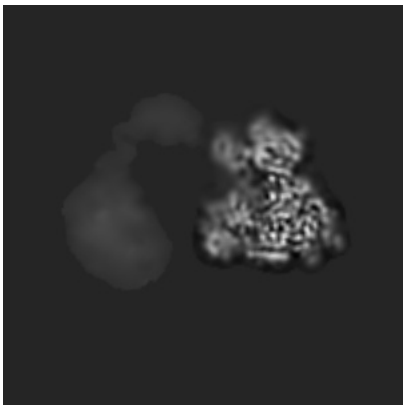

Z Index: 160

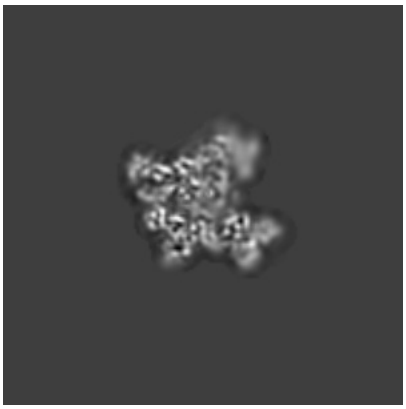
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

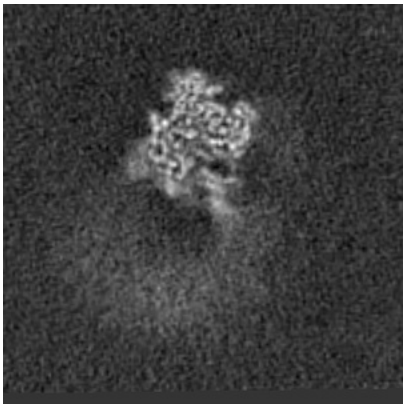
6.3.1 Primary map

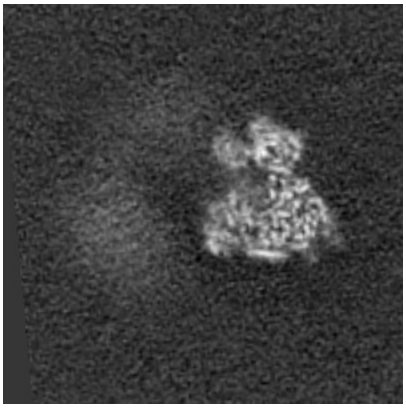

X Index: 147

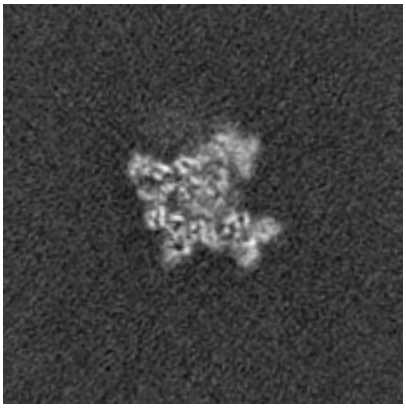

Y Index: 143


Z Index: 221

6.3.2 Raw map


X Index: 147

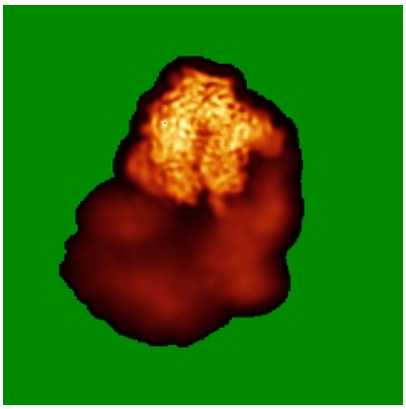

Y Index: 142


Z Index: 221

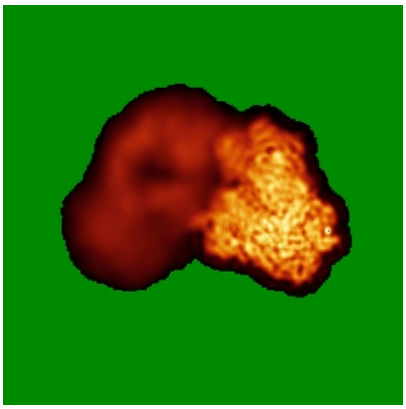
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X



