Full wwPDB EM Validation Report

Aug 6, 2026 – 08:42 PM JST

PDB ID	:	8WAP / pdb_00008wap
EMDB ID	:	EMD-37400
Title	:	Structure of transcribing complex 6 (TC6), the initially transcribing complex with Pol II positioned 6nt downstream of TSS.
Authors	:	Chen, X.; Liu, W.; Wang, Q.; Wang, X.; Ren, Y.; Qu, X.; Li, W.; Xu, Y.
Deposited on	:	2023-09-08
Resolution	:	5.85 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

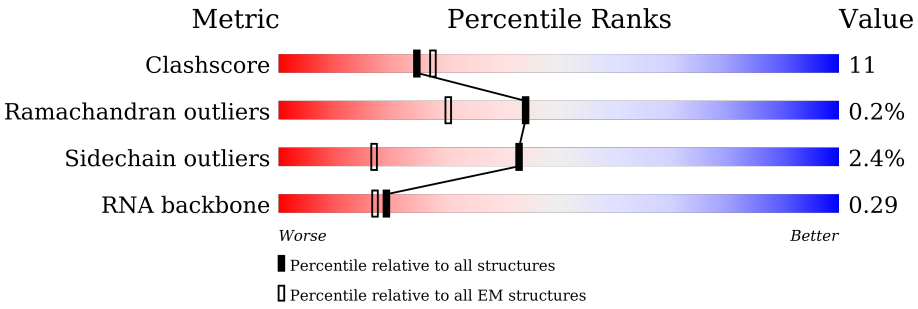
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

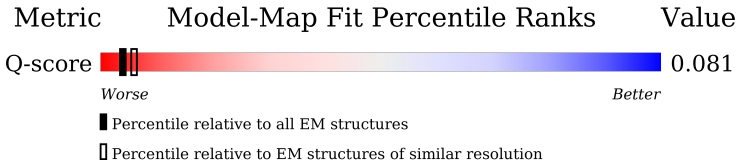
1 Overall quality at a glance

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

The reported resolution of this entry is 5.85 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	480 (5.35 - 6.35)

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	50% 38% 16% • 45%
2	1	548	15% 40% 8% 52%
3	2	395	7% 66% 17% 17%

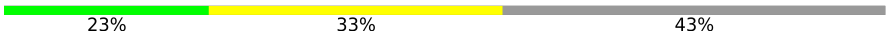
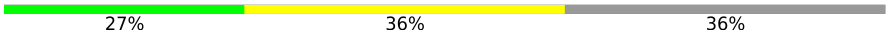
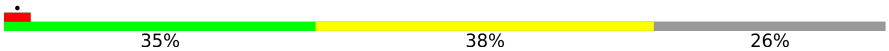
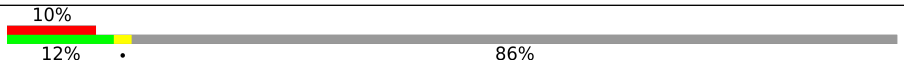
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Mol	Chain	Length	Quality of chain
4	3	308	10% 65% 19% 15%
5	4	462	20% 66% 18% 15%
6	5	71	37% 54% 18% 24%
7	6	782	28% 65% 13% 23%
8	7	760	24% 72% 22% 6%
9	N	8	25% 25% 50%
10	Z	6	33% 50% 17%
11	A	1872	22% 24% 5% 70%
12	B	1199	5% 69% 11% 20%
13	D	1085	10% 12% 85%
13	d	1085	15% 13% 85%
14	E	800	22% 55% 12% 32%
14	e	800	60% 56% 10% 33%
15	F	677	35% 44% 15% 39%
15	f	677	31% 48% 10% 40%
16	G	349	41% 36% 59%
17	H	310	10% 51% 14% 33%
18	I	264	24% 39% 6% 55%
18	i	264	41% 42% 54%
19	J	218	15% 32% 8% 59%
19	j	218	39% 36% 7% 56%
20	L	161	40% 32% 12% 53%
20	l	161	66% 59% 7% 34%
21	O	109	75% 16% 9%
22	P	339	47% 6% 47%

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Mol	Chain	Length	Quality of chain
23	Q	376	
24	R	316	
25	S	517	
26	T	249	
27	U	439	
28	V	291	
29	X	99	
30	Y	99	
31	c	929	
32	k	211	
33	m	124	
34	o	1970	
35	p	1174	
36	q	275	
37	r	142	
38	s	210	
39	t	127	
40	u	172	
41	v	150	
42	w	125	
43	x	67	
44	y	117	
45	z	58	

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 108642 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
7	6	605	Total	C	N	O	S	0	0
			4890	3127	848	885	30		

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

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

- Molecule 9 is a protein called Alpha-amanitin.

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

- Molecule 10 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Z	6	Total	C	N	O	P	0	0
			139	59	25	47	8		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	63	Total	C	N	O	P	0	0
			1304	616	248	377	63		

- Molecule 30 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	73	Total	C	N	O	P	0	0
			1484	706	266	439	73		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 45 is a protein called RPB12.

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

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

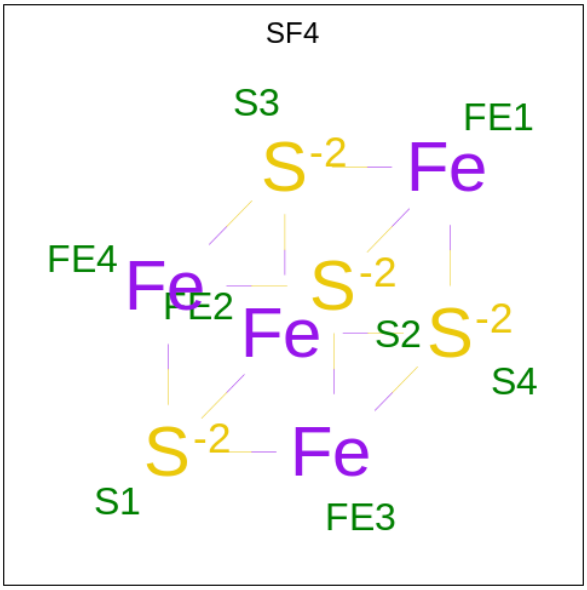
Mol	Chain	Residues	Atoms		AltConf
46	0	2	Total	Zn	0
			2	2	
46	2	3	Total	Zn	0
			3	3	
46	3	2	Total	Zn	0
			2	2	

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

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

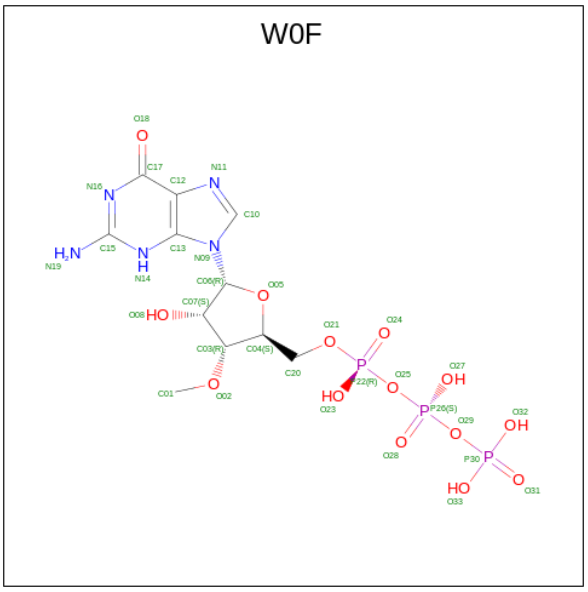


Mol	Chain	Residues	Atoms	AltConf
47	7	1	Total Fe S 8 4 4	0

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

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

- 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).



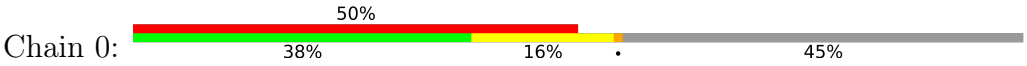
Mol	Chain	Residues	Atoms					AltConf
49	p	1	Total	C	N	O	P	0
			33	11	5	14	3	

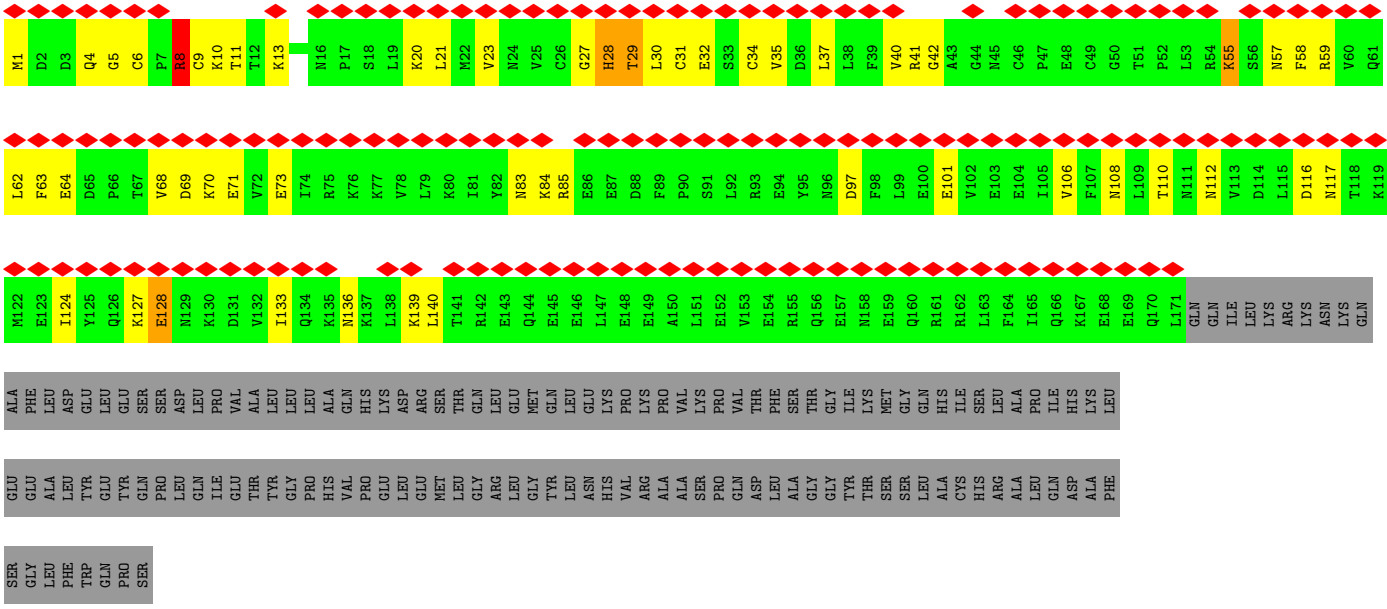
3 Residue-property plots (i)

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

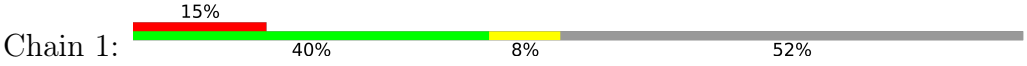
Chain 0:

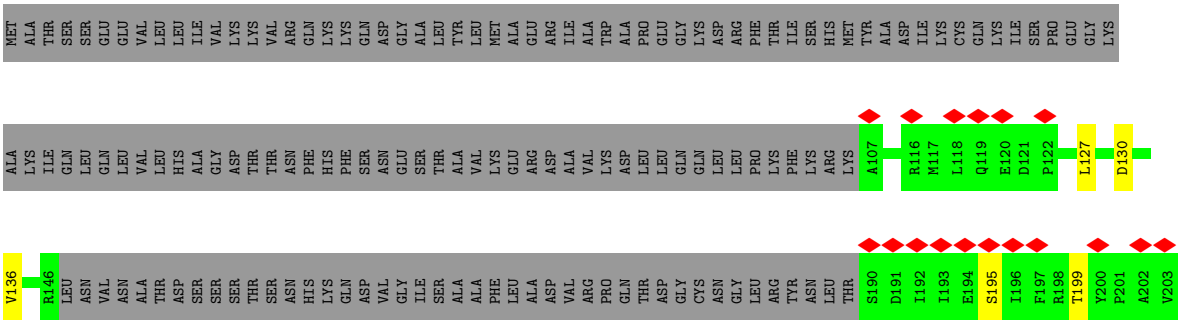


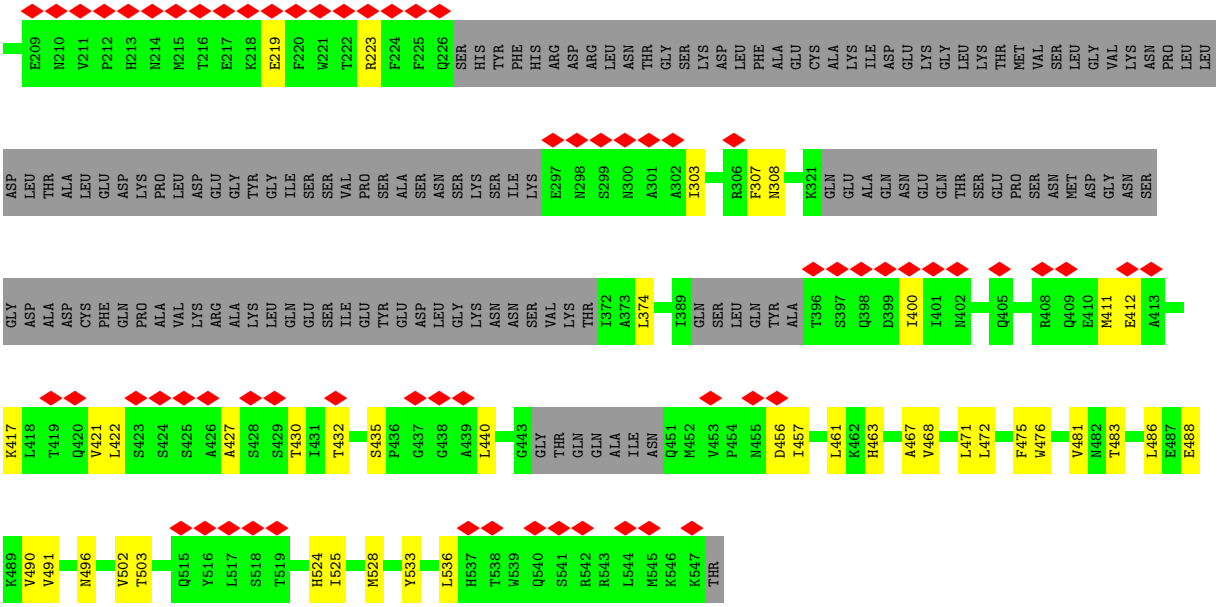


• Molecule 2: General transcription factor IIH subunit 1

Chain 1:

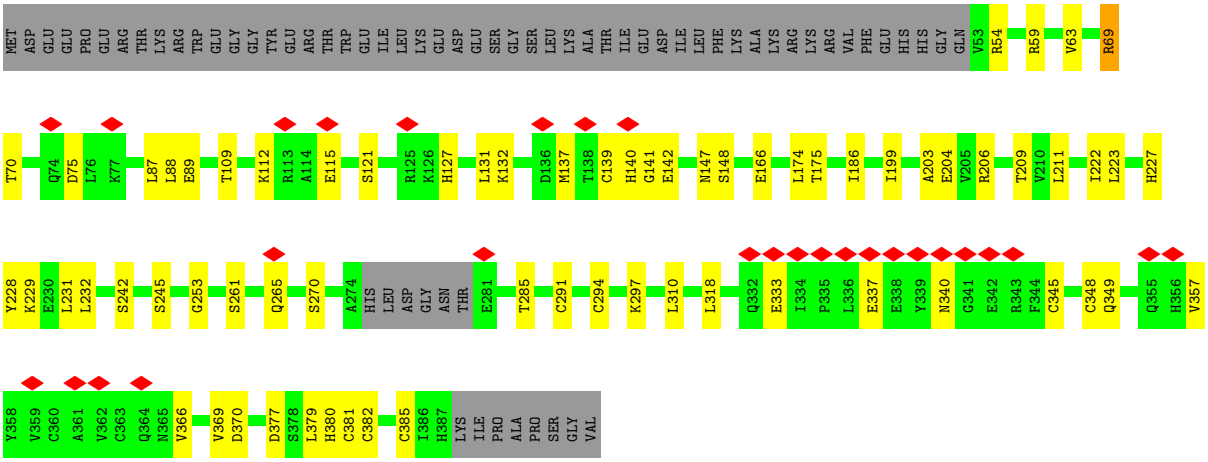






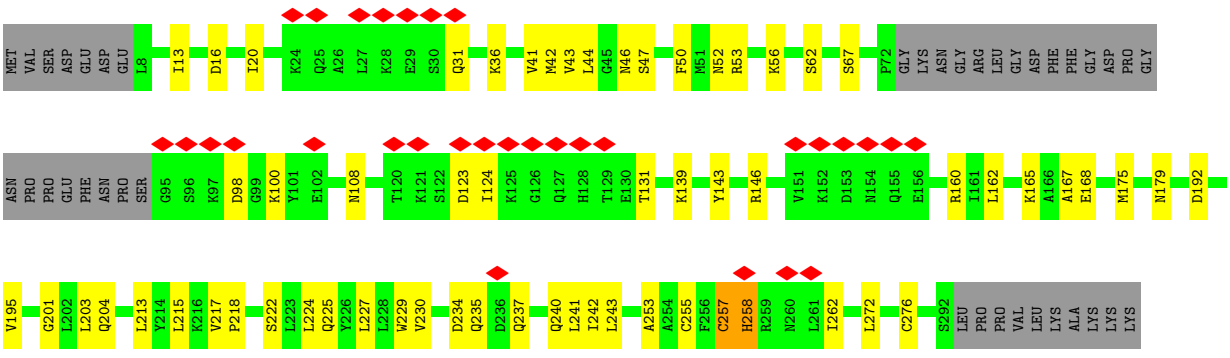
• Molecule 3: General transcription factor IIH subunit 2





• Molecule 4: General transcription factor IIH subunit 3

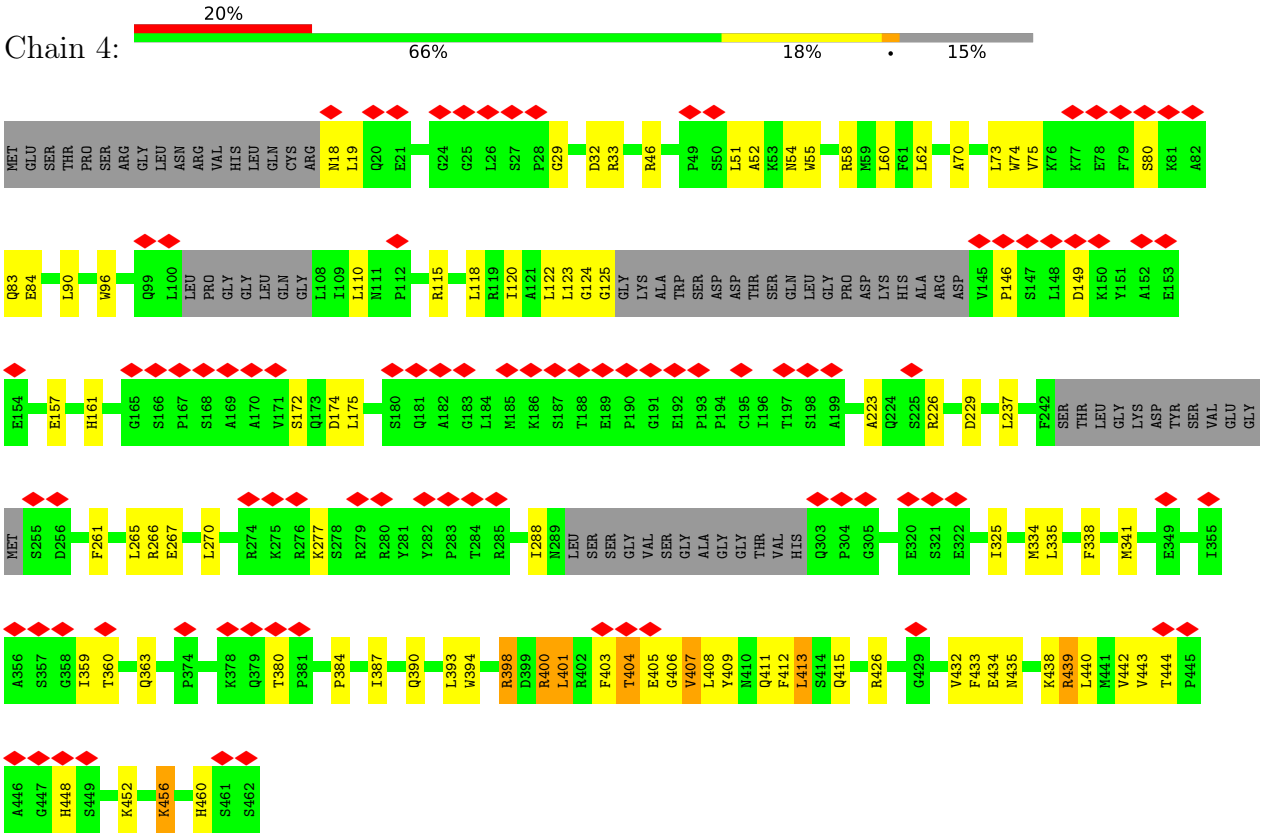






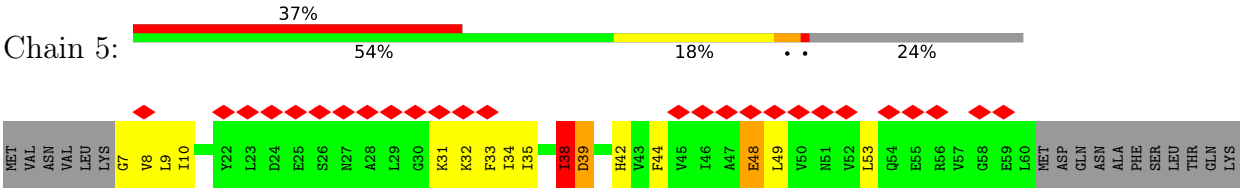
• Molecule 5: General transcription factor IIH subunit 4

Chain 4:



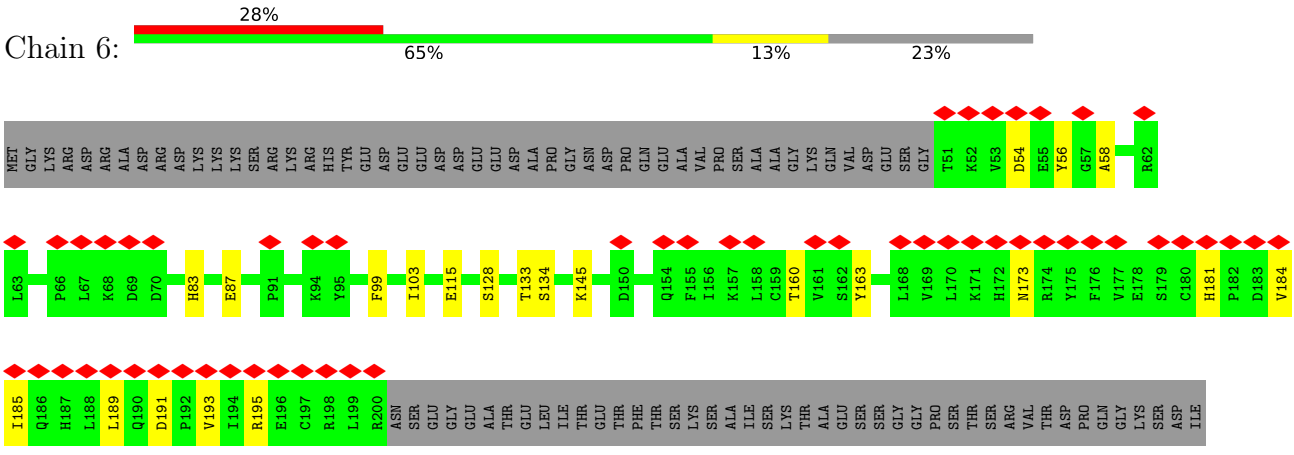
• Molecule 6: General transcription factor IIH subunit 5

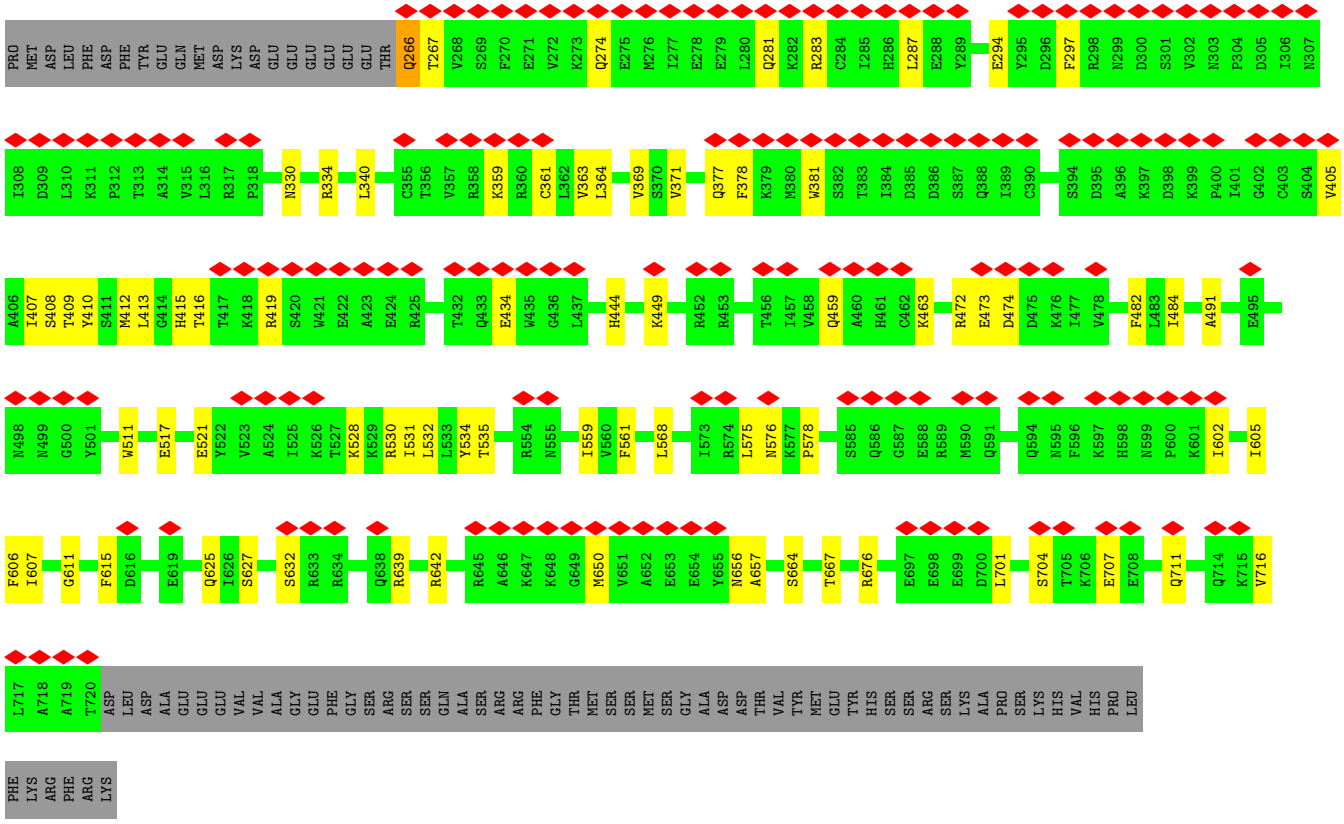
Chain 5:



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

Chain 6:

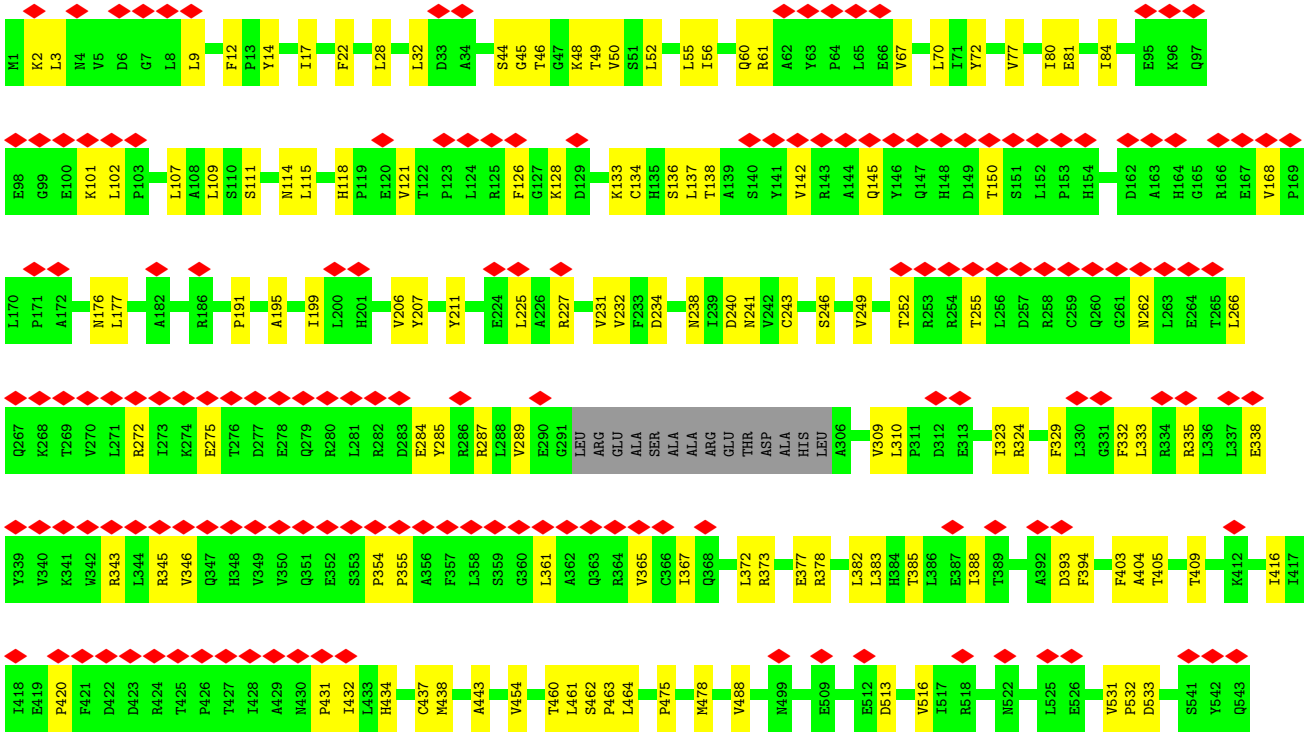


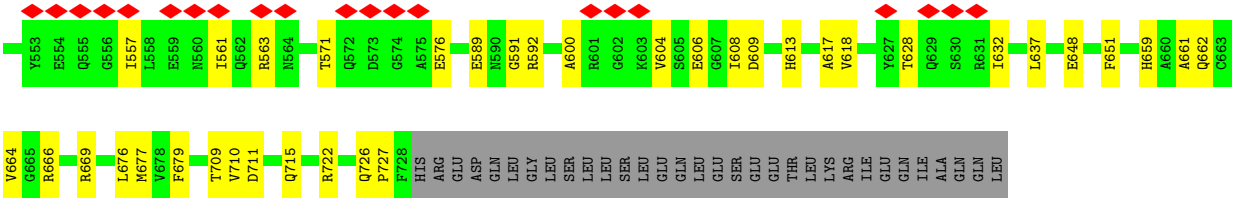


• Molecule 8: General transcription and DNA repair factor IIH helicase subunit XPD

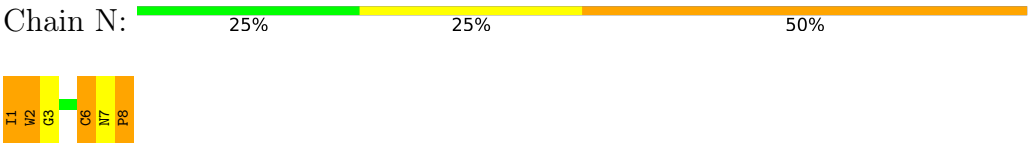
Chain 7:







