



Full wwPDB EM Validation Report ⓘ

Jul 10, 2026 – 04:20 AM JST

PDB ID : 9XA8 / pdb_00009xa8
EMDB ID : EMD-66678
Title : Cryo-EM structure of the 90S pre-ribosome (Enp1-Rrp12 WT) from *Chaetomium thermophilum*, state B1
Authors : Lau, B.; Li, Y.; Zhu, J.; Fischer, P.; Hong, X.; Yuan, R.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on : 2025-10-22
Resolution : 2.90 Å (reported)
Based on initial model : 6RXU

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

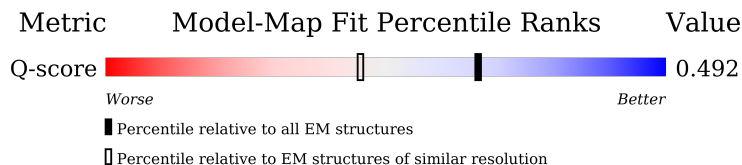
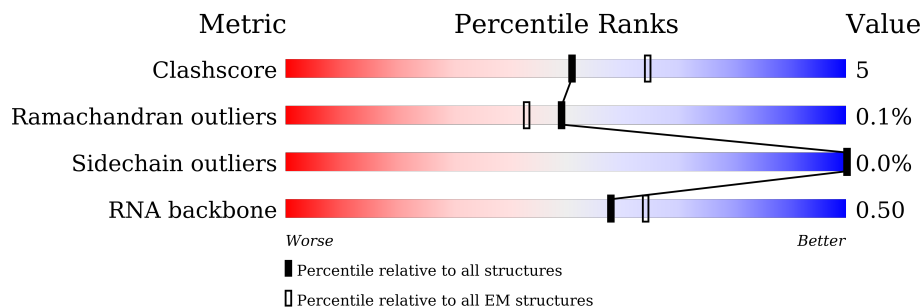
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.



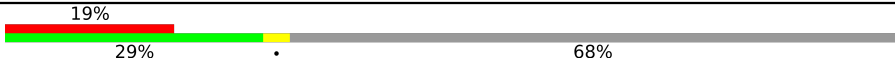
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	UA	904	
2	UB	907	

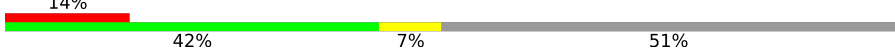
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Mol	Chain	Length	Quality of chain
3	UC	648	
4	UD	884	
5	UF	414	
6	UG	558	
7	UJ	1802	
8	UK	270	
9	UL	962	
10	UM	912	
11	UN	700	
12	UO	557	
13	UQ	960	
14	UR	618	
15	UU	1049	
16	UX	193	
17	UZ	391	
18	CA	313	
18	CB	313	
19	CC	523	
20	CD	582	
21	CE	127	
21	CF	127	
22	CG	630	
23	CH	411	
24	CI	1163	
25	CJ	183	

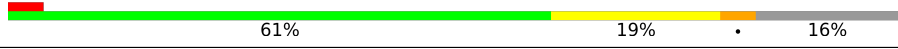
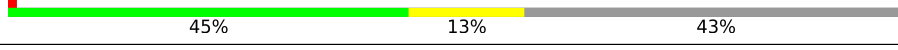
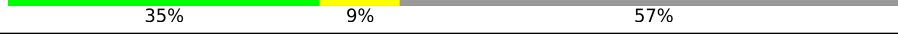
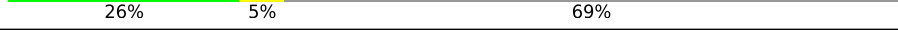
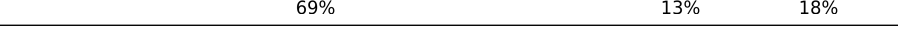
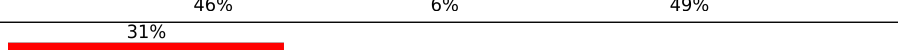
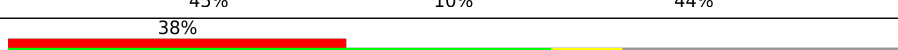
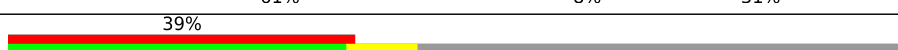
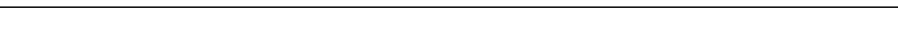
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Mol	Chain	Length	Quality of chain
26	CK	297	
27	CL	658	
28	CM	446	
29	CN	252	
29	CO	252	
30	CP	322	
31	CQ	259	
32	CR	1073	
32	CS	1073	
33	CT	203	
34	Ca	255	
35	Cb	264	
36	Cc	212	
37	Cd	239	
38	Ce	203	
39	Cf	202	
40	Cg	190	
41	Ch	151	
42	Ci	150	
43	Cj	143	
44	Ck	161	
45	Cm	130	
46	Cn	145	
47	Co	136	
48	Cp	68	

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Mol	Chain	Length	Quality of chain
49	CU	311	
50	C1	2311	
51	C2	274	
52	CW	668	
53	UT	2612	
54	UH	930	
55	UE	410	
55	UI	410	
56	US	549	
57	Cl	156	
58	CX	480	
59	CY	381	
60	CZ	609	
61	UP	364	

2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 227951 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 Periodic tryptophan protein 2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	UA	839	Total	C	N	O	P	S	
			6411	4118	1136	1132	1	24	0
									0

- Molecule 2 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	UB	566	Total	C	N	O	S		
			4506	2845	858	790	13	0	0

- Molecule 3 is a protein called Sas10 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	UC	205	Total	C	N	O	S		
			1633	1034	293	300	6	0	0

- Molecule 4 is a protein called UTP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	UD	777	Total	C	N	O	S		
			6108	3872	1099	1113	24	0	0

- Molecule 5 is a protein called U3 snoRNP protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	UF	331	Total	C	N	O	S		
			2599	1678	504	403	14	0	0

- Molecule 6 is a protein called U three protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	UG	479	Total	C	N	O	S		
			3765	2391	700	662	12	0	0

- Molecule 7 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	UJ	1637	Total	C	N	O	S	0	0
			12592	8061	2154	2326	51		

- Molecule 8 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	UK	217	Total	C	N	O	S	0	0
			1699	1068	351	275	5		

- Molecule 9 is a protein called Small-subunit processome Utp12 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	UL	785	Total	C	N	O	S	0	0
			6175	3940	1088	1130	17		

- Molecule 10 is a protein called U3 small nucleolar RNA-associated protein 13 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	UM	843	Total	C	N	O	S	0	0
			6545	4139	1151	1241	14		

- Molecule 11 is a protein called UTP14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	UN	177	Total	C	N	O	S	0	0
			1401	892	263	239	7		

- Molecule 12 is a protein called U3 small nucleolar RNA-associated protein 15 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	UO	503	Total	C	N	O	S	0	0
			3811	2417	698	683	13		

- Molecule 13 is a protein called UTP17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	UQ	789	Total	C	N	O	S	0	0
			6012	3834	1038	1119	21		

- Molecule 14 is a protein called UTP18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	UR	447	Total	C	N	O	P	S	
			3498	2210	656	621	1	10	
								0	0

- Molecule 15 is a protein called Putative U3 snoRNP protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	UU	908	Total	C	N	O	S		
			6778	4361	1243	1148	26		
								0	0

- Molecule 16 is a protein called UTP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	UX	190	Total	C	N	O	S		
			1480	938	286	246	10		
								0	0

- Molecule 17 is a protein called Ribosome biogenesis protein C8F11.04.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	UZ	235	Total	C	N	O	S		
			1815	1184	330	298	3		
								0	0

- Molecule 18 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CA	242	Total	C	N	O	S		
			1778	1149	327	293	9		
18	CB	237	Total	C	N	O	S		
			1816	1154	318	335	9		
								0	0

- Molecule 19 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	CC	387	Total	C	N	O	S		
			2866	1836	527	492	11		
								0	0

- Molecule 20 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	CD	446	Total	C	N	O	S		
			3355	2150	594	600	11		
								0	0

- Molecule 21 is a protein called H/ACA ribonucleoprotein complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CE	121	Total	C	N	O	S	0	0
			879	557	165	154	3		
21	CF	120	Total	C	N	O	S	0	0
			864	550	161	150	3		

- Molecule 22 is a protein called Ribosomal RNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CG	416	Total	C	N	O	S	0	0
			3245	2065	587	580	13		

- Molecule 23 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	CH	389	Total	C	N	O	S	0	0
			2888	1827	526	525	10		

- Molecule 24 is a protein called Bms1-type G domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	CI	841	Total	C	N	O	S	0	0
			6666	4277	1246	1113	30		

- Molecule 25 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	CJ	179	Total	C	N	O	S	0	0
			1434	918	283	226	7		

- Molecule 26 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	CK	297	Total	C	N	O	S	0	0
			2329	1476	445	400	8		

- Molecule 27 is a protein called Mpp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	CL	320	Total	C	N	O	S	0	0
			2466	1550	460	450	6		

- Molecule 28 is a protein called DDB1- and CUL4-associated factor 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	CM	445	Total	C	N	O	S	0	0
			3501	2195	672	619	15		

- Molecule 29 is a protein called Nucleolar essential protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	CN	226	Total	C	N	O	S	0	0
			1762	1119	306	327	10		
29	CO	215	Total	C	N	O	S	0	0
			1683	1067	293	313	10		

- Molecule 30 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	CP	233	Total	C	N	O	S	0	0
			1893	1209	340	335	9		

- Molecule 31 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	CQ	180	Total	C	N	O	S	0	0
			1413	898	257	251	7		

- Molecule 32 is a protein called RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	CR	846	Total	C	N	O	S	0	0
			6677	4278	1137	1233	29		
32	CS	836	Total	C	N	O	S	0	0
			6591	4217	1118	1228	28		

- Molecule 33 is a protein called Fcf2 pre-rRNA processing C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	CT	131	Total	C	N	O	S	0	0
			1035	656	197	178	4		

- Molecule 34 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ca	225	Total	C	N	O	S	0	0
			1821	1160	341	315	5		

- Molecule 35 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Cb	232	Total	C	N	O	S	0	0
			1851	1179	340	325	7		

- Molecule 36 is a protein called 40S ribosomal protein s5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Cc	192	Total	C	N	O	S	0	0
			1464	926	278	253	7		

- Molecule 37 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Cd	226	Total	C	N	O	S	0	0
			1819	1138	363	313	5		

- Molecule 38 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ce	159	Total	C	N	O		0	0
			1279	810	237	232			

- Molecule 39 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Cf	174	Total	C	N	O	S	0	0
			1398	872	283	242	1		

- Molecule 40 is a protein called 40S ribosomal protein s9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Cg	159	Total	C	N	O	S	0	0
			1248	804	258	184	2		

- Molecule 41 is a protein called 40S ribosomal protein S13-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	Ch	66	Total	C	N	O	0	0
			546	355	101	90		

- Molecule 42 is a protein called 40S ribosomal protein S14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ci	115	Total	C	N	O	S	0	0
			808	506	156	141	5		

- Molecule 43 is a protein called 40S ribosomal protein S16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Cj	126	Total	C	N	O	S	0	0
			943	613	177	151	2		

- Molecule 44 is a protein called 40S ribosomal protein S11-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ck	131	Total	C	N	O	S	0	0
			1082	695	210	172	5		

- Molecule 45 is a protein called 40S ribosomal protein S22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Cm	126	Total	C	N	O	S	0	0
			985	632	184	164	5		

- Molecule 46 is a protein called 40S ribosomal protein s23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Cn	96	Total	C	N	O	S	0	0
			702	456	134	110	2		

- Molecule 47 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Co	92	Total	C	N	O	S	0	0
			741	474	139	126	2		

- Molecule 48 is a protein called 40S ribosomal protein S28-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Cp	61	Total	C	N	O	S	0	0
			458	286	97	74	1		

- Molecule 49 is a protein called Faf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	CU	176	Total	C	N	O	S	0	0
			1337	822	265	244	6		

- Molecule 50 is a RNA chain called 35S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	C1	1587	Total	C	N	O	P	0	0
			33862	15109	6070	11096	1587		

- Molecule 51 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	C2	229	Total	C	N	O	P	0	0
			4869	2172	851	1617	229		

- Molecule 52 is a protein called Ribosome biogenesis protein ENP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	CW	383	Total	C	N	O	S	0	0
			2932	1862	531	525	14		

- Molecule 53 is a protein called UTP20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	UT	2027	Total	C	N	O	S	0	0
			15998	10300	2811	2819	68		

- Molecule 54 is a protein called UTP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	UH	799	Total	C	N	O	S	0	0
			6198	3903	1105	1171	19		

- Molecule 55 is a protein called Small-subunit processome Utp12 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	UE	178	Total	C	N	O	S	0	0
			1362	851	251	254	6		
55	UI	128	Total	C	N	O	S	0	0
			996	622	187	181	6		

- Molecule 56 is a protein called CCAAT-binding factor domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	US	451	Total	C	N	O	S	0	0
			3672	2389	608	660	15		

- Molecule 57 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Cl	80	Total	C	N	O	S	0	0
			633	400	115	117	1		

- Molecule 58 is a protein called Bystin-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	CX	267	Total	C	N	O	S	0	0
			2130	1384	374	362	10		

- Molecule 59 is a protein called U3 small nucleolar ribonucleoprotein protein lcp5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	CY	264	Total	C	N	O	S	0	0
			2095	1296	388	406	5		

- Molecule 60 is a protein called Protein BFR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	CZ	283	Total	C	N	O	S	0	0
			2270	1398	426	439	7		

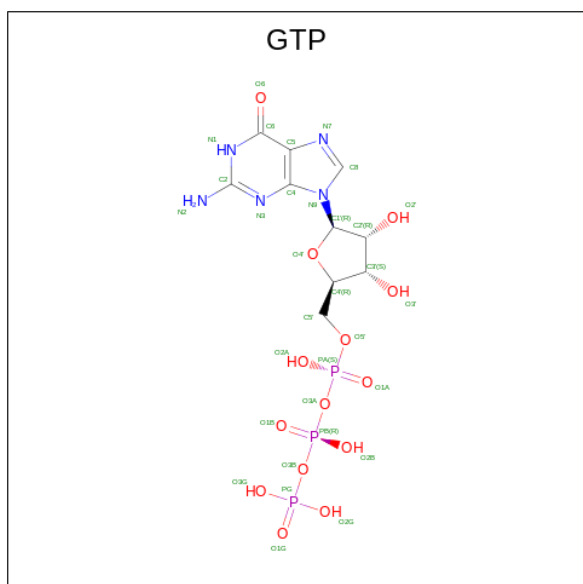
- Molecule 61 is a protein called UTP16.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	UP	54	Total	C	N	O	0	0
			422	264	88	70		

- Molecule 62 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
62	UX	1	Total	Zn	0
			1	1	

- Molecule 63 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

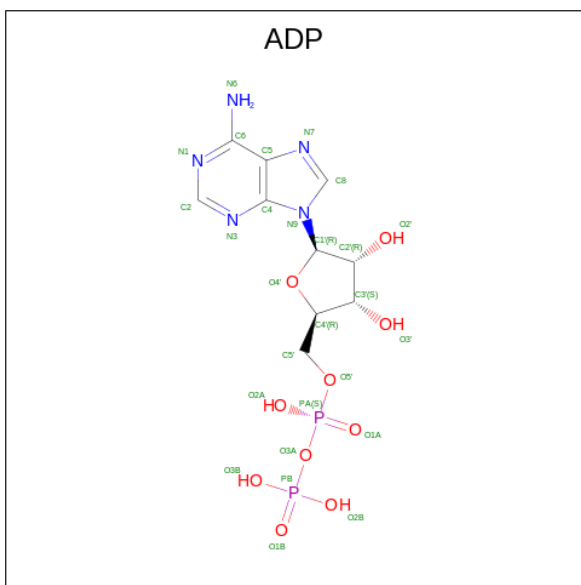


Mol	Chain	Residues	Atoms					AltConf
63	CI	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 64 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
64	CI	1	Total	Mg	0
			1	1	

- Molecule 65 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

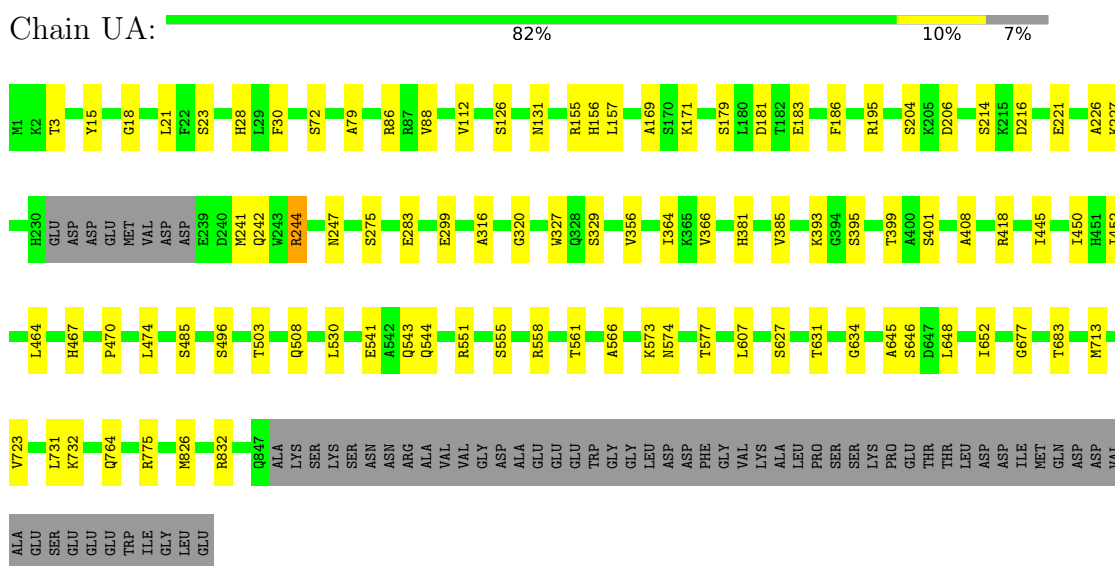


Mol	Chain	Residues	Atoms					AltConf
65	CS	1	Total	C	N	O	P	0
			27	10	5	10	2	

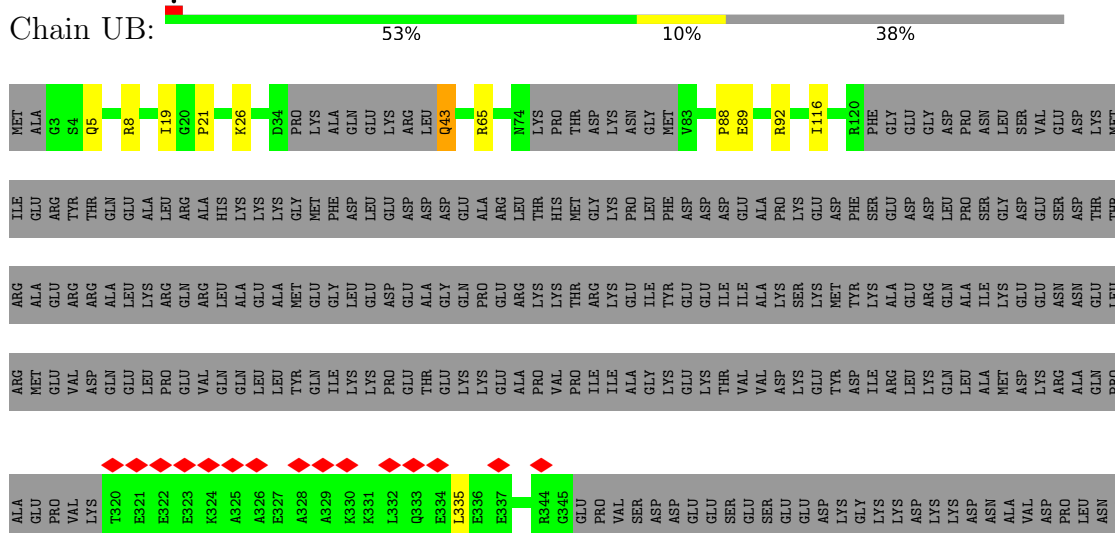
3 Residue-property plots

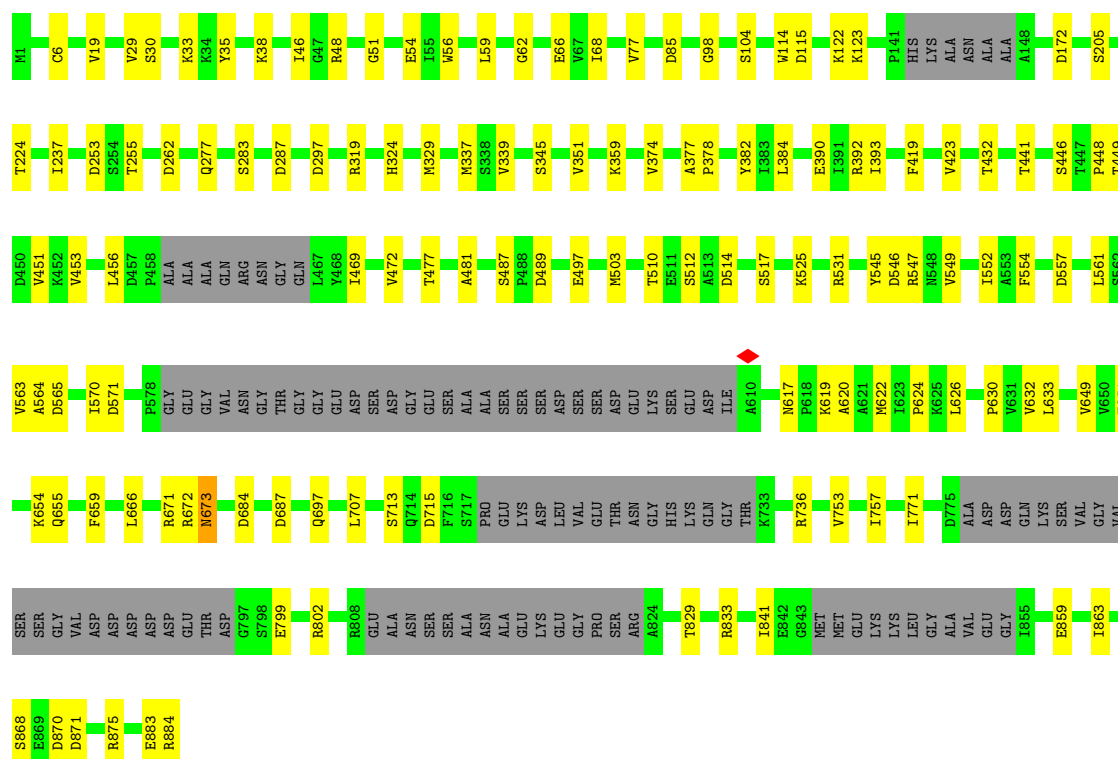
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Periodic tryptophan protein 2-like protein



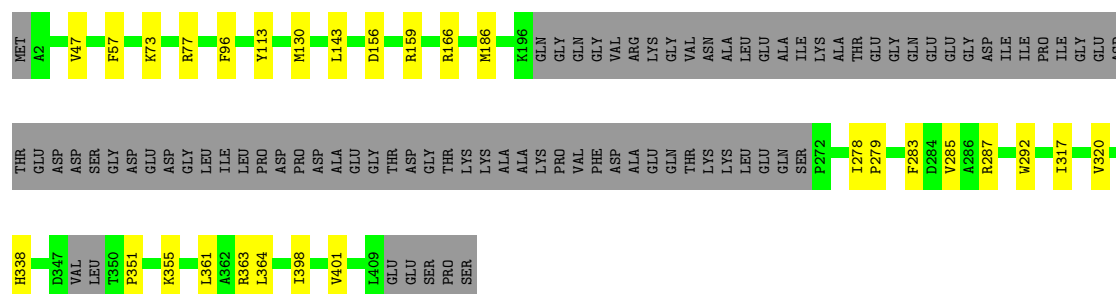
- Molecule 2: Nucleolar complex protein 14





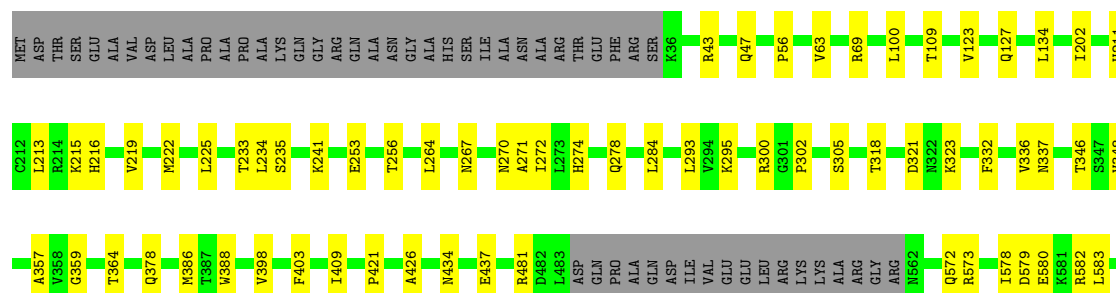
• Molecule 5: U3 snoRNP protein

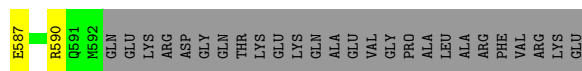
Chain UF: 73% 7% 20%



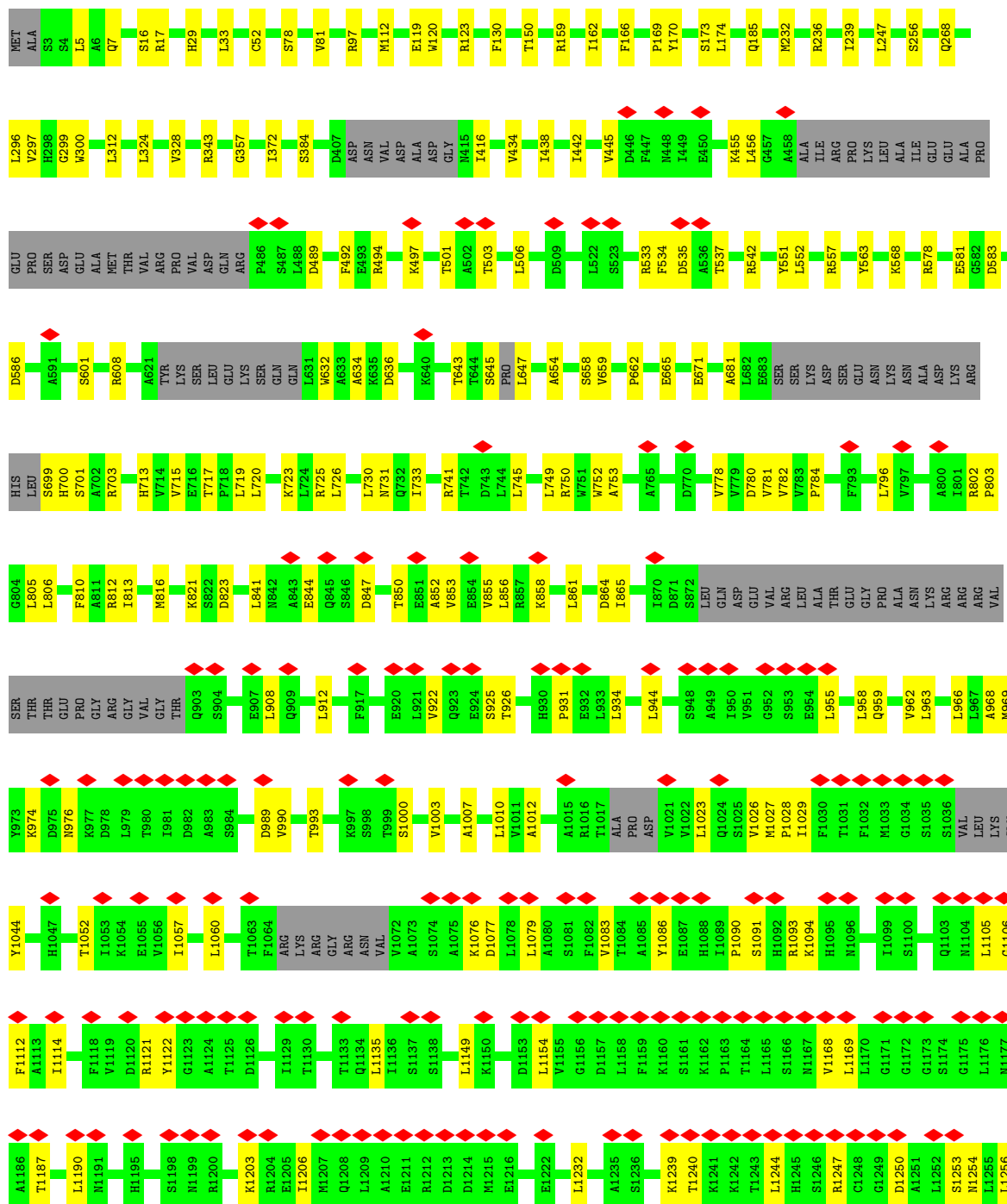
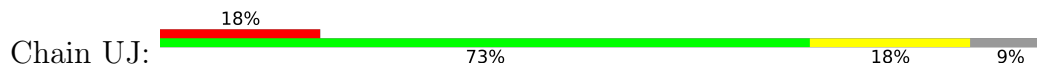
• Molecule 6: U three protein 7

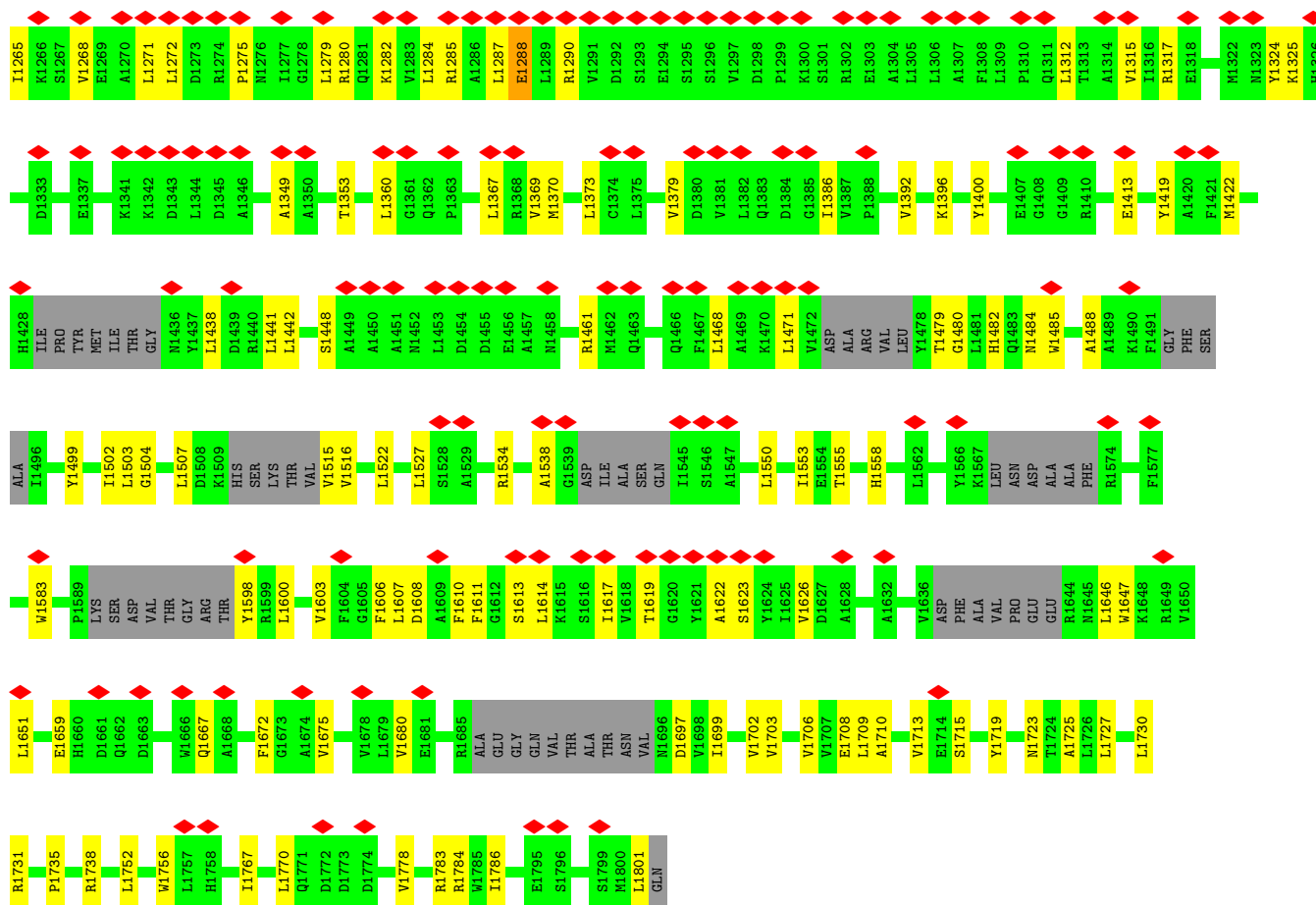
Chain UG: 74% 12% 14%





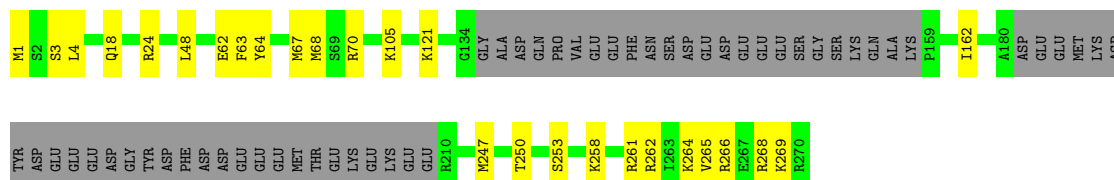
• Molecule 7: U3 small nucleolar RNA-associated protein 10





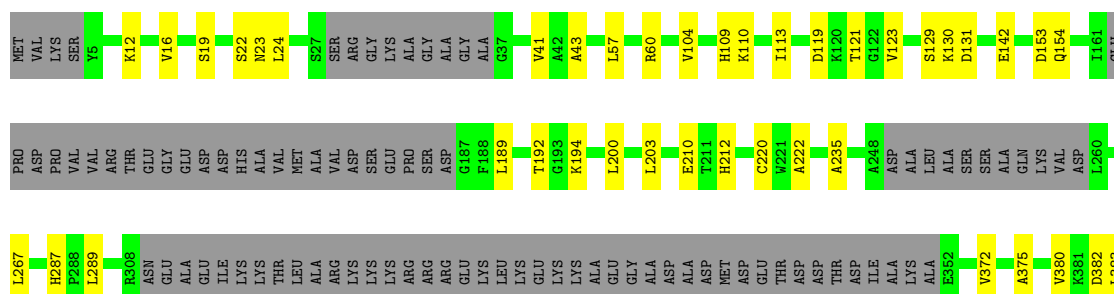
- Molecule 8: U3 small nucleolar RNA-associated protein 11

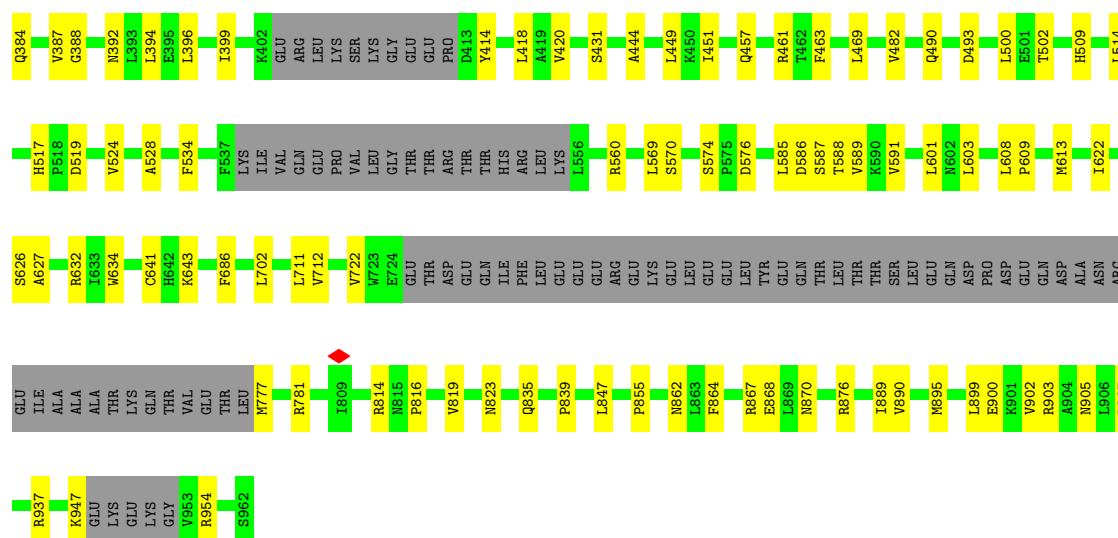
Chain UK: 71% 10% 20%



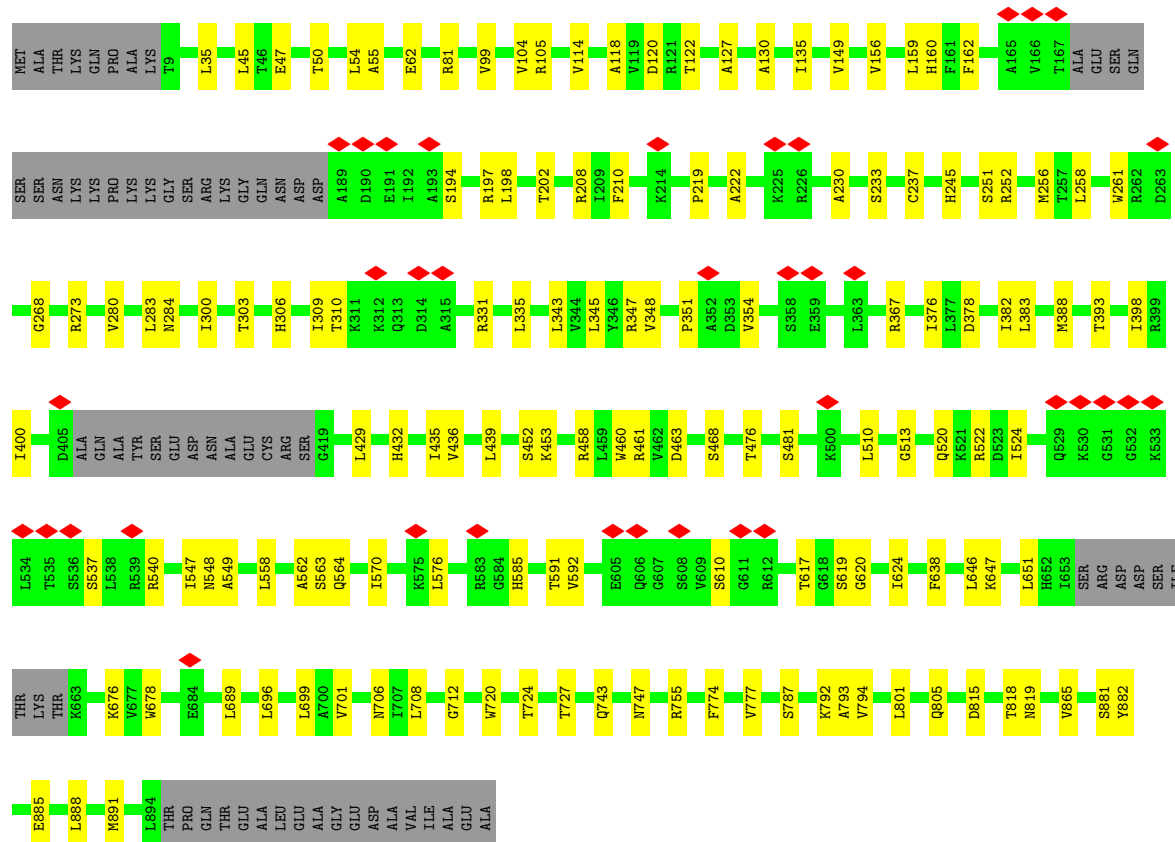
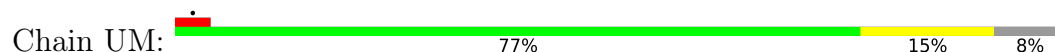
- Molecule 9: Small-subunit processome Utp12 domain-containing protein

Chain UL: 68% 13% 18%





- Molecule 10: U3 small nucleolar RNA-associated protein 13 C-terminal domain-containing protein

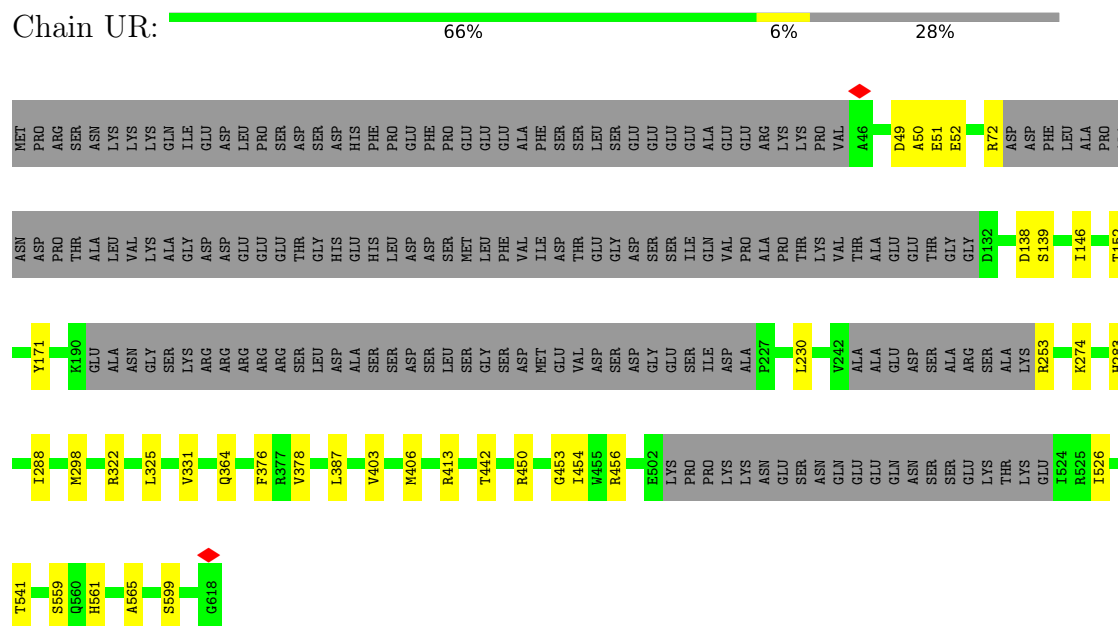


- Molecule 11: UTP14



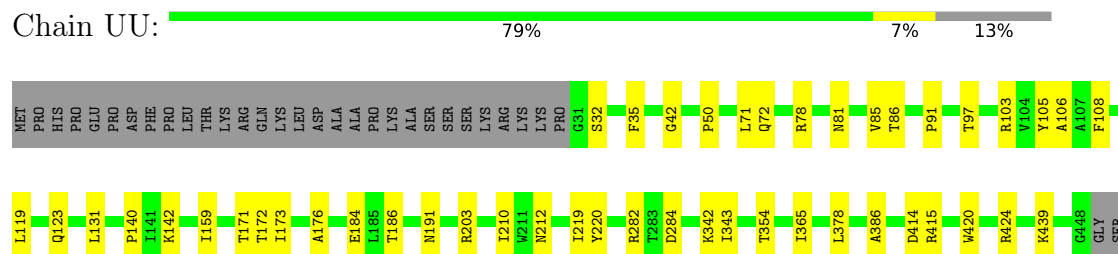
- Molecule 14: UTP18

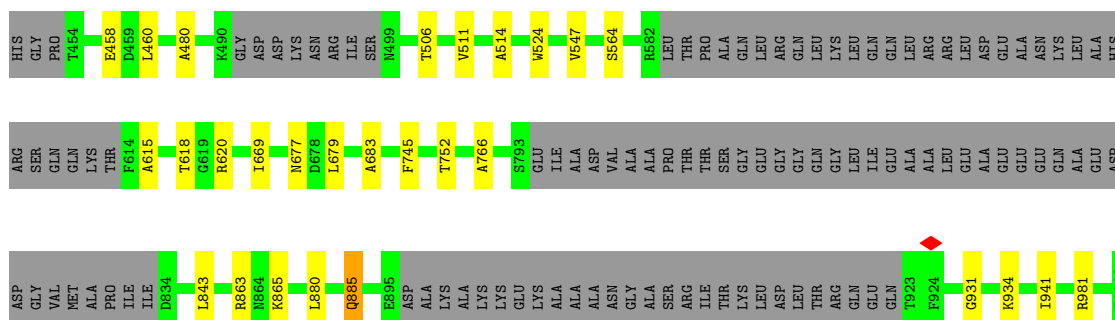
Chain UR:



- Molecule 15: Putative U3 snoRNP protein

Chain UU:





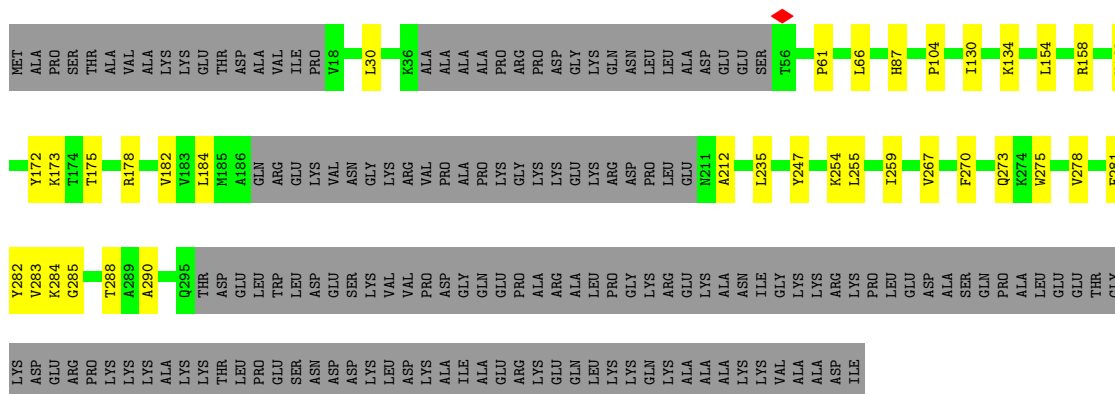
• Molecule 16: UTP24

Chain UX: 89% 10% .