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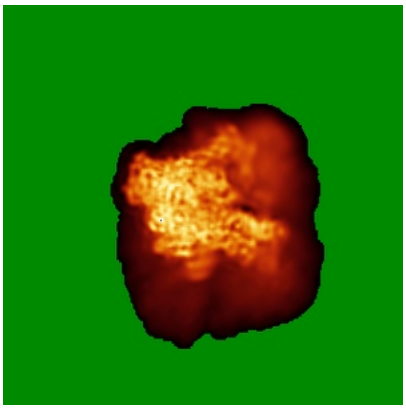
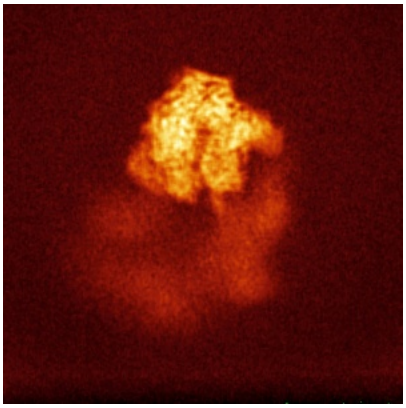
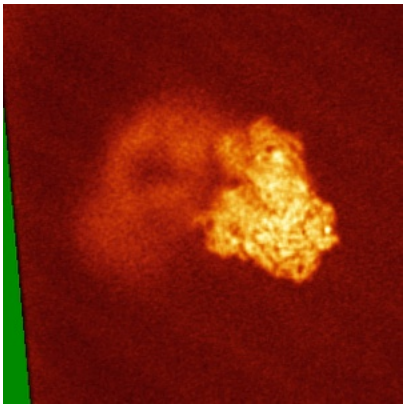


Z

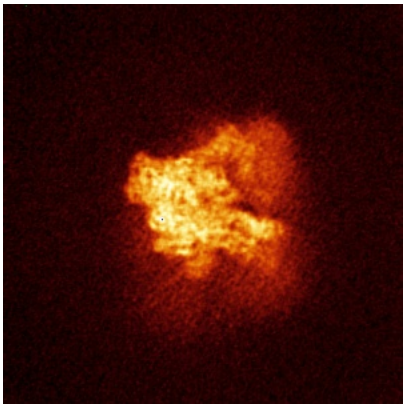
6.4.2 Raw map



X



Y

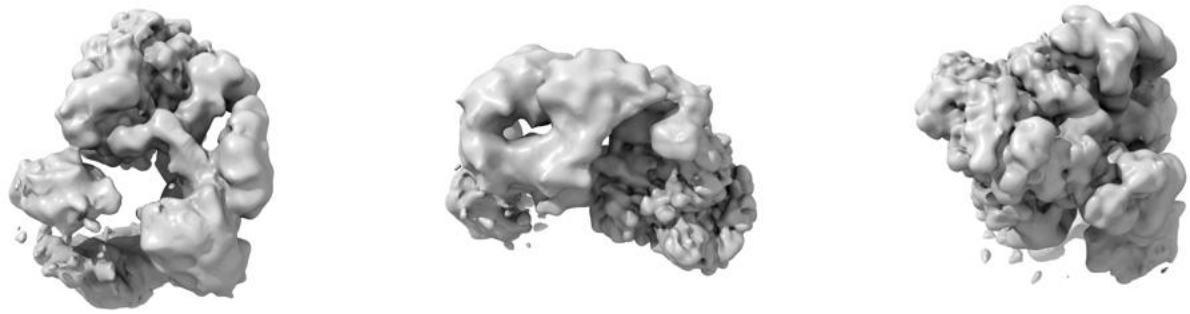


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.42. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