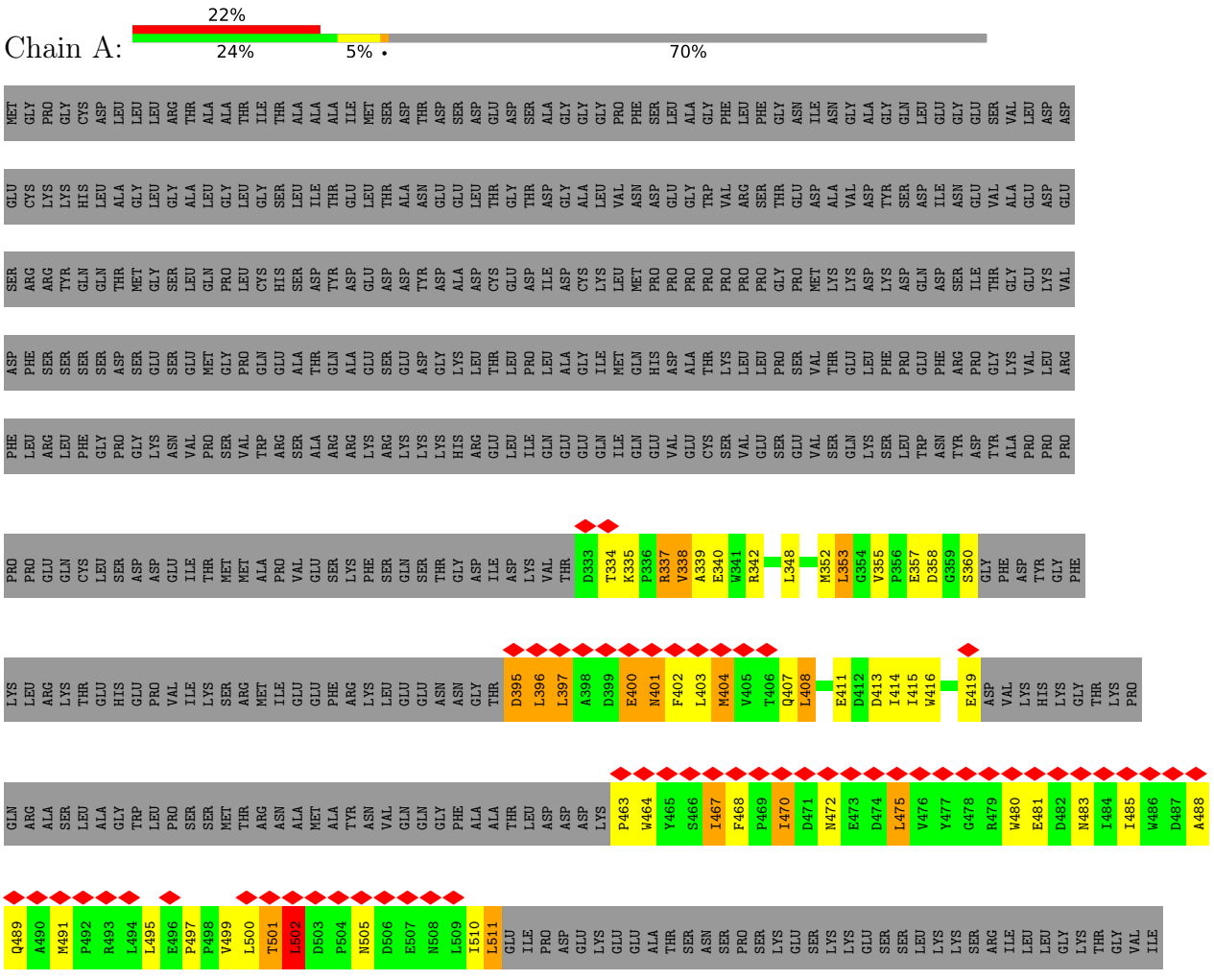
• Molecule 9: Alpha-amanitin

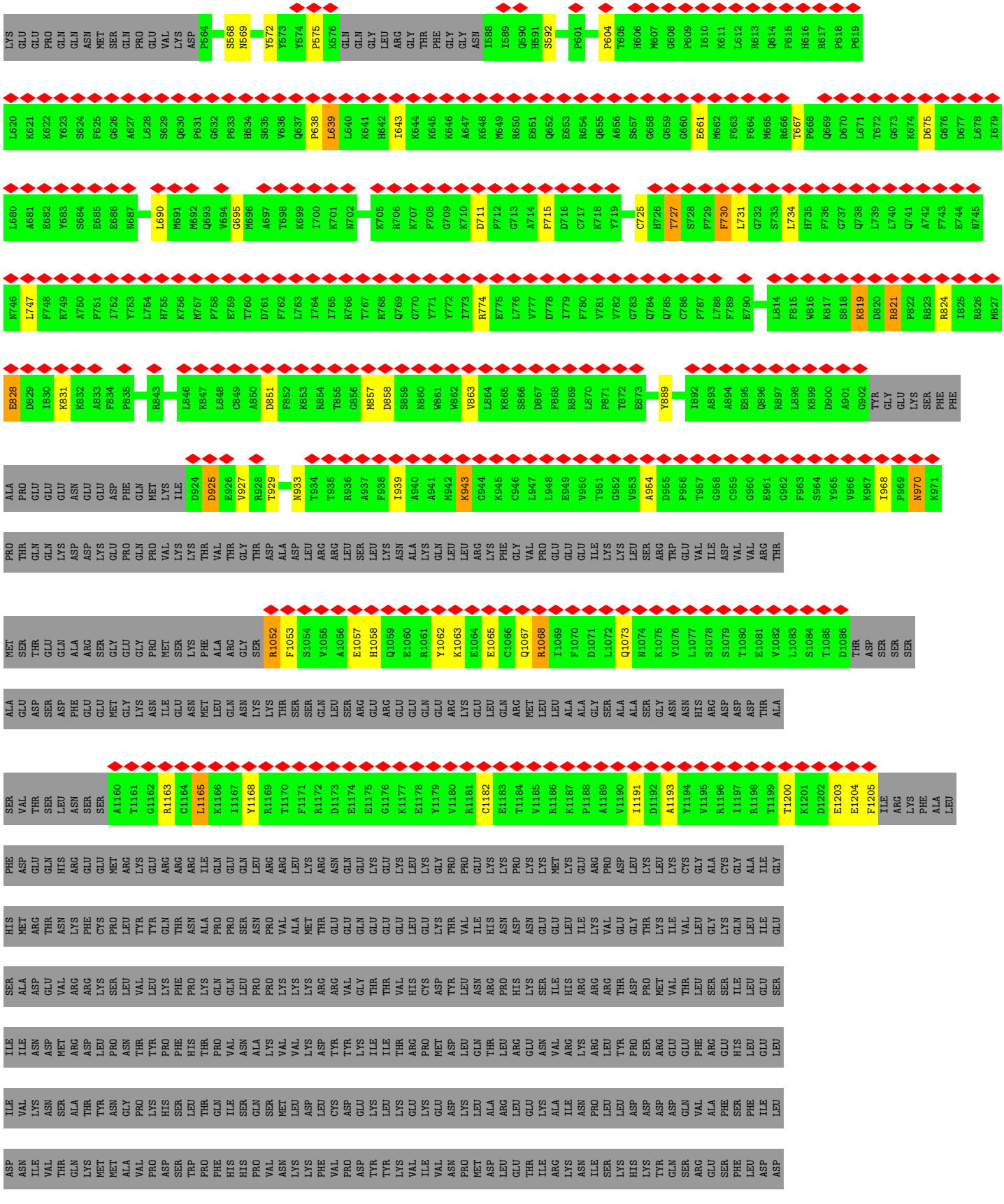


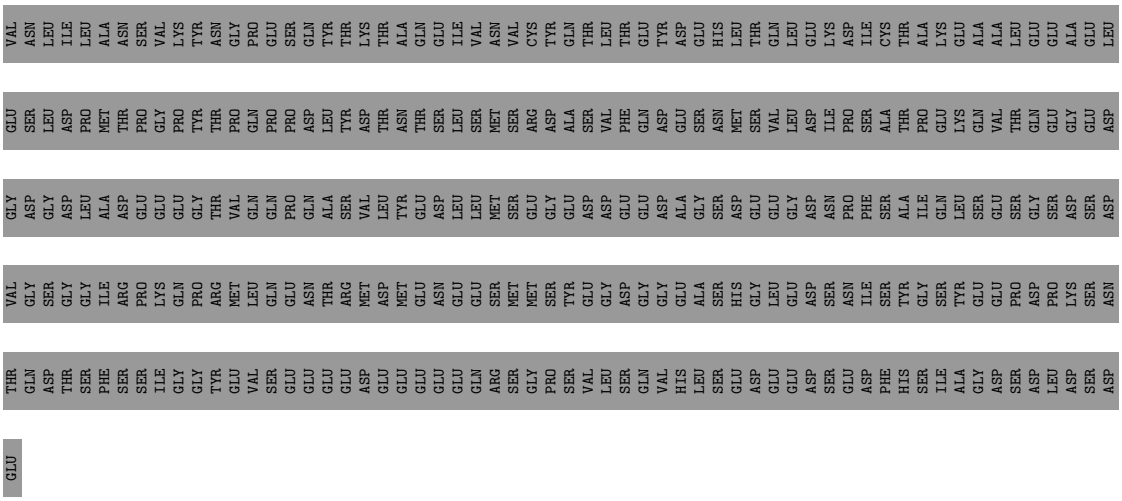
• Molecule 10: RNA



• Molecule 11: Transcription initiation factor TFIID subunit 1



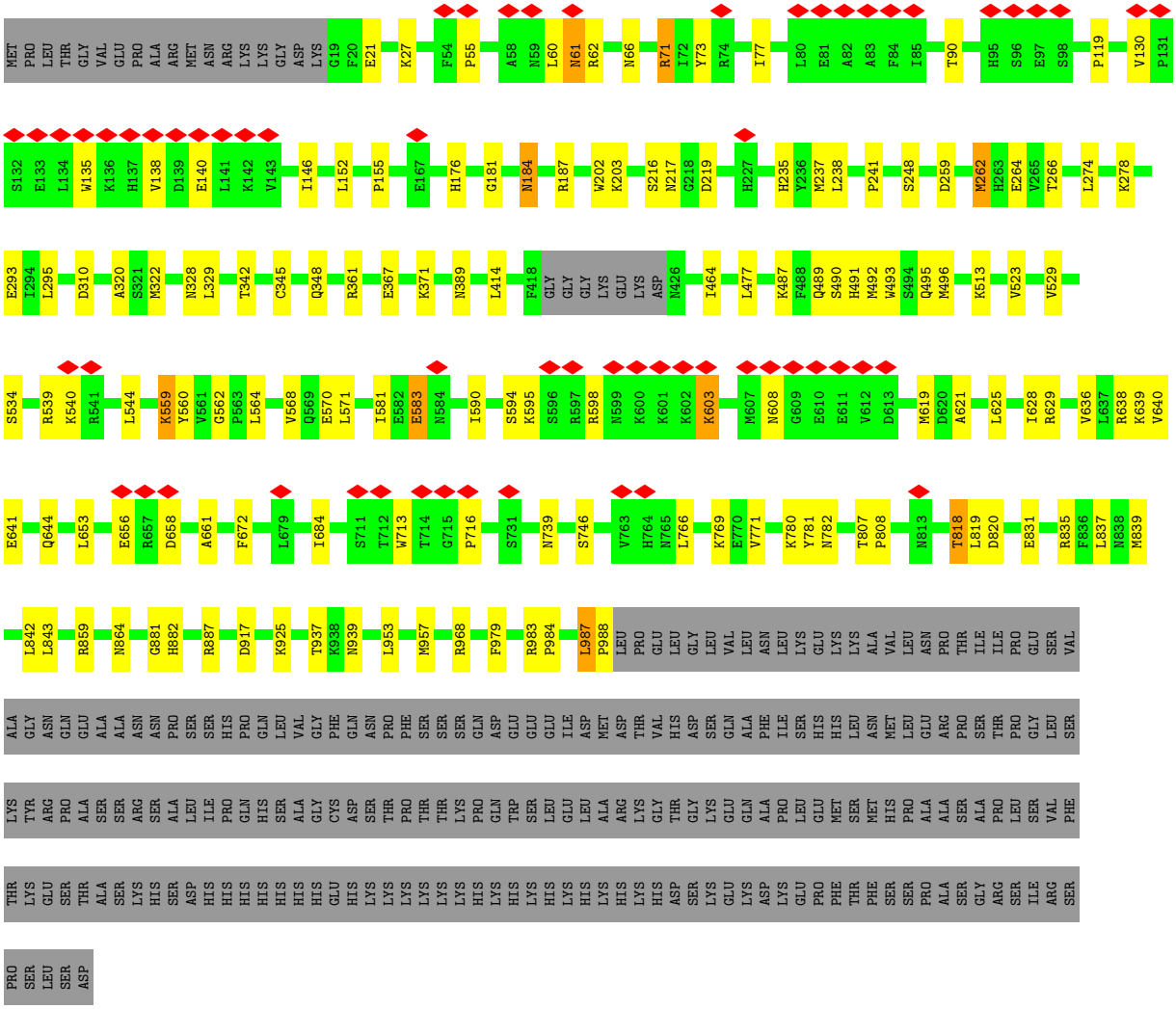

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L620 K621 K622 Y623 S624 F625 G626 A627 L628 S629 Q630 P631 G632 P633 H634 S635 V636 Q637 P638 L639 L640 K641 H642 I643 K644 K645 K646 A647 K648 M649 R650 E651 Q652 E653 R654 Q655 A656 S657 G658 G659 G660 E661 M662 F663 F664 M665 R666 T667 F668 Q669 D670 L671 T672 G673 K674 D675 G676 D677 L678 I679
L680 A681 E682 Y683 S684 E685 E686 N687 L690 M691 M692 Q693 V694 G695 M696 A697 T698 K699 I700 K701 N702 K705 R706 K707 P708 G709 K710 D711 P712 G713 A714 P715 D716 C717 K718 Y719 G725 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 P758 E759 T760 D761 F762 L763 I764 I765 R766 T767 R768 Q769 G770 Y771 Y772 I773 R774 E775 L776 V777 D778 I779 F780 V781 V782 G783 Q784 Q785 C786 P787 L788 F789 E790 L814 F815 W816 K817 S818 K819 D820 R821 P822 R823 R824 I825 R826 M827
E828 D829 I830 K831 K832 A833 F834 P835 R843 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 Y889 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 GLU ASP PHE GLN MET LYS ILE D924 D925 E926 V927 R928 T929 N933 T934 T935 R936 A937 F938 I939 A940 A941 N942 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 GLN GLN LYS ASP ASP LYS GLU PRO GLN PRO VAL LYS LYS THR VAL THR GLY THR ASP ALA ASP LEU ARG ARG LEU SER LEU LYS ASN ALA LYS GLN LEU LEU ARG LYS PHE GLY VAL PRO GLU GLU ILE LYS LYS LEU SER ARG TRP GLU VAL ILE ASP VAL VAL ARG THR
MET SER THR GLU GLN ALA ARG SER GLY GLU GLY PRO MET SER LYS PHE ALA ARG GLY SER R1052 F1053 S1054 V1055 A1056 E1057 H1058 Q1059 E1060 R1061 Y1062 K1063 E1064 E1065 C1066 Q1067 R1068 I1069 F1070 D1071 L1072 Q1073 N1074 K1075 V1076 L1077 S1078 S1079 T1080 E1081 V1082 L1083 S1084 T1085 D1086 THR ASP SER SER SER
ALA GLU ASP SER ASP PHE GLU GLU MET GLY LYS ASN ILE GLU ASN MET LEU GLN ASN LYS LYS THR SER SER GLN LEU SER ARG GLU ARG GLU GLU GLN GLU ARG LYS GLU LEU GLN ARG MET LEU LEU ALA ALA GLY SER ALA SER GLY ASN ASN HIS ARG ASP ASP THR ALA
SER VAL THR SER LEU ASN SER SER A1160 T1161 G1162 R1163 C1164 L1165 K1166 I1167 Y1168 R1169 T1170 F1171 R1172 D1173 E1174 E1175 G1176 K1177 E1178 Y1179 V1180 R1181 C1182 E1183 T1184 V1185 R1186 K1187 P1188 A1189 V1190 I1191 D1192 A1193 Y1194 V1195 R1196 I1197 R1198 T1199 T1200 K1201 D1202 E1203 E1204 F1205 ILE ARG LYS PHE ALA LEU
PHE ASP GLU GLN HIS ARG GLU GLU MET ARG LYS GLU ARG ARG ARG ILE GLN GLU GLN LEU ARG ARG LEU LYS ARG ASN GLN GLU LYS GLU LYS LEU LYS GLY PRO PRO GLU LYS LYS PRO LYS LYS MET LYS GLU ASP LEU LYS LEU LYS CYS GLY ALA CYS GLY ALA ILE GLY
HIS MET ARG THR ASN LYS PHE CYS PRO LEU TYR TYR GLN THR ASN ALA PRO PRO SER ASN PRO VAL ALA MET THR GLU GLN GLU GLU LEU GLU LYS THR VAL ILE HIS ASN ASP ASN GLU GLU LEU ILE LYS VAL GLU GLY THR LYS ILE VAL LEU GLY LYS GLN LEU ILE GLU
SER ALA ASP GLU VAL ARG ARG LYS SER LEU VAL LEU LYS PHE PRO LYS GLN GLN LEU PRO PRO PRO LYS LYS LYS ARG ARG VAL GLY THR THR VAL HIS CYS ASP TYR LEU ASN ARG PRO HIS LYS SER ILE HIS ARG ARG ARG THR ASP PRO MET VAL THR LEU SER SER ILE LEU GLU SER
ILE ILE ASN ASP MET ARG ASP LEU PRO ASN THR TYR PRO PHE HIS THR PRO VAL ASN ALA LYS VAL VAL LYS ASP TYR TYR LYS ILE ILE THR ARG PRO MET ASP LEU GLN THR LEU ARG GLU GLU ASN VAL ARG LYS ARG LEU TYR PRO SER ARG GLU GLU PHE ARG GLU HIS LEU GLU LEU
ILE VAL LYS ASN SER ALA THR TYR ASN GLY PRO LYS HIS SER LEU THR GLN ILE SER GLN SER MET LEU ASP LEU CYS ASP GLU LYS LEU LYS GLU GLU LYS GLU ASP LYS LEU ALA ARG LEU GLU GLU LYS ALA ILE ASN PRO LEU LEU ASP ASP ASP GLN VAL ALA PHE SER PHE ILE LEU
ASP ASN ILE VAL THR GLN LYS MET MET ALA VAL PRO ASP PRO HIS HIS PRO VAL ASN LYS LYS PHE VAL PRO ASP TYR TYR LYS VAL ILE VAL ASN PRO MET ASP LEU GLU THR ILE ARG LYS ASN ILE SER LYS HIS LYS TYR GLN SER GLU SER ARG GLU SER PHE LEU ASP ASP



• Molecule 12: Transcription initiation factor TFIID subunit 2

Chain B:

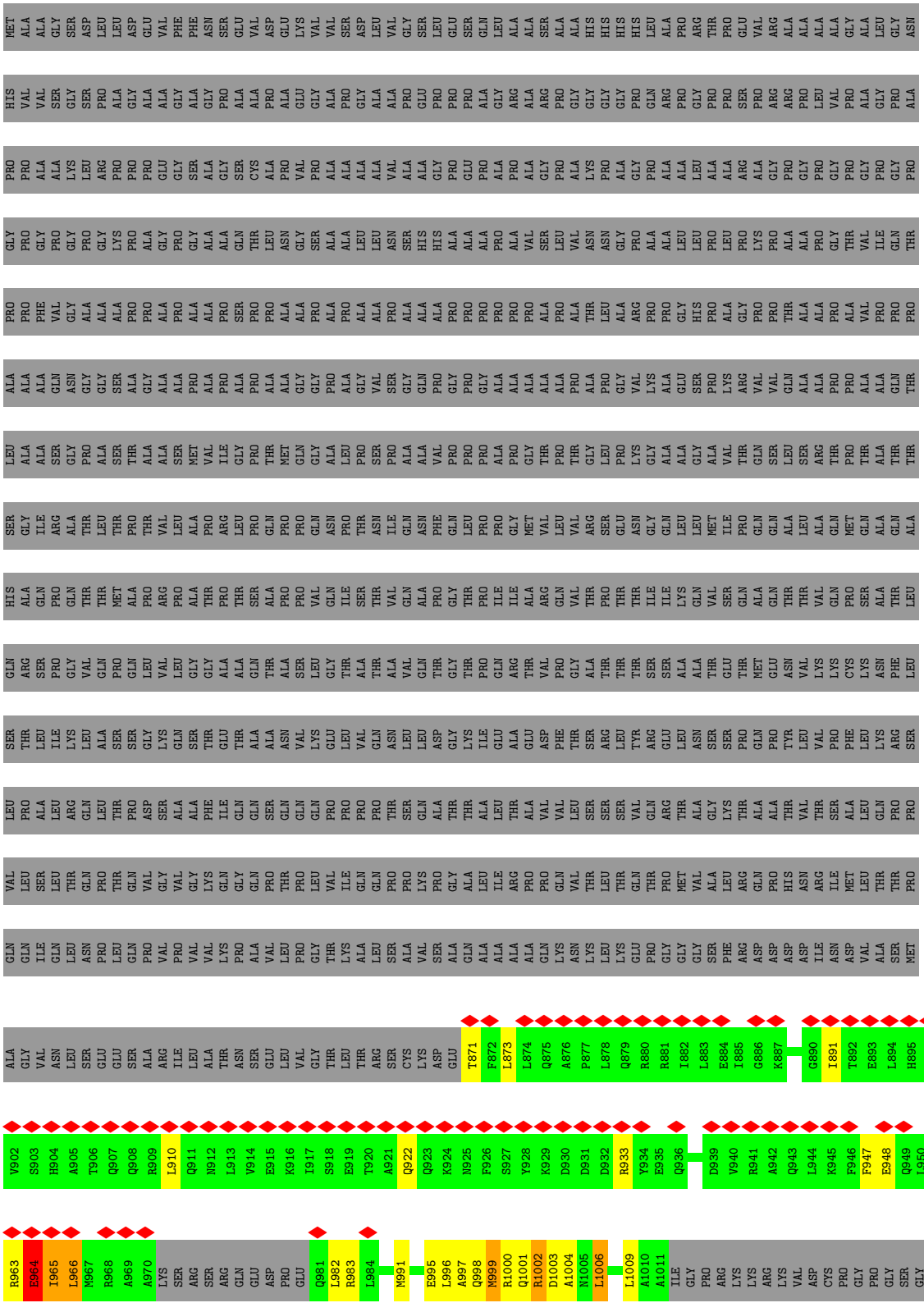


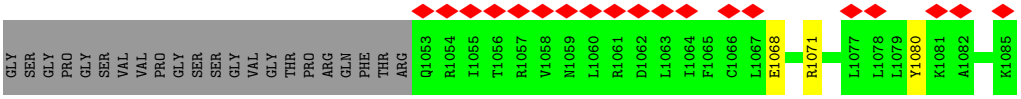


• Molecule 13: Transcription initiation factor TFIID subunit 4

Chain D:

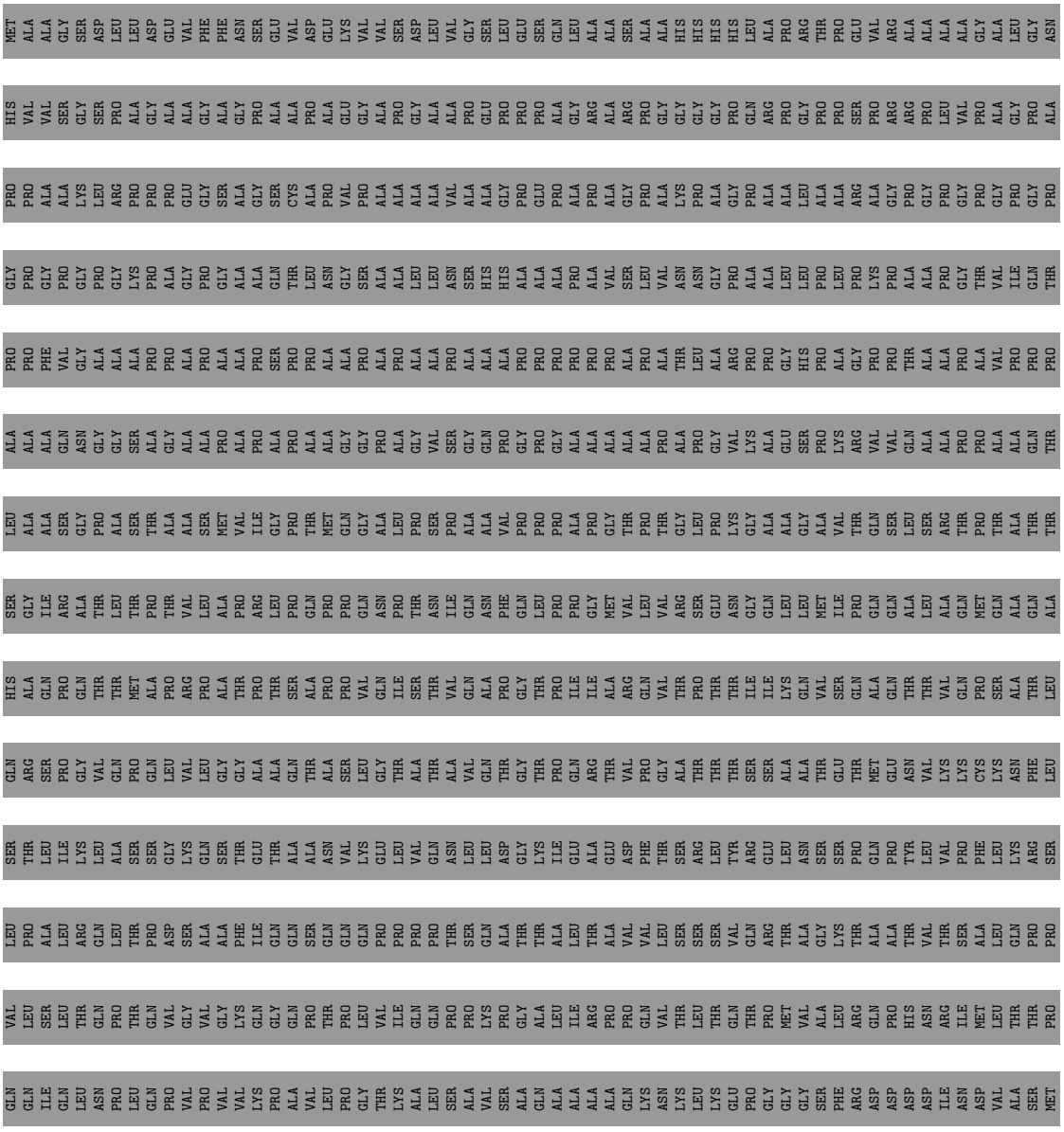

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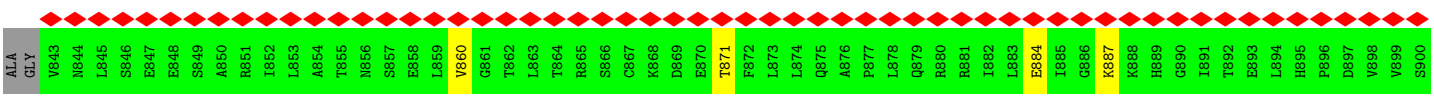

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HIS VAL VAL SER GLY SER PRO ALA GLY ALA ALA GLY ALA GLY PRO ALA ALA PRO ALA GLU ALA ALA PRO GLY GLY ALA ALA PRO PRO PRO PRO PRO PRO SER PRO ARG ARG PRO LEU VAL PRO ALA GLY PRO ALA
PRO PRO ALA ALA LYS LEU ARG PRO PRO PRO GLU GLY SER ALA GLY SER CYS ALA PRO VAL PRO ALA ALA ALA ALA VAL ALA ALA GLY PRO GLU PRO ALA PRO ALA GLY PRO ALA ALA ALA ARG ALA GLY PRO PRO GLY PRO GLY
GLY PRO GLY PRO GLY PRO GLY LYS PRO ALA GLY PRO GLY SER 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 PRO ALA ALA LEU LEU PRO PRO LEU PRO LYS PRO ALA ALA PRO GLY THR VAL ILE GLN THR
PRO PRO PHE VAL GLY GLY ALA ALA ALA PRO PRO ALA ALA PRO PRO PRO SER PRO ALA ALA PRO PRO PRO PRO PRO PRO ALA ALA ALA PRO ALA ALA PRO PRO PRO ALA ALA PRO PRO PRO PRO PRO PRO ALA GLY PRO THR ALA ALA PRO PRO
ALA ALA ALA GLN ASN GLY GLY GLY SER ALA GLY ALA ALA ALA ALA PRO ALA ALA PRO ALA ALA GLY VAL SER GLY GLN PRO GLY PRO GLY ALA ALA ALA ALA ALA ALA ALA ALA ALA PRO PRO PRO ALA ALA ALA ALA PRO ALA PRO GLY VAL LYS ALA GLU SER PRO LYS ARG VAL VAL GLN ALA ALA ALA PRO ALA GLN THR
LEU ALA ALA SER GLY PRO ALA SER THR ALA ALA ALA SER MET VAL ILE GLY PRO THR MET GLN GLY ALA LEU PRO SER PRO ALA ALA VAL PRO PRO PRO ALA PRO GLY THR PRO THR GLY LEU PRO LYS GLY ALA ALA GLY ALA VAL THR GLN SER LEU SER ARG THR PRO THR THR THR
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HIS ALA GLN PRO GLN THR THR MET ALA PRO ARG PRO ALA THR PRO THR PRO THR SER ALA PRO PRO PRO VAL GLN ILE SER THR VAL GLN ALA ALA ARG GLN VAL THR PRO 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 GLY ALA ALA GLN THR ALA SER LEU GLY THR ALA THR ALA VAL GLN THR GLY THR PRO PRO GLN GLY THR ALA ALA GLU THR THR THR SER SER ALA ALA THR GLU THR MET GLU ASN VAL VAL LYS LYS CYS LYS ASN PHE LEU
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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 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 I966 M967 R968 A969 A970 LYS SER ARG SER ARG GLN GLU ASP PRO GLU Q981 L982 R983 L984 M991 E995 L996 A997 Q998 M999 R1000 Q1001 R1002 D1003 A1004 N1005 L1006 L1009 A1010 A1011 ILE GLY PRO ARG LYS LYS ARG LYS VAL ASP CYS PRO GLY PRO GLY SER GLY ALA GLU

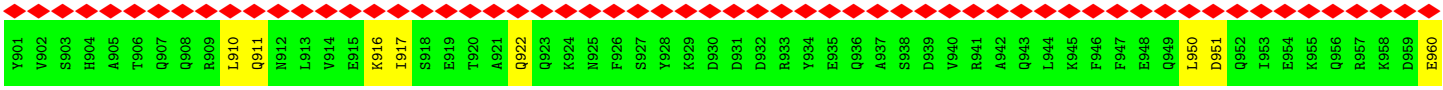


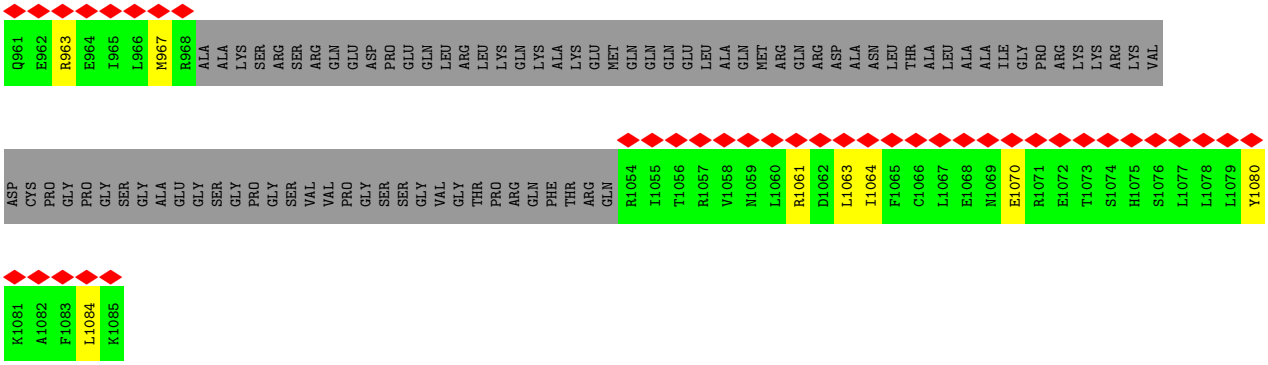
• Molecule 13: Transcription initiation factor TFIID subunit 4





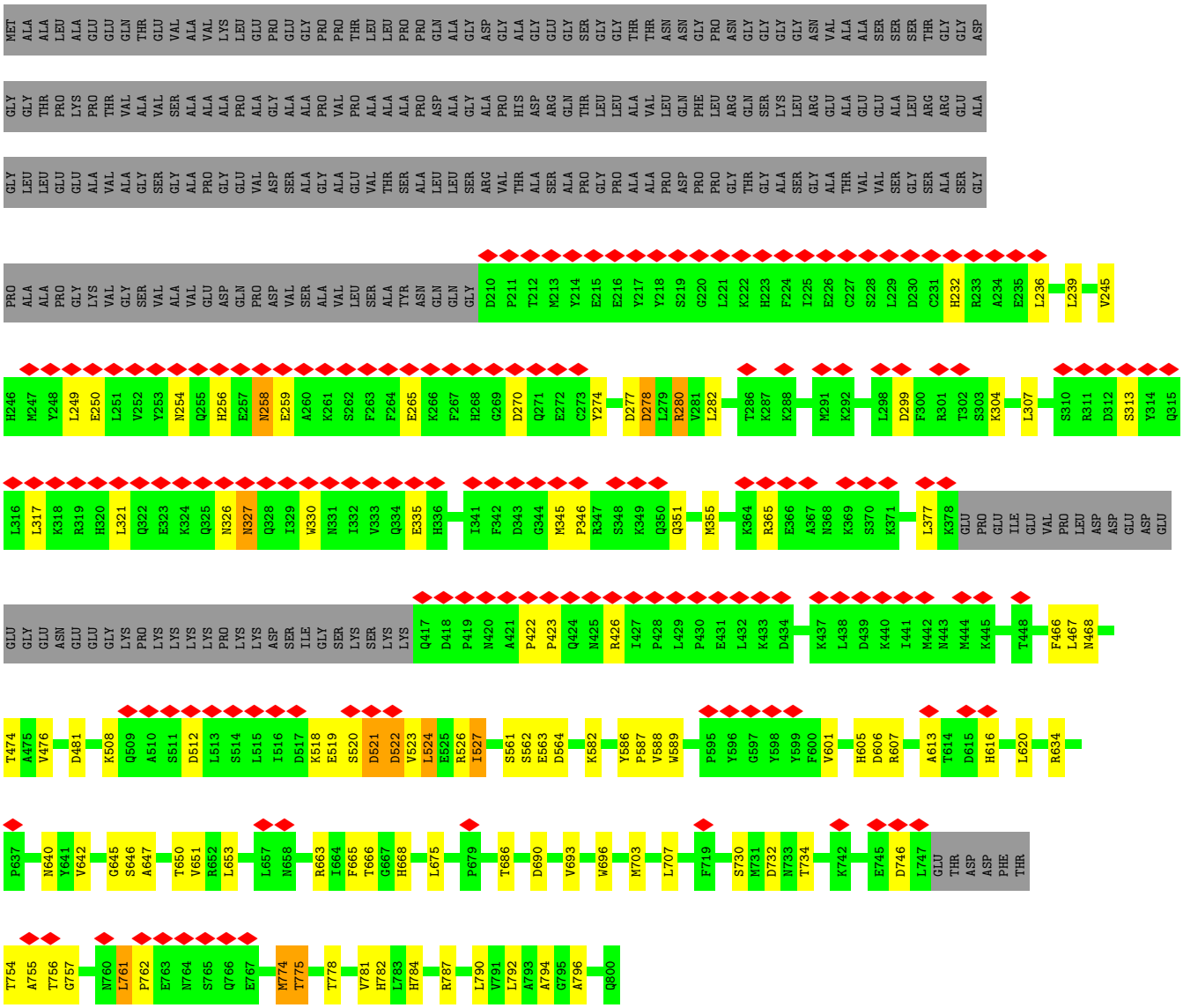






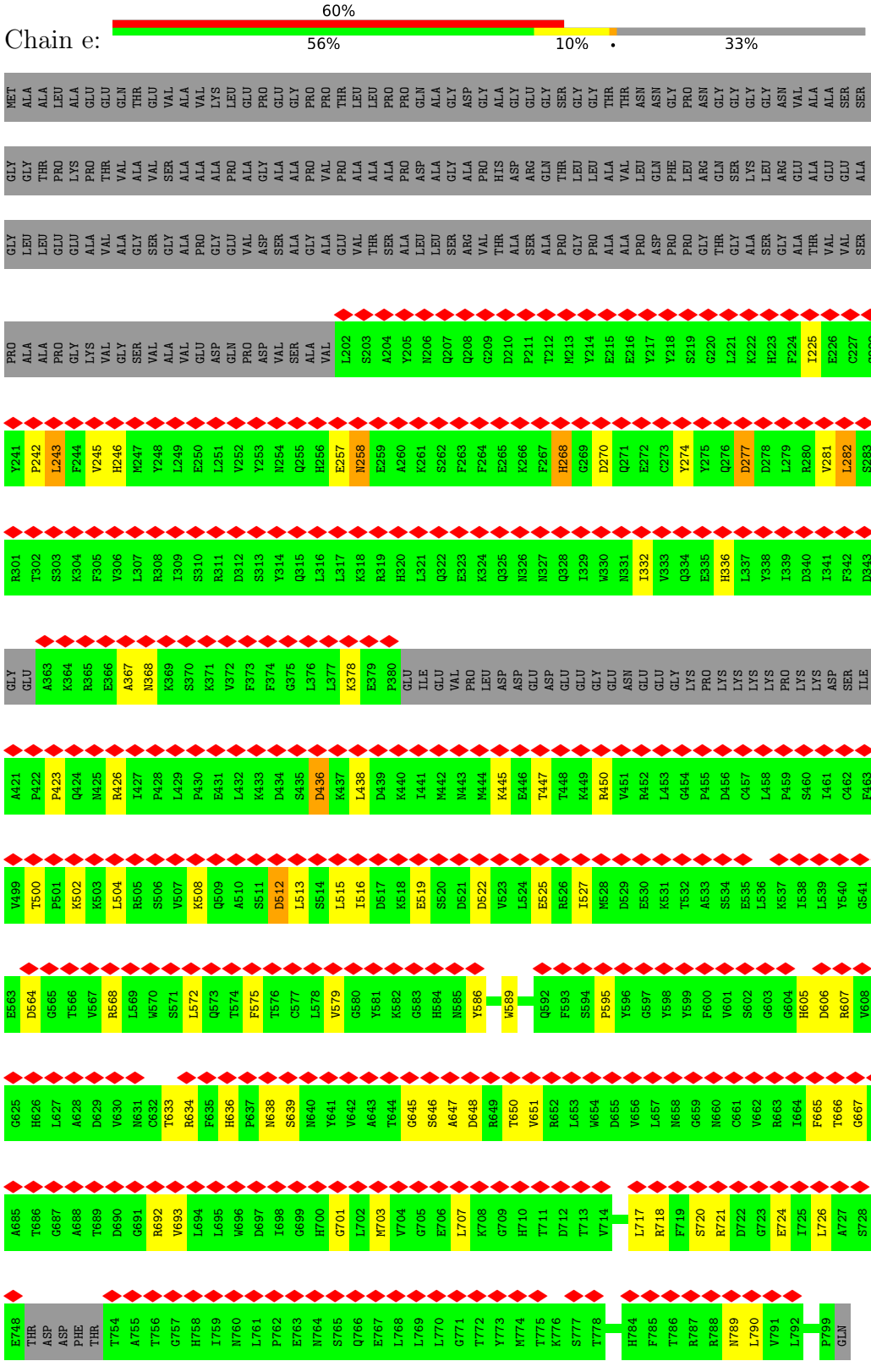
• Molecule 14: Transcription initiation factor TFIID subunit 5





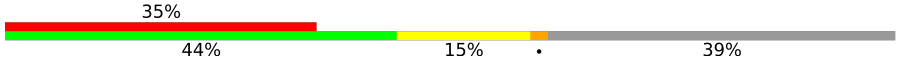
• Molecule 14: Transcription initiation factor TFIID subunit 5

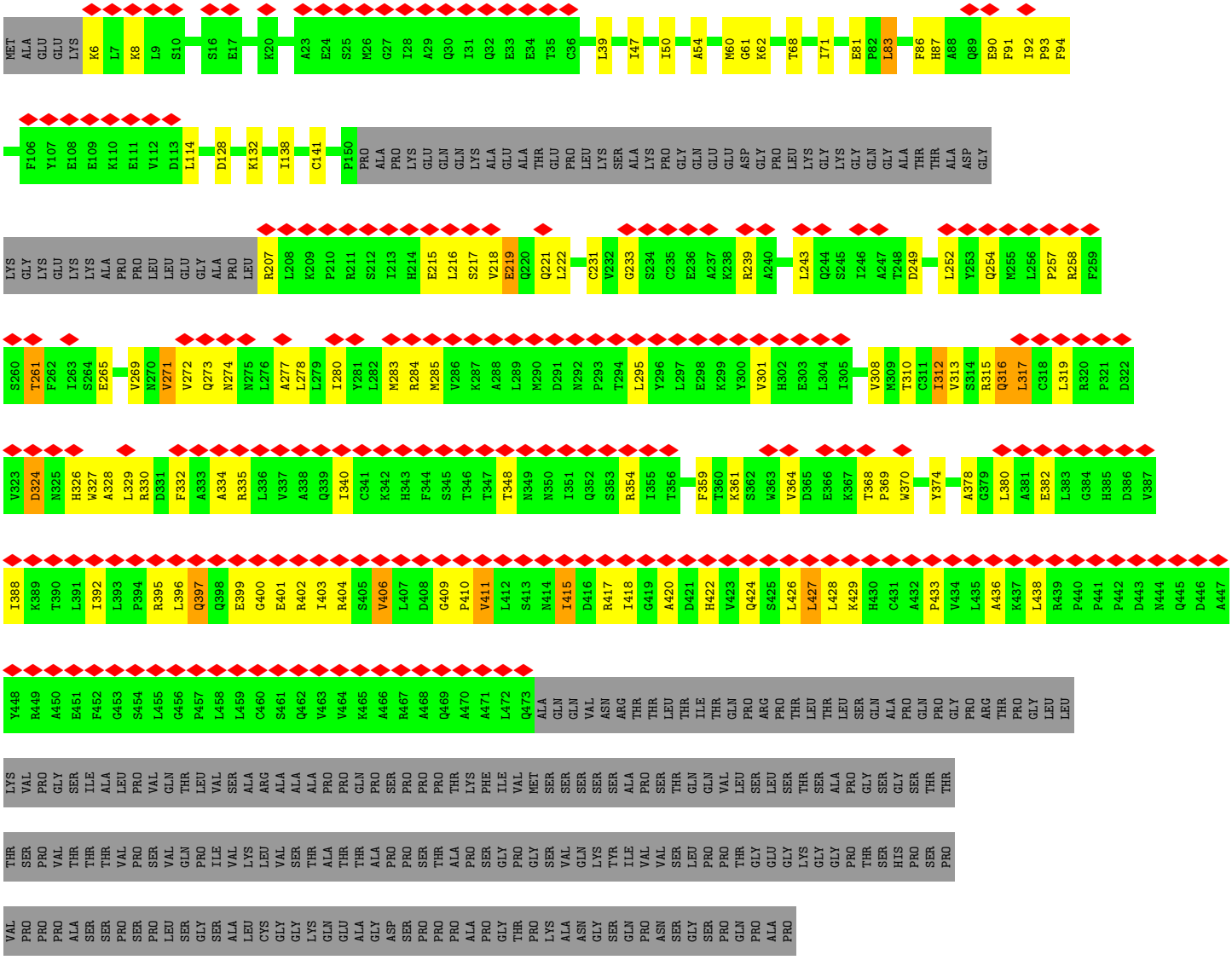
Chain e:



• Molecule 15: Transcription initiation factor TFIID subunit 6

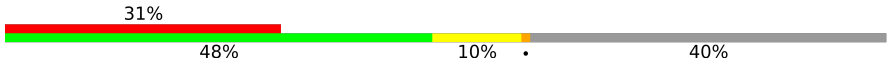
Chain F:

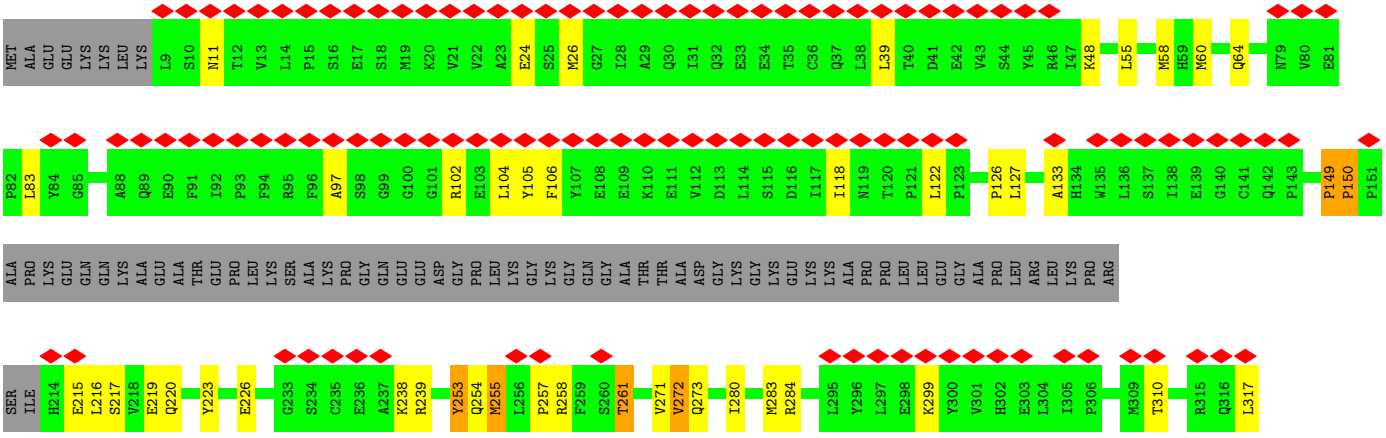


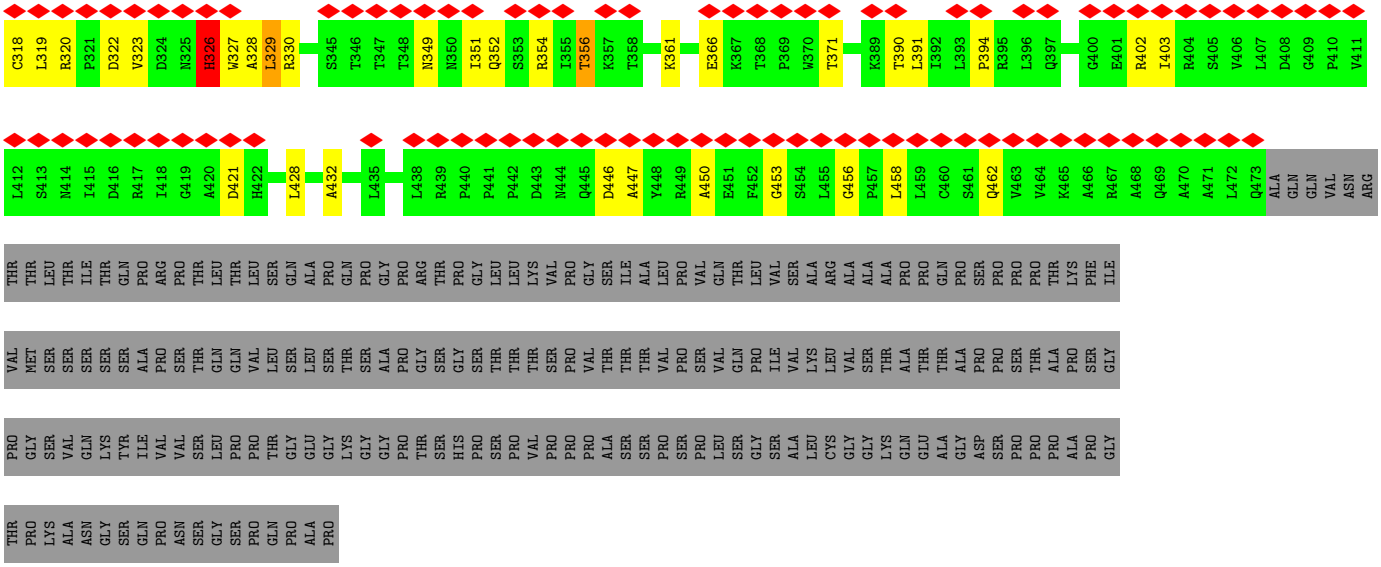


• Molecule 15: Transcription initiation factor TFIID subunit 6

Chain f:

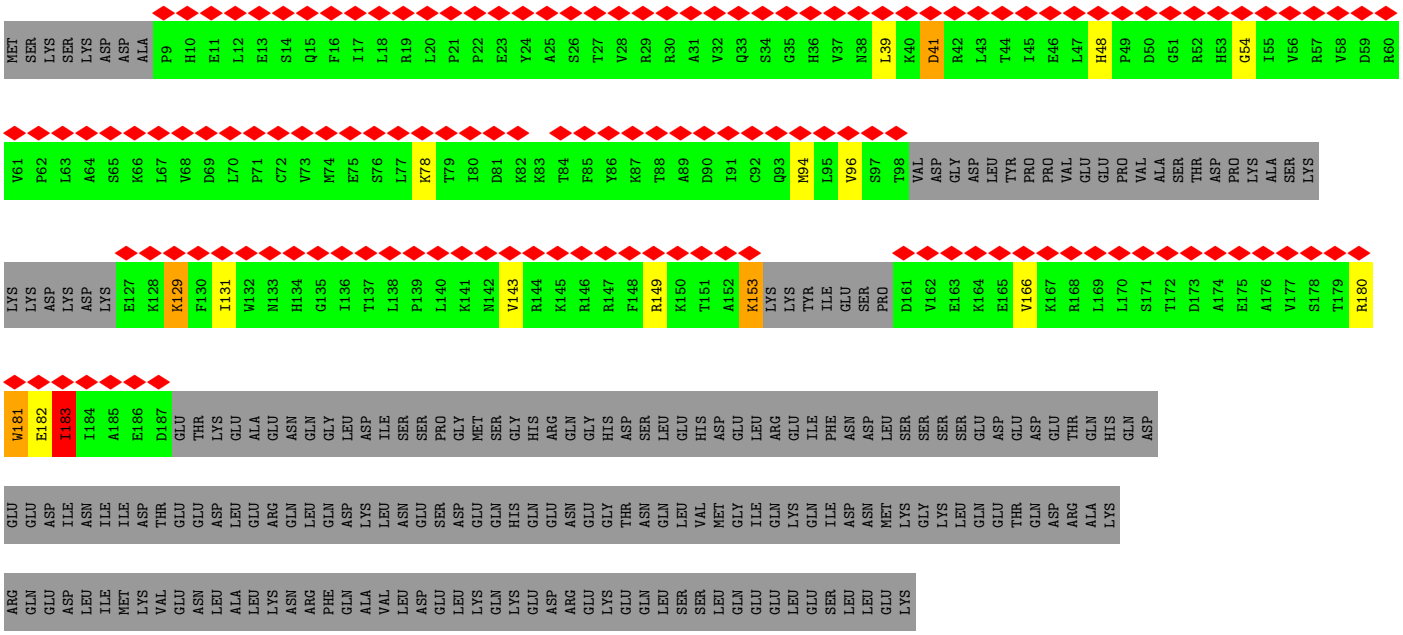






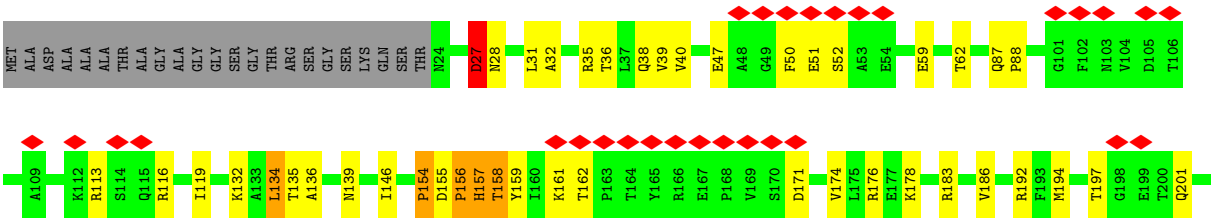
• Molecule 16: Transcription initiation factor TFIID subunit 7

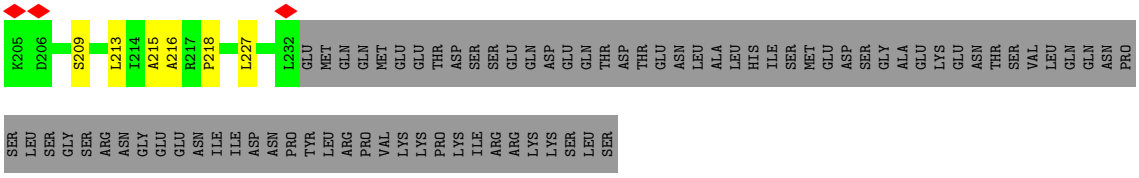




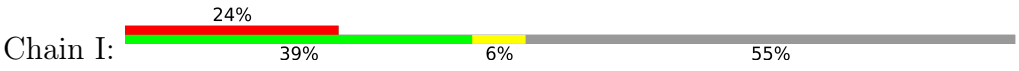
• Molecule 17: Transcription initiation factor TFIID subunit 8

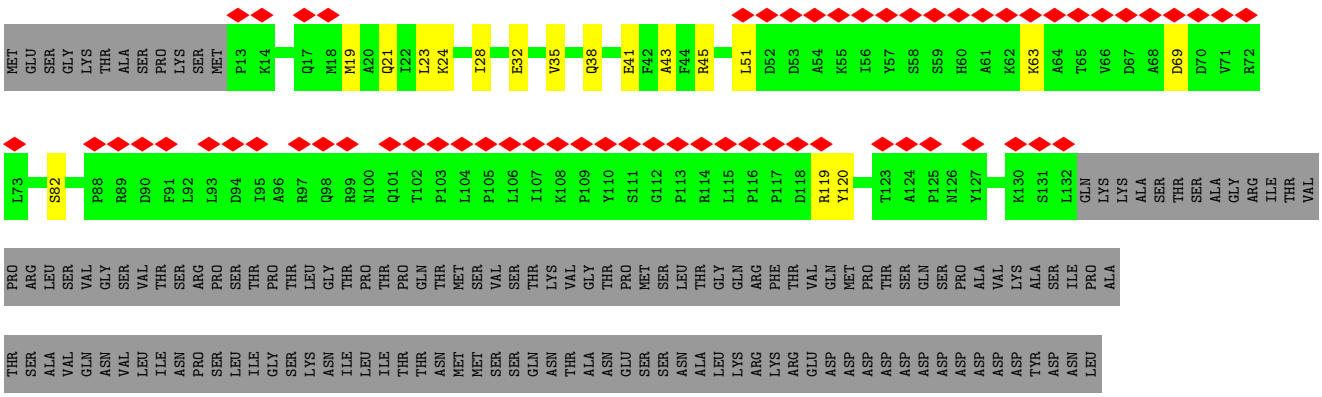




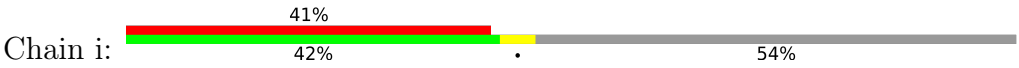


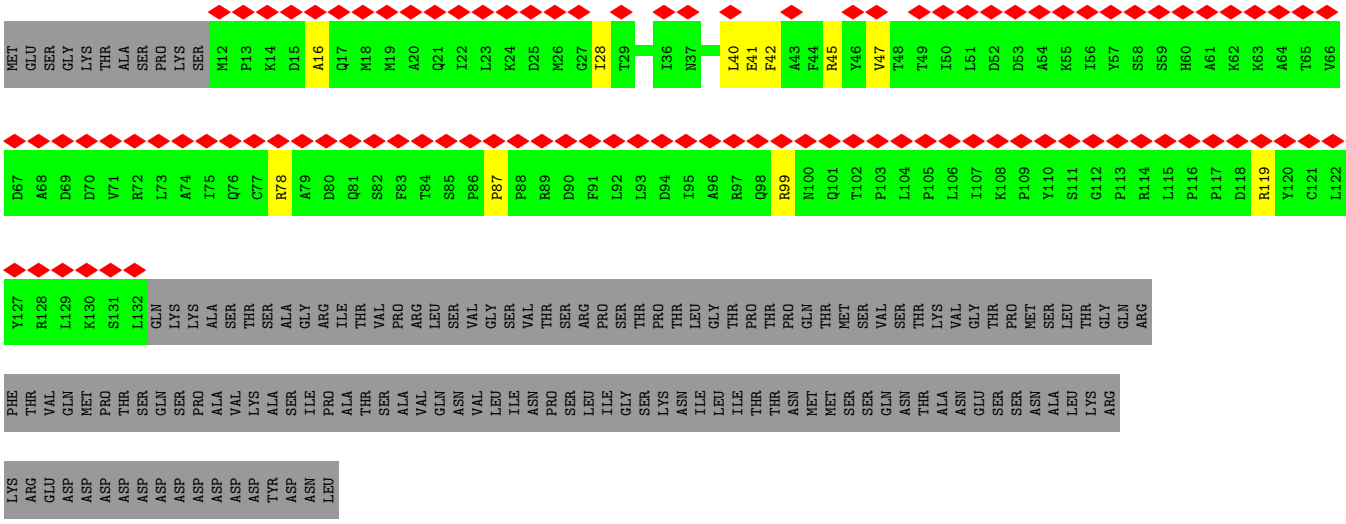
• Molecule 18: Transcription initiation factor TFIID subunit 9