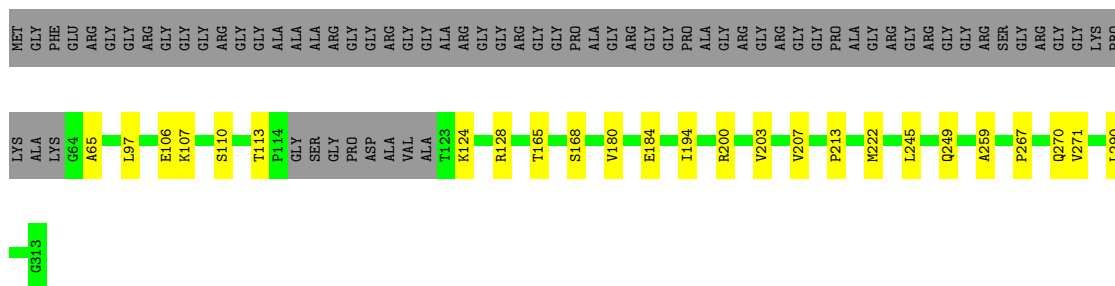
• Molecule 17: Ribosome biogenesis protein C8F11.04

Chain UZ: 51% 9% 40%



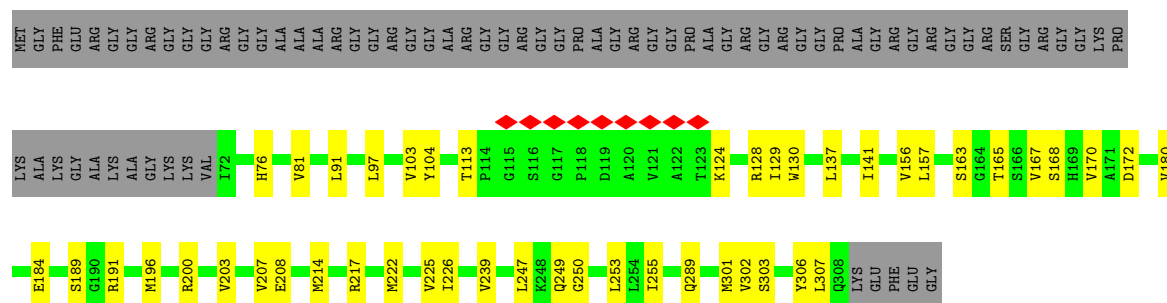
• Molecule 18: rRNA 2'-O-methyltransferase fibrillar

Chain CA: 69% 8% 23%



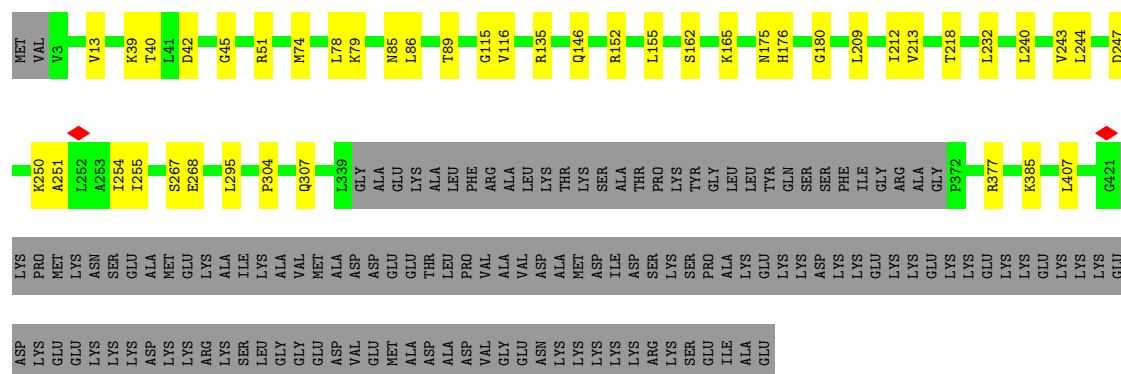
• Molecule 18: rRNA 2'-O-methyltransferase fibrillar

Chain CB: 61% 15% 24%



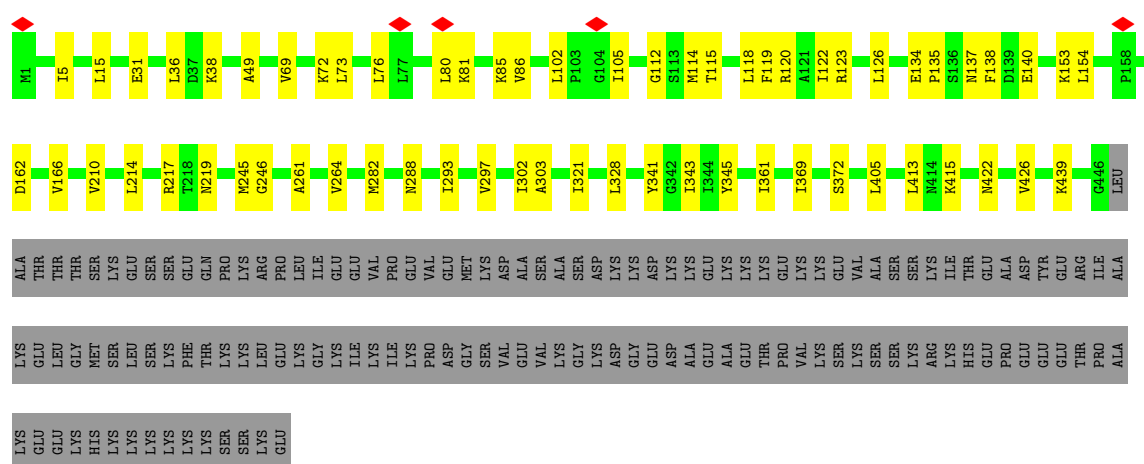
• Molecule 19: Nucleolar protein 56

Chain CC: 66% 8% 26%



• Molecule 20: Nucleolar protein 58

Chain CD: 66% 11% 23%

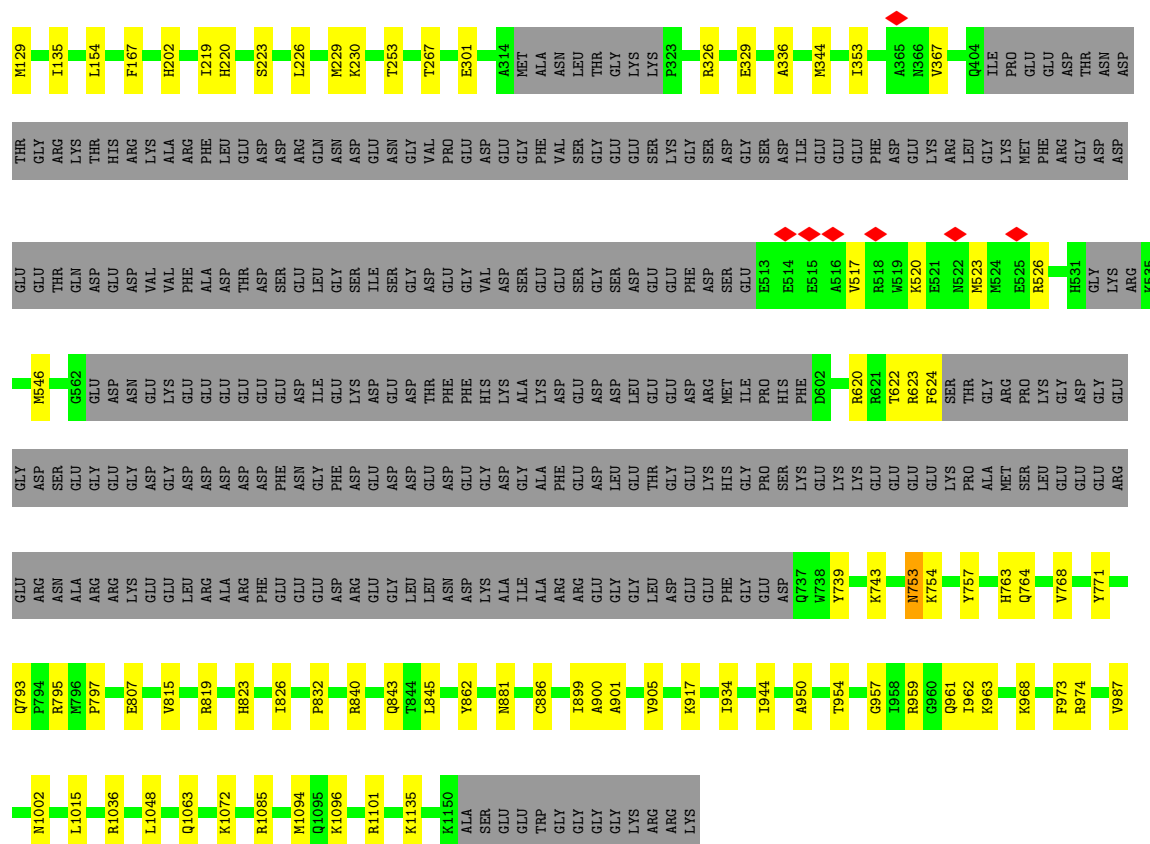


• Molecule 21: H/ACA ribonucleoprotein complex subunit 2

Chain CE: 80% 16% 5%

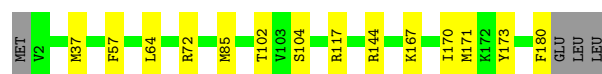


- | | | | |
|------|------|------|------|
| MET | ASP | SER | GLN | GLN | HIS | LYS | PRO | PRO | HIS | ARG | ARG | PRO | SER | LYS | THR | LYS | GLY | LYS | LYS | GLN | ASN | SER | GLY | GLY | ASN | PRO | LYS | ALA | PHE | ALA | VAL | ALA | ALA | ASN | PRO | GLY | LYS | LEU | LYS | ALA | V66 | P68 | R69 | L70 | V71 | S87 | K94 | I104 | S109 | R113 | I117 |
|------|------|------|------|



• Molecule 25: U3 small nucleolar ribonucleoprotein protein IMP3

Chain CJ: 90% 8%



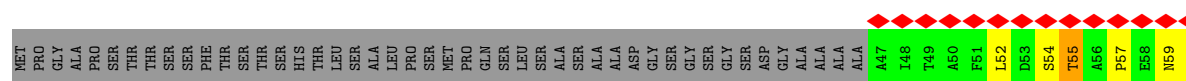
• Molecule 26: U3 small nucleolar ribonucleoprotein protein IMP4

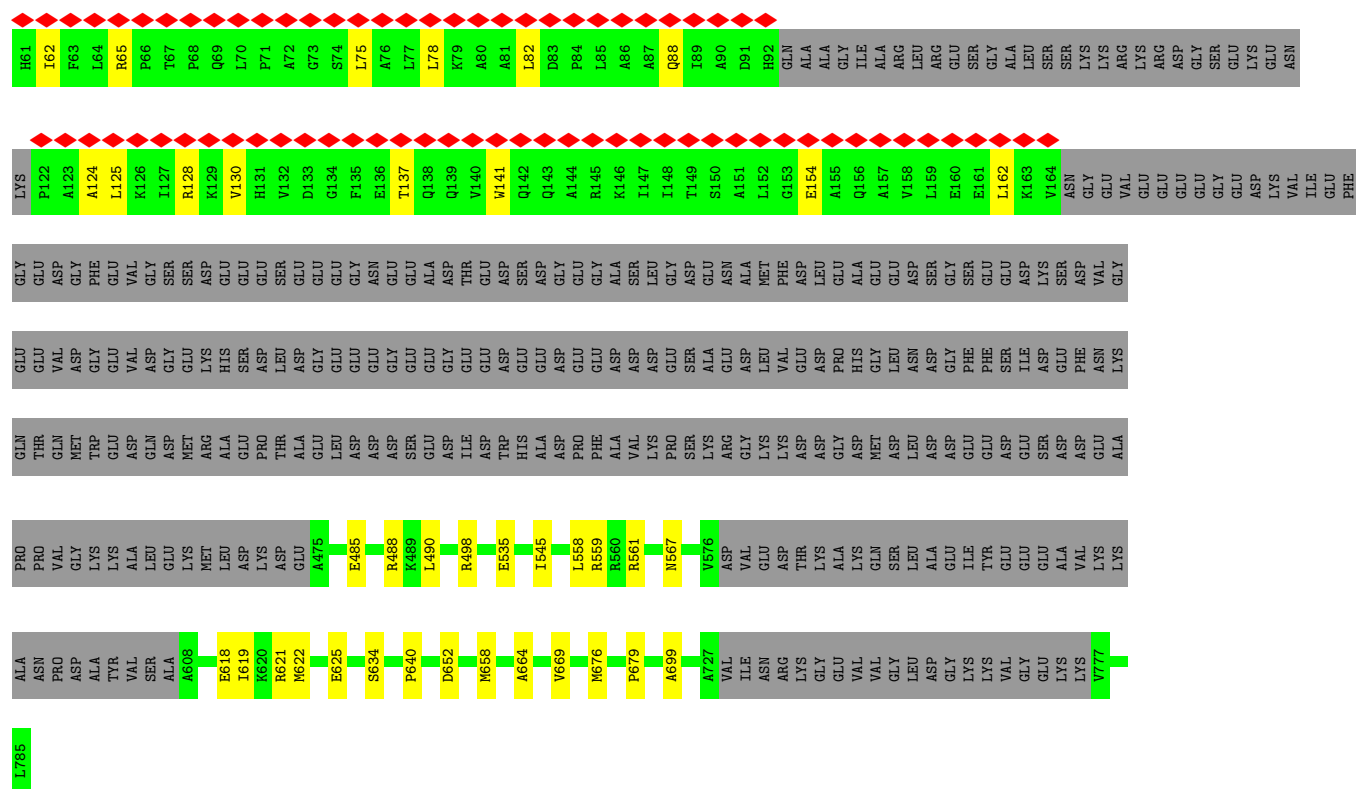
Chain CK: 87% 13%



• Molecule 27: Mpp10

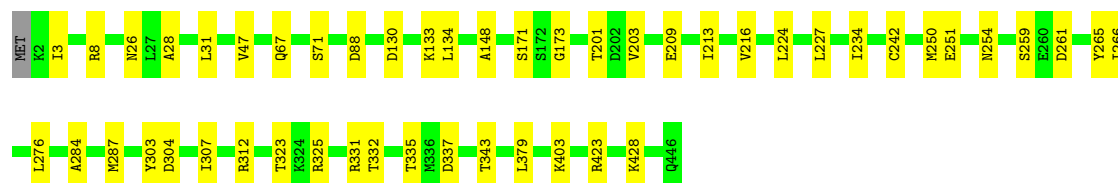
Chain CL: 14% 42% 7% 51%





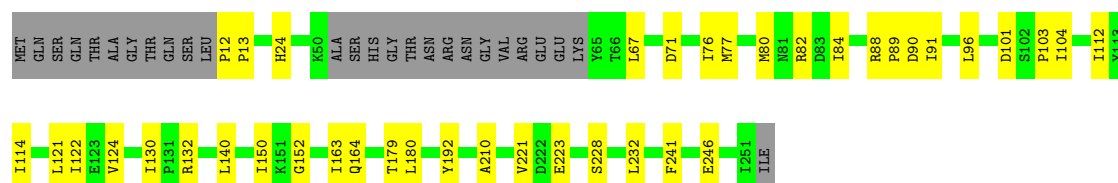
- Molecule 28: DDB1- and CUL4-associated factor 13

Chain CM: 89% 11%



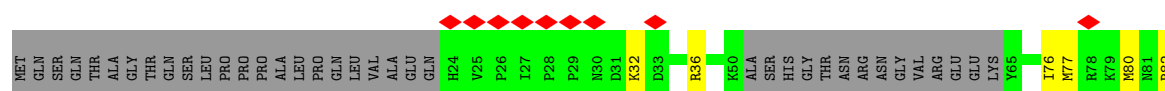
- Molecule 29: Nucleolar essential protein 1

Chain CN: 74% 16% 10%



- Molecule 29: Nucleolar essential protein 1

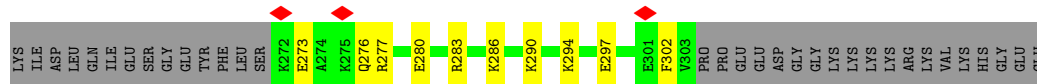
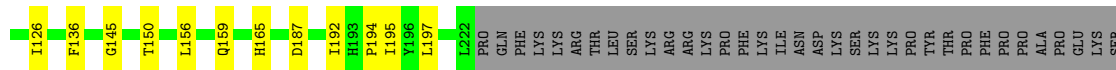
Chain CO: 73% 12% 15%





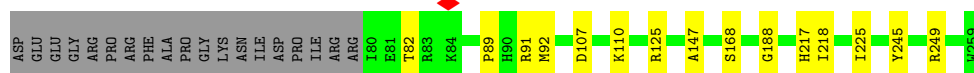
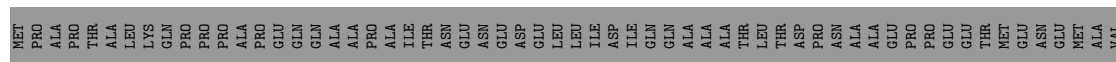
- Molecule 30: KRR1 small subunit processome component

Chain CP: 59% 13% 28%



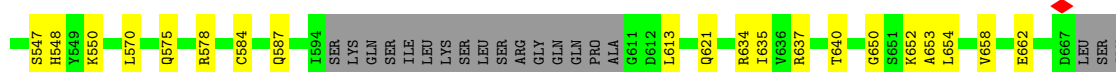
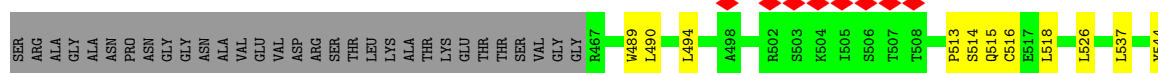
- Molecule 31: Pre-rRNA-processing protein PNO1

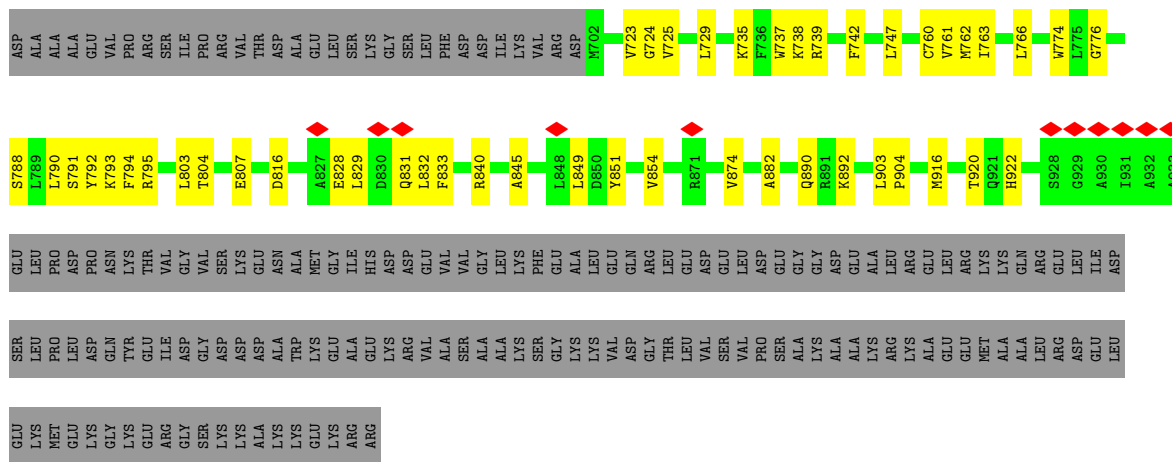
Chain CQ: 64% 6% 31%



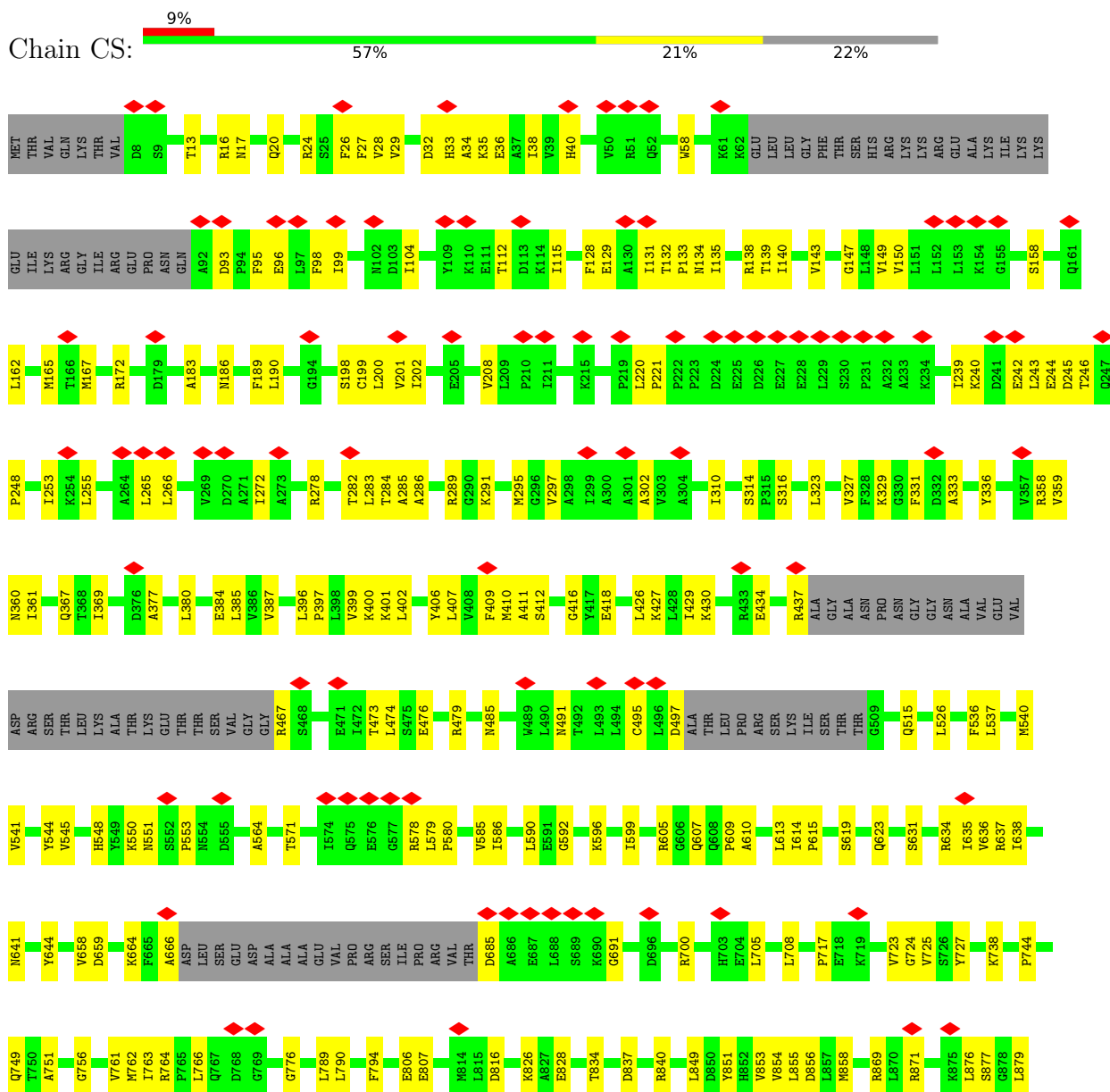
- Molecule 32: RNA cytidine acetyltransferase

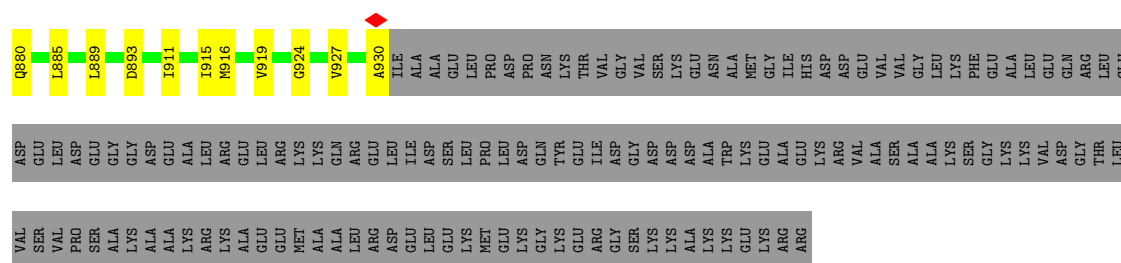
Chain CR: 63% 15% 21%





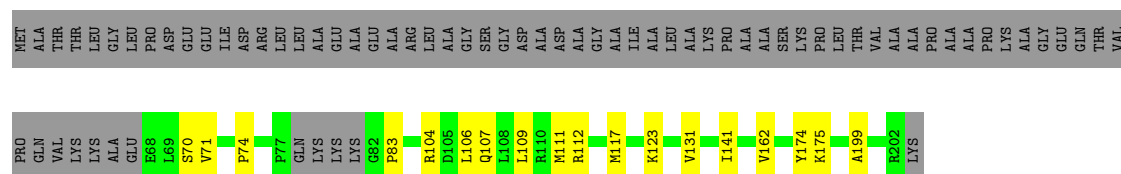
- Molecule 32: RNA cytidine acetyltransferase





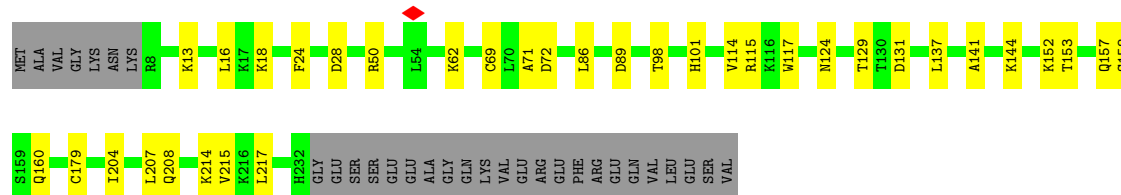
- Molecule 33: Fcf2 pre-rRNA processing C-terminal domain-containing protein

Chain CT: 56% 9% 35%



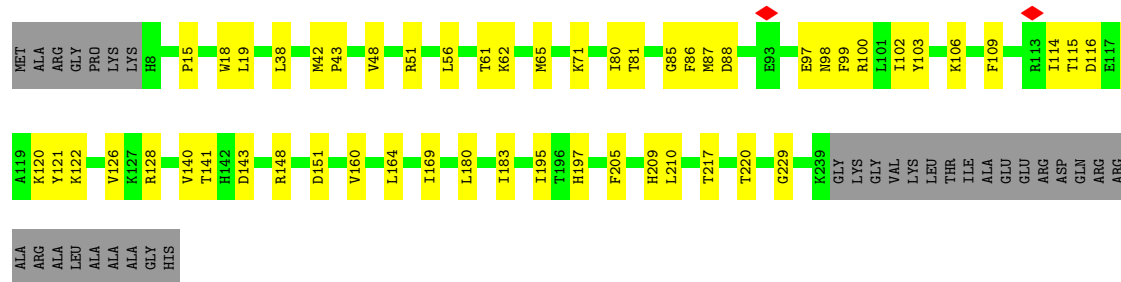
- Molecule 34: Small ribosomal subunit protein eS1

Chain Ca: 75% 14% 12%



- Molecule 35: 40S ribosomal protein S4

Chain Cb: 67% 20% 12%



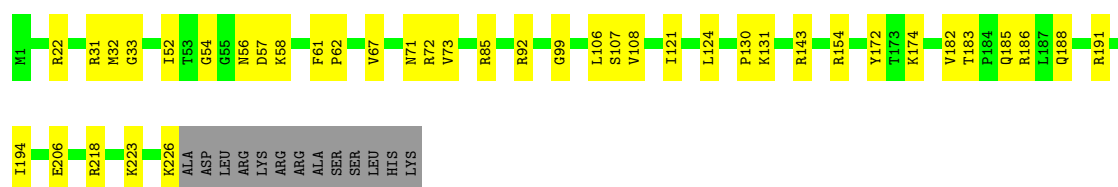
- Molecule 36: 40S ribosomal protein s5-like protein

Chain Cc: 83% 8% 9%



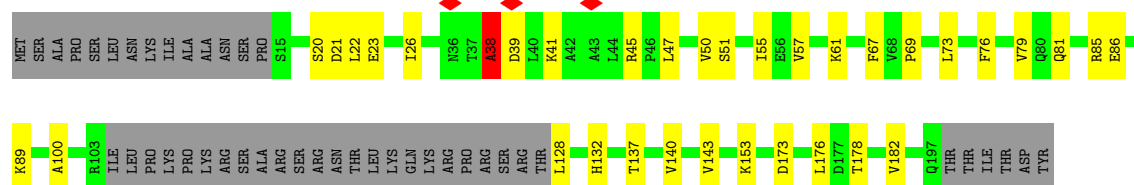
- Molecule 37: 40S ribosomal protein S6

Chain Cd:  78% 17% 5%



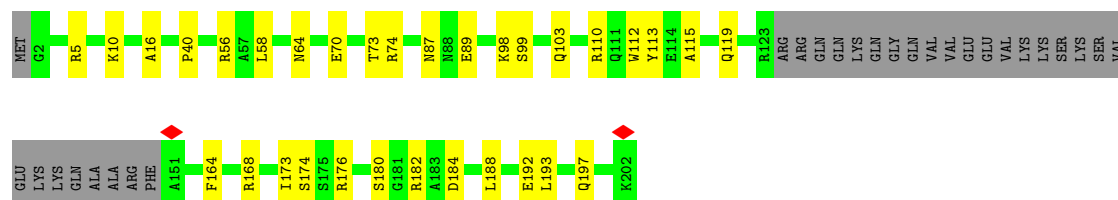
- Molecule 38: 40S ribosomal protein S7

Chain Ce:  61% 17% 22%



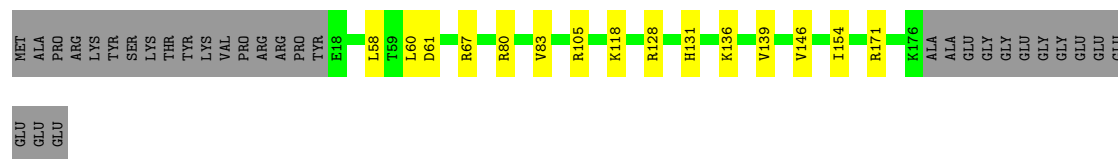
- Molecule 39: 40S ribosomal protein S8

Chain Cf:  70% 16% 14%



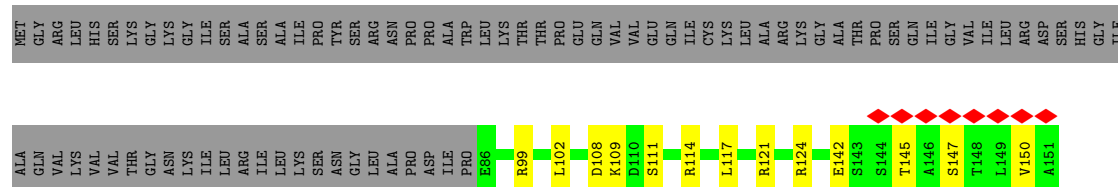
- Molecule 40: 40S ribosomal protein s9-like protein

Chain Cg:  76% 8% 16%



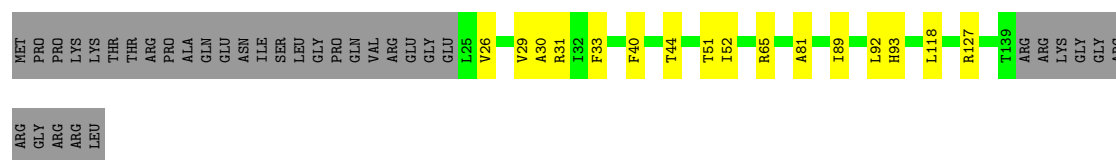
- Molecule 41: 40S ribosomal protein S13-like protein

Chain Ch:  5% 35% 9% 56%



- Molecule 42: 40S ribosomal protein S14-like protein

Chain Ci: 



- Molecule 43: 40S ribosomal protein S16-like protein

Chain Cj: 

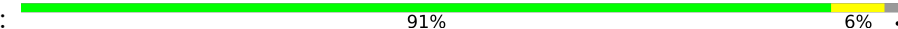


- Molecule 44: 40S ribosomal protein S11-like protein

Chain Ck: 



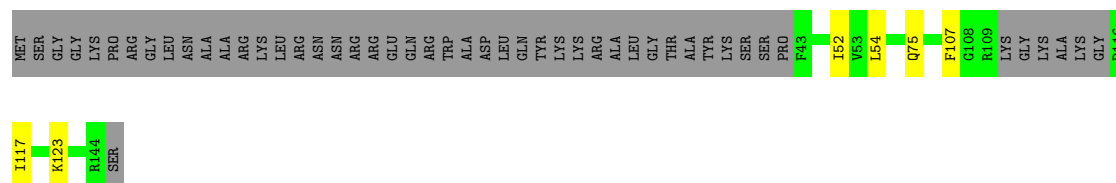
- Molecule 45: 40S ribosomal protein S22-like protein

Chain Cm: 



- Molecule 46: 40S ribosomal protein s23-like protein

Chain Cn: 



- Molecule 47: Small ribosomal subunit protein eS24

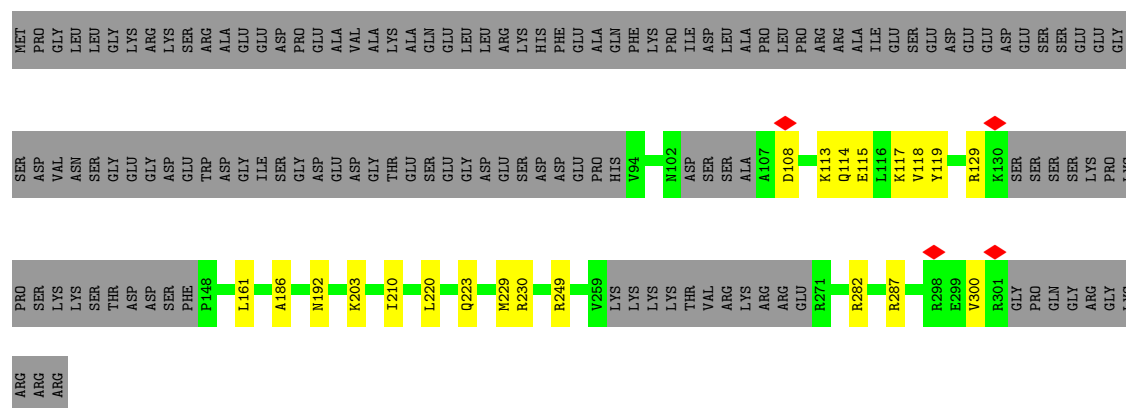
Chain Co: 



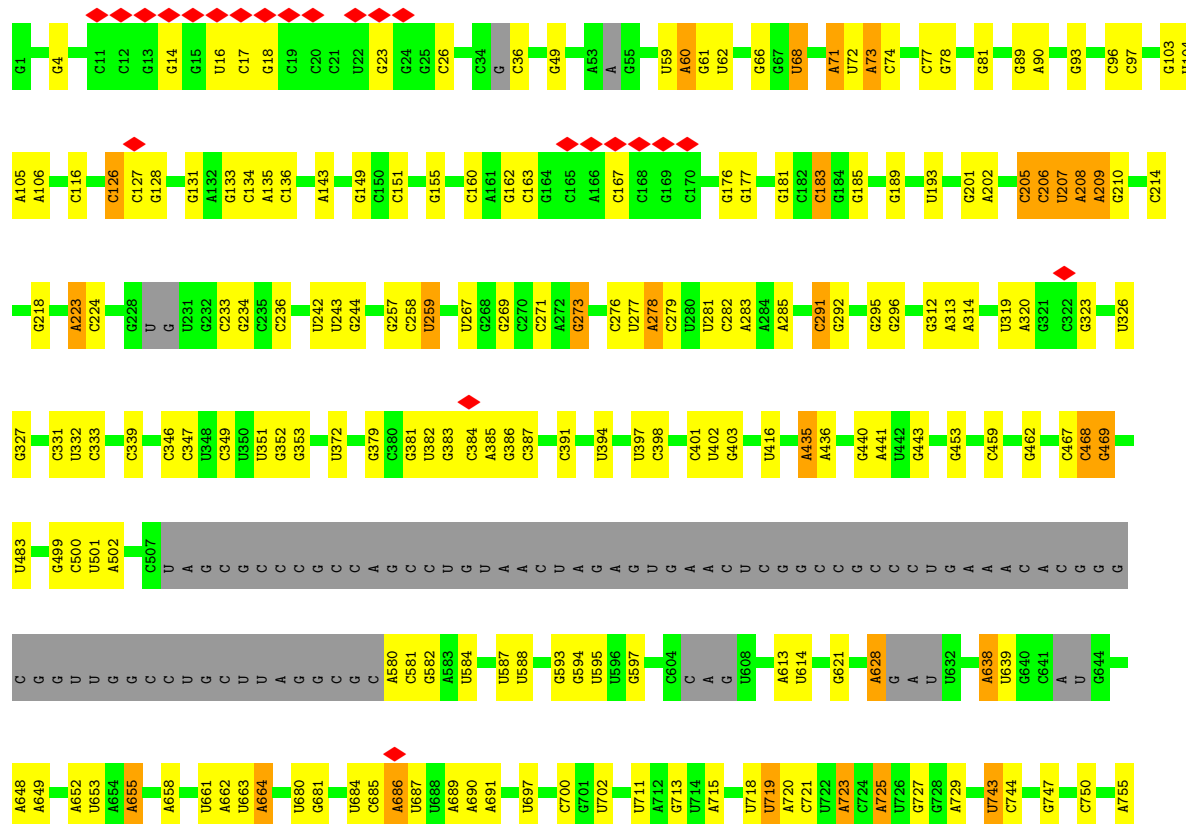
- Molecule 48: 40S ribosomal protein S28-like protein

MET	ASP	SER	SER	LYS	A6	V13	G25	R30	V45	R50	E51	N52	L55	R66	LEU	ARG
-----	-----	-----	-----	-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Chain CU:

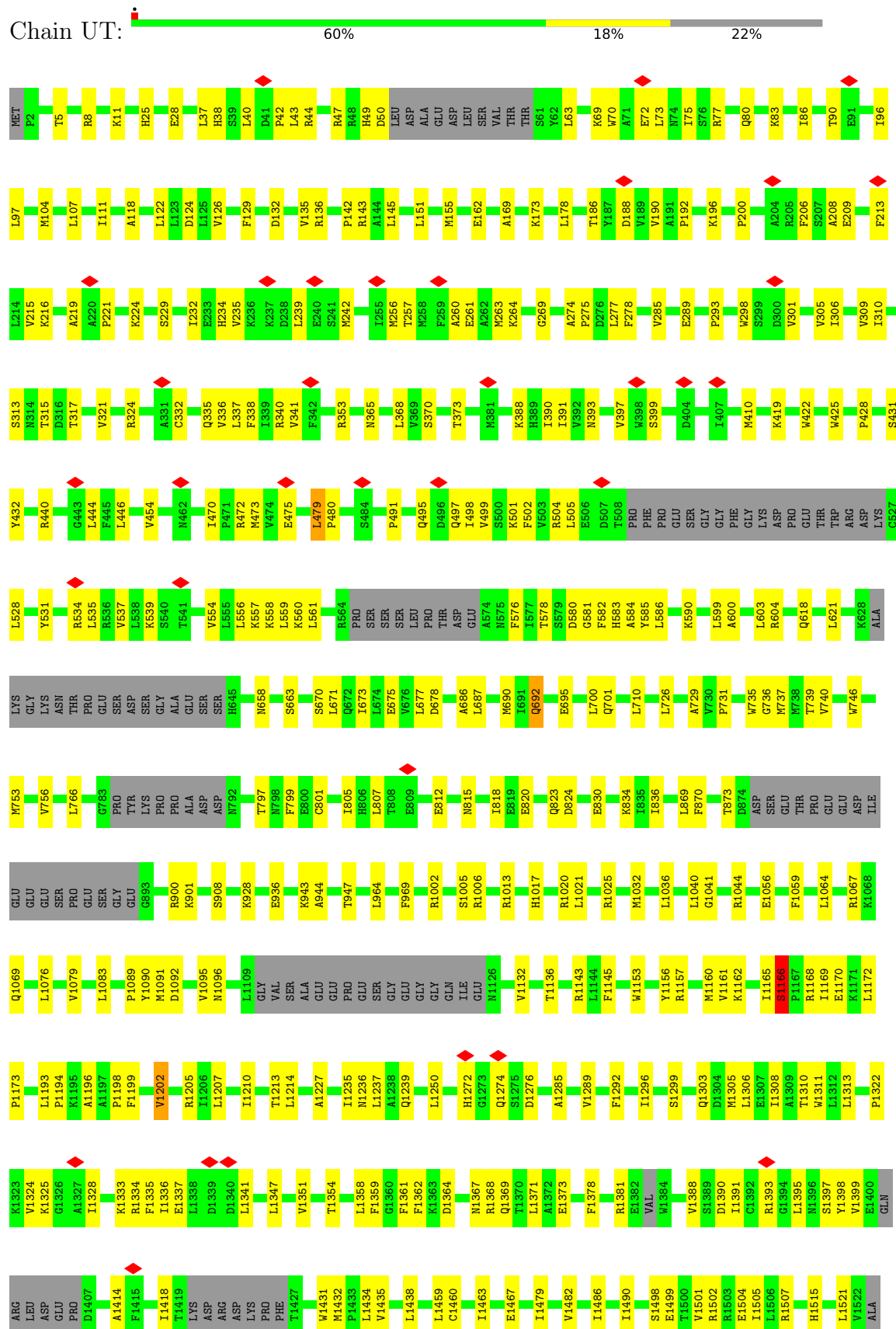


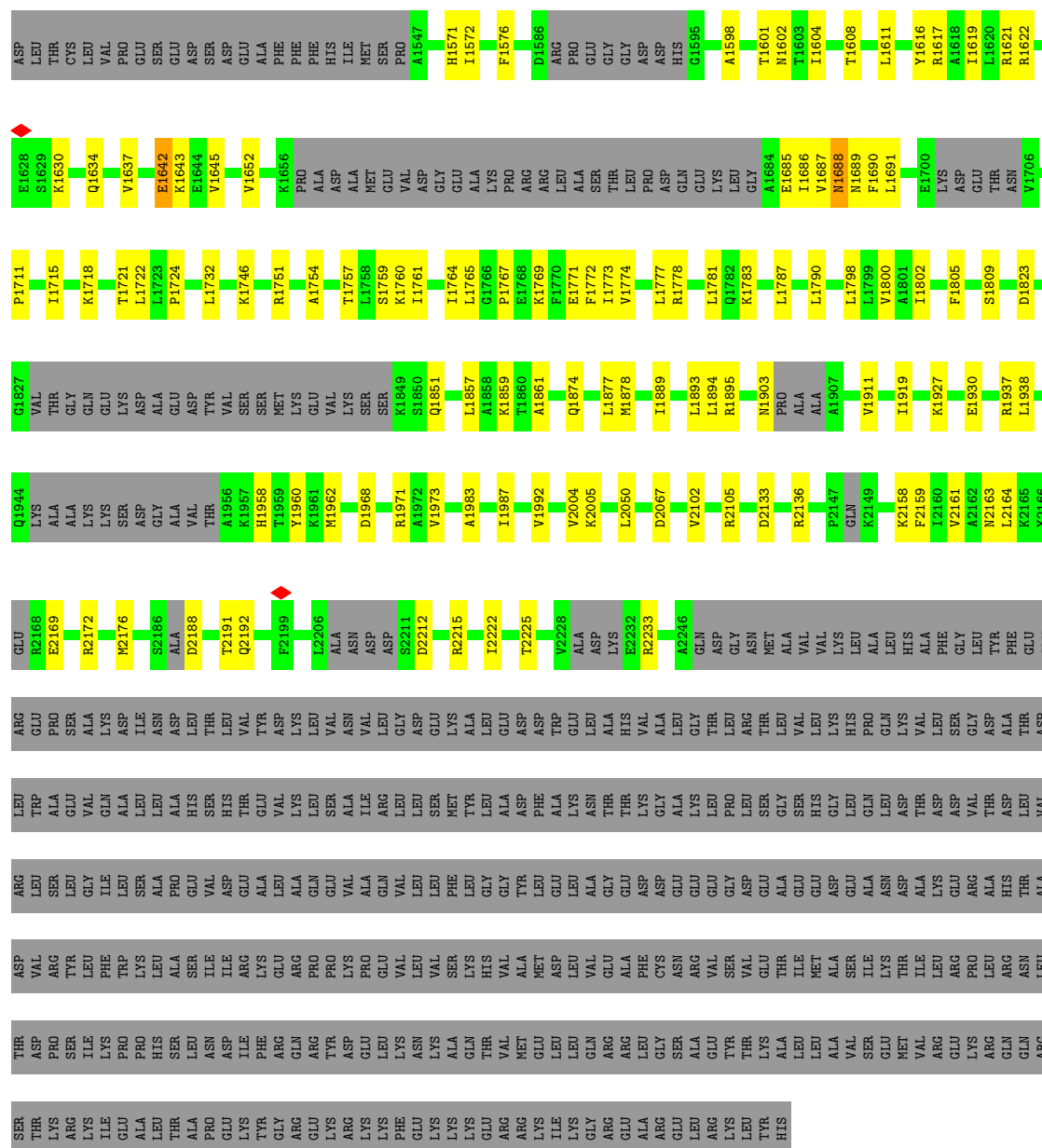
Chain C1:



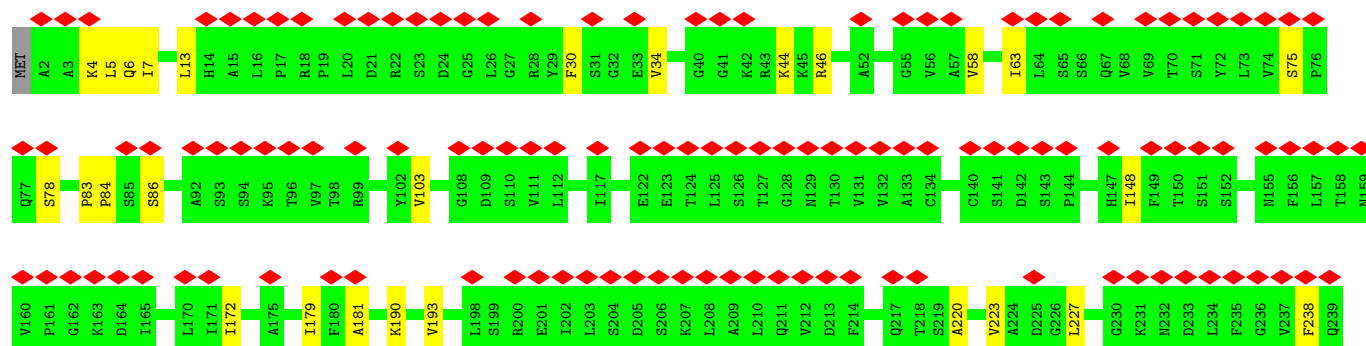
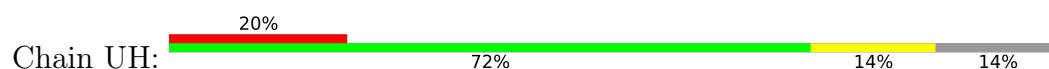