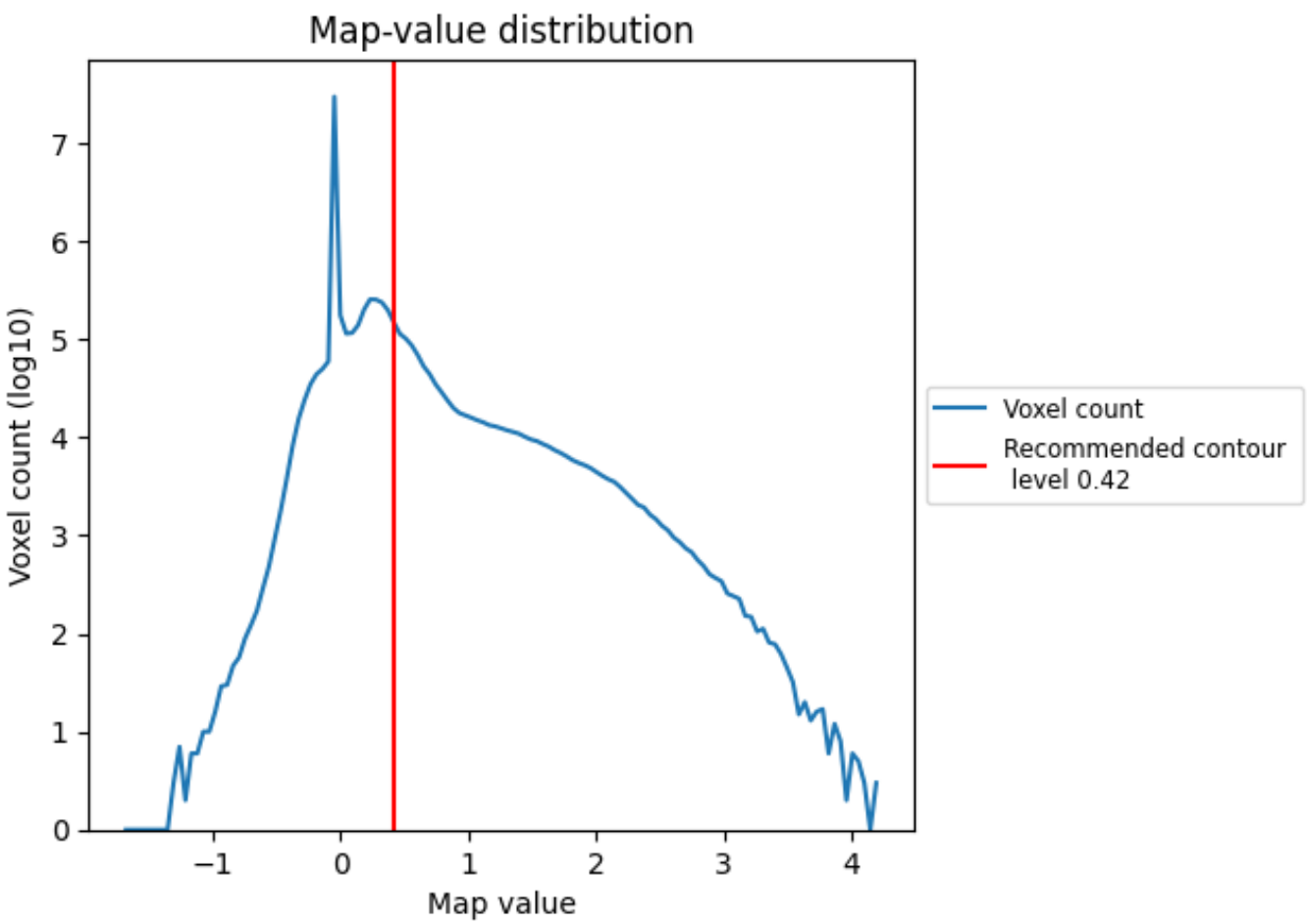
6.6 Mask visualisation (i)