• Molecule 18: Transcription initiation factor TFIID subunit 9

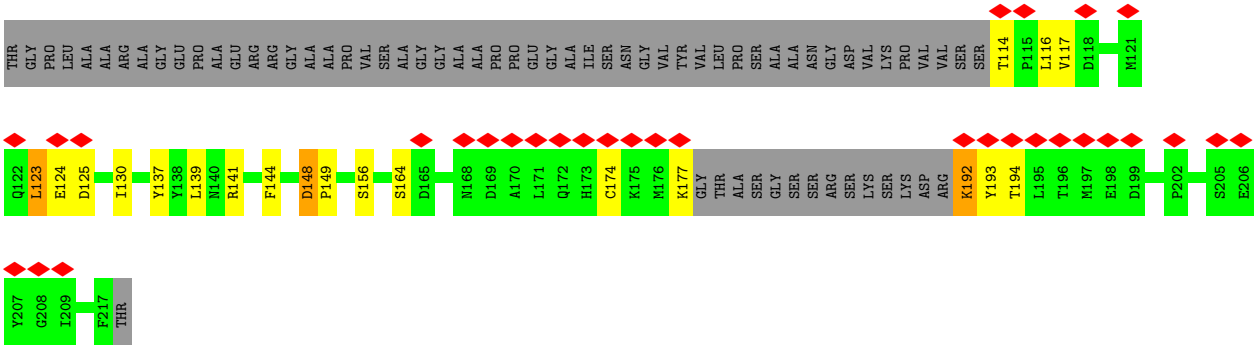




• Molecule 19: Transcription initiation factor TFIID subunit 10



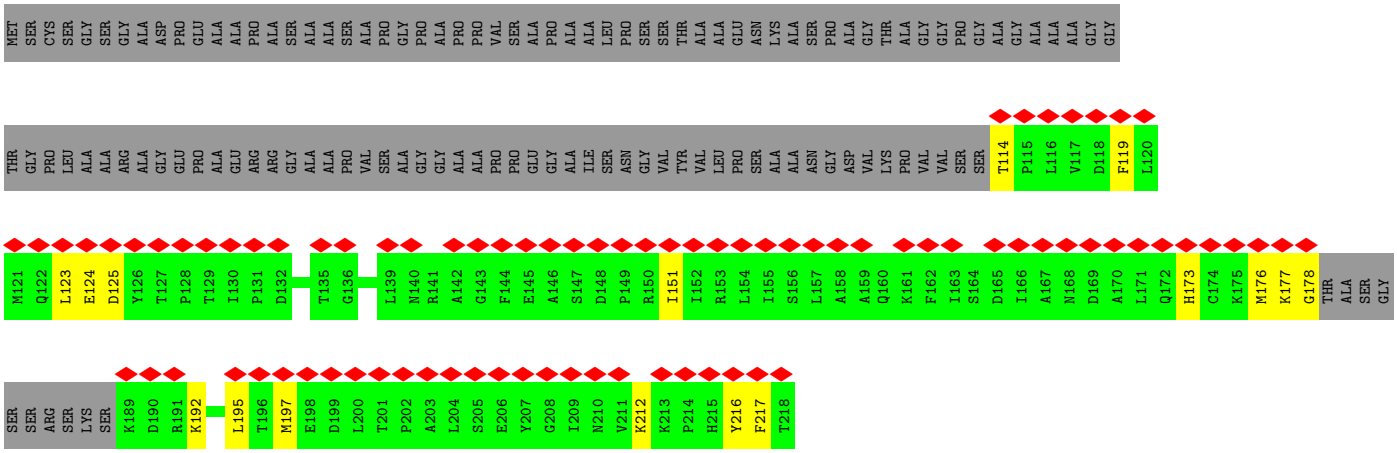




• Molecule 19: Transcription initiation factor TFIID subunit 10

Chain j:

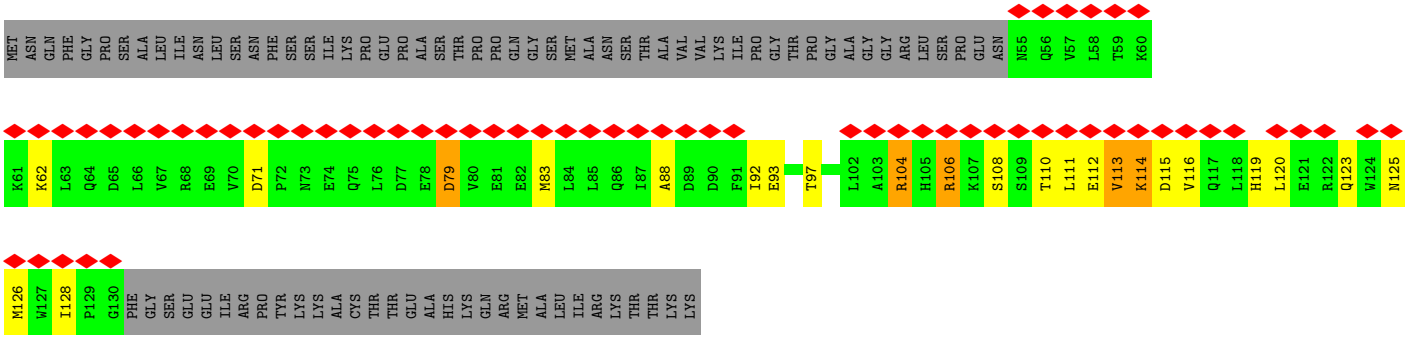




• Molecule 20: Transcription initiation factor TFIID subunit 12

Chain L:





• Molecule 20: Transcription initiation factor TFIID subunit 12

Chain l:





K61 K62 L63 Q64 D65 L66 V67 R68 E69 V70 D71 P72 N73 E74 Q75 L76 D77 E78 D79 V80 E81 E82 M83 L84 L85 Q86 I87 A88 D89 D90 F91 I92 E93 S94 V95 V96 T97 A98 A99 C100 Q101 L102 A103 R104 H105 R106 K107 S108 S109 T110 L111 E112 V113 K114 D115 V116 Q117 L118 H119 L120

E121 R122 Q123 W124 N125 M126 W127 I128 P129 G130 F131 G132 S133 E134 E135 I136 R137 P138 Y139 K140 K141 A142 C143 T144 T145 E146 A147 H148 K149 Q150 R151 M152 A153 L154 I155 R156 K157 T158 T159 K160 K161

- Molecule 21: Transcription initiation factor IIA subunit 2

Chain O: 75% 16% 9%

M1 L11 Q16 D20 Q24 T29 L32 I44 L48 R51 N57 F58 L62 N63 T64 Y65 D69 T73 L76 D99 GLY LYS ASN THR GLY SER ASN THR THR GLU

- Molecule 22: TATA-box-binding protein

Chain P: 47% 6% 47%

MET ASP GLN ASN ASN SER LEU PRO PRO TYR ALA GLN GLY LEU ALA SER PRO GLN GLY ALA MET THR PRO GLY ILE PRO ILE PHE SER PRO MET MET PRO TYR GLY THR GLY LEU THR PRO GLN PRO ILE GLN ASN THR ASN SER LEU SER ILE LEU GLU GLU GLN GLN ARG GLN GLN GLN

GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN ALA VAL ALA ALA ALA ALA VAL GLN GLN SER THR SER GLN GLN ALA THR GLN GLY THR SER GLY GLN ALA PRO GLN

LEU PHE HIS SER GLN THR LEU THR THR ALA PRO LEU PRO GLY THR THR PRO LEU TYR PRO SER PRO MET THR PRO MET THR PRO ILE THR PRO ALA THR PRO ALA SER GLU SER S159 V169 L174 L178 R186 A187 R188 R203 E206 P207 R208 T222 E227

K236 L244 M295 I296 K297 P298 R299 I300 R318 E323 K337 THR THR

- Molecule 23: Transcription initiation factor IIA beta chain

Chain Q: 27% 70%

MET ALA ASN SER ALA ASN THR ASN T9 R15 I18 E19 D20 V21 I22 D31 L39 W46 M51 GLN SER ARG ALA VAL ASP GLY PHE HIS SER GLU GLU GLN GLN LEU LEU LEU GLN VAL GLN GLN GLN HIS GLN PRO GLN GLN GLN GLN HIS HIS HIS HIS HIS HIS

HIS GLN GLN ALA GLN PRO GLN GLN THR VAL PRO GLN GLN ALA GLN THR GLN GLN VAL LEU ILE PRO ALA SER GLN GLN ALA THR ALA PRO GLN VAL ILE VAL PRO ASP SER LYS LEU ILE GLN HIS MET ASN ALA SER ASN MET SER ALA ALA ALA THR ALA ALA THR LEU ALA LEU PRO

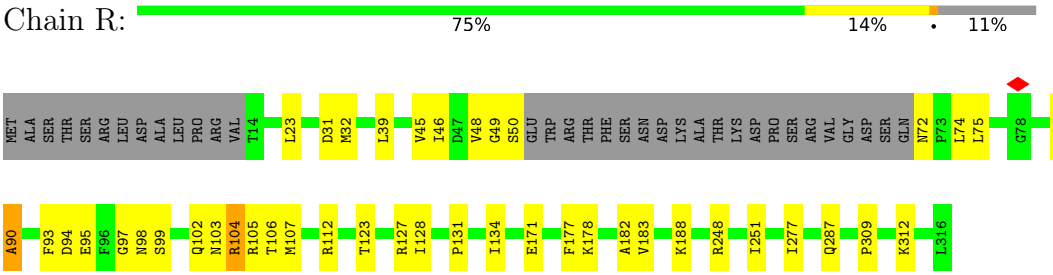
ALA GLY VAL THR PRO VAL GLN GLN ILE LEU THR ASN SER GLY GLN LEU LEU GLN VAL VAL ARG ALA ALA ASN GLY ALA GLN TYR ILE PHE GLN PRO GLN GLN SER VAL VAL LEU GLN GLN GLN VAL ILE PRO GLN MET GLN PRO GLY GLY VAL GLN ALA PRO VAL ILE GLN GLN VAL LEU

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

ALA PRO LEU VAL LEU GLN VAL ASP GLY THR GLY ASP THR SER SER GLU GLU ASP GLU ASP GLU GLU GLU ASP TYR ASP ASP ASP GLU GLU GLU ASP LYS GLU LYS ASP GLY ALA GLU ASP G307 Q308 V309 S321 D322 E332 K346 I366 W376

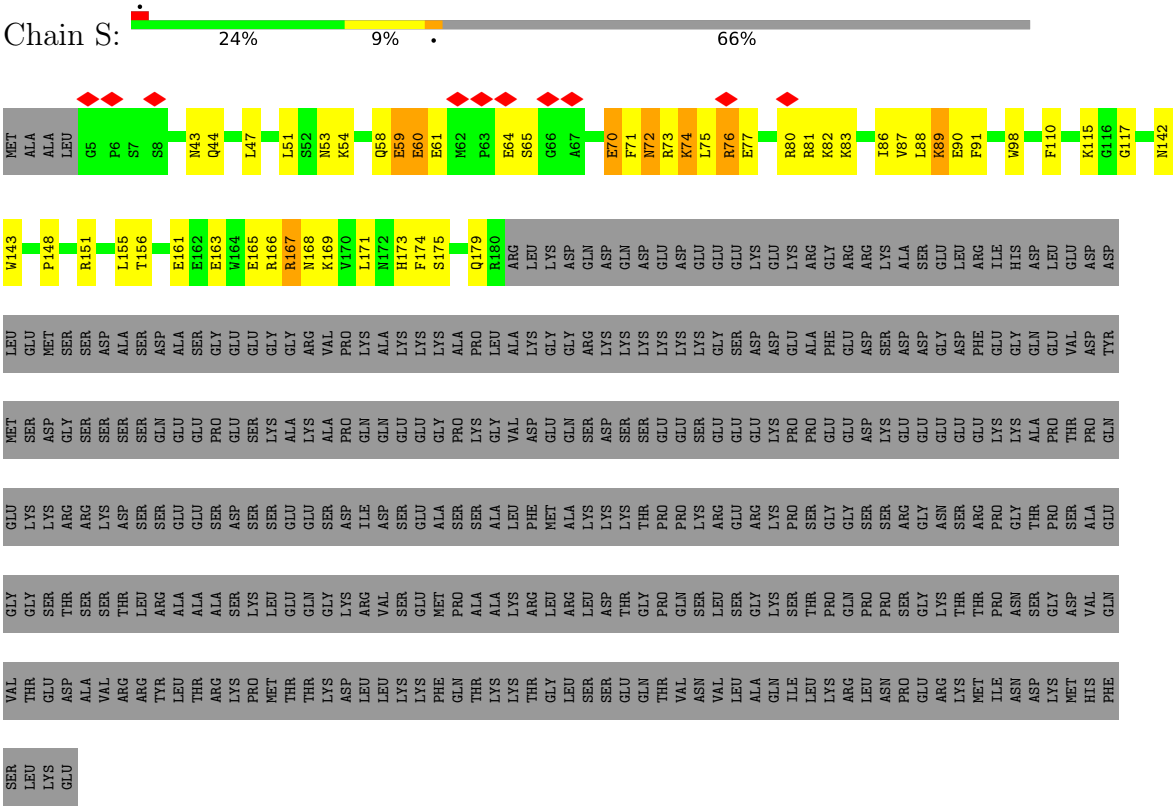
- Molecule 24: Transcription initiation factor IIB

Chain R:



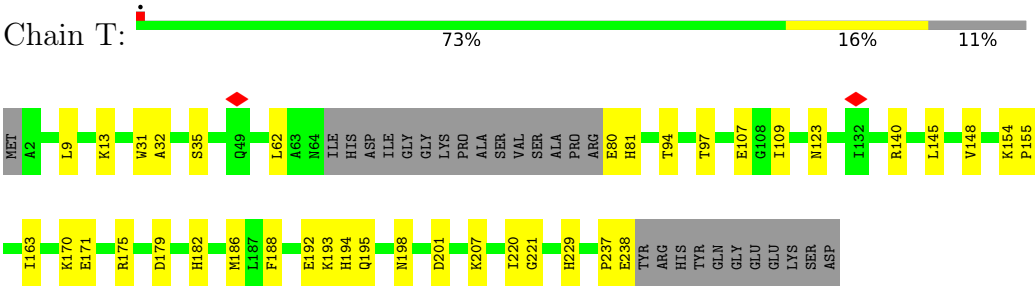
• Molecule 25: General transcription factor IIF subunit 1

Chain S:



• Molecule 26: General transcription factor IIF subunit 2

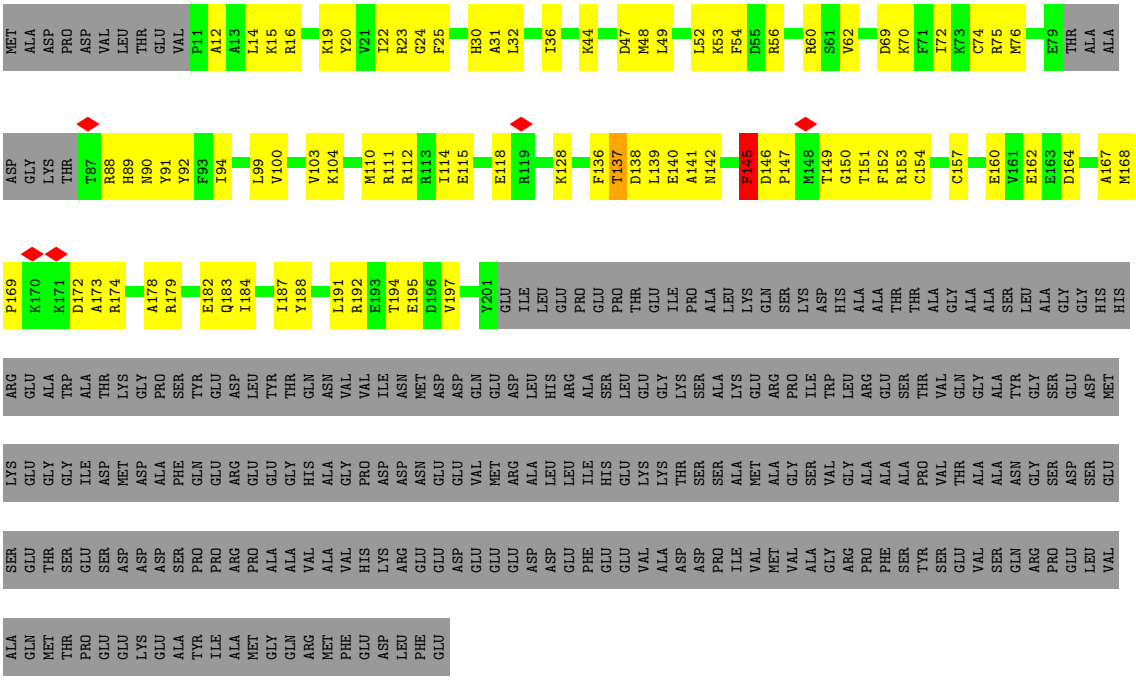
Chain T:



• Molecule 27: General transcription factor IIE subunit 1

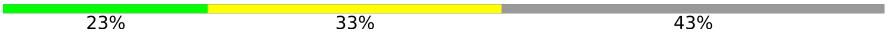
Chain U:

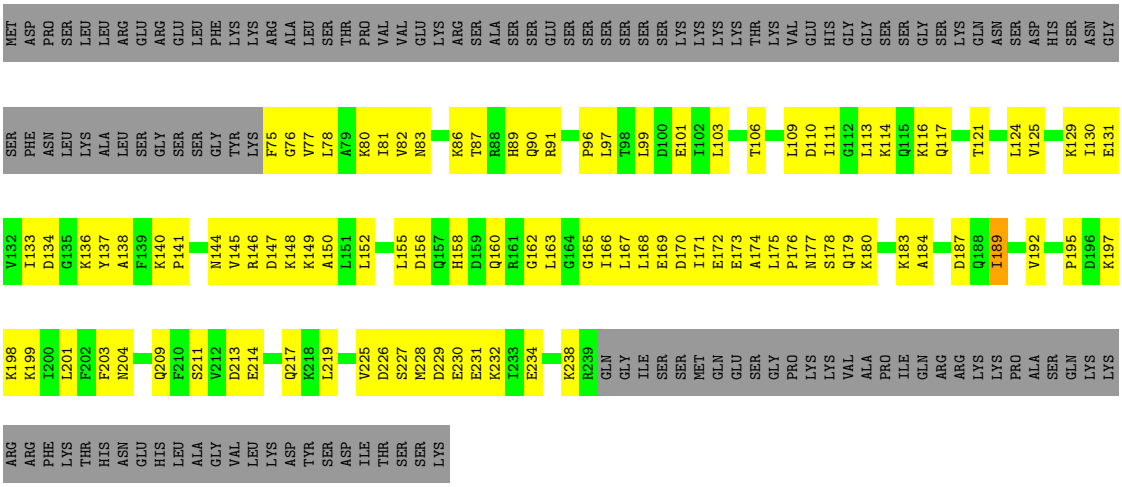




• Molecule 28: Transcription initiation factor IIE subunit beta

Chain V:

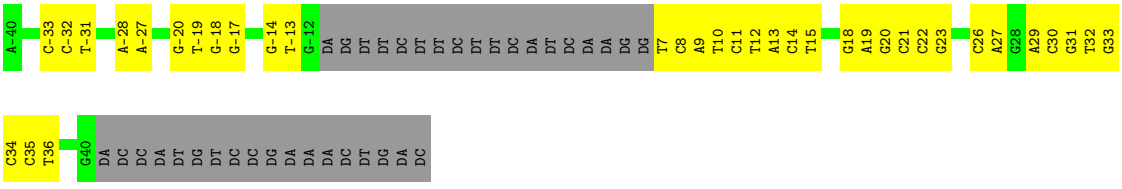




• Molecule 29: non-template DNA

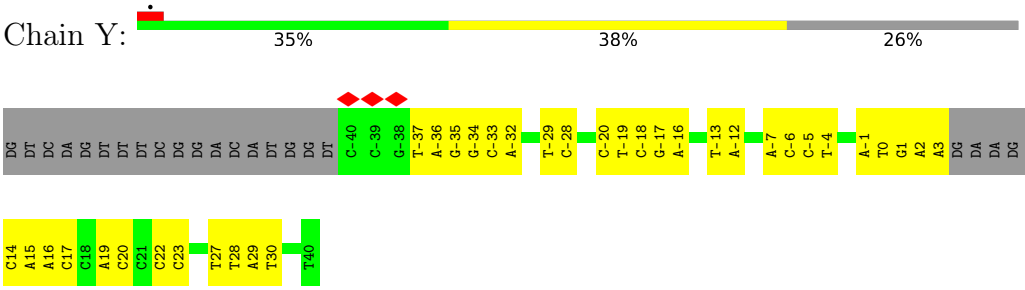
Chain X:





• Molecule 30: template DNA

Chain Y:



• Molecule 31: Transcription initiation factor TFIID subunit 3

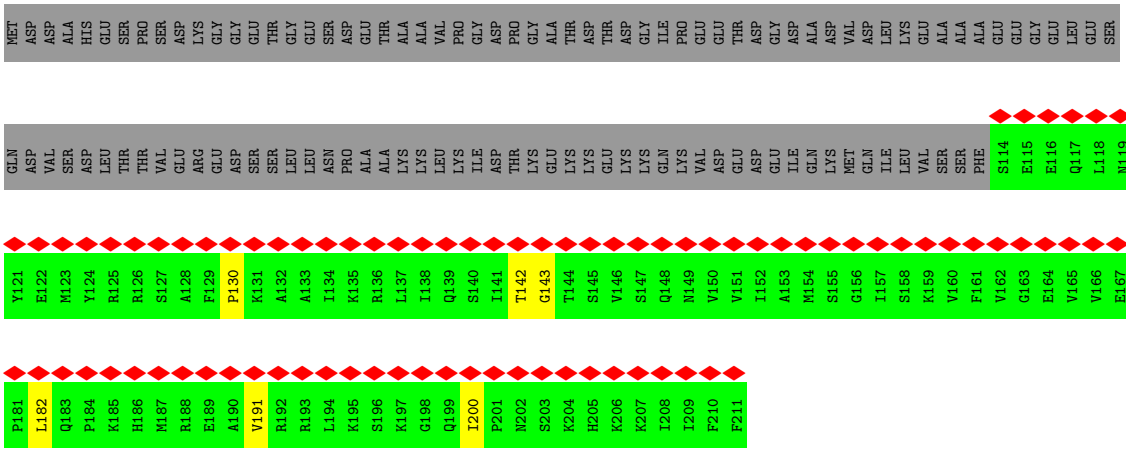
Chain c:





• Molecule 32: Transcription initiation factor TFIID subunit 11





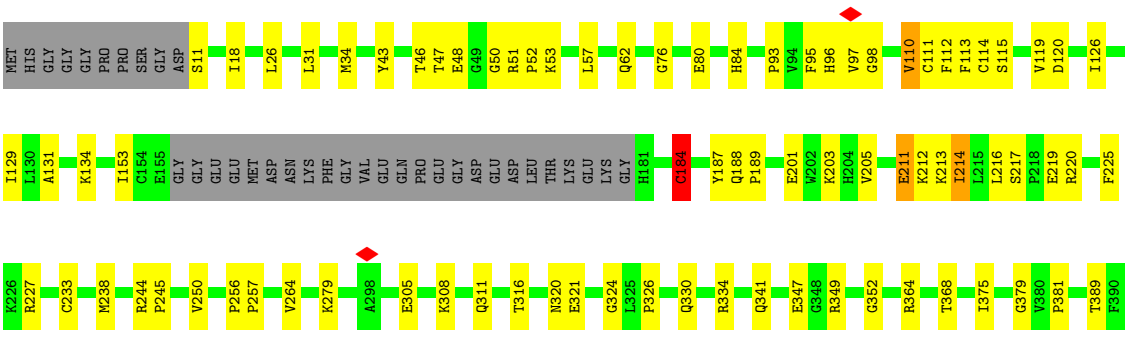
• Molecule 33: Transcription initiation factor TFIID subunit 13

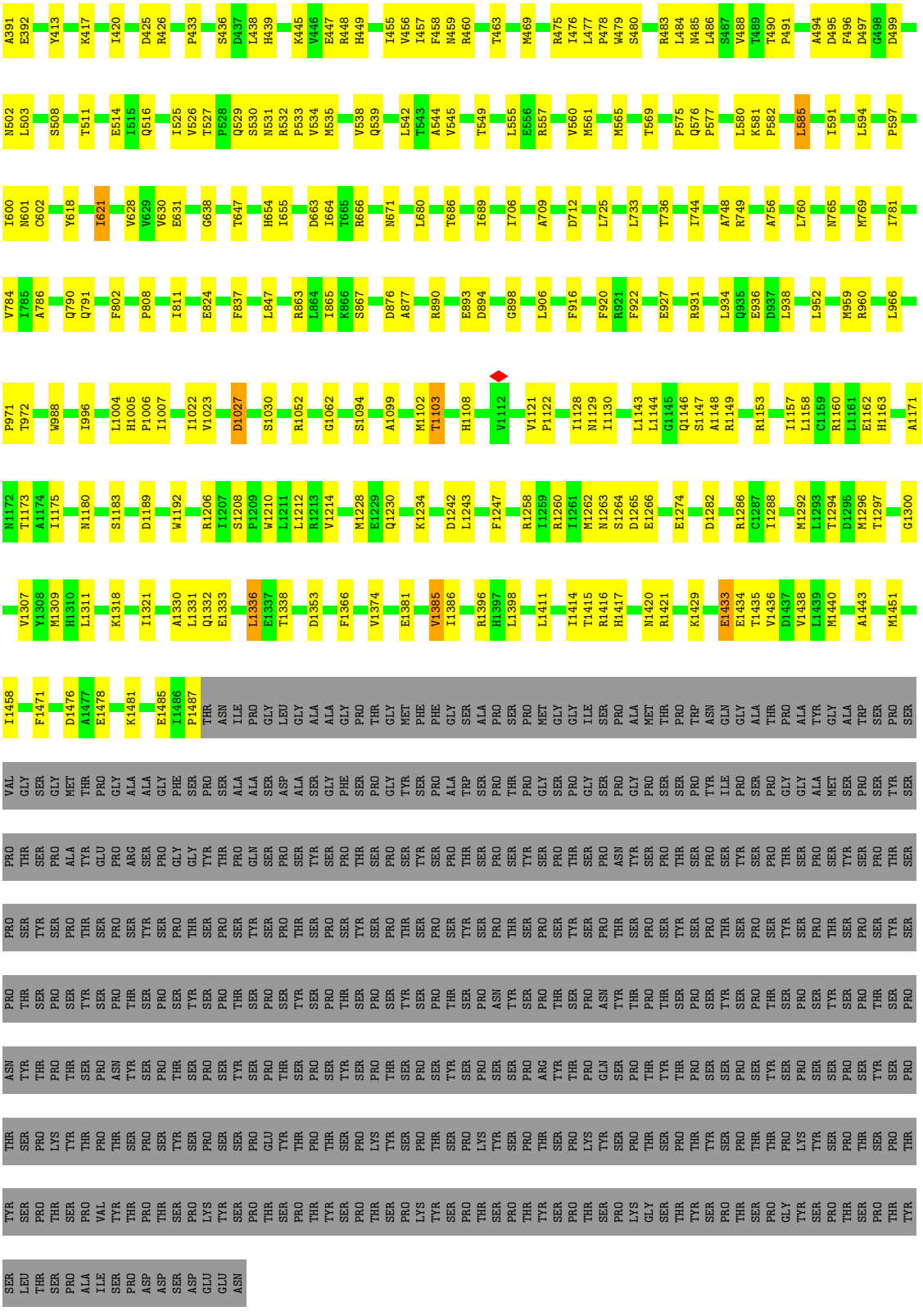




• Molecule 34: DNA-directed RNA polymerase subunit

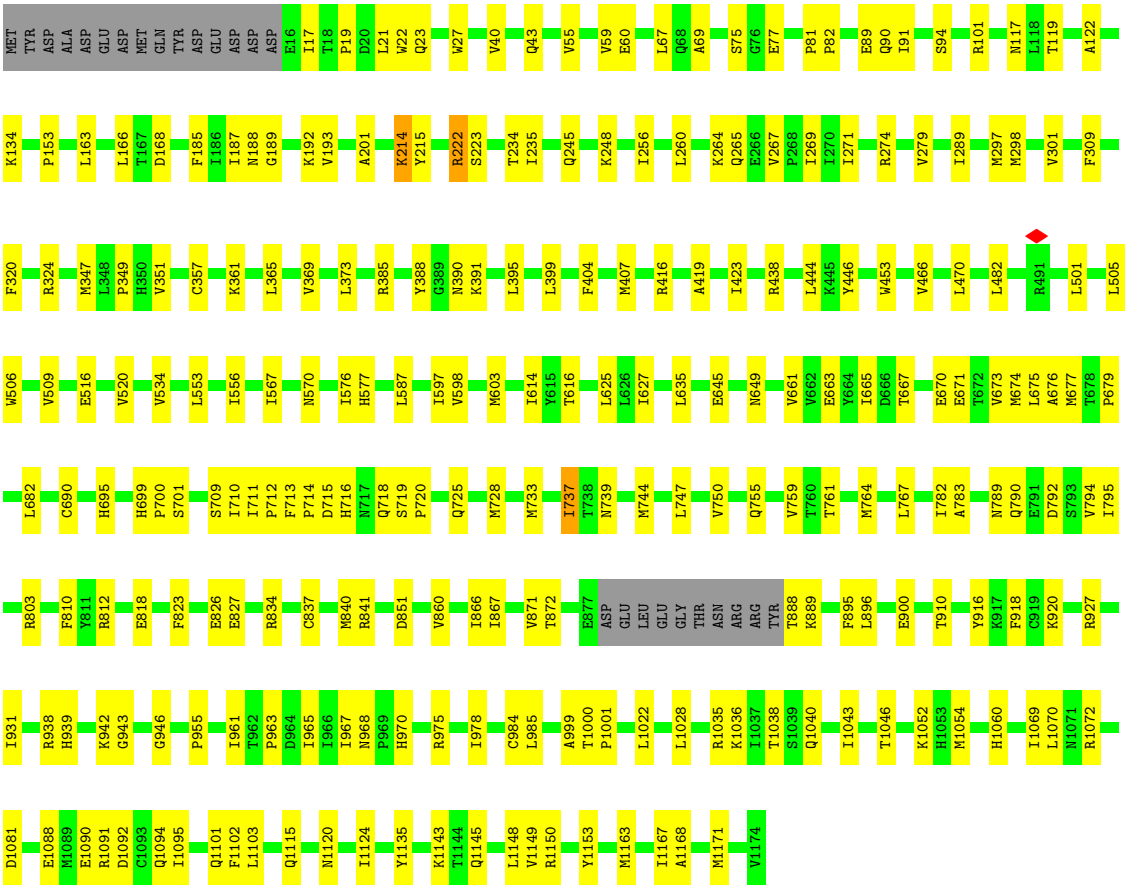






• Molecule 35: DNA-directed RNA polymerase subunit beta

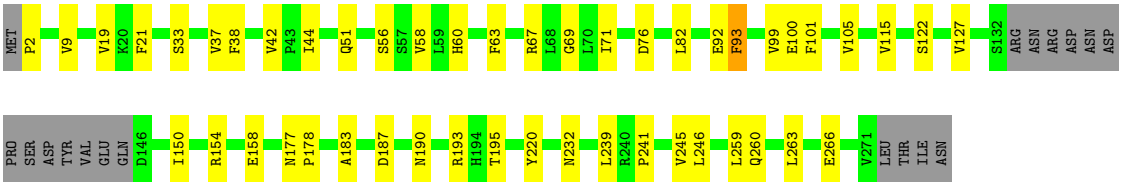
Chain p: 77% 21%



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

Chain q:

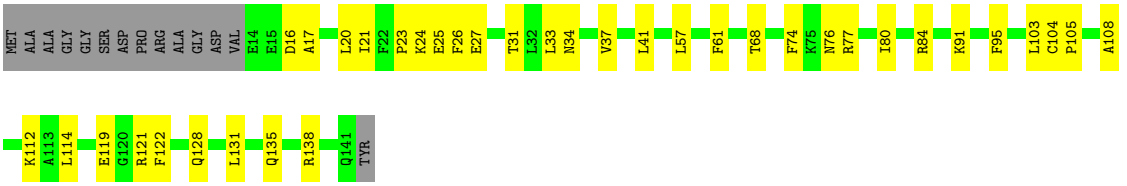




• Molecule 37: DNA-directed RNA polymerase II subunit RPB4

Chain r:

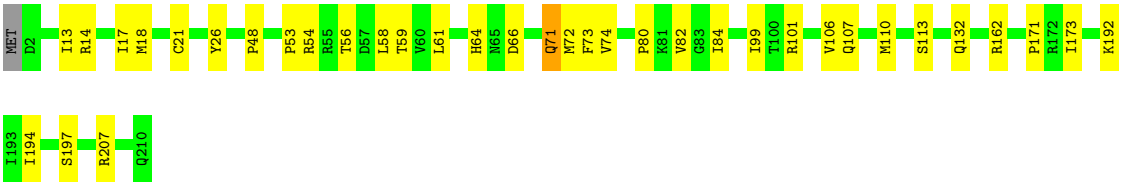




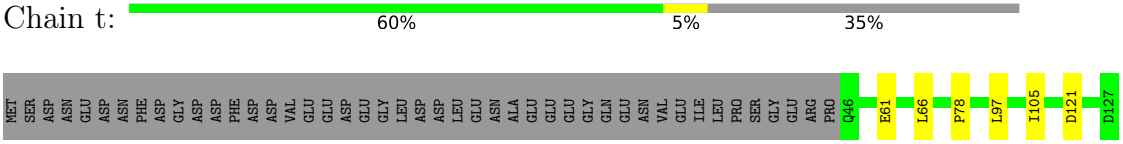
• Molecule 38: DNA-directed RNA polymerase II subunit E

Chain s:

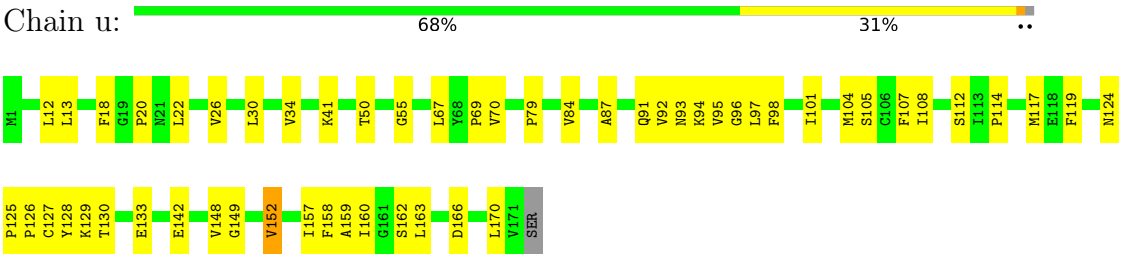




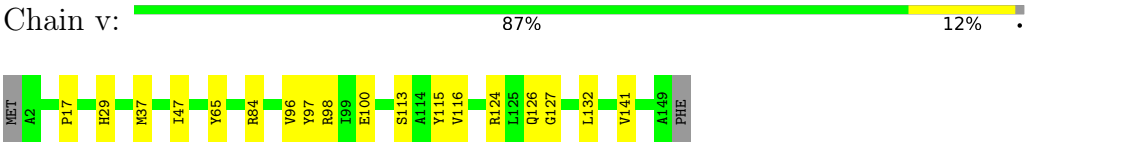
• Molecule 39: DNA-directed RNA polymerase II subunit F



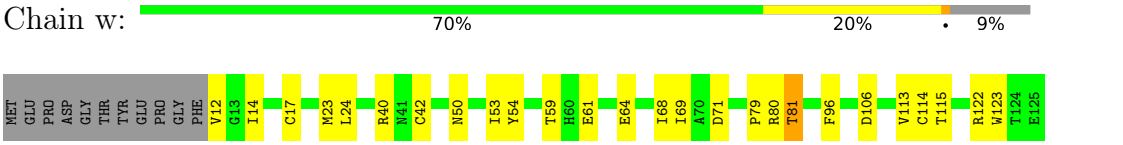
• Molecule 40: DNA-directed RNA polymerase II subunit RPB7



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



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



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



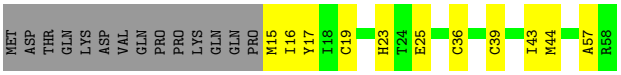
• Molecule 44: DNA-directed RNA polymerase II subunit RPB11-a





• Molecule 45: RPB12





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4867	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	4.331	Depositor
Minimum map value	-1.901	Depositor
Average map value	0.035	Depositor
Map value standard deviation	0.176	Depositor
Recommended contour level	0.48	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: ATP, CSX, HYP, MG, SF4, W0F, ILX, TRX, G2L, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >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	0.19	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	0.36	0/93	0.59	0/142
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	0.56	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	3/6069 (0.0%)
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	0.94	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	0.97	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	0.27	0/816	0.36	0/1105
22	P	0.12	0/1448	0.24	0/1948
23	Q	0.19	0/945	0.36	0/1274
24	R	0.18	0/2199	0.38	0/2967
25	S	0.19	0/1496	0.38	0/2013
26	T	0.15	0/1817	0.29	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	0.34	0/1464	0.61	0/2258
30	Y	0.38	0/1660	0.59	0/2554
31	c	0.48	0/1035	0.67	0/1406
32	k	0.28	0/799	0.53	1/1070 (0.1%)
33	m	0.84	0/733	1.18	1/977 (0.1%)
34	o	0.25	0/11723	0.38	0/15830
35	p	0.27	0/9358	0.37	0/12633
36	q	0.31	1/2102 (0.0%)	0.38	0/2857
37	r	0.11	0/1064	0.23	0/1428
38	s	0.24	0/1751	0.34	0/2366
39	t	0.22	0/667	0.31	0/901
40	u	0.19	0/1382	0.31	0/1874
41	v	0.22	0/1207	0.31	0/1628
42	w	0.20	0/948	0.31	0/1284
43	x	0.26	0/542	0.37	0/730
44	y	0.26	0/939	0.34	0/1271
45	z	0.22	0/377	0.34	0/500
All	All	0.38	8/110959 (0.0%)	0.59	48/150559 (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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	28	ASN	C-O	-7.45	1.15	1.24
17	H	27	ASP	C-O	-7.05	1.15	1.24
17	H	31	LEU	C-O	-6.31	1.16	1.24
12	B	61	ASN	C-O	-6.12	1.18	1.24
14	E	524	LEU	C-O	5.72	1.30	1.24
15	F	395	ARG	C-O	5.61	1.31	1.24
14	e	445	LYS	C-O	5.59	1.30	1.24
36	q	187	ASP	C-O	5.58	1.31	1.24

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	55	LYS	CB-CA-C	-11.48	94.97	111.85
12	B	491	HIS	N-CA-C	-9.46	100.97	111.28
15	f	149	PRO	O-C-N	9.13	125.51	121.31
14	E	756	THR	N-CA-C	-8.40	103.16	113.50
17	H	32	ALA	N-CA-C	-8.21	102.29	111.07
17	H	27	ASP	N-CA-C	-7.94	102.71	111.36
14	E	762	PRO	N-CA-C	7.36	124.20	114.27
15	F	271	VAL	N-CA-C	-7.30	105.89	112.90
11	A	715	PRO	N-CA-C	-7.05	100.17	111.03
12	B	495	GLN	N-CA-C	-7.04	104.69	113.28
6	5	38	ILE	N-CA-CB	-6.91	102.46	110.55
32	k	180	PRO	N-CA-C	6.78	118.97	110.70
1	0	8	ARG	N-CA-CB	-6.74	99.10	110.49
11	A	396	LEU	N-CA-C	-6.74	104.80	113.16
15	f	326	HIS	N-CA-C	-6.68	104.23	112.38
15	f	319	LEU	N-CA-C	-6.55	103.96	112.68
11	A	467	ILE	N-CA-C	-6.42	104.01	111.00
3	2	70	THR	N-CA-C	-6.33	104.48	111.82
11	A	1205	PHE	CA-CB-CG	-6.27	107.53	113.80
13	D	999	MET	N-CA-C	-6.23	104.40	111.07
5	4	439	ARG	CB-CA-C	6.19	122.74	110.42
13	D	964	GLU	N-CA-C	-6.16	97.68	110.80
17	H	27	ASP	CA-C-O	-6.13	113.92	120.42
19	J	148	ASP	CA-C-N	6.07	125.79	119.05
19	J	148	ASP	C-N-CA	6.07	125.79	119.05
15	f	255	MET	N-CA-C	-5.91	104.92	114.09
15	F	316	GLN	CB-CA-C	5.77	120.20	110.79
12	B	181	GLY	CA-C-O	-5.76	118.17	122.37
27	U	145	PHE	CA-CB-CG	5.75	119.56	113.80
12	B	583	GLU	CB-CA-C	-5.72	101.30	110.79
1	0	8	ARG	CB-CG-CD	-5.70	98.19	111.30
15	F	310	THR	CB-CA-C	5.69	120.24	110.79
15	F	330	ARG	N-CA-C	-5.65	105.12	111.28
15	F	324	ASP	N-CA-C	-5.65	105.22	111.71
15	f	150	PRO	N-CA-C	5.62	117.55	110.70
13	D	1002	ARG	CB-CA-C	5.57	122.07	110.32
12	B	264	GLU	N-CA-C	-5.55	106.18	113.17
33	m	71	LYS	CB-CA-C	5.44	119.82	110.79
14	E	270	ASP	CB-CA-C	5.42	119.14	110.09
16	G	183	ILE	N-CA-C	-5.39	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	105.16	110.62
12	B	491	HIS	CB-CA-C	5.27	119.53	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	L	106	ARG	N-CA-C	-5.22	106.94	113.15
17	H	134	LEU	CB-CA-C	-5.13	110.64	116.54
11	A	1067	GLN	CB-CA-C	5.13	119.30	110.79
17	H	51	GLU	CB-CA-C	-5.04	100.50	109.71
15	F	438	LEU	N-CA-C	5.02	118.48	111.30