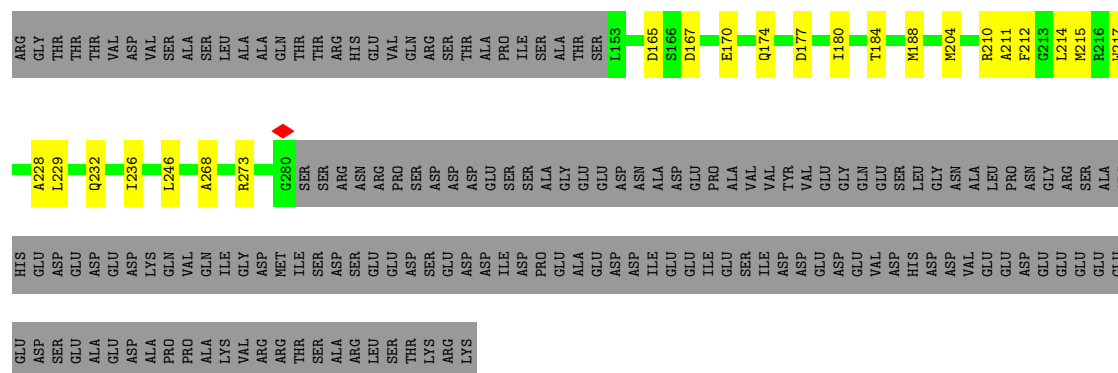
● Molecule 53: UTP20





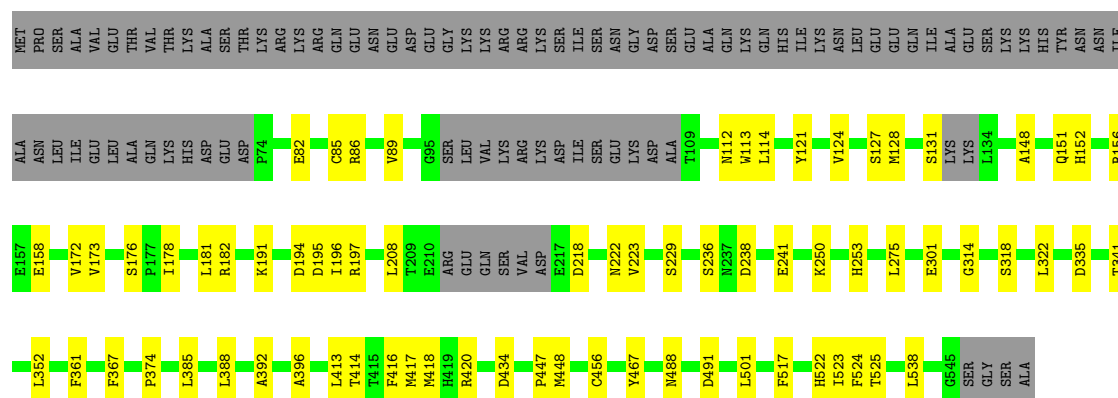
● Molecule 54: UTP8





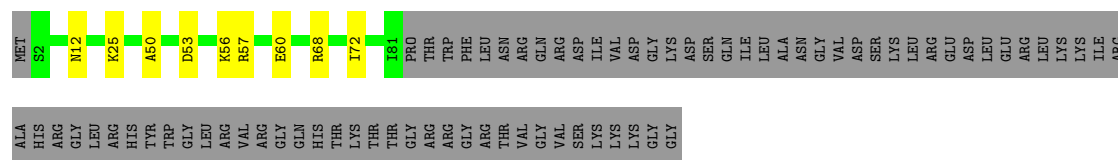
• Molecule 56: CCAAT-binding factor domain-containing protein

Chain US:



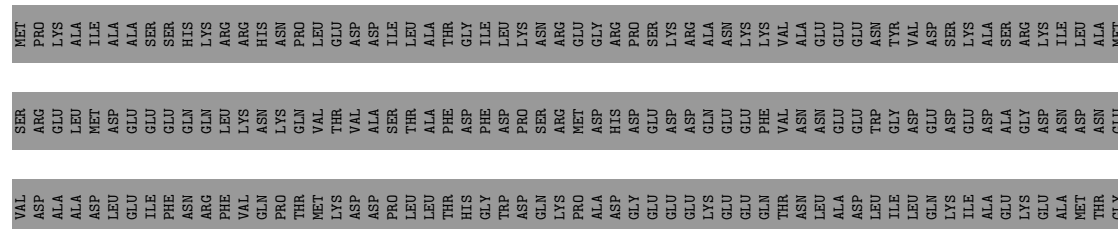
• Molecule 57: Putative ribosomal protein

Chain Cl:



• Molecule 58: Bystin-like protein

Chain CX:



- Molecule 61: UTP16



PRO	LYS	GLN	LEU	ASP	SER	ASN	GLY	MET
K308		ALA	ASP	VAL	ASP	ASN	GLY	
A319		GLU	GLU	THR	ARG	LYS	ARG	
R330		ASP	GLY	GLY	THR	LYS	SER	
Q337		GLN	PRO	GLU	ASP	GLN	LEU	
Q338		ARG	ARG	ALA	SER	GLU	LEU	
R356		THR	LEU	LEU	GLU	PRO	SER	
G357		PRO	PRO	LYS	GLU	ILE	ASP	
V361		ILE	ARG	ALA	PHE	GLN	ILE	
ASN		ARG	LEU	LYS	GLY	ASP	VAL	
LYS		GLU	LEU	ALA	THR	GLU	VAL	
ARG		LYS	PRO	GLN	ALA	LEU	VAL	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	436428	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Relion	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.783	Depositor
Minimum map value	-0.411	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	550.08, 550.08, 550.08	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.146, 1.146, 1.146	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ZN, SEP, A2M, GTP, OMC, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	UA	0.35	0/6555	0.59	0/8909
2	UB	0.23	0/4592	0.48	0/6178
3	UC	0.23	0/1661	0.44	0/2228
4	UD	0.24	0/6250	0.49	0/8465
5	UF	0.28	0/2665	0.51	0/3606
6	UG	0.36	0/3838	0.59	0/5181
7	UJ	0.26	0/12800	0.63	1/17357 (0.0%)
8	UK	0.31	0/1713	0.49	0/2266
9	UL	0.24	0/6299	0.52	0/8531
10	UM	0.21	0/6680	0.49	0/9090
11	UN	0.32	0/1425	0.50	0/1913
12	UO	0.29	0/3895	0.52	0/5302
13	UQ	0.26	1/6140 (0.0%)	0.51	2/8352 (0.0%)
14	UR	0.33	0/3560	0.54	0/4809
15	UU	0.33	0/6947	0.56	2/9452 (0.0%)
16	UX	0.33	0/1503	0.55	0/2022
17	UZ	0.22	0/1857	0.50	0/2526
18	CA	0.34	0/1814	0.57	0/2456
18	CB	0.21	0/1853	0.48	0/2511
19	CC	0.28	0/2911	0.52	0/3937
20	CD	0.25	0/3412	0.51	1/4617 (0.0%)
21	CE	0.31	0/891	0.55	0/1214
21	CF	0.24	0/876	0.49	0/1195
22	CG	0.22	0/3307	0.52	0/4462
23	CH	0.27	0/2939	0.49	0/3988
24	CI	0.29	0/6813	0.52	3/9182 (0.0%)
25	CJ	0.37	0/1462	0.57	0/1967
26	CK	0.35	0/2376	0.55	0/3214
27	CL	0.28	0/2504	0.52	0/3377
28	CM	0.34	0/3573	0.60	0/4829
29	CN	0.26	0/1797	0.51	0/2443
29	CO	0.21	0/1714	0.46	0/2325

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	CP	0.27	0/1923	0.58	2/2577 (0.1%)
31	CQ	0.23	0/1436	0.50	0/1932
32	CR	0.22	0/6809	0.55	1/9215 (0.0%)
32	CS	0.21	0/6722	0.56	0/9099
33	CT	0.31	0/1053	0.55	1/1413 (0.1%)
34	Ca	0.19	0/1850	0.46	0/2486
35	Cb	0.23	0/1890	0.64	0/2548
36	Cc	0.30	0/1485	0.51	0/2008
37	Cd	0.21	0/1850	0.52	1/2474 (0.0%)
38	Ce	0.24	0/1298	0.62	2/1750 (0.1%)
39	Cf	0.20	0/1429	0.49	0/1915
40	Cg	0.29	0/1265	0.47	0/1694
41	Ch	0.17	0/557	0.44	0/749
42	Ci	0.19	0/819	0.42	0/1107
43	Cj	0.37	0/958	0.57	0/1293
44	Ck	0.16	0/1107	0.44	0/1486
45	Cm	0.27	0/1001	0.54	0/1345
46	Cn	0.31	0/712	0.51	0/954
47	Co	0.28	0/754	0.70	0/1011
48	Cp	0.30	0/461	0.56	0/620
49	CU	0.25	0/1350	0.44	0/1810
50	C1	0.24	0/37786	0.30	1/58849 (0.0%)
51	C2	0.27	0/5434	0.31	0/8459
52	CW	0.19	0/3004	0.55	0/4085
53	UT	0.25	0/16312	0.64	6/22073 (0.0%)
54	UH	0.18	0/6301	0.47	0/8526
55	UE	0.25	0/1374	0.54	0/1852
55	UI	0.23	0/1005	0.50	0/1352
56	US	0.23	0/3765	0.54	0/5100
57	Cl	0.21	0/638	0.60	0/857
58	CX	0.24	0/2180	0.61	1/2956 (0.0%)
59	CY	0.20	0/2111	0.49	0/2816
60	CZ	0.18	0/2298	0.48	2/3080 (0.1%)
61	UP	0.23	0/428	0.50	0/570
All	All	0.26	1/235987 (0.0%)	0.51	26/327965 (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
1	UA	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	UQ	0	1
17	UZ	0	1
22	CG	0	1
27	CL	0	1
38	Ce	0	1
43	Cj	0	1
48	Cp	0	1
53	UT	0	1
58	CX	0	1
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	UQ	821	PRO	CG-CD	-6.38	1.29	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	UQ	821	PRO	CA-N-CD	-11.15	96.39	112.00
13	UQ	821	PRO	N-CD-CG	-8.79	90.02	103.20
24	CI	753	ASN	CA-C-N	7.98	136.78	121.54
24	CI	753	ASN	C-N-CA	7.98	136.78	121.54
38	Ce	38	ALA	CA-C-N	6.85	134.04	121.70
38	Ce	38	ALA	C-N-CA	6.85	134.04	121.70
53	UT	1688	ASN	CA-C-N	-6.77	111.49	122.26
53	UT	1688	ASN	C-N-CA	-6.77	111.49	122.26
24	CI	129	MET	CB-CG-SD	-6.14	94.29	112.70
32	CR	807	GLU	N-CA-CB	6.08	119.66	110.30
30	CP	297	GLU	N-CA-CB	5.67	119.64	110.40
53	UT	692	GLN	N-CA-CB	5.54	118.88	110.28
33	CT	83	PRO	CA-N-CD	-5.51	104.29	112.00
60	CZ	565	GLU	CA-C-N	5.40	131.85	121.54
60	CZ	565	GLU	C-N-CA	5.40	131.85	121.54
15	UU	171	THR	CA-C-N	5.33	129.51	121.40
15	UU	171	THR	C-N-CA	5.33	129.51	121.40
53	UT	1642	GLU	N-CA-CB	5.22	119.05	110.39
7	UJ	1288	GLU	N-CA-CB	5.21	117.78	110.12
20	CD	112	GLY	N-CA-C	5.16	116.58	111.21
58	CX	238	ARG	CA-CB-CG	5.12	124.34	114.10
30	CP	280	GLU	N-CA-CB	5.06	118.65	110.40
37	Cd	206	GLU	N-CA-CB	5.06	118.12	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	C1	2177	G	C4'-C3'-O3'	5.04	116.96	109.40
53	UT	584	ALA	CA-C-N	-5.03	112.35	121.14
53	UT	584	ALA	C-N-CA	-5.03	112.35	121.14

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	CG	348	GLY	Peptide
27	CL	55	THR	Peptide
58	CX	373	LYS	Peptide
38	Ce	38	ALA	Peptide
43	Cj	126	PRO	Peptide
48	Cp	50	ARG	Sidechain
1	UA	244	ARG	Sidechain
1	UA	283	GLU	Peptide
1	UA	645	ALA	Mainchain
13	UQ	849	ALA	Peptide
53	UT	1166	SER	Peptide
17	UZ	273	GLN	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	UA	6411	0	6306	55	0
2	UB	4506	0	4633	71	0
3	UC	1633	0	1696	16	0
4	UD	6108	0	6108	85	0
5	UF	2599	0	2650	17	0
6	UG	3765	0	3800	46	0
7	UJ	12592	0	12889	206	0
8	UK	1699	0	1832	22	0
9	UL	6175	0	6188	80	0
10	UM	6545	0	6547	91	0
11	UN	1401	0	1455	15	0
12	UO	3811	0	3861	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	UQ	6012	0	6044	79	0
14	UR	3498	0	3508	25	0
15	UU	6778	0	6782	43	0
16	UX	1480	0	1554	13	0
17	UZ	1815	0	1896	19	0
18	CA	1778	0	1830	15	0
18	CB	1816	0	1847	29	0
19	CC	2866	0	2960	31	0
20	CD	3355	0	3483	41	0
21	CE	879	0	918	12	0
21	CF	864	0	900	8	0
22	CG	3245	0	3262	36	0
23	CH	2888	0	2979	37	0
24	CI	6666	0	6826	65	0
25	CJ	1434	0	1482	12	0
26	CK	2329	0	2373	28	0
27	CL	2466	0	2532	34	0
28	CM	3501	0	3498	33	0
29	CN	1762	0	1807	24	0
29	CO	1683	0	1726	19	0
30	CP	1893	0	1993	31	0
31	CQ	1413	0	1479	8	0
32	CR	6677	0	6809	104	0
32	CS	6591	0	6674	150	0
33	CT	1035	0	1063	16	0
34	Ca	1821	0	1936	26	0
35	Cb	1851	0	1905	37	0
36	Cc	1464	0	1504	14	0
37	Cd	1819	0	1920	30	0
38	Ce	1279	0	1322	22	0
39	Cf	1398	0	1401	22	0
40	Cg	1248	0	1365	13	0
41	Ch	546	0	580	10	0
42	Ci	808	0	831	11	0
43	Cj	943	0	1002	12	0
44	Ck	1082	0	1138	8	0
45	Cm	985	0	1021	6	0
46	Cn	702	0	750	4	0
47	Co	741	0	785	15	0
48	Cp	458	0	489	7	0
49	CU	1337	0	1376	15	0
50	C1	33862	0	17147	173	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	C2	4869	0	2465	15	0
52	CW	2932	0	2866	58	0
53	UT	15998	0	16397	291	0
54	UH	6198	0	6272	82	0
55	UE	1362	0	1440	26	0
55	UI	996	0	1054	17	0
56	US	3672	0	3679	54	0
57	CI	633	0	676	7	0
58	CX	2130	0	2219	30	0
59	CY	2095	0	2185	32	0
60	CZ	2270	0	2273	45	0
61	UP	422	0	457	5	0
62	UX	1	0	0	0	0
63	CI	32	0	12	0	0
64	CI	1	0	0	0	0
65	CS	27	0	11	1	0
All	All	227951	0	212668	2383	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 5.