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

7 Map analysis (i)

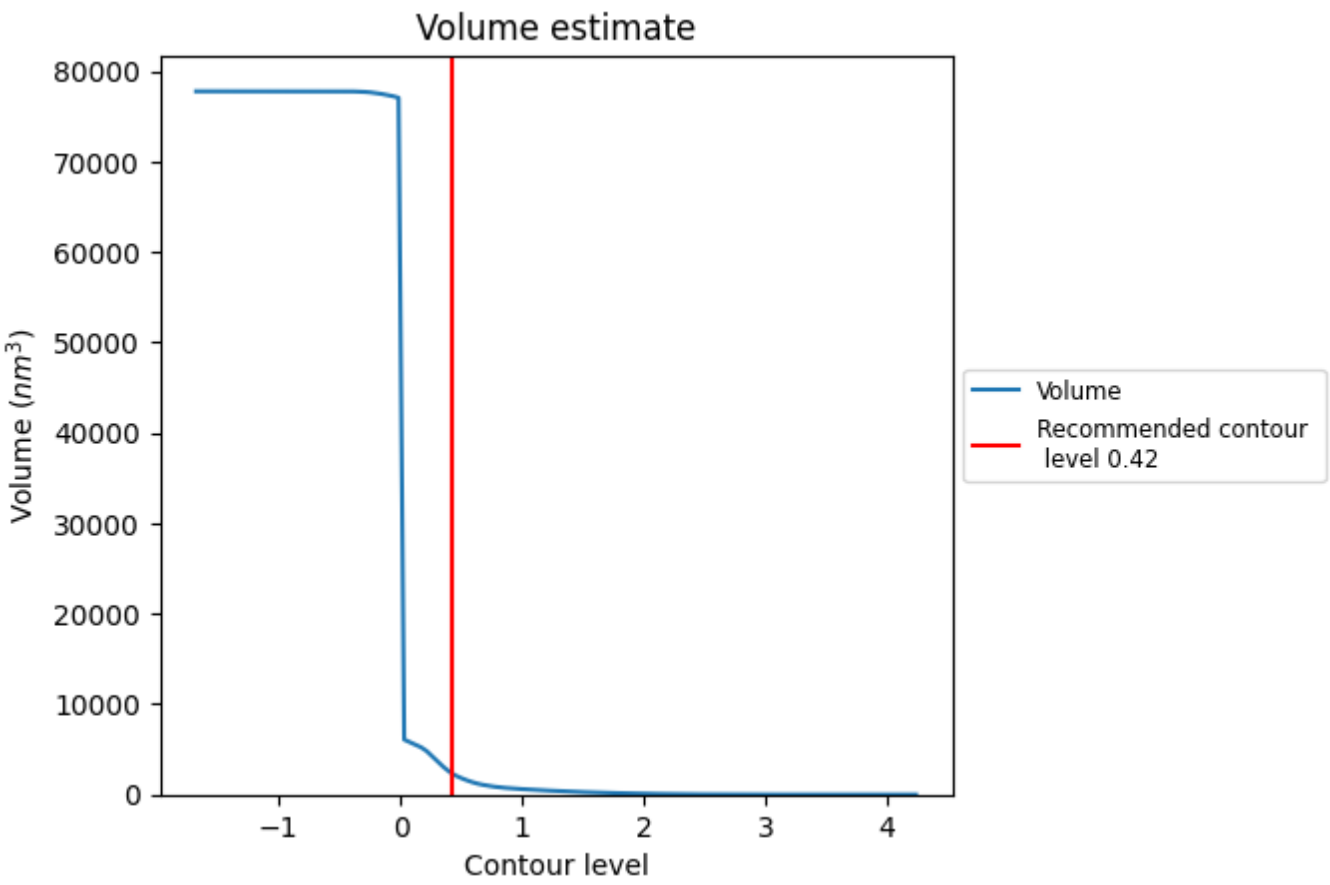
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