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	125	0
2	1	2167	0	2175	39	0
3	2	2567	0	2539	95	0
4	3	2066	0	2097	102	0
5	4	3189	0	3243	141	0
6	5	428	0	434	43	0
7	6	4890	0	4949	93	0
8	7	5751	0	5794	146	0
9	N	64	0	51	8	0
10	Z	139	0	64	4	0
11	A	4580	0	4502	99	0
12	B	7796	0	7751	117	0
13	D	1366	0	1390	73	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	99	0
15	f	3081	0	3012	71	0
16	G	1171	0	1222	15	0
17	H	1633	0	1621	36	0
18	I	959	0	969	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	i	967	0	977	10	0
19	J	720	0	719	12	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	17	0
23	Q	930	0	888	12	0
24	R	2167	0	2193	32	0
25	S	1461	0	1429	39	0
26	T	1788	0	1819	54	0
27	U	1520	0	1520	215	0
28	V	1357	0	1381	90	0
29	X	1304	0	708	44	0
30	Y	1484	0	822	45	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	239	0
35	p	9175	0	9196	178	0
36	q	2059	0	2007	30	0
37	r	1050	0	1033	23	0
38	s	1720	0	1737	22	0
39	t	657	0	684	6	0
40	u	1351	0	1358	133	0
41	v	1186	0	1147	12	0
42	w	927	0	860	23	0
43	x	533	0	553	12	0
44	y	920	0	942	16	0
45	z	372	0	378	9	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
47	7	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	o	1	0	0	0	0
49	p	33	0	0	8	0
All	All	108642	0	107204	2279	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 (2279) 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	1.23	1.65
27:U:139:LEU:HB2	40:u:160:ILE:CG1	1.22	1.58
1:0:41:ARG:CG	27:U:169:PRO:HG2	1.34	1.54
27:U:139:LEU:CB	40:u:160:ILE:HG12	1.41	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	1.46	1.44
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
27:U:141:ALA:CB	40:u:107:PHE:CD1	2.05	1.37
1:0:41:ARG:HG3	27:U:169:PRO:CG	1.56	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	1.95	1.33
13:D:960:GLU:CG	13:D:983:ARG:HG2	1.59	1.30
27:U:139:LEU:HB2	40:u:160:ILE:CD1	1.62	1.30
27:U:138:ASP:OD1	40:u:160:ILE:HD13	1.16	1.29
1:0:85:ARG:HH22	1:0:139:LYS:C	1.40	1.28
4:3:237:GLN:CD	5:4:51:LEU:CD2	2.08	1.27
27:U:142:ASN:ND2	40:u:105:SER:HB2	1.46	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	1.24
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
27:U:139:LEU:CD2	40:u:158:PHE:HD1	1.52	1.20
3:2:175:THR:HG23	8:7:592:ARG:CD	1.72	1.19
7:6:528:LYS:HG2	7:6:531:ILE:HD13	1.21	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
1:0:21:LEU:HD22	1:0:69:ASP:OD2	1.43	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	2.26	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	1.59	1.12
3:2:175:THR:HG23	8:7:592:ARG:HD2	1.17	1.12
4:3:229:TRP:CZ3	5:4:58:ARG:NH1	2.18	1.12
13:D:960:GLU:HG3	13:D:983:ARG:HG2	1.29	1.12
1:0:85:ARG:NH2	1:0:139:LYS:C	2.07	1.12
27:U:152:PHE:CD1	40:u:95:VAL:HB	1.84	1.12
3:2:175:THR:CG2	8:7:592:ARG:HD2	1.81	1.11
27:U:141:ALA:CB	40:u:107:PHE:CE1	2.33	1.11
4:3:237:GLN:CD	5:4:51:LEU:HD22	1.71	1.10
27:U:152:PHE:CZ	40:u:95:VAL:HB	1.85	1.10
27:U:141:ALA:CB	40:u:107:PHE:CG	2.35	1.10
6:5:33:PHE:CE1	6:5:49:LEU:CD1	2.34	1.10
11:A:1200:THR:O	11:A:1204:GLU:HG2	1.52	1.09
1:0:37:LEU:HD11	27:U:173:ALA:HA	1.34	1.09
27:U:139:LEU:HD21	40:u:158:PHE:C	1.77	1.09
27:U:141:ALA:HB3	40:u:107:PHE:CD1	1.87	1.08
4:3:237:GLN:CD	5:4:51:LEU:HD23	1.75	1.07
27:U:139:LEU:HD12	40:u:160:ILE:HG13	1.35	1.07
1:0:83:ASN:OD1	1:0:140:LEU:HD11	1.53	1.07
27:U:138:ASP:O	40:u:107:PHE:CD2	2.07	1.06
13:D:960:GLU:HG2	13:D:983:ARG:HG2	1.29	1.06
1:0:5:GLY:HA3	1:0:10:LYS:HB2	1.37	1.06
27:U:139:LEU:HA	40:u:160:ILE:HG12	1.37	1.05
27:U:139:LEU:HB2	40:u:160:ILE:HG13	1.31	1.04
1:0:84:LYS:HA	1:0:136:ASN:ND2	1.73	1.04
3:2:174:LEU:HD21	3:2:203:ALA:HB1	1.36	1.03
27:U:139:LEU:HD11	40:u:159:ALA:HA	1.39	1.03
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
27:U:141:ALA:HB1	40:u:107:PHE:CE1	1.94	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	2.42	1.02
27:U:141:ALA:HB3	40:u:107:PHE:CG	1.95	1.01
11:A:339:ALA:HB3	11:A:355:VAL:HG21	1.43	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
26:T:238:GLU:HB3	28:V:130:ILE:HG12	1.42	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	0.98
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
27:U:138:ASP:OD1	40:u:160:ILE:CD1	2.12	0.96
13:D:960:GLU:HG2	13:D:983:ARG:CG	1.92	0.96
27:U:139:LEU:CD1	40:u:160:ILE:HG13	1.94	0.96
3:2:174:LEU:HD21	3:2:203:ALA:CB	1.95	0.95
27:U:139:LEU:HB2	40:u:160:ILE:HD11	1.48	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:142:ASN:HD22	40:u:105:SER:HB2	1.14	0.94
1:0:37:LEU:HD13	27:U:173:ALA:CB	1.97	0.94
8:7:726:GLN:HG3	8:7:727:PRO:HD2	1.51	0.93
1:0:41:ARG:CD	27:U:169:PRO:HG2	1.99	0.93
10:Z:6:G2L:N1	30:Y:-5:DC:N3	2.16	0.93
27:U:141:ALA:HB2	40:u:107:PHE:CD1	2.01	0.93
27:U:139:LEU:HG	40:u:159:ALA:C	1.93	0.92
27:U:141:ALA:HB2	40:u:107:PHE:CD2	2.03	0.92
27:U:139:LEU:HD21	40:u:158:PHE:O	1.70	0.92
27:U:139:LEU:HD22	40:u:158:PHE:HD1	1.35	0.92
27:U:141:ALA:HB2	40:u:107:PHE:CG	2.01	0.92
9:N:1:ILX:HG23	34:o:791:GLN:HE22	1.34	0.92
27:U:141:ALA:HB1	40:u:107:PHE:CD1	1.99	0.92
4:3:229:TRP:CE3	5:4:58:ARG:NE	2.38	0.92
1:0:21:LEU:CD2	1:0:69:ASP:OD2	2.18	0.91
5:4:442:VAL:HG21	6:5:44:PHE:HZ	1.35	0.91
16:G:153:LYS:HD3	16:G:153:LYS:H	1.36	0.91
27:U:141:ALA:HB2	40:u:107:PHE:CE1	2.05	0.91
13:D:960:GLU:HG3	13:D:983:ARG:CG	1.97	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	1.33	0.91
27:U:140:GLU:OE2	40:u:158:PHE:HE1	1.53	0.90
34:o:497:ASP:OD2	49:p:1201:W0F:O33	1.89	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:726:GLN:CG	8:7:727:PRO:HD2	2.01	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
1:0:27:GLY:HA3	1:0:70:LYS:HD3	1.51	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
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
26:T:238:GLU:HB3	28:V:130:ILE:CG1	2.02	0.89
4:3:237:GLN:HE21	5:4:51:LEU:HD22	1.38	0.89
27:U:141:ALA:HB2	40:u:107:PHE:CE2	2.07	0.89
13:D:1006:LEU:HD13	21:O:69:ASP:CG	1.97	0.89
7:6:528:LYS:CG	7:6:531:ILE:HD11	2.00	0.88
27:U:141:ALA:HB2	40:u:107:PHE:CZ	2.08	0.88
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
13:D:1006:LEU:CD1	21:O:69:ASP:OD2	2.21	0.88
27:U:140:GLU:OE2	40:u:158:PHE:CE1	2.27	0.88
3:2:174:LEU:O	8:7:591:GLY:HA3	1.74	0.88
27:U:53:LYS:HD2	28:V:166:ILE:HD11	1.56	0.88
5:4:438:LYS:HE2	12:B:621:ALA:CB	2.04	0.87
5:4:442:VAL:HG21	6:5:44:PHE:CZ	2.09	0.87
27:U:145:PHE:CE1	27:U:149:THR:OG1	2.28	0.87
1:0:83:ASN:CG	1:0:140:LEU:CD1	2.47	0.87
27:U:152:PHE:CD1	40:u:95:VAL:CB	2.51	0.87
11:A:475:LEU:HD11	15:f:351:ILE:HD11	1.57	0.87
9:N:3:GLY:HA3	34:o:749:ARG:NH1	1.89	0.86
26:T:238:GLU:CB	28:V:130:ILE:HG12	2.04	0.86
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
3:2:174:LEU:HD11	3:2:203:ALA:HB3	1.57	0.86
7:6:528:LYS:CG	7:6:531:ILE:HD13	1.90	0.86
11:A:511:LEU:H	11:A:511:LEU:HD22	1.37	0.86
29:X:-14:DG:O6	30:Y:14:DC:N4	2.09	0.86
13:D:963:ARG:C	13:D:965:ILE:N	2.25	0.85
13:D:1006:LEU:HD11	21:O:69:ASP:HB3	1.58	0.85
4:3:100:LYS:HG2	5:4:124:GLY:O	1.76	0.84
1:0:37:LEU:CD1	27:U:173:ALA:HA	2.06	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)
29:X:9:DA:H4'	29:X:10:DT:H5'	1.58	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
3:2:175:THR:CG2	8:7:592:ARG:HE	1.92	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
1:0:55:LYS:HB2	40:u:166:ASP:OD2	1.79	0.83
4:3:50:PHE:CE2	5:4:118:LEU:HD11	2.13	0.83
35:p:975:ARG:NH2	49:p:1201:W0F:O32	2.10	0.83
2:1:503:THR:HG1	2:1:533:TYR:HH	1.20	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	0.83
27:U:138:ASP:O	40:u:107:PHE:HD2	1.62	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
26:T:188:PHE:CD2	28:V:80:LYS:HB2	2.14	0.82
11:A:821:ARG:CZ	11:A:821:ARG:HA	2.10	0.82
7:6:266:GLN:N	7:6:266:GLN:HE21	1.79	0.81
1:0:85:ARG:NH2	1:0:140:LEU:N	2.26	0.81
15:F:324:ASP:HA	15:F:327:TRP:HB3	1.63	0.81
27:U:139:LEU:CG	40:u:160:ILE:HG13	2.10	0.81
7:6:449:LYS:HD3	29:X:33:DG:OP1	1.81	0.81
13:D:960:GLU:HB3	13:D:983:ARG:HG3	1.63	0.81
15:f:447:ALA:HA	15:f:456:GLY:HA3	1.61	0.81
1:0:8:ARG:HD2	27:U:173:ALA:H	1.44	0.81
5:4:438:LYS:CE	12:B:621:ALA:H	1.94	0.80
14:E:327:ASN:HD22	14:E:327:ASN:H	1.30	0.80
27:U:139:LEU:HD23	40:u:158:PHE:HD1	1.44	0.80
33:m:77:ARG:HH11	33:m:77:ARG:HG2	1.45	0.80
13:D:1006:LEU:CD1	21:O:69:ASP:CG	2.55	0.80
1:0:8:ARG:NE	1:0:9:CYS:SG	2.54	0.80
30:Y:-1:DA:H2"	30:Y:0:DT:H5'	1.62	0.80
5:4:334:MET:SD	7:6:56:TYR:CD2	2.75	0.80
4:3:16:ASP:HA	4:3:62:SER:OG	1.82	0.79
27:U:56:ARG:NH1	27:U:60:ARG:NH1	2.30	0.79
1:0:42:GLY:N	27:U:168:MET:CE	2.44	0.79
1:0:83:ASN:OD1	1:0:140:LEU:CD1	2.31	0.79
2:1:430:THR:OG1	4:3:222:SER:OG	2.00	0.79
6:5:33:PHE:CZ	6:5:49:LEU:HD12	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:138:ASP:OD1	40:u:160:ILE:HG21	1.82	0.79
15:F:273:GLN:NE2	15:F:273:GLN:H	1.81	0.79
22:P:188:ARG:NH2	23:Q:321:SER:OG	2.16	0.79
27:U:139:LEU:CD1	40:u:159:ALA:HA	2.13	0.79
1:0:83:ASN:CG	1:0:140:LEU:HD11	2.07	0.79
14:E:774:MET:HE2	14:E:774:MET:H	1.46	0.79
3:2:174:LEU:CD2	3:2:203:ALA:CB	2.57	0.78
4:3:237:GLN:CG	5:4:51:LEU:CD2	2.60	0.78
27:U:139:LEU:CA	40:u:160:ILE:CG1	2.41	0.78
30:Y:28:DT:H2'	30:Y:29:DA:C8	2.19	0.78
33:m:31:LEU:HD23	33:m:31:LEU:H	1.47	0.78
14:e:747:LEU:HD23	14:e:747:LEU:H	1.47	0.78
27:U:139:LEU:HD22	40:u:158:PHE:CD1	2.16	0.78
27:U:151:THR:HG23	27:U:153:ARG:HD3	1.65	0.78
15:F:274:ASN:ND2	15:F:316:GLN:HA	1.99	0.78
26:T:192:GLU:HG3	28:V:75:PHE:HB3	1.65	0.78
5:4:393:LEU:HD21	7:6:511:TRP:CZ3	2.19	0.78
34:o:1242:ASP:HA	34:o:1262:MET:HB2	1.65	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
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
1:0:37:LEU:HD11	27:U:173:ALA:CA	2.14	0.77
1:0:85:ARG:HH22	1:0:140:LEU:CA	1.98	0.76
13:D:963:ARG:C	13:D:982:LEU:HD11	2.10	0.76
3:2:69:ARG:HD3	3:2:140:HIS:CD2	2.20	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	0.76
27:U:152:PHE:CD2	40:u:95:VAL:HG11	2.20	0.76
34:o:111:CYS:SG	34:o:188:GLN:NE2	2.59	0.75
15:F:429:LYS:O	15:F:433:PRO:HD2	1.85	0.75
11:A:467:ILE:H	15:F:221:GLN:HE21	1.33	0.75
1:0:42:GLY:H	27:U:168:MET:HE1	1.49	0.75
27:U:141:ALA:HB1	40:u:98:PHE:HE1	1.51	0.75
6:5:33:PHE:HE1	6:5:49:LEU:HD12	0.84	0.75
1:0:41:ARG:HB2	27:U:168:MET:SD	2.26	0.74
8:7:711:ASP:OD1	8:7:715:GLN:NE2	2.20	0.74
1:0:84:LYS:CA	1:0:136:ASN:ND2	2.49	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:47:SER:HA	5:4:122:LEU:HD11	1.68	0.74
27:U:48:MET:HE2	27:U:52:LEU:HB2	1.69	0.74
27:U:138:ASP:O	40:u:107:PHE:CE2	2.41	0.74
26:T:188:PHE:HE2	28:V:80:LYS:HG3	1.52	0.74
1:0:8:ARG:NH2	1:0:34:CYS:SG	2.61	0.74
11:A:970:ASN:OD1	11:A:970:ASN:N	2.21	0.74
9:N:3:GLY:HA3	34:o:749:ARG:HH12	1.50	0.74
27:U:152:PHE:CD1	40:u:95:VAL:CG2	2.70	0.74
5:4:438:LYS:HE2	12:B:621:ALA:HB3	1.70	0.74
27:U:147:PRO:HA	40:u:91:GLN:CD	2.13	0.73
34:o:585:LEU:HD22	41:v:47:ILE:HD11	1.70	0.73
6:5:31:LYS:HB3	12:B:540:LYS:CE	2.17	0.73
11:A:639:LEU:HD11	11:A:774:ARG:HG2	1.70	0.73
1:0:41:ARG:C	27:U:168:MET:HE1	2.13	0.73
11:A:488:ALA:HB1	15:f:271:VAL:HG23	1.70	0.73
15:F:359:PHE:HB3	15:F:380:LEU:HG	1.68	0.73
40:u:142:GLU:HB2	40:u:170:LEU:HD22	1.70	0.73
34:o:1307:VAL:HG13	34:o:1338:THR:HG22	1.71	0.73
8:7:231:VAL:HG13	8:7:454:VAL:HG23	1.70	0.73
9:N:8:HYP:HD23	34:o:1108:HIS:CE1	2.23	0.73
7:6:371:VAL:HG23	7:6:407:ILE:HG22	1.69	0.73
6:5:31:LYS:CG	12:B:540:LYS:HZ3	2.01	0.73
27:U:152:PHE:CZ	40:u:95:VAL:CB	2.62	0.73
4:3:237:GLN:OE1	5:4:54:ASN:OD1	2.07	0.73
34:o:922:PHE:H	34:o:1052:ARG:HD2	1.54	0.73
4:3:50:PHE:CD2	5:4:122:LEU:HD12	2.24	0.72
6:5:34:ILE:O	12:B:539:ARG:NH2	2.22	0.72
15:F:418:ILE:H	15:F:418:ILE:HD12	1.54	0.72
36:q:2:PRO:HB3	44:y:54:PRO:HD2	1.69	0.72
35:p:69:ALA:HB3	35:p:81:PRO:HB3	1.70	0.72
36:q:190:ASN:ND2	36:q:195:THR:O	2.22	0.72
1:0:23:VAL:HG21	1:0:73:GLU:HG3	1.71	0.72
28:V:131:GLU:HG3	28:V:140:LYS:HA	1.71	0.72
1:0:10:LYS:HZ2	27:U:178:ALA:HB1	1.55	0.72
25:S:64:GLU:O	25:S:81:ARG:NH2	2.20	0.72
5:4:120:ILE:HG23	5:4:125:GLY:HA2	1.72	0.72
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
11:A:353:LEU:HD21	15:f:272:VAL:HG21	1.72	0.71
34:o:46:THR:HG22	34:o:57:LEU:HB2	1.71	0.71
2:1:195:SER:O	2:1:199:THR:OG1	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:r:25:GLU:HG3	40:u:41:LYS:HE2	1.72	0.71
5:4:29:GLY:O	5:4:33:ARG:NE	2.24	0.71
35:p:625:LEU:HD13	35:p:675:LEU:HD21	1.71	0.71
40:u:92:VAL:HB	40:u:126:PRO:HB2	1.72	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
36:q:259:LEU:HD22	44:y:19:ILE:HD11	1.73	0.71
4:3:272:LEU:O	4:3:272:LEU:HD23	1.90	0.70
6:5:31:LYS:HB2	12:B:540:LYS:NZ	2.06	0.70
36:q:67:ARG:NH2	43:x:3:ILE:O	2.24	0.70
1:0:8:ARG:HH22	1:0:37:LEU:CB	2.04	0.70
1:0:120:LYS:O	1:0:124:ILE:HD12	1.91	0.70
12:B:241:PRO:HG2	12:B:496:MET:HE1	1.72	0.70
27:U:139:LEU:CB	40:u:160:ILE:HG13	1.94	0.70
13:D:960:GLU:HG2	13:D:983:ARG:CD	2.22	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
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
35:p:761:THR:H	35:p:764:MET:HE3	1.54	0.70
4:3:237:GLN:HG3	5:4:51:LEU:CD2	2.21	0.70
34:o:877:ALA:HB3	34:o:890:ARG:HH11	1.56	0.70
7:6:528:LYS:HE2	7:6:531:ILE:CD1	2.22	0.70
8:7:571:THR:OG1	8:7:576:GLU:OE1	2.08	0.70
9:N:1:ILX:HG23	34:o:791:GLN:NE2	2.04	0.70
28:V:197:LYS:HG3	28:V:198:LYS:HG3	1.72	0.70
24:R:72:ASN:HB2	24:R:75:LEU:HG	1.73	0.70
24:R:102:GLN:HE21	34:o:305:GLU:HG2	1.57	0.70
27:U:75:ARG:H	27:U:91:TYR:HB2	1.55	0.70
28:V:234:GLU:OE1	28:V:238:LYS:NZ	2.25	0.70
3:2:206:ARG:HB3	8:7:589:GLU:O	1.91	0.69
4:3:160:ARG:NH2	4:3:234:ASP:OD1	2.23	0.69
7:6:191:ASP:O	7:6:195:ARG:NH1	2.25	0.69
8:7:252:THR:HG22	8:7:432:ILE:HG22	1.74	0.69
29:X:-14:DG:C6	30:Y:14:DC:N4	2.60	0.69
2:1:468:VAL:HG21	2:1:525:ILE:HD11	1.74	0.69
16:G:129:LYS:O	16:G:129:LYS:NZ	2.23	0.69
27:U:36:ILE:HD11	28:V:163:LEU:HD22	1.74	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
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
27:U:152:PHE:CE2	40:u:95:VAL:CG1	2.76	0.69
35:p:827:GLU:HG2	35:p:871:VAL:HG22	1.75	0.69
4:3:242:ILE:HD11	5:4:75:VAL:C	2.17	0.68
12:B:490:SER:HA	12:B:493:TRP:HB2	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
7:6:56:TYR:C	7:6:58:ALA:H	2.01	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:139:LEU:CG	40:u:160:ILE:CG1	2.66	0.68
32:k:191:VAL:HG13	32:k:200:ILE:HD13	1.74	0.68
3:2:75:ASP:OD2	8:7:722:ARG:NH2	2.26	0.68
23:Q:346:LYS:NZ	30:Y:29:DA:OP1	2.27	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
15:F:83:LEU:CD1	15:F:83:LEU:H	2.06	0.68
34:o:1148:ALA:HB1	34:o:1333:GLU:HB2	1.75	0.68
13:D:998:GLN:NE2	26:T:186:MET:HA	2.08	0.68
34:o:560:VAL:HG22	34:o:591:ILE:HD11	1.75	0.68
35:p:193:VAL:HG21	35:p:470:LEU:HD13	1.74	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
35:p:910:THR:HG22	45:z:43:ILE:HA	1.75	0.68
14:e:645:GLY:H	14:e:675:LEU:HD11	1.59	0.68
35:p:407:MET:HE1	35:p:444:LEU:HG	1.75	0.68
35:p:866:ILE:HG22	35:p:867:ILE:HG13	1.76	0.68
35:p:975:ARG:NE	49:p:1201:W0F:O32	2.27	0.68
38:s:192:LYS:HE3	38:s:194:ILE:HD11	1.74	0.68
6:5:38:ILE:HG21	6:5:42:HIS:HB2	1.76	0.67
27:U:138:ASP:OD2	40:u:160:ILE:HG21	1.92	0.67
34:o:877:ALA:HB3	34:o:890:ARG:NH1	2.10	0.67
3:2:174:LEU:CD1	3:2:203:ALA:HB3	2.17	0.67
3:2:175:THR:HG23	8:7:592:ARG:HE	1.56	0.67
14:E:426:ARG:HH11	14:E:640:ASN:HD22	1.42	0.67
24:R:23:LEU:HD12	24:R:32:MET:HE2	1.76	0.67
1:0:37:LEU:CD1	27:U:173:ALA:CA	2.71	0.67
34:o:706:ILE:HD13	34:o:824:GLU:HG3	1.76	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
1:0:10:LYS:NZ	27:U:178:ALA:CB	2.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:88:LEU:CD2	3:2:131:LEU:HD21	2.24	0.67
4:3:46:ASN:OD1	5:4:123:LEU:CD2	2.42	0.67
14:E:365:ARG:HD3	14:E:757:GLY:CA	2.24	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:48:MET:HA	27:U:48:MET:HE3	1.75	0.67
27:U:152:PHE:CD1	40:u:95:VAL:HG21	2.30	0.67
30:Y:-19:DT:H1'	30:Y:-18:DC:H5'	1.76	0.67
1:0:85:ARG:NH1	1:0:140:LEU:CG	2.45	0.67
3:2:75:ASP:OD1	8:7:722:ARG:NH2	2.28	0.67
5:4:409:TYR:HB2	5:4:412:PHE:CZ	2.30	0.67
15:f:239:ARG:HD3	15:f:284:ARG:HH11	1.60	0.67
5:4:60:LEU:HD13	5:4:118:LEU:HD23	1.76	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
13:D:1002:ARG:HB2	26:T:182:HIS:CD2	2.30	0.66
27:U:141:ALA:HB1	40:u:98:PHE:CE1	2.30	0.66
28:V:141:PRO:HB2	28:V:144:ASN:HB3	1.76	0.66
28:V:227:SER:HB3	28:V:230:GLU:HB2	1.77	0.66
30:Y:-6:DC:O2	49:p:1201:W0F:N19	2.28	0.66
34:o:1286:ARG:HH21	42:w:53:ILE:HG22	1.60	0.66
4:3:237:GLN:OE1	5:4:51:LEU:HD23	1.94	0.66
13:D:1006:LEU:HD11	21:O:69:ASP:CB	2.25	0.66
2:1:432:THR:O	2:1:435:SER:OG	2.10	0.66
21:O:51:ARG:NH2	23:Q:20:ASP:OD2	2.28	0.66
37:r:77:ARG:HA	37:r:80:ILE:HD12	1.78	0.66
5:4:438:LYS:HE3	12:B:621:ALA:N	2.10	0.66
33:m:79:GLY:HA2	20:l:141:LYS:HE2	1.76	0.66
35:p:269:ILE:HD11	35:p:369:VAL:HG21	1.76	0.66
1:0:106:VAL:O	1:0:110:THR:HG23	1.95	0.66
4:3:229:TRP:CE3	5:4:58:ARG:HD2	2.31	0.66
34:o:733:LEU:HB3	42:w:106:ASP:HB2	1.78	0.66
19:j:123:LEU:C	19:j:125:ASP:H	2.03	0.66
4:3:229:TRP:CE3	5:4:58:ARG:CD	2.78	0.66
26:T:237:PRO:HB3	28:V:83:ASN:HD21	1.60	0.66
34:o:98:GLY:HA3	34:o:1440:MET:HE2	1.76	0.66
3:2:137:MET:SD	3:2:139:CYS:N	2.67	0.66
25:S:76:ARG:HH21	25:S:80:ARG:HD3	1.60	0.66
11:A:339:ALA:CB	11:A:355:VAL:HG21	2.22	0.65
35:p:365:LEU:O	35:p:369:VAL:HG23	1.96	0.65
40:u:92:VAL:HG13	40:u:128:TYR:CE2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:175:THR:HG22	8:7:592:ARG:CD	2.27	0.65
13:D:960:GLU:CB	13:D:983:ARG:HG3	2.26	0.65
30:Y:-5:DC:H2'	30:Y:-4:DT:C6	2.31	0.65
34:o:1146:GLN:HG2	34:o:1149:ARG:HH12	1.61	0.65
8:7:238:ASN:ND2	8:7:662:GLN:OE1	2.29	0.65
22:P:206:GLU:OE1	22:P:236:LYS:NZ	2.30	0.65
3:2:174:LEU:O	8:7:591:GLY:CA	2.43	0.65
11:A:821:ARG:HA	11:A:821:ARG:NH1	2.11	0.65
13:D:1006:LEU:CD1	21:O:69:ASP:CB	2.74	0.65
7:6:701:LEU:O	7:6:704:SER:OG	2.14	0.65
1:0:8:ARG:NE	27:U:173:ALA:HB2	2.10	0.65
4:3:229:TRP:HZ3	5:4:58:ARG:HH11	1.44	0.65
4:3:98:ASP:O	5:4:125:GLY:HA3	1.96	0.65
5:4:172:SER:OG	5:4:174:ASP:OD1	2.15	0.65
27:U:72:ILE:HG22	27:U:94:ILE:HA	1.78	0.65
3:2:174:LEU:HG	3:2:203:ALA:CB	2.27	0.65
37:r:103:LEU:HD13	37:r:114:LEU:HD13	1.76	0.65
6:5:38:ILE:CG2	6:5:42:HIS:HB2	2.27	0.65
27:U:139:LEU:HD12	40:u:149:GLY:O	1.98	0.64
28:V:144:ASN:HA	28:V:173:GLU:HB2	1.78	0.64
33:m:77:ARG:HH11	33:m:77:ARG:CG	2.10	0.64
34:o:890:ARG:HE	34:o:1023:VAL:HG22	1.63	0.64
15:F:83:LEU:HD12	15:F:83:LEU:N	2.12	0.64
36:q:42:VAL:HB	36:q:178:PRO:HG3	1.79	0.64
35:p:896:LEU:HD21	35:p:900:GLU:HB3	1.79	0.64
36:q:183:ALA:HB3	36:q:232:ASN:HB3	1.79	0.64
4:3:168:GLU:N	4:3:168:GLU:OE1	2.31	0.64
11:A:1168:TYR:HB2	16:G:180:ARG:HB3	1.78	0.64
26:T:188:PHE:CE2	28:V:80:LYS:HG3	2.31	0.64
27:U:145:PHE:HD1	27:U:149:THR:OG1	1.76	0.64
15:f:320:ARG:NH1	15:f:320:ARG:HB3	2.12	0.64
1:0:41:ARG:HG3	27:U:169:PRO:HG2	0.68	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:111:ARG:HD3	27:U:188:TYR:OH	1.97	0.64
4:3:229:TRP:HE3	5:4:58:ARG:NE	1.91	0.64
37:r:114:LEU:HD22	40:u:84:VAL:HG11	1.80	0.64
5:4:335:LEU:O	7:6:58:ALA:HA	1.98	0.64
34:o:11:SER:N	35:p:1135:TYR:HH	1.96	0.64
19:j:123:LEU:O	19:j:125:ASP:N	2.30	0.64
8:7:513:ASP:OD1	8:7:516:VAL:N	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:76:MET:HE3	27:U:88:ARG:HD2	1.80	0.64
3:2:377:ASP:O	3:2:380:HIS:NE2	2.30	0.64
7:6:517:GLU:O	7:6:521:GLU:OE1	2.16	0.64
14:E:522:ASP:HB2	14:E:526:ARG:HG2	1.80	0.64
27:U:139:LEU:CB	40:u:160:ILE:CD1	2.52	0.64
36:q:154:ARG:HD3	43:x:64:PRO:HD3	1.80	0.64
5:4:55:TRP:CZ2	5:4:83:GLN:NE2	2.66	0.63
6:5:31:LYS:HB2	12:B:540:LYS:HZ1	1.59	0.63
13:D:960:GLU:CB	13:D:983:ARG:CG	2.76	0.63
28:V:158:HIS:O	28:V:162:GLY:N	2.28	0.63
1:0:41:ARG:CB	27:U:169:PRO:HG2	2.24	0.63
8:7:726:GLN:HG2	8:7:727:PRO:HD2	1.80	0.63
35:p:851:ASP:HB3	45:z:15:MET:HE1	1.81	0.63
3:2:242:SER:O	3:2:245:SER:OG	2.17	0.63
7:6:266:GLN:HG2	7:6:267:THR:HG23	1.81	0.63
3:2:175:THR:HG21	8:7:592:ARG:NE	2.13	0.63
13:D:966:LEU:O	13:D:966:LEU:HD22	1.99	0.63
38:s:13:ILE:HD11	38:s:132:GLN:HG3	1.80	0.63
3:2:75:ASP:CG	8:7:722:ARG:NH2	2.57	0.63
3:2:175:THR:HG21	8:7:592:ARG:HE	1.63	0.63
7:6:528:LYS:NZ	29:X:36:DT:H5”	2.13	0.63
14:e:277:ASP:OD1	14:e:277:ASP:N	2.32	0.63
4:3:16:ASP:OD1	4:3:131:THR:OG1	2.16	0.63
27:U:139:LEU:N	40:u:160:ILE:HG12	2.12	0.63
27:U:152:PHE:CG	40:u:95:VAL:HG11	2.34	0.63
28:V:78:LEU:HD21	28:V:124:LEU:HD22	1.79	0.63
1:0:27:GLY:CA	1:0:70:LYS:HD3	2.26	0.63
7:6:528:LYS:HG2	7:6:528:LYS:O	1.97	0.63
29:X:31:DG:H2”	29:X:32:DT:C5	2.34	0.63
3:2:109:THR:OG1	3:2:148:SER:OG	2.06	0.63
17:H:50:PHE:HD1	19:J:193:TYR:O	1.82	0.63
3:2:87:LEU:HD22	3:2:232:LEU:HD12	1.81	0.62
4:3:240:GLN:HE21	5:4:51:LEU:HD21	1.61	0.62
1:0:71:GLU:OE2	8:7:335:ARG:NH1	2.32	0.62
1:0:83:ASN:ND2	1:0:140:LEU:HD12	2.14	0.62
4:3:229:TRP:HE3	5:4:58:ARG:CD	2.12	0.62
11:A:342:ARG:HG2	11:A:342:ARG:O	1.99	0.62
12:B:361:ARG:HD2	12:B:367:GLU:HB2	1.80	0.62
12:B:583:GLU:CD	12:B:583:GLU:H	2.06	0.62
7:6:128:SER:OG	7:6:163:TYR:OH	2.17	0.62
15:F:92:ILE:HG13	15:F:93:PRO:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:138:ASP:CG	40:u:160:ILE:CG2	2.62	0.62
37:r:23:PRO:HG2	37:r:26:PHE:HB2	1.79	0.62
3:2:112:LYS:O	3:2:147:ASN:ND2	2.32	0.62
27:U:152:PHE:CZ	40:u:95:VAL:CG1	2.82	0.62
27:U:152:PHE:CE2	40:u:95:VAL:HG12	2.35	0.62
1:0:41:ARG:HG3	27:U:169:PRO:CD	2.27	0.62
22:P:208:ARG:NH2	23:Q:346:LYS:O	2.32	0.62
27:U:100:VAL:O	27:U:104:LYS:HG2	1.99	0.62
34:o:577:PRO:HG2	34:o:580:LEU:HD23	1.82	0.62
13:D:960:GLU:CG	13:D:983:ARG:HG3	2.25	0.62
34:o:784:VAL:HG22	35:p:978:ILE:HD11	1.80	0.62
3:2:223:LEU:HD13	8:7:726:GLN:OE1	1.99	0.62
8:7:343:ARG:O	8:7:346:VAL:HG12	1.99	0.62
15:F:335:ARG:NE	15:F:382:GLU:OE1	2.33	0.62
8:7:2:LYS:HB3	8:7:9:LEU:HD11	1.81	0.62
27:U:139:LEU:CB	40:u:160:ILE:HD11	2.23	0.62
35:p:975:ARG:HH21	49:p:1201:W0F:P30	2.23	0.62
35:p:553:LEU:HA	35:p:556:ILE:HD12	1.81	0.62
13:d:884:GLU:HA	13:d:887:LYS:HE3	1.82	0.62
7:6:371:VAL:HG23	7:6:407:ILE:CG2	2.30	0.61
27:U:147:PRO:HA	40:u:91:GLN:NE2	2.14	0.61
35:p:153:PRO:HB3	35:p:187:ILE:HD11	1.81	0.61
36:q:19:VAL:HG23	36:q:241:PRO:HB2	1.82	0.61
34:o:769:MET:HE1	35:p:970:HIS:HA	1.81	0.61
34:o:1208:SER:HA	34:o:1266:GLU:HG3	1.82	0.61
25:S:70:GLU:HA	25:S:74:LYS:HB2	1.82	0.61
27:U:136:PHE:O	27:U:137:THR:OG1	2.13	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
15:F:114:LEU:HB2	17:H:52:SER:H	1.66	0.61
29:X:31:DG:H2"	29:X:32:DT:C6	2.36	0.61
3:2:206:ARG:HG2	8:7:589:GLU:HA	1.81	0.61
4:3:53:ARG:HG2	5:4:46:ARG:NH2	2.15	0.61
7:6:473:GLU:OE1	7:6:473:GLU:N	2.33	0.61
5:4:401:LEU:HD13	6:5:10:ILE:HD13	1.81	0.61
8:7:609:ASP:OD1	8:7:669:ARG:NH2	2.34	0.61
13:D:1002:ARG:HE	26:T:182:HIS:CD2	2.19	0.61
34:o:689:ILE:HD12	35:p:985:LEU:HD22	1.81	0.61
35:p:404:PHE:HA	35:p:407:MET:HE2	1.83	0.61
12:B:203:LYS:HD3	12:B:237:MET:HE3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:613:ALA:HB2	14:E:620:LEU:HD11	1.81	0.61
34:o:863:ARG:HH21	34:o:1415:THR:HG22	1.64	0.61
35:p:267:VAL:HG13	35:p:320:PHE:HE2	1.65	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
26:T:238:GLU:CG	28:V:130:ILE:HG12	2.30	0.61
28:V:171:ILE:HD13	28:V:177:ASN:HB3	1.83	0.61
40:u:93:ASN:O	40:u:128:TYR:OH	2.10	0.61
7:6:528:LYS:HZ3	29:X:36:DT:H5"	1.66	0.60
13:D:996:LEU:O	13:D:1000:ARG:HG3	2.01	0.60
31:c:18:CYS:O	31:c:23:TRP:HB2	2.00	0.60
33:m:75:ILE:HD11	19:j:176:MET:HE1	1.82	0.60
34:o:581:LYS:HG2	34:o:582:PRO:HA	1.81	0.60
8:7:461:LEU:HD23	8:7:464:LEU:CD2	2.31	0.60
28:V:121:THR:O	28:V:125:VAL:HG23	2.01	0.60
34:o:203:LYS:HG2	34:o:212:LYS:HE3	1.83	0.60
42:w:69:ILE:HG22	42:w:71:ASP:H	1.65	0.60
1:0:10:LYS:HZ3	27:U:178:ALA:HB1	1.66	0.60
27:U:25:PHE:O	28:V:217:GLN:NE2	2.33	0.60
44:y:12:LEU:HD11	44:y:18:LYS:HE2	1.83	0.60
5:4:18:ASN:OD1	5:4:19:LEU:N	2.35	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
8:7:628:THR:O	8:7:628:THR:HG22	2.02	0.60
14:E:754:THR:O	14:E:755:ALA:HB3	2.01	0.60
28:V:77:VAL:O	28:V:81:ILE:HG12	2.01	0.60
28:V:174:ALA:HB1	28:V:180:LYS:HZ1	1.67	0.60
29:X:7:DT:H3	30:Y:-7:DA:H2	1.50	0.60
31:c:99:PHE:HB2	31:c:100:PRO:HD3	1.83	0.60
35:p:834:ARG:HA	35:p:840:MET:HG3	1.84	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
1:0:55:LYS:HB2	40:u:166:ASP:CG	2.25	0.60
12:B:27:LYS:HE3	12:B:490:SER:HB3	1.84	0.60
34:o:433:PRO:HG2	34:o:438:LEU:HD21	1.84	0.60
37:r:16:ASP:H	37:r:21:ILE:HB	1.66	0.60
1:0:55:LYS:HE2	40:u:166:ASP:OD2	2.02	0.60
33:m:31:LEU:HD23	33:m:31:LEU:N	2.16	0.60
35:p:1120:ASN:HB2	35:p:1145:GLN:HB3	1.84	0.60
2:1:422:LEU:HD22	4:3:225:GLN:HE22	1.66	0.60
15:F:90:GLU:H	15:F:90:GLU:CD	2.08	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:150:GLY:HA2	40:u:93:ASN:OD1	2.01	0.60
5:4:438:LYS:HE2	12:B:621:ALA:HB2	1.82	0.59
3:2:174:LEU:HG	3:2:203:ALA:HB1	1.83	0.59
3:2:175:THR:HG22	8:7:592:ARG:HD2	1.80	0.59
7:6:707:GLU:O	7:6:711:GLN:OE1	2.20	0.59
30:Y:-13:DT:H2"	30:Y:-12:DA:C8	2.37	0.59
34:o:938:LEU:HD22	34:o:1005:HIS:HD1	1.67	0.59
34:o:1262:MET:HE2	34:o:1264:SER:HB3	1.83	0.59
11:A:475:LEU:HD13	15:f:349:ASN:OD1	2.02	0.59
38:s:82:VAL:HG23	38:s:106:VAL:HG13	1.84	0.59
4:3:242:ILE:HD13	5:4:74:TRP:C	2.27	0.59
34:o:26:LEU:HD13	34:o:31:LEU:HD21	1.84	0.59
35:p:222:ARG:HB3	35:p:234:THR:HG22	1.83	0.59
1:0:83:ASN:HD21	1:0:140:LEU:HD13	1.66	0.59
36:q:56:SER:HB2	36:q:158:GLU:H	1.67	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
33:m:88:PHE:C	33:m:88:PHE:CD1	2.81	0.59
6:5:48:GLU:HG3	6:5:49:LEU:HG	1.84	0.59
27:U:15:LYS:NZ	27:U:94:ILE:O	2.31	0.59
2:1:130:ASP:OD2	2:1:463:HIS:NE2	2.33	0.59
7:6:266:GLN:N	7:6:266:GLN:NE2	2.49	0.59
7:6:528:LYS:HE2	7:6:531:ILE:HD13	1.84	0.59
8:7:372:LEU:HD11	8:7:404:ALA:HB1	1.84	0.59
11:A:1193:ALA:HB3	16:G:166:VAL:HG21	1.83	0.59
34:o:1173:THR:HG22	34:o:1214:VAL:HG22	1.85	0.59
40:u:108:ILE:HG21	40:u:163:LEU:HG	1.84	0.59
38:s:171:PRO:HB2	38:s:207:ARG:HD3	1.84	0.59
15:f:349:ASN:HB3	15:f:351:ILE:HG13	1.84	0.59
3:2:88:LEU:HD22	3:2:131:LEU:HD21	1.83	0.59
4:3:195:VAL:HG12	4:3:203:LEU:HD23	1.85	0.59
5:4:401:LEU:HG	6:5:53:LEU:HD23	1.85	0.59
8:7:262:ASN:O	8:7:266:LEU:HD23	2.03	0.59
15:F:312:ILE:HG13	15:F:334:ALA:CB	2.33	0.59
35:p:627:ILE:HD11	35:p:663:GLU:HB2	1.85	0.59
1:0:84:LYS:HA	1:0:136:ASN:CG	2.28	0.58
2:1:417:LYS:HA	2:1:421:VAL:HG23	1.84	0.58
8:7:405:THR:O	8:7:409:THR:OG1	2.16	0.58
15:f:330:ARG:HH22	15:f:371:THR:HB	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:98:ASP:HB2	4:3:100:LYS:HE3	1.84	0.58
11:A:470:ILE:O	11:A:470:ILE:HG22	2.02	0.58
1:0:35:VAL:HG13	1:0:58:PHE:CE2	2.39	0.58
3:2:69:ARG:CD	8:7:563:ARG:HH21	2.15	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:20:DG:H2"	29:X:21:DC:C6	2.39	0.58
2:1:471:LEU:HD12	2:1:472:LEU:HD22	1.84	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	1.86	0.58
25:S:58:GLN:C	25:S:60:GLU:H	2.10	0.58
31:c:12:VAL:HG23	15:f:118:ILE:HA	1.86	0.58
35:p:826:GLU:H	35:p:872:THR:HG22	1.67	0.58
27:U:36:ILE:HG21	27:U:48:MET:HE1	1.84	0.58
40:u:152:VAL:HB	40:u:157:ILE:HG12	1.85	0.58
11:A:929:THR:HG22	11:A:954:ALA:HA	1.86	0.58
15:F:207:ARG:HD2	15:F:207:ARG:N	2.18	0.58
22:P:299:ARG:NH2	29:X:-27:DA:OP1	2.37	0.58
35:p:55:VAL:HG12	35:p:91:ILE:HD13	1.85	0.58
7:6:56:TYR:C	7:6:58:ALA:N	2.61	0.58
27:U:70:LYS:HE2	28:V:226:ASP:HA	1.86	0.58
27:U:145:PHE:HB2	27:U:153:ARG:HG2	1.85	0.58
33:m:67:GLU:HA	33:m:67:GLU:OE1	2.02	0.58
34:o:1158:LEU:HD11	34:o:1309:MET:HB2	1.86	0.58
1:0:8:ARG:O	27:U:178:ALA:HB2	2.04	0.58
28:V:163:LEU:HG	28:V:201:LEU:HD21	1.85	0.58
34:o:1230:GLN:HG2	34:o:1234:LYS:HE3	1.85	0.58
14:e:513:LEU:HD21	14:e:527:ILE:HG23	1.86	0.58
3:2:345:CYS:O	3:2:349:GLN:N	2.36	0.58
11:A:340:GLU:N	11:A:497:PRO:HG2	2.19	0.58
24:R:103:ASN:HB3	30:Y:12:DC:H5'	1.84	0.58
29:X:8:DC:H2"	29:X:9:DA:H2'	1.84	0.58
31:c:21:LEU:HD12	31:c:21:LEU:C	2.29	0.58
13:d:967:MET:HA	13:d:967:MET:HE2	1.85	0.58
4:3:52:ASN:OD1	4:3:53:ARG:N	2.37	0.57
4:3:241:LEU:HD23	4:3:243:LEU:HD11	1.86	0.57
7:6:528:LYS:CG	7:6:531:ILE:HD12	2.29	0.57
11:A:1063:LYS:HD3	11:A:1063:LYS:C	2.29	0.57
14:E:522:ASP:O	14:E:524:LEU:N	2.37	0.57
34:o:756:ALA:HB2	34:o:786:ALA:HB2	1.86	0.57
34:o:1147:SER:HA	34:o:1153:ARG:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:p:22:TRP:CE2	35:p:679:PRO:HG3	2.39	0.57
21:O:29:THR:HG23	21:O:32:LEU:H	1.70	0.57
14:e:484:LEU:HD21	14:e:504:LEU:HD21	1.86	0.57
1:0:1:MET:SD	8:7:345:ARG:HD3	2.45	0.57
34:o:555:LEU:HD13	34:o:591:ILE:HD12	1.86	0.57
4:3:215:LEU:HD22	4:3:230:VAL:HG21	1.87	0.57
14:E:586:TYR:HB3	14:E:605:HIS:HB3	1.85	0.57
29:X:8:DC:H2"	29:X:9:DA:C8	2.40	0.57
11:A:334:THR:HA	11:A:489:GLN:O	2.04	0.57
25:S:71:PHE:CE2	26:T:194:HIS:HB3	2.39	0.57
34:o:347:GLU:HA	34:o:352:GLY:HA3	1.87	0.57
1:0:8:ARG:NH2	1:0:37:LEU:HB3	2.12	0.57
8:7:252:THR:HG1	8:7:255:THR:HG1	1.51	0.57
15:F:315:ARG:CZ	15:F:369:PRO:HB3	2.35	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
12:B:629:ARG:NH1	12:B:658:ASP:OD2	2.37	0.57
15:F:81:GLU:HB3	15:F:83:LEU:HD13	1.85	0.57
25:S:115:LYS:NZ	25:S:117:GLY:O	2.34	0.57
1:0:84:LYS:CB	1:0:136:ASN:ND2	2.68	0.57
12:B:837:LEU:HD22	17:H:213:LEU:HD22	1.86	0.57
25:S:73:ARG:CZ	25:S:76:ARG:HD2	2.34	0.57
34:o:760:LEU:HD11	34:o:781:ILE:HG21	1.85	0.57
43:x:3:ILE:HD12	43:x:4:PRO:HD2	1.87	0.57
1:0:41:ARG:CD	27:U:169:PRO:CG	2.74	0.57
7:6:625:GLN:OE1	7:6:639:ARG:NH1	2.36	0.57
8:7:240:ASP:OD1	8:7:241:ASN:N	2.37	0.57
21:O:62:LEU:HA	21:O:76:LEU:HD23	1.86	0.57
14:e:257:GLU:CD	14:e:257:GLU:N	2.63	0.57
1:0:1:MET:SD	8:7:345:ARG:CD	2.93	0.57
12:B:769:LYS:O	12:B:769:LYS:HG3	2.03	0.57
27:U:160:GLU:OE2	27:U:162:GLU:N	2.38	0.57
38:s:73:PHE:HD2	38:s:99:ILE:HD13	1.70	0.57
15:f:219:GLU:OE1	15:f:219:GLU:N	2.25	0.57
15:f:320:ARG:CB	15:f:320:ARG:HH11	2.17	0.57
13:D:960:GLU:HB3	13:D:983:ARG:CG	2.35	0.56
15:F:335:ARG:HH21	15:F:378:ALA:HB1	1.69	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:420:ILE:HG12	34:o:426:ARG:HG3	1.87	0.56
35:p:82:PRO:HB3	35:p:134:LYS:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:41:ARG:CB	27:U:169:PRO:CG	2.81	0.56
34:o:189:PRO:HA	34:o:205:VAL:HG21	1.85	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
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
22:P:297:LYS:NZ	22:P:323:GLU:OE2	2.38	0.56
26:T:94:THR:HG22	26:T:109:ILE:HG22	1.87	0.56
28:V:192:VAL:HG21	28:V:203:PHE:HB3	1.86	0.56
30:Y:19:DA:H2"	30:Y:20:DC:H5'	1.87	0.56
30:Y:28:DT:H2'	30:Y:29:DA:N7	2.19	0.56
30:Y:29:DA:H2'	30:Y:30:DT:C6	2.40	0.56
34:o:460:ARG:HD2	34:o:494:ALA:HB2	1.87	0.56
35:p:67:LEU:HD21	35:p:416:ARG:HG3	1.87	0.56
35:p:984:CYS:SG	35:p:1046:THR:OG1	2.51	0.56
10:Z:6:G2L:H2'	49:p:1201:W0F:C10	2.35	0.56
11:A:851:ASP:OD1	11:A:851:ASP:N	2.38	0.56
14:E:345:MET:HE3	14:E:346:PRO:HD2	1.88	0.56
14:e:527:ILE:HG22	14:e:527:ILE:O	2.05	0.56
3:2:261:SER:OG	3:2:265:GLN:O	2.23	0.56
4:3:108:ASN:HD21	5:4:123:LEU:HD22	1.71	0.56
5:4:433:PHE:CE2	6:5:38:ILE:HG23	2.41	0.56
7:6:54:ASP:HB2	7:6:58:ALA:HB3	1.87	0.56
11:A:401:ASN:H	11:A:401:ASN:HD22	1.53	0.56
12:B:259:ASP:HB3	12:B:262:MET:O	2.06	0.56
20:L:113:VAL:O	20:L:114:LYS:C	2.49	0.56
28:V:86:LYS:NZ	28:V:140:LYS:HD2	2.21	0.56
13:d:910:LEU:HD11	20:l:88:ALA:HB2	1.87	0.56
13:D:956:GLN:HA	13:D:956:GLN:HE21	1.69	0.56
27:U:152:PHE:CD2	40:u:95:VAL:CG1	2.88	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
35:p:975:ARG:CZ	49:p:1201:W0F:O32	2.53	0.56
38:s:48:PRO:HA	38:s:53:PRO:HG2	1.86	0.56
12:B:27:LYS:CE	12:B:490:SER:HB3	2.35	0.56
12:B:560:TYR:CD2	12:B:581:ILE:HD11	2.40	0.56
25:S:168:ASN:HA	35:p:248:LYS:HD2	1.88	0.56
41:v:37:MET:HE3	41:v:127:GLY:HA3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:B:61:ASN:O	12:B:130:VAL:HG23	2.06	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
15:f:280:ILE:O	15:f:284:ARG:HG3	2.05	0.56
4:3:242:ILE:C	4:3:243:LEU:HD12	2.31	0.56
14:E:468:ASN:ND2	15:F:128:ASP:O	2.39	0.56
38:s:21:CYS:SG	38:s:26:TYR:HB2	2.45	0.56
2:1:456:ASP:OD1	2:1:457:ILE:HD12	2.06	0.55
5:4:393:LEU:HD21	7:6:511:TRP:CH2	2.41	0.55
1:0:20:LYS:HE3	1:0:62:LEU:HD13	1.87	0.55
4:3:44:LEU:HD21	4:3:162:LEU:HD13	1.89	0.55
28:V:155:LEU:HD21	28:V:204:ASN:H	1.71	0.55
3:2:59:ARG:NH2	3:2:166:GLU:OE1	2.38	0.55
8:7:309:VAL:HG12	8:7:309:VAL:O	2.07	0.55
15:F:83:LEU:CD1	15:F:83:LEU:N	2.67	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
22:P:186:ARG:NH1	22:P:244:LEU:O	2.39	0.55
27:U:56:ARG:NH1	27:U:60:ARG:HH11	2.02	0.55
34:o:1210:TRP:HZ3	42:w:53:ILE:HG13	1.71	0.55
34:o:1294:THR:HG21	35:p:245:GLN:NE2	2.21	0.55
7:6:444:HIS:O	7:6:472:ARG:NH1	2.39	0.55
7:6:528:LYS:CE	7:6:531:ILE:HD13	2.35	0.55
11:A:511:LEU:HD22	11:A:511:LEU:N	2.11	0.55
20:l:99:ALA:HB1	20:l:111:LEU:HD11	1.87	0.55
7:6:361:CYS:SG	7:6:405:VAL:HG13	2.46	0.55
7:6:664:SER:O	7:6:667:THR:OG1	2.25	0.55
13:D:964:GLU:HA	13:D:982:LEU:HG	1.87	0.55
26:T:194:HIS:CG	26:T:195:GLN:H	2.24	0.55
27:U:30:HIS:CD2	27:U:62:VAL:HG13	2.42	0.55
28:V:170:ASP:OD1	28:V:171:ILE:N	2.40	0.55
34:o:131:ALA:HA	34:o:134:LYS:HE2	1.89	0.55
15:f:253:TYR:O	15:f:254:GLN:HB3	2.06	0.55
5:4:407:VAL:N	5:4:443:VAL:O	2.37	0.55
8:7:114:ASN:C	8:7:114:ASN:HD22	2.15	0.55
25:S:167:ARG:HH11	25:S:168:ASN:H	1.53	0.55