All (2383) 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)
4:UD:441:THR:HA	4:UD:456:LEU:O	1.30	1.26
54:UH:555:GLY:O	54:UH:567:LEU:HA	1.42	1.18
52:CW:206:VAL:O	52:CW:219:PHE:HA	1.55	1.06
52:CW:208:ALA:O	52:CW:217:CYS:HA	1.52	1.06
12:UO:333:HIS:HA	12:UO:346:ARG:O	1.58	1.01
12:UO:335:ALA:HA	12:UO:344:SER:O	1.63	0.99
15:UU:159:ILE:O	15:UU:172:THR:HA	1.70	0.91
29:CO:121:LEU:HB3	29:CO:163:ILE:O	1.71	0.91
35:Cb:98:ASN:HB2	35:Cb:114:ILE:O	1.75	0.86
14:UR:559:SER:O	14:UR:565:ALA:HB3	1.77	0.83
53:UT:673:ILE:O	53:UT:677:LEU:HB2	1.78	0.83
47:Co:360:HIS:O	47:Co:398:GLY:HA2	1.78	0.82
60:CZ:414:VAL:O	60:CZ:418:ARG:HB2	1.81	0.81
55:UI:211:ALA:HB1	55:UI:214:LEU:HB2	1.63	0.80
56:US:172:VAL:O	56:US:176:SER:HB3	1.83	0.79
12:UO:546:MET:HE1	55:UE:219:GLN:HG2	1.65	0.79
55:UI:184:THR:O	55:UI:188:MET:HB2	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CR:361:ILE:HB	32:CR:367:GLN:HB2	1.66	0.77
32:CS:286:ALA:H	32:CS:289:ARG:HD3	1.52	0.74
2:UB:43:GLN:N	2:UB:43:GLN:HE21	1.85	0.73
55:UI:229:LEU:HB3	55:UI:236:ILE:HD11	1.71	0.73
32:CS:641:ASN:HB3	32:CS:644:TYR:HB2	1.71	0.73
38:Ce:50:VAL:HG21	38:Ce:69:PRO:HD3	1.71	0.73
22:CG:262:VAL:HG12	22:CG:272:VAL:HG12	1.71	0.72
18:CA:180:VAL:HB	18:CA:203:VAL:HG12	1.72	0.72
32:CR:845:ALA:HA	32:CR:916:MET:HE1	1.71	0.72
4:UD:35:TYR:HA	4:UD:38:LYS:HE3	1.72	0.72
20:CD:282:MET:HE1	20:CD:302:ILE:HD12	1.71	0.72
53:UT:275:PRO:HG3	53:UT:321:VAL:HG22	1.71	0.72
20:CD:122:ILE:O	20:CD:126:LEU:HB2	1.89	0.71
23:CH:219:ARG:NE	49:CU:115:GLU:OE2	2.24	0.71
53:UT:1759:SER:HB2	53:UT:1800:VAL:HG21	1.72	0.71
8:UK:253:SER:HB3	8:UK:265:VAL:H	1.56	0.70
32:CR:387:VAL:HG12	32:CR:409:PHE:HB2	1.72	0.70
13:UQ:759:ASP:OD2	54:UH:435:ARG:NH1	2.23	0.70
35:Cb:100:ARG:NH2	35:Cb:118:GLU:O	2.24	0.70
9:UL:835:GLN:HE21	9:UL:870:ASN:HD22	1.38	0.70
53:UT:1652:VAL:HG11	53:UT:1722:LEU:HD11	1.73	0.70
13:UQ:450:ALA:HB2	13:UQ:458:PRO:HB2	1.72	0.70
24:CI:1101:ARG:HD2	33:CT:111:MET:HG2	1.74	0.70
2:UB:65:ARG:HH21	50:C1:2047:G:H5"	1.57	0.70
23:CH:339:MET:HE1	23:CH:349:LEU:HB2	1.74	0.69
50:C1:2168:U:H3	50:C1:2194:A:H2	1.41	0.69
7:UJ:971:PRO:HA	7:UJ:974:LYS:HG2	1.73	0.69
6:UG:364:THR:HG22	6:UG:388:TRP:HB3	1.74	0.69
32:CR:570:LEU:HB3	32:CR:584:CYS:HB3	1.73	0.69
1:UA:408:ALA:HB3	1:UA:418:ARG:HB2	1.75	0.69
32:CR:851:TYR:HA	32:CR:854:VAL:HG12	1.75	0.69
8:UK:268:ARG:HE	21:CE:95:SER:HB3	1.57	0.69
50:C1:928:G:N7	60:CZ:537:ARG:NH2	2.40	0.69
53:UT:1781:LEU:HB2	53:UT:1790:LEU:HD12	1.75	0.69
32:CR:276:THR:HG22	32:CR:278:ARG:H	1.58	0.68
53:UT:1168:ARG:O	53:UT:1172:LEU:HB2	1.93	0.68
7:UJ:1659:GLU:HB3	7:UJ:1708:GLU:HB3	1.75	0.68
18:CB:222:MET:HG2	20:CD:123:ARG:HG2	1.75	0.68
37:Cd:57:ASP:HA	37:Cd:106:LEU:HA	1.76	0.68
15:UU:159:ILE:HB	15:UU:173:ILE:HB	1.74	0.68
52:CW:40:GLU:O	52:CW:44:ASN:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:UJ:720:LEU:HD23	7:UJ:723:LYS:HZ2	1.58	0.68
27:CL:498:ARG:NH1	50:C1:1161:G:OP1	2.27	0.68
42:CI:29:VAL:HG12	42:CI:93:HIS:HB2	1.76	0.68
9:UL:589:VAL:HB	9:UL:603:LEU:HB2	1.76	0.68
15:UU:78:ARG:O	15:UU:81:ASN:ND2	2.26	0.68
32:CR:23:LYS:O	32:CR:146:GLY:N	2.26	0.68
32:CS:744:PRO:HA	32:CS:762:MET:HG2	1.76	0.68
10:UM:513:GLY:HA3	10:UM:547:ILE:HD11	1.75	0.68
39:Cf:193:LEU:HD12	39:Cf:197:GLN:HE22	1.58	0.67
54:UH:793:MET:HE1	55:UI:273:ARG:HH12	1.59	0.67
15:UU:564:SER:HB3	15:UU:620:ARG:HH21	1.58	0.67
25:CJ:117:ARG:HG3	50:C1:353:G:H4'	1.76	0.67
53:UT:1482:VAL:O	53:UT:1486:ILE:HB	1.94	0.67
53:UT:2161:VAL:HA	53:UT:2164:LEU:HD23	1.76	0.67
55:UE:156:VAL:HG21	56:US:301:GLU:HB3	1.77	0.67
13:UQ:401:ASN:HB2	13:UQ:414:HIS:HB3	1.78	0.66
50:C1:628:A:H61	50:C1:1050:U:H3	1.42	0.66
53:UT:219:ALA:HB1	53:UT:277:LEU:HD21	1.78	0.66
53:UT:535:LEU:HD22	53:UT:580:ASP:HB2	1.77	0.66
4:UD:19:VAL:HG12	4:UD:46:ILE:HG12	1.78	0.66
55:UE:210:ARG:HB3	55:UE:214:LEU:HD13	1.76	0.66
32:CS:24:ARG:NH1	32:CS:140:ILE:O	2.28	0.66
10:UM:429:LEU:HB3	10:UM:460:TRP:HZ3	1.61	0.66
32:CS:418:GLU:HB2	32:CS:550:LYS:HE3	1.78	0.66
53:UT:1851:GLN:HB3	53:UT:1895:ARG:HG3	1.77	0.66
39:Cf:98:LYS:HB3	50:C1:913:G:H5''	1.78	0.66
1:UA:21:LEU:HB2	1:UA:30:PHE:HB2	1.78	0.66
42:CI:65:ARG:HB3	50:C1:1490:A:H5'	1.76	0.65
53:UT:1036:LEU:HD21	53:UT:1079:VAL:HG11	1.78	0.65
47:Co:358:ILE:O	47:Co:399:LYS:HA	1.96	0.65
24:CI:1085:ARG:NE	50:C1:391:C:OP1	2.29	0.65
50:C1:950:G:H1	50:C1:959:U:H3	1.43	0.65
21:CE:35:LYS:HB2	21:CE:102:SER:HB3	1.79	0.65
29:CN:76:ILE:HG22	29:CN:80:MET:HE2	1.79	0.65
38:Ce:51:SER:HB3	38:Ce:67:PHE:HB2	1.78	0.65
1:UA:316:ALA:O	1:UA:320:GLY:O	2.15	0.65
5:UF:285:VAL:HG11	11:UN:369:LEU:HB2	1.78	0.65
32:CR:587:GLN:HB3	32:CR:637:ARG:HB3	1.79	0.65
53:UT:753:MET:HA	53:UT:756:VAL:HG12	1.78	0.65
10:UM:104:VAL:HG12	10:UM:105:ARG:HG2	1.79	0.65
12:UO:417:ARG:NH2	50:C1:78:G:O6	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CR:252:LEU:HB3	32:CR:265:LEU:HD21	1.77	0.65
32:CR:840:ARG:HH22	32:CS:623:GLN:HB2	1.61	0.65
12:UO:180:THR:HG22	12:UO:181:ARG:HD2	1.79	0.64
18:CB:180:VAL:HB	18:CB:203:VAL:HG12	1.79	0.64
32:CS:749:GLN:HE21	32:CS:789:LEU:HD21	1.61	0.64
56:US:85:CYS:SG	56:US:121:TYR:OH	2.52	0.64
14:UR:442:THR:HG22	14:UR:454:ILE:HG12	1.77	0.64
32:CR:311:PHE:HB2	32:CR:386:VAL:HG12	1.78	0.64
7:UJ:1026:VAL:HA	7:UJ:1029:ILE:HD12	1.80	0.64
20:CD:361:ILE:HG13	20:CD:405:LEU:HD13	1.80	0.64
32:CS:255:LEU:HD22	32:CS:329:LYS:HE2	1.78	0.64
53:UT:870:PHE:HA	53:UT:873:THR:HG22	1.80	0.64
19:CC:244:LEU:HD12	19:CC:250:LYS:HE2	1.78	0.64
32:CS:879:LEU:HD11	52:CW:299:PRO:HG2	1.78	0.64
7:UJ:506:LEU:HD12	7:UJ:557:ARG:HH21	1.61	0.64
27:CL:621:ARG:NH1	27:CL:625:GLU:OE2	2.31	0.64
59:CY:47:LEU:HG	60:CZ:418:ARG:HE	1.63	0.64
18:CB:156:VAL:HG12	18:CB:225:VAL:HB	1.78	0.64
32:CR:742:PHE:HB3	32:CR:762:MET:HB3	1.80	0.64
45:Cm:19:LYS:NZ	50:C1:1666:C:O3'	2.31	0.64
50:C1:60:A:H62	54:UH:876:LYS:HA	1.63	0.64
38:Ce:23:GLU:HA	38:Ce:26:ILE:HG12	1.79	0.64
1:UA:826:MET:HE1	15:UU:843:LEU:HD11	1.79	0.63
53:UT:422:TRP:HD1	53:UT:425:TRP:HE1	1.45	0.63
1:UA:329:SER:O	15:UU:865:LYS:NZ	2.30	0.63
2:UB:587:THR:O	2:UB:591:LEU:HB2	1.97	0.63
15:UU:863:ARG:NH2	27:CL:664:ALA:O	2.30	0.63
17:UZ:169:LYS:O	17:UZ:172:TYR:C	2.41	0.63
53:UT:1432:MET:HA	53:UT:1435:VAL:HG12	1.78	0.63
22:CG:557:ARG:HD2	22:CG:598:ARG:HE	1.63	0.63
23:CH:219:ARG:HA	23:CH:251:HIS:O	1.98	0.63
54:UH:267:ARG:HH12	54:UH:302:CYS:HB2	1.64	0.63
19:CC:212:ILE:HG23	19:CC:213:VAL:HG23	1.80	0.63
27:CL:485:GLU:OE2	27:CL:488:ARG:NH2	2.32	0.63
28:CM:171:SER:HB3	28:CM:203:VAL:HB	1.79	0.63
58:CX:371:LEU:HD21	58:CX:417:PHE:HB2	1.80	0.63
32:CR:516:CYS:HB3	32:CR:570:LEU:HD11	1.80	0.63
50:C1:926:C:H5''	52:CW:194:GLY:HA3	1.81	0.63
54:UH:372:LEU:HD23	54:UH:600:ARG:HH12	1.62	0.63
26:CK:53:ARG:HD3	49:CU:210:ILE:HG21	1.80	0.63
32:CR:310:ILE:HD12	32:CR:385:LEU:HD23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:UM:547:ILE:HG22	10:UM:563:SER:HB2	1.79	0.63
30:CP:156:LEU:O	30:CP:159:GLN:NE2	2.32	0.63
32:CS:186:ASN:HA	32:CS:189:PHE:HB3	1.80	0.63
55:UI:170:GLU:O	55:UI:174:GLN:NE2	2.32	0.63
7:UJ:29:HIS:O	7:UJ:123:ARG:NH1	2.30	0.63
40:Cg:136:LYS:H	59:CY:250:GLY:HA3	1.63	0.63
53:UT:77:ARG:NH2	53:UT:80:GLN:OE1	2.32	0.63
56:US:208:LEU:HD21	56:US:223:VAL:HG11	1.79	0.63
56:US:388:LEU:O	56:US:392:ALA:HB2	1.98	0.63
7:UJ:654:ALA:O	7:UJ:658:SER:HB2	1.98	0.62
56:US:314:GLY:HA2	56:US:318:SER:HB3	1.81	0.62
4:UD:456:LEU:HG	4:UD:469:ILE:HG12	1.80	0.62
7:UJ:1600:LEU:HD23	7:UJ:1646:LEU:HB2	1.81	0.62
53:UT:42:PRO:O	53:UT:47:ARG:NH2	2.32	0.62
1:UA:364:ILE:HG12	1:UA:399:THR:HG21	1.81	0.62
1:UA:558:ARG:NH2	51:C2:62:A:OP2	2.32	0.62
9:UL:380:VAL:HG22	9:UL:382:ASP:H	1.63	0.62
13:UQ:383:GLN:NE2	14:UR:364:GLN:O	2.32	0.62
55:UE:220:TRP:HA	55:UE:223:VAL:HG12	1.80	0.62
13:UQ:88:ARG:HD3	13:UQ:441:VAL:HG21	1.82	0.62
38:Ce:73:LEU:HD22	38:Ce:100:ALA:HB2	1.81	0.62
57:Cl:12:ASN:HB2	57:Cl:25:LYS:HD3	1.82	0.62
5:UF:130:MET:HE1	5:UF:143:LEU:HD22	1.82	0.62
6:UG:426:ALA:O	28:CM:8:ARG:NH1	2.33	0.62
18:CB:76:HIS:HB3	18:CB:81:VAL:HG23	1.81	0.62
24:Cl:944:ILE:HD13	24:Cl:973:PHE:HB3	1.82	0.62
27:CL:52:LEU:O	27:CL:55:THR:C	2.42	0.62
53:UT:104:MET:HE1	53:UT:143:ARG:HD3	1.81	0.62
10:UM:345:LEU:HB2	10:UM:367:ARG:HB3	1.80	0.62
32:CS:592:GLY:HA3	32:CS:631:SER:HA	1.82	0.62
37:Cd:131:LYS:HD3	53:UT:700:LEU:HD11	1.81	0.62
17:UZ:130:ILE:HG13	17:UZ:134:LYS:HE2	1.82	0.62
60:CZ:374:ARG:HH22	60:CZ:414:VAL:HG21	1.65	0.62
2:UB:497:VAL:HA	2:UB:500:LEU:HD23	1.82	0.61
32:CS:854:VAL:HG12	32:CS:858:MET:HE3	1.82	0.61
50:C1:205:C:O2'	50:C1:206:C:O2	2.18	0.61
54:UH:371:SER:HA	54:UH:437:GLY:HA2	1.82	0.61
10:UM:335:LEU:HD11	10:UM:343:LEU:HB3	1.81	0.61
53:UT:83:LYS:HA	53:UT:86:ILE:HG22	1.81	0.61
7:UJ:551:TYR:HD2	7:UJ:552:LEU:HD12	1.64	0.61
9:UL:210:GLU:HG2	9:UL:267:LEU:HD13	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:UO:206:VAL:HG21	12:UO:247:LEU:HD11	1.80	0.61
24:CI:819:ARG:NH1	24:CI:823:HIS:O	2.33	0.61
50:C1:718:U:OP2	53:UT:1020:ARG:NH2	2.32	0.61
9:UL:375:ALA:HB3	9:UL:384:GLN:HB2	1.81	0.61
12:UO:104:CYS:O	12:UO:116:ALA:HA	2.00	0.61
40:Cg:146:VAL:HG11	40:Cg:154:ILE:HD11	1.82	0.61
41:Ch:124:ARG:NH2	50:C1:1551:A:OP2	2.34	0.61
53:UT:559:LEU:HD21	53:UT:581:GLY:HA3	1.82	0.61
59:CY:106:LYS:HB2	60:CZ:433:ASN:HB2	1.82	0.61
39:Cf:16:ALA:HB2	50:C1:938:C:H5"	1.82	0.61
32:CR:317:PRO:HA	32:CR:320:LEU:HB2	1.82	0.61
37:Cd:33:GLY:N	37:Cd:52:ILE:O	2.33	0.61
40:Cg:139:VAL:HG13	59:CY:257:GLY:HA3	1.83	0.61
50:C1:372:U:H3	50:C1:394:U:H3	1.48	0.61
54:UH:340:VAL:HG11	54:UH:356:THR:HG21	1.81	0.61
7:UJ:1783:ARG:NH1	53:UT:49:HIS:O	2.34	0.61
56:US:178:ILE:HG22	56:US:181:LEU:H	1.65	0.61
15:UU:72:GLN:HG2	15:UU:85:VAL:HG22	1.83	0.61
53:UT:315:THR:HB	53:UT:353:ARG:HA	1.83	0.61
56:US:218:ASP:O	56:US:222:ASN:ND2	2.34	0.61
58:CX:325:SER:HB2	58:CX:369:VAL:HG11	1.83	0.61
2:UB:584:LEU:HD22	2:UB:625:LYS:HB2	1.82	0.60
19:CC:243:VAL:HG12	19:CC:244:LEU:HG	1.81	0.60
24:CI:807:GLU:O	24:CI:840:ARG:NH2	2.34	0.60
26:CK:264:ARG:NH2	50:C1:2180:A:O2'	2.34	0.60
32:CR:635:ILE:HB	32:CR:725:VAL:HG22	1.83	0.60
55:UE:229:LEU:HD23	55:UE:239:LEU:HD11	1.82	0.60
10:UM:540:ARG:HD3	10:UM:576:LEU:HD22	1.83	0.60
15:UU:752:THR:N	15:UU:766:ALA:O	2.30	0.60
35:Cb:43:PRO:HB3	35:Cb:81:THR:HG23	1.83	0.60
55:UE:178:LEU:HD13	55:UE:216:ARG:HD2	1.82	0.60
1:UA:731:LEU:HD13	1:UA:764:GLN:HG3	1.82	0.60
6:UG:63:VAL:O	6:UG:69:ARG:NH1	2.34	0.60
26:CK:89:LEU:HD11	26:CK:117:LEU:HB2	1.83	0.60
38:Ce:57:VAL:O	38:Ce:61:LYS:HB3	2.01	0.60
53:UT:256:MET:HE1	53:UT:305:VAL:HA	1.83	0.60
13:UQ:540:LYS:HB2	13:UQ:553:ILE:HB	1.83	0.60
24:CI:959:ARG:NH1	26:CK:287:TYR:O	2.34	0.60
27:CL:54:SER:O	27:CL:59:ASN:ND2	2.34	0.60
35:Cb:56:LEU:HD21	59:CY:280:PHE:HB2	1.84	0.60
59:CY:39:SER:OG	60:CZ:425:TRP:NE1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:UL:372:VAL:HG12	9:UL:387:VAL:HG12	1.83	0.60
10:UM:520:GLN:OE1	10:UM:522:ARG:NH2	2.32	0.60
15:UU:140:PRO:HB2	15:UU:142:LYS:HE3	1.83	0.60
32:CS:246:THR:HG22	32:CS:248:PRO:HD2	1.84	0.60
53:UT:278:PHE:HD2	53:UT:324:ARG:HH22	1.49	0.60
53:UT:600:ALA:O	53:UT:604:ARG:HB2	2.02	0.60
53:UT:1771:GLU:HA	53:UT:1774:VAL:HG12	1.83	0.60
13:UQ:499:LEU:HD22	13:UQ:513:LYS:HE2	1.84	0.60
26:CK:40:LYS:NZ	26:CK:41:PRO:O	2.35	0.60
48:Cp:13:VAL:O	48:Cp:52:ASN:N	2.34	0.60
50:C1:718:U:OP1	53:UT:1006:ARG:NH1	2.34	0.60
9:UL:899:LEU:HA	9:UL:902:VAL:HG12	1.84	0.60
9:UL:129:SER:OG	9:UL:131:ASP:OD1	2.19	0.60
10:UM:233:SER:OG	34:Ca:50:ARG:NH2	2.34	0.60
24:CI:517:VAL:HG12	32:CR:277:LEU:HD23	1.82	0.60
35:Cb:62:LYS:HD3	35:Cb:80:ILE:HD11	1.84	0.60
1:UA:221:GLU:OE1	1:UA:247:ASN:ND2	2.32	0.60
7:UJ:1000:SER:HB3	7:UJ:1003:VAL:HG22	1.84	0.60
32:CS:416:GLY:O	32:CS:551:ASN:ND2	2.34	0.60
52:CW:298:THR:HB	52:CW:302:GLU:HB2	1.84	0.60
53:UT:1092:ASP:O	53:UT:1096:ASN:ND2	2.35	0.60
56:US:218:ASP:OD1	56:US:222:ASN:ND2	2.35	0.60
13:UQ:466:LEU:HB3	13:UQ:833:SER:HB2	1.84	0.60
16:UX:11:ASP:OD1	51:C2:48:G:O2'	2.20	0.60
21:CE:94:VAL:HG12	21:CE:96:ARG:H	1.67	0.60
25:CJ:85:MET:HE3	27:CL:634:SER:HB3	1.82	0.60
29:CN:228:SER:HB3	29:CN:232:LEU:HD11	1.83	0.60
53:UT:97:LEU:HD13	53:UT:136:ARG:HH21	1.67	0.60
2:UB:577:GLU:OE1	2:UB:581:HIS:NE2	2.30	0.59
9:UL:109:HIS:HD1	9:UL:129:SER:HG	1.48	0.59
12:UO:531:ASN:OD1	55:UE:260:LYS:NZ	2.28	0.59
52:CW:292:ASN:ND2	52:CW:336:VAL:O	2.35	0.59
53:UT:740:VAL:O	53:UT:746:TRP:NE1	2.30	0.59
9:UL:19:SER:OG	9:UL:43:ALA:O	2.20	0.59
29:CO:114:ILE:HB	29:CO:122:ILE:HB	1.82	0.59
39:Cf:73:THR:O	39:Cf:74:ARG:NH1	2.35	0.59
7:UJ:162:ILE:HD12	20:CD:426:VAL:HB	1.84	0.59
8:UK:262:ARG:HH12	8:UK:264:LYS:HD2	1.67	0.59
4:UD:554:PHE:HE1	4:UD:561:LEU:HD13	1.67	0.59
29:CN:121:LEU:HB3	29:CN:163:ILE:O	2.02	0.59
40:Cg:128:ARG:HG3	50:C1:1059:A:H5'	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:UG:403:PHE:O	28:CM:8:ARG:NH2	2.32	0.59
7:UJ:926:THR:HG22	7:UJ:968:ALA:HB1	1.85	0.59
53:UT:209:GLU:HB2	53:UT:261:GLU:HG2	1.84	0.59
15:UU:212:ASN:HB2	15:UU:219:ILE:HD11	1.84	0.59
15:UU:480:ALA:O	15:UU:506:THR:OG1	2.17	0.59
22:CG:127:GLU:HB3	22:CG:130:ARG:HH21	1.68	0.59
38:Ce:41:LYS:HD3	38:Ce:45:ARG:HD2	1.85	0.59
50:C1:1613:C:H4'	50:C1:1614:U:H5'	1.85	0.59
53:UT:232:ILE:HA	53:UT:235:VAL:HG12	1.85	0.59
53:UT:2159:PHE:O	53:UT:2163:ASN:ND2	2.36	0.59
15:UU:119:LEU:HD22	15:UU:131:LEU:HD22	1.84	0.59
17:UZ:169:LYS:O	17:UZ:172:TYR:O	2.20	0.59
23:CH:152:THR:O	23:CH:156:ALA:HB3	2.03	0.59
26:CK:87:ARG:NH2	26:CK:134:GLU:O	2.36	0.59
28:CM:251:GLU:OE1	28:CM:254:ASN:ND2	2.35	0.59
32:CS:36:GLU:O	32:CS:40:HIS:ND1	2.35	0.59
50:C1:809:U:H3	53:UT:1622:ARG:HH21	1.50	0.59
4:UD:875:ARG:NH1	4:UD:883:GLU:OE2	2.36	0.59
8:UK:1:MET:HE3	8:UK:4:LEU:HG	1.84	0.59
8:UK:64:TYR:HD1	8:UK:67:MET:HE3	1.68	0.59
19:CC:240:LEU:HB3	19:CC:250:LYS:HB3	1.83	0.59
24:CI:520:LYS:O	32:CR:275:LYS:NZ	2.36	0.59
19:CC:218:THR:HB	19:CC:244:LEU:HD11	1.85	0.59
32:CR:776:GLY:HA3	32:CR:816:ASP:HB2	1.84	0.59
53:UT:621:LEU:HB3	53:UT:673:ILE:HG22	1.84	0.59
55:UE:229:LEU:HA	55:UE:235:LEU:HD12	1.85	0.59
7:UJ:150:THR:HG22	33:CT:74:PRO:HD3	1.85	0.58
15:UU:71:LEU:H	15:UU:86:THR:HB	1.66	0.58
18:CB:128:ARG:NH1	18:CB:172:ASP:OD2	2.36	0.58
19:CC:377:ARG:NH2	51:C2:197:C:OP2	2.36	0.58
32:CS:708:LEU:HD13	60:CZ:296:ILE:HD11	1.85	0.58
18:CA:222:MET:HG2	19:CC:135:ARG:HG2	1.85	0.58
24:CI:754:LYS:HA	24:CI:757:TYR:HB2	1.84	0.58
9:UL:189:LEU:HB2	9:UL:203:LEU:HD11	1.85	0.58
32:CS:27:PHE:HB2	32:CS:150:VAL:HG12	1.85	0.58
7:UJ:1442:LEU:HD22	7:UJ:1484:ASN:HB2	1.85	0.58
53:UT:1341:LEU:HB3	53:UT:1381:ARG:HH22	1.69	0.58
10:UM:549:ALA:HB3	10:UM:562:ALA:HB3	1.85	0.58
16:UX:54:PRO:HB3	16:UX:85:ALA:HB1	1.86	0.58
37:Cd:85:ARG:NH2	50:C1:743:U:O2	2.36	0.58
54:UH:832:LEU:HD23	55:UI:204:MET:HE1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:Cl:50:ALA:O	57:Cl:68:ARG:NH1	2.37	0.58
2:UB:641:ILE:HG21	56:US:538:LEU:HD13	1.84	0.58
15:UU:343:ILE:HG22	15:UU:354:THR:HG22	1.86	0.58
18:CB:250:GLY:N	18:CB:306:TYR:O	2.37	0.58
32:CR:283:LEU:HD23	32:CR:295:MET:HE2	1.86	0.58
34:Ca:214:LYS:NZ	50:C1:1471:U:OP1	2.35	0.58
3:UC:230:ASP:OD1	27:CL:60:ARG:NH2	2.36	0.58
4:UD:624:PRO:HD2	4:UD:659:PHE:HE2	1.68	0.58
13:UQ:815:ASN:HB2	13:UQ:822:LYS:HG3	1.86	0.58
23:CH:216:ARG:NH2	24:Cl:624:PHE:O	2.36	0.58
38:Ce:81:GLN:HE22	38:Ce:85:ARG:HD2	1.68	0.58
53:UT:1877:LEU:HD22	53:UT:1958:HIS:HB2	1.85	0.58
32:CS:596:LYS:HA	32:CS:599:ILE:HD12	1.85	0.58
32:CS:806:GLU:OE2	32:CS:871:ARG:NH2	2.37	0.58
4:UD:619:LYS:O	4:UD:622:MET:HB2	2.04	0.58
7:UJ:1713:VAL:HG12	7:UJ:1715:SER:H	1.68	0.58
15:UU:511:VAL:HB	15:UU:524:TRP:HB2	1.85	0.58
32:CS:725:VAL:O	32:CS:761:VAL:HA	2.04	0.58
34:Ca:24:PHE:HZ	42:Cl:52:ILE:HA	1.67	0.58
47:Co:352:LYS:NZ	53:UT:72:GLU:O	2.37	0.58
5:UF:166:ARG:NH2	11:UN:358:GLN:O	2.36	0.58
58:CX:418:ALA:O	58:CX:422:ARG:NH2	2.37	0.58
10:UM:547:ILE:HA	10:UM:563:SER:HA	1.86	0.57
10:UM:647:LYS:HD2	10:UM:699:LEU:H	1.67	0.57
21:CF:41:THR:HG23	21:CF:102:SER:HB2	1.84	0.57
23:CH:284:GLU:OE2	49:CU:119:TYR:OH	2.22	0.57
32:CS:700:ARG:HH21	32:CS:705:LEU:HD23	1.70	0.57
56:US:173:VAL:O	56:US:182:ARG:NH2	2.37	0.57
9:UL:394:LEU:HB2	9:UL:420:VAL:HB	1.86	0.57
28:CM:251:GLU:OE2	28:CM:312:ARG:NH1	2.37	0.57
32:CR:112:THR:HA	32:CR:115:ILE:HG12	1.85	0.57
32:CR:133:PRO:HB3	32:CR:494:LEU:HD22	1.85	0.57
37:Cd:31:ARG:NH2	52:CW:42:LEU:O	2.37	0.57
52:CW:304:LYS:NZ	52:CW:317:ASP:OD1	2.37	0.57
1:UA:832:ARG:HH21	27:CL:669:VAL:HG13	1.69	0.57
10:UM:458:ARG:HB3	10:UM:460:TRP:HE1	1.69	0.57
12:UO:145:GLN:HE22	56:US:413:LEU:HG	1.70	0.57
32:CR:392:ALA:HB1	32:CR:420:THR:HB	1.86	0.57
33:CT:107:GLN:HG3	33:CT:111:MET:HE2	1.86	0.57
48:Cp:25:GLY:H	50:C1:1746:C:H4'	1.70	0.57
59:CY:39:SER:HG	60:CZ:425:TRP:HE1	1.50	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:UD:697:GLN:HG3	4:UD:713:SER:HB3	1.86	0.57
7:UJ:810:PHE:HA	7:UJ:813:ILE:HG12	1.86	0.57
7:UJ:955:LEU:HD23	7:UJ:958:LEU:HD12	1.85	0.57
7:UJ:1370:MET:HA	7:UJ:1373:LEU:HD23	1.87	0.57
9:UL:509:HIS:HB3	9:UL:528:ALA:HB3	1.86	0.57
26:CK:29:ARG:HG3	26:CK:56:PHE:HD1	1.68	0.57
52:CW:210:ALA:HB3	52:CW:215:GLY:H	1.70	0.57
53:UT:1787:LEU:HD21	53:UT:1823:ASP:HB3	1.86	0.57
56:US:191:LYS:NZ	56:US:229:SER:O	2.37	0.57
7:UJ:1023:LEU:HA	7:UJ:1026:VAL:HG12	1.85	0.57
9:UL:192:THR:OG1	9:UL:220:CYS:SG	2.61	0.57
14:UR:453:GLY:HA3	14:UR:526:ILE:HG13	1.87	0.57
32:CR:793:LYS:NZ	32:CS:893:ASP:OD2	2.38	0.57
2:UB:843:ARG:NH1	50:C1:2044:C:OP2	2.37	0.57
6:UG:267:ASN:HB2	6:UG:274:HIS:HE2	1.68	0.57
32:CR:24:ARG:NH1	32:CR:140:ILE:O	2.37	0.57
53:UT:216:LYS:NZ	53:UT:264:LYS:O	2.30	0.57
9:UL:712:VAL:HG12	9:UL:722:VAL:HG22	1.87	0.57
29:CN:103:PRO:HG3	29:CO:232:LEU:HD21	1.86	0.57
38:Ce:47:LEU:HD22	38:Ce:76:PHE:HZ	1.69	0.57
50:C1:761:U:O2	50:C1:762:G:N2	2.36	0.57
2:UB:550:GLU:HG3	56:US:523:ILE:HB	1.86	0.57
4:UD:481:ALA:HA	4:UD:497:GLU:HA	1.86	0.57
7:UJ:1442:LEU:HD11	7:UJ:1488:ALA:HB2	1.86	0.57
53:UT:1272:HIS:HA	53:UT:1311:TRP:HZ3	1.67	0.57
60:CZ:378:MET:HE1	60:CZ:414:VAL:HG11	1.87	0.57
14:UR:152:THR:HG21	50:C1:273:G:H21	1.70	0.57
20:CD:69:VAL:HG13	20:CD:73:LEU:HB3	1.87	0.57
32:CS:540:MET:HG2	32:CS:585:VAL:HG11	1.87	0.57
52:CW:254:ARG:HH22	52:CW:296:LEU:HA	1.69	0.57
53:UT:1170:GLU:OE2	53:UT:1205:ARG:NH1	2.38	0.57
53:UT:2192:GLN:HB3	53:UT:2233:ARG:HH22	1.68	0.57
2:UB:479:PHE:HB2	2:UB:507:ILE:HD13	1.87	0.57
6:UG:580:GLU:HA	6:UG:583:LEU:HD13	1.86	0.57
36:Cc:57:ILE:HD11	43:Cj:47:LYS:HG2	1.87	0.57
53:UT:1333:LYS:NZ	53:UT:1373:GLU:OE1	2.38	0.57
9:UL:862:ASN:OD1	9:UL:905:ASN:ND2	2.36	0.56
19:CC:175:ASN:OD1	19:CC:176:HIS:N	2.38	0.56
32:CS:426:LEU:HA	32:CS:429:ILE:HG22	1.87	0.56
5:UF:278:ILE:HG23	11:UN:373:ILE:HD12	1.87	0.56
7:UJ:812:ARG:HH12	7:UJ:816:MET:HB3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:UQ:809:SER:HB3	13:UQ:830:VAL:HA	1.85	0.56
15:UU:365:ILE:HB	15:UU:378:LEU:HD22	1.86	0.56
53:UT:1013:ARG:O	53:UT:1017:HIS:CB	2.53	0.56
54:UH:34:VAL:HG22	54:UH:86:SER:HB3	1.88	0.56
4:UD:531:ARG:NH2	4:UD:571:ASP:OD1	2.37	0.56
4:UD:651:THR:O	4:UD:654:LYS:N	2.39	0.56
16:UX:1:ALA:HB1	25:CJ:37:MET:HE1	1.87	0.56
26:CK:94:ARG:NH2	50:C1:2189:C:OP2	2.36	0.56
32:CS:28:VAL:HB	32:CS:201:VAL:HG12	1.88	0.56
53:UT:1013:ARG:O	53:UT:1017:HIS:HB3	2.05	0.56
56:US:194:ASP:OD1	56:US:197:ARG:NH2	2.39	0.56
5:UF:338:HIS:O	5:UF:363:ARG:NH1	2.39	0.56
9:UL:210:GLU:OE2	9:UL:212:HIS:NE2	2.38	0.56
28:CM:287:MET:HE3	28:CM:303:TYR:HB2	1.88	0.56
59:CY:98:LYS:HB3	60:CZ:441:LEU:HD22	1.87	0.56
2:UB:661:LEU:HD23	2:UB:733:LEU:HG	1.87	0.56
7:UJ:1392:VAL:O	7:UJ:1396:LYS:NZ	2.35	0.56
12:UO:490:ALA:O	55:UE:249:ARG:NH2	2.38	0.56
20:CD:341:TYR:HB3	20:CD:345:TYR:HB2	1.87	0.56
32:CS:291:LYS:NZ	32:CS:412:SER:O	2.38	0.56
34:Ca:62:LYS:NZ	34:Ca:89:ASP:O	2.39	0.56
47:Co:345:ARG:O	47:Co:345:ARG:NH1	2.37	0.56
56:US:250:LYS:HD3	56:US:253:HIS:HD2	1.70	0.56
1:UA:72:SER:O	1:UA:79:ALA:HA	2.04	0.56
7:UJ:608:ARG:HD3	7:UJ:671:GLU:HB3	1.87	0.56
13:UQ:453:ARG:HG3	13:UQ:457:ARG:HH21	1.70	0.56
32:CR:526:LEU:HG	32:CR:537:LEU:HD12	1.87	0.56
32:CS:255:LEU:HD11	32:CS:333:ALA:HB2	1.88	0.56
37:Cd:143:ARG:NH2	50:C1:727:G:OP1	2.37	0.56
53:UT:446:LEU:HD11	53:UT:480:PRO:HD3	1.88	0.56
2:UB:550:GLU:OE2	2:UB:554:ARG:NH2	2.38	0.56
29:CN:179:THR:HB	29:CN:221:VAL:HG11	1.87	0.56
32:CS:13:THR:HA	32:CS:16:ARG:HE	1.71	0.56
54:UH:402:VAL:HG12	54:UH:411:VAL:HG22	1.86	0.56
1:UA:3:THR:HG21	1:UA:607:LEU:HD13	1.86	0.56
7:UJ:855:VAL:HA	7:UJ:858:LYS:HG2	1.87	0.56
7:UJ:959:GLN:HA	7:UJ:962:VAL:HG22	1.87	0.56
20:CD:49:ALA:HB1	20:CD:72:LYS:HE2	1.87	0.56
53:UT:534:ARG:HA	53:UT:537:VAL:HG22	1.87	0.56
4:UD:54:GLU:HG3	4:UD:56:TRP:HE1	1.71	0.56
4:UD:757:ILE:HB	4:UD:771:ILE:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:UL:847:LEU:O	48:Cp:30:ARG:NH2	2.39	0.56
19:CC:385:LYS:HD3	19:CC:407:LEU:HD22	1.88	0.56
27:CL:561:ARG:NH2	27:CL:567:ASN:O	2.38	0.56
32:CR:792:TYR:HA	32:CR:795:ARG:HH21	1.71	0.56
34:Ca:13:LYS:HB2	34:Ca:16:LEU:HD13	1.87	0.56
53:UT:1196:ALA:HA	53:UT:1199:PHE:HD2	1.71	0.56
24:Cl:1135:LYS:NZ	51:C2:13:U:OP2	2.39	0.56
26:CK:134:GLU:HG3	43:Cj:128:LYS:HD3	1.88	0.56
41:Ch:108:ASP:HB3	41:Ch:111:SER:HB2	1.87	0.56
54:UH:6:GLN:HB2	54:UH:415:GLU:HB3	1.87	0.56
56:US:522:HIS:ND1	56:US:525:THR:OG1	2.39	0.56
1:UA:544:GLN:OE1	43:Cj:114:ARG:NH1	2.36	0.55
8:UK:1:MET:HE1	8:UK:3:SER:HB3	1.88	0.55
15:UU:677:ASN:HB3	15:UU:679:LEU:HG	1.87	0.55
18:CB:97:LEU:HD13	18:CB:172:ASP:HA	1.88	0.55
53:UT:944:ALA:O	53:UT:947:THR:OG1	2.23	0.55
19:CC:247:ASP:O	19:CC:251:ALA:HB2	2.06	0.55
22:CG:256:GLN:HE22	22:CG:298:ARG:HA	1.69	0.55
29:CO:112:ILE:HB	29:CO:124:VAL:HB	1.88	0.55
32:CS:172:ARG:HH22	32:CS:609:PRO:HB2	1.70	0.55
36:Cc:52:ARG:NH2	36:Cc:73:ASN:OD1	2.40	0.55
52:CW:230:ASP:OD1	52:CW:232:ARG:NH1	2.39	0.55
53:UT:1919:ILE:HD13	53:UT:1992:VAL:HG11	1.86	0.55
55:UE:158:ASN:HD21	55:UE:188:MET:HA	1.71	0.55
7:UJ:659:VAL:HG11	7:UJ:681:ALA:HB2	1.87	0.55
7:UJ:1272:LEU:HD13	7:UJ:1315:VAL:HG21	1.87	0.55
7:UJ:1752:LEU:HD23	7:UJ:1756:TRP:HE1	1.70	0.55
8:UK:24:ARG:NH2	33:CT:199:ALA:O	2.39	0.55
18:CB:157:LEU:HB3	18:CB:226:ILE:HG12	1.88	0.55
28:CM:173:GLY:O	38:Cc:153:LYS:NZ	2.36	0.55
29:CO:76:ILE:HG22	29:CO:80:MET:HE3	1.88	0.55
32:CR:738:LYS:NZ	32:CR:804:THR:O	2.40	0.55
32:CS:132:THR:OG1	32:CS:134:ASN:OD1	2.25	0.55
37:Cd:121:ILE:HG21	37:Cd:124:LEU:HD12	1.88	0.55
53:UT:556:LEU:HG	53:UT:560:LYS:HE2	1.88	0.55
53:UT:2212:ASP:OD1	53:UT:2215:ARG:NH2	2.37	0.55
54:UH:84:PRO:HB3	54:UH:103:VAL:HG12	1.89	0.55
54:UH:340:VAL:HB	54:UH:343:LEU:HB2	1.87	0.55
7:UJ:97:ARG:NH2	14:UR:72:ARG:O	2.40	0.55
7:UJ:1438:LEU:HD13	7:UJ:1441:LEU:HD21	1.89	0.55
19:CC:180:GLY:HA3	19:CC:295:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CS:32:ASP:O	32:CS:35:LYS:NZ	2.34	0.55
36:Cc:63:ARG:HH11	43:Cj:122:ARG:HD3	1.71	0.55
53:UT:1418:ILE:HD12	53:UT:1434:LEU:HD23	1.87	0.55
7:UJ:1767:ILE:HG21	7:UJ:1786:ILE:HD13	1.87	0.55
13:UQ:383:GLN:OE1	13:UQ:386:THR:OG1	2.23	0.55
18:CA:249:GLN:HG2	19:CC:39:LYS:HD2	1.87	0.55
29:CN:114:ILE:HB	29:CN:122:ILE:HB	1.87	0.55
29:CO:180:LEU:HD21	29:CO:241:PHE:HE2	1.71	0.55
54:UH:258:GLN:O	54:UH:265:ASN:HA	2.07	0.55
2:UB:26:LYS:NZ	9:UL:110:LYS:O	2.40	0.55
4:UD:870:ASP:HA	61:UP:356:ARG:HD3	1.88	0.55
24:CI:117:ILE:HD11	24:CI:797:PRO:HB3	1.87	0.55
36:Cc:86:MET:HE1	50:C1:2194:A:H8	1.71	0.55
53:UT:310:ILE:HD12	53:UT:353:ARG:HG3	1.89	0.55
53:UT:1368:ARG:HA	53:UT:1371:LEU:HG	1.87	0.55
5:UF:156:ASP:OD2	5:UF:159:ARG:NH1	2.39	0.55
10:UM:548:ASN:ND2	10:UM:564:GLN:OE1	2.38	0.55
11:UN:341:PHE:HE1	28:CM:250:MET:HE2	1.71	0.55
22:CG:167:ARG:HD3	22:CG:598:ARG:HD3	1.87	0.55
24:CI:56:VAL:HG22	46:Cn:52:ILE:HG12	1.89	0.55
47:Co:358:ILE:HD11	47:Co:371:LEU:HD11	1.88	0.55
58:CX:244:PRO:HB2	58:CX:287:HIS:HB2	1.89	0.55
26:CK:214:PRO:HG2	27:CL:559:ARG:HE	1.71	0.55
56:US:208:LEU:HD23	56:US:275:LEU:HD21	1.88	0.55
60:CZ:566:GLU:HA	60:CZ:569:ILE:HG12	1.89	0.55
4:UD:384:LEU:HD12	4:UD:393:ILE:HG12	1.89	0.55
7:UJ:236:ARG:HD2	7:UJ:239:ILE:HD12	1.89	0.55
7:UJ:1706:VAL:HA	7:UJ:1709:LEU:HG	1.88	0.55
9:UL:24:LEU:HG	9:UL:41:VAL:HG12	1.89	0.55
23:CH:240:ARG:HH22	49:CU:108:ASP:HB2	1.71	0.55
32:CR:60:TYR:OH	50:C1:1000:A:N1	2.35	0.55
32:CS:659:ASP:HB2	32:CS:664:LYS:HG3	1.89	0.55
53:UT:663:SER:HB2	53:UT:836:ILE:HG21	1.89	0.55
54:UH:728:ARG:HG3	54:UH:729:LEU:HG	1.89	0.55
60:CZ:419:ARG:HE	60:CZ:450:VAL:HG13	1.71	0.55
7:UJ:232:MET:HE1	7:UJ:247:LEU:HB2	1.89	0.55
10:UM:135:ILE:HB	10:UM:149:VAL:HB	1.87	0.55
30:CP:83:THR:HG22	30:CP:85:LYS:H	1.71	0.55
50:C1:927:C:H2'	50:C1:928:G:H8	1.72	0.55
52:CW:99:ASN:ND2	52:CW:115:LEU:O	2.40	0.55
52:CW:331:VAL:HG21	52:CW:349:ASN:HD22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:UL:287:HIS:HE1	9:UL:383:LEU:HD22	1.72	0.54
13:UQ:713:VAL:HG22	13:UQ:725:VAL:HG22	1.88	0.54
24:CI:917:LYS:NZ	50:C1:1142:U:OP1	2.35	0.54
29:CO:104:ILE:HG22	29:CO:251:ILE:HD11	1.88	0.54
32:CR:788:SER:OG	32:CS:856:ASP:O	2.22	0.54
50:C1:1241:U:H3	50:C1:1258:A:H61	1.54	0.54
53:UT:1336:ILE:O	53:UT:1381:ARG:NH1	2.40	0.54
2:UB:584:LEU:HB3	2:UB:625:LYS:HD3	1.88	0.54
4:UD:684:ASP:OD1	4:UD:736:ARG:NH2	2.41	0.54
6:UG:386:MET:HE1	6:UG:421:PRO:HD2	1.88	0.54
7:UJ:741:ARG:O	7:UJ:745:LEU:HB2	2.07	0.54
8:UK:63:PHE:HB2	25:CJ:170:ILE:HD11	1.89	0.54
10:UM:198:LEU:HD23	10:UM:210:PHE:HB3	1.89	0.54
13:UQ:218:ILE:HD12	13:UQ:235:HIS:HB3	1.90	0.54
54:UH:555:GLY:O	54:UH:567:LEU:CA	2.35	0.54
58:CX:267:GLU:HA	58:CX:271:LEU:HD23	1.89	0.54
4:UD:374:VAL:HG11	4:UD:863:ILE:HD13	1.89	0.54
6:UG:284:LEU:O	6:UG:293:LEU:N	2.39	0.54
6:UG:398:VAL:HG12	6:UG:409:ILE:HG12	1.89	0.54
37:Cd:183:THR:OG1	37:Cd:185:GLN:OE1	2.24	0.54
53:UT:1390:ASP:HA	53:UT:1393:ARG:HE	1.71	0.54
53:UT:1608:THR:HA	53:UT:1611:LEU:HD13	1.89	0.54
58:CX:335:VAL:HG23	58:CX:375:TYR:HB3	1.88	0.54
2:UB:759:HIS:O	2:UB:765:ASN:ND2	2.35	0.54
6:UG:305:SER:OG	6:UG:318:THR:OG1	2.24	0.54
32:CS:289:ARG:HH21	32:CS:474:LEU:HB3	1.72	0.54
36:Cc:129:PRO:HA	36:Cc:201:LYS:HE3	1.89	0.54
7:UJ:535:ASP:OD2	7:UJ:542:ARG:NH1	2.40	0.54
53:UT:1783:LYS:O	53:UT:1787:LEU:N	2.40	0.54
9:UL:449:LEU:HB3	9:UL:463:PHE:HB2	1.90	0.54
29:CN:101:ASP:OD2	29:CN:132:ARG:NH2	2.37	0.54
53:UT:1236:ASN:O	53:UT:1239:GLN:C	2.50	0.54
12:UO:42:TRP:NE1	57:Cl:60:GLU:OE1	2.38	0.54
13:UQ:591:GLY:O	13:UQ:594:GLN:N	2.40	0.54
14:UR:541:THR:HG21	14:UR:561:HIS:HB2	1.90	0.54
32:CS:13:THR:O	32:CS:17:ASN:ND2	2.41	0.54
53:UT:1968:ASP:OD1	53:UT:1971:ARG:NH1	2.40	0.54
58:CX:266:MET:HE3	58:CX:302:PHE:HA	1.90	0.54
58:CX:275:ARG:NH1	58:CX:320:GLU:OE1	2.41	0.54
60:CZ:316:LYS:HD2	60:CZ:319:ARG:HH21	1.73	0.54
1:UA:204:SER:OG	1:UA:206:ASP:O	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:UL:109:HIS:ND1	9:UL:129:SER:OG	2.36	0.54
9:UL:200:LEU:HB3	9:UL:210:GLU:HB3	1.89	0.54
10:UM:331:ARG:O	10:UM:347:ARG:NH1	2.41	0.54
12:UO:171:LEU:HD13	12:UO:205:LEU:HD11	1.90	0.54
30:CP:273:GLU:HB3	30:CP:277:ARG:HH12	1.73	0.54
32:CS:112:THR:HA	32:CS:115:ILE:HG12	1.89	0.54
32:CS:284:THR:HB	32:CS:473:THR:HG22	1.89	0.54
47:Co:372:ARG:HA	47:Co:386:VAL:HG11	1.90	0.54
2:UB:726:LEU:HD22	2:UB:773:LEU:HD21	1.90	0.54
5:UF:77:ARG:NH1	14:UR:52:GLU:OE2	2.41	0.54
52:CW:114:HIS:HB3	52:CW:116:GLN:HE22	1.72	0.54
53:UT:1021:LEU:O	53:UT:1025:ARG:HG3	2.08	0.54
1:UA:393:LYS:HG3	1:UA:395:SER:H	1.73	0.54
1:UA:558:ARG:HB2	1:UA:566:ALA:HB2	1.90	0.54
7:UJ:78:SER:HA	7:UJ:81:VAL:HG12	1.90	0.54
7:UJ:563:TYR:O	7:UJ:568:LYS:NZ	2.40	0.54
7:UJ:912:LEU:HB3	7:UJ:958:LEU:HD11	1.89	0.54
7:UJ:1090:PRO:HD2	7:UJ:1093:ARG:HD2	1.88	0.54
7:UJ:1727:LEU:O	7:UJ:1731:ARG:HB2	2.07	0.54
40:Cg:128:ARG:HE	50:C1:1059:A:H4'	1.73	0.54
46:Cn:54:LEU:HD11	46:Cn:75:GLN:HB2	1.90	0.54
50:C1:181:G:O2'	50:C1:183:C:N4	2.40	0.54
53:UT:1765:LEU:HD22	53:UT:1773:ILE:HD11	1.89	0.54
7:UJ:1109:ASP:OD1	7:UJ:1109:ASP:N	2.41	0.53
9:UL:900:GLU:OE2	9:UL:903:ARG:NH2	2.42	0.53
26:CK:94:ARG:HA	26:CK:119:ARG:HG2	1.90	0.53
35:Cb:183:ILE:HG12	35:Cb:220:THR:HG21	1.90	0.53
44:Ck:108:ARG:NH1	50:C1:936:A:OP1	2.39	0.53
52:CW:290:ILE:HA	52:CW:309:ASP:HB3	1.89	0.53
56:US:82:GLU:OE1	56:US:86:ARG:NH1	2.41	0.53
12:UO:247:LEU:HD22	12:UO:258:LEU:HD12	1.88	0.53
14:UR:322:ARG:NH1	50:C1:133:G:H22	2.06	0.53
21:CE:29:SER:HB2	21:CE:34:LEU:HD22	1.91	0.53
32:CS:58:TRP:HB2	32:CS:104:ILE:HD11	1.89	0.53
1:UA:452:ILE:HG13	1:UA:464:LEU:HD13	1.90	0.53
2:UB:590:ASP:HA	2:UB:593:ILE:HG22	1.90	0.53
7:UJ:1187:THR:HA	7:UJ:1244:LEU:HD21	1.89	0.53
18:CB:239:VAL:HG21	18:CB:255:ILE:HD12	1.90	0.53
22:CG:196:LYS:HB2	22:CG:227:ILE:HD11	1.89	0.53
22:CG:270:LEU:HD11	22:CG:294:LEU:HD21	1.89	0.53
32:CS:24:ARG:HG2	32:CS:147:GLY:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:CU:186:ALA:O	49:CU:192:ASN:ND2	2.38	0.53
53:UT:1306:LEU:HD21	53:UT:1335:PHE:HB3	1.91	0.53
18:CB:208:GLU:OE1	20:CD:153:LYS:NZ	2.42	0.53
32:CR:137:ALA:HA	32:CR:490:LEU:HD21	1.90	0.53
54:UH:349:LEU:HD21	54:UH:355:LEU:HG	1.90	0.53
7:UJ:1623:SER:HA	7:UJ:1626:VAL:HG22	1.90	0.53
13:UQ:521:PRO:HG3	55:UE:26:THR:HG21	1.90	0.53
23:CH:375:TRP:O	24:CI:763:HIS:NE2	2.41	0.53
24:CI:223:SER:HA	24:CI:226:LEU:HG	1.88	0.53
56:US:322:LEU:HD21	56:US:367:PHE:HE2	1.74	0.53
1:UA:555:SER:HB2	1:UA:573:LYS:HD3	1.90	0.53
2:UB:554:ARG:HH21	56:US:523:ILE:HG13	1.73	0.53
9:UL:816:PRO:HA	9:UL:819:VAL:HG22	1.90	0.53
25:CJ:57:PHE:HD1	27:CL:622:MET:HE2	1.73	0.53
53:UT:1604:ILE:O	53:UT:1608:THR:OG1	2.20	0.53
59:CY:64:ARG:HH12	60:CZ:399:ALA:HA	1.73	0.53
6:UG:332:PHE:HB3	11:UN:869:VAL:HG11	1.89	0.53
8:UK:68:MET:HG3	51:C2:58:A:H4'	1.89	0.53
10:UM:222:ALA:HB2	10:UM:230:ALA:HA	1.89	0.53
27:CL:59:ASN:HB3	27:CL:62:ILE:HG22	1.89	0.53
32:CR:143:VAL:HG21	32:CR:149:VAL:HG22	1.90	0.53
32:CR:829:LEU:O	32:CR:832:LEU:C	2.51	0.53
35:Cb:151:ASP:OD2	37:Cd:218:ARG:NH1	2.41	0.53
53:UT:1296:ILE:O	53:UT:1334:ARG:NH2	2.42	0.53
56:US:341:THR:HG22	56:US:447:PRO:HD2	1.90	0.53
6:UG:219:VAL:HA	6:UG:235:SER:HA	1.91	0.53
10:UM:283:LEU:HD21	10:UM:348:VAL:HG21	1.91	0.53
10:UM:376:ILE:HA	10:UM:393:THR:HG22	1.89	0.53
13:UQ:392:LEU:HD22	13:UQ:428:MET:HE3	1.89	0.53
23:CH:227:VAL:O	50:C1:1714:G:N2	2.42	0.53
24:CI:963:LYS:NZ	50:C1:2181:U:OP2	2.37	0.53
51:C2:101:G:H1	51:C2:251:U:H3	1.55	0.53
53:UT:69:LYS:O	53:UT:73:LEU:HB2	2.08	0.53
53:UT:309:VAL:O	53:UT:313:SER:OG	2.27	0.53
7:UJ:16:SER:O	7:UJ:159:ARG:NH2	2.40	0.53
9:UL:954:ARG:HB2	27:CL:652:ASP:HB2	1.91	0.53
17:UZ:104:PRO:HG2	17:UZ:212:ALA:HB2	1.90	0.53
26:CK:178:LYS:NZ	50:C1:1743:C:O2'	2.42	0.53
30:CP:66:GLY:O	30:CP:86:THR:OG1	2.24	0.53
35:Cb:19:LEU:HD23	35:Cb:51:ARG:HH12	1.74	0.53
39:Cf:40:PRO:HB3	52:CW:21:ARG:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:C1:729:A:OP1	52:CW:36:LYS:NZ	2.42	0.53
53:UT:70:TRP:NE1	53:UT:124:ASP:OD2	2.42	0.53
53:UT:869:LEU:HA	53:UT:900:ARG:HH12	1.74	0.53
4:UD:671:ARG:NH2	7:UJ:662:PRO:O	2.42	0.53
6:UG:215:LYS:HG2	50:C1:291:C:C2	2.44	0.53
7:UJ:861:LEU:HD12	7:UJ:865:ILE:HG21	1.91	0.53
9:UL:864:PHE:O	9:UL:867:ARG:O	2.27	0.53
10:UM:237:CYS:HB3	10:UM:280:VAL:HG12	1.90	0.53
20:CD:137:ASN:HA	20:CD:140:GLU:HG3	1.90	0.53
37:CD:131:LYS:NZ	50:C1:750:C:OP1	2.42	0.53
53:UT:1334:ARG:NH1	53:UT:1337:GLU:OE2	2.42	0.53
3:UC:305:MET:N	3:UC:305:MET:SD	2.82	0.52
4:UD:30:SER:H	4:UD:33:LYS:HD2	1.74	0.52
5:UF:361:LEU:HD23	5:UF:364:LEU:HD12	1.91	0.52
7:UJ:733:ILE:O	7:UJ:741:ARG:NH1	2.42	0.52
7:UJ:1651:LEU:HD13	7:UJ:1702:VAL:HB	1.90	0.52
7:UJ:1667:GLN:HE22	7:UJ:1713:VAL:HG22	1.75	0.52
14:UR:376:PHE:HB3	14:UR:387:LEU:HD23	1.91	0.52
29:CN:77:MET:HG3	29:CN:82:ARG:HB2	1.91	0.52
32:CR:165:MET:HE1	32:CR:187:GLU:HA	1.91	0.52
34:Ca:86:LEU:HB3	34:Ca:98:THR:HB	1.91	0.52
39:Cf:87:ASN:HB3	39:Cf:89:GLU:HG2	1.91	0.52
50:C1:103:G:N2	50:C1:106:A:OP2	2.42	0.52
50:C1:1122:A:H5'	50:C1:1127:C:H41	1.74	0.52
54:UH:743:ARG:NH2	54:UH:818:GLU:OE2	2.42	0.52
4:UD:549:VAL:HA	4:UD:565:ASP:HA	1.91	0.52
10:UM:651:LEU:HB3	10:UM:706:ASN:HD21	1.75	0.52
29:CN:104:ILE:N	29:CN:246:GLU:OE2	2.42	0.52
38:Ce:128:LEU:O	38:Ce:132:HIS:ND1	2.40	0.52
53:UT:37:LEU:HD21	53:UT:162:GLU:HB2	1.91	0.52
53:UT:1761:ILE:O	53:UT:1765:LEU:HB3	2.10	0.52
54:UH:5:LEU:HD23	54:UH:364:VAL:HG11	1.91	0.52
60:CZ:491:ASP:N	60:CZ:491:ASP:OD1	2.42	0.52
4:UD:48:ARG:NE	4:UD:54:GLU:OE2	2.36	0.52
4:UD:487:SER:OG	4:UD:489:ASP:OD1	2.23	0.52
10:UM:777:VAL:HG21	10:UM:794:VAL:HG21	1.91	0.52
18:CA:65:ALA:O	18:CA:107:LYS:NZ	2.35	0.52
22:CG:123:PHE:O	35:Cb:106:LYS:NZ	2.42	0.52
29:CN:77:MET:HE3	29:CN:84:ILE:HG22	1.91	0.52
29:CN:96:LEU:HD23	29:CN:130:ILE:HD12	1.91	0.52
29:CO:80:MET:SD	29:CO:82:ARG:NH2	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CQ:107:ASP:O	31:CQ:110:LYS:NZ	2.40	0.52
32:CR:295:MET:HE3	32:CR:411:ALA:HB2	1.91	0.52
34:Ca:157:GLN:HB2	34:Ca:160:GLN:HG3	1.90	0.52
42:Ci:31:ARG:NH1	42:Ci:44:THR:OG1	2.42	0.52
52:CW:208:ALA:O	52:CW:217:CYS:CA	2.44	0.52
53:UT:188:ASP:HB3	53:UT:234:HIS:HE2	1.73	0.52
2:UB:550:GLU:HB2	56:US:524:PHE:HB2	1.91	0.52
2:UB:730:THR:HG23	2:UB:780:LEU:HD22	1.92	0.52
7:UJ:1360:LEU:N	7:UJ:1400:TYR:OH	2.40	0.52
10:UM:563:SER:OG	10:UM:564:GLN:N	2.41	0.52
24:CI:104:ILE:HG23	24:CI:336:ALA:HB2	1.92	0.52
30:CP:187:ASP:HB3	30:CP:192:ILE:HB	1.92	0.52
46:Cn:107:PHE:HD2	46:Cn:123:LYS:HB3	1.74	0.52
53:UT:151:LEU:HG	53:UT:155:MET:HE1	1.91	0.52
53:UT:1173:PRO:HA	53:UT:1213:THR:HB	1.92	0.52
54:UH:292:PHE:HE1	54:UH:294:ALA:HB2	1.75	0.52
54:UH:436:ARG:HG3	54:UH:600:ARG:HG2	1.89	0.52
59:CY:52:LEU:HD21	60:CZ:328:ARG:HD2	1.90	0.52
6:UG:234:LEU:HD12	6:UG:264:LEU:HB2	1.91	0.52
22:CG:565:LEU:HG	22:CG:578:VAL:HG12	1.92	0.52
24:CI:326:ARG:NH1	50:C1:639:U:O4	2.43	0.52
32:CS:33:HIS:ND1	32:CS:33:HIS:O	2.42	0.52
32:CS:402:LEU:O	32:CS:406:TYR:OH	2.24	0.52
52:CW:206:VAL:O	52:CW:219:PHE:CA	2.45	0.52
53:UT:658:ASN:OD1	53:UT:670:SER:OG	2.27	0.52
53:UT:1642:GLU:HA	53:UT:1645:VAL:HG12	1.91	0.52
54:UH:646:LYS:HB2	54:UH:730:PHE:HE1	1.75	0.52
1:UA:275:SER:HB2	1:UA:299:GLU:HG3	1.91	0.52
1:UA:356:VAL:HG22	1:UA:366:VAL:HG22	1.90	0.52
2:UB:801:HIS:NE2	56:US:418:MET:HE2	2.24	0.52
4:UD:115:ASP:HB2	4:UD:122:LYS:HB2	1.90	0.52
7:UJ:1284:LEU:HA	7:UJ:1287:LEU:HD12	1.92	0.52
30:CP:294:LYS:NZ	50:C1:901:C:OP1	2.42	0.52
39:Cf:110:ARG:NH2	39:Cf:164:PHE:O	2.42	0.52
53:UT:1630:LYS:O	53:UT:1634:GLN:NE2	2.32	0.52
55:UE:223:VAL:HG21	55:UI:268:ALA:HB3	1.91	0.52
55:UI:214:LEU:HA	55:UI:217:TRP:HB2	1.91	0.52
6:UG:123:VAL:O	6:UG:127:GLN:HG3	2.09	0.52
10:UM:724:THR:HA	10:UM:727:THR:HG22	1.91	0.52
17:UZ:267:VAL:HG22	17:UZ:278:VAL:HG21	1.91	0.52
24:CI:1096:LYS:HE2	33:CT:175:LYS:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:UT:554:VAL:HA	53:UT:557:LYS:HG2	1.92	0.52
54:UH:348:ARG:HH12	54:UH:351:LYS:HA	1.74	0.52
7:UJ:324:LEU:HD13	7:UJ:357:GLY:HA3	1.91	0.52
12:UO:6:VAL:HG23	55:UE:27:ARG:HH21	1.75	0.52
13:UQ:813:ILE:HB	13:UQ:823:LEU:HB3	1.90	0.52
24:CI:826:ILE:HD12	24:CI:862:TYR:HB3	1.92	0.52
32:CS:35:LYS:HA	32:CS:38:ILE:HD12	1.92	0.52
32:CS:515:GLN:HG3	59:CY:116:ARG:HB3	1.91	0.52
54:UH:591:VAL:HG21	54:UH:609:ILE:HG21	1.92	0.52
58:CX:422:ARG:O	58:CX:430:ARG:NH2	2.43	0.52
7:UJ:174:LEU:HD13	33:CT:74:PRO:HB2	1.92	0.52
10:UM:619:SER:OG	10:UM:620:GLY:N	2.42	0.52
12:UO:554:VAL:HG23	55:UE:230:VAL:HG13	1.92	0.52
13:UQ:632:ASP:OD2	13:UQ:636:ARG:NH2	2.43	0.52
18:CB:196:MET:HE1	18:CB:203:VAL:HG11	1.92	0.52
36:Cc:69:PHE:HB3	48:Cp:50:ARG:NH2	2.25	0.52
39:Cf:5:ARG:NH2	50:C1:918:U:O4	2.38	0.52
53:UT:528:LEU:HA	53:UT:531:TYR:HD2	1.74	0.52
60:CZ:419:ARG:HH21	60:CZ:450:VAL:HA	1.74	0.52
7:UJ:112:MET:HE1	33:CT:71:VAL:HG23	1.92	0.52
7:UJ:803:PRO:HA	7:UJ:806:LEU:HG	1.92	0.52
10:UM:743:GLN:NE2	10:UM:747:ASN:OD1	2.43	0.52
32:CR:38:ILE:HD11	32:CR:152:LEU:HD21	1.91	0.52
42:Ci:30:ALA:HB2	42:Ci:92:LEU:HD13	1.92	0.52
52:CW:183:GLN:O	52:CW:229:TYR:OH	2.27	0.52
53:UT:428:PRO:HG2	53:UT:818:ILE:HD12	1.91	0.52
2:UB:639:LEU:HD23	2:UB:642:LEU:HD12	1.91	0.51
32:CS:526:LEU:HB3	32:CS:537:LEU:HD21	1.91	0.51
32:CS:605:ARG:NH1	32:CS:607:GLN:OE1	2.42	0.51
52:CW:216:LEU:HD11	52:CW:228:PHE:HB3	1.92	0.51
52:CW:228:PHE:HB2	52:CW:238:ALA:HB3	1.92	0.51
53:UT:5:THR:HG22	53:UT:8:ARG:HH21	1.75	0.51
15:UU:931:GLY:O	15:UU:934:LYS:C	2.54	0.51
18:CA:113:THR:HG21	18:CA:124:LYS:HE3	1.91	0.51
21:CE:36:LYS:HD3	21:CE:92:CYS:HB3	1.93	0.51
27:CL:82:LEU:HD13	27:CL:130:VAL:HG21	1.91	0.51
32:CS:427:LYS:HD3	32:CS:430:LYS:HE3	1.90	0.51
2:UB:792:ARG:HH12	56:US:434:ASP:HB2	1.74	0.51
13:UQ:636:ARG:NH1	55:UE:41:LEU:O	2.43	0.51
26:CK:166:SER:OG	50:C1:2180:A:N3	2.44	0.51
34:Ca:137:LEU:HD22	34:Ca:215:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:UT:221:PRO:HA	53:UT:224:LYS:HB2	1.92	0.51
56:US:89:VAL:HG12	56:US:148:ALA:HB2	1.91	0.51
7:UJ:372:ILE:HD11	7:UJ:416:ILE:HG12	1.92	0.51
7:UJ:717:THR:HG22	7:UJ:719:LEU:H	1.76	0.51
18:CB:91:LEU:HD13	18:CB:129:ILE:HG21	1.93	0.51
32:CR:518:LEU:HD12	32:CR:570:LEU:HD13	1.92	0.51
32:CS:885:LEU:HG	32:CS:889:LEU:HD12	1.92	0.51
33:CT:117:MET:HE3	33:CT:174:TYR:HD1	1.76	0.51
36:Cc:63:ARG:NH1	43:Cj:122:ARG:HD3	2.26	0.51
53:UT:310:ILE:HG23	53:UT:353:ARG:HG3	1.92	0.51
53:UT:1438:LEU:HD21	53:UT:1459:LEU:HB2	1.91	0.51
4:UD:453:VAL:HB	4:UD:472:VAL:HB	1.92	0.51
25:CJ:102:THR:HG22	25:CJ:104:SER:H	1.75	0.51
37:Cd:182:VAL:HG12	50:C1:725:A:H8	1.76	0.51
39:Cf:10:LYS:NZ	50:C1:921:G:O2'	2.44	0.51
54:UH:267:ARG:HB2	54:UH:296:LEU:O	2.10	0.51
58:CX:390:LEU:HD11	58:CX:432:ALA:HB1	1.93	0.51
1:UA:445:ILE:HA	1:UA:470:PRO:HB3	1.91	0.51
2:UB:528:GLN:O	2:UB:532:HIS:ND1	2.40	0.51
7:UJ:552:LEU:HD22	7:UJ:632:TRP:HZ3	1.75	0.51
7:UJ:847:ASP:HA	7:UJ:850:THR:HG22	1.93	0.51
7:UJ:990:VAL:HA	7:UJ:993:THR:HG22	1.93	0.51
12:UO:125:VAL:HB	12:UO:138:LYS:HB3	1.92	0.51
16:UX:112:ILE:HD11	45:Cm:96:ALA:HB2	1.93	0.51
28:CM:224:LEU:HB2	28:CM:234:ILE:HG22	1.92	0.51
32:CR:307:TYR:O	32:CR:367:GLN:NE2	2.44	0.51
36:Cc:209:LYS:HG3	36:Cc:212:ARG:HE	1.76	0.51
39:Cf:103:GLN:HG2	39:Cf:168:ARG:HB3	1.91	0.51
41:Ch:109:LYS:NZ	50:C1:1561:G:OP1	2.39	0.51
42:Ci:33:PHE:HB3	42:Ci:40:PHE:HB2	1.92	0.51
47:Co:342:LYS:HB2	47:Co:355:VAL:HG12	1.93	0.51
52:CW:63:SER:OG	52:CW:107:GLN:O	2.29	0.51
7:UJ:1527:LEU:HD21	7:UJ:1583:TRP:HD1	1.76	0.51
10:UM:638:PHE:HB3	10:UM:678:TRP:CZ3	2.46	0.51
19:CC:45:GLY:HA3	50:C1:435:A:N1	2.26	0.51
23:CH:405:ASN:HD21	23:CH:408:ARG:HB2	1.76	0.51
32:CR:34:ALA:HB1	32:CR:152:LEU:HD22	1.93	0.51
32:CS:331:PHE:HB3	32:CS:336:TYR:HB2	1.93	0.51
34:Ca:101:HIS:HA	34:Ca:217:LEU:HD12	1.91	0.51
39:Cf:99:SER:N	39:Cf:173:ILE:O	2.44	0.51
49:CU:249:ARG:HD2	50:C1:1519:C:H5	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:UT:454:VAL:HA	53:UT:491:PRO:HG3	1.93	0.51
56:US:416:PHE:O	56:US:420:ARG:HB2	2.10	0.51
1:UA:627:SER:O	16:UX:-5:LYS:NZ	2.40	0.51
4:UD:392:ARG:HB3	4:UD:419:PHE:HE1	1.76	0.51
4:UD:449:THR:HA	61:UP:330:ARG:HH21	1.75	0.51
4:UD:570:ILE:HD11	4:UD:626:LEU:HD11	1.93	0.51
7:UJ:1077:ASP:HB2	7:UJ:1168:VAL:HG21	1.93	0.51
13:UQ:731:LYS:HB3	13:UQ:749:ASP:HB2	1.93	0.51
23:CH:225:THR:O	23:CH:275:ILE:HA	2.11	0.51
24:CI:523:MET:HA	24:CI:526:ARG:HE	1.75	0.51
32:CR:514:SER:OG	32:CR:515:GLN:OE1	2.29	0.51
38:Ce:86:GLU:HA	38:Ce:89:LYS:HG2	1.93	0.51
38:Ce:173:ASP:HA	38:Ce:176:LEU:HG	1.92	0.51
53:UT:1746:LYS:HA	53:UT:1751:ARG:HH21	1.75	0.51
60:CZ:392:ARG:NH1	60:CZ:406:THR:OG1	2.43	0.51
4:UD:390:GLU:OE2	4:UD:392:ARG:NE	2.31	0.51
7:UJ:1727:LEU:HA	7:UJ:1730:LEU:HD23	1.92	0.51
10:UM:815:ASP:O	10:UM:818:THR:OG1	2.26	0.51
13:UQ:791:LEU:HD23	13:UQ:812:LEU:HD12	1.92	0.51
30:CP:42:LEU:HB3	34:Ca:115:ARG:HD3	1.93	0.51
32:CR:234:LYS:HA	32:CR:237:LYS:HE3	1.93	0.51