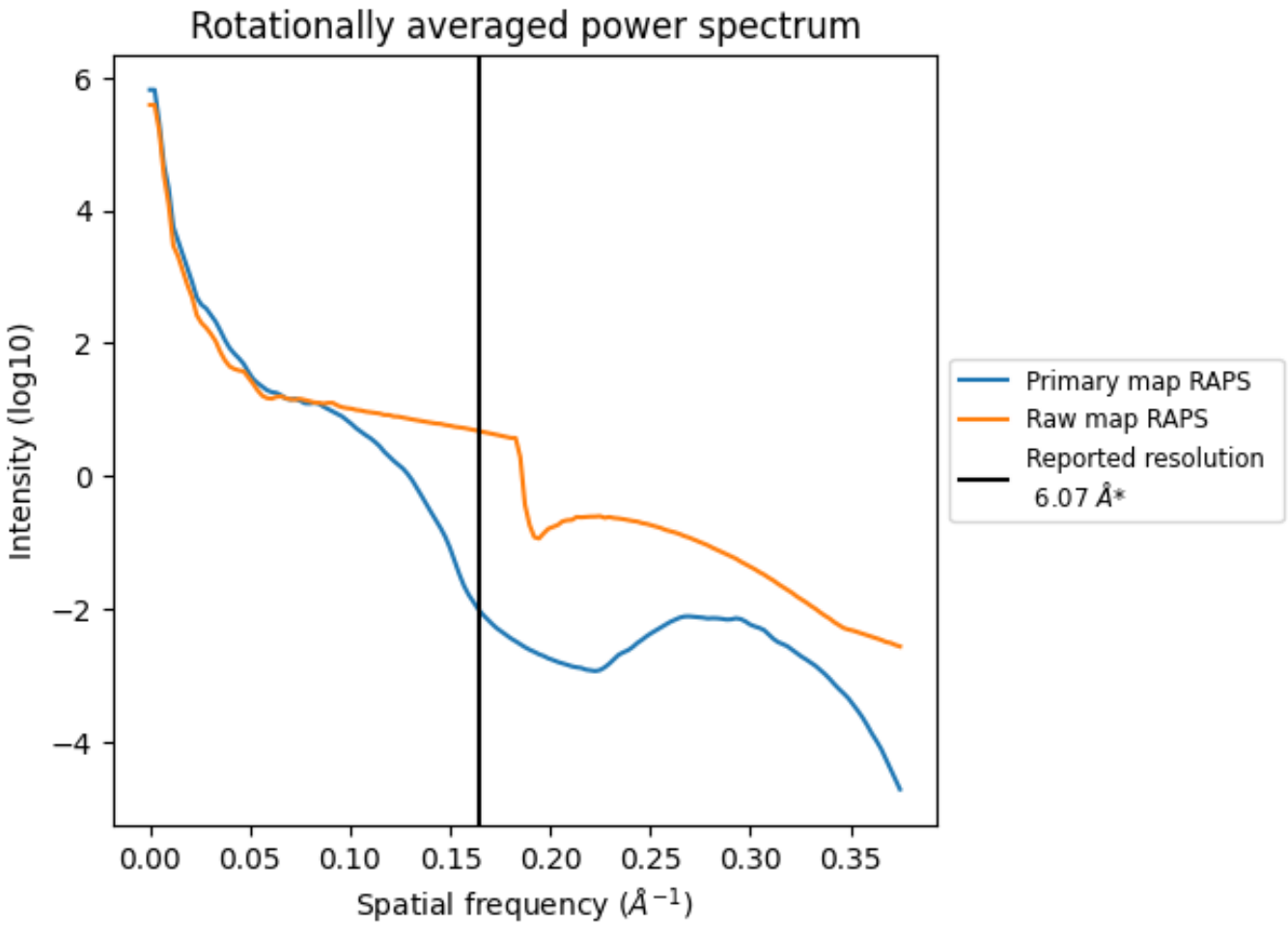
7.2 Volume estimate (i)



The volume at the recommended contour level is 2397 nm^3; this corresponds to an approximate mass of 2165 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