28:V:149:LYS:HA	28:V:152:LEU:HD12	1.87	0.55
30:Y:16:DA:H2"	30:Y:17:DC:OP2	2.06	0.55
34:o:1128:ILE:HG23	34:o:1414:ILE:HB	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:8:ARG:CZ	1:0:34:CYS:SG	2.94	0.55
3:2:174:LEU:C	8:7:591:GLY:O	2.49	0.55
14:E:474:THR:HG22	15:F:61:GLY:HA2	1.88	0.55
27:U:14:LEU:HD11	27:U:194:THR:HG23	1.87	0.55
34:o:321:GLU:HG3	34:o:341:GLN:HE21	1.72	0.55
34:o:381:PRO:HB3	34:o:480:SER:HA	1.88	0.55
34:o:1189:ASP:HA	34:o:1192:TRP:CE2	2.41	0.55
35:p:783:ALA:O	35:p:789:ASN:ND2	2.40	0.55
38:s:59:THR:HB	38:s:73:PHE:HE1	1.72	0.55
13:d:960:GLU:HG2	13:d:963:ARG:HH21	1.70	0.55
15:F:71:ILE:HD11	18:I:35:VAL:HG13	1.89	0.55
15:F:86:PHE:CD1	15:F:86:PHE:N	2.75	0.55
24:R:134:ILE:HG12	24:R:171:GLU:HG3	1.87	0.55
41:v:124:ARG:HD3	41:v:126:GLN:HG3	1.88	0.55
7:6:83:HIS:ND1	7:6:115:GLU:OE2	2.40	0.55
7:6:528:LYS:CD	7:6:531:ILE:CD1	2.85	0.55
11:A:1052:ARG:HD2	11:A:1052:ARG:O	2.07	0.55
28:V:234:GLU:HB3	28:V:238:LYS:HZ3	1.72	0.55
14:E:561:SER:HB2	14:E:588:VAL:HB	1.88	0.55
15:F:87:HIS:HB2	18:I:45:ARG:HE	1.71	0.55
25:S:72:ASN:HB3	26:T:201:ASP:OD2	2.07	0.55
34:o:375:ILE:HD13	34:o:485:ASN:HD22	1.72	0.55
34:o:1381:GLU:O	34:o:1385:VAL:HG13	2.07	0.55
38:s:26:TYR:HA	38:s:64:HIS:HA	1.88	0.55
11:A:489:GLN:NE2	11:A:489:GLN:H	2.04	0.54
11:A:1200:THR:C	11:A:1204:GLU:HG2	2.31	0.54
15:F:433:PRO:HA	15:F:436:ALA:HB3	1.90	0.54
28:V:213:ASP:O	28:V:217:GLN:N	2.39	0.54
34:o:458:PHE:HE2	34:o:484:LEU:HD23	1.72	0.54
5:4:393:LEU:CD2	7:6:511:TRP:CH2	2.91	0.54
11:A:355:VAL:O	11:A:355:VAL:HG23	2.07	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
21:O:16:GLN:NE2	21:O:20:ASP:OD2	2.40	0.54
28:V:170:ASP:HA	28:V:173:GLU:HG2	1.89	0.54
7:6:87:GLU:OE2	7:6:145:LYS:NZ	2.40	0.54
8:7:17:ILE:HD11	8:7:22:PHE:CZ	2.42	0.54
27:U:32:LEU:O	27:U:36:ILE:HG12	2.08	0.54
28:V:147:ASP:HB3	28:V:150:ALA:H	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:365:VAL:HG22	8:7:365:VAL:O	2.08	0.54
22:P:206:GLU:HB3	22:P:207:PRO:HD3	1.90	0.54
26:T:188:PHE:HB3	28:V:76:GLY:O	2.06	0.54
30:Y:14:DC:N4	30:Y:15:DA:C6	2.75	0.54
34:o:628:VAL:HA	34:o:638:GLY:HA3	1.88	0.54
34:o:1436:VAL:O	34:o:1440:MET:HG2	2.08	0.54
35:p:265:GLN:OE1	35:p:324:ARG:NH1	2.39	0.54
1:0:8:ARG:NH2	1:0:37:LEU:HD22	2.21	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
14:E:524:LEU:O	14:E:527:ILE:HG12	2.08	0.54
15:F:418:ILE:HD12	15:F:418:ILE:N	2.20	0.54
35:p:570:ASN:ND2	35:p:616:THR:OG1	2.39	0.54
14:e:368:ASN:ND2	14:e:701:GLY:HA3	2.23	0.54
5:4:80:SER:O	5:4:84:GLU:OE1	2.25	0.54
8:7:437:CYS:SG	8:7:438:MET:N	2.81	0.54
24:R:50:SER:C	35:p:1069:ILE:HG13	2.33	0.54
38:s:106:VAL:HG21	38:s:110:MET:HG3	1.89	0.54
13:d:911:GLN:NE2	20:l:69:GLU:OE2	2.41	0.54
15:f:390:THR:HG23	15:f:391:LEU:HD22	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
4:3:108:ASN:OD1	5:4:123:LEU:CD1	2.51	0.54
12:B:544:LEU:HD23	12:B:590:ILE:HD11	1.88	0.54
12:B:571:LEU:HD21	12:B:619:MET:HE1	1.89	0.54
23:Q:15:ARG:HA	23:Q:18:ILE:HD12	1.89	0.54
34:o:769:MET:HE3	35:p:970:HIS:CD2	2.43	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
15:F:403:ILE:O	15:F:406:VAL:HG22	2.08	0.54
28:V:89:HIS:NE2	28:V:138:ALA:O	2.38	0.54
30:Y:3:DA:H2"	35:p:446:TYR:CD2	2.42	0.54
40:u:55:GLY:HA3	40:u:69:PRO:HG2	1.90	0.54
1:0:85:ARG:HH12	1:0:140:LEU:N	2.06	0.54
3:2:69:ARG:HB2	8:7:563:ARG:NH2	2.23	0.54
4:3:242:ILE:CD1	5:4:75:VAL:C	2.81	0.54
7:6:377:GLN:OE1	7:6:381:TRP:NE1	2.40	0.54
13:D:963:ARG:C	13:D:982:LEU:CD1	2.79	0.54
28:V:156:ASP:O	28:V:160:GLN:HG2	2.08	0.54
15:f:352:GLN:O	15:f:356:THR:OG1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:j:123:LEU:C	19:j:125:ASP:N	2.66	0.54
5:4:265:LEU:HD12	5:4:270:LEU:HD12	1.89	0.54
5:4:408:LEU:HD21	5:4:440:LEU:HD22	1.89	0.54
12:B:808:PRO:HA	12:B:864:ASN:HB3	1.91	0.54
26:T:238:GLU:HB3	28:V:130:ILE:CD1	2.38	0.54
27:U:76:MET:HG2	27:U:88:ARG:HB3	1.89	0.54
34:o:1004:LEU:HD13	34:o:1062:GLY:HA2	1.90	0.54
34:o:1294:THR:HG21	35:p:245:GLN:HE22	1.73	0.54
4:3:195:VAL:CG1	4:3:203:LEU:HD23	2.38	0.53
13:D:998:GLN:HG3	13:D:1002:ARG:NH1	2.22	0.53
16:G:149:ARG:O	16:G:149:ARG:HG3	2.08	0.53
14:E:563:GLU:HG2	14:E:587:PRO:HG3	1.90	0.53
24:R:90:ALA:HB3	34:o:324:GLY:HA2	1.90	0.53
26:T:188:PHE:HB3	28:V:76:GLY:C	2.33	0.53
26:T:238:GLU:OE1	28:V:82:VAL:HG11	2.08	0.53
8:7:289:VAL:HG22	8:7:324:ARG:NH1	2.23	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
14:E:653:LEU:HB2	14:E:663:ARG:HB2	1.90	0.53
34:o:217:SER:HB3	34:o:220:ARG:HG3	1.90	0.53
34:o:479:TRP:HB2	34:o:483:ARG:HH21	1.73	0.53
42:w:17:CYS:HB2	42:w:24:LEU:HD21	1.91	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
13:D:922:GLN:NE2	20:L:71:ASP:OD2	2.41	0.53
14:E:645:GLY:H	14:E:675:LEU:HD11	1.73	0.53
24:R:87:GLY:HA3	34:o:326:PRO:HA	1.90	0.53
30:Y:-6:DC:H2'	30:Y:-5:DC:C6	2.44	0.53
31:c:33:LEU:HD13	19:j:197:MET:HE1	1.91	0.53
34:o:784:VAL:HG13	35:p:978:ILE:HD11	1.90	0.53
35:p:918:PHE:HE2	35:p:920:LYS:HE3	1.73	0.53
14:e:646:SER:OG	14:e:647:ALA:N	2.40	0.53
1:0:8:ARG:HB2	27:U:172:ASP:OD2	2.08	0.53
1:0:85:ARG:HH22	1:0:140:LEU:HA	1.72	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
8:7:44: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
27:U:139:LEU:CD1	40:u:149:GLY:O	2.56	0.53
30:Y:19:DA:H8	30:Y:19:DA:OP2	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:o:43:TYR:HB3	34:o:53:LYS:HE3	1.91	0.53
34:o:375:ILE:HG21	34:o:535:MET:HE1	1.91	0.53
7:6:528:LYS:CD	7:6:531:ILE:HD11	2.39	0.53
8:7:133:LYS:O	8:7:137:LEU:HD23	2.07	0.53
11:A:395:ASP:OD1	11:A:395:ASP:N	2.41	0.53
12:B:937:THR:HG23	12:B:939:ASN:H	1.74	0.53
13:D:910:LEU:HD11	20:L:88:ALA:HB2	1.91	0.53
22:P:295:MET:HG2	22:P:298:PRO:HD2	1.89	0.53
49:p:1201:W0F:C01	49:p:1201:W0F:C20	2.85	0.53
4:3:44:LEU:HD22	4:3:227:LEU:HB3	1.90	0.53
6:5:38:ILE:HG22	6:5:39:ASP:N	2.24	0.53
8:7:488:VAL:HG23	8:7:488:VAL:O	2.09	0.53
34:o:1030:SER:HB3	38:s:162:ARG:HE	1.73	0.53
35:p:841:ARG:HD2	35:p:895:PHE:CZ	2.43	0.53
14:e:423:PRO:HG2	14:e:426:ARG:HB2	1.91	0.53
14:e:610:ARG:HD3	14:e:619:PRO:HG3	1.89	0.53
2:1:127:LEU:HD12	2:1:467:ALA:HA	1.91	0.53
12:B:66:ASN:HD21	12:B:119:PRO:HB3	1.73	0.53
15:F:335:ARG:HD2	15:F:382:GLU:HB2	1.90	0.53
15:f:283:MET:HG3	15:f:329:LEU:HD11	1.91	0.53
4:3:50:PHE:HZ	5:4:118:LEU:HD13	1.62	0.53
7:6:528:LYS:HG3	7:6:531:ILE:HD12	1.88	0.53
11:A:675:ASP:OD1	16:G:78:LYS:NZ	2.37	0.53
35:p:75:SER:O	35:p:77:GLU:HG2	2.09	0.53
44:y:88:THR:O	44:y:92:THR:HG23	2.08	0.53
3:2:174:LEU:HD21	3:2:203:ALA:HB2	1.89	0.53
13:D:960:GLU:HG2	13:D:983:ARG:HD3	1.91	0.53
4:3:108:ASN:CG	5:4:123:LEU:HD13	2.33	0.52
5:4:32:ASP:OD1	5:4:33:ARG:N	2.42	0.52
8:7:28:LEU:HD22	8:7:55:LEU:HD23	1.91	0.52
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
33:m:110:LEU:N	33:m:110:LEU:HD23	2.23	0.52
6:5:31:LYS:HB3	12:B:540:LYS:HZ1	1.44	0.52
14:E:304:LYS:NZ	14:E:335:GLU:O	2.42	0.52
34:o:1487:PRO:HG2	39:t:78:PRO:HA	1.90	0.52
5:4:172:SER:OG	5:4:267:GLU:OE2	2.13	0.52
8:7:393:ASP:OD1	8:7:394:PHE:N	2.42	0.52
12:B:202:TRP:HB2	12:B:238:LEU:HB3	1.92	0.52
14:E:562:SER:OG	14:E:564:ASP:OD1	2.28	0.52
30:Y:27:DT:C6	30:Y:28:DT:H72	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:o:1005:HIS:HD2	34:o:1007:ILE:HG22	1.74	0.52
1:0:83:ASN:CG	1:0:140:LEU:HD12	2.34	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
27:U:146:ASP:HB2	27:U:147:PRO:HD2	1.90	0.52
34:o:927:GLU:O	34:o:931:ARG:HG2	2.09	0.52
15:f:447:ALA:O	15:f:453:GLY:HA2	2.09	0.52
7:6:340:LEU:HD23	7:6:491:ALA:HB2	1.91	0.52
7:6:449:LYS:HB3	29:X:33:DG:OP1	2.10	0.52
15:F:273:GLN:H	15:F:273:GLN:CD	2.17	0.52
27:U:184:ILE:HG23	27:U:187:ILE:HB	1.91	0.52
30:Y:-35:DG:H2"	30:Y:-34:DG:C8	2.44	0.52
34:o:26:LEU:HG	35:p:1168:ALA:HB2	1.91	0.52
34:o:1311:LEU:HD11	34:o:1332:GLN:HB3	1.92	0.52
41:v:113:SER:HB3	41:v:126:GLN:HG2	1.91	0.52
15:f:318:CYS:SG	15:f:326:HIS:HB3	2.49	0.52
5:4:438:LYS:HE2	12:B:621:ALA:H	1.74	0.52
34:o:894:ASP:O	34:o:1022:ILE:HD13	2.10	0.52
15:F:39:LEU:HD11	18:I:51:LEU:HD21	1.92	0.52
28:V:175:LEU:HB2	28:V:180:LYS:HE2	1.91	0.52
35:p:201:ALA:N	35:p:390:ASN:O	2.42	0.52
5:4:413:LEU:HB2	12:B:672:PHE:HE1	1.74	0.52
7:6:181:HIS:O	7:6:184:VAL:HG12	2.10	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
25:S:73:ARG:NH1	26:T:229:HIS:HB2	2.25	0.52
14:e:595:PRO:HD2	14:e:639:SER:HB3	1.92	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
12:B:529:VAL:HG11	12:B:560:TYR:HB2	1.91	0.52
14:E:278:ASP:OD1	14:E:278:ASP:N	2.43	0.52
27:U:48:MET:O	27:U:52:LEU:N	2.42	0.52
28:V:117:GLN:O	28:V:121:THR:OG1	2.18	0.52
14:e:607:ARG:NH1	18:i:87:PRO:O	2.43	0.52
11:A:339:ALA:HA	11:A:497:PRO:HG3	1.92	0.52
12:B:66:ASN:OD1	12:B:187:ARG:NH1	2.43	0.52
14:E:522:ASP:OD1	14:E:522:ASP:N	2.42	0.52
15:F:219:GLU:HG2	17:H:156:PRO:C	2.35	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
30:Y:12:DC:H2"	30:Y:13:DA:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
27:U:128:LYS:O	27:U:162:GLU:HB3	2.10	0.51
27:U:139:LEU:CG	40:u:159:ALA:C	2.76	0.51
35:p:298:MET:HB3	42:w:14:ILE:HD12	1.91	0.51
14:e:747:LEU:HG	14:e:747:LEU:O	2.09	0.51
12:B:489:GLN:OE1	12:B:489:GLN:N	2.34	0.51
14:E:423:PRO:HG2	14:E:426:ARG:HB2	1.92	0.51
33:m:28:ARG:HH21	33:m:31:LEU:HD21	1.76	0.51
35:p:297:MET:O	35:p:301:VAL:HG23	2.10	0.51
42:w:59:THR:HB	42:w:61:GLU:HG3	1.92	0.51
1:0:8:ARG:NE	27:U:173:ALA:CB	2.73	0.51
2:1:471:LEU:HD13	2:1:475:PHE:HE2	1.75	0.51
3:2:54:ARG:NH2	3:2:245:SER:O	2.42	0.51
11:A:338:VAL:HG12	11:A:497:PRO:HD3	1.91	0.51
11:A:828:GLU:HA	11:A:831:LYS:HB2	1.92	0.51
15:F:243:LEU:HD21	15:F:284:ARG:HB3	1.92	0.51
28:V:97:LEU:HG	28:V:101:GLU:CD	2.35	0.51
41:v:17:PRO:HG3	41:v:29:HIS:NE2	2.25	0.51
8:7:126:PHE:CE2	8:7:128:LYS:HB2	2.46	0.51
12:B:656:GLU:HG2	12:B:661:ALA:HB3	1.92	0.51
24:R:127:ARG:HD2	24:R:183:VAL:HB	1.92	0.51
25:S:73:ARG:CZ	26:T:229:HIS:HB2	2.41	0.51
29:X:-14:DG:N2	29:X:-13:DT:O4'	2.44	0.51
1:0:41:ARG:C	27:U:168:MET:CE	2.81	0.51
8:7:709:THR:HG22	8:7:710:VAL:N	2.25	0.51
12:B:780:LYS:O	17:H:183:ARG:NH1	2.44	0.51
12:B:983:ARG:HH11	12:B:983:ARG:HG3	1.75	0.51
16:G:181:TRP:CD2	16:G:181:TRP:C	2.87	0.51
27:U:139:LEU:CD1	40:u:159:ALA:CA	2.86	0.51
34:o:1386:ILE:HD12	34:o:1398:LEU:HD21	1.92	0.51
14:e:650:THR:HG22	14:e:666:THR:HG22	1.93	0.51
15:f:320:ARG:NH1	15:f:320:ARG:CB	2.73	0.51
3:2:204:GLU:OE1	3:2:209:THR:OG1	2.28	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
21:O:57:ASN:OD1	21:O:58:PHE:N	2.44	0.51
22:P:169:VAL:HG21	29:X:-27:DA:C2	2.46	0.51
31:c:21:LEU:HD12	31:c:21:LEU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:o:597:PRO:HD2	34:o:600:ILE:HD12	1.91	0.51
44:y:41:THR:O	44:y:45:ILE:HG13	2.11	0.51
44:y:45:ILE:HG22	44:y:94:LEU:HD22	1.93	0.51
17:H:52:SER:O	19:J:194:THR:HA	2.10	0.51
27:U:139:LEU:CD2	40:u:158:PHE:O	2.53	0.51
4:3:165:LYS:NZ	4:3:167:ALA:O	2.38	0.51
5:4:266:ARG:HE	5:4:277:LYS:HZ2	1.56	0.51
14:E:746:ASP:OD1	14:E:746:ASP:N	2.42	0.51
30:Y:-6:DC:C2	30:Y:-5:DC:C5	2.98	0.51
34:o:538:VAL:HG22	34:o:539:GLN:HG2	1.93	0.51
34:o:1440:MET:SD	35:p:1167:ILE:HD11	2.51	0.51
35:p:40:VAL:HG11	35:p:482:LEU:HD13	1.93	0.51
5:4:409:TYR:HB2	5:4:412:PHE:HZ	1.74	0.51
8:7:3:LEU:O	8:7:9:LEU:HD12	2.11	0.51
27:U:74:CYS:HA	27:U:91:TYR:O	2.11	0.51
30:Y:-33:DC:H2"	30:Y:-32:DA:C8	2.46	0.51
31:c:1:MET:HG3	15:f:126:PRO:HB3	1.93	0.51
4:3:100:LYS:HG2	5:4:124:GLY:C	2.35	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
28:V:179:GLN:O	28:V:183:LYS:HB2	2.10	0.51
29:X:-20:DG:H2"	29:X:-19:DT:OP2	2.11	0.51
29:X:11:DC:H4'	34:o:1417:HIS:CG	2.46	0.51
34:o:110:VAL:HG13	34:o:115:SER:HA	1.93	0.51
34:o:459:ASN:HD22	34:o:469:MET:HE3	1.75	0.51
34:o:863:ARG:NH2	34:o:1415:THR:HG22	2.26	0.51
34:o:890:ARG:HH21	34:o:1023:VAL:HG13	1.76	0.51
15:f:24:GLU:HG2	20:l:145:THR:HG21	1.93	0.51
7:6:274:GLN:OE1	7:6:459:GLN:NE2	2.44	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
8:7:726:GLN:CG	8:7:727:PRO:CD	2.84	0.50
11:A:510:ILE:HB	11:A:511:LEU:HD13	1.93	0.50
22:P:297:LYS:HB3	22:P:298:PRO:HD3	1.93	0.50
27:U:164:ASP:HB2	27:U:167:ALA:HA	1.93	0.50
35:p:810:PHE:CB	35:p:927:ARG:HE	2.24	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
22:P:174:LEU:HD12	22:P:178:LEU:HD11	1.92	0.50
28:V:227:SER:O	28:V:231:GLU:HG2	2.11	0.50
35:p:43:GLN:NE2	35:p:482:LEU:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:p:794:VAL:HG22	35:p:967:ILE:HG22	1.93	0.50
36:q:101:PHE:CE2	36:q:122:SER:HB3	2.46	0.50
14:e:500:THR:HG22	14:e:502:LYS:H	1.76	0.50
5:4:390:GLN:HE21	5:4:394:TRP:NE1	2.09	0.50
8:7:284:GLU:HA	8:7:287:ARG:HG2	1.94	0.50
12:B:274:LEU:HG	12:B:278:LYS:HE2	1.93	0.50
20:L:126:MET:HE3	20:L:128:ILE:HD11	1.93	0.50
34:o:1366:PHE:HB2	34:o:1374:VAL:HG21	1.93	0.50
35:p:709:SER:HB2	35:p:767:LEU:HD11	1.93	0.50
14:e:527:ILE:O	14:e:527:ILE:CG2	2.59	0.50
3:2:121:SER:OG	3:2:127:HIS:NE2	2.39	0.50
12:B:983:ARG:HG3	12:B:983:ARG:NH1	2.26	0.50
27:U:139:LEU:HD11	40:u:158:PHE:O	2.11	0.50
30:Y:-33:DC:H2"	30:Y:-32:DA:H8	1.76	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
2:1:471:LEU:HD13	2:1:475:PHE:CE2	2.47	0.50
4:3:108:ASN:ND2	5:4:123:LEU:HD22	2.26	0.50
25:S:174:PHE:HD1	42:w:40:ARG:HA	1.77	0.50
26:T:160:GLN:O	26:T:163:ILE:HG12	2.12	0.50
30:Y:-37:DT:H2"	30:Y:-36:DA:C8	2.46	0.50
31:c:77:LEU:HD23	31:c:77:LEU:O	2.11	0.50
34:o:863:ARG:NH2	34:o:1129:ASN:OD1	2.44	0.50
36:q:263:LEU:HD22	44:y:87:PHE:HD2	1.77	0.50
2:1:524:HIS:ND1	3:2:270:SER:OG	2.38	0.50
7:6:369:VAL:HG11	7:6:615:PHE:HA	1.93	0.50
29:X:9:DA:H1'	29:X:10:DT:C6	2.46	0.50
35:p:309:PHE:CE2	42:w:40:ARG:HB2	2.47	0.50
13:d:1080:TYR:OH	14:e:606:ASP:OD2	2.26	0.50
15:F:316:GLN:NE2	15:F:319:LEU:O	2.45	0.50
17:H:113:ARG:O	17:H:116:ARG:NH1	2.44	0.50
20:L:93:GLU:O	20:L:97:THR:HG23	2.11	0.50
35:p:117:ASN:HA	35:p:189:GLY:HA3	1.93	0.50
36:q:260:GLN:HE22	44:y:92:THR:HG22	1.76	0.50
38:s:14:ARG:O	38:s:18:MET:HG2	2.10	0.50
5:4:438:LYS:CE	12:B:621:ALA:HB2	2.42	0.50
8:7:118:HIS:HB3	8:7:121:VAL:HG22	1.94	0.50
15:F:71:ILE:HD12	18:I:38:GLN:HE21	1.76	0.50
25:S:169:LYS:HD2	25:S:173:HIS:CD2	2.47	0.50
27:U:145:PHE:HB2	27:U:153:ARG:CG	2.41	0.50
35:p:755:GLN:HE22	43:x:48:MET:HE2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:u:94:LYS:HA	40:u:119:PHE:HB3	1.94	0.50
7:6:578:PRO:HG3	7:6:602:ILE:HD11	1.94	0.50
12:B:820:ASP:OD1	12:B:820:ASP:N	2.37	0.50
12:B:882:HIS:HE1	17:H:216:ALA:HB1	1.77	0.50
14:E:327:ASN:H	14:E:327:ASN:ND2	2.05	0.50
19:J:139:LEU:HB3	19:J:144:PHE:HB3	1.93	0.50
21:O:73:THR:O	21:O:73:THR:HG22	2.12	0.50
27:U:139:LEU:HD23	40:u:158:PHE:CD1	2.29	0.50
28:V:87:THR:O	28:V:91:ARG:HG2	2.11	0.50
28:V:113:LEU:HA	28:V:116:LYS:HE2	1.94	0.50
33:m:69:THR:HG22	33:m:73:MET:HE2	1.94	0.50
34:o:495:ASP:OD1	34:o:495:ASP:N	2.44	0.50
34:o:811:ILE:HG21	42:w:79:PRO:HB3	1.94	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
34:o:95:PHE:HB2	34:o:311:GLN:HE22	1.77	0.49
34:o:349:ARG:HH21	35:p:1070:LEU:HD21	1.77	0.49
36:q:99:VAL:HG21	36:q:127:VAL:HG21	1.94	0.49
14:e:586:TYR:HB3	14:e:605:HIS:HB3	1.94	0.49
1:0:27:GLY:HA3	1:0:70:LYS:CD	2.34	0.49
2:1:374:LEU:HD12	2:1:374:LEU:O	2.13	0.49
34:o:392:GLU:HB2	34:o:448:ARG:NH1	2.27	0.49
43:x:8:PHE:CD2	43:x:48:MET:HE1	2.47	0.49
5:4:406:GLY:HA2	5:4:444:THR:HA	1.94	0.49
7:6:650:MET:SD	7:6:656:ASN:ND2	2.82	0.49
13:D:965:ILE:C	13:D:965:ILE:HD13	2.37	0.49
27:U:30:HIS:CE1	27:U:62:VAL:HG22	2.47	0.49
34:o:525:ILE:HG12	34:o:535:MET:HE2	1.95	0.49
40:u:12:LEU:HD11	40:u:67:LEU:HD12	1.95	0.49
15:f:97:ALA:HB2	15:f:106:PHE:HE1	1.77	0.49
3:2:69:ARG:CG	3:2:141:GLY:H	2.23	0.49
8:7:284:GLU:HG2	8:7:385:THR:HG21	1.94	0.49
34:o:51:ARG:HB2	34:o:52:PRO:HD3	1.94	0.49
34:o:1258:ARG:HH22	34:o:1260:ARG:HH21	1.59	0.49
34:o:1434:GLU:C	34:o:1435:THR:HG1	2.17	0.49
40:u:93:ASN:N	40:u:128:TYR:OH	2.42	0.49
3:2:87:LEU:HD11	3:2:229:LYS:CG	2.43	0.49
12:B:818:THR:OG1	12:B:819:LEU:N	2.44	0.49
14:E:481:ASP:HB3	14:E:787:ARG:HH22	1.78	0.49
15:F:312:ILE:HG22	15:F:313:VAL:HG13	1.94	0.49
26:T:188:PHE:CE2	28:V:80:LYS:HB2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:p:715:ASP:OD1	35:p:715:ASP:N	2.44	0.49
36:q:105:VAL:HG11	36:q:115:VAL:HG22	1.93	0.49
5:4:405:GLU:O	5:4:444:THR:HG22	2.11	0.49
11:A:821:ARG:HA	11:A:821:ARG:NE	2.25	0.49
11:A:927:VAL:O	11:A:933:ASN:ND2	2.45	0.49
13:D:998:GLN:NE2	26:T:186:MET:SD	2.86	0.49
26:T:238:GLU:OE1	28:V:130:ILE:HG13	2.13	0.49
27:U:99:LEU:O	27:U:103:VAL:HG23	2.13	0.49
34:o:1153:ARG:O	34:o:1157:ILE:HG12	2.13	0.49
35:p:674:MET:HE2	35:p:690:CYS:SG	2.53	0.49
35:p:955:PRO:HB2	35:p:1028:LEU:HD13	1.94	0.49
35:p:1115:GLN:HG2	35:p:1150:ARG:HG2	1.94	0.49
41:v:65:TYR:HD1	41:v:84:ARG:HG2	1.76	0.49
4:3:237:GLN:HG3	5:4:51:LEU:HD21	1.94	0.49
5:4:338:PHE:N	5:4:341:MET:O	2.44	0.49
11:A:468:PHE:CE1	15:F:216:LEU:HD12	2.47	0.49
14:E:693:VAL:HB	14:E:707:LEU:HB2	1.94	0.49
16:G:94:MET:HE3	16:G:96:VAL:HG22	1.94	0.49
29:X:-32:DC:H6	29:X:-32:DC:H5'	1.78	0.49
34:o:575:PRO:HG3	34:o:594:LEU:HD11	1.95	0.49
34:o:1481:LYS:HG2	40:u:20:PRO:HA	1.94	0.49
35:p:792:ASP:O	35:p:943:GLY:HA3	2.12	0.49
3:2:63:VAL:HG11	3:2:88:LEU:HD11	1.95	0.49
14:E:232:HIS:HD1	14:E:313:SER:HG	1.58	0.49
15:F:273:GLN:CD	15:F:273:GLN:N	2.70	0.49
16:G:48:HIS:HD2	16:G:54:GLY:HA2	1.78	0.49
26:T:238:GLU:CD	28:V:130:ILE:HG12	2.37	0.49
32:k:191:VAL:HG13	32:k:200:ILE:CD1	2.41	0.49
34:o:48:GLU:HB2	34:o:53:LYS:HD2	1.94	0.49
42:w:114:CYS:HB2	42:w:123:TRP:HZ3	1.77	0.49
8:7:243:CYS:SG	8:7:443:ALA:HB3	2.53	0.49
25:S:142:ASN:OD1	25:S:143:TRP:N	2.45	0.49
27:U:139:LEU:HD11	40:u:159:ALA:CA	2.26	0.49
34:o:392:GLU:HB2	34:o:448:ARG:HH11	1.78	0.49
35:p:75:SER:OG	35:p:77:GLU:OE2	2.28	0.49
37:r:33:LEU:HG	37:r:84:ARG:NH2	2.27	0.49
14:e:651:VAL:HG13	14:e:665:PHE:HB2	1.95	0.49
1:0:4:GLN:OE1	1:0:10:LYS:HD3	2.13	0.49
3:2:69:ARG:HD2	8:7:563:ARG:NH2	2.28	0.49
8:7:134:CYS:O	8:7:138:THR:HG22	2.13	0.49
8:7:136:SER:O	8:7:142:VAL:HG21	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:589:TRP:CE3	15:F:60:MET:HG3	2.48	0.49
22:P:227:GLU:OE1	22:P:318:ARG:NH2	2.44	0.49
34:o:1471:PHE:CZ	39:t:61:GLU:HA	2.48	0.49
35:p:764:MET:HE1	35:p:938:ARG:NH1	2.28	0.49
14:e:525:GLU:OE1	14:e:525:GLU:N	2.41	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
2:1:456:ASP:OD1	2:1:456:ASP:N	2.47	0.48
3:2:69:ARG:HG2	3:2:141:GLY:H	1.78	0.48
11:A:569:ASN:HB3	11:A:572:TYR:HD2	1.78	0.48
12:B:560:TYR:HD2	12:B:581:ILE:HD11	1.78	0.48
14:E:467:LEU:HD11	15:F:132:LYS:HD3	1.94	0.48
34:o:115:SER:OG	34:o:227:ARG:HB2	2.13	0.48
35:p:759:VAL:HG12	35:p:999:ALA:HB2	1.94	0.48
38:s:17:ILE:HD13	38:s:74:VAL:HG11	1.94	0.48
3:2:348:CYS:O	4:3:146:ARG:NH2	2.45	0.48
4:3:13:ILE:HD13	4:3:41:VAL:HG13	1.94	0.48
11:A:337:ARG:HH11	11:A:338:VAL:H	1.60	0.48
13:D:1068:GLU:OE2	14:E:582:LYS:NZ	2.45	0.48
14:E:651:VAL:HB	14:E:665:PHE:HB2	1.95	0.48
15:F:409:GLY:O	15:F:417:ARG:NH2	2.46	0.48
20:L:113:VAL:O	20:L:116:VAL:N	2.46	0.48
30:Y:16:DA:H1'	30:Y:17:DC:O5'	2.13	0.48
34:o:1429:LYS:HB2	34:o:1438:VAL:HG11	1.94	0.48
40:u:114:PRO:HD3	40:u:163:LEU:HB2	1.95	0.48
14:e:633:THR:O	14:e:634:ARG:NH2	2.45	0.48
5:4:174:ASP:OD1	5:4:175:LEU:N	2.45	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
12:B:329:LEU:HB3	12:B:342:THR:HG23	1.96	0.48
12:B:598:ARG:HH11	12:B:619:MET:HE3	1.77	0.48
14:E:256:HIS:HB3	14:E:259:GLU:CG	2.44	0.48
20:L:106:ARG:O	20:L:106:ARG:HG2	2.14	0.48
28:V:110:ASP:OD1	28:V:114:LYS:HD3	2.12	0.48
30:Y:-5:DC:H2'	30:Y:-4:DT:H6	1.76	0.48
34:o:201:GLU:HG3	34:o:213:LYS:HG3	1.95	0.48
1:0:8:ARG:NH2	1:0:34:CYS:HA	2.28	0.48
17:H:197:THR:HB	15:f:238:LYS:HG2	1.95	0.48
24:R:248:ARG:NH2	24:R:287:GLN:OE1	2.46	0.48
28:V:176:PRO:O	28:V:178:SER:N	2.46	0.48
29:X:18:DG:H4'	29:X:19:DA:H5'	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:o:62:GLN:HG3	34:o:84:HIS:O	2.14	0.48
34:o:1243:LEU:HD21	34:o:1288:ILE:HD13	1.95	0.48
35:p:667:THR:HA	35:p:670:GLU:HB2	1.94	0.48
35:p:733:MET:HE3	35:p:1052:LYS:HA	1.95	0.48
35:p:1028:LEU:HD11	35:p:1043:ILE:HD11	1.94	0.48
36:q:38:PHE:HE1	36:q:245:VAL:HA	1.78	0.48
7:6:363:VAL:HG21	7:6:378:PHE:CE2	2.47	0.48
12:B:559:LYS:HZ3	12:B:559:LYS:HB2	1.78	0.48
12:B:570:GLU:HA	12:B:625:LEU:HA	1.95	0.48
14:E:703:MET:HE2	14:E:761:LEU:HD21	1.95	0.48
23:Q:18:ILE:HD11	23:Q:46:TRP:CZ3	2.48	0.48
25:S:54:LYS:HG2	25:S:59:GLU:OE1	2.13	0.48
27:U:139:LEU:HD21	40:u:158:PHE:CD1	2.42	0.48
29:X:14:DC:H2"	29:X:15:DT:H72	1.95	0.48
31:c:119:GLU:HG3	14:e:790:LEU:HD11	1.96	0.48
35:p:725:GLN:HA	35:p:728:MET:HE2	1.95	0.48
36:q:38:PHE:CE1	36:q:245:VAL:HA	2.48	0.48
37:r:112:LYS:HB3	37:r:119:GLU:HG2	1.95	0.48
40:u:30:LEU:HD22	40:u:70:VAL:HG11	1.95	0.48
2:1:481:VAL:HG23	2:1:483:THR:HG23	1.94	0.48
5:4:438:LYS:CE	12:B:621:ALA:CB	2.86	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
27:U:30:HIS:NE2	27:U:62:VAL:HA	2.28	0.48
34:o:455:ILE:HD13	34:o:516:GLN:HB2	1.95	0.48
34:o:1443:ALA:HB2	35:p:1167:ILE:HG23	1.96	0.48
35:p:737:ILE:HG22	35:p:739:ASN:H	1.79	0.48
44:y:84:GLN:O	44:y:88:THR:HG23	2.13	0.48
15:f:257:PRO:O	15:f:261:THR:OG1	2.31	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	1.96	0.48
11:A:338:VAL:HG13	11:A:360:SER:HB2	1.96	0.48
14:E:299:ASP:OD2	14:E:607:ARG:NH2	2.38	0.48
17:H:39:VAL:HG12	17:H:119:ILE:HG12	1.96	0.48
27:U:44:LYS:HG3	27:U:89:HIS:CD2	2.48	0.48
27:U:150:GLY:C	40:u:93:ASN:OD1	2.57	0.48
29:X:12:DT:H2"	29:X:13:DA:C8	2.49	0.48
34:o:330:GLN:HE21	34:o:334:ARG:HE	1.60	0.48
35:p:269:ILE:HD11	35:p:369:VAL:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:e:693:VAL:HB	14:e:707:LEU:HB2	1.94	0.48
12:B:636:VAL:HG23	12:B:638:ARG:HB3	1.96	0.48
34:o:486:LEU:HD13	35:p:790:GLN:CD	2.39	0.48
34:o:733:LEU:HA	34:o:736:THR:HG22	1.96	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
27:U:114:ILE:O	27:U:174:ARG:NH2	2.47	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
27:U:76:MET:HB2	27:U:90:ASN:OD1	2.14	0.48
28:V:234:GLU:HB3	28:V:238:LYS:NZ	2.28	0.48
35:p:516:GLU:HA	35:p:520:VAL:HG22	1.96	0.48
12:B:135:TRP:HA	12:B:138:VAL:HG12	1.95	0.47
26:T:80:GLU:OE1	26:T:81:HIS:N	2.45	0.47
26:T:179:ASP:N	26:T:179:ASP:OD1	2.46	0.47
40:u:92:VAL:HG12	40:u:119:PHE:CD1	2.49	0.47
42:w:68:ILE:HB	42:w:122:ARG:HD2	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
15:f:39:LEU:HD22	18:i:47:VAL:HG13	1.95	0.47
15:f:254:GLN:O	15:f:258:ARG:NH2	2.47	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
5:4:398:ARG:HA	5:4:398:ARG:HE	1.79	0.47
7:6:449:LYS:HD3	29:X:33:DG:P	2.53	0.47
11:A:501:THR:O	11:A:502:LEU:C	2.57	0.47
11:A:639:LEU:O	11:A:643:ILE:HG13	2.13	0.47
11:A:824:ARG:HB3	11:A:863:VAL:HG12	1.95	0.47
24:R:177:PHE:HB3	24:R:188:LYS:HG3	1.95	0.47
27:U:56:ARG:HD3	27:U:60:ARG:CZ	2.44	0.47
27:U:141:ALA:O	40:u:98:PHE:CZ	2.67	0.47
30:Y:22:DC:H2"	30:Y:23:DC:C6	2.48	0.47
32:k:173:CYS:SG	32:k:179:MET:O	2.72	0.47
35:p:168:ASP:N	35:p:168:ASP:OD1	2.47	0.47
35:p:789:ASN:O	35:p:968:ASN:HB2	2.14	0.47
7:6:605:ILE:HD12	7:6:607:ILE:HD11	1.96	0.47
13:D:998:GLN:HG2	13:D:999:MET:N	2.29	0.47
15:F:317:LEU:N	15:F:317:LEU:HD23	2.30	0.47
18:I:63:LYS:NZ	18:I:69:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:o:508:SER:HB3	34:o:511:THR:HG22	1.94	0.47
34:o:597:PRO:HB3	34:o:664:ILE:HG22	1.95	0.47
34:o:808:PRO:HB2	35:p:675:LEU:HD12	1.96	0.47
34:o:1228:MET:HE3	34:o:1247:PHE:HB2	1.95	0.47
34:o:1321:ILE:HD12	34:o:1331:LEU:HD12	1.97	0.47
37:r:108:ALA:HB2	37:r:128:GLN:HB2	1.96	0.47
42:w:12:VAL:HG23	42:w:50:ASN:HD21	1.78	0.47
42:w:81:THR:HG23	42:w:96:PHE:CE1	2.49	0.47
1:0:41:ARG:HD2	27:U:169:PRO:CG	2.44	0.47
5:4:360:THR:HG22	5:4:363:GLN:OE1	2.13	0.47
11:A:475:LEU:O	15:f:354:ARG:NH2	2.46	0.47
11:A:485:ILE:HB	15:f:310:THR:HG23	1.94	0.47
11:A:730:PHE:CD1	11:A:730:PHE:N	2.82	0.47
14:E:634:ARG:HG3	14:E:675:LEU:HB2	1.95	0.47
15:F:90:GLU:CD	15:F:90:GLU:N	2.72	0.47
24:R:39:LEU:HD11	34:o:425:ASP:HB3	1.95	0.47
29:X:-18:DG:C2	29:X:-17:DG:C5	3.02	0.47
33:m:67:GLU:O	33:m:71:LYS:HG2	2.14	0.47
34:o:557:ARG:O	34:o:561:MET:HG2	2.15	0.47
38:s:80:PRO:HA	38:s:107:GLN:HB2	1.96	0.47
2:1:422:LEU:HD13	4:3:225:GLN:NE2	2.29	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
7:6:297:PHE:O	7:6:359:LYS:NZ	2.38	0.47
24:R:123:THR:O	24:R:127:ARG:HG3	2.14	0.47
27:U:14:LEU:HD13	27:U:197:VAL:HG22	1.96	0.47
35:p:185:PHE:HB3	35:p:187:ILE:HD13	1.96	0.47
35:p:818:GLU:HG3	35:p:827:GLU:O	2.14	0.47
35:p:1090:GLU:N	35:p:1090:GLU:OE1	2.48	0.47
37:r:131:LEU:O	37:r:135:GLN:HG2	2.14	0.47
14:e:589:TRP:HB3	15:f:60:MET:HE3	1.96	0.47
14:E:696:TRP:HA	14:E:703:MET:HA	1.96	0.47
14:E:774:MET:HE2	14:E:774:MET:N	2.22	0.47
27:U:140:GLU:OE1	27:U:140:GLU:N	2.48	0.47
28:V:103:LEU:HA	28:V:106:THR:HG22	1.96	0.47
35:p:320:PHE:HE1	35:p:324:ARG:HE	1.62	0.47
37:r:57:LEU:HD13	37:r:61:PHE:CE2	2.50	0.47
40:u:148:VAL:N	40:u:160:ILE:O	2.42	0.47
14:e:474:THR:OG1	14:e:546:VAL:O	2.28	0.47
14:e:556:ASN:HA	14:e:572:LEU:HB2	1.96	0.47
15:f:330:ARG:NH1	15:f:371:THR:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:20:ILE:H	4:3:20:ILE:HD12	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
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
27:U:49:LEU:O	27:U:53:LYS:HA	2.15	0.47
27:U:69:ASP:OD1	27:U:69:ASP:N	2.39	0.47
28:V:225:VAL:HG13	28:V:226:ASP:OD2	2.15	0.47
29:X:-33:DC:C2	29:X:-32:DC:C5	3.02	0.47
33:m:56:ILE:HG23	20:l:129:PRO:HB2	1.97	0.47
34:o:712:ASP:HB3	34:o:744:ILE:HD13	1.96	0.47
35:p:59:VAL:HG21	35:p:91:ILE:HD12	1.96	0.47
35:p:1094:GLN:HB2	35:p:1103:LEU:HD13	1.97	0.47
38:s:54:ARG:C	38:s:56:THR:H	2.21	0.47
38:s:64:HIS:HD2	38:s:66:ASP:H	1.62	0.47
40:u:124:ASN:HB2	40:u:125:PRO:HD3	1.97	0.47
13:d:916:LYS:NZ	13:d:1070:GLU:OE2	2.42	0.47
3:2:291:CYS:SG	3:2:294:CYS:N	2.82	0.47
11:A:575:PRO:HD3	12:B:608:ASN:HD22	1.79	0.47
18:I:119:ARG:NH1	18:I:120:TYR:OH	2.48	0.47
24:R:31:ASP:OD1	24:R:31:ASP:N	2.47	0.47
24:R:128:ILE:HG23	24:R:183:VAL:HG11	1.97	0.47
31:c:26:VAL:HG23	19:j:195:LEU:HB3	1.96	0.47
34:o:18:ILE:HG12	35:p:1171:MET:HB2	1.97	0.47
34:o:526:VAL:HA	34:o:533:PRO:HA	1.97	0.47
35:p:289:ILE:HD11	35:p:301:VAL:HG21	1.97	0.47
37:r:105:PRO:HG2	37:r:131:LEU:HD22	1.97	0.47
5:4:404:THR:O	6:5:8:VAL:HG22	2.15	0.47
11:A:1165:LEU:HB2	11:A:1191:ILE:HG12	1.97	0.47
12:B:71:ARG:HD3	12:B:73:TYR:CE1	2.50	0.47
12:B:564:LEU:HB2	12:B:581:ILE:HD13	1.97	0.47
15:F:424:GLN:O	15:F:428:LEU:HG	2.15	0.47
23:Q:321:SER:OG	23:Q:322:ASP:N	2.48	0.47
28:V:99:LEU:HD23	28:V:114:LYS:HZ2	1.80	0.47
34:o:530:SER:O	34:o:532:ARG:HG3	2.15	0.47
35:p:385:ARG:O	35:p:391:LYS:HE3	2.15	0.47
1:0:8:ARG:CZ	1:0:9:CYS:SG	3.02	0.47
8:7:617:ALA:HB2	8:7:676:LEU:HD21	1.97	0.47
15:F:411:VAL:HG13	15:F:411:VAL:O	2.15	0.47
22:P:203:ARG:NH1	30:Y:27:DT:OP1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:36:ILE:HG21	27:U:48:MET:CE	2.45	0.47
27:U:179:ARG:HA	27:U:182:GLU:HG2	1.96	0.47
4:3:44:LEU:HD21	4:3:162:LEU:CD1	2.45	0.46
12:B:781:TYR:O	17:H:176:ARG:NH2	2.47	0.46
13:D:963:ARG:O	13:D:966:LEU:N	2.48	0.46
15:F:215:GLU:O	15:F:254:GLN:NE2	2.39	0.46
26:T:31:TRP:HD1	26:T:62:LEU:HD21	1.80	0.46
29:X:11:DC:H4'	34:o:1417:HIS:CD2	2.50	0.46
35:p:665:ILE:HD11	35:p:695:HIS:NE2	2.30	0.46
15:f:102:ARG:HD3	20:l:151:ARG:HG3	1.95	0.46
11:A:397:LEU:HD21	15:f:361:LYS:HB3	1.97	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:47:ILE:HD13	18:I:19:MET:HE1	1.96	0.46
15:F:418:ILE:H	15:F:418:ILE:CD1	2.26	0.46
24:R:107:MET:O	24:R:112:ARG:NH2	2.47	0.46
34:o:478:PRO:O	44:y:4:PRO:HD3	2.15	0.46
35:p:223:SER:HB2	35:p:349:PRO:HD2	1.96	0.46
35:p:271:ILE:HG21	35:p:320:PHE:CD2	2.50	0.46
35:p:665:ILE:HD13	35:p:673:VAL:HG21	1.97	0.46
42:w:64:GLU:O	42:w:68:ILE:HG12	2.16	0.46
15:f:326:HIS:ND1	15:f:326:HIS:N	2.64	0.46
15:f:326:HIS:O	15:f:330:ARG:HG2	2.15	0.46
1:0:28:HIS:HB3	1:0:30:LEU:HG	1.96	0.46
25:S:73:ARG:HD2	25:S:73:ARG:HA	1.64	0.46
27:U:139:LEU:HD12	40:u:160:ILE:N	2.31	0.46
27:U:150:GLY:O	40:u:93:ASN:OD1	2.34	0.46
29:X:-19:DT:C2	29:X:-18:DG:C5	3.03	0.46
41:v:96:VAL:HG22	41:v:116:VAL:HG22	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
15:f:328:ALA:C	15:f:330:ARG:N	2.72	0.46
4:3:229:TRP:CH2	5:4:58:ARG:NH1	2.79	0.46
11:A:470:ILE:O	15:f:299:LYS:NZ	2.49	0.46
12:B:217:ASN:ND2	12:B:320:ALA:O	2.35	0.46
16:G:41:ASP:OD1	16:G:41:ASP:N	2.48	0.46
34:o:544:ALA:HB2	34:o:680:LEU:HD13	1.97	0.46
34:o:931:ARG:NH1	34:o:936:GLU:HG3	2.31	0.46
34:o:1171:ALA:HA	42:w:59:THR:HG23	1.96	0.46
37:r:34:ASN:O	37:r:68:THR:OG1	2.33	0.46
45:z:17:TYR:HB3	45:z:44:MET:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:382:CYS:HB3	3:2:385:CYS:HB3	1.96	0.46
4:3:13:ILE:HG21	4:3:41:VAL:HG13	1.97	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
8:7:28:LEU:O	8:7:32:LEU:HD23	2.16	0.46
24:R:105:ARG:NH1	30:Y:13:DA:N7	2.59	0.46
24:R:182:ALA:HB2	26:T:155:PRO:HA	1.97	0.46
27:U:112:ARG:O	27:U:115:GLU:HG2	2.16	0.46
27:U:152:PHE:CZ	40:u:96:GLY:N	2.84	0.46
34:o:93:PRO:HD2	34:o:219:GLU:HG2	1.98	0.46
34:o:364:ARG:NH1	34:o:502:ASN:OD1	2.48	0.46
34:o:413:TYR:O	34:o:449:HIS:HD2	1.99	0.46
34:o:490:THR:OG1	34:o:491:PRO:HD3	2.15	0.46
34:o:1143:LEU:HD21	34:o:1336:LEU:HD11	1.98	0.46
34:o:1292:MET:O	34:o:1296:MET:HB2	2.15	0.46
35:p:645:GLU:O	35:p:649:ASN:HB2	2.15	0.46
15:f:58:MET:HE3	15:f:64:GLN:HA	1.98	0.46
4:3:53:ARG:HD2	5:4:46:ARG:HH12	1.80	0.46
11:A:404:MET:O	11:A:408:LEU:HB2	2.16	0.46
14:E:277:ASP:O	14:E:280:ARG:HG2	2.16	0.46
15:F:83:LEU:H	15:F:83:LEU:HD12	1.71	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
25:S:43:ASN:OD1	25:S:44:GLN:N	2.48	0.46
25:S:71:PHE:CZ	26:T:194:HIS:HB3	2.51	0.46
31:c:80:LEU:HB3	19:j:119:PHE:CZ	2.50	0.46
35:p:744:MET:HE3	35:p:744:MET:HB3	1.80	0.46
35:p:860:VAL:HG12	35:p:896:LEU:HD22	1.98	0.46
35:p:1088:GLU:O	35:p:1091:ARG:HG2	2.14	0.46
37:r:104:CYS:SG	37:r:138:ARG:HD2	2.56	0.46
42:w:14:ILE:HG21	42:w:23:MET:HE2	1.97	0.46
14:e:717:LEU:HD22	14:e:726:LEU:HD11	1.98	0.46
1:0:8:ARG:CD	27:U:172:ASP:HB2	2.45	0.46
1:0:8:ARG:HH21	1:0:37:LEU:HD22	1.80	0.46
3:2:357:VAL:CG1	3:2:366:VAL:HG23	2.45	0.46
4:3:50:PHE:CZ	5:4:118:LEU:HD12	2.38	0.46
25:S:65:SER:HA	25:S:81:ARG:NH1	2.15	0.46
28:V:168:LEU:O	28:V:172:GLU:HG2	2.16	0.46
34:o:368:THR:HG21	35:p:931:ILE:O	2.16	0.46
35:p:399:LEU:HB3	35:p:453:TRP:NE1	2.30	0.46
35:p:810:PHE:HB2	35:p:927:ARG:HE	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:p:1038:THR:HA	36:q:195:THR:HA	1.98	0.46
40:u:112:SER:HB3	40:u:162:SER:HA	1.98	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
1:0:37:LEU:O	1:0:40:VAL:HG12	2.16	0.46
2:1:427:ALA:HB1	5:4:62:LEU:HD11	1.98	0.46
7:6:656:ASN:OD1	7:6:657:ALA:N	2.49	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
27:U:150:GLY:CA	40:u:93:ASN:OD1	2.64	0.46
29:X:-20:DG:C8	29:X:-19:DT:H72	2.51	0.46
34:o:532:ARG:NH1	34:o:647:THR:O	2.49	0.46
34:o:1206:ARG:H	34:o:1263:ASN:HB3	1.81	0.46
39:t:66:LEU:HD21	39:t:97:LEU:HB2	1.98	0.46
1:0:31:CYS:SG	1:0:34:CYS:HB2	2.56	0.46
1:0:128:GLU:HB3	1:0:133:ILE:HG12	1.98	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
34:o:459:ASN:HD21	35:p:1090:GLU:HG3	1.81	0.46
14:e:519:GLU:O	14:e:519:GLU:HG3	2.16	0.46
15:f:327:TRP:O	15:f:330:ARG:HB2	2.15	0.46
1:0:5:GLY:HA3	1:0:10:LYS:CB	2.25	0.46
7:6:185:ILE:HG22	7:6:189:LEU:HD13	1.97	0.46
15:F:141:CYS:SG	17:H:158:THR:HB	2.56	0.46
43:x:66:GLU:HA	45:z:23:HIS:HB3	1.97	0.46
19:J:123:LEU:HD12	19:J:123:LEU:HA	1.73	0.45
27:U:54:PHE:CE1	28:V:195:PRO:HG3	2.51	0.45
34:o:686:THR:HG21	35:p:1040:GLN:O	2.16	0.45
34:o:725:LEU:HB3	34:o:733:LEU:HD11	1.97	0.45
35:p:712:PRO:HG2	35:p:939:HIS:CE1	2.52	0.45
40:u:97:LEU:HD23	40:u:108:ILE:HD13	1.98	0.45
4:3:31:GLN:OE1	4:3:36:LYS:NZ	2.42	0.45
4:3:98:ASP:CB	4:3:100:LYS:HE3	2.47	0.45
8:7:329:PHE:O	8:7:333:LEU:HD23	2.17	0.45
8:7:361:LEU:O	8:7:365:VAL:HG12	2.16	0.45
13:D:871:THR:HG21	13:D:910:LEU:HD12	1.98	0.45
15:F:426:LEU:C	15:F:426:LEU:HD23	2.41	0.45
34:o:420:ILE:HB	34:o:445:LYS:HB2	1.99	0.45
34:o:486:LEU:HD23	34:o:496:PHE:HE2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:e:258:ASN:OD1	14:e:258:ASN:N	2.38	0.45
14:e:718:ARG:HD3	14:e:718:ARG:HA	1.76	0.45
5:4:334:MET:SD	7:6:56:TYR:CE2	3.09	0.45
5:4:435:ASN:HB3	5:4:440:LEU:HB2	1.97	0.45
8:7:109:LEU:HD12	8:7:207:TYR:CD2	2.51	0.45
8:7:137:LEU:O	8:7:142:VAL:HG11	2.15	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
14:E:730:SER:OG	14:E:732:ASP:OD1	2.33	0.45
34:o:463:THR:HG21	35:p:1090:GLU:HG3	1.97	0.45
35:p:505:LEU:HD22	35:p:509:VAL:HB	1.99	0.45
35:p:711:ILE:HG12	35:p:725:GLN:HG2	1.98	0.45
1:0:55:LYS:C	1:0:57:ASN:H	2.24	0.45
2:1:457:ILE:HG22	2:1:461:LEU:HD13	1.98	0.45
2:1:472:LEU:HD12	2:1:476:TRP:CD1	2.52	0.45
14:E:245:VAL:HG13	14:E:282:LEU:HD11	1.97	0.45
17:H:186:VAL:HG21	15:f:220:GLN:HB3	1.97	0.45
28:V:97:LEU:O	28:V:137:TYR:HE1	2.00	0.45
29:X:11:DC:H2'	29:X:12:DT:H71	1.98	0.45
35:p:17:ILE:O	35:p:19:PRO:HD3	2.16	0.45
14:e:243:LEU:HD13	14:e:243:LEU:HA	1.73	0.45
15:f:219:GLU:H	15:f:219:GLU:CD	2.21	0.45
2:1:308:ASN:ND2	8:7:576:GLU:OE2	2.49	0.45
5:4:411:GLN:HE22	12:B:534:SER:HB2	1.82	0.45
11:A:857:MET:HE3	11:A:858:ASP:H	1.81	0.45