53:UT:1064:LEU:O	53:UT:1069:GLN:NE2	2.44	0.51
1:UA:327:TRP:HZ3	15:UU:880:LEU:HD13	1.76	0.51
9:UL:493:ASP:HB2	9:UL:500:LEU:HD11	1.91	0.51
28:CM:130:ASP:OD2	28:CM:133:LYS:NZ	2.43	0.51
32:CS:877:SER:HB3	52:CW:361:ASN:HD22	1.76	0.51
38:Ce:38:ALA:HA	38:Ce:39:ASP:HB2	1.93	0.51
39:Cf:182:ARG:NH2	50:C1:789:U:O2	2.41	0.51
52:CW:216:LEU:O	52:CW:252:TYR:OH	2.25	0.51
53:UT:335:GLN:HA	53:UT:338:PHE:HB2	1.93	0.51
4:UD:510:THR:OG1	4:UD:517:SER:OG	2.28	0.50
7:UJ:1534:ARG:HB2	7:UJ:1598:TYR:HB3	1.93	0.50
10:UM:135:ILE:HD11	10:UM:156:VAL:HG21	1.93	0.50
28:CM:323:THR:HG22	28:CM:325:ARG:H	1.76	0.50
30:CP:72:ASP:OD2	30:CP:75:GLU:N	2.42	0.50
32:CR:240:LYS:HG2	32:CR:253:ILE:HG22	1.92	0.50
32:CR:271:ALA:O	32:CR:279:ASN:ND2	2.44	0.50
32:CR:547:SER:OG	32:CR:640:THR:O	2.29	0.50
32:CS:128:PHE:HA	32:CS:131:ILE:HG12	1.91	0.50
32:CS:143:VAL:HG21	32:CS:149:VAL:HG22	1.92	0.50
35:Cb:42:MET:HB3	35:Cb:109:PHE:CE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Cb:126:VAL:HG22	35:Cb:141:THR:HG22	1.92	0.50
39:Cf:58:LEU:HD11	52:CW:75:TYR:HB2	1.93	0.50
53:UT:1041:GLY:HA2	53:UT:1044:ARG:HH21	1.75	0.50
53:UT:1460:CYS:HA	53:UT:1463:ILE:HG12	1.93	0.50
53:UT:1617:ARG:O	53:UT:1621:ARG:HG2	2.12	0.50
7:UJ:1379:VAL:HG22	7:UJ:1386:ILE:HG21	1.93	0.50
10:UM:429:LEU:HB3	10:UM:460:TRP:CZ3	2.45	0.50
12:UO:227:MET:HE1	12:UO:260:LEU:HB3	1.92	0.50
12:UO:479:ILE:O	12:UO:483:ARG:HG3	2.12	0.50
20:CD:297:VAL:HG13	20:CD:343:ILE:HG22	1.93	0.50
21:CF:21:LEU:HD23	21:CF:118:LEU:HD13	1.93	0.50
22:CG:191:TYR:HE1	22:CG:231:LYS:HD3	1.76	0.50
34:Ca:152:LYS:HG3	34:Ca:153:THR:HG23	1.93	0.50
43:Cj:50:GLU:O	43:Cj:54:ILE:HG13	2.11	0.50
50:C1:785:U:OP1	53:UT:1013:ARG:NH2	2.41	0.50
53:UT:1521:LEU:HD12	53:UT:1571:HIS:HE1	1.75	0.50
4:UD:868:SER:OG	4:UD:871:ASP:OD2	2.29	0.50
7:UJ:1203:LYS:HD3	7:UJ:1258:LEU:HA	1.93	0.50
9:UL:113:ILE:HD13	9:UL:129:SER:HB3	1.93	0.50
24:CI:974:ARG:NH1	50:C1:2183:A:OP2	2.44	0.50
32:CR:725:VAL:O	32:CR:761:VAL:HA	2.11	0.50
32:CS:29:VAL:HG11	32:CS:38:ILE:HD11	1.94	0.50
32:CS:240:LYS:HA	32:CS:253:ILE:HD12	1.93	0.50
32:CS:578:ARG:NH1	32:CS:579:LEU:O	2.44	0.50
43:Cj:94:ALA:HB2	43:Cj:102:LYS:HG3	1.92	0.50
2:UB:88:PRO:O	2:UB:92:ARG:HB2	2.12	0.50
7:UJ:1448:SER:O	7:UJ:1461:ARG:NH2	2.44	0.50
9:UL:431:SER:OG	9:UL:469:LEU:O	2.28	0.50
13:UQ:116:THR:HA	13:UQ:432:MET:HG3	1.92	0.50
15:UU:439:LYS:HE2	15:UU:460:LEU:HD22	1.92	0.50
30:CP:40:MET:HA	30:CP:78:MET:O	2.11	0.50
37:Cd:67:VAL:HG21	37:Cd:73:VAL:HG11	1.92	0.50
53:UT:1313:LEU:HD12	53:UT:1358:LEU:HG	1.93	0.50
53:UT:1805:PHE:HD2	53:UT:1809:SER:HB3	1.76	0.50
7:UJ:268:GLN:NE2	7:UJ:299:GLY:O	2.41	0.50
7:UJ:1190:LEU:HD12	7:UJ:1244:LEU:HD13	1.93	0.50
7:UJ:1268:VAL:HG21	7:UJ:1287:LEU:HD21	1.92	0.50
10:UM:388:MET:HE3	10:UM:400:ILE:HG22	1.93	0.50
12:UO:463:ARG:NH1	13:UQ:524:VAL:O	2.37	0.50
27:CL:125:LEU:HD13	27:CL:128:ARG:HH21	1.76	0.50
49:CU:203:LYS:HE3	49:CU:220:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:UT:309:VAL:O	53:UT:313:SER:CB	2.60	0.50
60:CZ:495:TYR:HA	60:CZ:498:LEU:HD23	1.93	0.50
1:UA:15:TYR:OH	1:UA:18:GLY:O	2.27	0.50
7:UJ:1534:ARG:HA	7:UJ:1538:ALA:HB3	1.93	0.50
20:CD:81:LYS:HE2	20:CD:105:ILE:HG23	1.93	0.50
23:CH:7:GLU:HA	23:CH:32:HIS:HB2	1.93	0.50
26:CK:100:LEU:HD13	26:CK:144:GLU:HB3	1.93	0.50
29:CO:122:ILE:HD12	29:CO:144:LEU:HD21	1.94	0.50
31:CQ:245:TYR:O	31:CQ:249:ARG:HG3	2.12	0.50
32:CR:832:LEU:HG	32:CR:833:PHE:H	1.75	0.50
40:Cg:60:LEU:HD23	40:Cg:67:ARG:HB2	1.93	0.50
52:CW:183:GLN:O	52:CW:236:ARG:NH2	2.42	0.50
53:UT:505:LEU:HB2	53:UT:531:TYR:HE1	1.76	0.50
54:UH:542:ASP:HB3	54:UH:545:TRP:HD1	1.77	0.50
2:UB:490:ASN:HA	2:UB:493:LYS:HG2	1.94	0.50
4:UD:122:LYS:HG2	4:UD:123:LYS:HG3	1.93	0.50
7:UJ:645:SER:O	7:UJ:647:LEU:N	2.45	0.50
14:UR:403:VAL:HA	14:UR:406:MET:HE2	1.93	0.50
24:CI:226:LEU:HA	24:CI:229:MET:HE2	1.94	0.50
24:CI:886:CYS:O	24:CI:900:ALA:N	2.38	0.50
54:UH:220:ALA:HB1	54:UH:242:ILE:HD13	1.94	0.50
54:UH:774:GLN:NE2	54:UH:778:ASP:OD2	2.45	0.50
58:CX:284:LEU:HD11	58:CX:288:LEU:HD22	1.93	0.50
7:UJ:33:LEU:HB3	7:UJ:119:GLU:OE1	2.12	0.50
7:UJ:1480:GLY:O	7:UJ:1484:ASN:ND2	2.45	0.50
24:CI:68:PRO:HB3	24:CI:113:ARG:HG3	1.93	0.50
32:CS:310:ILE:HB	32:CS:369:ILE:HG22	1.93	0.50
53:UT:1032:MET:HG2	53:UT:1083:LEU:HD11	1.94	0.50
53:UT:1310:THR:HB	53:UT:1354:THR:HG21	1.93	0.50
53:UT:1572:ILE:HA	53:UT:1576:PHE:HD1	1.75	0.50
53:UT:1602:ASN:HB2	53:UT:1643:LYS:HZ3	1.77	0.50
54:UH:223:VAL:HG13	54:UH:227:LEU:HD12	1.93	0.50
56:US:352:LEU:HD22	56:US:396:ALA:HB1	1.94	0.50
2:UB:813:PRO:HA	29:CN:152:GLY:HA2	1.94	0.50
9:UL:777:MET:HG3	9:UL:781:ARG:HH21	1.77	0.50
10:UM:120:ASP:OD2	10:UM:122:THR:OG1	2.28	0.50
24:CI:1072:LYS:NZ	50:C1:218:G:O6	2.32	0.50
53:UT:422:TRP:CD1	53:UT:425:TRP:HE1	2.27	0.50
60:CZ:456:GLN:O	60:CZ:460:SER:HB2	2.12	0.50
1:UA:112:VAL:HG13	1:UA:157:LEU:HD13	1.93	0.49
10:UM:300:ILE:HG23	10:UM:309:ILE:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:UX:154:LYS:HG2	16:UX:165:ILE:HG21	1.92	0.49
29:CO:84:ILE:HA	29:CO:87:ALA:HB3	1.92	0.49
32:CS:278:ARG:HB3	32:CS:467:ARG:HG2	1.93	0.49
35:Cb:197:HIS:HB3	35:Cb:209:HIS:HB2	1.93	0.49
44:Ck:11:ARG:NH2	50:C1:926:C:O2'	2.41	0.49
1:UA:683:THR:O	1:UA:775:ARG:NH2	2.45	0.49
2:UB:900:LYS:HG3	2:UB:903:ARG:HH21	1.76	0.49
3:UC:209:VAL:HB	27:CL:65:ARG:HB2	1.93	0.49
7:UJ:586:ASP:OD1	7:UJ:586:ASP:N	2.43	0.49
7:UJ:1023:LEU:HD12	7:UJ:1060:LEU:HB3	1.94	0.49
7:UJ:1369:VAL:HG11	7:UJ:1413:GLU:HB3	1.93	0.49
7:UJ:1485:TRP:HB3	7:UJ:1503:LEU:HD22	1.94	0.49
22:CG:351:ASP:N	22:CG:351:ASP:OD1	2.45	0.49
23:CH:232:ASN:O	23:CH:236:ILE:HG12	2.12	0.49
23:CH:405:ASN:HD21	23:CH:408:ARG:HD2	1.77	0.49
40:Cg:80:ARG:NH1	59:CY:309:GLU:OE1	2.45	0.49
53:UT:1056:GLU:HA	53:UT:1059:PHE:HB2	1.93	0.49
53:UT:1686:ILE:O	53:UT:1690:PHE:HB2	2.13	0.49
58:CX:199:VAL:HG22	58:CX:236:LEU:HD11	1.94	0.49
7:UJ:823:ASP:OD1	7:UJ:823:ASP:N	2.46	0.49
7:UJ:1608:ASP:HA	7:UJ:1611:PHE:HD2	1.77	0.49
53:UT:239:LEU:O	53:UT:242:MET:C	2.55	0.49
54:UH:348:ARG:HA	54:UH:354:VAL:HG12	1.94	0.49
2:UB:8:ARG:NH2	26:CK:180:ILE:O	2.46	0.49
2:UB:335:LEU:HD21	56:US:517:PHE:HB3	1.94	0.49
3:UC:321:LEU:HD21	27:CL:162:LEU:HD13	1.93	0.49
7:UJ:1600:LEU:HA	7:UJ:1603:VAL:HG22	1.95	0.49
8:UK:261:ARG:NH2	50:C1:206:C:O2'	2.45	0.49
12:UO:121:GLY:HA2	12:UO:147:VAL:HG23	1.93	0.49
20:CD:321:ILE:HD12	20:CD:328:LEU:HD22	1.93	0.49
22:CG:583:GLY:HA2	22:CG:599:CYS:HA	1.94	0.49
28:CM:67:GLN:OE1	45:Cm:68:ARG:NH2	2.46	0.49
32:CS:240:LYS:O	32:CS:244:GLU:HB2	2.12	0.49
32:CS:434:GLU:OE2	32:CS:437:ARG:NH2	2.45	0.49
32:CS:790:LEU:HD23	32:CS:794:PHE:HB3	1.93	0.49
42:Ci:81:ALA:HB2	42:Ci:118:LEU:HD23	1.94	0.49
53:UT:710:LEU:HD21	53:UT:737:MET:HG3	1.94	0.49
53:UT:2067:ASP:OD1	53:UT:2067:ASP:N	2.44	0.49
54:UH:44:LYS:HB2	54:UH:46:ARG:HH12	1.77	0.49
1:UA:561:THR:OG1	25:CJ:144:ARG:NH1	2.45	0.49
9:UL:287:HIS:HD2	9:UL:289:LEU:H	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:CM:242:CYS:HA	28:CM:259:SER:HA	1.94	0.49
30:CP:145:GLY:HA3	30:CP:150:THR:HG22	1.94	0.49
35:Cb:100:ARG:HB2	35:Cb:114:ILE:HG13	1.95	0.49
53:UT:1305:MET:HA	53:UT:1308:ILE:HG12	1.93	0.49
54:UH:277:GLU:OE2	54:UH:281:ARG:NH2	2.43	0.49
58:CX:369:VAL:HA	58:CX:372:GLU:HG3	1.93	0.49
9:UL:57:LEU:HD21	9:UL:60:ARG:HG3	1.95	0.49
10:UM:303:THR:O	10:UM:306:HIS:ND1	2.45	0.49
10:UM:510:LEU:HB2	10:UM:524:ILE:HD11	1.95	0.49
24:CI:845:LEU:HD11	27:CL:490:LEU:HD21	1.95	0.49
29:CO:178:VAL:HG21	29:CO:225:ILE:HD12	1.95	0.49
30:CP:46:TYR:HE2	34:Ca:117:TRP:HE1	1.59	0.49
53:UT:388:LYS:NZ	53:UT:812:GLU:OE1	2.45	0.49
53:UT:432:TYR:OH	53:UT:807:LEU:O	2.29	0.49
53:UT:1091:MET:O	53:UT:1095:VAL:HB	2.13	0.49
53:UT:1322:PRO:HA	53:UT:1325:LYS:HE2	1.93	0.49
56:US:195:ASP:OD1	56:US:196:ILE:HD12	2.13	0.49
60:CZ:331:LEU:HD21	60:CZ:366:LEU:HD21	1.93	0.49
2:UB:820:ASP:OD1	2:UB:823:LYS:HG2	2.11	0.49
13:UQ:658:LEU:HD11	55:UE:32:ARG:HD2	1.95	0.49
14:UR:253:ARG:HH12	14:UR:599:SER:HB2	1.78	0.49
18:CA:110:SER:HB3	33:CT:141:ILE:HD11	1.94	0.49
24:CI:301:GLU:HG3	24:CI:771:TYR:HD1	1.77	0.49
32:CS:112:THR:HB	32:CS:138:ARG:HD3	1.93	0.49
35:Cb:97:GLU:HG3	35:Cb:99:PHE:HE1	1.78	0.49
53:UT:1336:ILE:HD12	53:UT:1378:PHE:HB2	1.93	0.49
4:UD:51:GLY:HA2	4:UD:77:VAL:HG23	1.94	0.49
10:UM:351:PRO:HA	10:UM:354:VAL:HG12	1.93	0.49
10:UM:624:ILE:HB	10:UM:638:PHE:HB2	1.94	0.49
13:UQ:84:PRO:HG3	13:UQ:853:TRP:CH2	2.47	0.49
20:CD:80:LEU:HD22	20:CD:86:VAL:HG21	1.95	0.49
22:CG:124:ASP:HB3	22:CG:127:GLU:HG3	1.95	0.49
32:CS:586:ILE:HD12	32:CS:638:ILE:HD12	1.94	0.49
35:Cb:102:ILE:HG22	35:Cb:103:TYR:H	1.78	0.49
53:UT:1467:GLU:HG2	53:UT:1515:HIS:HB3	1.94	0.49
59:CY:21:THR:OG1	60:CZ:365:LYS:NZ	2.45	0.49
7:UJ:343:ARG:HH21	7:UJ:384:SER:HA	1.76	0.49
7:UJ:636:ASP:OD1	7:UJ:636:ASP:N	2.46	0.49
7:UJ:753:ALA:HB3	7:UJ:796:LEU:HD23	1.95	0.49
9:UL:16:VAL:HA	9:UL:392:ASN:HD21	1.76	0.49
19:CC:74:MET:HE3	19:CC:79:LYS:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:CI:1094:MET:HE2	33:CT:104:ARG:HG3	1.95	0.49
32:CR:791:SER:O	32:CR:795:ARG:NH2	2.46	0.49
50:C1:1029:A:H61	50:C1:1046:G:H1'	1.78	0.49
53:UT:830:GLU:HB3	53:UT:834:LYS:HE3	1.94	0.49
54:UH:571:LEU:HB3	54:UH:574:SER:HB2	1.95	0.49
2:UB:829:ARG:NH1	2:UB:833:GLU:OE2	2.39	0.49
4:UD:283:SER:HB2	4:UD:329:MET:HG3	1.95	0.49
6:UG:100:LEU:HD13	6:UG:421:PRO:HG2	1.95	0.49
7:UJ:170:TYR:O	7:UJ:173:SER:O	2.31	0.49
10:UM:689:LEU:HD23	10:UM:720:TRP:CD2	2.48	0.49
19:CC:152:ARG:NH1	20:CD:245:MET:HE3	2.28	0.49
23:CH:170:ARG:HB2	23:CH:198:SER:HB3	1.94	0.49
32:CS:586:ILE:HD11	32:CS:635:ILE:HD12	1.94	0.49
32:CS:723:VAL:HG23	32:CS:766:LEU:HD21	1.94	0.49
36:Cc:68:ARG:HD2	50:C1:2198:C:H3'	1.94	0.49
49:CU:229:MET:HE1	50:C1:296:G:H21	1.77	0.49
53:UT:142:PRO:HA	53:UT:145:LEU:HG	1.95	0.49
53:UT:399:SER:O	53:UT:440:ARG:NH1	2.44	0.49
53:UT:1502:ARG:HA	53:UT:1505:ILE:HG22	1.95	0.49
54:UH:148:ILE:HG22	54:UH:172:ILE:HG12	1.95	0.49
57:CI:12:ASN:HA	57:CI:25:LYS:HB3	1.95	0.49
9:UL:937:ARG:HH21	9:UL:947:LYS:HB3	1.78	0.48
10:UM:476:THR:O	10:UM:522:ARG:NH2	2.42	0.48
11:UN:323:LEU:HD23	28:CM:209:GLU:HG3	1.95	0.48
13:UQ:264:GLY:HA2	13:UQ:280:ARG:O	2.13	0.48
17:UZ:169:LYS:O	17:UZ:173:LYS:HB3	2.13	0.48
26:CK:143:HIS:HB2	26:CK:151:ALA:HB3	1.93	0.48
36:Cc:36:ASP:OD1	36:Cc:36:ASP:N	2.46	0.48
37:Cd:72:ARG:NH2	50:C1:1003:G:O5'	2.46	0.48
50:C1:1223:U:N3	50:C1:1225:G:OP2	2.42	0.48
53:UT:1272:HIS:HA	53:UT:1311:TRP:CZ3	2.47	0.48
56:US:488:ASN:HB3	56:US:491:ASP:HB2	1.95	0.48
7:UJ:1515:VAL:HG13	7:UJ:1516:VAL:HG23	1.95	0.48
9:UL:22:SER:OG	9:UL:23:ASN:N	2.46	0.48
13:UQ:560:GLU:HB3	13:UQ:573:GLN:HB3	1.95	0.48
18:CB:172:ASP:OD1	18:CB:200:ARG:NH1	2.46	0.48
22:CG:298:ARG:HH22	22:CG:473:PRO:HG2	1.78	0.48
24:CI:793:GLN:OE1	24:CI:795:ARG:NH2	2.46	0.48
32:CS:96:GLU:HA	32:CS:99:ILE:HG12	1.95	0.48
50:C1:1169:A:H4'	50:C1:1170:G:H5'	1.94	0.48
52:CW:119:ARG:NH1	52:CW:135:ILE:O	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:UT:129:PHE:HA	53:UT:132:ASP:HB2	1.94	0.48
53:UT:1857:LEU:O	53:UT:1861:ALA:HB2	2.13	0.48
57:CI:68:ARG:O	57:CI:72:ILE:HD12	2.13	0.48
6:UG:587:GLU:OE1	6:UG:590:ARG:NH2	2.41	0.48
13:UQ:915:ASP:OD1	13:UQ:915:ASP:N	2.45	0.48
21:CF:11:LYS:HA	21:CF:81:TYR:HB2	1.95	0.48
24:CI:69:ARG:NH1	24:CI:230:LYS:O	2.46	0.48
30:CP:273:GLU:HB3	30:CP:277:ARG:NH1	2.28	0.48
32:CR:386:VAL:HG22	32:CR:406:TYR:HE2	1.78	0.48
50:C1:809:U:O4	53:UT:1622:ARG:NH2	2.47	0.48
53:UT:1732:LEU:HD11	53:UT:1765:LEU:HD11	1.96	0.48
3:UC:616:ARG:NH1	50:C1:1086:U:OP1	2.43	0.48
6:UG:300:ARG:HE	11:UN:866:LEU:HD22	1.78	0.48
9:UL:153:ASP:HB3	9:UL:194:LYS:HB3	1.94	0.48
9:UL:626:SER:OG	9:UL:627:ALA:N	2.46	0.48
10:UM:194:SER:O	10:UM:197:ARG:NH2	2.46	0.48
22:CG:438:LEU:HA	22:CG:463:PRO:HA	1.96	0.48
28:CM:335:THR:OG1	28:CM:337:ASP:OD1	2.28	0.48
30:CP:104:ARG:O	30:CP:165:HIS:NE2	2.46	0.48
32:CS:666:ALA:HB2	32:CS:717:PRO:HD2	1.94	0.48
50:C1:1148:G:N2	50:C1:2179:C:OP2	2.46	0.48
58:CX:377:LEU:HD23	58:CX:382:ILE:HG13	1.96	0.48
7:UJ:501:THR:HG22	7:UJ:503:THR:H	1.78	0.48
7:UJ:1667:GLN:HE22	7:UJ:1713:VAL:HG13	1.78	0.48
10:UM:47:GLU:OE1	10:UM:50:THR:N	2.35	0.48
10:UM:819:ASN:ND2	27:CL:699:ALA:O	2.36	0.48
11:UN:334:ARG:NH2	28:CM:251:GLU:OE1	2.40	0.48
27:CL:124:ALA:HB1	27:CL:125:LEU:HD23	1.95	0.48
28:CM:261:ASP:OD2	28:CM:265:TYR:OH	2.25	0.48
32:CS:29:VAL:HG22	32:CS:34:ALA:HB1	1.95	0.48
32:CS:242:GLU:HG3	32:CS:243:LEU:HG	1.96	0.48
37:Cd:56:ASN:HB2	37:Cd:108:VAL:HG12	1.95	0.48
40:Cg:61:ASP:N	40:Cg:61:ASP:OD1	2.46	0.48
50:C1:1177:U:H4'	50:C1:1179:G:H4'	1.95	0.48
53:UT:1798:LEU:O	53:UT:1802:ILE:HG12	2.13	0.48
59:CY:96:LEU:O	59:CY:100:THR:OG1	2.30	0.48
59:CY:317:GLY:O	59:CY:320:ARG:HG2	2.13	0.48
55:UI:177:ASP:HB3	55:UI:180:ILE:HD13	1.94	0.48
2:UB:574:ARG:HG2	2:UB:593:ILE:HD13	1.94	0.48
4:UD:104:SER:HB3	4:UD:114:TRP:HE1	1.78	0.48
7:UJ:534:PHE:O	7:UJ:537:THR:OG1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:UJ:731:ASN:HD21	7:UJ:781:VAL:HA	1.79	0.48
7:UJ:812:ARG:NH1	7:UJ:816:MET:HB3	2.27	0.48
7:UJ:1253:SER:HA	7:UJ:1256:LEU:HD12	1.95	0.48
7:UJ:1735:PRO:HA	7:UJ:1738:ARG:HB2	1.96	0.48
10:UM:54:LEU:HD12	10:UM:99:VAL:HG23	1.94	0.48
10:UM:245:HIS:ND1	10:UM:261:TRP:HB2	2.27	0.48
17:UZ:61:PRO:HA	17:UZ:247:TYR:HA	1.96	0.48
18:CB:214:MET:O	18:CB:217:ARG:NH1	2.46	0.48
22:CG:307:SER:OG	22:CG:308:LYS:N	2.47	0.48
26:CK:73:ILE:HG23	26:CK:75:ASP:HB2	1.95	0.48
51:C2:31:A:O2'	51:C2:33:U:O4	2.31	0.48
53:UT:586:LEU:HA	53:UT:590:LYS:HD3	1.96	0.48
3:UC:639:LYS:HG2	33:CT:123:LYS:HD3	1.95	0.48
7:UJ:1610:PHE:HA	7:UJ:1613:SER:HB2	1.95	0.48
7:UJ:1672:PHE:HA	7:UJ:1675:VAL:HG12	1.95	0.48
13:UQ:494:ALA:HB3	13:UQ:534:ILE:HD13	1.96	0.48
13:UQ:725:VAL:O	54:UH:589:SER:OG	2.29	0.48
22:CG:176:VAL:HB	22:CG:581:VAL:HG21	1.96	0.48
24:CI:843:GLN:HB3	24:CI:1002:ASN:HB3	1.95	0.48
26:CK:289:ARG:NH1	50:C1:1145:G:N7	2.62	0.48
28:CM:71:SER:HA	28:CM:331:ARG:HD2	1.95	0.48
53:UT:431:SER:HA	53:UT:473:MET:HE1	1.94	0.48
55:UI:167:ASP:N	55:UI:167:ASP:OD1	2.47	0.48
2:UB:747:ILE:HA	2:UB:788:LEU:HD22	1.96	0.48
7:UJ:297:VAL:HG11	7:UJ:328:VAL:HG23	1.95	0.48
12:UO:169:VAL:HB	12:UO:183:PHE:HB2	1.95	0.48
22:CG:413:SER:OG	22:CG:415:ASN:OD1	2.30	0.48
23:CH:151:ASP:OD2	23:CH:178:ARG:NH2	2.36	0.48
24:CI:94:LYS:NZ	24:CI:329:GLU:OE1	2.38	0.48
32:CS:479:ARG:HG3	65:CS:1101:ADP:H4'	1.96	0.48
37:CD:183:THR:HG23	37:CD:186:ARG:H	1.79	0.48
50:C1:1623:U:H5''	50:C1:1624:A:H2'	1.96	0.48
53:UT:1310:THR:HG21	53:UT:1351:VAL:HG12	1.95	0.48
56:US:236:SER:OG	56:US:238:ASP:OD1	2.29	0.48
60:CZ:407:MET:HE3	60:CZ:411:GLU:HG2	1.94	0.48
2:UB:512:HIS:O	2:UB:519:ASN:ND2	2.42	0.48
6:UG:43:ARG:O	6:UG:47:GLN:HG3	2.13	0.48
6:UG:270:ASN:HB3	6:UG:272:ILE:HG12	1.96	0.48
6:UG:579:ASP:HB3	6:UG:582:ARG:HG2	1.96	0.48
13:UQ:608:THR:OG1	13:UQ:609:LYS:N	2.47	0.48
28:CM:332:THR:HG22	28:CM:343:THR:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CN:112:ILE:HB	29:CN:124:VAL:HB	1.95	0.48
40:Cg:118:LYS:HE3	50:C1:1063:U:H4'	1.95	0.48
53:UT:1274:GLN:HG3	53:UT:1276:ASP:H	1.78	0.48
56:US:112:ASN:OD1	56:US:113:TRP:N	2.47	0.48
2:UB:21:PRO:HB3	50:C1:1732:C:H1'	1.96	0.48
2:UB:590:ASP:OD1	2:UB:590:ASP:N	2.47	0.48
18:CB:113:THR:H	18:CB:124:LYS:HG3	1.79	0.48
32:CR:258:THR:HG23	32:CR:261:GLN:H	1.79	0.48
32:CR:654:LEU:HD21	32:CR:737:TRP:HZ3	1.79	0.48
32:CS:397:PRO:HA	32:CS:400:LYS:HG2	1.95	0.48
38:Ce:76:PHE:O	38:Ce:79:VAL:C	2.57	0.48
52:CW:170:ARG:HB2	52:CW:179:LEU:HB2	1.96	0.48
52:CW:250:LEU:HB3	52:CW:259:LEU:HD11	1.95	0.48
53:UT:2172:ARG:O	53:UT:2176:MET:HG3	2.14	0.48
1:UA:242:GLN:HG2	1:UA:244:ARG:HH12	1.79	0.47
7:UJ:853:VAL:HA	7:UJ:856:LEU:HG	1.96	0.47
7:UJ:1801:LEU:O	53:UT:44:ARG:NE	2.45	0.47
9:UL:431:SER:HB2	9:UL:444:ALA:HB3	1.97	0.47
9:UL:449:LEU:HD11	9:UL:482:VAL:HG21	1.96	0.47
10:UM:558:LEU:HB3	10:UM:570:ILE:HD11	1.95	0.47
11:UN:343:LEU:HD11	28:CM:250:MET:HE1	1.96	0.47
12:UO:149:VAL:HG12	12:UO:163:CYS:HB2	1.96	0.47
32:CS:579:LEU:HD12	32:CS:580:PRO:HD2	1.96	0.47
36:Cc:82:ASN:O	50:C1:2194:A:O2'	2.32	0.47
53:UT:229:SER:HA	53:UT:232:ILE:HG22	1.95	0.47
53:UT:969:PHE:CE1	53:UT:1002:ARG:HG2	2.49	0.47
53:UT:1388:VAL:HA	53:UT:1391:ILE:HG12	1.96	0.47
53:UT:1718:LYS:O	53:UT:1721:THR:OG1	2.28	0.47
53:UT:1859:LYS:O	53:UT:1903:ASN:ND2	2.46	0.47
54:UH:238:PHE:HE1	54:UH:275:PRO:HB3	1.79	0.47
54:UH:754:ARG:HA	55:UI:210:ARG:HB2	1.96	0.47
1:UA:183:GLU:HB2	1:UA:186:PHE:HB3	1.96	0.47
4:UD:884:ARG:NH2	50:C1:71:A:O2'	2.39	0.47
7:UJ:966:LEU:HA	7:UJ:969:MET:HG3	1.95	0.47
17:UZ:235:LEU:HD11	17:UZ:270:PHE:HB3	1.95	0.47
18:CA:165:THR:O	18:CA:168:SER:OG	2.29	0.47
20:CD:15:LEU:HB2	20:CD:76:LEU:HD11	1.96	0.47
21:CE:60:GLN:OE1	21:CE:85:LYS:NZ	2.44	0.47
22:CG:345:VAL:HG23	22:CG:403:MET:HE2	1.96	0.47
53:UT:1504:GLU:HA	53:UT:1507:ARG:HG2	1.96	0.47
59:CY:235:ILE:HA	59:CY:239:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UA:156:HIS:HB3	1:UA:169:ALA:HB3	1.96	0.47
7:UJ:578:ARG:NH1	7:UJ:583:ASP:OD1	2.43	0.47
9:UL:287:HIS:CD2	9:UL:289:LEU:H	2.32	0.47
9:UL:586:ASP:OD1	9:UL:588:THR:OG1	2.28	0.47
9:UL:814:ARG:NH1	9:UL:823:ASN:OD1	2.47	0.47
14:UR:253:ARG:NH1	14:UR:599:SER:O	2.48	0.47
20:CD:31:GLU:O	20:CD:38:LYS:NZ	2.38	0.47
23:CH:209:ASN:O	23:CH:350:ARG:NH1	2.40	0.47
31:CQ:188:GLY:O	50:C1:2350:G:O2'	2.31	0.47
52:CW:208:ALA:HB3	52:CW:218:ALA:HB3	1.96	0.47
53:UT:289:GLU:HA	53:UT:293:PRO:HD3	1.95	0.47
53:UT:388:LYS:HD3	53:UT:815:ASN:HB2	1.96	0.47
9:UL:490:GLN:HG2	9:UL:502:THR:HG23	1.95	0.47
19:CC:250:LYS:HA	19:CC:254:ILE:HD12	1.96	0.47
28:CM:307:ILE:HG12	28:CM:343:THR:HG21	1.97	0.47
28:CM:403:LYS:HE2	50:C1:1664:U:H4'	1.96	0.47
35:Cb:116:ASP:OD2	35:Cb:120:LYS:NZ	2.48	0.47
50:C1:808:A:H61	50:C1:821:C:H2'	1.80	0.47
53:UT:206:PHE:HA	53:UT:209:GLU:HG2	1.97	0.47
1:UA:226:ALA:HA	1:UA:241:MET:HG2	1.96	0.47
9:UL:632:ARG:NH1	9:UL:641:CYS:SG	2.87	0.47
10:UM:461:ARG:HE	10:UM:463:ASP:HB2	1.79	0.47
18:CA:106:GLU:OE2	18:CA:128:ARG:NH1	2.46	0.47
32:CS:245:ASP:OD1	32:CS:245:ASP:N	2.47	0.47
35:Cb:180:LEU:N	35:Cb:229:GLY:O	2.47	0.47
38:Ce:57:VAL:HG11	38:Ce:178:THR:HG23	1.96	0.47
50:C1:381:G:H21	50:C1:385:A:H62	1.61	0.47
53:UT:1145:PHE:HZ	53:UT:1160:MET:HE1	1.80	0.47
54:UH:30:PHE:HB3	54:UH:83:PRO:HA	1.96	0.47
58:CX:250:ALA:O	58:CX:254:PHE:HB2	2.14	0.47
1:UA:216:ASP:OD1	1:UA:216:ASP:N	2.48	0.47
2:UB:43:GLN:N	2:UB:43:GLN:NE2	2.57	0.47
4:UD:277:GLN:HG3	4:UD:297:ASP:HB3	1.97	0.47
4:UD:547:ARG:NH1	4:UD:565:ASP:OD2	2.47	0.47
7:UJ:1232:LEU:HD22	7:UJ:1282:LYS:HD2	1.97	0.47
13:UQ:671:VAL:HG22	54:UH:718:PRO:HD3	1.96	0.47
15:UU:159:ILE:O	15:UU:172:THR:CA	2.52	0.47
15:UU:885:GLN:HA	15:UU:885:GLN:HE21	1.80	0.47
32:CR:735:LYS:NZ	32:CR:739:ARG:HH12	2.13	0.47
32:CS:29:VAL:HA	32:CS:202:ILE:O	2.15	0.47
32:CS:840:ARG:HH11	32:CS:853:VAL:HG12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Cb:160:VAL:HG11	35:Cb:169:ILE:HD12	1.95	0.47
48:Cp:13:VAL:O	48:Cp:52:ASN:CA	2.63	0.47
48:Cp:13:VAL:O	48:Cp:52:ASN:HA	2.15	0.47
50:C1:713:G:N3	50:C1:767:U:O2'	2.46	0.47
58:CX:328:LEU:HA	58:CX:331:ILE:HG22	1.97	0.47
1:UA:577:THR:HG21	1:UA:677:GLY:HA2	1.96	0.47
1:UA:723:VAL:HG11	1:UA:732:LYS:HG2	1.95	0.47
2:UB:886:GLN:HB2	46:Cn:117:ILE:HG23	1.95	0.47
4:UD:6:CYS:HB2	4:UD:863:ILE:HG13	1.96	0.47
6:UG:434:ASN:HB3	6:UG:437:GLU:HB3	1.96	0.47
7:UJ:750:ARG:HA	7:UJ:796:LEU:HD21	1.96	0.47
7:UJ:1699:ILE:HA	7:UJ:1702:VAL:HG12	1.97	0.47
9:UL:222:ALA:HB3	9:UL:235:ALA:HB3	1.97	0.47
9:UL:534:PHE:HB2	9:UL:560:ARG:HB2	1.97	0.47
10:UM:118:ALA:HB3	10:UM:127:ALA:HB3	1.97	0.47
10:UM:452:SER:OG	10:UM:453:LYS:N	2.45	0.47
18:CA:97:LEU:HD23	18:CA:200:ARG:HG2	1.97	0.47
18:CA:267:PRO:HG2	18:CA:270:GLN:HG2	1.96	0.47
18:CB:167:VAL:HA	18:CB:170:VAL:HG22	1.96	0.47
29:CO:77:MET:HE3	29:CO:87:ALA:HB2	1.97	0.47
32:CR:70:HIS:HB3	32:CR:73:LYS:HB3	1.97	0.47
32:CR:845:ALA:HB2	32:CR:920:THR:HG21	1.97	0.47
32:CS:162:LEU:HA	32:CS:165:MET:HG2	1.96	0.47
32:CS:495:CYS:HB3	32:CS:541:VAL:HG21	1.95	0.47
50:C1:68:U:H3	54:UH:883:ARG:HH21	1.62	0.47
50:C1:189:G:N2	61:UP:338:GLN:OE1	2.40	0.47
53:UT:63:LEU:HD13	53:UT:129:PHE:HB3	1.95	0.47
53:UT:599:LEU:HB3	53:UT:603:LEU:HD23	1.97	0.47
53:UT:1359:PHE:CD1	53:UT:1371:LEU:HD13	2.50	0.47
53:UT:1391:ILE:HG21	53:UT:1434:LEU:HD11	1.96	0.47
54:UH:179:ILE:HB	54:UH:193:VAL:HB	1.97	0.47
56:US:113:TRP:HE3	56:US:114:LEU:HD22	1.80	0.47
55:UI:184:THR:O	55:UI:188:MET:CB	2.58	0.47
2:UB:587:THR:O	2:UB:591:LEU:CB	2.63	0.47
3:UC:255:ALA:HA	3:UC:260:VAL:HG11	1.97	0.47
7:UJ:1710:ALA:HB1	7:UJ:1719:TYR:HE1	1.80	0.47
10:UM:801:LEU:HD22	10:UM:805:GLN:HB3	1.97	0.47
21:CE:63:SER:HA	21:CE:66:LEU:HB2	1.96	0.47
31:CQ:218:ILE:HG22	31:CQ:225:ILE:HG12	1.97	0.47
32:CR:141:GLU:OE2	32:CR:287:ARG:NH1	2.48	0.47
37:Cd:223:LYS:HA	37:Cd:226:LYS:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:C2:49:U:H2'	51:C2:50:G:H8	1.79	0.47
52:CW:270:ILE:HG22	52:CW:280:LEU:HB3	1.96	0.47
52:CW:300:THR:OG1	52:CW:302:GLU:OE1	2.30	0.47
53:UT:1194:PRO:HA	53:UT:1237:LEU:HD11	1.97	0.47
53:UT:1685:GLU:HA	53:UT:1688:ASN:HD21	1.80	0.47
55:UI:165:ASP:OD1	55:UI:165:ASP:N	2.48	0.47
2:UB:672:ARG:NH2	2:UB:684:GLU:OE2	2.48	0.47
21:CE:53:VAL:O	21:CE:79:TYR:HA	2.15	0.47
24:CI:934:ILE:HD12	24:CI:987:VAL:HG21	1.97	0.47
32:CR:385:LEU:HD13	32:CR:407:LEU:HD12	1.96	0.47
32:CR:385:LEU:HA	32:CR:407:LEU:O	2.15	0.47
35:Cb:100:ARG:NH2	35:Cb:121:TYR:O	2.43	0.47
47:Co:344:ILE:HB	47:Co:353:GLN:HB2	1.97	0.47
50:C1:661:U:O2'	53:UT:11:LYS:NZ	2.48	0.47
52:CW:261:LEU:HB2	52:CW:269:ARG:HB2	1.97	0.47
53:UT:498:ILE:HG23	53:UT:534:ARG:HD3	1.97	0.47
53:UT:1778:ARG:HA	53:UT:1790:LEU:HD11	1.97	0.47
53:UT:2005:LYS:HD2	53:UT:2050:LEU:HD11	1.97	0.47
2:UB:618:ILE:HG23	2:UB:639:LEU:HB3	1.95	0.47
2:UB:723:ILE:HG23	2:UB:773:LEU:HD22	1.97	0.47
2:UB:798:LEU:HD13	56:US:456:CYS:HB3	1.96	0.47
10:UM:156:VAL:HA	10:UM:202:THR:HA	1.97	0.47
10:UM:208:ARG:HD3	10:UM:219:PRO:HA	1.97	0.47
10:UM:436:VAL:HA	10:UM:452:SER:HA	1.97	0.47
12:UO:122:ARG:HB2	12:UO:141:HIS:HD2	1.78	0.47
12:UO:449:ASP:HB3	12:UO:452:ILE:HB	1.97	0.47
12:UO:528:ALA:O	12:UO:532:ARG:HG2	2.15	0.47
13:UQ:395:LEU:HD12	13:UQ:399:ILE:HD11	1.96	0.47
13:UQ:754:TYR:OH	13:UQ:759:ASP:OD1	2.32	0.47
19:CC:247:ASP:O	19:CC:251:ALA:CB	2.63	0.47
34:Ca:129:THR:HG23	34:Ca:131:ASP:H	1.80	0.47
34:Ca:158:SER:OG	50:C1:1461:G:OP1	2.31	0.47
37:Cd:191:ARG:HA	37:Cd:194:ILE:HG12	1.96	0.47
39:Cf:70:GLU:HG3	39:Cf:112:TRP:HE1	1.79	0.47
42:CI:44:THR:HG22	42:CI:51:THR:HA	1.96	0.47
53:UT:1157:ARG:HE	53:UT:1161:VAL:HG23	1.79	0.47
2:UB:561:LYS:HZ3	56:US:517:PHE:HD1	1.63	0.46
4:UD:707:LEU:HB3	4:UD:829:THR:HG22	1.97	0.46
8:UK:67:MET:HG2	25:CJ:173:TYR:CD2	2.50	0.46
9:UL:591:VAL:HB	9:UL:601:LEU:HB2	1.97	0.46
13:UQ:847:ASP:OD1	13:UQ:847:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:UU:50:PRO:HB2	15:UU:342:LYS:HD2	1.96	0.46
32:CR:849:LEU:HD21	32:CS:623:GLN:HE22	1.80	0.46
32:CS:289:ARG:NH2	32:CS:476:GLU:O	2.48	0.46
32:CS:571:THR:HG21	32:CS:580:PRO:HB2	1.96	0.46
53:UT:2133:ASP:OD1	53:UT:2136:ARG:NH2	2.47	0.46
7:UJ:802:ARG:HG3	7:UJ:805:LEU:H	1.80	0.46
12:UO:415:ARG:NH1	50:C1:131:G:N7	2.62	0.46
13:UQ:196:GLU:HB3	13:UQ:201:VAL:HG12	1.96	0.46
18:CB:249:GLN:NE2	18:CB:307:LEU:O	2.46	0.46
25:CJ:167:LYS:O	25:CJ:171:MET:HG2	2.15	0.46
32:CR:650:GLY:O	32:CR:654:LEU:HD12	2.15	0.46
32:CS:285:ALA:HB2	32:CS:474:LEU:HB2	1.97	0.46
35:Cb:86:PHE:CE1	35:Cb:87:MET:HG2	2.50	0.46
36:Cc:86:MET:HE1	50:C1:2194:A:C8	2.50	0.46
50:C1:149:G:H5''	61:UP:337:LYS:HE3	1.96	0.46
50:C1:906:G:H4'	50:C1:907:A:H5'	1.96	0.46
56:US:176:SER:O	56:US:182:ARG:NH2	2.45	0.46
59:CY:48:LEU:HD11	60:CZ:325:LEU:HD12	1.96	0.46
1:UA:23:SER:HB3	1:UA:28:HIS:HB2	1.98	0.46
1:UA:214:SER:OG	1:UA:216:ASP:OD1	2.27	0.46
3:UC:239:LEU:HB3	3:UC:266:LEU:HD11	1.98	0.46
7:UJ:1499:TYR:HA	7:UJ:1502:ILE:HG22	1.97	0.46
8:UK:258:LYS:NZ	50:C1:214:C:OP2	2.49	0.46
19:CC:74:MET:HG3	19:CC:78:LEU:HD23	1.97	0.46
20:CD:80:LEU:HD13	20:CD:86:VAL:HG11	1.96	0.46
32:CR:169:VAL:O	32:CR:172:ARG:NH1	2.36	0.46
32:CR:312:ILE:HA	32:CR:387:VAL:HG23	1.97	0.46
32:CS:220:LEU:HD12	32:CS:221:PRO:HD2	1.97	0.46
32:CS:387:VAL:HG12	32:CS:409:PHE:HB2	1.97	0.46
50:C1:781:G:H2'	50:C1:782:G:H8	1.80	0.46
1:UA:364:ILE:HD11	1:UA:381:HIS:HD2	1.80	0.46
6:UG:100:LEU:HD23	6:UG:109:THR:HB	1.98	0.46
7:UJ:864:ASP:OD1	7:UJ:864:ASP:N	2.48	0.46
13:UQ:104:ILE:HG12	13:UQ:113:VAL:HG12	1.98	0.46
13:UQ:637:PHE:O	13:UQ:664:SER:N	2.48	0.46
13:UQ:803:LEU:HD22	13:UQ:807:THR:HG21	1.96	0.46
24:CI:220:HIS:HE2	50:C1:639:U:HO2'	1.64	0.46
26:CK:241:HIS:HD1	26:CK:258:GLY:HA3	1.80	0.46
30:CP:78:MET:HE1	30:CP:102:LEU:HB3	1.97	0.46
30:CP:194:PRO:HA	30:CP:197:LEU:HD12	1.98	0.46
32:CR:575:GLN:HB3	32:CR:578:ARG:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CR:613:LEU:HA	37:Cd:22:ARG:HH12	1.81	0.46
32:CS:751:ALA:HB1	32:CS:756:GLY:HA2	1.98	0.46
34:Ca:71:ALA:HB3	42:Ci:127:ARG:HH12	1.81	0.46
39:Cf:56:ARG:HH22	50:C1:915:G:H5''	1.81	0.46
52:CW:58:ASN:ND2	52:CW:99:ASN:O	2.42	0.46
52:CW:170:ARG:NH1	52:CW:180:ARG:O	2.40	0.46
59:CY:98:LYS:HE3	60:CZ:456:GLN:HE22	1.80	0.46
7:UJ:1076:LYS:HB3	7:UJ:1169:LEU:HG	1.96	0.46
32:CS:536:PHE:HD1	32:CS:579:LEU:HD21	1.80	0.46
32:CS:828:GLU:OE2	32:CS:869:ARG:NH2	2.48	0.46
41:Ch:142:GLU:HG2	41:Ch:145:THR:H	1.80	0.46
50:C1:1744:A:H2'	50:C1:1745:C:C6	2.51	0.46
52:CW:359:ILE:HG22	52:CW:362:LEU:H	1.80	0.46
53:UT:269:GLY:HA2	53:UT:317:THR:HG21	1.97	0.46
53:UT:419:LYS:HD2	53:UT:422:TRP:HZ3	1.79	0.46
5:UF:73:LYS:HE3	14:UR:51:GLU:HB3	1.98	0.46
7:UJ:654:ALA:O	7:UJ:658:SER:CB	2.62	0.46
7:UJ:715:VAL:HG11	7:UJ:745:LEU:HA	1.98	0.46
10:UM:676:LYS:HB3	10:UM:678:TRP:HE1	1.81	0.46
13:UQ:248:ALA:HB3	13:UQ:309:LEU:HD12	1.98	0.46
20:CD:261:ALA:HA	20:CD:264:VAL:HG12	1.97	0.46
21:CF:34:LEU:HD11	21:CF:101:VAL:HB	1.98	0.46
44:Ck:111:ASN:HD22	50:C1:932:U:H5''	1.80	0.46
52:CW:147:GLN:HE22	60:CZ:560:ASP:HA	1.79	0.46
52:CW:147:GLN:HE22	60:CZ:561:ARG:H	1.64	0.46
52:CW:347:THR:HB	52:CW:355:HIS:HB2	1.98	0.46
53:UT:1196:ALA:HA	53:UT:1199:PHE:CD2	2.50	0.46
53:UT:1687:VAL:HA	53:UT:1691:LEU:HD23	1.98	0.46
8:UK:18:GLN:O	24:CI:1036:ARG:NH2	2.47	0.46
9:UL:12:LYS:HB2	9:UL:722:VAL:HB	1.96	0.46
10:UM:591:THR:OG1	10:UM:646:LEU:O	2.33	0.46
14:UR:146:ILE:HG13	14:UR:171:TYR:CD2	2.51	0.46
22:CG:110:LYS:HE2	59:CY:328:LYS:HE3	1.98	0.46
22:CG:151:ARG:NH1	22:CG:494:GLU:OE1	2.46	0.46
28:CM:284:ALA:HB3	28:CM:304:ASP:H	1.81	0.46
7:UJ:442:ILE:HA	7:UJ:445:VAL:HG12	1.98	0.46
7:UJ:601:SER:HB3	7:UJ:725:ARG:HD3	1.98	0.46
7:UJ:1265:ILE:HG23	7:UJ:1290:ARG:HH12	1.80	0.46
10:UM:256:MET:SD	10:UM:273:ARG:NH2	2.89	0.46
11:UN:921:PRO:HG2	11:UN:924:ILE:HD13	1.98	0.46
12:UO:210:TYR:HA	12:UO:234:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:UQ:81:VAL:HG22	13:UQ:855:ILE:HG12	1.98	0.46
13:UQ:195:ILE:HD12	13:UQ:204:VAL:HG21	1.97	0.46
13:UQ:557:GLN:HB3	13:UQ:581:ARG:HG2	1.97	0.46
28:CM:266:ILE:O	28:CM:276:LEU:N	2.49	0.46
32:CS:840:ARG:HH12	32:CS:854:VAL:HA	1.80	0.46
37:Cd:58:LYS:HA	37:Cd:107:SER:HB3	1.98	0.46
47:Co:345:ARG:HG2	53:UT:75:ILE:HG22	1.97	0.46
53:UT:1002:ARG:NH2	53:UT:1005:SER:OG	2.47	0.46
53:UT:1166:SER:HB2	53:UT:1168:ARG:HG2	1.98	0.46
53:UT:1767:PRO:HB2	53:UT:1809:SER:HB2	1.98	0.46
54:UH:7:ILE:HD11	54:UH:364:VAL:HG23	1.97	0.46
1:UA:508:GLN:O	43:Cj:114:ARG:NH2	2.49	0.46
2:UB:19:ILE:HD13	26:CK:247:THR:HA	1.97	0.46
5:UF:398:ILE:HA	5:UF:401:VAL:HG22	1.97	0.46
6:UG:573:ARG:HG2	6:UG:582:ARG:HH22	1.81	0.46
7:UJ:1264:PHE:HB3	7:UJ:1290:ARG:NH2	2.31	0.46
8:UK:121:LYS:HD2	51:C2:260:G:H5"	1.97	0.46
14:UR:298:MET:HG3	14:UR:325:LEU:HD13	1.97	0.46
23:CH:245:GLN:O	24:CI:620:ARG:NH2	2.40	0.46
24:CI:753:ASN:O	24:CI:754:LYS:HG2	2.15	0.46
31:CQ:82:THR:HG22	31:CQ:125:ARG:HG3	1.98	0.46
32:CS:93:ASP:OD1	32:CS:93:ASP:N	2.44	0.46
32:CS:243:LEU:HD13	32:CS:266:LEU:HD21	1.98	0.46
32:CS:255:LEU:HD13	32:CS:329:LYS:HG3	1.98	0.46
32:CS:635:ILE:HB	32:CS:725:VAL:HG23	1.98	0.46
53:UT:1757:THR:O	53:UT:1761:ILE:HG12	2.16	0.46
56:US:374:PRO:HG2	56:US:448:MET:HE1	1.98	0.46
1:UA:227:LYS:HG2	1:UA:244:ARG:HH22	1.80	0.46
4:UD:85:ASP:O	4:UD:98:GLY:CA	2.65	0.46
7:UJ:17:ARG:HD3	7:UJ:130:PHE:CE2	2.51	0.46
7:UJ:1247:ARG:NH1	7:UJ:1250:ASP:OD2	2.49	0.46
7:UJ:1325:LYS:HE2	7:UJ:1367:LEU:HD21	1.98	0.46
10:UM:114:VAL:HA	10:UM:130:ALA:HA	1.98	0.46
32:CS:724:GLY:HA2	32:CS:763:ILE:HA	1.98	0.46
38:Ce:20:SER:H	38:Ce:23:GLU:CD	2.23	0.46
53:UT:1983:ALA:O	53:UT:1987:ILE:HG12	2.16	0.46
54:UH:544:ARG:HA	54:UH:547:VAL:HG22	1.98	0.46
54:UH:618:ALA:HB1	54:UH:624:MET:HE1	1.98	0.46
13:UQ:417:ASP:OD1	13:UQ:419:SER:OG	2.29	0.45
15:UU:184:GLU:HG3	15:UU:186:THR:HG23	1.98	0.45
27:CL:658:MET:HG2	27:CL:676:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CS:396:LEU:HA	32:CS:399:VAL:HG12	1.97	0.45
32:CS:776:GLY:HA3	32:CS:816:ASP:HB2	1.98	0.45
35:Cb:148:ARG:HD2	50:C1:711:U:H5'	1.97	0.45
53:UT:1927:LYS:HB2	53:UT:1930:GLU:HG2	1.98	0.45
58:CX:284:LEU:HD13	58:CX:323:ILE:HD12	1.98	0.45
6:UG:481:ARG:HH12	50:C1:588:U:P	2.39	0.45
7:UJ:1468:LEU:HA	7:UJ:1471:LEU:HG	1.98	0.45
9:UL:903:ARG:HD3	10:UM:885:GLU:HG3	1.98	0.45
17:UZ:255:LEU:O	17:UZ:259:ILE:HG12	2.16	0.45
21:CE:8:ALA:HB3	21:CE:11:LYS:HE3	1.97	0.45
24:CI:167:PHE:HD1	24:CI:202:HIS:HB2	1.81	0.45
28:CM:213:ILE:HD12	28:CM:227:LEU:HD11	1.98	0.45
28:CM:423:ARG:NH1	28:CM:428:LYS:O	2.49	0.45
37:Cd:67:VAL:HG13	37:Cd:99:GLY:HA2	1.97	0.45
52:CW:282:LYS:NZ	52:CW:321:GLY:O	2.41	0.45
53:UT:2169:GLU:OE2	53:UT:2172:ARG:NH2	2.49	0.45
54:UH:13:LEU:HD11	54:UH:63:ILE:HG23	1.98	0.45
2:UB:616:LEU:HD23	56:US:501:LEU:HG	1.97	0.45
4:UD:633:LEU:HD12	4:UD:649:VAL:HG22	1.98	0.45
7:UJ:1603:VAL:HA	7:UJ:1606:PHE:CD2	2.51	0.45
9:UL:109:HIS:CE1	9:UL:129:SER:HG	2.32	0.45
10:UM:865:VAL:HG12	27:CL:679:PRO:HG3	1.97	0.45
15:UU:282:ARG:HE	15:UU:284:ASP:HB3	1.81	0.45
17:UZ:30:LEU:HD22	17:UZ:283:VAL:HG12	1.98	0.45
19:CC:86:LEU:HD13	19:CC:116:VAL:HG21	1.99	0.45
19:CC:89:THR:HG23	19:CC:115:GLY:HA3	1.98	0.45
22:CG:176:VAL:HG12	22:CG:562:ASP:HB3	1.99	0.45
23:CH:83:THR:HA	23:CH:125:LYS:HB3	1.98	0.45
30:CP:290:LYS:NZ	50:C1:900:A:O5'	2.47	0.45
32:CS:200:LEU:HD23	32:CS:208:VAL:HG11	1.98	0.45
33:CT:106:LEU:HD13	33:CT:131:VAL:HA	1.97	0.45
35:Cb:141:THR:OG1	35:Cb:143:ASP:OD1	2.31	0.45
38:Ce:76:PHE:O	38:Ce:79:VAL:O	2.34	0.45
49:CU:223:GLN:O	49:CU:230:ARG:NH2	2.48	0.45
52:CW:115:LEU:HB2	52:CW:142:LEU:HD11	1.97	0.45
53:UT:1358:LEU:HD12	53:UT:1362:PHE:CE2	2.52	0.45
54:UH:397:SER:O	54:UH:425:ARG:NH1	2.49	0.45
59:CY:39:SER:HG	60:CZ:425:TRP:NE1	2.11	0.45
2:UB:599:THR:HG23	2:UB:600:THR:HG23	1.98	0.45
7:UJ:492:PHE:HB3	7:UJ:533:ARG:HH21	1.82	0.45
13:UQ:665:ARG:HD3	13:UQ:720:GLY:HA3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CB:156:VAL:HA	18:CB:225:VAL:O	2.16	0.45
29:CN:180:LEU:HD11	29:CN:241:PHE:CE2	2.51	0.45
32:CR:544:TYR:CE1	32:CR:637:ARG:HG2	2.51	0.45
32:CS:265:LEU:HD13	32:CS:297:VAL:HG23	1.98	0.45
32:CS:614:ILE:H	32:CS:634:ARG:NH2	2.14	0.45
53:UT:1145:PHE:HB3	53:UT:1193:LEU:HD11	1.98	0.45
2:UB:530:LEU:O	2:UB:534:ILE:HD12	2.16	0.45
2:UB:550:GLU:CD	56:US:524:PHE:H	2.24	0.45
4:UD:487:SER:HA	4:UD:554:PHE:HD2	1.82	0.45
5:UF:351:PRO:O	5:UF:355:LYS:NZ	2.50	0.45
6:UG:202:ILE:HB	6:UG:211:HIS:HB2	1.97	0.45
7:UJ:922:VAL:O	7:UJ:925:SER:C	2.59	0.45
7:UJ:1079:LEU:HD22	7:UJ:1114:ILE:HD13	1.97	0.45
9:UL:396:LEU:HD23	9:UL:418:LEU:HD12	1.99	0.45
9:UL:702:LEU:HD11	9:UL:711:LEU:HD12	1.99	0.45
9:UL:890:VAL:HA	10:UM:891:MET:HG2	1.99	0.45
14:UR:456:ARG:HE	14:UR:456:ARG:HB3	1.66	0.45
20:CD:293:ILE:HG21	20:CD:369:ILE:HD11	1.98	0.45
23:CH:170:ARG:NH1	23:CH:197:ALA:O	2.49	0.45
23:CH:222:ALA:HB2	23:CH:279:LEU:HD13	1.97	0.45
24:CI:344:MET:SD	32:CR:40:HIS:ND1	2.90	0.45
24:CI:954:THR:O	24:CI:957:GLY:N	2.36	0.45
30:CP:283:ARG:NE	50:C1:899:A:O2'	2.49	0.45
32:CR:790:LEU:HA	32:CR:794:PHE:HB2	1.98	0.45
32:CS:162:LEU:HD21	32:CS:190:LEU:HD11	1.97	0.45
32:CS:384:GLU:O	32:CS:406:TYR:HB2	2.17	0.45
52:CW:14:VAL:HG11	52:CW:372:LEU:HD21	1.98	0.45
53:UT:1754:ALA:HA	53:UT:1757:THR:HG22	1.99	0.45
6:UG:278:GLN:HA	6:UG:302:PRO:HB3	1.99	0.45
7:UJ:542:ARG:NH2	7:UJ:581:GLU:OE2	2.48	0.45
7:UJ:1448:SER:OG	7:UJ:1461:ARG:NH2	2.50	0.45
10:UM:463:ASP:HB3	10:UM:468:SER:HB3	1.98	0.45
24:CI:815:VAL:HG12	24:CI:905:VAL:HG22	1.98	0.45
24:CI:881:ASN:N	24:CI:905:VAL:O	2.50	0.45
32:CR:249:ILE:HD13	32:CR:269:VAL:HG21	1.97	0.45
32:CR:548:HIS:ND1	32:CR:550:LYS:O	2.49	0.45
32:CS:358:ARG:HE	32:CS:360:ASN:HD21	1.65	0.45
41:Ch:99:ARG:HA	41:Ch:99:ARG:HD2	1.84	0.45
50:C1:379:G:H1	50:C1:387:C:H42	1.65	0.45
53:UT:583:HIS:HA	53:UT:586:LEU:HG	1.99	0.45
54:UH:575:SER:HA	54:UH:578:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:Cl:57:ARG:HB2	57:Cl:60:GLU:HG3	1.99	0.45
59:CY:106:LYS:HG3	60:CZ:429:VAL:HG12	1.98	0.45
4:UD:564:ALA:HB1	4:UD:630:PRO:HG2	1.99	0.45
4:UD:833:ARG:NH1	50:C1:62:U:O2'	2.49	0.45
6:UG:222:MET:HG2	6:UG:233:THR:HG22	1.99	0.45
7:UJ:1079:LEU:HD13	7:UJ:1114:ILE:HB	1.99	0.45
13:UQ:922:ALA:HB3	13:UQ:925:ARG:HG2	1.99	0.45
20:CD:119:PHE:HA	20:CD:122:ILE:HG12	1.98	0.45
28:CM:134:LEU:HB3	28:CM:148:ALA:HB3	1.97	0.45
34:Ca:69:CYS:SG	42:Ci:127:ARG:NH1	2.89	0.45
39:Cf:176:ARG:NH2	50:C1:914:G:OP2	2.41	0.45
43:Cj:22:CYS:HB2	43:Cj:88:SER:OG	2.16	0.45
44:Ck:38:ARG:NH2	44:Ck:58:TYR:O	2.41	0.45
45:Cm:88:LYS:HA	45:Cm:91:THR:HG22	1.98	0.45
53:UT:256:MET:HE3	53:UT:260:ALA:HB2	1.99	0.45
53:UT:472:ARG:HA	53:UT:475:GLU:HG3	1.98	0.45
53:UT:692:GLN:HA	53:UT:695:GLU:HG2	1.99	0.45
53:UT:1161:VAL:HG21	53:UT:1202:VAL:HG11	1.99	0.45
53:UT:1598:ALA:O	53:UT:1643:LYS:NZ	2.50	0.45
53:UT:1960:TYR:HB2	53:UT:2004:VAL:HG21	1.99	0.45
55:UE:154:GLY:HA3	55:UE:187:ARG:HG3	1.97	0.45
4:UD:666:LEU:O	4:UD:671:ARG:NH1	2.50	0.45
7:UJ:1479:THR:OG1	7:UJ:1480:GLY:N	2.50	0.45
12:UO:5:VAL:HA	13:UQ:522:THR:HG21	1.99	0.45
23:CH:22:VAL:HG21	23:CH:116:PRO:HB3	1.99	0.45
32:CR:828:GLU:HA	32:CR:831:GLN:HG3	1.98	0.45
37:Cd:32:MET:HE3	37:Cd:54:GLY:HA2	1.99	0.45
55:UE:215:MET:HE1	55:UE:249:ARG:HG2	1.99	0.45
55:UE:306:VAL:O	55:UE:311:GLN:NE2	2.49	0.45
1:UA:155:ARG:HE	1:UA:155:ARG:HB3	1.55	0.45
1:UA:385:VAL:HA	1:UA:401:SER:HB2	1.97	0.45
2:UB:591:LEU:HD11	2:UB:638:TYR:HD2	1.82	0.45
7:UJ:297:VAL:HG12	7:UJ:300:TRP:CZ3	2.51	0.45
8:UK:62:GLU:HG3	8:UK:67:MET:HE1	1.99	0.45
9:UL:576:ASP:OD1	9:UL:576:ASP:N	2.48	0.45
9:UL:587:SER:HA	9:UL:609:PRO:HA	1.98	0.45
9:UL:855:PRO:HG3	9:UL:895:MET:HE2	1.99	0.45
13:UQ:100:GLU:OE1	13:UQ:405:SER:OG	2.34	0.45
18:CB:250:GLY:CA	18:CB:306:TYR:O	2.65	0.45
21:CF:53:VAL:O	21:CF:79:TYR:HA	2.17	0.45
34:Ca:124:ASN:HA	34:Ca:137:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Ca:129:THR:OG1	34:Ca:179:CYS:O	2.33	0.45
37:Cd:130:PRO:HB3	53:UT:701:GLN:HA	1.99	0.45
50:C1:467:C:H4'	50:C1:468:C:H5'	1.98	0.45
53:UT:38:HIS:CE1	53:UT:40:LEU:HG	2.52	0.45
53:UT:118:ALA:HB1	53:UT:122:LEU:HD23	1.99	0.45
53:UT:1601:THR:HA	53:UT:1604:ILE:HG12	1.99	0.45
54:UH:712:SER:HA	54:UH:775:LEU:HD11	1.99	0.45
4:UD:29:VAL:HB	4:UD:33:LYS:HB2	1.98	0.45
4:UD:59:LEU:HD22	4:UD:62:GLY:HA3	1.98	0.45
4:UD:799:GLU:HA	4:UD:802:ARG:HG2	1.99	0.45
7:UJ:813:ILE:HA	7:UJ:816:MET:HG2	1.99	0.45
7:UJ:1279:LEU:HA	7:UJ:1282:LYS:HE2	1.98	0.45
7:UJ:1285:ARG:HA	7:UJ:1288:GLU:OE1	2.17	0.45
9:UL:907:ARG:HH22	10:UM:881:SER:HB2	1.80	0.45
11:UN:282:LEU:HD11	53:UT:2158:LYS:HG2	1.97	0.45
15:UU:32:SER:HB3	15:UU:745:PHE:CD1	2.52	0.45
15:UU:71:LEU:HD11	15:UU:106:ALA:HB2	1.99	0.45
17:UZ:284:LYS:NZ	17:UZ:285:GLY:O	2.43	0.45
28:CM:201:THR:N	28:CM:216:VAL:O	2.51	0.45
32:CR:803:LEU:HD21	32:CR:882:ALA:HA	1.98	0.45
41:Ch:114:ARG:NH2	50:C1:1524:A:OP1	2.50	0.45
53:UT:370:SER:O	53:UT:373:THR:OG1	2.29	0.45
53:UT:1479:ILE:HA	53:UT:1482:VAL:HG22	1.98	0.45
4:UD:324:HIS:ND1	4:UD:345:SER:HB2	2.32	0.44
7:UJ:169:PRO:HB2	20:CD:413:LEU:HD23	1.98	0.44
10:UM:283:LEU:HD12	10:UM:284:ASN:H	1.82	0.44
13:UQ:266:LEU:HD21	13:UQ:271:LEU:HD11	1.98	0.44
18:CB:253:LEU:O	18:CB:303:SER:HA	2.16	0.44
19:CC:51:ARG:NH1	19:CC:85:ASN:O	2.51	0.44
22:CG:198:GLN:NE2	22:CG:221:LYS:HE2	2.32	0.44
32:CR:874:VAL:HG13	32:CR:922:HIS:HD2	1.82	0.44
32:CS:685:ASP:OD1	32:CS:685:ASP:N	2.49	0.44
35:Cb:38:LEU:HG	50:C1:882:C:H5''	1.99	0.44
53:UT:263:MET:HE3	53:UT:309:VAL:HG22	1.99	0.44
53:UT:501:LYS:HA	53:UT:504:ARG:HG2	1.98	0.44
53:UT:908:SER:OG	53:UT:943:LYS:NZ	2.35	0.44
53:UT:928:LYS:HB2	53:UT:928:LYS:HE3	1.79	0.44
6:UG:241:LYS:HG2	6:UG:253:GLU:HG2	1.98	0.44
13:UQ:369:TYR:CE2	13:UQ:383:GLN:HG2	2.52	0.44
16:UX:99:LEU:HD23	16:UX:102:LEU:HD12	1.99	0.44
18:CB:289:GLN:HG2	18:CB:302:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:CC:232:LEU:HD22	19:CC:255:ILE:HG23	1.99	0.44
22:CG:491:ARG:NH1	22:CG:500:GLU:OE2	2.50	0.44
32:CS:738:LYS:NZ	32:CS:807:GLU:OE1	2.37	0.44
45:Cm:85:GLU:HA	49:CU:300:VAL:HG21	1.98	0.44
50:C1:155:G:H1	50:C1:183:C:H42	1.64	0.44
50:C1:1052:A:N1	50:C1:1178:A:O2'	2.46	0.44
53:UT:390:ILE:HG22	53:UT:391:ILE:HD13	1.99	0.44
53:UT:470:ILE:HG23	53:UT:479:LEU:HD21	1.99	0.44
53:UT:820:GLU:HB3	53:UT:823:GLN:HB2	1.98	0.44
53:UT:1499:GLU:HB3	53:UT:1502:ARG:HH21	1.82	0.44
53:UT:1877:LEU:HD12	53:UT:1962:MET:HE3	1.99	0.44
1:UA:496:SER:HB2	1:UA:503:THR:HB	1.99	0.44
4:UD:205:SER:HA	4:UD:237:ILE:HA	1.99	0.44
7:UJ:1044:TYR:HB2	20:CD:36:LEU:HD21	1.99	0.44
7:UJ:1280:ARG:HB3	7:UJ:1324:TYR:HE1	1.81	0.44
7:UJ:1709:LEU:O	7:UJ:1713:VAL:HG23	2.17	0.44
7:UJ:1784:ARG:NH2	53:UT:50:ASP:O	2.48	0.44
9:UL:104:VAL:HG11	9:UL:142:GLU:HG2	2.00	0.44
9:UL:517:HIS:ND1	9:UL:519:ASP:OD1	2.50	0.44
12:UO:470:LEU:O	12:UO:509:TYR:OH	2.28	0.44
13:UQ:762:LEU:HD22	54:UH:440:ARG:NH2	2.33	0.44
13:UQ:765:TYR:OH	13:UQ:819:GLU:O	2.31	0.44
15:UU:615:ALA:O	15:UU:618:THR:OG1	2.31	0.44
22:CG:557:ARG:HH11	22:CG:598:ARG:HE	1.65	0.44
30:CP:283:ARG:HA	30:CP:286:LYS:HZ2	1.82	0.44
32:CS:172:ARG:NH2	32:CS:610:ALA:O	2.50	0.44
32:CS:183:ALA:HB1	32:CS:186:ASN:HD21	1.82	0.44
32:CS:377:ALA:O	32:CS:380:LEU:HG	2.17	0.44
47:Co:381:ALA:HB1	47:Co:385:GLN:HE21	1.82	0.44
53:UT:1364:ASP:HB3	53:UT:1367:ASN:HB2	2.00	0.44
53:UT:1878:MET:HE3	53:UT:1878:MET:HB3	1.82	0.44
53:UT:1911:VAL:HG11	53:UT:1973:VAL:HG11	1.98	0.44
1:UA:551:ARG:HG2	1:UA:573:LYS:HB3	2.00	0.44
4:UD:377:ALA:HB3	4:UD:382:TYR:HB2	1.99	0.44
6:UG:134:LEU:HD21	7:UJ:5:LEU:HB2	1.99	0.44
6:UG:346:THR:N	6:UG:359:GLY:O	2.50	0.44
6:UG:481:ARG:NH1	50:C1:587:U:O2'	2.50	0.44
11:UN:327:ILE:HD11	50:C1:580:A:C8	2.52	0.44
20:CD:114:MET:HG2	20:CD:115:THR:HG23	2.00	0.44
20:CD:162:ASP:N	20:CD:162:ASP:OD1	2.49	0.44
21:CE:105:SER:OG	21:CE:112:ASN:OD1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:CF:63:SER:HA	21:CF:66:LEU:HD12	1.99	0.44
27:CL:52:LEU:O	27:CL:57:PRO:HD2	2.17	0.44
32:CS:282:THR:HA	32:CS:410:MET:HB2	1.99	0.44
35:Cb:210:LEU:O	35:Cb:217:THR:HA	2.17	0.44
50:C1:207:U:H5'	50:C1:208:A:C5	2.52	0.44
50:C1:1665:A:N3	50:C1:1666:C:N4	2.66	0.44
54:UH:399:GLU:HB3	54:UH:414:ILE:HG13	1.98	0.44
54:UH:724:LYS:HD3	54:UH:728:ARG:HH21	1.82	0.44
56:US:208:LEU:HB3	56:US:275:LEU:HD21	1.99	0.44
2:UB:711:ASP:OD1	2:UB:711:ASP:N	2.44	0.44
6:UG:267:ASN:HB2	6:UG:274:HIS:NE2	2.31	0.44
7:UJ:781:VAL:HG23	7:UJ:782:VAL:HG23	1.99	0.44
7:UJ:1091:SER:HA	7:UJ:1094:LYS:HG2	2.00	0.44
7:UJ:1271:LEU:HD22	7:UJ:1275:PRO:HG3	1.99	0.44
7:UJ:1607:LEU:HD13	7:UJ:1610:PHE:CZ	2.53	0.44
9:UL:399:ILE:HD13	9:UL:414:TYR:HB3	1.98	0.44
19:CC:267:SER:OG	19:CC:268:GLU:N	2.51	0.44
26:CK:128:VAL:HG13	26:CK:157:PHE:HE2	1.82	0.44