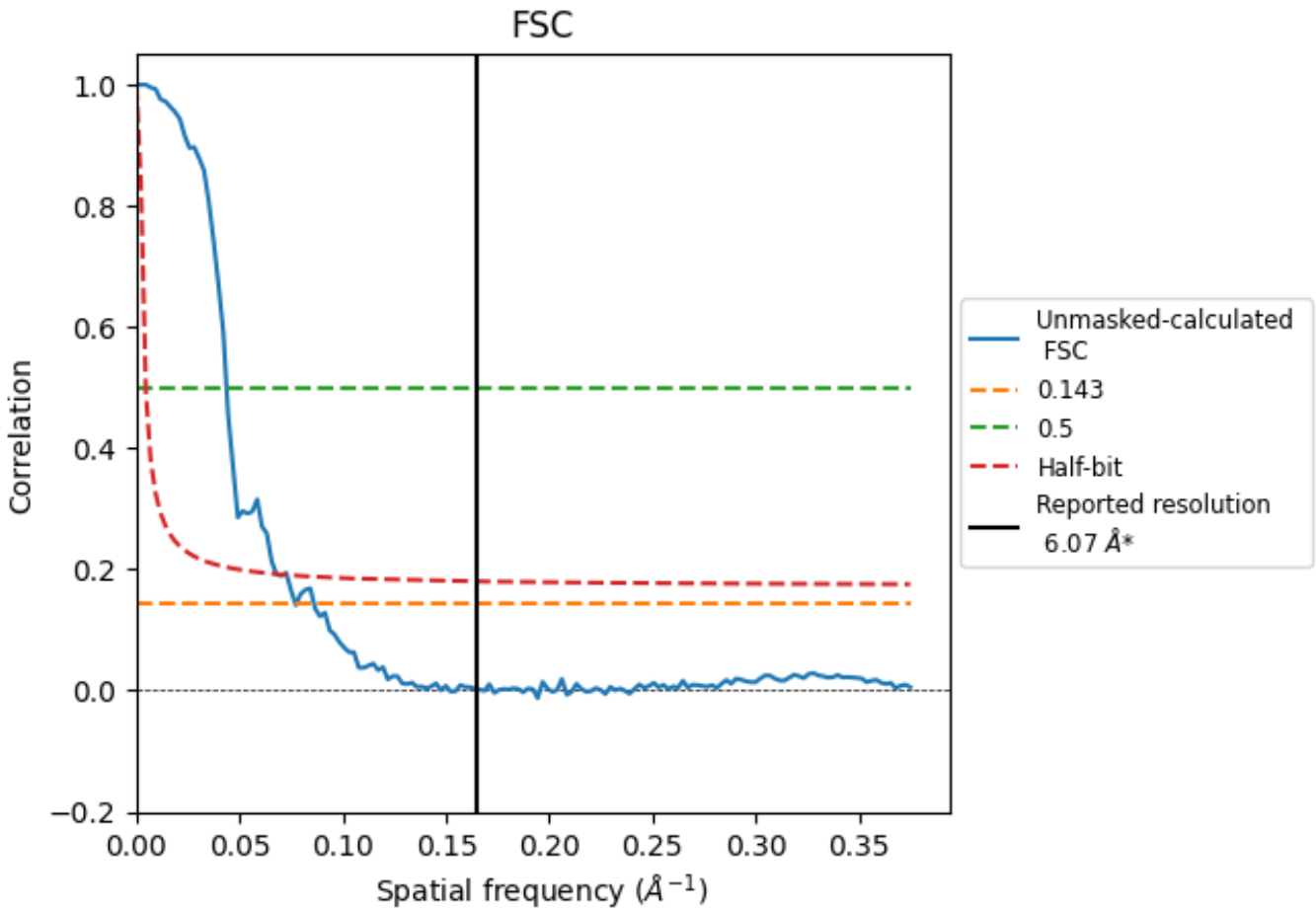


*Reported resolution corresponds to spatial frequency of 0.165 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.165 Å^{-1}

8.2 Resolution estimates (i)

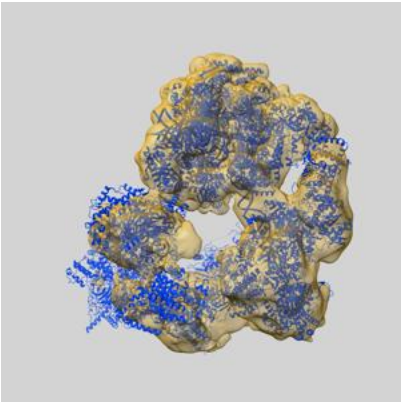
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.07	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	12.97	22.88	14.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 12.97 differs from the reported value 6.07 by more than 10 %

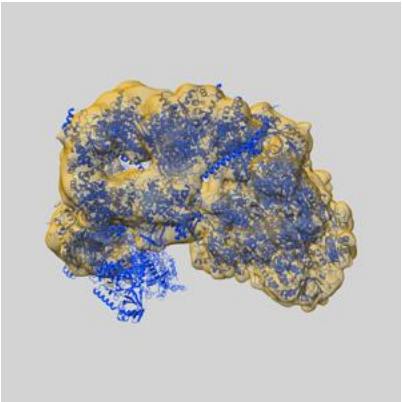
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-37398 and PDB model 8WAN. Per-residue inclusion information can be found in section 3 on page 15.