17:H:27:ASP:OD1	17:H:27:ASP:N	2.48	0.45
17:H:87:GLN:HA	17:H:88:PRO:HD3	1.82	0.45
23:Q:22:ILE:HG22	23:Q:39:LEU:HD11	1.98	0.45
29:X:-28:DA:H2'	29:X:-27:DA:C8	2.51	0.45
30:Y:-6:DC:H2'	30:Y:-5:DC:H6	1.80	0.45
33:m:84:GLU:H	33:m:84:GLU:HG3	1.42	0.45
34:o:569:THR:HG23	34:o:671:ASN:HD21	1.81	0.45
35:p:260:LEU:HD22	35:p:347:MET:SD	2.56	0.45
39:t:121:ASP:OD1	39:t:121:ASP:N	2.49	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
5:4:406:GLY:O	6:5:7:GLY:N	2.49	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
27:U:76:MET:CG	27:U:88:ARG:HB3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:m:47:GLN:HG2	13:d:860:VAL:HA	1.98	0.45
34:o:920:PHE:CD1	34:o:959:MET:HE1	2.52	0.45
35:p:119:THR:HG23	35:p:187:ILE:HA	1.98	0.45
38:s:82:VAL:HB	38:s:110:MET:HG2	1.98	0.45
15:f:83:LEU:HD22	18:i:41:GLU:HG2	1.99	0.45
4:3:201:GLY:O	4:3:204:GLN:HG2	2.17	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: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	2.43	0.45
23:Q:332:GLU:OE1	23:Q:332:GLU:N	2.49	0.45
27:U:179:ARG:HH21	27:U:183:GLN:HG3	1.81	0.45
29:X:8:DC:C2'	29:X:9:DA:C8	3.00	0.45
34:o:153:ILE:HG12	34:o:187:TYR:CD1	2.52	0.45
34:o:971:PRO:O	34:o:972:THR:OG1	2.29	0.45
44:y:49:GLN:HB2	44:y:94:LEU:HD21	1.99	0.45
8:7:460:THR:HB	8:7:661:ALA:HB1	1.98	0.45
11:A:475:LEU:HD23	11:A:480:TRP:HE1	1.82	0.45
13:D:947:PHE:HE1	14:E:527:ILE:HD12	1.82	0.45
25:S:175:SER:O	25:S:179:GLN:HG2	2.17	0.45
27:U:112:ARG:HA	27:U:115:GLU:OE2	2.16	0.45
29:X:29:DA:H2"	29:X:30:DC:C6	2.52	0.45
30:Y:-17:DG:C6	30:Y:-16:DA:C6	3.05	0.45
34:o:18:ILE:HD11	35:p:1149:VAL:HG11	1.99	0.45
34:o:459:ASN:HD21	34:o:463:THR:HG21	1.81	0.45
40:u:129:LYS:HD2	40:u:133:GLU:HG2	1.99	0.45
42:w:106:ASP:OD1	42:w:106:ASP:N	2.48	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
3:2:242:SER:N	3:2:245:SER:OG	2.50	0.45
8:7:373:ARG:O	8:7:405:THR:OG1	2.24	0.45
10:Z:6:G2L:O2'	34:o:460:ARG:NH2	2.50	0.45
13:D:966:LEU:HD22	13:D:966:LEU:C	2.42	0.45
24:R:251:ILE:H	24:R:251:ILE:HD12	1.82	0.45
25:S:47:LEU:HD11	25:S:98:TRP:HB3	1.99	0.45
28:V:86:LYS:HZ2	28:V:140:LYS:HD2	1.81	0.45
34:o:527:THR:HB	34:o:534:VAL:HG22	1.99	0.45
37:r:20:LEU:HD12	37:r:121:ARG:HH22	1.81	0.45
40:u:22:LEU:O	40:u:26:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:199:ILE:CG2	3:2:222:ILE:HD11	2.47	0.45
14:E:784:HIS:HB3	14:E:792:LEU:HB2	1.99	0.45
27:U:12:ALA:O	27:U:16:ARG:HG2	2.18	0.45
28:V:130:ILE:HD12	28:V:140:LYS:HG3	1.99	0.45
35:p:718:GLN:HG2	35:p:720:PRO:HD2	1.98	0.45
35:p:837:CYS:SG	35:p:889:LYS:HD3	2.56	0.45
38:s:72:MET:HG3	38:s:101:ARG:HD2	1.99	0.45
13:d:1084:LEU:HB3	18:i:99:ARG:HH21	1.81	0.45
1:0:6:CYS:O	1:0:10:LYS:HE3	2.17	0.44
5:4:325:ILE:H	5:4:325:ILE:HD12	1.82	0.44
7:6:133:THR:HB	7:6:160:THR:HG21	2.00	0.44
7:6:528:LYS:CD	7:6:531:ILE:HD13	2.47	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	2.50	0.44
27:U:145:PHE:HB3	27:U:153:ARG:H	1.82	0.44
34:o:96:HIS:HB2	34:o:250:VAL:HG23	1.99	0.44
35:p:713:PHE:HB3	35:p:716:HIS:HD2	1.82	0.44
35:p:955:PRO:O	35:p:963:PRO:HD2	2.16	0.44
14:e:245:VAL:HG12	14:e:282:LEU:HD11	1.99	0.44
19:j:176:MET:O	19:j:178:GLY:N	2.43	0.44
4:3:42:MET:SD	4:3:108:ASN:ND2	2.86	0.44
4:3:123:ASP:OD1	4:3:124:ILE:N	2.45	0.44
8:7:475:PRO:HG3	8:7:478:MET:HE2	1.99	0.44
16:G:129:LYS:HA	16:G:129:LYS:HD2	1.76	0.44
26:T:194:HIS:CG	26:T:195:GLN:N	2.83	0.44
34:o:1160:ARG:O	34:o:1300:GLY:HA2	2.16	0.44
35:p:556:ILE:HD11	35:p:576:ILE:HG12	1.98	0.44
35:p:714:PRO:HD2	35:p:1001:PRO:HA	1.99	0.44
8:7:600:ALA:HB1	8:7:659:HIS:HD2	1.82	0.44
11:A:1063:LYS:HD3	11:A:1063:LYS:O	2.16	0.44
13:D:991:MET:HE1	26:T:192:GLU:HG2	1.98	0.44
21:O:65:TYR:OH	22:P:203:ARG:NE	2.50	0.44
24:R:46:ILE:O	24:R:49:GLY:N	2.50	0.44
26:T:159:HIS:O	26:T:163:ILE:HG23	2.18	0.44
26:T:170:LYS:HE3	26:T:170:LYS:HB3	1.72	0.44
28:V:129:LYS:HA	28:V:129:LYS:HE3	1.97	0.44
33:m:57:LEU:HA	33:m:57:LEU:HD23	1.73	0.44
35:p:1060:HIS:HE1	35:p:1081:ASP:HA	1.82	0.44
14:e:525:GLU:N	14:e:525:GLU:CD	2.76	0.44
1:0:1:MET:SD	8:7:345:ARG:HD2	2.57	0.44
3:2:175:THR:HA	8:7:591:GLY:C	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:242:ILE:CD1	5:4:75:VAL:N	2.80	0.44
6:5:35:ILE:C	12:B:539:ARG:HD3	2.42	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:463:PRO:O	15:F:218:VAL:HG23	2.17	0.44
11:A:1053:PHE:HB2	11:A:1057:GLU:HB2	2.00	0.44
24:R:93:PHE:HB2	24:R:97:GLY:HA2	1.99	0.44
24:R:102:GLN:HE21	34:o:305:GLU:CG	2.29	0.44
25:S:73:ARG:NE	25:S:76:ARG:HH11	2.16	0.44
28:V:96:PRO:HB3	28:V:136:LYS:HD2	1.98	0.44
29:X:-32:DC:H2'	29:X:-31:DT:H71	1.98	0.44
34:o:952:LEU:HD21	34:o:1006:PRO:HB2	2.00	0.44
37:r:74:PHE:HB2	37:r:80:ILE:HG12	2.00	0.44
1:0:8:ARG:CG	27:U:172:ASP:HB2	2.47	0.44
2:1:400:ILE:H	2:1:400:ILE:HD12	1.82	0.44
5:4:52:ALA:HB1	5:4:90:LEU:HD21	1.99	0.44
7:6:415:HIS:HD2	7:6:419:ARG:HH22	1.65	0.44
8:7:107:LEU:HD12	8:7:195:ALA:HB1	1.98	0.44
8:7:726:GLN:HG2	8:7:727:PRO:CD	2.47	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	2.17	0.44
14:E:249:LEU:HD21	14:E:282:LEU:HD22	2.00	0.44
14:E:650:THR:HG22	14:E:666:THR:HG22	2.00	0.44
15:F:328:ALA:O	15:F:332:PHE:N	2.50	0.44
15:F:361:LYS:HA	15:F:364:VAL:HG22	1.99	0.44
22:P:298:PRO:HB2	22:P:300:ILE:HG12	1.98	0.44
24:R:131:PRO:HG3	35:p:101:ARG:HG3	1.98	0.44
27:U:152:PHE:CZ	40:u:95:VAL:HG12	2.49	0.44
34:o:618:TYR:HA	34:o:621:ILE:HG13	2.00	0.44
36:q:69:GLY:HA3	45:z:57:ALA:HB1	1.98	0.44
44:y:82:SER:HB3	44:y:85:GLU:HG3	1.99	0.44
14:e:542:HIS:CE1	14:e:568:ARG:HG3	2.53	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
12:B:492:MET:HE3	12:B:492:MET:HB2	1.85	0.44
12:B:653:LEU:HG	12:B:684:ILE:HG13	1.99	0.44
25:S:53:ASN:HB2	25:S:91:PHE:CZ	2.53	0.44
26:T:220:ILE:HG13	26:T:221:GLY:H	1.82	0.44
30:Y:15:DA:C2'	30:Y:16:DA:C8	3.01	0.44
34:o:233:CYS:SG	34:o:238:MET:HB2	2.57	0.44
34:o:1417:HIS:O	34:o:1421:ARG:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:p:677:MET:CE	35:p:700:PRO:HB3	2.47	0.44
36:q:92:GLU:HG3	36:q:93:PHE:H	1.82	0.44
20:l:113:VAL:O	20:l:113:VAL:HG22	2.17	0.44
4:3:242:ILE:CD1	5:4:74:TRP:C	2.91	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
11:A:1165:LEU:HD22	11:A:1165:LEU:HA	1.87	0.44
12:B:859:ARG:HA	12:B:859:ARG:HD2	1.80	0.44
12:B:925:LYS:HD3	12:B:925:LYS:HA	1.78	0.44
13:D:1080:TYR:OH	14:E:606:ASP:OD2	2.30	0.44
15:F:47:ILE:HD11	18:I:43:ALA:HB2	1.98	0.44
28:V:111:ILE:O	28:V:114:LYS:N	2.51	0.44
28:V:214:GLU:HA	28:V:217:GLN:HB3	1.99	0.44
34:o:733:LEU:CB	42:w:106:ASP:HB2	2.48	0.44
35:p:419:ALA:O	35:p:423:ILE:HG12	2.17	0.44
40:u:30:LEU:O	40:u:34:VAL:HG22	2.17	0.44
43:x:2:ILE:HD12	43:x:56:ILE:HD13	1.99	0.44
45:z:36:CYS:HB3	45:z:39:CYS:SG	2.57	0.44
6:5:9:LEU:HD11	6:5:42:HIS:HD2	1.83	0.44
17:H:59:GLU:HA	17:H:62:THR:HG22	1.99	0.44
27:U:53:LYS:O	28:V:199:LYS:HE2	2.18	0.44
34:o:379:GLY:HA2	34:o:475:ARG:O	2.18	0.44
34:o:459:ASN:OD1	34:o:460:ARG:N	2.51	0.44
35:p:728:MET:SD	35:p:942:LYS:HB3	2.58	0.44
35:p:794:VAL:HG13	35:p:965:ILE:HG23	1.99	0.44
40:u:13:LEU:HD11	40:u:26:VAL:HG22	2.00	0.44
3:2:87:LEU:HD23	3:2:87:LEU:O	2.18	0.44
3:2:369:VAL:HG13	3:2:370:ASP:N	2.32	0.44
8:7:332:PHE:CZ	8:7:367:ILE:HG23	2.53	0.44
12:B:414:LEU:HB2	12:B:523:VAL:HG13	2.00	0.44
13:D:933:ARG:HD2	19:J:117:VAL:HG11	2.00	0.44
13:D:1071:ARG:HH22	18:I:82:SER:HA	1.83	0.44
15:F:400:GLY:O	15:F:404:ARG:HG2	2.18	0.44
20:L:113:VAL:C	20:L:115:ASP:N	2.75	0.44
27:U:139:LEU:N	40:u:160:ILE:CD1	2.81	0.44
34:o:48:GLU:HB3	34:o:53:LYS:HA	1.99	0.44
34:o:279:LYS:HE2	34:o:316:THR:HB	2.00	0.44
34:o:514:GLU:CD	35:p:1101:GLN:HB2	2.42	0.44
34:o:663:ASP:OD1	34:o:666:ARG:NH1	2.44	0.44
34:o:1180:ASN:O	34:o:1183:SER:OG	2.24	0.44
35:p:19:PRO:C	35:p:21:LEU:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:p:163:LEU:HA	35:p:166:LEU:HD12	2.00	0.44
35:p:635:LEU:HD13	35:p:661:VAL:HG11	1.99	0.44
35:p:710:ILE:HA	35:p:764:MET:HE2	2.00	0.44
35:p:1135:TYR:H	35:p:1143:LYS:HZ3	1.66	0.44
36:q:71:ILE:HD11	36:q:150:ILE:HG12	1.99	0.44
40:u:87:ALA:HB2	40:u:101:ILE:HG12	1.99	0.44
15:f:447:ALA:CB	15:f:456:GLY:HA3	2.48	0.44
13:D:997:ALA:O	13:D:1001:GLN:N	2.48	0.43
23:Q:18:ILE:HD11	23:Q:46:TRP:CH2	2.53	0.43
28:V:229:ASP:HA	28:V:232:LYS:HE2	1.99	0.43
31:c:24:ASP:CB	19:j:192:LYS:HD2	2.48	0.43
34:o:211:GLU:H	34:o:211:GLU:HG3	1.48	0.43
34:o:436:SER:HA	34:o:439:HIS:HD2	1.80	0.43
35:p:357:CYS:SG	35:p:361:LYS:NZ	2.91	0.43
35:p:1060:HIS:CE1	35:p:1081:ASP:HA	2.53	0.43
40:u:96:GLY:O	40:u:128:TYR:OH	2.36	0.43
7:6:99:PHE:CZ	7:6:103:ILE:HD13	2.53	0.43
11:A:400:GLU:HG3	11:A:401:ASN:N	2.33	0.43
12:B:328:ASN:HA	17:H:227:LEU:HD21	2.00	0.43
14:E:377:LEU:HD21	14:E:422:PRO:HG2	2.00	0.43
14:E:564:ASP:OD1	14:E:564:ASP:N	2.51	0.43
15:F:6:LYS:HE2	15:F:8:LYS:HG3	2.01	0.43
15:F:283:MET:HE1	15:F:308:VAL:HG12	2.00	0.43
18:I:23:LEU:HD22	18:I:28:ILE:HD12	2.00	0.43
20:L:83:MET:HE3	20:L:83:MET:HB3	1.61	0.43
25:S:72:ASN:ND2	26:T:198:ASN:H	2.16	0.43
28:V:78:LEU:O	28:V:82:VAL:HG23	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
3:2:206:ARG:CB	8:7:589:GLU:O	2.63	0.43
8:7:354:PRO:HB2	8:7:355:PRO:HD3	2.00	0.43
12:B:603:LYS:H	12:B:603:LYS:HG2	1.64	0.43
15:F:427:LEU:HD12	15:F:427:LEU:HA	1.72	0.43
21:O:48:LEU:HG	23:Q:366:ILE:HD11	2.00	0.43
25:S:70:GLU:CA	25:S:74:LYS:HB2	2.47	0.43
32:k:179:MET:HB3	32:k:180:PRO:HD2	2.01	0.43
33:m:87:VAL:HG13	33:m:97:PHE:HE1	1.83	0.43
34:o:34:MET:SD	35:p:1124:ILE:HG21	2.58	0.43
34:o:225:PHE:HB3	34:o:245:PRO:HB2	2.00	0.43
34:o:769:MET:HB3	34:o:769:MET:HE2	1.65	0.43
35:p:256:ILE:HD11	35:p:373:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:p:789:ASN:HB3	35:p:795:ILE:HG13	1.99	0.43
41:v:65:TYR:HE1	41:v:84:ARG:HH11	1.66	0.43
1:0:68:VAL:HG11	8:7:338:GLU:HG2	2.00	0.43
8:7:67:VAL:HG23	8:7:67:VAL:O	2.19	0.43
12:B:766:LEU:HA	12:B:807:THR:HG21	2.00	0.43
14:E:481:ASP:N	14:E:481:ASP:OD1	2.41	0.43
24:R:83:MET:HB2	24:R:104:ARG:HH11	1.83	0.43
25:S:89:LYS:HE2	25:S:89:LYS:HB2	1.78	0.43
34:o:631:GLU:HG2	34:o:988:TRP:HZ2	1.84	0.43
34:o:1144:LEU:HG	34:o:1353:ASP:HA	2.00	0.43
35:p:713:PHE:HB3	35:p:716:HIS:CD2	2.53	0.43
36:q:76:ASP:HA	36:q:239:LEU:HD23	1.99	0.43
14:e:268:HIS:O	14:e:268:HIS:CG	2.70	0.43
7:6:133:THR:HG23	7:6:134:SER:N	2.33	0.43
11:A:340:GLU:H	11:A:497:PRO:HG2	1.84	0.43
14:E:351:GLN:HG2	14:E:355:MET:HE2	2.01	0.43
28:V:184:ALA:O	28:V:189:ILE:HG23	2.19	0.43
34:o:865:ILE:HG21	35:p:1092:ASP:CG	2.43	0.43
15:f:11:ASN:OD1	15:f:48:LYS:NZ	2.51	0.43
3:2:112:LYS:N	3:2:142:GLU:O	2.41	0.43
7:6:184:VAL:HG13	7:6:185:ILE:N	2.33	0.43
13:D:891:ILE:HG21	20:L:111:LEU:HB2	2.01	0.43
13:D:963:ARG:O	13:D:965:ILE:N	2.52	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
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
18:I:21:GLN:HE22	18:I:24:LYS:HE2	1.84	0.43
19:J:124:GLU:O	19:J:125:ASP:HB3	2.16	0.43
34:o:1162:GLU:O	34:o:1300:GLY:HA3	2.18	0.43
34:o:1485:GLU:HG2	40:u:20:PRO:HD3	2.01	0.43
35:p:803:ARG:HH21	36:q:177:ASN:HD22	1.67	0.43
35:p:927:ARG:HD3	35:p:1054:MET:SD	2.59	0.43
18:i:16:ALA:HB2	18:i:40:LEU:HD11	2.00	0.43
11:A:639:LEU:O	11:A:639:LEU:CD1	2.67	0.43
13:D:958:LYS:HD2	13:D:958:LYS:HA	1.62	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
17:H:194:MET:HE2	17:H:194:MET:HB2	1.85	0.43
30:Y:-20:DC:H2"	30:Y:-19:DT:C5'	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:o:76:GLY:HA2	34:o:80:GLU:HB3	2.00	0.43
34:o:456:VAL:HG21	34:o:503:LEU:HD11	2.01	0.43
34:o:1099:ALA:HA	34:o:1102:MET:HG2	2.01	0.43
35:p:81:PRO:HA	35:p:82:PRO:HD3	1.91	0.43
39:t:66:LEU:HD23	39:t:66:LEU:HA	1.83	0.43
43:x:7:CYS:HB2	43:x:48:MET:HG3	2.00	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
5:4:426:ARG:NH2	5:4:434:GLU:OE1	2.52	0.43
7:6:193:VAL:HG11	7:6:283:ARG:CD	2.49	0.43
8:7:168:VAL:O	8:7:168:VAL:HG13	2.19	0.43
11:A:1052:ARG:O	11:A:1052:ARG:CG	2.67	0.43
27:U:16:ARG:HA	27:U:16:ARG:HD2	1.94	0.43
31:c:101:VAL:HG22	15:f:127:LEU:HA	2.00	0.43
34:o:477:LEU:HB2	34:o:483:ARG:NH1	2.33	0.43
34:o:1416:ARG:HB3	34:o:1433:GLU:OE1	2.19	0.43
35:p:603:MET:HG3	35:p:614:ILE:HG12	2.01	0.43
15:f:55:LEU:HD13	18:i:28:ILE:HG12	2.01	0.43
7:6:532:LEU:HD23	7:6:532:LEU:O	2.19	0.43
31:c:124:ILE:HD11	15:f:133:ALA:HB1	2.00	0.43
34:o:216:LEU:HD12	34:o:216:LEU:HA	1.87	0.43
34:o:893:GLU:OE1	38:s:197:SER:OG	2.29	0.43
35:p:274:ARG:HG2	35:p:279:VAL:HA	2.01	0.43
35:p:1115:GLN:HB3	35:p:1148:LEU:HD11	2.01	0.43
37:r:17:ALA:HB1	37:r:95:PHE:CZ	2.53	0.43
38:s:61:LEU:HB2	38:s:73:PHE:CE2	2.54	0.43
7:6:532:LEU:CD2	7:6:716:VAL:HG13	2.49	0.43
9:N:6:CSX:HB2	9:N:7:ASN:H	1.42	0.43
13:D:995:GLU:OE2	26:T:193:LYS:HD2	2.19	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
19:J:148:ASP:HA	19:J:149:PRO:HD2	1.80	0.43
26:T:32:ALA:HA	26:T:35:SER:HB2	2.00	0.43
31:c:21:LEU:HD11	31:c:23:TRP:CD1	2.54	0.43
34:o:47:THR:HB	34:o:50:GLY:O	2.19	0.43
34:o:244:ARG:HH11	34:o:245:PRO:HD2	1.84	0.43
35:p:1035:ARG:NH1	35:p:1036:LYS:O	2.52	0.43
36:q:9:VAL:HG11	44:y:105:PHE:CD1	2.54	0.43
36:q:60:HIS:CE1	36:q:63:PHE:HB2	2.54	0.43
40:u:117:MET:HA	40:u:130:THR:HA	2.01	0.43
13:d:871:THR:O	20:l:62:LYS:NZ	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:A:727:THR:HG23	11:A:727:THR:O	2.19	0.42
11:A:925:ASP:N	11:A:925:ASP:OD1	2.52	0.42
14:E:327:ASN:HD22	14:E:327:ASN:N	2.07	0.42
15:F:401:GLU:C	15:F:401:GLU:CD	2.87	0.42
19:J:192:LYS:N	19:J:192:LYS:CE	2.66	0.42
27:U:56:ARG:HH11	27:U:60:ARG:HH11	1.60	0.42
31:c:66:VAL:HG21	19:j:151:ILE:HG23	2.01	0.42
33:m:91:ARG:HG2	33:m:92:LYS:N	2.34	0.42
37:r:91:LYS:H	37:r:122:PHE:HZ	1.67	0.42
14:e:667:GLY:O	14:e:692: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
8:7:49:THR:HG23	8:7:50:VAL:N	2.34	0.42
8:7:109:LEU:HD11	8:7:199:ILE:HD11	2.01	0.42
8:7:111:SER:N	8:7:211:TYR:OH	2.52	0.42
11:A:357:GLU:HB3	11:A:358:ASP:H	1.61	0.42
12:B:831:GLU:OE1	12:B:835:ARG:NH2	2.52	0.42
12:B:882:HIS:CE1	17:H:216:ALA:HB1	2.54	0.42
15:F:397:GLN:H	15:F:397:GLN:HG3	1.60	0.42
22:P:169:VAL:HG22	22:P:222:THR:HG22	2.00	0.42
27:U:74:CYS:SG	27:U:92:TYR:HA	2.60	0.42
32:k:182:LEU:HD23	32:k:182:LEU:HA	1.85	0.42
34:o:120:ASP:O	34:o:126:ILE:HG13	2.19	0.42
34:o:1282:ASP:N	34:o:1282:ASP:OD1	2.52	0.42
35:p:1163:MET:HA	35:p:1167:ILE:O	2.18	0.42
38:s:71:GLN:O	38:s:99:ILE:HG23	2.19	0.42
43:x:47:ARG:CZ	43:x:48:MET:HE3	2.49	0.42
45:z:16:ILE:HG22	45:z:25:GLU:HB3	2.00	0.42
15:f:223:TYR:CD2	15:f:255:MET:HE1	2.52	0.42
1:0:64:GLU:OE1	8:7:345:ARG:NH2	2.52	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
8:7:249:VAL:HG21	8:7:403:PHE:HB2	2.00	0.42
11:A:353:LEU:HD22	15:f:273:GLN:HE22	1.85	0.42
17:H:38:GLN:HG2	17:H:62:THR:HG21	2.01	0.42
24:R:50:SER:O	34:o:264:VAL:HA	2.19	0.42
27:U:188:TYR:O	27:U:191:LEU:HG	2.20	0.42
29:X:14:DC:H1'	29:X:15:DT:C6	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:19:DA:C6	29:X:20:DG:C6	3.07	0.42
34:o:876:ASP:O	34:o:890:ARG:NH1	2.53	0.42
34:o:1158:LEU:HD23	34:o:1336:LEU:HD13	2.01	0.42
35:p:676:ALA:HA	35:p:682:LEU:HD22	2.00	0.42
14:e:447:THR:O	14:e:450:ARG:HB2	2.19	0.42
15:f:317:LEU:HG	15:f:330:ARG:HE	1.83	0.42
2:1:496:ASN:HB3	2:1:536:LEU:HD11	2.02	0.42
4:3:53:ARG:HG3	5:4:46:ARG:CZ	2.50	0.42
10:Z:2:U:H2'	10:Z:3:C:C6	2.54	0.42
11:A:468:PHE:HE1	15:F:221:GLN:HG3	1.85	0.42
15:F:233:GLY:HA2	15:F:239:ARG:HE	1.83	0.42
26:T:175:ARG:HD2	26:T:207:LYS:HA	2.01	0.42
27:U:44:LYS:HB2	27:U:47:ASP:OD1	2.19	0.42
27:U:188:TYR:O	27:U:192:ARG:HG2	2.20	0.42
28:V:228:MET:O	28:V:232:LYS:HG3	2.20	0.42
29:X:29:DA:H2"	29:X:30:DC:C5	2.54	0.42
34:o:1143:LEU:HB2	34:o:1148:ALA:HB2	2.00	0.42
37:r:41:LEU:HD22	37:r:61:PHE:CE1	2.55	0.42
40:u:92:VAL:HG11	40:u:127:CYS:N	2.34	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
15:F:410:PRO:O	15:F:411:VAL:C	2.63	0.42
25:S:166:ARG:O	25:S:169:LYS:HG2	2.19	0.42
34:o:279:LYS:HD2	34:o:279:LYS:HA	1.92	0.42
34:o:1416:ARG:O	34:o:1420:ASN:HB2	2.19	0.42
40:u:18:PHE:HA	40:u:22:LEU:HD13	2.01	0.42
15:f:432:ALA:HB1	15:f:462:GLN:CB	2.49	0.42
2:1:524:HIS:NE2	2:1:528:MET:SD	2.93	0.42
5:4:415:GLN:HB2	5:4:439:ARG:HH21	1.85	0.42
5:4:456:LYS:HA	5:4:456:LYS:HD2	1.50	0.42
8:7:557:ILE:HG22	8:7:561:ILE:HD12	2.01	0.42
12:B:562:GLY:O	12:B:581:ILE:HG12	2.19	0.42
14:E:476:VAL:HB	14:E:782:HIS:HB2	2.01	0.42
17:H:178:LYS:HD3	17:H:178:LYS:HA	1.82	0.42
20:L:120:LEU:HD23	20:L:128:ILE:HG12	2.01	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:211:GLU:HB2	34:o:214:ILE:HG12	2.01	0.42
35:p:567:ILE:HD11	35:p:577:HIS:HB2	2.01	0.42
14:e:225:ILE:HD12	14:e:236:LEU:HB3	2.02	0.42
14:e:504:LEU:HD22	14:e:575:PHE:HZ	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:374:LEU:HD12	2:1:374:LEU:C	2.45	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
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
9:N:2:TRX:CE3	34:o:749:ARG:HD2	2.50	0.42
11:A:464:TRP:CD1	11:A:464:TRP:C	2.96	0.42
11:A:468:PHE:CE1	15:F:221:GLN:HG3	2.54	0.42
12:B:216:SER:OG	12:B:217:ASN:N	2.52	0.42
12:B:487:LYS:O	12:B:487:LYS:CG	2.67	0.42
25:S:161:GLU:O	25:S:165:GLU:HG2	2.19	0.42
27:U:154:CYS:HB3	27:U:157:CYS:O	2.19	0.42
28:V:165:GLY:HA2	28:V:169:GLU:OE1	2.18	0.42
34:o:320:ASN:HB3	34:o:341:GLN:NE2	2.35	0.42
41:v:98:ARG:HD3	41:v:100:GLU:HG3	2.02	0.42
1:0:8:ARG:HG3	27:U:173:ALA:N	2.34	0.42
5:4:261:PHE:CZ	5:4:265:LEU:HD21	2.54	0.42
7:6:412:MET:HA	7:6:415:HIS:CD2	2.55	0.42
7:6:559:ILE:HG22	7:6:561:PHE:CE1	2.55	0.42
8:7:462:SER:OG	8:7:463:PRO:CD	2.66	0.42
12:B:594:SER:OG	12:B:595:LYS:N	2.52	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
17:H:154:PRO:HB2	17:H:155:ASP:H	1.46	0.42
25:S:77:GLU:OE2	25:S:81:ARG:NH2	2.52	0.42
31:c:94:HIS:CD2	15:f:122:LEU:HD22	2.54	0.42
34:o:916:PHE:HE2	34:o:960:ARG:HG2	1.84	0.42
34:o:1163:HIS:CE1	34:o:1297:THR:HG23	2.55	0.42
15:f:104:LEU:HD22	19:j:216:TYR:HB2	2.02	0.42
1:0:85:ARG:NH2	1:0:139:LYS:HB3	2.34	0.42
3:2:174:LEU:CD2	3:2:203:ALA:HB2	2.42	0.42
11:A:968:ILE:HD12	11:A:968:ILE:HA	1.94	0.42
12:B:496:MET:HE3	12:B:496:MET:HB2	1.83	0.42
20:L:62:LYS:HD2	20:L:62:LYS:HA	1.87	0.42
20:L:120:LEU:O	20:L:125:ASN:N	2.53	0.42
28:V:145:VAL:C	28:V:146:ARG:HD2	2.45	0.42
34:o:114:CYS:SG	34:o:184:CYS:HB3	2.59	0.42
34:o:531:ASN:HB3	34:o:898:GLY:O	2.20	0.42
34:o:802:PHE:HD2	35:p:671:GLU:HG2	1.83	0.42
36:q:9:VAL:HG11	44:y:105:PHE:HD1	1.85	0.42
36:q:193:ARG:HG2	36:q:220:TYR:HD1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:r:24:LYS:HA	37:r:27:GLU:CD	2.45	0.42
15:f:26:MET:HE3	15:f:26:MET:HB3	1.77	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
14:E:790:LEU:HD13	17:H:146:ILE:HG12	2.01	0.42
15:F:329:LEU:HA	15:F:332:PHE:HB3	2.01	0.42
21:O:11:LEU:HD23	21:O:44:ILE:HD12	2.02	0.42
25:S:73:ARG:NH2	26:T:229:HIS:HB2	2.35	0.42
25:S:173:HIS:HB2	42:w:40:ARG:HD3	2.01	0.42
27:U:14:LEU:HD12	27:U:194:THR:HA	2.02	0.42
28:V:231:GLU:OE1	28:V:231:GLU:HA	2.18	0.42
30:Y:1:DG:C6	30:Y:2:DA:C6	3.07	0.42
32:k:179:MET:HB3	32:k:180:PRO:CD	2.50	0.42
34:o:256:PRO:HA	34:o:257:PRO:HD3	1.94	0.42
34:o:565:MET:HE1	44:y:74:ARG:HB2	2.02	0.42
34:o:867:SER:HB3	34:o:1414:ILE:HG23	2.01	0.42
34:o:906:LEU:HD13	34:o:966:LEU:HD22	2.02	0.42
35:p:501:LEU:HD12	35:p:505:LEU:HD12	2.01	0.42
35:p:587:LEU:HD22	35:p:597:ILE:HD11	2.01	0.42
35:p:1028:LEU:HD23	35:p:1028:LEU:HA	1.84	0.42
41:v:37:MET:HE2	41:v:37:MET:HB3	1.84	0.42
45:z:43:ILE:O	45:z:44:MET:HE2	2.20	0.42
14:e:332:ILE:HA	14:e:336:HIS:HD2	1.84	0.42
1:0:85:ARG:NH1	1:0:140:LEU:N	2.68	0.41
2:1:503:THR:OG1	2:1:533:TYR:OH	2.01	0.41
4:3:42:MET:HE3	4:3:108:ASN:HA	2.02	0.41
8:7:114:ASN:C	8:7:114:ASN:ND2	2.78	0.41
12:B:371:LYS:HA	12:B:371:LYS:HD3	1.87	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
26:T:154:LYS:HE3	26:T:154:LYS:HB2	1.95	0.41
27:U:44:LYS:HA	27:U:44:LYS:HD3	1.85	0.41
27:U:76:MET:HG3	27:U:89:HIS:C	2.45	0.41
34:o:709:ALA:HB2	34:o:748:ALA:HB2	2.02	0.41
34:o:1027:ASP:N	34:o:1027:ASP:OD1	2.52	0.41
34:o:1130:ILE:HD13	34:o:1411:LEU:HD22	2.02	0.41
35:p:21:LEU:HD12	35:p:21:LEU:HA	1.92	0.41
35:p:264:LYS:HE2	35:p:264:LYS:HB3	1.87	0.41
15:f:428:LEU:HD13	15:f:458:LEU:CB	2.49	0.41
1:0:85:ARG:CZ	1:0:140:LEU:HG	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:174:LEU:HD23	8:7:533:ASP:OD2	2.20	0.41
4:3:175:MET:HE3	4:3:179:ASN:CG	2.45	0.41
4:3:253:ALA:O	4:3:262:ILE:N	2.42	0.41
4:3:257:CYS:HB2	4:3:258:HIS:CD2	2.54	0.41
8:7:323:ILE:O	8:7:378:ARG:NH1	2.53	0.41
13:D:963:ARG:HA	13:D:966:LEU:H	1.84	0.41
15:F:249:ASP:HB3	15:F:252:LEU:HB2	2.02	0.41
24:R:94:ASP:O	24:R:97:GLY:N	2.36	0.41
26:T:192:GLU:HG3	28:V:75:PHE:CB	2.44	0.41
28:V:109:LEU:HD23	28:V:109:LEU:H	1.84	0.41
34:o:214:ILE:H	34:o:214:ILE:HG13	1.44	0.41
35:p:737:ILE:HG21	35:p:737:ILE:HD13	1.62	0.41
41:v:97:TYR:CZ	41:v:115:TYR:HB3	2.55	0.41
1:0:8:ARG:CZ	1:0:37:LEU:HD13	2.50	0.41
5:4:237:LEU:HD21	5:4:261:PHE:HZ	1.86	0.41
5:4:403:PHE:HA	6:5:8:VAL:HG13	2.01	0.41
8:7:354:PRO:HA	8:7:416:ILE:HD12	2.03	0.41
11:A:464:TRP:CD1	11:A:464:TRP:O	2.73	0.41
12:B:176:HIS:HE1	12:B:310:ASP:H	1.68	0.41
12:B:367:GLU:OE2	12:B:371:LYS:NZ	2.40	0.41
12:B:713:TRP:NE1	12:B:716:PRO:O	2.50	0.41
26:T:123:ASN:OD1	26:T:123:ASN:N	2.52	0.41
28:V:166:ILE:HG22	28:V:167:LEU:H	1.86	0.41
33:m:70:HIS:HA	33:m:73:MET:HE3	2.02	0.41
33:m:93:ASP:OD1	33:m:93:ASP:C	2.64	0.41
34:o:1374:VAL:HG11	34:o:1411:LEU:HD21	2.02	0.41
35:p:794:VAL:O	35:p:946:GLY:N	2.48	0.41
40:u:91:GLN:HB3	40:u:98:PHE:HB2	2.01	0.41
15:f:402:ARG:HH22	15:f:403:ILE:HD12	1.85	0.41
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
5:4:400:ARG:NE	5:4:400:ARG:HA	2.36	0.41
7:6:173:ASN:N	7:6:434:GLU:OE2	2.49	0.41
7:6:193:VAL:HG11	7:6:283:ARG:HD3	2.01	0.41
8:7:383:LEU:HD21	8:7:388:ILE:HD11	2.02	0.41
11:A:639:LEU:O	11:A:639:LEU:HD13	2.20	0.41
12:B:62:ARG:H	12:B:62:ARG:HG2	1.57	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:110:PHE:CE2	25:S:148:PRO:HB3	2.54	0.41
28:V:229:ASP:HA	28:V:232:LYS:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y:15:DA:H5"	30:Y:15:DA:H8	1.85	0.41
30:Y:27:DT:H2'	30:Y:28:DT:C6	2.55	0.41
34:o:529:GLN:HG3	34:o:1094:SER:HB3	2.02	0.41
34:o:602:CYS:HB2	34:o:655:ILE:HD12	2.02	0.41
36:q:19:VAL:HG12	36:q:21:PHE:HD1	1.85	0.41
45:z:36:CYS:HB2	45:z:44:MET:HE1	2.03	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
7:6:364:LEU:HD23	7:6:410:TYR:CD1	2.56	0.41
8:7:618:VAL:HG11	8:7:664:VAL:HA	2.03	0.41
11:A:337:ARG:HD3	11:A:338:VAL:H	1.85	0.41
11:A:819:LYS:HE2	11:A:819:LYS:HB2	1.94	0.41
14:E:476:VAL:HG11	14:E:794:ALA:HB3	2.02	0.41
15:F:388:ILE:HA	15:F:392:ILE:HG12	2.03	0.41
24:R:178:LYS:HE3	26:T:157:ALA:HB2	2.01	0.41
26:T:31:TRP:CD1	26:T:62:LEU:HD21	2.56	0.41
27:U:104:LYS:HE3	27:U:191:LEU:HB2	2.01	0.41
27:U:172:ASP:OD1	27:U:172:ASP:N	2.51	0.41
27:U:172:ASP:O	27:U:173:ALA:C	2.64	0.41
34:o:389:THR:HG21	34:o:417:LYS:HB2	2.03	0.41
35:p:1091:ARG:O	35:p:1095:ILE:HG13	2.20	0.41
42:w:113:VAL:HG22	42:w:122:ARG:HG2	2.01	0.41
14:e:378:LYS:HZ3	14:e:378:LYS:HG2	1.61	0.41
14:e:703:MET:HE2	14:e:703:MET:HB3	1.83	0.41
15:f:83:LEU:HD11	18:i:42:PHE:HB2	2.03	0.41
1:0:8:ARG:NH1	1:0:9:CYS:SG	2.94	0.41
5:4:359:ILE:HG22	5:4:360:THR:N	2.35	0.41
13:D:1002:ARG:HB2	26:T:182:HIS:HD2	1.79	0.41
14:E:508:LYS:HB3	14:E:512:ASP:HB2	2.02	0.41
26:T:140:ARG:NH2	35:p:89:GLU:HB2	2.35	0.41
27:U:194:THR:O	27:U:195:GLU:HG3	2.21	0.41
28:V:187:ASP:HB2	28:V:189:ILE:HG22	2.02	0.41
34:o:576:GLN:HG3	34:o:577:PRO:HD2	2.02	0.41
34:o:890:ARG:HH21	34:o:1023:VAL:HG22	1.84	0.41
34:o:1121:VAL:N	34:o:1122:PRO:HD2	2.35	0.41
34:o:1262:MET:HB3	34:o:1265:ASP:CB	2.50	0.41
34:o:1478:GLU:HA	34:o:1481:LYS:HE2	2.02	0.41
40:u:92:VAL:HG13	40:u:128:TYR:CD2	2.55	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	2.49	0.41
15:f:320:ARG:HH11	15:f:320:ARG:HB2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:3:255:CYS:HB2	4:3:276:CYS:N	2.36	0.41
5:4:146:PRO:HA	5:4:149:ASP:OD2	2.21	0.41
7:6:128:SER:O	7:6:334:ARG:NH2	2.51	0.41
11:A:463:PRO:HD2	15:F:218:VAL:HG22	2.03	0.41
12:B:639:LYS:NZ	12:B:641:GLU:OE2	2.43	0.41
13:D:960:GLU:OE1	13:D:960:GLU:N	2.53	0.41
14:E:668:HIS:NE2	14:E:686:THR:OG1	2.42	0.41
15:F:396:LEU:HA	15:F:399:GLU:OE1	2.20	0.41
24:R:94:ASP:H	24:R:98:ASN:H	1.69	0.41
25:S:51:LEU:O	25:S:54:LYS:HG3	2.20	0.41
29:X:34:DC:H2"	29:X:35:DC:C5	2.55	0.41
36:q:33:SER:O	36:q:37:VAL:HG23	2.20	0.41
36:q:193:ARG:HA	36:q:193:ARG:HD3	1.77	0.41
37:r:31:THR:HG21	37:r:95:PHE:HA	2.03	0.41
15:f:216:LEU:HD21	15:f:254:GLN:O	2.21	0.41
2:1:422:LEU:HD21	4:3:224:LEU:HB3	2.02	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
5:4:96:TRP:HB3	5:4:110:LEU:HD23	2.03	0.41
11:A:335:LYS:HE2	11:A:495:LEU:HB2	2.03	0.41
12:B:887:ARG:NH2	12:B:917:ASP:OD2	2.49	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
20:L:110:THR:HG23	20:L:112:GLU:HG3	2.02	0.41
24:R:102:GLN:NE2	34:o:305:GLU:HG2	2.28	0.41
25:S:76:ARG:NH2	25:S:77:GLU:OE1	2.53	0.41
26:T:9:LEU:O	26:T:13:LYS:HG2	2.20	0.41
27:U:139:LEU:HA	40:u:160:ILE:CG1	2.28	0.41
30:Y:-29:DT:H2"	30:Y:-28:DC:C5	2.56	0.41
30:Y:0:DT:H2"	30:Y:1:DG:H5'	2.03	0.41
35:p:782:ILE:HG12	35:p:967:ILE:HD11	2.03	0.41
36:q:246:LEU:HD23	36:q:246:LEU:HA	1.88	0.41
38:s:84:ILE:HD11	38:s:113:SER:HB3	2.03	0.41
40:u:79:PRO:HG3	40:u:104:MET:SD	2.61	0.41
43:x:49:LEU:HD23	43:x:49:LEU:HA	1.80	0.41
19:j:173:HIS:HA	19:j:176:MET:HE3	2.02	0.41
1:0:84:LYS:CB	1:0:136:ASN:HD21	2.33	0.41
4:3:217:VAL:O	4:3:217:VAL:HG23	2.20	0.41
5:4:229:ASP:OD1	5:4:229:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:384:PRO:HB2	5:4:387:ILE:HG12	2.03	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
11:A:352:MET:HE3	11:A:352:MET:HB3	1.81	0.41
11:A:413:ASP:O	11:A:414:ILE:C	2.63	0.41
12:B:55:PRO:HB3	12:B:60:LEU:HD22	2.03	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:544:LEU:HD22	12:B:625:LEU:HD22	2.03	0.41
14:E:236:LEU:HD21	14:E:317:LEU:HB2	2.03	0.41
14:E:265:GLU:OE1	14:E:265:GLU:HA	2.20	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	1.85	0.41
25:S:58:GLN:C	25:S:60:GLU:N	2.76	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:-18:DG:H2"	29:X:-17:DG:H8	1.86	0.41
29:X:-18:DG:H2"	29:X:-17:DG:C8	2.56	0.41
29:X:10:DT:H2"	29:X:11:DC:C6	2.56	0.41
29:X:26:DC:H2"	29:X:27:DA:N7	2.35	0.41
30:Y:3:DA:O5'	35:p:188:ASN:ND2	2.53	0.41
33:m:52:GLU:OE1	33:m:52:GLU:N	2.40	0.41
34:o:129:ILE:HD13	34:o:129:ILE:HA	1.96	0.41
34:o:514:GLU:OE2	35:p:1101:GLN:HB2	2.21	0.41
34:o:1189:ASP:HA	34:o:1192:TRP:CZ2	2.56	0.41
34:o:1318:LYS:HE2	34:o:1330:ALA:HB1	2.03	0.41
35:p:214:LYS:H	35:p:214:LYS:HD3	1.86	0.41
35:p:699:HIS:CD2	35:p:701:SER:H	2.39	0.41
35:p:810:PHE:HZ	35:p:812:ARG:HE	1.67	0.41
37:r:37:VAL:O	37:r:41:LEU:HG	2.20	0.41
37:r:76:ASN:O	37:r:80:ILE:HG13	2.21	0.41
43:x:22:LEU:O	43:x:26:GLN:HG2	2.20	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:149:PRO:HA	15:f:150:PRO:HD3	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:229:TRP:CZ3	5:4:58:ARG:CD	3.03	0.41
4:3:237:GLN:HG3	5:4:51:LEU:HD22	1.93	0.41
8:7:12:PHE:CE2	8:7:14:TYR:HB2	2.56	0.41
8:7:195:ALA:O	8:7:199:ILE:HG12	2.21	0.41
8:7:225:LEU:O	8:7:227:ARG:NH1	2.53	0.41
14:E:651:VAL:HG21	14:E:686:THR:HG21	2.01	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
23:Q:19:GLU:O	23:Q:22:ILE:HG12	2.21	0.41
25:S:44:GLN:HE21	25:S:44:GLN:HB3	1.66	0.41
27:U:19:LYS:HA	27:U:22:ILE:HB	2.03	0.41
29:X:22:DC:H2"	29:X:23:DG:C8	2.56	0.41
32:k:142:THR:OG1	32:k:143:GLY:N	2.55	0.41
33:m:77:ARG:CZ	33:m:77:ARG:HB3	2.51	0.41
34:o:457:ILE:HD12	35:p:1102:PHE:CE2	2.56	0.41
15:f:254:GLN:O	15:f:254:GLN:HG3	2.21	0.41
3:2:318:LEU:HD12	4:3:272:LEU:CD2	2.51	0.40
4:3:46:ASN:OD1	5:4:123:LEU:HD23	2.20	0.40
4:3:242:ILE:HD13	5:4:73:LEU:O	2.21	0.40
7:6:340:LEU:CD2	7:6:491:ALA:HB2	2.51	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
8:7:243:CYS:O	8:7:246:SER:OG	2.37	0.40
11:A:1068:ARG:HD2	11:A:1068:ARG:C	2.46	0.40
12:B:295:LEU:HD13	12:B:477:LEU:HD11	2.03	0.40
13:D:998:GLN:HE22	26:T:186:MET:HA	1.82	0.40
15:F:370:TRP:CH2	15:F:402:ARG:HB3	2.56	0.40
22:P:169:VAL:HG21	29:X:-27:DA:H2	1.85	0.40
24:R:74:LEU:HD21	35:p:823:PHE:H	1.86	0.40
27:U:139:LEU:HD12	40:u:160:ILE:H	1.85	0.40
27:U:192:ARG:O	27:U:195:GLU:HB3	2.21	0.40
28:V:166:ILE:HG22	28:V:167:LEU:N	2.36	0.40
28:V:189:ILE:HB	28:V:204:ASN:HB2	2.03	0.40
34:o:533:PRO:HD3	34:o:654:HIS:CD2	2.56	0.40
34:o:542:LEU:O	34:o:545:VAL:HG12	2.21	0.40
34:o:1175:ILE:HG12	34:o:1212:LEU:HD13	2.02	0.40
35:p:23:GLN:O	35:p:27:TRP:HD1	2.02	0.40
35:p:395:LEU:HD23	35:p:395:LEU:HA	1.95	0.40
35:p:1072:ARG:HD2	35:p:1153:TYR:CE1	2.56	0.40
14:e:467:LEU:HD23	14:e:467:LEU:HA	1.93	0.40
2:1:411:MET:HG2	2:1:411:MET:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:62:LEU:O	5:4:115:ARG:NH2	2.54	0.40
6:5:32:LYS:HE3	12:B:539:ARG:NH2	2.36	0.40
9:N:2:TRX:O	34:o:790:GLN:N	2.54	0.40
11:A:604:PRO:O	11:A:889:TYR:OH	2.34	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
12:B:464:ILE:HG12	12:B:513:LYS:HE2	2.02	0.40
12:B:957:MET:O	12:B:968:ARG:NH1	2.53	0.40
12:B:987:LEU:HG	12:B:988:PRO:HD2	2.03	0.40
15:F:329:LEU:HA	15:F:332:PHE:CB	2.52	0.40
27:U:139:LEU:HG	40:u:159:ALA:CA	2.50	0.40
27:U:141:ALA:HB3	40:u:107:PHE:CB	2.47	0.40
34:o:112:PHE:HB3	34:o:113:PHE:CD1	2.57	0.40
34:o:837:PHE:HB2	35:p:506:TRP:HZ3	1.86	0.40
34:o:1476:ASP:HB2	39:t:105:ILE:HG23	2.03	0.40
1:0:1:MET:HG3	8:7:345:ARG:NH1	2.36	0.40
1:0:32:GLU:OE1	1:0:32:GLU:N	2.47	0.40
2:1:303:ILE:HG22	2:1:307:PHE:HE2	1.87	0.40
5:4:223:ALA:HA	5:4:226:ARG:HG2	2.02	0.40
5:4:448:HIS:CD2	5:4:452:LYS:HE3	2.56	0.40
8:7:28:LEU:HD22	8:7:55:LEU:CD2	2.52	0.40
8:7:604:VAL:O	8:7:608:ILE:HG22	2.21	0.40
11:A:411:GLU:H	11:A:411:GLU:HG3	1.64	0.40
11:A:511:LEU:N	11:A:511:LEU:HD13	2.36	0.40
11:A:592:SER:OG	11:A:695:GLY:O	2.31	0.40
11:A:731:LEU:HD23	11:A:731:LEU:HA	1.92	0.40
12:B:881:GLY:HA3	17:H:218:PRO:HB3	2.03	0.40
15:F:312:ILE:HG22	15:F:313:VAL:CG1	2.50	0.40
30:Y:15:DA:H2"	30:Y:16:DA:C8	2.56	0.40
34:o:391:ALA:HA	34:o:447:GLU:HA	2.02	0.40
34:o:601:ASN:HA	34:o:630:VAL:O	2.21	0.40
34:o:1286:ARG:NH2	42:w:54:TYR:HB2	2.36	0.40
44:y:98:LEU:O	44:y:102:GLU:HG3	2.20	0.40
14:e:479:THR:OG1	14:e:481:ASP:O	2.32	0.40
15:f:446:ASP:O	15:f:450:ALA:N	2.54	0.40
18:i:78:ARG:HD3	18:i:78:ARG:HA	1.78	0.40
1:0:85:ARG:HH12	1:0:140:LEU:H	1.67	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
7:6:530:ARG:O	7:6:534:TYR:CD2	2.75	0.40
8:7:72:TYR:HB3	8:7:206:VAL:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:963:ARG:C	13:D:966:LEU:H	2.29	0.40
14:E:239:LEU:HB3	14:E:307:LEU:HD21	2.03	0.40
15:F:324:ASP:CA	15:F:327:TRP:HB3	2.44	0.40
17:H:132:LYS:HG3	17:H:134:LEU:H	1.86	0.40
30:Y:0:DT:H5"	35:p:747:LEU:HD12	2.03	0.40
31:c:105:ASN:OD1	31:c:105:ASN:N	2.55	0.40
34:o:765:ASN:O	34:o:769:MET:HG3	2.22	0.40
34:o:784:VAL:HG13	35:p:978:ILE:CD1	2.52	0.40
34:o:1451:MET:HE3	34:o:1451:MET:HB3	1.93	0.40
35:p:94:SER:O	35:p:122:ALA:HB1	2.22	0.40
35:p:818:GLU:O	35:p:916:TYR:HB3	2.22	0.40
41:v:37:MET:HE1	41:v:132:LEU:HD21	2.03	0.40
1:0:84:LYS:HB3	1:0:136:ASN:ND2	2.36	0.40
3:2:174:LEU:HD23	8:7:533:ASP:CG	2.47	0.40
3:2:227:HIS:CE1	3:2:231:LEU:HD11	2.57	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
11:A:939:ILE:HG22	11:A:943:LYS:NZ	2.37	0.40
12:B:842:LEU:HD21	17:H:194:MET:HG2	2.03	0.40
13:D:1001:GLN:HG2	21:O:1:MET:HB3	2.04	0.40
17:H:47:GLU:OE1	17:H:113:ARG:NH2	2.54	0.40
17:H:201:GLN:HG3	17:H:215:ALA:HA	2.04	0.40
24:R:309:PRO:HG2	24:R:312:LYS:HB2	2.03	0.40
26:T:97:THR:OG1	26:T:107:GLU:OE2	2.27	0.40
27:U:32:LEU:HD12	27:U:54:PHE:HZ	1.86	0.40
27:U:152:PHE:HZ	40:u:96:GLY:N	2.17	0.40
28:V:133:ILE:HG22	28:V:134:ASP:N	2.36	0.40
30:Y:-19:DT:H2"	30:Y:-18:DC:O5'	2.21	0.40
34:o:847:LEU:HD11	35:p:720:PRO:HB3	2.03	0.40
34:o:1180:ASN:HB2	34:o:1183:SER:HB3	2.04	0.40
35:p:961:ILE:HG23	43:x:9:THR:HG21	2.03	0.40
40:u:119:PHE:HB2	40:u:128:TYR:CE1	2.57	0.40
15:f:217:SER:H	15:f:220:GLN:HE21	1.70	0.40
15:f:284:ARG:HH21	15:f:284:ARG:HD2	1.76	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%)	156 (92%)	13 (8%)	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%)	573 (95%)	27 (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
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%)	392 (96%)	15 (4%)	1 (0%)	43 77
15	f	399/677 (59%)	379 (95%)	20 (5%)	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 26
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 28
20	L	74/161 (46%)	72 (97%)	2 (3%)	0	100 100
20	l	105/161 (65%)	100 (95%)	5 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	263 (95%)	13 (5%)	2 (1%)	18	55
25	S	174/517 (34%)	163 (94%)	10 (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%)	1398 (96%)	46 (3%)	4 (0%)	36	72
35	p	1145/1174 (98%)	1106 (97%)	39 (3%)	0	100	100
36	q	253/275 (92%)	245 (97%)	8 (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%)	166 (98%)	3 (2%)	0	100	100
41	v	146/150 (97%)	141 (97%)	5 (3%)	0	100	100
42	w	112/125 (90%)	109 (97%)	3 (3%)	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%)	565 (4%)	22 (0%)	44	77