27:CL:52:LEU:HD23	27:CL:52:LEU:HA	1.86	0.44
28:CM:28:ALA:HB3	28:CM:31:LEU:HD13	1.99	0.44
30:CP:273:GLU:O	30:CP:276:GLN:HG3	2.17	0.44
32:CS:361:ILE:HB	32:CS:367:GLN:HB2	2.00	0.44
32:CS:634:ARG:HD2	32:CS:636:VAL:HG22	2.00	0.44
32:CS:924:GLY:HA2	32:CS:927:VAL:HG12	1.99	0.44
51:C2:49:U:H2'	51:C2:50:G:C8	2.52	0.44
57:Cl:53:ASP:HB3	57:Cl:56:LYS:HG3	1.99	0.44
7:UJ:813:ILE:HG22	7:UJ:816:MET:HE2	1.99	0.44
10:UM:382:ILE:HG13	10:UM:383:LEU:HG	2.00	0.44
12:UO:532:ARG:HH21	55:UE:212:PHE:HE2	1.63	0.44
13:UQ:222:ASN:HD22	13:UQ:225:MET:HE2	1.83	0.44
13:UQ:453:ARG:NH1	54:UH:880:GLU:OE2	2.42	0.44
20:CD:210:VAL:O	20:CD:214:LEU:HB3	2.17	0.44
22:CG:174:THR:HB	22:CG:587:ARG:HG3	2.00	0.44
24:CI:353:ILE:HD11	32:CR:206:LEU:HD12	1.99	0.44
32:CS:26:PHE:O	32:CS:199:CYS:HA	2.17	0.44
35:Cb:205:PHE:HE2	50:C1:697:U:H5'	1.82	0.44
50:C1:313:A:N6	50:C1:327:G:O2'	2.51	0.44
50:C1:686:A:H2'	50:C1:687:U:H4'	2.00	0.44
52:CW:344:MET:HE3	52:CW:346:LEU:HD21	2.00	0.44
53:UT:735:TRP:HE1	53:UT:766:LEU:HD13	1.82	0.44
1:UA:631:THR:OG1	1:UA:634:GLY:O	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:UB:618:ILE:HG12	2:UB:639:LEU:HD22	2.00	0.44
4:UD:287:ASP:OD1	4:UD:287:ASP:N	2.41	0.44
4:UD:423:VAL:HG13	55:UE:307:TYR:HD2	1.83	0.44
4:UD:546:ASP:OD1	4:UD:546:ASP:N	2.51	0.44
9:UL:570:SER:HB3	9:UL:613:MET:HE2	2.00	0.44
10:UM:160:HIS:CE1	10:UM:162:PHE:HB3	2.53	0.44
23:CH:202:LEU:HD13	23:CH:343:SER:HB3	1.99	0.44
32:CR:318:GLU:O	32:CR:321:LYS:NZ	2.41	0.44
32:CS:198:SER:HB2	32:CS:485:ASN:HB2	2.00	0.44
35:Cb:195:ILE:HA	35:Cb:210:LEU:HG	2.00	0.44
39:Cf:64:ASN:O	39:Cf:184:ASP:HA	2.17	0.44
39:Cf:113:TYR:OH	39:Cf:119:GLN:NE2	2.46	0.44
42:Ci:26:VAL:HB	42:Ci:89:ILE:HA	1.98	0.44
53:UT:104:MET:HA	53:UT:107:LEU:HB2	1.99	0.44
53:UT:192:PRO:HA	53:UT:196:LYS:HB3	1.99	0.44
53:UT:675:GLU:HA	53:UT:687:LEU:HD21	1.98	0.44
53:UT:1774:VAL:HA	53:UT:1777:LEU:HD12	2.00	0.44
1:UA:713:MET:HE2	1:UA:713:MET:HB3	1.86	0.44
4:UD:262:ASP:OD1	14:UR:450:ARG:NH1	2.51	0.44
4:UD:512:SER:OG	4:UD:514:ASP:OD1	2.29	0.44
13:UQ:142:HIS:CE1	13:UQ:445:ARG:HH12	2.36	0.44
20:CD:219:ASN:O	20:CD:219:ASN:ND2	2.51	0.44
23:CH:102:ILE:HD12	23:CH:137:VAL:HG22	2.00	0.44
24:CI:886:CYS:HB2	24:CI:901:ALA:HB3	2.00	0.44
32:CS:272:ILE:HD13	32:CS:302:ALA:HB2	1.99	0.44
32:CS:283:LEU:HD11	32:CS:474:LEU:HG	1.99	0.44
32:CS:619:SER:O	32:CS:623:GLN:HA	2.18	0.44
37:Cd:172:TYR:OH	50:C1:658:A:N6	2.51	0.44
50:C1:719:U:OP2	53:UT:1067:ARG:NH2	2.51	0.44
52:CW:154:PRO:HB3	52:CW:204:VAL:HG12	1.99	0.44
53:UT:215:VAL:O	53:UT:219:ALA:HB2	2.17	0.44
60:CZ:436:LEU:HD23	60:CZ:436:LEU:HA	1.88	0.44
2:UB:579:GLU:HG3	56:US:501:LEU:HD13	1.99	0.44
5:UF:317:ILE:HA	5:UF:320:VAL:HG12	2.00	0.44
7:UJ:434:VAL:O	7:UJ:438:ILE:HG12	2.18	0.44
7:UJ:494:ARG:HD2	7:UJ:497:LYS:HZ3	1.82	0.44
7:UJ:1012:ALA:HB2	7:UJ:1052:THR:HG23	1.99	0.44
7:UJ:1697:ASP:N	7:UJ:1697:ASP:OD1	2.50	0.44
13:UQ:635:VAL:HG23	13:UQ:669:LEU:HD11	2.00	0.44
15:UU:97:THR:HA	15:UU:105:TYR:O	2.17	0.44
17:UZ:154:LEU:HB3	17:UZ:182:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:CL:75:LEU:HD23	27:CL:78:LEU:HD12	1.99	0.44
31:CQ:89:PRO:HA	31:CQ:92:MET:HB3	1.99	0.44
32:CR:396:LEU:HA	32:CR:399:VAL:HG12	2.00	0.44
37:Cd:92:ARG:O	50:C1:989:C:O2'	2.27	0.44
52:CW:23:LEU:HD22	52:CW:27:LEU:HD23	2.00	0.44
53:UT:135:VAL:HA	53:UT:178:LEU:HD12	2.00	0.44
53:UT:736:GLY:O	53:UT:739:THR:OG1	2.26	0.44
53:UT:1769:LYS:HA	53:UT:1772:PHE:HD2	1.82	0.44
54:UH:275:PRO:HB2	54:UH:279:GLU:HB2	1.99	0.44
54:UH:344:SER:OG	54:UH:357:SER:O	2.26	0.44
1:UA:648:LEU:O	1:UA:652:ILE:HD12	2.18	0.43
3:UC:210:THR:H	3:UC:213:MET:HE2	1.83	0.43
4:UD:841:ILE:HG13	4:UD:859:GLU:HB2	1.99	0.43
7:UJ:852:ALA:HA	7:UJ:855:VAL:HG12	2.00	0.43
8:UK:105:LYS:HD2	8:UK:247:MET:HE1	1.98	0.43
12:UO:171:LEU:O	12:UO:180:THR:N	2.46	0.43
13:UQ:615:PHE:H	13:UQ:630:GLY:HA2	1.83	0.43
18:CA:259:ALA:HA	18:CA:271:VAL:HG11	2.00	0.43
26:CK:183:THR:HG21	50:C1:2205:G:O2'	2.17	0.43
32:CS:20:GLN:HG2	32:CS:220:LEU:HD11	1.98	0.43
32:CS:724:GLY:HA2	32:CS:762:MET:O	2.18	0.43
32:CS:911:ILE:O	32:CS:915:ILE:HG12	2.18	0.43
38:Ce:55:ILE:HG21	38:Ce:182:VAL:HG22	2.00	0.43
39:Cf:115:ALA:O	53:UT:1143:ARG:NH2	2.51	0.43
52:CW:294:ILE:HD13	52:CW:306:LEU:HD22	2.00	0.43
54:UH:58:VAL:HG21	54:UH:103:VAL:HG11	1.99	0.43
54:UH:559:GLN:O	54:UH:563:ASN:HB2	2.18	0.43
56:US:128:MET:HA	56:US:131:SER:HB3	2.00	0.43
56:US:151:GLN:OE1	56:US:152:HIS:ND1	2.51	0.43
58:CX:328:LEU:HD11	58:CX:333:ILE:HD13	2.01	0.43
6:UG:225:LEU:HD13	6:UG:271:ALA:HB1	2.00	0.43
7:UJ:720:LEU:HA	7:UJ:723:LYS:HG2	2.00	0.43
7:UJ:784:PRO:HG3	7:UJ:816:MET:HB2	2.01	0.43
7:UJ:1770:LEU:HD21	7:UJ:1778:VAL:HG12	2.00	0.43
9:UL:130:LYS:HA	9:UL:154:GLN:HB2	1.99	0.43
15:UU:514:ALA:HB2	15:UU:547:VAL:HG13	2.00	0.43
24:CI:253:THR:HB	24:CI:267:THR:H	1.83	0.43
30:CP:283:ARG:HH21	50:C1:899:A:H1'	1.83	0.43
30:CP:302:PHE:CZ	60:CZ:543:LYS:HE2	2.53	0.43
32:CS:541:VAL:HA	32:CS:544:TYR:HB3	2.00	0.43
35:Cb:122:LYS:HD2	35:Cb:164:LEU:HD21	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Cf:188:LEU:HD22	39:Cf:192:GLU:HB3	1.99	0.43
41:Ch:102:LEU:HD23	41:Ch:102:LEU:HA	1.89	0.43
50:C1:1097:U:H2'	50:C1:1098:G:C8	2.53	0.43
54:UH:4:LYS:NZ	54:UH:601:GLU:O	2.51	0.43
2:UB:769:LEU:HD22	2:UB:773:LEU:HD23	2.01	0.43
4:UD:441:THR:CA	4:UD:456:LEU:O	2.27	0.43
7:UJ:112:MET:HE3	33:CT:70:SER:HA	2.00	0.43
7:UJ:713:HIS:O	7:UJ:717:THR:OG1	2.26	0.43
10:UM:378:ASP:OD2	10:UM:439:LEU:N	2.51	0.43
12:UO:335:ALA:HB1	12:UO:343:LEU:HD11	2.01	0.43
13:UQ:814:PHE:CE1	13:UQ:821:PRO:HD3	2.53	0.43
20:CD:134:GLU:H	20:CD:137:ASN:HD21	1.66	0.43
29:CN:12:PRO:HA	29:CN:13:PRO:HD3	1.90	0.43
32:CR:19:LEU:HD13	32:CR:49:ASP:HB2	1.99	0.43
32:CS:295:MET:HE3	32:CS:411:ALA:HB2	2.00	0.43
32:CS:359:VAL:HB	32:CS:369:ILE:HG12	2.00	0.43
32:CS:406:TYR:O	32:CS:467:ARG:NH2	2.51	0.43
34:Ca:141:ALA:HB1	34:Ca:207:LEU:HD13	1.99	0.43
40:Cg:83:VAL:HG12	40:Cg:105:ARG:HG3	2.00	0.43
45:Cm:11:LEU:HD12	45:Cm:74:VAL:HG13	1.99	0.43
50:C1:462:G:N7	59:CY:374:ARG:NH1	2.66	0.43
53:UT:1169:ILE:HD13	53:UT:1172:LEU:HD13	2.01	0.43
53:UT:1236:ASN:O	53:UT:1239:GLN:O	2.35	0.43
54:UH:734:GLU:HA	54:UH:737:VAL:HG12	2.01	0.43
54:UH:891:ARG:HE	54:UH:891:ARG:HB2	1.71	0.43
56:US:156:ARG:HG2	56:US:158:GLU:H	1.82	0.43
2:UB:759:HIS:O	2:UB:762:THR:OG1	2.27	0.43
7:UJ:52:CYS:HB3	7:UJ:120:TRP:HB2	1.99	0.43
7:UJ:166:PHE:CD1	7:UJ:185:GLN:HG2	2.54	0.43
7:UJ:1614:LEU:HD13	7:UJ:1617:ILE:H	1.84	0.43
13:UQ:222:ASN:H	13:UQ:225:MET:HE3	1.82	0.43
22:CG:401:VAL:HG23	22:CG:411:THR:HG22	2.00	0.43
24:CI:622:THR:HG23	24:CI:623:ARG:HG2	2.00	0.43
27:CL:137:THR:HG22	27:CL:141:TRP:HD1	1.82	0.43
29:CO:171:LEU:HD23	29:CO:177:LYS:HD2	1.99	0.43
32:CR:386:VAL:HG23	32:CR:408:VAL:HG23	2.00	0.43
33:CT:104:ARG:HD3	33:CT:162:VAL:HG21	1.99	0.43
34:Ca:28:ASP:OD1	34:Ca:50:ARG:NE	2.51	0.43
50:C1:314:A:H61	50:C1:326:U:H3	1.66	0.43
50:C1:1070:G:H1	50:C1:1085:U:H3	1.66	0.43
53:UT:1431:TRP:HA	53:UT:1434:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:UH:357:SER:HB2	54:UH:391:PHE:CZ	2.53	0.43
59:CY:40:LEU:HB2	60:CZ:425:TRP:CD2	2.53	0.43
59:CY:62:LYS:HB3	60:CZ:341:PHE:HD2	1.83	0.43
6:UG:336:VAL:HG22	6:UG:378:GLN:HB2	2.01	0.43
10:UM:45:LEU:HD12	10:UM:55:ALA:HB3	2.00	0.43
12:UO:274:LYS:HE2	56:US:335:ASP:HB3	2.00	0.43
19:CC:165:LYS:HE2	19:CC:165:LYS:HB2	1.83	0.43
49:CU:114:GLN:O	49:CU:118:VAL:HG23	2.19	0.43
53:UT:528:LEU:HD12	53:UT:576:PHE:HE2	1.84	0.43
53:UT:1616:TYR:HA	53:UT:1619:ILE:HG22	2.01	0.43
53:UT:1711:PRO:O	53:UT:1715:ILE:HG12	2.18	0.43
54:UH:538:TYR:OH	54:UH:582:ASP:OD2	2.36	0.43
60:CZ:466:LYS:O	60:CZ:469:THR:OG1	2.36	0.43
3:UC:239:LEU:HD23	3:UC:242:LEU:HD12	2.01	0.43
3:UC:264:TRP:HZ3	27:CL:154:GLU:HG2	1.83	0.43
4:UD:253:ASP:OD1	4:UD:255:THR:OG1	2.35	0.43
6:UG:321:ASP:O	6:UG:323:LYS:N	2.46	0.43
7:UJ:489:ASP:OD1	7:UJ:489:ASP:N	2.51	0.43
8:UK:48:LEU:HG	24:CI:1048:LEU:HD11	2.01	0.43
8:UK:250:THR:OG1	8:UK:269:LYS:NZ	2.45	0.43
9:UL:24:LEU:HD11	9:UL:388:GLY:HA3	1.99	0.43
13:UQ:413:LEU:HD12	13:UQ:421:MET:HE3	2.01	0.43
13:UQ:736:ALA:HB3	13:UQ:747:LEU:HB3	2.00	0.43
15:UU:91:PRO:HD2	15:UU:108:PHE:CE2	2.53	0.43
15:UU:386:ALA:HB3	15:UU:414:ASP:N	2.34	0.43
18:CB:163:SER:N	18:CB:189:SER:OG	2.47	0.43
18:CB:184:GLU:O	18:CB:207:VAL:HA	2.18	0.43
23:CH:284:GLU:OE1	49:CU:129:ARG:NH2	2.52	0.43
26:CK:288:THR:HG23	50:C1:1146:G:C5	2.54	0.43
28:CM:26:ASN:HB3	28:CM:31:LEU:HD22	2.00	0.43
32:CR:203:ASP:OD1	32:CR:204:ASP:N	2.49	0.43
53:UT:1490:ILE:HA	53:UT:1505:ILE:HD11	2.00	0.43
54:UH:700:ASP:OD1	54:UH:700:ASP:N	2.51	0.43
54:UH:833:LYS:HB2	55:UI:246:LEU:HB3	2.00	0.43
58:CX:203:THR:HA	58:CX:238:ARG:HH12	1.84	0.43
4:UD:123:LYS:HE3	4:UD:172:ASP:HA	2.00	0.43
4:UD:359:LYS:HG3	4:UD:753:VAL:HG21	1.99	0.43
4:UD:632:VAL:O	4:UD:649:VAL:HA	2.19	0.43
4:UD:654:LYS:NZ	4:UD:687:ASP:O	2.37	0.43
4:UD:672:ARG:NH1	4:UD:715:ASP:OD1	2.52	0.43
7:UJ:752:TRP:CD1	7:UJ:778:VAL:HG21	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:UJ:1555:THR:HA	7:UJ:1558:HIS:ND1	2.34	0.43
7:UJ:1680:VAL:HG11	7:UJ:1725:ALA:HB1	2.01	0.43
8:UK:70:ARG:NH2	24:CI:1063:GLN:OE1	2.52	0.43
9:UL:622:ILE:HG23	9:UL:634:TRP:HB2	2.00	0.43
9:UL:864:PHE:O	9:UL:868:GLU:HA	2.18	0.43
15:UU:32:SER:OG	15:UU:35:PHE:O	2.36	0.43
21:CF:40:GLU:OE2	51:C2:194:G:N1	2.51	0.43
23:CH:405:ASN:ND2	23:CH:408:ARG:HB2	2.34	0.43
32:CS:95:PHE:HA	32:CS:98:PHE:CE2	2.53	0.43
32:CS:644:TYR:HE1	60:CZ:571:ARG:HH11	1.66	0.43
35:Cb:15:PRO:HD2	35:Cb:18:TRP:CZ3	2.54	0.43
37:Cd:61:PHE:HA	37:Cd:62:PRO:HD3	1.90	0.43
39:Cf:98:LYS:NZ	39:Cf:174:SER:O	2.39	0.43
53:UT:173:LYS:HD2	53:UT:213:PHE:CE2	2.54	0.43
53:UT:285:VAL:HG21	53:UT:337:LEU:HD22	2.00	0.43
4:UD:66:GLU:OE1	4:UD:545:TYR:OH	2.30	0.43
7:UJ:1260:SER:O	7:UJ:1290:ARG:NE	2.52	0.43
9:UL:451:ILE:HB	9:UL:461:ARG:HB2	1.99	0.43
10:UM:882:TYR:HA	10:UM:885:GLU:OE1	2.19	0.43
11:UN:915:PHE:O	11:UN:919:THR:OG1	2.26	0.43
28:CM:47:VAL:HB	28:CM:379:LEU:HD21	2.01	0.43
32:CS:849:LEU:HD12	32:CS:853:VAL:HG11	2.00	0.43
34:Ca:114:VAL:HG11	50:C1:1515:A:H2'	2.01	0.43
37:Cd:174:LYS:NZ	50:C1:655:A:OP2	2.38	0.43
48:Cp:45:VAL:HG22	48:Cp:55:LEU:HD21	2.00	0.43
53:UT:1089:PRO:HB2	53:UT:1090:TYR:CD1	2.53	0.43
4:UD:324:HIS:HD1	4:UD:345:SER:HB2	1.84	0.43
4:UD:514:ASP:OD1	4:UD:514:ASP:N	2.52	0.43
5:UF:47:VAL:HG13	5:UF:57:PHE:CE1	2.53	0.43
7:UJ:989:ASP:OD1	7:UJ:989:ASP:N	2.48	0.43
7:UJ:1619:THR:HA	7:UJ:1622:ALA:HB2	2.00	0.43
10:UM:755:ARG:HG3	10:UM:793:ALA:HB1	2.00	0.43
12:UO:413:HIS:HB3	12:UO:417:ARG:H	1.83	0.43
15:UU:669:ILE:N	15:UU:683:ALA:O	2.42	0.43
24:CI:950:ALA:O	24:CI:961:GLN:HA	2.19	0.43
29:CO:192:TYR:OH	29:CO:223:GLU:OE2	2.34	0.43
32:CR:890:GLN:HE21	32:CR:892:LYS:NZ	2.16	0.43
40:Cg:58:LEU:HD23	40:Cg:58:LEU:HA	1.86	0.43
41:Ch:121:ARG:HH12	50:C1:1452:G:H5''	1.84	0.43
50:C1:1230:U:H5'	53:UT:1894:LEU:HD21	2.01	0.43
53:UT:1162:LYS:HA	53:UT:1165:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:UT:1358:LEU:HD13	53:UT:1361:PHE:HB3	2.01	0.43
2:UB:784:LEU:HD23	2:UB:784:LEU:HA	1.90	0.43
4:UD:339:VAL:HG13	4:UD:351:VAL:HG13	2.01	0.43
7:UJ:455:LYS:HD3	7:UJ:456:LEU:HD22	2.01	0.43
7:UJ:749:LEU:HD22	7:UJ:781:VAL:HG21	2.00	0.43
13:UQ:403:VAL:HB	13:UQ:412:ALA:HB3	2.01	0.43
19:CC:155:LEU:HD23	20:CD:245:MET:HE1	2.00	0.43
23:CH:121:ALA:HB1	23:CH:196:PHE:CD2	2.54	0.43
24:CI:109:SER:HA	50:C1:638:A:H5'	1.99	0.43
29:CO:167:ILE:HG13	29:CO:171:LEU:HD13	2.00	0.43
31:CQ:91:ARG:HG2	31:CQ:147:ALA:HA	2.01	0.43
35:Cb:128:ARG:HB3	35:Cb:140:VAL:HB	2.01	0.43
50:C1:860:C:O2'	50:C1:862:U:OP2	2.34	0.43
51:C2:4:G:H2'	51:C2:5:A:C8	2.54	0.43
53:UT:824:ASP:N	53:UT:824:ASP:OD1	2.52	0.43
54:UH:347:LEU:HD23	54:UH:355:LEU:HB2	2.00	0.43
58:CX:344:THR:O	58:CX:347:ASP:C	2.62	0.43
10:UM:35:LEU:HD21	10:UM:343:LEU:HD13	2.01	0.42
10:UM:696:LEU:HA	10:UM:712:GLY:HA3	2.01	0.42
16:UX:69:VAL:HG21	16:UX:109:ALA:HA	2.01	0.42
23:CH:292:TYR:HB3	23:CH:320:VAL:HG12	2.01	0.42
29:CO:152:GLY:HA2	29:CO:159:LEU:HG	2.01	0.42
30:CP:75:GLU:O	34:Ca:115:ARG:NH1	2.52	0.42
30:CP:105:SER:O	30:CP:105:SER:OG	2.32	0.42
32:CR:126:GLN:O	32:CR:154:LYS:NZ	2.52	0.42
32:CR:201:VAL:HG12	32:CR:209:LEU:HD12	2.01	0.42
32:CS:314:SER:OG	32:CS:316:SER:O	2.37	0.42
53:UT:90:THR:HG23	53:UT:96:ILE:HD11	2.00	0.42
53:UT:1198:PRO:HG3	53:UT:1250:LEU:HD22	2.00	0.42
53:UT:1874:GLN:O	53:UT:1878:MET:HG2	2.19	0.42
54:UH:322:LEU:HD23	54:UH:338:LEU:HD21	2.00	0.42
54:UH:345:SER:HB3	54:UH:357:SER:HB3	2.01	0.42
56:US:385:LEU:HD23	56:US:385:LEU:HA	1.86	0.42
1:UA:450:ILE:HG12	1:UA:474:LEU:HD21	2.01	0.42
1:UA:467:HIS:HE2	1:UA:485:SER:HG	1.65	0.42
4:UD:617:ASN:HB3	4:UD:620:ALA:HB2	2.01	0.42
7:UJ:1121:ARG:HH11	7:UJ:1122:TYR:H	1.67	0.42
14:UR:138:ASP:OD2	15:UU:212:ASN:ND2	2.50	0.42
16:UX:41:PRO:HB2	16:UX:44:MET:HG2	2.01	0.42
18:CB:191:ARG:HG2	20:CD:154:LEU:HD13	2.00	0.42
22:CG:426:LYS:NZ	59:CY:237:ASP:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:CP:58:VAL:HG13	30:CP:98:LEU:HD21	2.02	0.42
32:CR:308:SER:N	32:CR:384:GLU:OE2	2.52	0.42
49:CU:113:LYS:O	49:CU:117:LYS:HG3	2.19	0.42
50:C1:1240:G:H1	50:C1:1259:C:H42	1.66	0.42
53:UT:2222:ILE:HA	53:UT:2225:THR:HG22	2.00	0.42
59:CY:324:LEU:C	59:CY:328:LYS:HZ2	2.26	0.42
60:CZ:536:ARG:HD2	60:CZ:536:ARG:HA	1.87	0.42
3:UC:300:ARG:HA	3:UC:305:MET:HE3	2.01	0.42
9:UL:574:SER:OG	9:UL:576:ASP:O	2.30	0.42
10:UM:774:PHE:HA	10:UM:777:VAL:HG12	2.01	0.42
13:UQ:727:SER:OG	54:UH:635:GLN:OE1	2.33	0.42
32:CS:564:ALA:HB1	32:CS:590:LEU:HB2	2.02	0.42
35:Cb:114:ILE:HG23	35:Cb:118:GLU:HB3	2.00	0.42
37:Cd:154:ARG:NH1	50:C1:664:A:OP1	2.53	0.42
50:C1:1131:U:O2'	50:C1:1180:C:O2'	2.31	0.42
50:C1:1701:U:H2'	50:C1:1702:G:C8	2.54	0.42
53:UT:37:LEU:HD12	53:UT:37:LEU:HA	1.88	0.42
53:UT:964:LEU:HD23	53:UT:964:LEU:HA	1.82	0.42
53:UT:1634:GLN:HA	53:UT:1637:VAL:HG12	2.01	0.42
53:UT:2102:VAL:O	53:UT:2105:ARG:C	2.63	0.42
58:CX:217:LEU:HD11	58:CX:249:ALA:HB1	2.01	0.42
2:UB:89:GLU:HB3	27:CL:535:GLU:HG2	2.01	0.42
4:UD:337:MET:HE2	4:UD:339:VAL:HG21	2.02	0.42
4:UD:651:THR:HG22	4:UD:655:GLN:HB2	2.01	0.42
5:UF:287:ARG:HA	5:UF:292:TRP:CD2	2.54	0.42
7:UJ:1651:LEU:HD22	7:UJ:1702:VAL:HG23	2.01	0.42
9:UL:899:LEU:HB3	10:UM:888:LEU:HD11	2.01	0.42
17:UZ:282:TYR:HB3	17:UZ:290:ALA:HB1	2.02	0.42
22:CG:418:LEU:HD12	22:CG:418:LEU:HA	1.90	0.42
32:CR:723:VAL:HG23	32:CR:766:LEU:HD11	2.00	0.42
50:C1:223:A:O2'	50:C1:224:C:O4'	2.33	0.42
53:UT:797:THR:HG23	53:UT:799:PHE:H	1.83	0.42
60:CZ:331:LEU:HD23	60:CZ:331:LEU:HA	1.82	0.42
55:UI:210:ARG:HE	55:UI:212:PHE:HE1	1.66	0.42
2:UB:640:SER:HB2	2:UB:657:MET:HG3	2.02	0.42
4:UD:54:GLU:HB3	4:UD:68:ILE:HG12	2.01	0.42
4:UD:432:THR:N	4:UD:446:SER:O	2.46	0.42
6:UG:337:ASN:OD1	50:C1:279:C:N4	2.40	0.42
7:UJ:1149:LEU:HD23	7:UJ:1149:LEU:HA	1.89	0.42
11:UN:329:THR:HG23	11:UN:937:MET:HB2	2.01	0.42
15:UU:210:ILE:HD12	15:UU:220:TYR:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:CH:410:VAL:HG11	24:CI:881:ASN:HB2	2.01	0.42
24:CI:154:LEU:HD23	24:CI:154:LEU:HA	1.88	0.42
30:CP:283:ARG:NH2	50:C1:900:A:O4'	2.52	0.42
32:CR:903:LEU:HA	32:CR:904:PRO:HD3	1.92	0.42
32:CS:129:GLU:HA	32:CS:167:MET:HG3	2.00	0.42
32:CS:834:THR:HG23	32:CS:837:ASP:H	1.83	0.42
44:Ck:111:ASN:ND2	50:C1:933:G:OP2	2.52	0.42
50:C1:648:A:N6	50:C1:649:A:N1	2.68	0.42
51:C2:246:G:H3'	51:C2:247:G:H5''	2.01	0.42
52:CW:152:LEU:HD22	52:CW:170:ARG:HG2	2.01	0.42
53:UT:410:MET:HE1	53:UT:444:LEU:HD21	2.00	0.42
53:UT:726:LEU:HA	53:UT:729:ALA:HB3	2.01	0.42
54:UH:181:ALA:O	54:UH:190:LYS:N	2.52	0.42
59:CY:94:LEU:HD21	60:CZ:463:LEU:HD13	2.02	0.42
1:UA:179:SER:OG	1:UA:181:ASP:O	2.28	0.42
2:UB:471:ASP:OD2	2:UB:506:ARG:NH2	2.41	0.42
7:UJ:700:HIS:HA	7:UJ:701:SER:HA	1.72	0.42
7:UJ:1083:VAL:HA	7:UJ:1086:TYR:HB3	2.01	0.42
10:UM:638:PHE:HB3	10:UM:678:TRP:HZ3	1.84	0.42
13:UQ:455:VAL:HA	54:UH:888:ILE:HD11	2.00	0.42
17:UZ:87:HIS:CE1	17:UZ:254:LYS:HG2	2.55	0.42
27:CL:618:GLU:OE2	27:CL:621:ARG:NH2	2.36	0.42
29:CN:90:ASP:OD1	29:CN:91:ILE:N	2.53	0.42
32:CR:27:PHE:HB2	32:CR:150:VAL:HG22	2.02	0.42
32:CS:134:ASN:OD1	32:CS:135:ILE:HD12	2.20	0.42
32:CS:876:LEU:HD12	32:CS:880:GLN:HB3	2.01	0.42
32:CS:916:MET:HA	32:CS:919:VAL:HG22	2.01	0.42
34:Ca:144:LYS:HG3	34:Ca:208:GLN:HG3	2.02	0.42
50:C1:934:A:H5''	50:C1:936:A:H5'	2.01	0.42
51:C2:90:C:O2'	51:C2:91:G:OP2	2.37	0.42
52:CW:206:VAL:O	52:CW:218:ALA:O	2.37	0.42
53:UT:111:ILE:HG12	53:UT:151:LEU:HD11	2.00	0.42
54:UH:393:SER:OG	54:UH:394:TYR:N	2.52	0.42
54:UH:723:VAL:HG13	54:UH:786:ALA:HA	2.02	0.42
4:UD:224:THR:OG1	14:UR:413:ARG:NH2	2.47	0.42
4:UD:552:ILE:HG12	4:UD:563:VAL:HG12	2.01	0.42
7:UJ:821:LYS:HA	7:UJ:821:LYS:HD2	1.81	0.42
7:UJ:1027:MET:SD	7:UJ:1028:PRO:HD3	2.60	0.42
13:UQ:698:SER:HB2	54:UH:431:THR:HG23	2.02	0.42
16:UX:91:ILE:HG12	16:UX:118:TRP:CE3	2.54	0.42
18:CB:103:VAL:HG23	18:CB:104:TYR:HD1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:CH:209:ASN:HD21	23:CH:348:ARG:NH2	2.17	0.42
29:CN:88:ARG:HG3	29:CN:210:ALA:HB2	2.01	0.42
29:CN:192:TYR:OH	29:CN:223:GLU:OE2	2.24	0.42
32:CR:88:GLU:HB2	32:CR:91:GLN:HB2	2.02	0.42
32:CR:729:LEU:HD11	32:CR:747:LEU:HD21	2.01	0.42
52:CW:349:ASN:OD1	52:CW:349:ASN:N	2.53	0.42
53:UT:1285:ALA:O	53:UT:1289:VAL:HG23	2.20	0.42
58:CX:333:ILE:HG13	58:CX:375:TYR:HE2	1.85	0.42
58:CX:442:HIS:CD2	58:CX:445:ILE:HG22	2.55	0.42
55:UI:211:ALA:O	55:UI:215:MET:HG2	2.20	0.42
7:UJ:1349:ALA:O	7:UJ:1353:THR:HG23	2.19	0.42
8:UK:266:ARG:HH12	50:C1:205:C:N4	2.17	0.42
10:UM:476:THR:N	10:UM:522:ARG:HH12	2.18	0.42
17:UZ:288:THR:O	50:C1:2081:G:O2'	2.35	0.42
19:CC:212:ILE:HD13	19:CC:254:ILE:HG12	2.02	0.42
20:CD:217:ARG:NH2	20:CD:246:GLY:O	2.53	0.42
24:CI:520:LYS:NZ	32:CR:274:GLU:O	2.53	0.42
32:CR:747:LEU:HD13	32:CR:760:CYS:HB2	2.01	0.42
32:CS:29:VAL:HG23	32:CS:202:ILE:HG23	2.02	0.42
32:CS:384:GLU:O	32:CS:407:LEU:HD23	2.20	0.42
32:CS:658:VAL:HG21	32:CS:764:ARG:HD3	2.02	0.42
38:Ce:50:VAL:HG13	38:Ce:51:SER:H	1.85	0.42
52:CW:208:ALA:O	52:CW:216:LEU:O	2.38	0.42
54:UH:730:PHE:HE2	54:UH:738:LEU:HD22	1.85	0.42
59:CY:318:ALA:HA	59:CY:321:ILE:HD12	2.01	0.42
60:CZ:455:GLU:HA	60:CZ:458:MET:HE2	2.00	0.42
1:UA:541:GLU:O	1:UA:543:GLN:N	2.53	0.42
2:UB:65:ARG:NH1	50:C1:1752:U:O2	2.47	0.42
3:UC:642:LEU:HD23	16:UX:35:ARG:HB3	2.00	0.42
7:UJ:841:LEU:HA	7:UJ:844:GLU:HB2	2.02	0.42
10:UM:522:ARG:HG2	10:UM:537:SER:HA	2.02	0.42
10:UM:558:LEU:HD12	10:UM:570:ILE:HG13	2.01	0.42
12:UO:162:SER:HB3	12:UO:172:TRP:HE1	1.84	0.42
13:UQ:598:LEU:O	55:UE:33:THR:OG1	2.32	0.42
19:CC:13:VAL:HG21	19:CC:146:GLN:NE2	2.35	0.42
24:CI:739:TYR:CZ	24:CI:743:LYS:HD2	2.55	0.42
24:CI:823:HIS:CD2	24:CI:900:ALA:HA	2.55	0.42
25:CJ:72:ARG:HA	25:CJ:72:ARG:HD2	1.85	0.42
26:CK:123:ILE:HG12	26:CK:126:ASP:HB2	2.02	0.42
31:CQ:168:SER:OG	31:CQ:217:HIS:ND1	2.47	0.42
32:CR:425:SER:HA	32:CR:428:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CR:658:VAL:O	32:CR:662:GLU:HG2	2.19	0.42
32:CS:613:LEU:H	32:CS:634:ARG:HH22	1.68	0.42
32:CS:826:LYS:HE3	32:CS:930:ALA:HB3	2.01	0.42
35:Cb:115:THR:OG1	35:Cb:116:ASP:N	2.52	0.42
44:Ck:118:PRO:O	44:Ck:121:ARG:NH1	2.51	0.42
49:CU:282:ARG:HE	49:CU:287:ARG:HH22	1.68	0.42
53:UT:305:VAL:O	53:UT:309:VAL:HG23	2.20	0.42
53:UT:495:GLN:O	53:UT:499:VAL:HG23	2.19	0.42
53:UT:1165:ILE:HG13	53:UT:1166:SER:H	1.84	0.42
53:UT:1685:GLU:OE1	53:UT:1689:ASN:ND2	2.53	0.42
55:UE:185:ILE:HG21	55:UE:221:THR:HA	2.02	0.42
59:CY:21:THR:HB	60:CZ:369:THR:HG21	2.01	0.42
59:CY:57:PHE:HA	59:CY:60:LEU:HD23	2.02	0.42
2:UB:608:HIS:HB3	2:UB:611:CYS:HB3	2.01	0.42
2:UB:652:ARG:HD2	56:US:467:TYR:HA	2.02	0.42
4:UD:503:MET:HE2	4:UD:525:LYS:HB2	2.01	0.42
6:UG:348:VAL:HA	6:UG:357:ALA:O	2.20	0.42
9:UL:514:LEU:HA	9:UL:524:VAL:O	2.20	0.42
10:UM:62:GLU:HB3	10:UM:81:ARG:HB3	2.02	0.42
11:UN:275:ASP:HA	11:UN:278:ARG:HB2	2.02	0.42
20:CD:69:VAL:HG11	20:CD:102:LEU:HD11	2.02	0.42
20:CD:166:VAL:HG22	20:CD:303:ALA:HA	2.00	0.42
22:CG:339:LEU:HD23	22:CG:339:LEU:HA	1.81	0.42
25:CJ:64:LEU:HD11	27:CL:619:ILE:HG13	2.00	0.42
29:CN:164:GLN:HB3	50:C1:2158:G:H5'	2.01	0.42
32:CR:118:ASN:O	32:CR:142:THR:OG1	2.28	0.42
32:CR:544:TYR:HE1	32:CR:637:ARG:HG2	1.85	0.42
32:CS:35:LYS:H	32:CS:35:LYS:HG2	1.66	0.42
32:CS:133:PRO:HB2	32:CS:553:PRO:HB2	2.02	0.42
32:CS:385:LEU:HD13	32:CS:407:LEU:HG	2.02	0.42
35:Cb:85:GLY:N	35:Cb:88:ASP:OD2	2.53	0.42
36:Cc:35:TYR:CD1	36:Cc:54:PRO:HB3	2.54	0.42
43:Cj:107:GLN:O	43:Cj:111:GLN:HG3	2.20	0.42
50:C1:1238:C:H2'	50:C1:1239:G:H8	1.85	0.42
53:UT:393:ASN:O	53:UT:397:VAL:HG23	2.20	0.42
53:UT:901:LYS:HE2	53:UT:936:GLU:HB2	2.02	0.42
53:UT:1324:VAL:O	53:UT:1328:ILE:HD12	2.19	0.42
2:UB:570:ALA:HA	2:UB:573:MET:SD	2.60	0.41
3:UC:645:SER:HB3	18:CA:290:LEU:HB2	2.01	0.41
6:UG:579:ASP:O	6:UG:582:ARG:N	2.53	0.41
7:UJ:296:LEU:HD22	7:UJ:312:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:UJ:780:ASP:HA	7:UJ:812:ARG:HE	1.84	0.41
7:UJ:1106:GLY:HA2	7:UJ:1107:PRO:HD3	1.92	0.41
7:UJ:1312:LEU:HA	7:UJ:1315:VAL:HG12	2.02	0.41
7:UJ:1419:TYR:HA	7:UJ:1422:MET:HG3	2.01	0.41
7:UJ:1482:HIS:CD2	7:UJ:1522:LEU:HD13	2.55	0.41
10:UM:251:SER:OG	10:UM:252:ARG:N	2.53	0.41
10:UM:787:SER:HB3	10:UM:792:LYS:HD3	2.02	0.41
15:UU:176:ALA:O	15:UU:203:ARG:NH2	2.46	0.41
17:UZ:66:LEU:HD13	17:UZ:281:PHE:CZ	2.55	0.41
18:CA:194:ILE:HD11	19:CC:162:SER:HB3	2.02	0.41
20:CD:415:LYS:HB2	20:CD:415:LYS:HE2	1.88	0.41
24:CI:87:SER:HB3	24:CI:219:ILE:HG13	2.01	0.41
24:CI:546:MET:HE3	24:CI:546:MET:HB2	1.92	0.41
26:CK:217:PRO:HB3	27:CL:558:LEU:HD22	2.01	0.41
35:Cb:42:MET:HB3	35:Cb:109:PHE:HE2	1.83	0.41
36:Cc:99:ARG:NH1	50:C1:2111:U:OP1	2.34	0.41
37:Cd:71:ASN:OD1	37:Cd:71:ASN:N	2.52	0.41
41:Ch:117:LEU:HD21	41:Ch:121:ARG:HH21	1.85	0.41
50:C1:176:G:H2'	50:C1:177:G:H8	1.84	0.41
53:UT:498:ILE:O	53:UT:502:PHE:HB2	2.20	0.41
53:UT:582:PHE:HA	53:UT:585:TYR:CE1	2.55	0.41
53:UT:2188:ASP:O	53:UT:2191:THR:OG1	2.37	0.41
1:UA:86:ARG:O	1:UA:88:VAL:N	2.53	0.41
7:UJ:944:LEU:HD22	7:UJ:955:LEU:HD22	2.01	0.41
13:UQ:177:ASP:N	13:UQ:177:ASP:OD1	2.50	0.41
19:CC:304:PRO:HA	19:CC:307:GLN:HG2	2.02	0.41
21:CF:60:GLN:HA	21:CF:61:PRO:HA	1.92	0.41
23:CH:9:LEU:HD12	23:CH:9:LEU:HA	1.93	0.41
23:CH:293:ALA:HB3	23:CH:328:MET:HE1	2.02	0.41
32:CR:575:GLN:HG3	32:CR:578:ARG:HE	1.85	0.41
51:C2:135:U:H4'	51:C2:136:C:H4'	2.02	0.41
52:CW:316:TRP:CD1	52:CW:323:LEU:HA	2.55	0.41
53:UT:1368:ARG:NH1	53:UT:1369:GLN:HG3	2.35	0.41
53:UT:1395:LEU:O	53:UT:1399:VAL:HG22	2.19	0.41
58:CX:290:ASN:HA	58:CX:293:LYS:HB2	2.02	0.41
2:UB:116:ILE:HG13	23:CH:58:GLU:HG3	2.02	0.41
4:UD:451:VAL:H	4:UD:477:THR:HG21	1.85	0.41
6:UG:100:LEU:HD12	28:CM:3:ILE:HG12	2.02	0.41
7:UJ:931:PRO:HA	7:UJ:934:LEU:HD13	2.01	0.41
7:UJ:1703:VAL:HA	7:UJ:1706:VAL:HG22	2.03	0.41
9:UL:12:LYS:HD3	9:UL:457:GLN:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CG:269:ARG:HG2	22:CG:285:THR:HG22	2.02	0.41
35:Cb:71:LYS:HE3	35:Cb:71:LYS:HB3	1.77	0.41
41:Ch:147:SER:HA	41:Ch:150:VAL:HG22	2.02	0.41
47:Co:336:VAL:HG22	47:Co:363:ARG:HH21	1.85	0.41
50:C1:208:A:O2'	50:C1:209:A:O4'	2.32	0.41
52:CW:136:PRO:HG2	60:CZ:544:LEU:HG	2.01	0.41
53:UT:186:THR:O	53:UT:190:VAL:HG22	2.21	0.41
53:UT:1296:ILE:HD11	53:UT:1299:SER:HB3	2.01	0.41
53:UT:1398:TYR:HB3	53:UT:1414:ALA:HB3	2.02	0.41
53:UT:1937:ARG:HG3	53:UT:1938:LEU:HD12	2.02	0.41
53:UT:2188:ASP:N	53:UT:2188:ASP:OD1	2.50	0.41
56:US:208:LEU:HD11	56:US:223:VAL:HG21	2.02	0.41
1:UA:171:LYS:HB3	1:UA:171:LYS:HE2	1.72	0.41
3:UC:247:GLN:HB3	27:CL:88:GLN:HE21	1.86	0.41
7:UJ:256:SER:HB2	14:UR:230:LEU:HD23	2.02	0.41
7:UJ:699:SER:HB2	7:UJ:703:ARG:HG3	2.02	0.41
7:UJ:972:THR:O	7:UJ:976:ASN:HB2	2.20	0.41
7:UJ:1007:ALA:HA	7:UJ:1010:LEU:HG	2.02	0.41
7:UJ:1550:LEU:HA	7:UJ:1553:ILE:HG22	2.02	0.41
10:UM:135:ILE:HD12	10:UM:159:LEU:HD21	2.02	0.41
10:UM:453:LYS:HA	10:UM:481:SER:HB2	2.01	0.41
17:UZ:175:THR:HA	17:UZ:178:ARG:HG3	2.02	0.41
18:CB:130:TRP:HZ3	18:CB:141:ILE:HD12	1.86	0.41
21:CE:96:ARG:HA	21:CE:96:ARG:HD2	1.85	0.41
26:CK:229:THR:HG21	27:CL:545:ILE:HD11	2.01	0.41
29:CN:71:ASP:N	29:CN:71:ASP:OD1	2.54	0.41
53:UT:559:LEU:HD11	53:UT:578:THR:HA	2.03	0.41
53:UT:671:LEU:HD11	53:UT:690:MET:HB3	2.02	0.41
53:UT:1486:ILE:O	53:UT:1490:ILE:HG12	2.21	0.41
54:UH:75:SER:HB3	54:UH:78:SER:HB3	2.03	0.41
56:US:352:LEU:HA	56:US:352:LEU:HD23	1.85	0.41
2:UB:805:PRO:HB2	29:CN:24:HIS:CD2	2.55	0.41
4:UD:487:SER:HA	4:UD:554:PHE:CD2	2.56	0.41
7:UJ:1206:ILE:HG21	7:UJ:1259:LEU:HD12	2.03	0.41
10:UM:300:ILE:HG22	10:UM:310:THR:HG23	2.02	0.41
18:CB:165:THR:O	18:CB:168:SER:OG	2.31	0.41
20:CD:288:ASN:HB3	20:CD:372:SER:HB3	2.02	0.41
25:CJ:180:PHE:CD2	43:Cj:87:LYS:HD2	2.55	0.41
30:CP:302:PHE:HZ	60:CZ:543:LYS:HE2	1.85	0.41
32:CR:196:CYS:HB2	32:CR:489:TRP:CD1	2.55	0.41
32:CR:723:VAL:O	32:CR:763:ILE:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Ce:137:THR:O	38:Ce:140:VAL:C	2.64	0.41
47:Co:380:LYS:NZ	53:UT:49:HIS:HA	2.34	0.41
50:C1:278:A:OP2	50:C1:278:A:H8	2.03	0.41
53:UT:801:CYS:O	53:UT:805:ILE:HG12	2.21	0.41
53:UT:1621:ARG:NH1	53:UT:1689:ASN:O	2.38	0.41
56:US:414:THR:HB	56:US:417:MET:HE2	2.03	0.41
58:CX:303:PHE:O	58:CX:307:LEU:HG	2.20	0.41
2:UB:742:LYS:HD2	2:UB:742:LYS:HA	1.92	0.41
3:UC:250:ALA:HB1	3:UC:260:VAL:HG22	2.02	0.41
4:UD:378:PRO:HA	4:UD:841:ILE:HG22	2.02	0.41
5:UF:96:PHE:CD1	5:UF:113:TYR:HB2	2.56	0.41
5:UF:186:MET:HE2	5:UF:279:PRO:HG2	2.03	0.41
6:UG:572:GLN:HG3	6:UG:582:ARG:HD2	2.03	0.41
10:UM:398:ILE:HD11	10:UM:436:VAL:HG11	2.02	0.41
12:UO:235:ILE:HD13	12:UO:251:SER:HB3	2.03	0.41
15:UU:941:ILE:HG13	15:UU:981:ARG:HD3	2.02	0.41
20:CD:439:LYS:HE3	20:CD:439:LYS:HB3	1.91	0.41
22:CG:487:ILE:HD13	22:CG:580:VAL:HG21	2.03	0.41
24:CI:968:LYS:HD2	24:CI:968:LYS:HA	1.76	0.41
32:CR:399:VAL:HA	32:CR:402:LEU:HB2	2.02	0.41
32:CS:491:ASN:HD21	32:CS:497:ASP:HB2	1.85	0.41
38:Ce:21:ASP:OD1	38:Ce:22:LEU:N	2.54	0.41
44:Ck:77:THR:HG22	44:Ck:129:VAL:HG22	2.03	0.41
53:UT:43:LEU:HD11	53:UT:169:ALA:HB1	2.02	0.41
53:UT:497:GLN:O	53:UT:501:LYS:HG2	2.21	0.41
53:UT:558:LYS:HD2	53:UT:561:LEU:HD21	2.02	0.41
53:UT:618:GLN:HA	53:UT:621:LEU:HG	2.01	0.41
55:UE:228:ALA:HA	55:UE:231:THR:HG22	2.03	0.41
60:CZ:328:ARG:HE	60:CZ:494:PHE:HE2	1.68	0.41
2:UB:713:LEU:HD13	2:UB:717:GLU:HB2	2.03	0.41
7:UJ:634:ALA:HA	7:UJ:643:THR:HG22	2.03	0.41
10:UM:701:VAL:HG12	10:UM:708:LEU:HD23	2.03	0.41
13:UQ:109:THR:HG22	13:UQ:129:LEU:HG	2.03	0.41
14:UR:49:ASP:OD1	14:UR:50:ALA:N	2.54	0.41
17:UZ:267:VAL:HG11	17:UZ:275:TRP:CE2	2.55	0.41
21:CE:58:ASP:O	21:CE:85:LYS:NZ	2.53	0.41
30:CP:195:ILE:HG23	49:CU:161:LEU:HD21	2.01	0.41
32:CR:35:LYS:HB3	32:CR:95:PHE:CD1	2.55	0.41
32:CS:158:SER:HB2	32:CS:691:GLY:HA3	2.01	0.41
35:Cb:98:ASN:HD22	35:Cb:115:THR:C	2.28	0.41
50:C1:723:A:N6	50:C1:759:G:O2'	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:C1:2358:U:H3	50:C1:2369:G:H1	1.69	0.41
53:UT:332:CYS:O	53:UT:335:GLN:NE2	2.54	0.41
53:UT:1132:VAL:O	53:UT:1136:THR:HG22	2.20	0.41
4:UD:319:ARG:NH2	50:C1:66:G:OP1	2.53	0.41
4:UD:432:THR:HG23	4:UD:448:PRO:HD3	2.01	0.41
5:UF:283:PHE:CZ	5:UF:320:VAL:HG23	2.55	0.41
7:UJ:1057:ILE:HG22	7:UJ:1105:LEU:HD21	2.02	0.41
7:UJ:1504:GLY:HA2	7:UJ:1507:LEU:HD23	2.03	0.41
7:UJ:1647:TRP:O	7:UJ:1651:LEU:HG	2.20	0.41
10:UM:435:ILE:HD11	34:Ca:18:LYS:HG2	2.03	0.41
17:UZ:158:ARG:NH2	17:UZ:184:LEU:O	2.54	0.41
18:CA:184:GLU:O	18:CA:207:VAL:HA	2.20	0.41
18:CB:247:LEU:O	20:CD:120:ARG:NH1	2.41	0.41
22:CG:330:GLN:HB2	22:CG:351:ASP:HB3	2.02	0.41
33:CT:117:MET:HE3	33:CT:174:TYR:CD1	2.55	0.41
39:Cf:176:ARG:O	39:Cf:180:SER:N	2.39	0.41
53:UT:336:VAL:O	53:UT:340:ARG:HG2	2.21	0.41
53:UT:1303:GLN:HB2	53:UT:1347:LEU:HD21	2.02	0.41
53:UT:1397:SER:HB3	53:UT:1414:ALA:HB2	2.03	0.41
54:UH:301:THR:O	54:UH:303:ARG:NH1	2.53	0.41
56:US:124:VAL:O	56:US:127:SER:OG	2.26	0.41
58:CX:264:ARG:O	58:CX:268:MET:HG3	2.21	0.41
2:UB:5:GLN:OE1	26:CK:255:SER:OG	2.39	0.41
2:UB:641:ILE:HD13	2:UB:641:ILE:HA	1.92	0.41
4:UD:673:ASN:O	4:UD:673:ASN:ND2	2.53	0.41
7:UJ:908:LEU:O	7:UJ:912:LEU:HG	2.21	0.41
7:UJ:1111:LEU:HD11	7:UJ:1135:LEU:HD13	2.02	0.41
7:UJ:1112:PHE:CE1	7:UJ:1154:LEU:HD23	2.56	0.41
9:UL:23:ASN:N	9:UL:23:ASN:OD1	2.54	0.41
9:UL:569:LEU:HD11	9:UL:585:LEU:HD12	2.02	0.41
9:UL:839:PRO:HB3	9:UL:876:ARG:HH12	1.85	0.41
10:UM:258:LEU:O	10:UM:268:GLY:HA2	2.21	0.41
12:UO:429:ARG:NH2	50:C1:73:A:OP2	2.54	0.41
13:UQ:238:ASP:N	13:UQ:238:ASP:OD1	2.54	0.41
13:UQ:620:ASP:HA	13:UQ:621:PRO:HD3	1.93	0.41
13:UQ:670:PRO:HD2	13:UQ:713:VAL:HG21	2.03	0.41
13:UQ:710:ALA:HB3	13:UQ:730:PHE:HD2	1.85	0.41
13:UQ:782:VAL:HG12	13:UQ:789:PHE:HB3	2.03	0.41
14:UR:274:LYS:HD3	14:UR:274:LYS:HA	1.76	0.41
15:UU:42:GLY:HA2	15:UU:420:TRP:CH2	2.56	0.41
15:UU:103:ARG:HG2	15:UU:123:GLN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:UU:424:ARG:HA	50:C1:259:U:C2	2.56	0.41
23:CH:110:ILE:HD12	23:CH:110:ILE:HA	1.87	0.41
24:CI:899:ILE:HD13	24:CI:899:ILE:HG21	1.88	0.41
26:CK:164:MET:HB2	26:CK:267:SER:HB3	2.03	0.41
29:CO:77:MET:SD	29:CO:82:ARG:HB3	2.61	0.41
30:CP:126:ILE:HG13	30:CP:136:PHE:HE1	1.85	0.41
32:CR:513:PRO:HB3	32:CR:652:LYS:HD3	2.02	0.41
32:CS:139:THR:O	32:CS:143:VAL:HG23	2.21	0.41
34:Ca:204:ILE:O	50:C1:1648:G:O2'	2.39	0.41
47:Co:386:VAL:HG22	47:Co:406:ILE:HD13	2.03	0.41
50:C1:81:G:H1	50:C1:126:C:H42	1.69	0.41
50:C1:801:A:N3	53:UT:1322:PRO:HB2	2.35	0.41
50:C1:1038:A:N7	53:UT:25:HIS:HB2	2.36	0.41
50:C1:1644:U:O2'	50:C1:1645:U:O2	2.30	0.41
53:UT:126:VAL:HA	53:UT:129:PHE:CE2	2.56	0.41
53:UT:298:TRP:HA	53:UT:301:VAL:HB	2.03	0.41
53:UT:365:ASN:HA	53:UT:368:LEU:HG	2.03	0.41
53:UT:1498:SER:HB3	53:UT:1501:VAL:HG22	2.02	0.41
53:UT:1760:LYS:O	53:UT:1764:ILE:HG12	2.21	0.41
54:UH:477:ASN:HA	54:UH:480:MET:HE2	2.03	0.41
54:UH:592:LYS:HE2	54:UH:592:LYS:HB3	1.85	0.41
59:CY:43:VAL:HG11	60:CZ:421:VAL:HG11	2.03	0.41
4:UD:557:ASP:OD1	4:UD:557:ASP:N	2.53	0.41
4:UD:671:ARG:NE	7:UJ:665:GLU:OE2	2.55	0.41
6:UG:256:THR:O	6:UG:256:THR:OG1	2.37	0.41
7:UJ:7:GLN:HG2	20:CD:422:ASN:HB2	2.03	0.41
7:UJ:962:VAL:HG23	7:UJ:963:LEU:HD12	2.03	0.41
7:UJ:1667:GLN:NE2	7:UJ:1713:VAL:HG22	2.36	0.41
9:UL:119:ASP:OD1	9:UL:119:ASP:N	2.49	0.41
9:UL:643:LYS:HG2	9:UL:686:PHE:HB3	2.03	0.41
12:UO:513:VAL:HG23	54:UH:869:LEU:HD13	2.02	0.41
13:UQ:606:HIS:HB3	13:UQ:632:ASP:HB2	2.03	0.41
14:UR:331:VAL:HG22	14:UR:378:VAL:HG21	2.03	0.41
15:UU:415:ARG:NE	15:UU:458:GLU:O	2.54	0.41
16:UX:154:LYS:HG2	16:UX:165:ILE:HD13	2.02	0.41
19:CC:209:LEU:HA	19:CC:209:LEU:HD12	1.88	0.41
24:CI:764:GLN:HA	24:CI:768:VAL:HB	2.02	0.41
24:CI:832:PRO:HG2	24:CI:1015:LEU:HD12	2.03	0.41
30:CP:94:LYS:HB3	30:CP:115:LEU:HD23	2.03	0.41
32:CS:239:ILE:HG23	32:CS:243:LEU:HD12	2.04	0.41
32:CS:323:LEU:O	32:CS:327:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CS:545:VAL:HA	32:CS:548:HIS:ND1	2.36	0.41
34:Ca:72:ASP:OD1	34:Ca:72:ASP:N	2.53	0.41
50:C1:331:C:N4	50:C1:332:U:O4	2.54	0.41
50:C1:468:C:O2'	50:C1:469:G:O4'	2.39	0.41
50:C1:1243:C:H2'	50:C1:1244:G:C8	2.56	0.41
52:CW:277:ARG:HH11	59:CY:123:ARG:HH21	1.69	0.41
54:UH:346:TYR:HA	54:UH:355:LEU:O	2.21	0.41
56:US:385:LEU:HD23	56:US:388:LEU:HD12	2.03	0.41
1:UA:126:SER:OG	1:UA:131:ASN:OD1	2.27	0.40
6:UG:213:LEU:HB3	6:UG:216:HIS:CD2	2.56	0.40
6:UG:295:LYS:HE3	6:UG:295:LYS:HB2	1.92	0.40
7:UJ:1239:LYS:HG2	7:UJ:1240:THR:HG23	2.03	0.40
16:UX:67:ARG:HD2	16:UX:149:ASN:ND2	2.36	0.40
19:CC:40:THR:HG22	19:CC:42:ASP:H	1.86	0.40
20:CD:5:ILE:HD12	20:CD:118:LEU:HD21	2.02	0.40
22:CG:356:TYR:HB3	22:CG:365:LEU:HB2	2.03	0.40
22:CG:556:VAL:HG12	22:CG:602:VAL:HG21	2.03	0.40
24:CI:71:VAL:HG22	24:CI:135:ILE:HB	2.03	0.40
24:CI:962:ILE:HG12	24:CI:973:PHE:CE1	2.56	0.40
29:CN:67:LEU:HD23	29:CN:89:PRO:HB3	2.02	0.40
29:CO:32:LYS:HD3	29:CO:36:ARG:HH22	1.86	0.40
32:CR:402:LEU:O	32:CR:406:TYR:OH	2.33	0.40
32:CR:518:LEU:HD11	32:CR:653:ALA:HA	2.03	0.40
32:CR:634:ARG:HA	32:CR:724:GLY:O	2.22	0.40
35:Cb:48:VAL:HG21	35:Cb:65:MET:HE1	2.04	0.40
37:Cd:33:GLY:CA	37:Cd:52:ILE:O	2.70	0.40
37:Cd:188:GLN:HA	37:Cd:191:ARG:HG2	2.03	0.40
43:Cj:97:VAL:HG12	43:Cj:98:ASP:H	1.86	0.40
50:C1:747:G:OP2	50:C1:747:G:N2	2.40	0.40
50:C1:2046:C:H2'	50:C1:2047:G:C8	2.56	0.40
52:CW:37:TYR:HD2	52:CW:39:PRO:HD3	1.86	0.40
53:UT:1040:LEU:HD11	53:UT:1076:LEU:HD21	2.03	0.40
53:UT:1877:LEU:HG	53:UT:1889:ILE:HD13	2.02	0.40
54:UH:417:PRO:HB2	54:UH:420:ARG:HG3	2.04	0.40
55:UE:197:LEU:HD11	55:UE:229:LEU:HD21	2.03	0.40
58:CX:373:LYS:HD2	58:CX:373:LYS:HA	1.84	0.40
60:CZ:414:VAL:HA	60:CZ:417:HIS:CE1	2.56	0.40
1:UA:530:LEU:HD12	1:UA:574:ASN:ND2	2.36	0.40
7:UJ:552:LEU:HD22	7:UJ:632:TRP:CZ3	2.54	0.40
10:UM:432:HIS:CE1	10:UM:458:ARG:HD2	2.56	0.40
13:UQ:189:ASP:OD1	13:UQ:190:MET:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:UQ:359:HIS:HA	13:UQ:448:LYS:HD3	2.03	0.40
20:CD:135:PRO:HA	20:CD:138:PHE:HD2	1.86	0.40
22:CG:172:THR:OG1	22:CG:585:GLU:OE1	2.29	0.40
23:CH:153:PHE:O	23:CH:157:VAL:HG22	2.22	0.40
28:CM:88:ASP:OD1	28:CM:88:ASP:N	2.46	0.40
32:CS:266:LEU:HD23	32:CS:266:LEU:HA	1.93	0.40
35:Cb:61:THR:O	35:Cb:65:MET:HG2	2.21	0.40
52:CW:310:LYS:HA	52:CW:333:LEU:HB2	2.04	0.40
53:UT:1207:LEU:HA	53:UT:1210:ILE:HG22	2.02	0.40
53:UT:1214:LEU:HD13	53:UT:1227:ALA:HB3	2.04	0.40
53:UT:1893:LEU:HD21	53:UT:1962:MET:HE1	2.03	0.40
55:UE:200:LEU:HD13	55:UE:218:ILE:HG13	2.03	0.40
55:UI:228:ALA:O	55:UI:232:GLN:OE1	2.38	0.40
6:UG:578:ILE:HG23	6:UG:578:ILE:HD12	1.82	0.40
7:UJ:726:LEU:O	7:UJ:730:LEU:HB2	2.22	0.40
8:UK:261:ARG:HE	8:UK:261:ARG:HB3	1.55	0.40
9:UL:121:THR:HG23	9:UL:123:VAL:HG23	2.04	0.40
29:CN:121:LEU:HD12	29:CN:121:LEU:HA	1.88	0.40
30:CP:58:VAL:HA	30:CP:112:LEU:HD21	2.03	0.40
32:CR:312:ILE:HG23	32:CR:371:TYR:HA	2.01	0.40
32:CR:829:LEU:HA	32:CR:832:LEU:HB3	2.03	0.40
33:CT:109:LEU:HA	33:CT:112:ARG:HG3	2.03	0.40
40:Cg:131:HIS:CE1	50:C1:1097:U:H5'	2.57	0.40
44:Ck:71:ILE:HG23	50:C1:830:G:H22	1.86	0.40
47:Co:365:ASN:ND2	50:C1:1105:A:N3	2.69	0.40
53:UT:539:LYS:HE2	53:UT:539:LYS:HB3	1.93	0.40
53:UT:1153:TRP:HA	53:UT:1156:TYR:HD2	1.85	0.40
53:UT:1235:ILE:HG21	53:UT:1292:PHE:HA	2.03	0.40
54:UH:307:LEU:HD11	54:UH:327:PHE:HE2	1.86	0.40
56:US:361:PHE:HD1	56:US:361:PHE:HA	1.74	0.40
58:CX:240:ASP:OD1	58:CX:240:ASP:N	2.55	0.40
58:CX:266:MET:O	58:CX:270:ILE:HB	2.21	0.40
1:UA:195:ARG:O	6:UG:278:GLN:NE2	2.53	0.40
2:UB:571:TYR:CG	2:UB:597:ILE:HD11	2.57	0.40
7:UJ:1723:ASN:HD21	7:UJ:1756:TRP:HZ3	1.70	0.40
10:UM:585:HIS:NE2	10:UM:617:THR:OG1	2.42	0.40
10:UM:610:SER:O	50:C1:2243:A:O2'	2.39	0.40
13:UQ:127:LEU:HD23	13:UQ:127:LEU:HA	1.94	0.40
13:UQ:615:PHE:N	13:UQ:629:ILE:O	2.52	0.40
14:UR:283:HIS:HB2	14:UR:288:ILE:HB	2.02	0.40
23:CH:152:THR:O	23:CH:156:ALA:CB	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:CH:328:MET:HE3	23:CH:330:ALA:HB3	2.04	0.40
32:CR:774:TRP:CD1	32:CR:774:TRP:H	2.37	0.40
32:CS:548:HIS:HE2	32:CS:637:ARG:HD3	1.85	0.40
32:CS:614:ILE:HG13	32:CS:615:PRO:HD3	2.03	0.40
38:Ce:140:VAL:HB	38:Ce:143:VAL:HG23	2.04	0.40
47:Co:415:LYS:HB2	53:UT:25:HIS:NE2	2.37	0.40
53:UT:208:ALA:HB3	53:UT:257:THR:HG23	2.04	0.40
53:UT:306:ILE:HD12	53:UT:341:VAL:HG13	2.03	0.40
53:UT:505:LEU:HB2	53:UT:531:TYR:CE1	2.55	0.40
58:CX:288:LEU:HD23	58:CX:292:LEU:HD23	2.02	0.40
7:UJ:1254:ASN:C	7:UJ:1254:ASN:HD22	2.28	0.40
7:UJ:1317:ARG:HH12	7:UJ:1353:THR:HG22	1.86	0.40
8:UK:162:ILE:HG12	61:UP:319:ALA:HB3	2.04	0.40
9:UL:608:LEU:HB3	9:UL:627:ALA:HB3	2.03	0.40
9:UL:889:ILE:HG12	9:UL:895:MET:SD	2.62	0.40
10:UM:592:VAL:HG22	10:UM:617:THR:HG22	2.03	0.40
18:CA:213:PRO:HG2	18:CA:245:LEU:HD12	2.04	0.40
18:CB:137:LEU:HA	18:CB:301:MET:HE1	2.03	0.40
20:CD:85:LYS:HD3	20:CD:85:LYS:HA	1.96	0.40
29:CN:140:LEU:HD11	29:CN:150:ILE:HG21	2.03	0.40
29:CO:218:ASP:OD1	29:CO:218:ASP:N	2.55	0.40
30:CP:41:THR:HG22	30:CP:99:ILE:HG22	2.03	0.40
32:CR:621:GLN:HE22	32:CS:853:VAL:HG22	1.86	0.40
32:CS:377:ALA:HB3	32:CS:401:LYS:HD3	2.04	0.40
32:CS:727:TYR:OH	32:CS:762:MET:HE2	2.21	0.40
32:CS:851:TYR:O	32:CS:855:LEU:HG	2.22	0.40
40:Cg:171:ARG:HE	50:C1:1095:A:H5'	1.85	0.40
52:CW:84:THR:HB	52:CW:368:TRP:CD2	2.56	0.40
53:UT:731:PRO:HB3	53:UT:766:LEU:HD22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	UA	834/904 (92%)	803 (96%)	31 (4%)	0	100	100
2	UB	556/907 (61%)	538 (97%)	18 (3%)	0	100	100
3	UC	201/648 (31%)	194 (96%)	7 (4%)	0	100	100
4	UD	761/884 (86%)	726 (95%)	35 (5%)	0	100	100
5	UF	325/414 (78%)	317 (98%)	8 (2%)	0	100	100
6	UG	475/558 (85%)	458 (96%)	16 (3%)	1 (0%)	43	72
7	UJ	1599/1802 (89%)	1521 (95%)	77 (5%)	1 (0%)	48	77
8	UK	211/270 (78%)	210 (100%)	1 (0%)	0	100	100
9	UL	767/962 (80%)	728 (95%)	39 (5%)	0	100	100
10	UM	835/912 (92%)	797 (95%)	38 (5%)	0	100	100
11	UN	171/700 (24%)	167 (98%)	4 (2%)	0	100	100
12	UO	497/557 (89%)	477 (96%)	19 (4%)	1 (0%)	43	72
13	UQ	775/960 (81%)	734 (95%)	40 (5%)	1 (0%)	48	77
14	UR	436/618 (71%)	426 (98%)	10 (2%)	0	100	100
15	UU	896/1049 (85%)	857 (96%)	39 (4%)	0	100	100
16	UX	188/193 (97%)	180 (96%)	8 (4%)	0	100	100
17	UZ	229/391 (59%)	214 (93%)	15 (7%)	0	100	100
18	CA	238/313 (76%)	225 (94%)	13 (6%)	0	100	100
18	CB	235/313 (75%)	221 (94%)	14 (6%)	0	100	100
19	CC	383/523 (73%)	370 (97%)	13 (3%)	0	100	100
20	CD	444/582 (76%)	431 (97%)	13 (3%)	0	100	100
21	CE	119/127 (94%)	114 (96%)	5 (4%)	0	100	100
21	CF	118/127 (93%)	115 (98%)	3 (2%)	0	100	100
22	CG	402/630 (64%)	384 (96%)	18 (4%)	0	100	100
23	CH	383/411 (93%)	371 (97%)	12 (3%)	0	100	100
24	CI	829/1163 (71%)	804 (97%)	24 (3%)	1 (0%)	48	77
25	CJ	177/183 (97%)	176 (99%)	1 (1%)	0	100	100
26	CK	295/297 (99%)	285 (97%)	10 (3%)	0	100	100
27	CL	310/658 (47%)	298 (96%)	11 (4%)	1 (0%)	36	65
28	CM	443/446 (99%)	427 (96%)	16 (4%)	0	100	100
29	CN	222/252 (88%)	213 (96%)	9 (4%)	0	100	100
29	CO	211/252 (84%)	203 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	CP	227/322 (70%)	220 (97%)	7 (3%)	0	100	100
31	CQ	178/259 (69%)	177 (99%)	1 (1%)	0	100	100
32	CR	836/1073 (78%)	804 (96%)	32 (4%)	0	100	100
32	CS	826/1073 (77%)	785 (95%)	41 (5%)	0	100	100
33	CT	127/203 (63%)	119 (94%)	8 (6%)	0	100	100
34	Ca	223/255 (88%)	210 (94%)	13 (6%)	0	100	100
35	Cb	230/264 (87%)	215 (94%)	15 (6%)	0	100	100
36	Cc	188/212 (89%)	180 (96%)	7 (4%)	1 (0%)	24	54
37	Cd	224/239 (94%)	219 (98%)	5 (2%)	0	100	100
38	Ce	155/203 (76%)	143 (92%)	12 (8%)	0	100	100
39	Cf	170/202 (84%)	167 (98%)	3 (2%)	0	100	100
40	Cg	157/190 (83%)	152 (97%)	5 (3%)	0	100	100
41	Ch	64/151 (42%)	63 (98%)	1 (2%)	0	100	100
42	Ci	113/150 (75%)	109 (96%)	4 (4%)	0	100	100
43	Cj	124/143 (87%)	117 (94%)	7 (6%)	0	100	100
44	Ck	127/161 (79%)	123 (97%)	4 (3%)	0	100	100
45	Cm	122/130 (94%)	116 (95%)	6 (5%)	0	100	100
46	Cn	92/145 (63%)	90 (98%)	2 (2%)	0	100	100
47	Co	90/136 (66%)	78 (87%)	11 (12%)	1 (1%)	11	36
48	Cp	59/68 (87%)	53 (90%)	6 (10%)	0	100	100
49	CU	168/311 (54%)	164 (98%)	4 (2%)	0	100	100
52	CW	381/668 (57%)	358 (94%)	23 (6%)	0	100	100
53	UT	1981/2612 (76%)	1874 (95%)	98 (5%)	9 (0%)	24	54
54	UH	787/930 (85%)	763 (97%)	23 (3%)	1 (0%)	48	77
55	UE	172/410 (42%)	158 (92%)	14 (8%)	0	100	100
55	UI	126/410 (31%)	120 (95%)	6 (5%)	0	100	100
56	US	443/549 (81%)	423 (96%)	19 (4%)	1 (0%)	43	72
57	Cl	78/156 (50%)	72 (92%)	6 (8%)	0	100	100
58	CX	265/480 (55%)	247 (93%)	18 (7%)	0	100	100
59	CY	258/381 (68%)	252 (98%)	6 (2%)	0	100	100
60	CZ	279/609 (46%)	270 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	UP	52/364 (14%)	48 (92%)	4 (8%)	0	100	100
All	All	23887/32465 (74%)	22873 (96%)	995 (4%)	19 (0%)	49	77