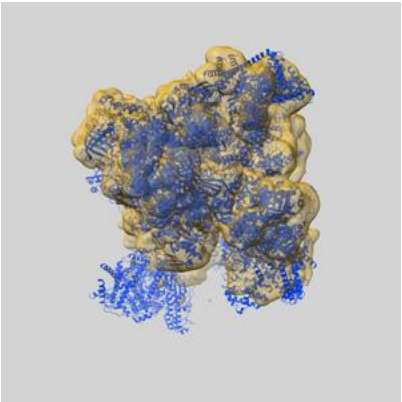
9.1 Map-model overlay (i)



X



Y



Z

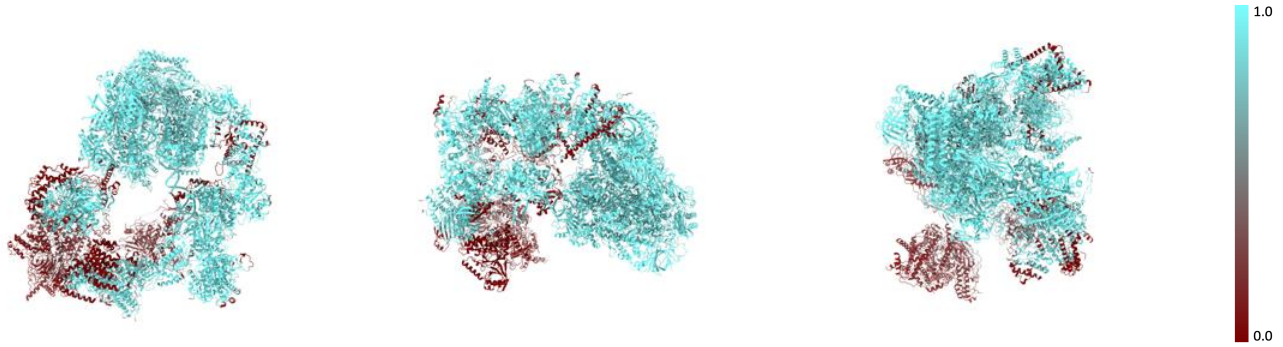
The images above show the 3D surface view of the map at the recommended contour level 0.42 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