All (22) 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
34	o	1274	GLU

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Mol	Chain	Res	Type
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
17	H	158	THR
27	U	137	THR
34	o	184	CYS

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 27
12	B	876/1083 (81%)	862 (98%)	14 (2%)	55 69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	D	147/815 (18%)	136 (92%)	11 (8%)	12 32
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 54
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 27
19	j	83/154 (54%)	82 (99%)	1 (1%)	63 74
20	L	71/141 (50%)	66 (93%)	5 (7%)	14 35
20	l	98/141 (70%)	97 (99%)	1 (1%)	68 77
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%)	233 (98%)	5 (2%)	47 65
25	S	154/448 (34%)	134 (87%)	20 (13%)	4 15
26	T	196/218 (90%)	193 (98%)	3 (2%)	57 71
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 67
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%)	1259 (98%)	21 (2%)	55 69
35	p	1004/1027 (98%)	987 (98%)	17 (2%)	53 68
36	q	234/252 (93%)	227 (97%)	7 (3%)	36 56
37	r	118/126 (94%)	118 (100%)	0	100 100
38	s	191/192 (100%)	188 (98%)	3 (2%)	55 69
39	t	71/111 (64%)	71 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	u	152/153 (99%)	150 (99%)	2 (1%)	61 73
41	v	129/131 (98%)	128 (99%)	1 (1%)	73 79
42	w	103/112 (92%)	99 (96%)	4 (4%)	28 49
43	x	56/56 (100%)	53 (95%)	3 (5%)	20 40
44	y	104/106 (98%)	101 (97%)	3 (3%)	37 57
45	z	41/55 (74%)	40 (98%)	1 (2%)	43 63
All	All	11634/19174 (61%)	11357 (98%)	277 (2%)	43 63

All (277) 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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	45	VAL
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

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Mol	Chain	Res	Type
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
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	119	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

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Mol	Chain	Res	Type
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	1027	ASP
34	o	1103	THR
34	o	1336	LEU
34	o	1385	VAL
34	o	1396	ARG
34	o	1458	ILE
35	p	90	GLN
35	p	192	LYS
35	p	214	LYS
35	p	215	TYR
35	p	222	ARG
35	p	235	ILE
35	p	351	VAL
35	p	388	TYR
35	p	438	ARG
35	p	466	VAL
35	p	534	VAL
35	p	598	VAL
35	p	719	SER
35	p	737	ILE
35	p	750	VAL
35	p	888	THR
35	p	1022	LEU
36	q	44	ILE
36	q	51	GLN
36	q	58	VAL
36	q	82	LEU
36	q	93	PHE
36	q	100	GLU
36	q	266	GLU
38	s	58	LEU
38	s	71	GLN
38	s	173	ILE
40	u	50	THR
40	u	152	VAL
41	v	141	VAL

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Mol	Chain	Res	Type
42	w	42	CYS
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
44	y	45	ILE
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
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 (207) 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	560	ASN
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	860	ASN
11	A	896	GLN
11	A	1073	GLN
12	B	30	HIS
12	B	36	ASN
12	B	137	HIS

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Mol	Chain	Res	Type
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
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	79	ASN
15	F	89	GLN
15	F	119	ASN
15	F	221	GLN
15	F	270	ASN

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Mol	Chain	Res	Type
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
24	R	98	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
26	T	64	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

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Mol	Chain	Res	Type
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	539	GLN
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	839	HIS
34	o	861	GLN
34	o	904	GLN
34	o	1032	GLN
34	o	1105	ASN
34	o	1163	HIS
34	o	1263	ASN
34	o	1410	HIS
35	p	72	GLN
35	p	90	GLN
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	699	HIS
35	p	725	GLN
35	p	755	GLN
35	p	986	GLN
35	p	1007	ASN
35	p	1021	HIS
35	p	1025	ASN

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Mol	Chain	Res	Type
35	p	1030	ASN
35	p	1097	HIS
36	q	18	ASN
36	q	260	GLN
36	q	265	HIS
37	r	48	ASN
37	r	76	ASN
37	r	129	GLN
38	s	64	HIS
38	s	71	GLN
38	s	210	GLN
41	v	131	ASN
42	w	41	ASN
42	w	50	ASN
44	y	22	ASN
44	y	36	ASN
44	y	69	HIS
45	z	26	ASN
13	d	912	ASN
13	d	943	GLN
14	e	246	HIS
14	e	320	HIS
14	e	336	HIS
14	e	368	ASN
14	e	420	ASN
14	e	424	GLN
15	f	30	GLN
15	f	64	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	4/6 (66%)	2 (50%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	Z	4	A
10	Z	6	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	$\#\|Z\| > 2$
10	G2L	Z	6	30,10,48	23,26,30	1.20	3 (13%)	32,38,44	2.06	7 (21%)
9	HYP	N	8	9	6,8,9	0.77	0	5,10,12	2.19	2 (40%)
9	TRX	N	2	9	15,16,17	1.00	1 (6%)	19,22,24	1.54	2 (10%)
9	CSX	N	6	9	3,6,7	1.06	0	1,6,8	2.25	1 (100%)
9	ILX	N	1	9	8,9,10	0.61	0	9,11,13	1.32	2 (22%)

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
10	G2L	Z	6	30,10,48	-	2/9/27/31	0/3/3/3
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
9	CSX	N	6	9	-	1/1/5/7	-
9	ILX	N	1	9	-	7/11/12/14	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Z	6	G2L	C5-C4	3.13	1.47	1.38
10	Z	6	G2L	C6-N1	-2.37	1.34	1.38
10	Z	6	G2L	C5-N7	-2.14	1.34	1.39
9	N	2	TRX	CD2-CE2	2.08	1.44	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	Z	6	G2L	C5-C4-N3	-6.14	118.50	128.46
9	N	2	TRX	CA-CB-CG	5.20	123.45	113.51
10	Z	6	G2L	C2-N3-C4	4.89	121.02	112.30
10	Z	6	G2L	N9-C4-N3	4.57	135.11	125.94
9	N	8	HYP	O-C-CA	-3.28	116.19	124.78
10	Z	6	G2L	C6-C5-N7	3.14	136.08	130.25
9	N	8	HYP	CB-CG-CD	3.11	107.08	103.27
9	N	1	ILX	OD1-CD1-CG1	-2.86	104.84	111.07
10	Z	6	G2L	C3'-C2'-C1'	2.69	105.85	99.89
10	Z	6	G2L	C4-C5-N7	-2.62	106.57	110.72
9	N	6	CSX	CA-CB-SG	2.25	118.27	113.36
10	Z	6	G2L	O6-C6-C5	-2.07	121.11	126.60
9	N	2	TRX	CZ3-CH2-CZ2	2.05	122.42	120.17
9	N	1	ILX	CB-CA-C	-2.03	110.19	112.94

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	6	G2L	C3'-C4'-C5'-O5'
9	N	2	TRX	CA-CB-CG-CD2
10	Z	6	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 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	Z	6	G2L	3	0
9	N	8	HYP	1	0
9	N	2	TRX	2	0
9	N	6	CSX	1	0
9	N	1	ILX	2	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	2.89	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	-9.40	1.27	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	p	1201	W0F	O05-C04	6.83	1.60	1.45
49	p	1201	W0F	O05-C06	-5.84	1.28	1.42
49	p	1201	W0F	C12-C13	5.70	1.47	1.38
49	p	1201	W0F	C13-N09	-3.12	1.34	1.37
49	p	1201	W0F	C07-C03	-2.87	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	2.13	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	-14.44	75.37	108.36
49	p	1201	W0F	C07-C06-N09	8.15	136.31	113.22
49	p	1201	W0F	O05-C04-C03	-5.66	92.74	104.87
49	p	1201	W0F	O05-C04-C20	4.79	125.13	109.37
49	p	1201	W0F	O05-C06-C07	-4.10	97.70	106.64
49	p	1201	W0F	O21-C20-C04	3.93	122.52	108.99
49	p	1201	W0F	O32-P30-O29	3.90	117.72	104.64
49	p	1201	W0F	O33-P30-O31	-3.31	97.73	110.68
49	p	1201	W0F	C06-N09-C10	-3.23	117.51	126.70
49	p	1201	W0F	P26-O25-P22	-3.11	122.17	132.83
49	p	1201	W0F	O08-C07-C06	2.94	119.85	110.02
49	p	1201	W0F	P26-O29-P30	2.73	142.21	132.83
49	p	1201	W0F	O33-P30-O29	2.67	113.58	104.64
49	p	1201	W0F	O21-P22-O24	-2.36	99.85	109.07
49	p	1201	W0F	C10-N09-C13	2.05	108.42	106.71
49	p	1201	W0F	C13-C12-N11	-2.05	106.57	109.23

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

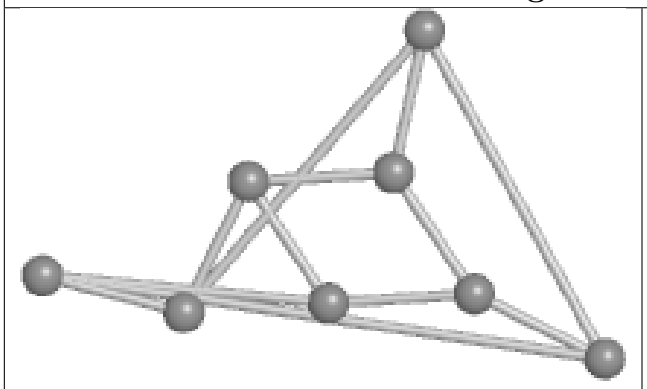
There are no ring outliers.

1 monomer is involved in 8 short contacts:

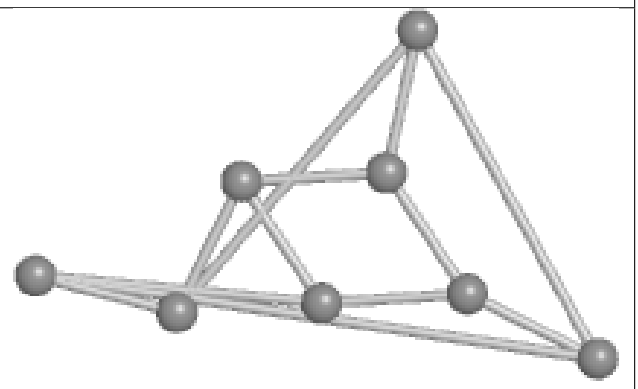
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	p	1201	W0F	8	0

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.