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
53	UT	200	PRO
53	UT	678	ASP
53	UT	1202	VAL
6	UG	56	PRO
12	UO	130	GLN
36	Cc	88	GLY
53	UT	274	ALA
53	UT	686	ALA
53	UT	1166	SER
56	US	241	GLU
53	UT	28	GLU
54	UH	754	ARG
7	UJ	1263	GLU
24	CI	367	VAL
13	UQ	447	SER
47	Co	367	SER
27	CL	640	PRO
53	UT	1724	PRO
53	UT	479	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	UA	662/774 (86%)	662 (100%)	0	100	100
2	UB	474/788 (60%)	473 (100%)	1 (0%)	87	96
3	UC	176/536 (33%)	176 (100%)	0	100	100
4	UD	657/738 (89%)	656 (100%)	1 (0%)	87	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	UF	250/341 (73%)	250 (100%)	0	100	100
6	UG	386/474 (81%)	386 (100%)	0	100	100
7	UJ	1364/1526 (89%)	1364 (100%)	0	100	100
8	UK	162/227 (71%)	162 (100%)	0	100	100
9	UL	667/821 (81%)	667 (100%)	0	100	100
10	UM	712/770 (92%)	712 (100%)	0	100	100
11	UN	146/568 (26%)	146 (100%)	0	100	100
12	UO	403/456 (88%)	403 (100%)	0	100	100
13	UQ	651/817 (80%)	651 (100%)	0	100	100
14	UR	360/523 (69%)	360 (100%)	0	100	100
15	UU	677/863 (78%)	675 (100%)	2 (0%)	86	96
16	UX	152/167 (91%)	152 (100%)	0	100	100
17	UZ	186/329 (56%)	186 (100%)	0	100	100
18	CA	175/228 (77%)	175 (100%)	0	100	100
18	CB	195/228 (86%)	195 (100%)	0	100	100
19	CC	287/435 (66%)	287 (100%)	0	100	100
20	CD	344/489 (70%)	344 (100%)	0	100	100
21	CE	91/108 (84%)	91 (100%)	0	100	100
21	CF	88/108 (82%)	88 (100%)	0	100	100
22	CG	331/525 (63%)	331 (100%)	0	100	100
23	CH	303/320 (95%)	303 (100%)	0	100	100
24	CI	681/1009 (68%)	681 (100%)	0	100	100
25	CJ	147/169 (87%)	147 (100%)	0	100	100
26	CK	245/266 (92%)	245 (100%)	0	100	100
27	CL	251/535 (47%)	251 (100%)	0	100	100
28	CM	364/383 (95%)	364 (100%)	0	100	100
29	CN	202/223 (91%)	202 (100%)	0	100	100
29	CO	193/223 (86%)	193 (100%)	0	100	100
30	CP	202/287 (70%)	202 (100%)	0	100	100
31	CQ	151/215 (70%)	151 (100%)	0	100	100
32	CR	731/916 (80%)	731 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	CS	722/916 (79%)	722 (100%)	0	100	100
33	CT	108/167 (65%)	108 (100%)	0	100	100
34	Ca	198/223 (89%)	198 (100%)	0	100	100
35	Cb	199/221 (90%)	199 (100%)	0	100	100
36	Cc	149/178 (84%)	149 (100%)	0	100	100
37	Cd	192/204 (94%)	192 (100%)	0	100	100
38	Ce	137/177 (77%)	137 (100%)	0	100	100
39	Cf	139/164 (85%)	139 (100%)	0	100	100
40	Cg	123/162 (76%)	123 (100%)	0	100	100
41	Ch	58/130 (45%)	58 (100%)	0	100	100
42	Ci	78/117 (67%)	78 (100%)	0	100	100
43	Cj	92/115 (80%)	92 (100%)	0	100	100
44	Ck	117/143 (82%)	116 (99%)	1 (1%)	70	90
45	Cm	103/113 (91%)	103 (100%)	0	100	100
46	Cn	70/116 (60%)	70 (100%)	0	100	100
47	Co	79/115 (69%)	79 (100%)	0	100	100
48	Cp	47/61 (77%)	47 (100%)	0	100	100
49	CU	137/260 (53%)	137 (100%)	0	100	100
52	CW	310/587 (53%)	310 (100%)	0	100	100
53	UT	1725/2276 (76%)	1725 (100%)	0	100	100
54	UH	674/788 (86%)	674 (100%)	0	100	100
55	UE	148/346 (43%)	148 (100%)	0	100	100
55	UI	108/346 (31%)	108 (100%)	0	100	100
56	US	404/493 (82%)	404 (100%)	0	100	100
57	Cl	71/135 (53%)	71 (100%)	0	100	100
58	CX	227/411 (55%)	227 (100%)	0	100	100
59	CY	225/322 (70%)	225 (100%)	0	100	100
60	CZ	238/519 (46%)	238 (100%)	0	100	100
61	UP	44/314 (14%)	44 (100%)	0	100	100
All	All	19988/27504 (73%)	19983 (100%)	5 (0%)	100	100