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

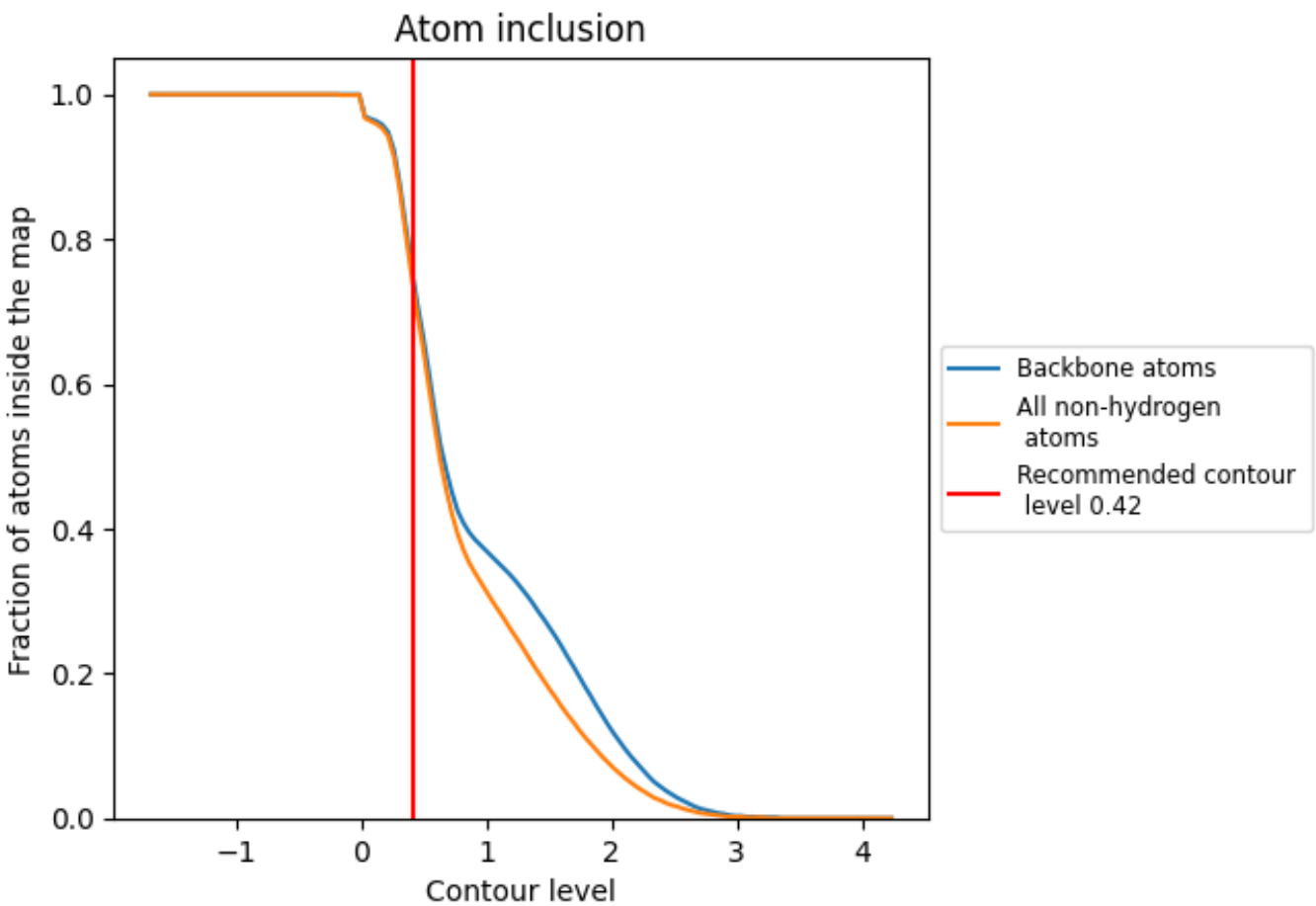
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.42).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.42) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7310	0.0770
0	0.3880	0.0450
1	0.7710	0.0480
2	0.9220	0.0580
3	0.9480	0.0450
4	0.9470	0.0610
5	0.6330	0.0140
6	0.7810	0.0390
7	0.9050	0.0520
A	0.1060	0.0200
B	0.8440	0.0360
D	0.4220	0.0220
E	0.6580	0.0410
F	0.3410	0.0300
G	0.0000	-0.0160
H	0.7700	0.0360
I	0.5970	0.0240
J	0.8570	0.0450
L	0.1980	0.0320
N	0.9840	0.1450
O	0.9780	0.0710
P	0.9980	0.1200
Q	0.9510	0.0870
R	0.9700	0.1450
S	0.9730	0.0920
T	0.9810	0.1270
U	0.9880	0.0950
V	0.9870	0.1150
X	0.9940	0.1690
Y	0.9790	0.1630
Z	0.9580	0.2140
c	0.0710	0.0170
d	0.0000	-0.0160
e	0.0580	0.0200
f	0.4670	0.0460

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Chain	Atom inclusion	Q-score
i	0.0020	0.0020
j	0.0050	0.0090
k	0.0010	-0.0170
l	0.0000	0.0120
m	0.0000	0.0110
o	0.9630	0.1450
p	0.9540	0.1370
q	0.9780	0.1560
r	0.9880	0.1380
s	0.9790	0.1590
t	0.9720	0.1520
u	0.9900	0.1180
v	0.9750	0.1500
w	0.9800	0.1320
x	0.9690	0.1370
y	0.9810	0.1630
z	0.9890	0.1510