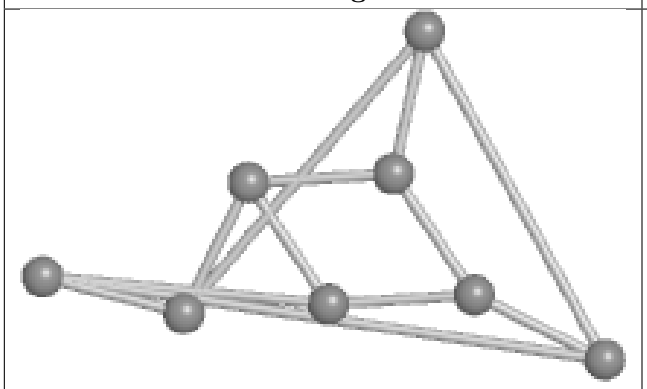
Ligand SF4 7 1000



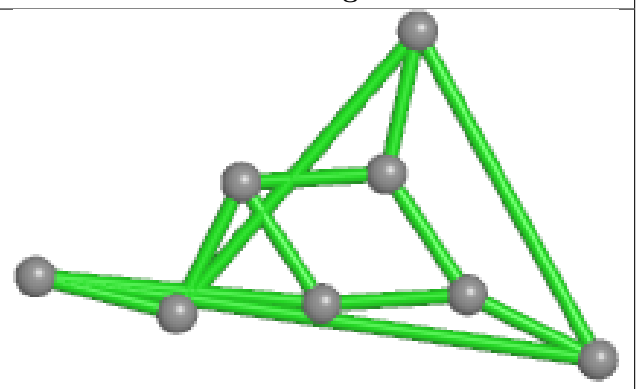
Bond lengths



Bond angles

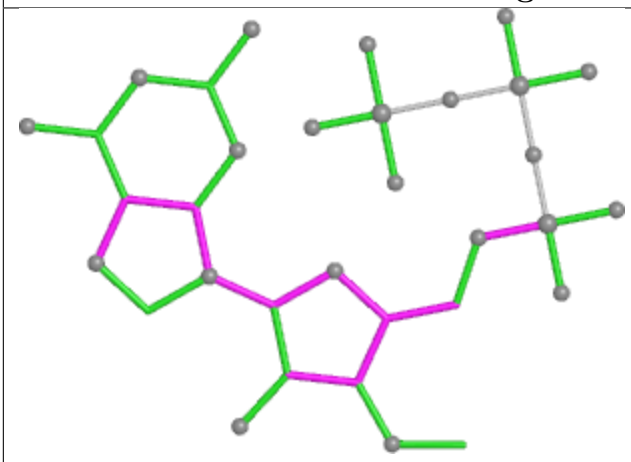


Torsions

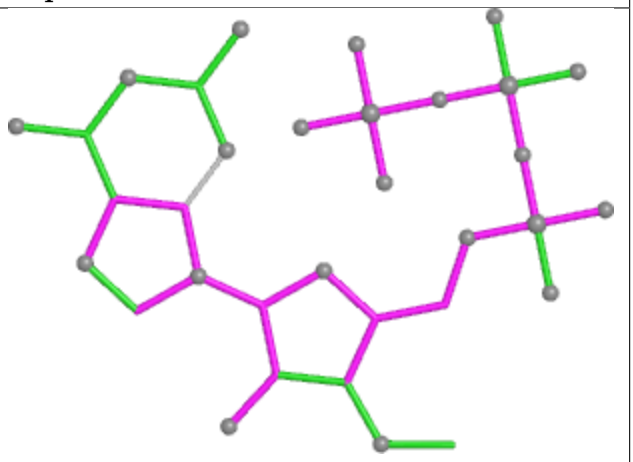


Rings

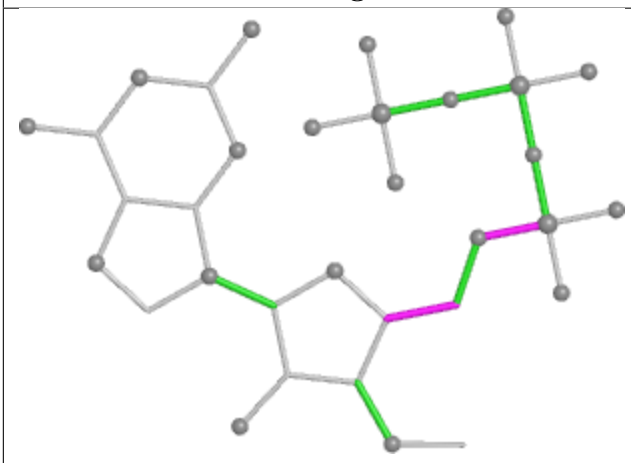
Ligand W0F p 1201



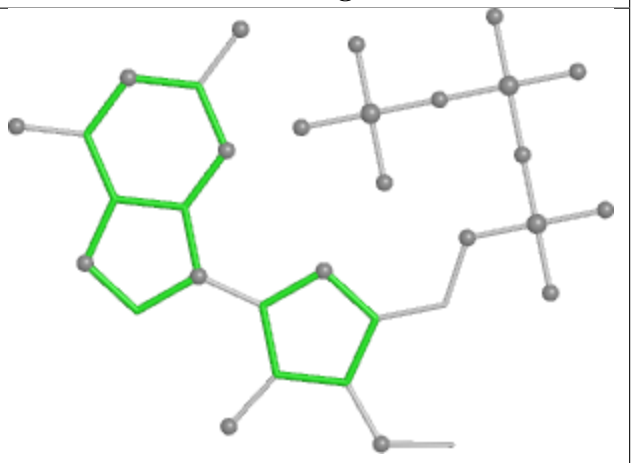
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

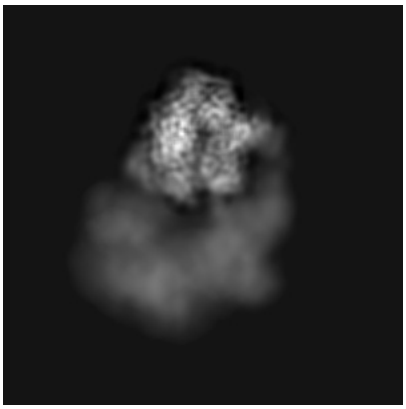
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37400. These allow visual inspection of the internal detail of the map and identification of artifacts.

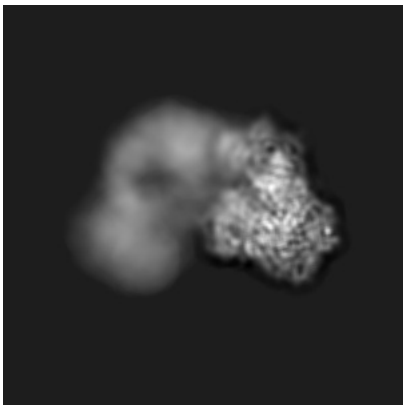
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

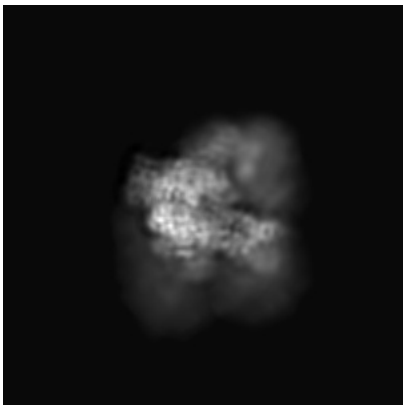
6.1.1 Primary map



X

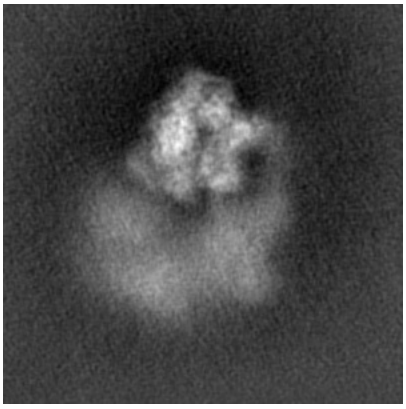


Y

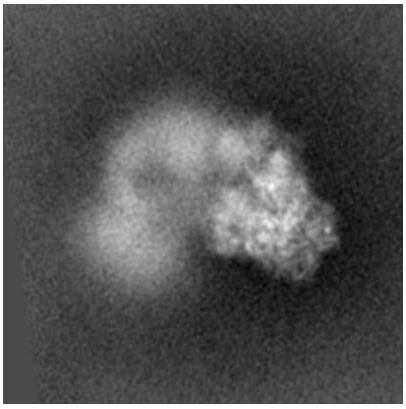


Z

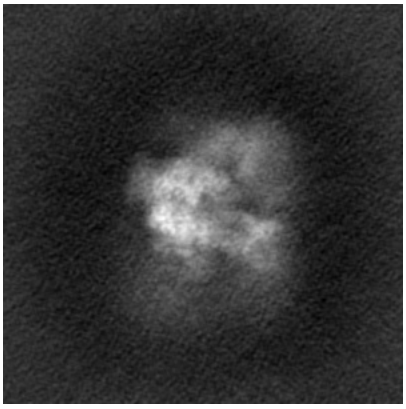
6.1.2 Raw map



X



Y

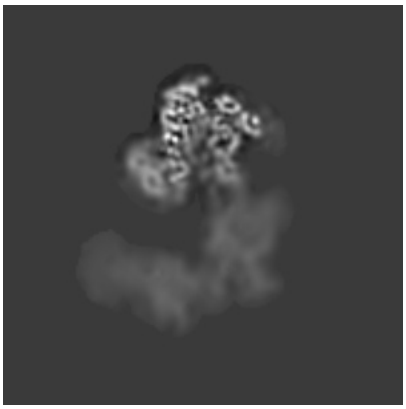


Z

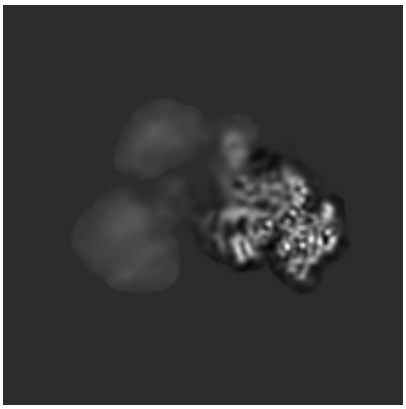
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

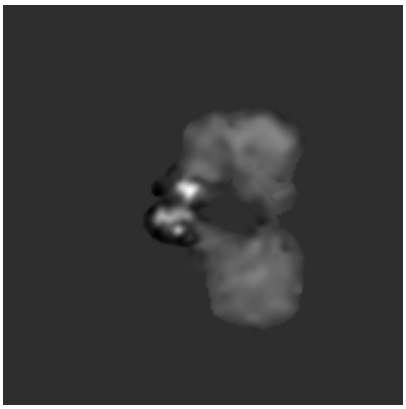
6.2.1 Primary map



X Index: 160

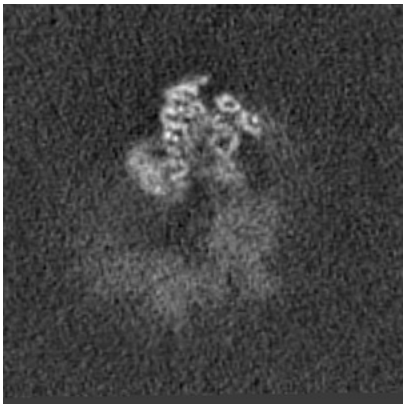


Y Index: 160

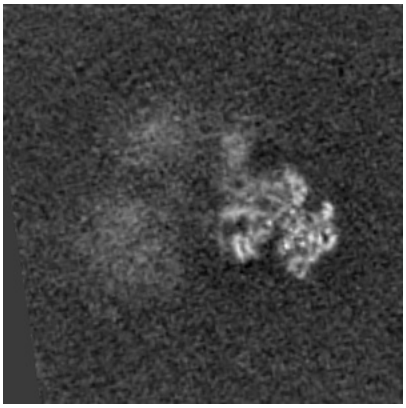


Z Index: 160

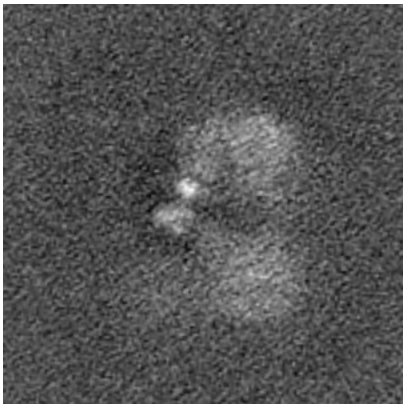
6.2.2 Raw map



X Index: 160



Y Index: 160

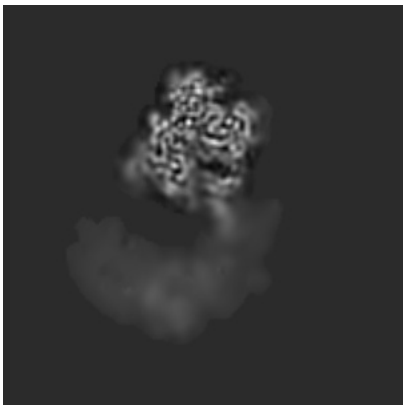


Z Index: 160

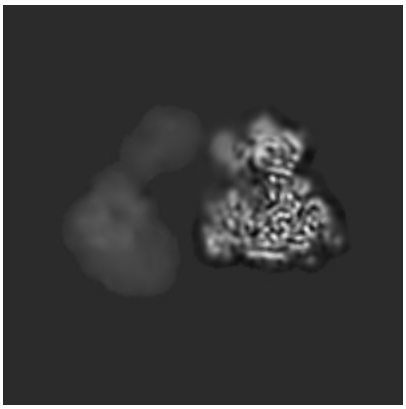
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 146

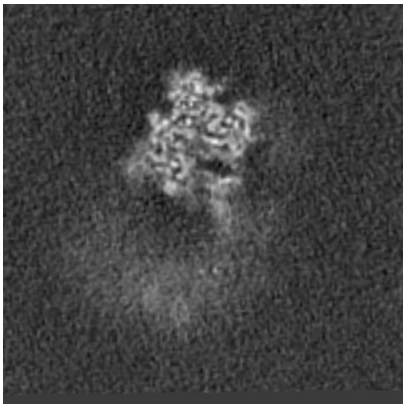


Y Index: 142

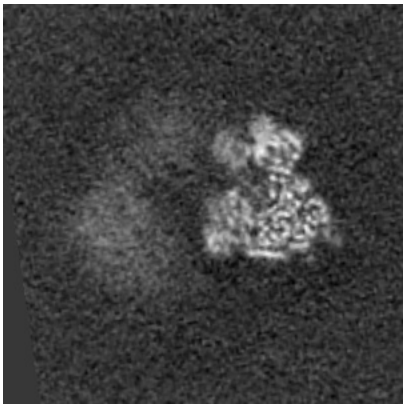


Z Index: 221

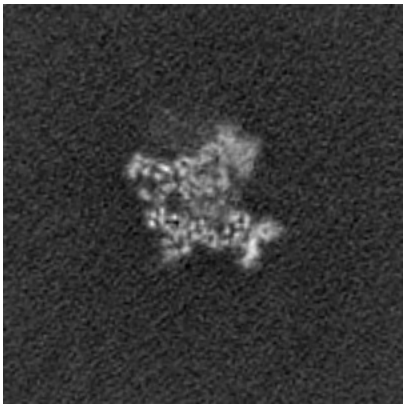
6.3.2 Raw map



X Index: 146



Y Index: 142

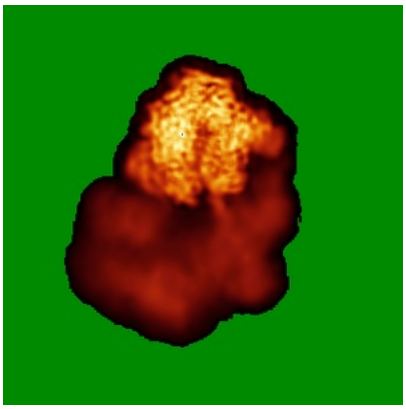


Z Index: 220

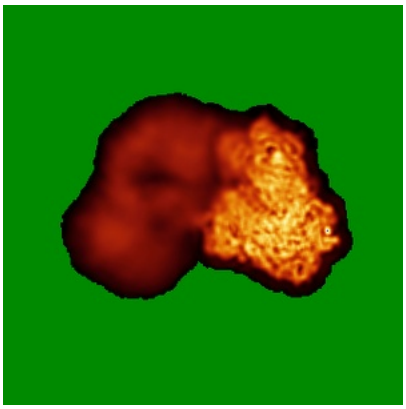
The images above show the largest variance slices of the map in three orthogonal directions.

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

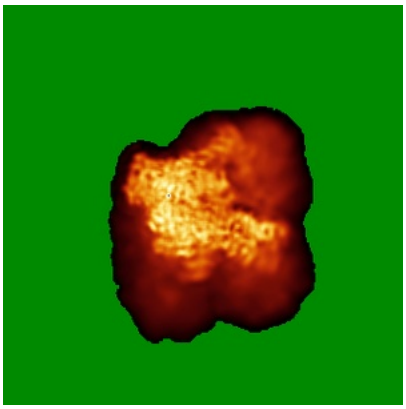
6.4.1 Primary map



X

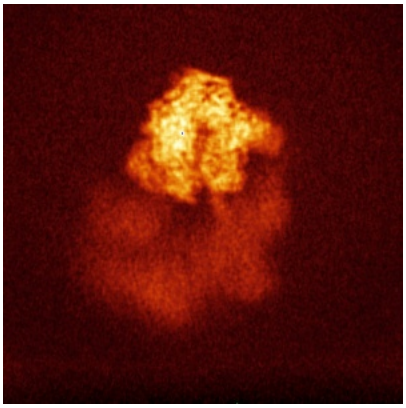


Y

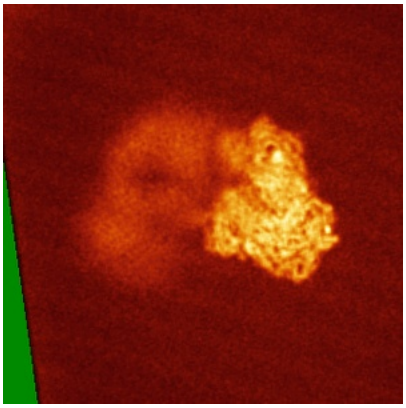


Z

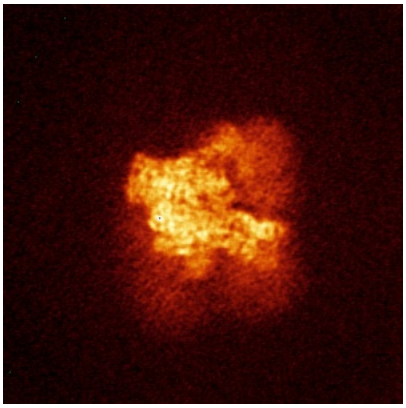
6.4.2 Raw map



X



Y

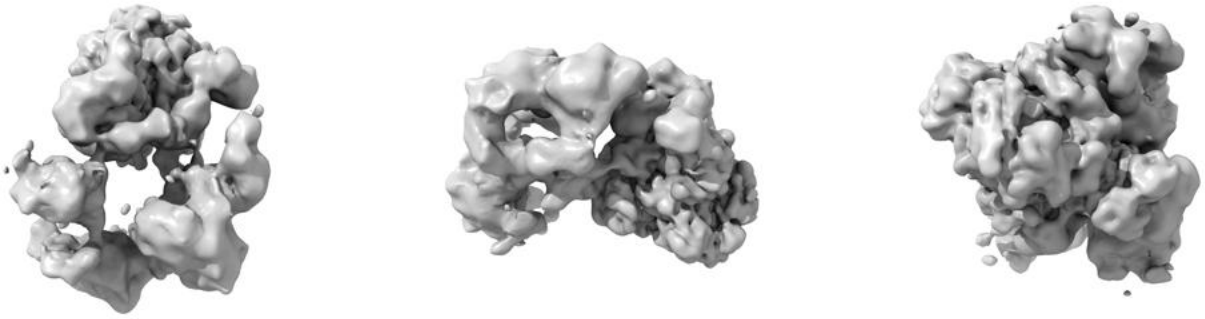


Z

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)

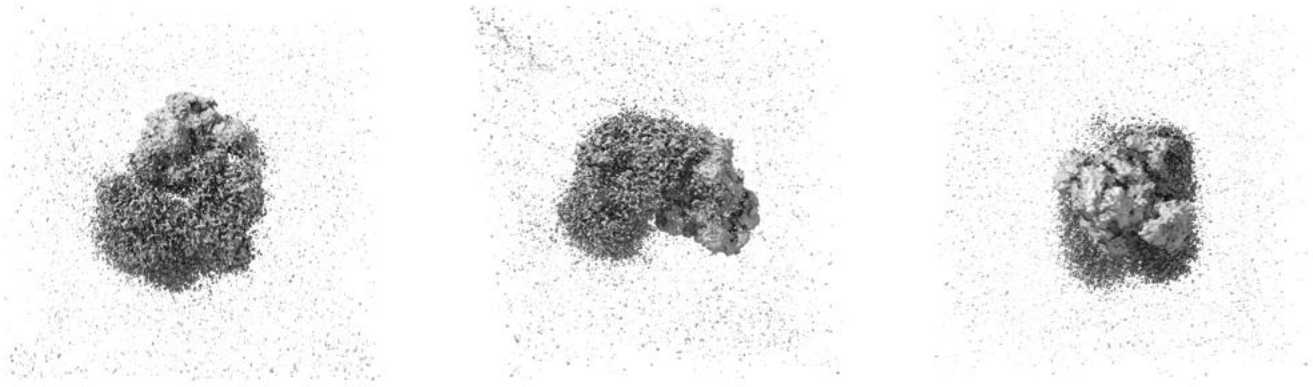
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.48. 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.

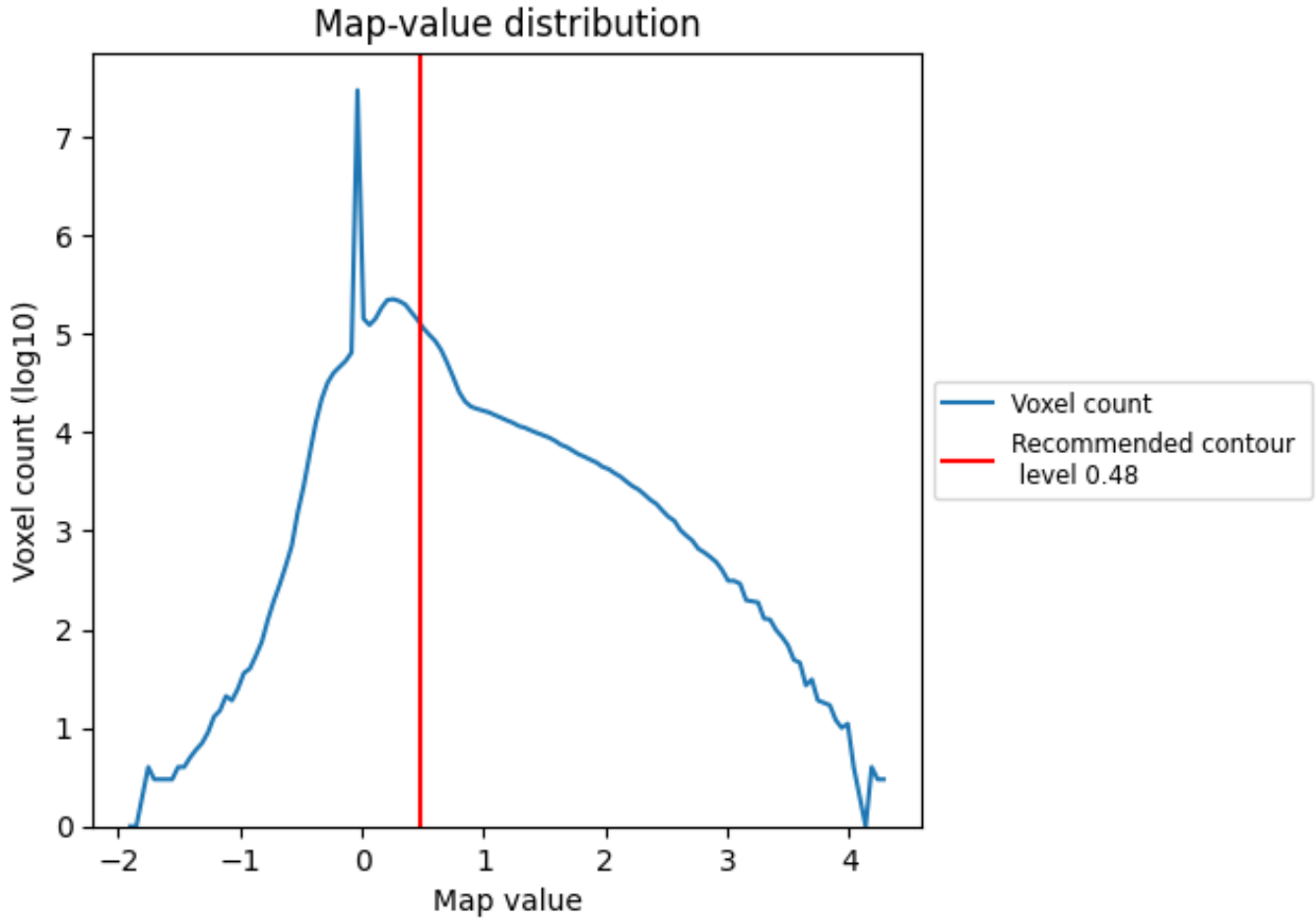
6.6 Mask visualisation (i)

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

7 Map analysis

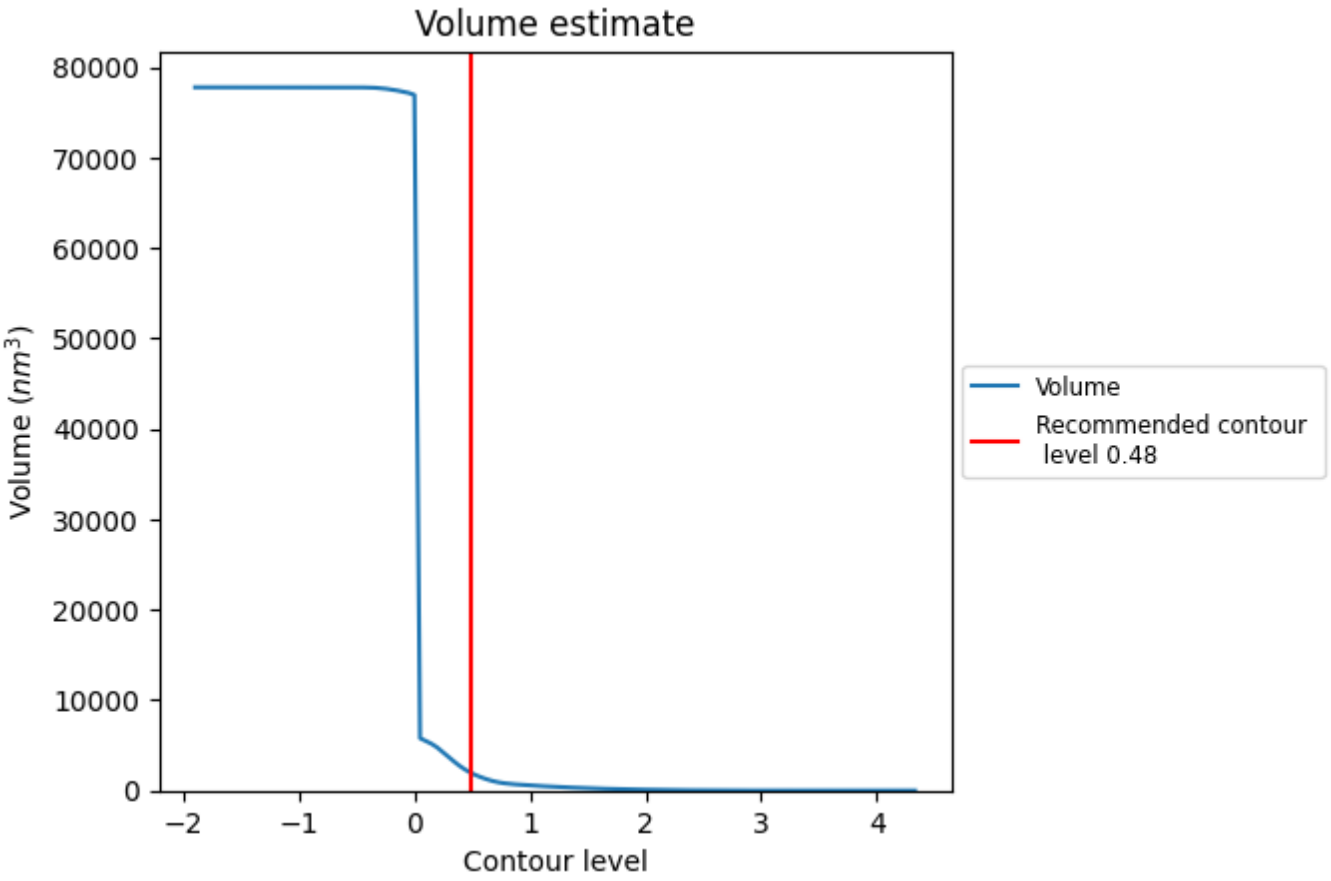
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

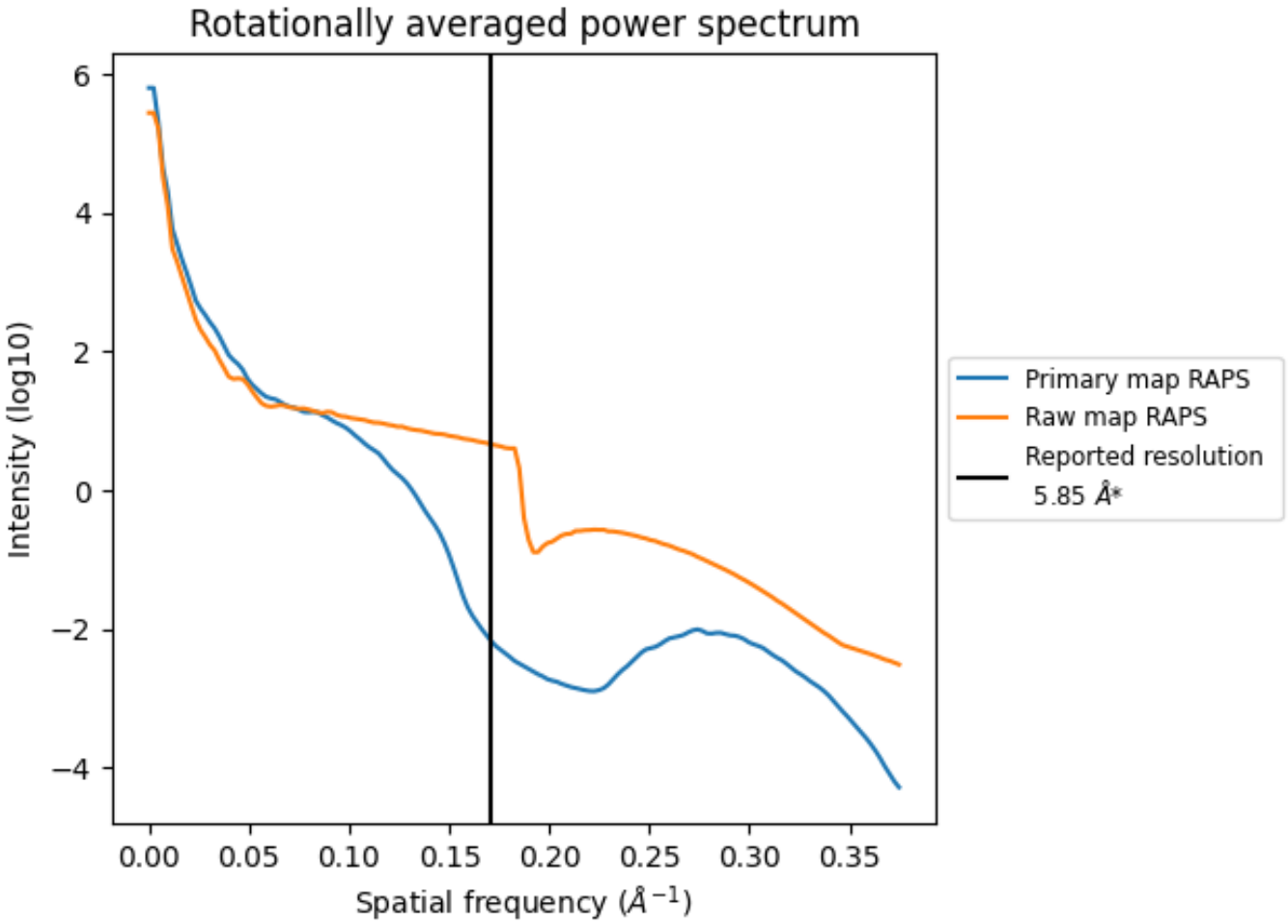
7.2 Volume estimate



The volume at the recommended contour level is 2009 nm^3; this corresponds to an approximate mass of 1814 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)

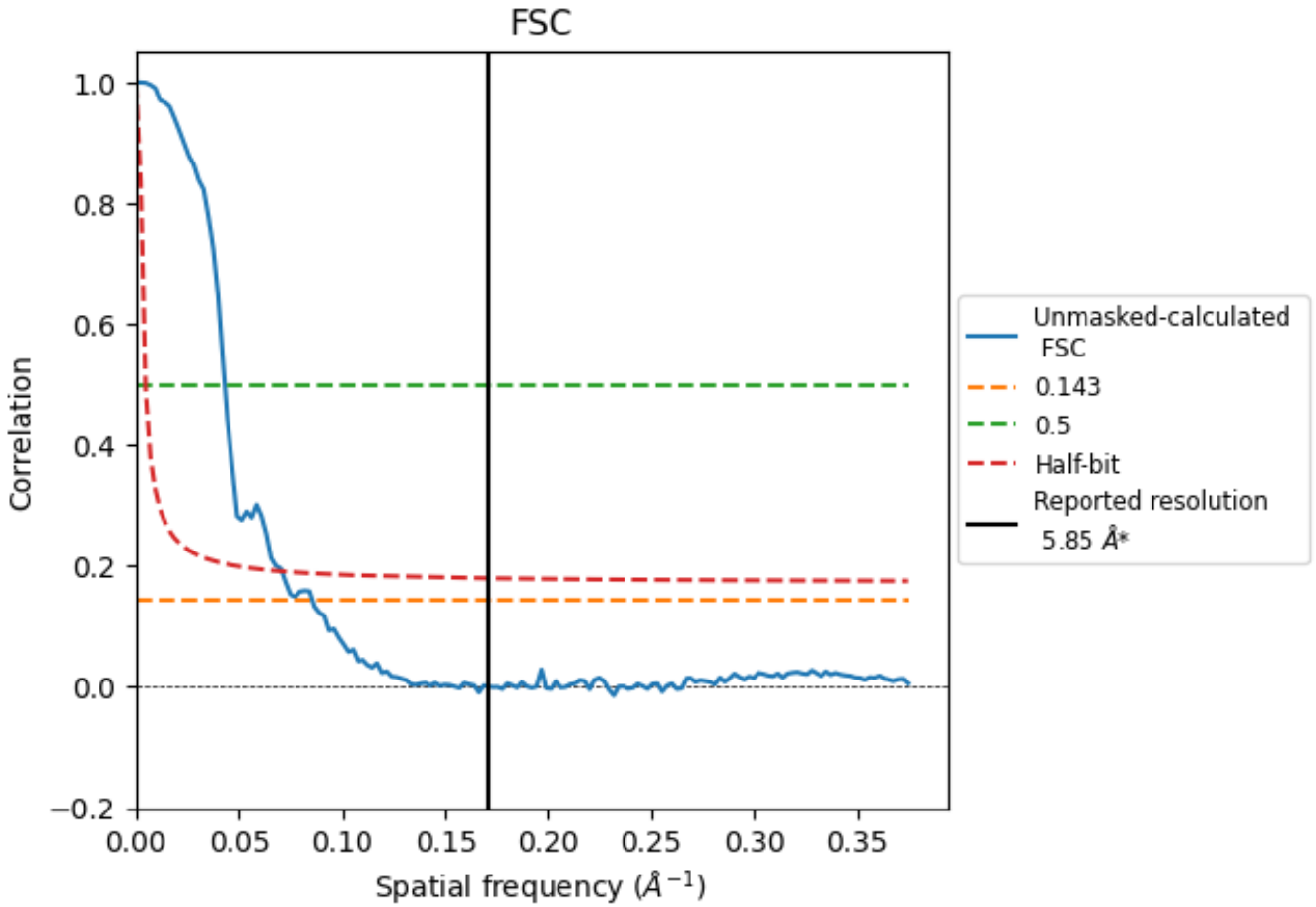


*Reported resolution corresponds to spatial frequency of 0.171 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.171 Å^{-1}

8.2 Resolution estimates (i)

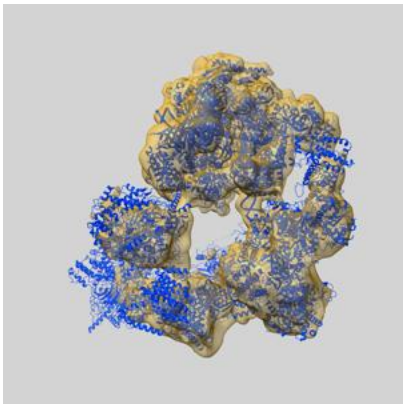
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.85	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	11.67	23.20	14.14

*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 11.67 differs from the reported value 5.85 by more than 10 %

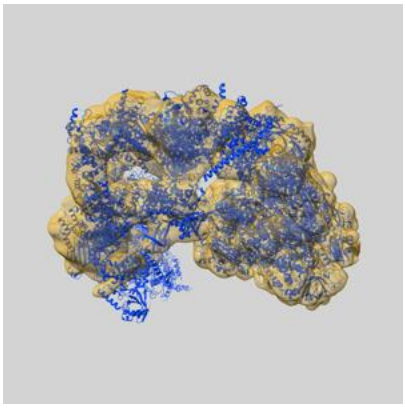
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37400 and PDB model 8WAP. Per-residue inclusion information can be found in section 3 on page 14.

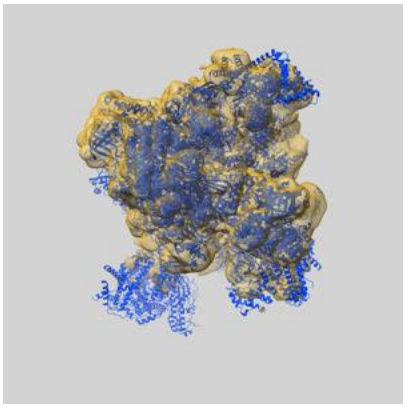
9.1 Map-model overlay



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.48 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.

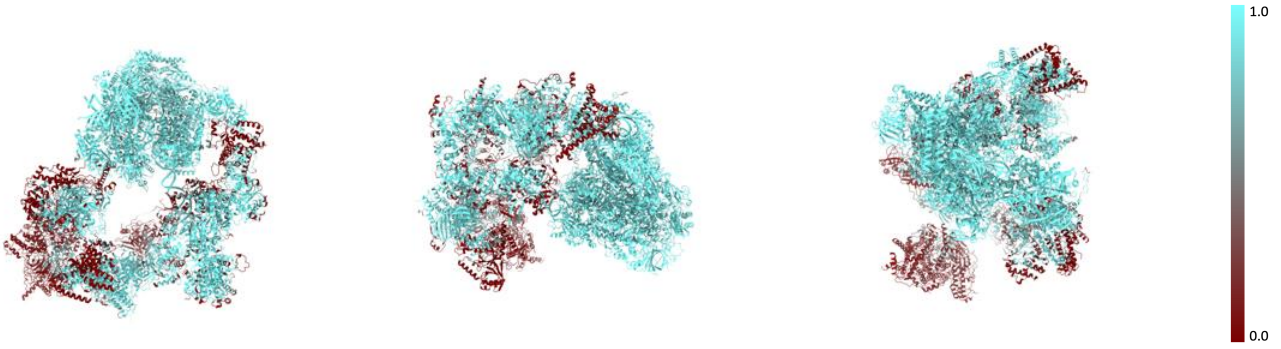
9.2 Q-score mapped to coordinate model (i)



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.

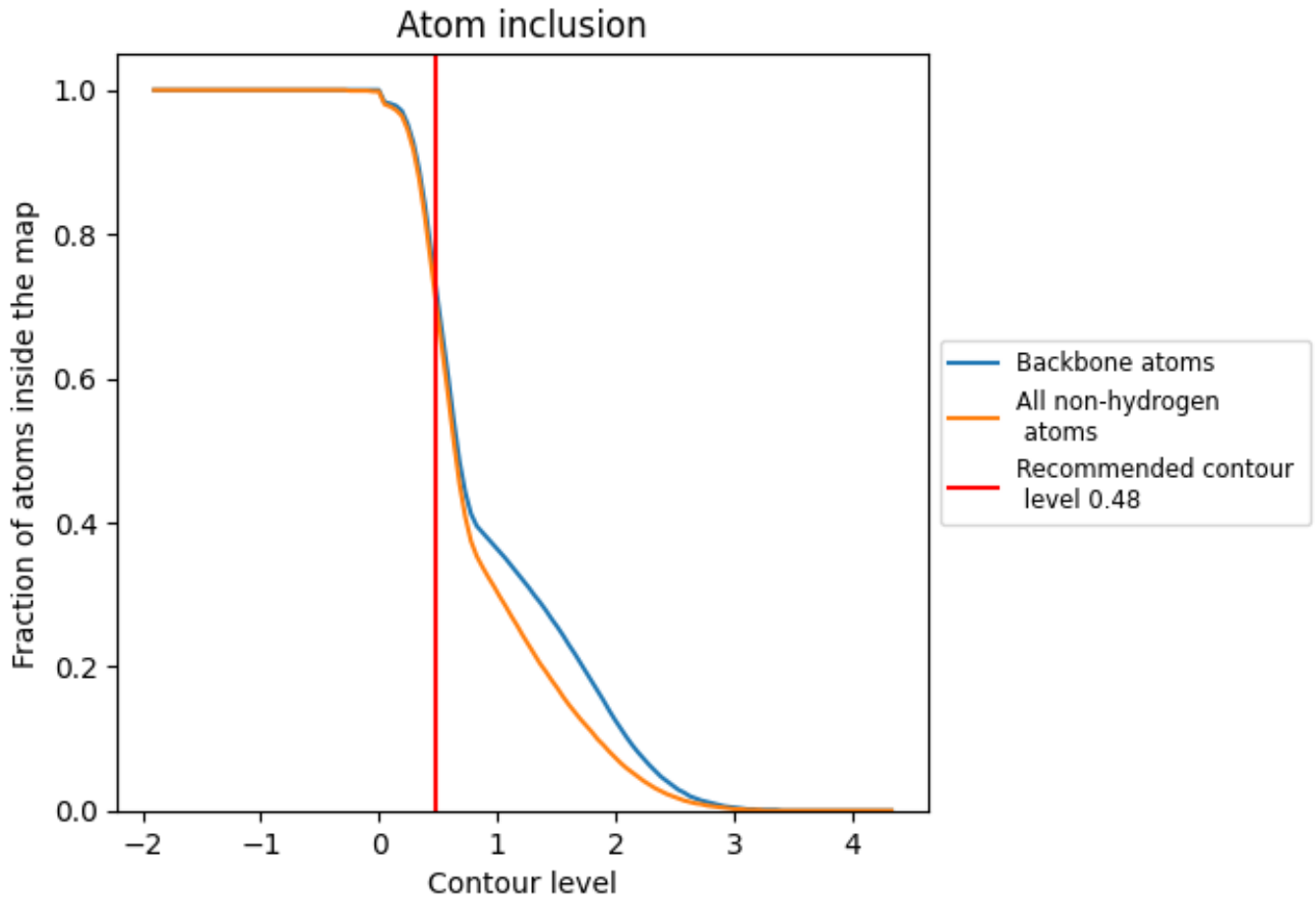
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.48).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.48) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7070	0.0810
0	0.0850	0.0580
1	0.6720	0.0530
2	0.9000	0.0640
3	0.8560	0.0400
4	0.7540	0.0630
5	0.5150	0.0160
6	0.6080	0.0420
7	0.7250	0.0570
A	0.2400	0.0310
B	0.9210	0.0510
D	0.3090	0.0290
E	0.6590	0.0430
F	0.4410	0.0270
G	0.0060	0.0170
H	0.8210	0.0420
I	0.4600	0.0240
J	0.6430	0.0680
L	0.1310	0.0450
N	0.9680	0.1310
O	0.9630	0.0830
P	0.9880	0.1260
Q	0.9510	0.1080
R	0.9600	0.1440
S	0.9270	0.0970
T	0.9660	0.1290
U	0.9530	0.0850
V	0.9700	0.1040
X	0.9870	0.1710
Y	0.9310	0.1480
Z	0.8990	0.1510
c	0.2340	0.0380
d	0.0000	0.0040
e	0.0980	0.0150
f	0.4770	0.0540



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.1270	0.0230
j	0.1030	0.0390
k	0.0000	-0.0130
l	0.0020	0.0420
m	0.0000	-0.0040
o	0.9420	0.1420
p	0.9310	0.1390
q	0.9610	0.1560
r	0.9860	0.1340
s	0.9670	0.1590
t	0.9670	0.1550
u	0.9830	0.1100
v	0.9680	0.1590
w	0.9630	0.1380
x	0.9420	0.1270
y	0.9580	0.1560
z	0.9780	0.1610