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	UB	43	GLN
4	UD	673	ASN
15	UU	191	ASN
15	UU	885	GLN
44	Ck	97	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (186) such sidechains are listed below:

Mol	Chain	Res	Type
1	UA	110	HIS
1	UA	147	HIS
1	UA	156	HIS
1	UA	337	GLN
1	UA	459	GLN
1	UA	510	GLN
1	UA	533	GLN
1	UA	592	ASN
1	UA	626	ASN
2	UB	483	GLN
2	UB	490	ASN
2	UB	511	HIS
2	UB	528	GLN
2	UB	606	HIS
2	UB	663	ASN
2	UB	789	GLN
2	UB	857	GLN
3	UC	597	GLN
4	UD	277	GLN
4	UD	673	ASN
5	UF	35	ASN
5	UF	319	HIS
5	UF	330	ASN
6	UG	190	GLN
6	UG	266	GLN
6	UG	452	ASN
6	UG	572	GLN
7	UJ	11	GLN
7	UJ	250	GLN
7	UJ	909	GLN
7	UJ	1281	GLN
7	UJ	1667	GLN
8	UK	23	GLN
8	UK	244	GLN

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Mol	Chain	Res	Type
9	UL	151	HIS
9	UL	262	GLN
9	UL	504	ASN
9	UL	661	ASN
9	UL	688	GLN
9	UL	706	HIS
9	UL	832	ASN
9	UL	870	ASN
9	UL	886	HIS
10	UM	267	GLN
10	UM	274	HIS
10	UM	455	ASN
10	UM	501	ASN
10	UM	505	HIS
10	UM	644	ASN
10	UM	706	ASN
10	UM	743	GLN
11	UN	348	HIS
12	UO	24	GLN
12	UO	145	GLN
12	UO	271	ASN
12	UO	296	HIS
13	UQ	142	HIS
13	UQ	487	GLN
14	UR	348	HIS
14	UR	472	ASN
14	UR	553	GLN
14	UR	561	HIS
15	UU	81	ASN
15	UU	191	ASN
15	UU	727	GLN
15	UU	740	HIS
15	UU	886	ASN
15	UU	1014	GLN
16	UX	49	ASN
17	UZ	22	GLN
17	UZ	90	ASN
17	UZ	150	HIS
18	CA	277	GLN
18	CB	76	HIS
19	CC	22	HIS
19	CC	146	GLN

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Mol	Chain	Res	Type
19	CC	242	ASN
19	CC	246	GLN
19	CC	264	GLN
19	CC	307	GLN
19	CC	394	ASN
20	CD	28	ASN
20	CD	91	HIS
20	CD	219	ASN
20	CD	357	ASN
21	CE	26	GLN
22	CG	256	GLN
22	CG	341	GLN
23	CH	49	HIS
23	CH	177	GLN
23	CH	405	ASN
24	CI	55	HIS
24	CI	282	GLN
24	CI	350	HIS
24	CI	747	GLN
24	CI	749	GLN
24	CI	767	GLN
24	CI	1070	GLN
25	CJ	39	GLN
26	CK	5	GLN
26	CK	168	HIS
26	CK	232	ASN
27	CL	88	GLN
27	CL	143	GLN
27	CL	476	HIS
27	CL	662	GLN
28	CM	446	GLN
29	CN	23	GLN
29	CN	93	HIS
29	CN	199	ASN
29	CO	69	ASN
29	CO	170	HIS
30	CP	215	HIS
32	CR	170	HIS
32	CR	339	HIS
32	CR	522	ASN
32	CR	538	GLN
32	CR	770	ASN

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Mol	Chain	Res	Type
32	CR	890	GLN
32	CS	261	GLN
32	CS	370	GLN
32	CS	587	GLN
32	CS	734	HIS
32	CS	749	GLN
32	CS	770	ASN
34	Ca	211	HIS
35	Cb	130	GLN
35	Cb	216	ASN
36	Cc	211	ASN
37	Cd	10	ASN
38	Ce	74	GLN
38	Ce	81	GLN
38	Ce	197	GLN
39	Cf	44	HIS
39	Cf	64	ASN
40	Cg	137	GLN
43	Cj	8	GLN
43	Cj	107	GLN
44	Ck	18	HIS
44	Ck	22	ASN
44	Ck	132	GLN
45	Cm	80	ASN
46	Cn	89	ASN
52	CW	107	GLN
52	CW	116	GLN
52	CW	147	GLN
52	CW	183	GLN
52	CW	284	GLN
52	CW	374	ASN
53	UT	38	HIS
53	UT	140	HIS
53	UT	333	GLN
53	UT	436	GLN
53	UT	495	GLN
53	UT	497	GLN
53	UT	544	HIS
53	UT	658	ASN
53	UT	709	HIS
53	UT	768	ASN
53	UT	896	ASN

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Mol	Chain	Res	Type
53	UT	978	GLN
53	UT	1017	HIS
53	UT	1026	GLN
53	UT	1233	ASN
53	UT	1259	ASN
53	UT	1274	GLN
53	UT	1437	ASN
53	UT	1562	ASN
53	UT	1571	HIS
53	UT	2033	HIS
53	UT	2192	GLN
54	UH	14	HIS
54	UH	339	GLN
54	UH	366	ASN
54	UH	612	GLN
54	UH	740	ASN
56	US	184	HIS
56	US	253	HIS
56	US	281	GLN
56	US	333	ASN
56	US	372	HIS
56	US	468	HIS
56	US	481	GLN
56	US	488	ASN
55	UI	158	ASN
55	UI	174	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	C1	1563/2311 (67%)	320 (20%)	21 (1%)
51	C2	225/274 (82%)	53 (23%)	1 (0%)
All	All	1788/2585 (69%)	373 (20%)	22 (1%)

All (373) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	C1	4	G
50	C1	14	G
50	C1	16	U
50	C1	17	C

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Mol	Chain	Res	Type
50	C1	18	G
50	C1	23	G
50	C1	26	C
50	C1	36	C
50	C1	49	G
50	C1	59	U
50	C1	60	A
50	C1	61	G
50	C1	68	U
50	C1	71	A
50	C1	72	U
50	C1	73	A
50	C1	74	C
50	C1	77	C
50	C1	90	A
50	C1	93	G
50	C1	96	C
50	C1	97	C
50	C1	104	U
50	C1	105	A
50	C1	116	C
50	C1	126	C
50	C1	127	C
50	C1	128	G
50	C1	134	C
50	C1	136	C
50	C1	143	A
50	C1	151	C
50	C1	160	C
50	C1	162	G
50	C1	163	C
50	C1	167	C
50	C1	183	C
50	C1	185	G
50	C1	193	U
50	C1	201	G
50	C1	202	A
50	C1	205	C
50	C1	206	C
50	C1	207	U
50	C1	208	A
50	C1	209	A

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Mol	Chain	Res	Type
50	C1	210	G
50	C1	223	A
50	C1	233	C
50	C1	234	G
50	C1	236	C
50	C1	242	U
50	C1	243	U
50	C1	244	G
50	C1	257	G
50	C1	258	C
50	C1	259	U
50	C1	267	U
50	C1	269	G
50	C1	271	C
50	C1	273	G
50	C1	276	C
50	C1	277	U
50	C1	278	A
50	C1	281	U
50	C1	282	C
50	C1	283	A
50	C1	285	A
50	C1	291	C
50	C1	292	G
50	C1	295	G
50	C1	312	G
50	C1	319	U
50	C1	320	A
50	C1	323	G
50	C1	333	C
50	C1	339	C
50	C1	346	C
50	C1	347	C
50	C1	349	C
50	C1	351	U
50	C1	352	G
50	C1	382	U
50	C1	383	G
50	C1	384	C
50	C1	386	G
50	C1	397	U
50	C1	398	C

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Mol	Chain	Res	Type
50	C1	401	C
50	C1	402	U
50	C1	403	G
50	C1	416	U
50	C1	435	A
50	C1	436	A
50	C1	440	G
50	C1	441	A
50	C1	443	G
50	C1	453	G
50	C1	459	C
50	C1	468	C
50	C1	469	G
50	C1	483	U
50	C1	499	G
50	C1	500	C
50	C1	501	U
50	C1	502	A
50	C1	581	C
50	C1	582	G
50	C1	584	U
50	C1	594	G
50	C1	595	U
50	C1	597	G
50	C1	613	A
50	C1	614	U
50	C1	621	G
50	C1	628	A
50	C1	638	A
50	C1	652	A
50	C1	653	U
50	C1	655	A
50	C1	662	A
50	C1	663	U
50	C1	664	A
50	C1	680	U
50	C1	681	G
50	C1	685	C
50	C1	686	A
50	C1	690	A
50	C1	691	A
50	C1	700	C

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Mol	Chain	Res	Type
50	C1	702	U
50	C1	715	A
50	C1	719	U
50	C1	720	A
50	C1	721	C
50	C1	723	A
50	C1	725	A
50	C1	743	U
50	C1	744	C
50	C1	755	A
50	C1	758	U
50	C1	760	C
50	C1	762	G
50	C1	763	A
50	C1	764	A
50	C1	772	A
50	C1	774	U
50	C1	775	U
50	C1	776	C
50	C1	778	G
50	C1	779	A
50	C1	786	G
50	C1	798	U
50	C1	801	A
50	C1	802	A
50	C1	803	A
50	C1	806	C
50	C1	807	A
50	C1	808	A
50	C1	841	A
50	C1	845	C
50	C1	849	A
50	C1	850	A
50	C1	861	U
50	C1	897	U
50	C1	900	A
50	C1	904	U
50	C1	907	A
50	C1	921	G
50	C1	922	C
50	C1	930	G
50	C1	934	A

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Mol	Chain	Res	Type
50	C1	935	C
50	C1	936	A
50	C1	943	A
50	C1	970	G
50	C1	972	A
50	C1	984	A
50	C1	985	A
50	C1	986	C
50	C1	1000	A
50	C1	1002	G
50	C1	1007	G
50	C1	1023	U
50	C1	1024	U
50	C1	1025	A
50	C1	1028	C
50	C1	1029	A
50	C1	1037	C
50	C1	1043	G
50	C1	1044	A
50	C1	1052	A
50	C1	1059	A
50	C1	1061	A
50	C1	1069	A
50	C1	1070	G
50	C1	1076	U
50	C1	1078	U
50	C1	1079	C
50	C1	1080	G
50	C1	1085	U
50	C1	1086	U
50	C1	1088	U
50	C1	1089	A
50	C1	1095	A
50	C1	1096	A
50	C1	1098	G
50	C1	1103	C
50	C1	1111	A
50	C1	1116	U
50	C1	1122	A
50	C1	1123	G
50	C1	1124	G
50	C1	1125	A

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Mol	Chain	Res	Type
50	C1	1126	A
50	C1	1129	A
50	C1	1138	C
50	C1	1141	G
50	C1	1148	G
50	C1	1149	C
50	C1	1154	A
50	C1	1156	C
50	C1	1158	G
50	C1	1159	C
50	C1	1163	A
50	C1	1164	A
50	C1	1167	C
50	C1	1169	A
50	C1	1170	G
50	C1	1178	A
50	C1	1179	G
50	C1	1218	G
50	C1	1219	A
50	C1	1220	A
50	C1	1223	U
50	C1	1254	G
50	C1	1256	G
50	C1	1257	C
50	C1	1258	A
50	C1	1265	G
50	C1	1444	A
50	C1	1448	A
50	C1	1449	U
50	C1	1461	G
50	C1	1466	G
50	C1	1481	U
50	C1	1483	A
50	C1	1491	A
50	C1	1497	U
50	C1	1498	G
50	C1	1499	G
50	C1	1518	A
50	C1	1519	C
50	C1	1520	U
50	C1	1527	G
50	C1	1529	A

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Mol	Chain	Res	Type
50	C1	1530	U
50	C1	1544	U
50	C1	1551	A
50	C1	1555	A
50	C1	1613	C
50	C1	1614	U
50	C1	1624	A
50	C1	1625	G
50	C1	1642	A
50	C1	1643	U
50	C1	1645	U
50	C1	1665	A
50	C1	1666	C
50	C1	1667	G
50	C1	1668	A
50	C1	1710	G
50	C1	1711	G
50	C1	1712	C
50	C1	1713	U
50	C1	1733	G
50	C1	1735	A
50	C1	1742	C
50	C1	1744	A
50	C1	1750	G
50	C1	1762	G
50	C1	1763	G
50	C1	2044	C
50	C1	2055	C
50	C1	2056	U
50	C1	2070	A
50	C1	2072	U
50	C1	2074	C
50	C1	2076	C
50	C1	2086	A
50	C1	2087	G
50	C1	2107	A
50	C1	2109	A
50	C1	2118	U
50	C1	2119	G
50	C1	2120	C
50	C1	2121	U
50	C1	2156	A

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Mol	Chain	Res	Type
50	C1	2157	G
50	C1	2167	G
50	C1	2173	G
50	C1	2177	G
50	C1	2178	U
50	C1	2184	G
50	C1	2185	C
50	C1	2197	A
50	C1	2201	C
50	C1	2205	G
50	C1	2208	C
50	C1	2214	A
50	C1	2215	C
50	C1	2220	C
50	C1	2221	G
50	C1	2227	C
50	C1	2234	A
50	C1	2351	G
50	C1	2362	U
50	C1	2363	G
50	C1	2364	A
50	C1	2373	A
51	C2	15	A
51	C2	26	U
51	C2	28	U
51	C2	29	A
51	C2	31	A
51	C2	32	G
51	C2	33	U
51	C2	34	A
51	C2	37	U
51	C2	39	U
51	C2	48	G
51	C2	58	A
51	C2	62	A
51	C2	63	G
51	C2	90	C
51	C2	91	G
51	C2	103	G
51	C2	104	C
51	C2	105	C
51	C2	111	G

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Mol	Chain	Res	Type
51	C2	125	U
51	C2	127	A
51	C2	128	C
51	C2	133	G
51	C2	135	U
51	C2	136	C
51	C2	142	G
51	C2	153	G
51	C2	156	C
51	C2	160	U
51	C2	163	C
51	C2	165	C
51	C2	166	G
51	C2	167	U
51	C2	177	G
51	C2	178	U
51	C2	179	A
51	C2	180	U
51	C2	181	A
51	C2	187	U
51	C2	188	G
51	C2	189	G
51	C2	190	C
51	C2	198	U
51	C2	199	G
51	C2	200	U
51	C2	201	A
51	C2	247	G
51	C2	255	U
51	C2	256	G
51	C2	260	G
51	C2	261	U
51	C2	262	C

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	C1	89	G
50	C1	135	A
50	C1	209	A
50	C1	277	U
50	C1	281	U

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Mol	Chain	Res	Type
50	C1	397	U
50	C1	441	A
50	C1	593	G
50	C1	684	U
50	C1	689	A
50	C1	771	G
50	C1	802	A
50	C1	1001	A
50	C1	1068	C
50	C1	1087	G
50	C1	1163	A
50	C1	1256	G
50	C1	1734	G
50	C1	2156	A
50	C1	2177	G
50	C1	2219	C
51	C2	255	U

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

4 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
1	SEP	UA	646	1	8,9,10	1.51	1 (12%)	8,12,14	1.71	2 (25%)
14	SEP	UR	139	14	8,9,10	1.50	1 (12%)	8,12,14	1.45	2 (25%)
50	A2M	C1	1004	50	22,25,26	3.40	9 (40%)	31,36,39	2.53	9 (29%)
50	OMC	C1	998	50	19,22,23	2.94	8 (42%)	26,31,34	0.68	0

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
1	SEP	UA	646	1	-	1/5/8/10	-
14	SEP	UR	139	14	-	0/5/8/10	-
50	A2M	C1	1004	50	-	0/9/27/28	0/3/3/3
50	OMC	C1	998	50	-	0/9/27/28	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	C1	1004	A2M	C2'-C1'	-8.55	1.31	1.53
50	C1	1004	A2M	O4'-C1'	8.48	1.62	1.42
50	C1	1004	A2M	O4'-C4'	-6.27	1.31	1.45
50	C1	998	OMC	C2-N3	6.22	1.49	1.36
50	C1	998	OMC	C6-C5	5.91	1.48	1.35
50	C1	998	OMC	C4-N3	5.03	1.44	1.34
50	C1	998	OMC	C4-N4	4.78	1.45	1.33
50	C1	1004	A2M	C6-N6	4.43	1.45	1.34
50	C1	998	OMC	C2-N1	4.23	1.49	1.40
1	UA	646	SEP	P-O1P	3.31	1.61	1.50
14	UR	139	SEP	P-O1P	3.26	1.61	1.50
50	C1	998	OMC	C6-N1	3.11	1.45	1.38
50	C1	1004	A2M	O3'-C3'	-2.98	1.35	1.43
50	C1	1004	A2M	C5-C4	-2.80	1.33	1.39
50	C1	998	OMC	O2-C2	-2.74	1.18	1.23
50	C1	1004	A2M	O2'-C2'	2.74	1.49	1.42
50	C1	1004	A2M	C5-N7	-2.68	1.34	1.39
50	C1	998	OMC	C5-C4	2.32	1.48	1.42
50	C1	1004	A2M	C8-N9	-2.10	1.33	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	C1	1004	A2M	N6-C6-N1	-6.14	104.91	118.35
50	C1	1004	A2M	N3-C2-N1	-5.67	119.73	128.60
50	C1	1004	A2M	C5-C4-N3	-5.33	119.80	126.75
50	C1	1004	A2M	C5-C6-N6	5.27	134.89	123.43
50	C1	1004	A2M	N9-C8-N7	-4.03	108.41	113.91
50	C1	1004	A2M	C2-N3-C4	3.64	120.36	111.75
1	UA	646	SEP	P-OG-CB	-3.45	108.78	118.30
50	C1	1004	A2M	N3-C4-N9	3.15	132.28	127.08
50	C1	1004	A2M	C5-N7-C8	3.00	107.78	103.51
14	UR	139	SEP	P-OG-CB	-2.96	110.15	118.30
1	UA	646	SEP	OG-CB-CA	2.90	110.97	108.14
14	UR	139	SEP	OG-CB-CA	2.30	110.38	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	C1	1004	A2M	C4-C5-N7	-2.02	108.15	110.62

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	UA	646	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 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	$\# Z > 2$
63	GTP	CI	1201	64	30,34,34	0.88	1 (3%)	46,54,54	1.76	11 (23%)
65	ADP	CS	1101	-	27,29,29	3.06	9 (33%)	42,45,45	2.42	13 (30%)

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
63	GTP	CI	1201	64	-	5/22/38/38	0/3/3/3
65	ADP	CS	1101	-	-	0/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	CS	1101	ADP	O4'-C1'	8.65	1.62	1.42
65	CS	1101	ADP	C2'-C1'	-6.91	1.31	1.53
65	CS	1101	ADP	O4'-C4'	-6.78	1.29	1.45
65	CS	1101	ADP	O2'-C2'	4.72	1.54	1.43
65	CS	1101	ADP	C6-N6	3.73	1.43	1.34
65	CS	1101	ADP	C5-N7	-2.68	1.34	1.39
65	CS	1101	ADP	O3'-C3'	-2.65	1.36	1.43
65	CS	1101	ADP	C5'-C4'	2.58	1.59	1.51
65	CS	1101	ADP	C8-N7	2.12	1.35	1.31
63	CI	1201	GTP	C2-N3	2.02	1.38	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	CS	1101	ADP	N6-C6-N1	-6.96	103.12	118.35
65	CS	1101	ADP	C5-C6-N6	6.10	136.71	123.43
65	CS	1101	ADP	N3-C2-N1	-5.66	119.75	128.60
65	CS	1101	ADP	C5-C4-N3	-5.38	119.73	126.75
63	CI	1201	GTP	C5-C4-N3	-4.92	120.47	128.46
63	CI	1201	GTP	C2-N3-C4	4.41	120.16	112.30
65	CS	1101	ADP	N9-C8-N7	-4.25	108.10	113.91
63	CI	1201	GTP	PB-O3B-PG	-3.84	119.66	132.83
65	CS	1101	ADP	C2-N3-C4	3.64	120.36	111.75
65	CS	1101	ADP	N3-C4-N9	3.26	132.45	127.08
65	CS	1101	ADP	C5-N7-C8	3.18	108.03	103.51
63	CI	1201	GTP	N9-C4-N3	3.15	132.26	125.94
63	CI	1201	GTP	C2-N1-C6	-2.98	119.66	125.10
63	CI	1201	GTP	N9-C8-N7	-2.64	108.42	113.39
63	CI	1201	GTP	C5-C6-N1	2.59	119.77	113.19
63	CI	1201	GTP	C8-N7-C5	2.50	108.77	104.24
65	CS	1101	ADP	PA-O3A-PB	-2.43	124.48	132.83
63	CI	1201	GTP	O6-C6-C5	-2.35	120.37	126.60
63	CI	1201	GTP	PA-O3A-PB	-2.26	125.07	132.83
65	CS	1101	ADP	C3'-C2'-C1'	2.26	105.71	101.43
63	CI	1201	GTP	C3'-C2'-C1'	2.25	105.71	101.43
65	CS	1101	ADP	C4-N9-C1'	-2.17	121.41	126.59
65	CS	1101	ADP	C4-C5-N7	-2.04	108.14	110.62
65	CS	1101	ADP	C4-N9-C8	2.01	107.91	105.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

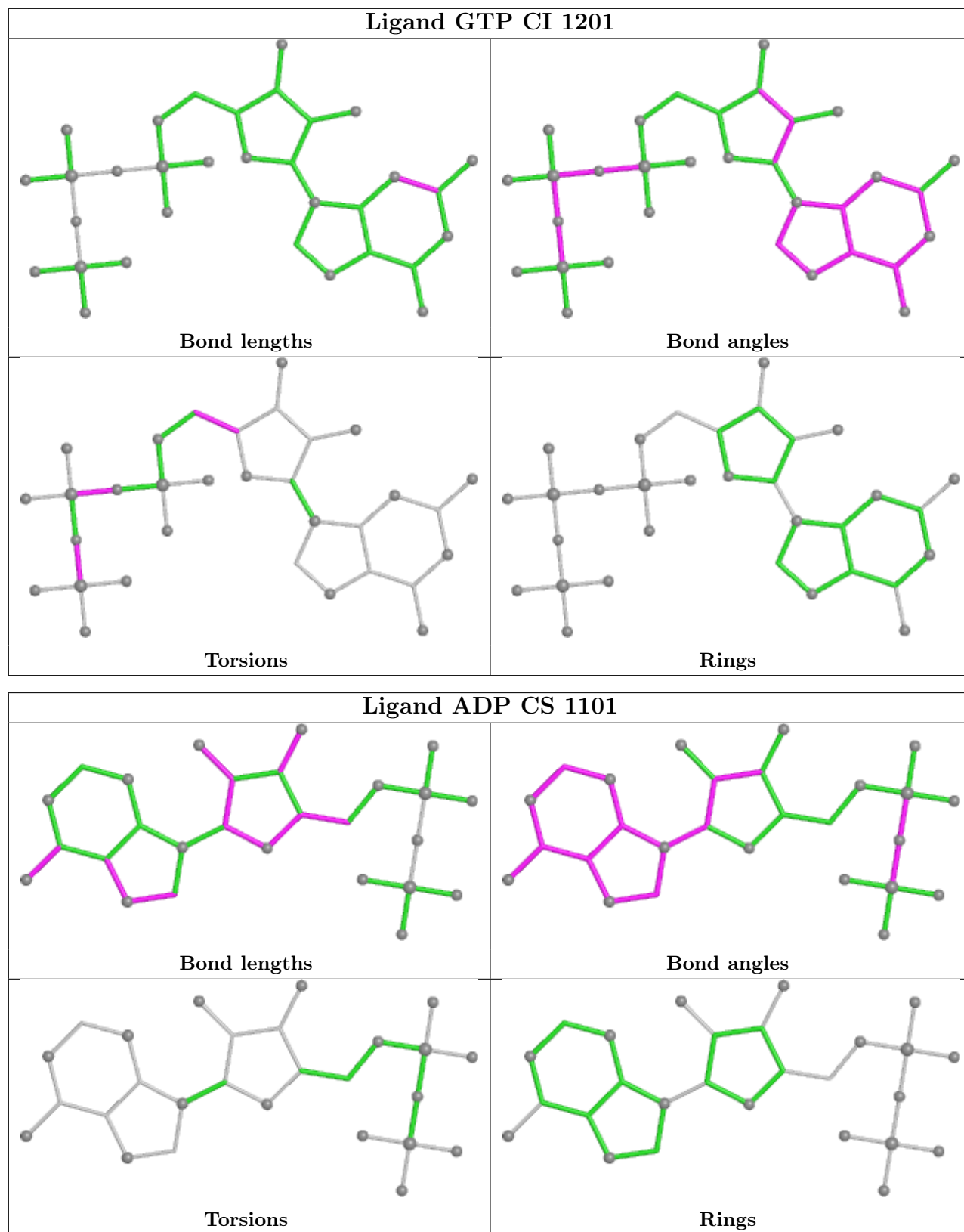
Mol	Chain	Res	Type	Atoms
63	CI	1201	GTP	PB-O3B-PG-O2G
63	CI	1201	GTP	PB-O3B-PG-O3G
63	CI	1201	GTP	PA-O3A-PB-O1B
63	CI	1201	GTP	PB-O3B-PG-O1G
63	CI	1201	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
65	CS	1101	ADP	1	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 than 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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

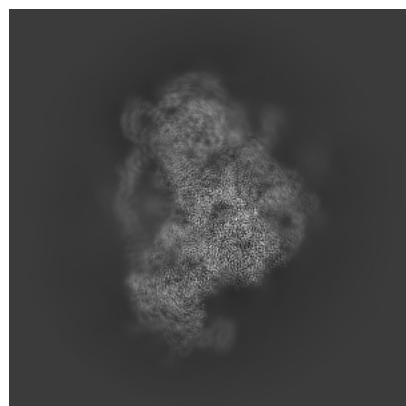
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66678. These allow visual inspection of the internal detail of the map and identification of artifacts.

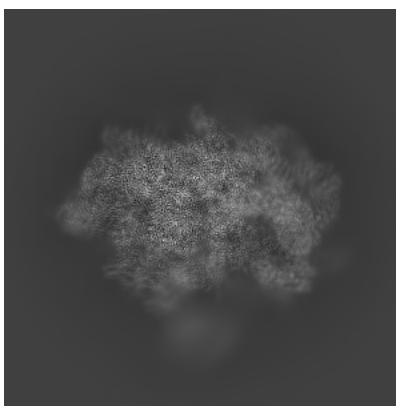
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

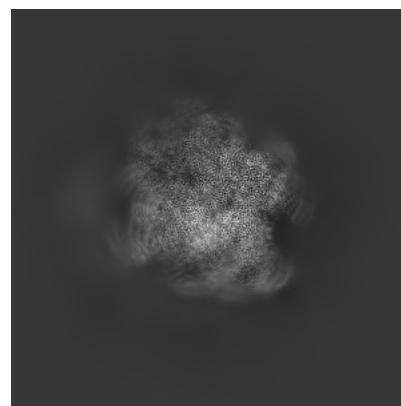
6.1.1 Primary map



X

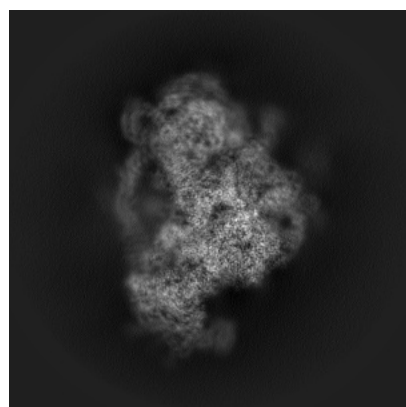


Y

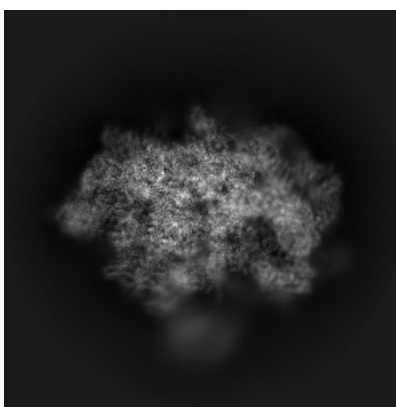


Z

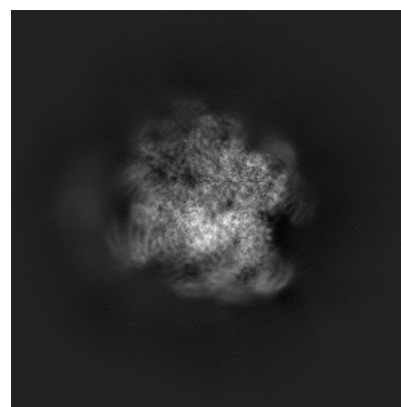
6.1.2 Raw map



X



Y

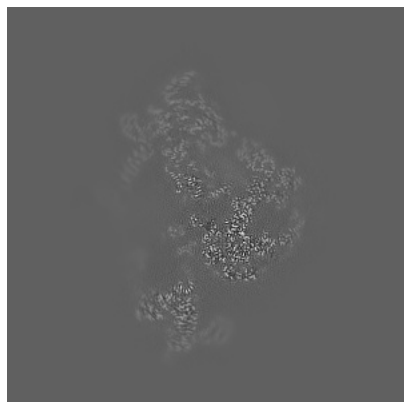


Z

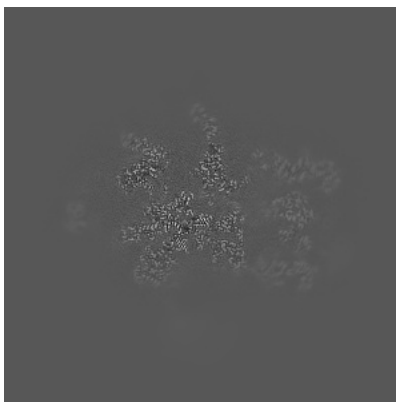
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

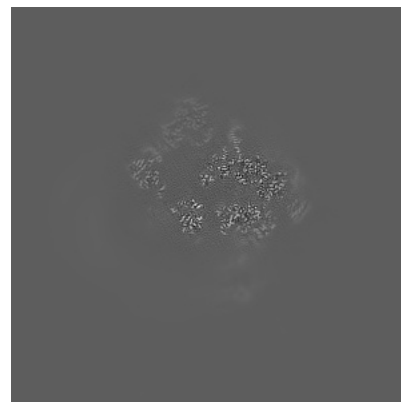
6.2.1 Primary map



X Index: 240

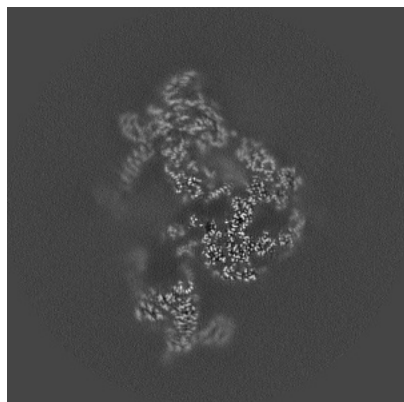


Y Index: 240

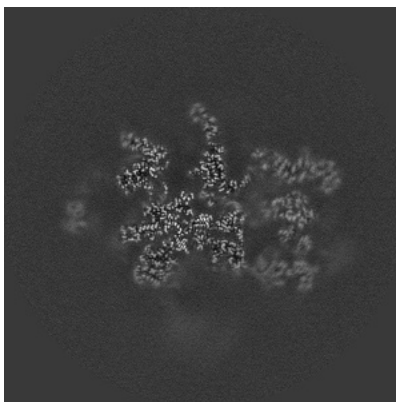


Z Index: 240

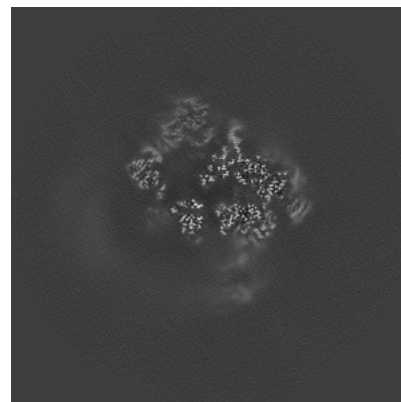
6.2.2 Raw map



X Index: 240



Y Index: 240

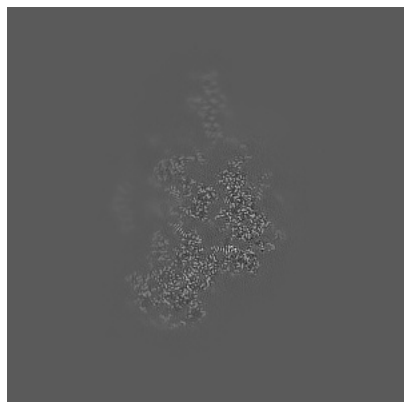


Z Index: 240

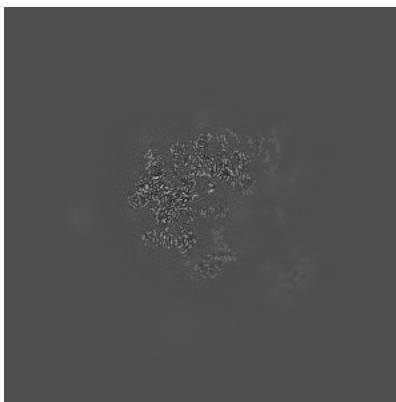
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 279

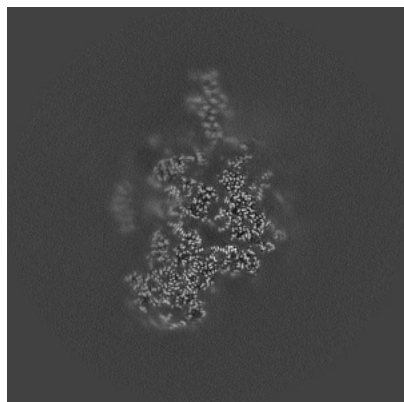


Y Index: 268

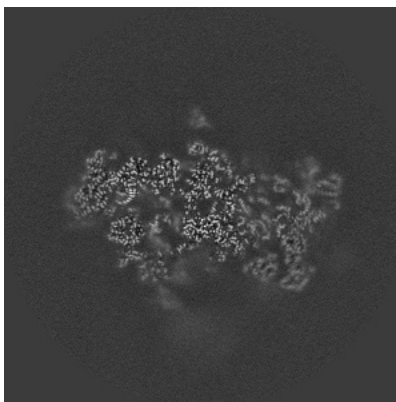


Z Index: 187

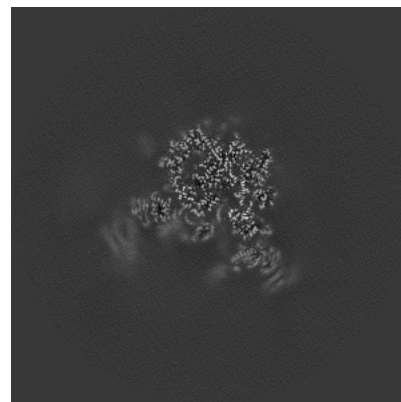
6.3.2 Raw map



X Index: 279



Y Index: 224

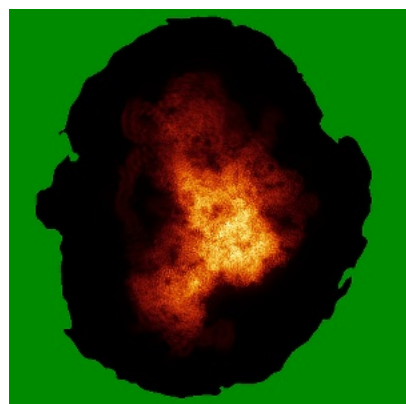


Z Index: 187

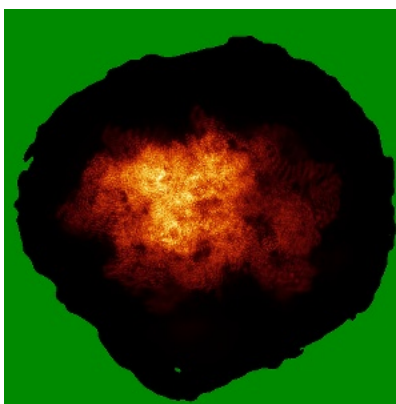
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

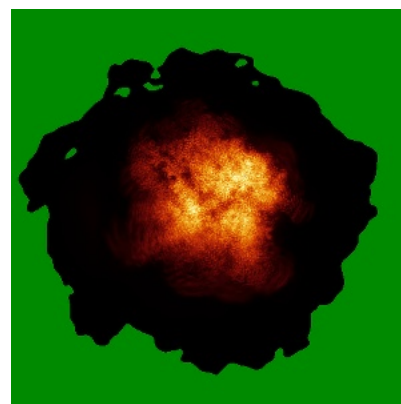
6.4.1 Primary map



X

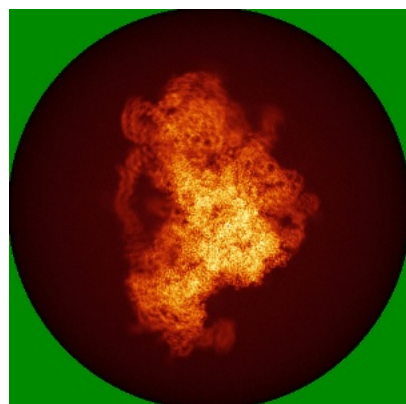


Y

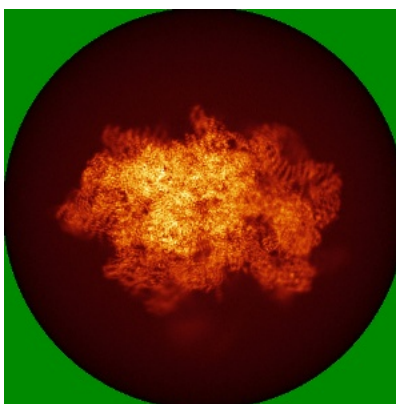


Z

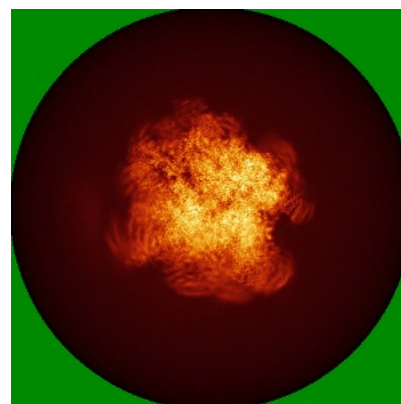
6.4.2 Raw map



X



Y

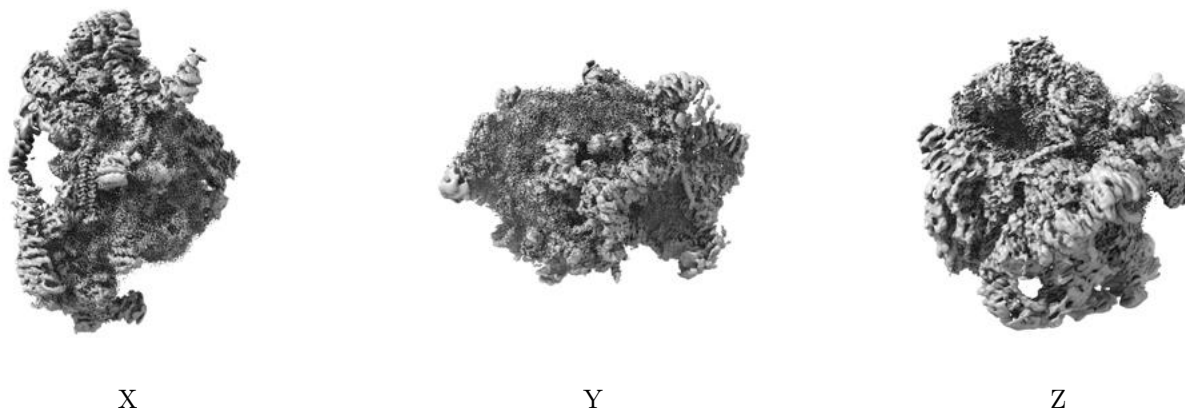


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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



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

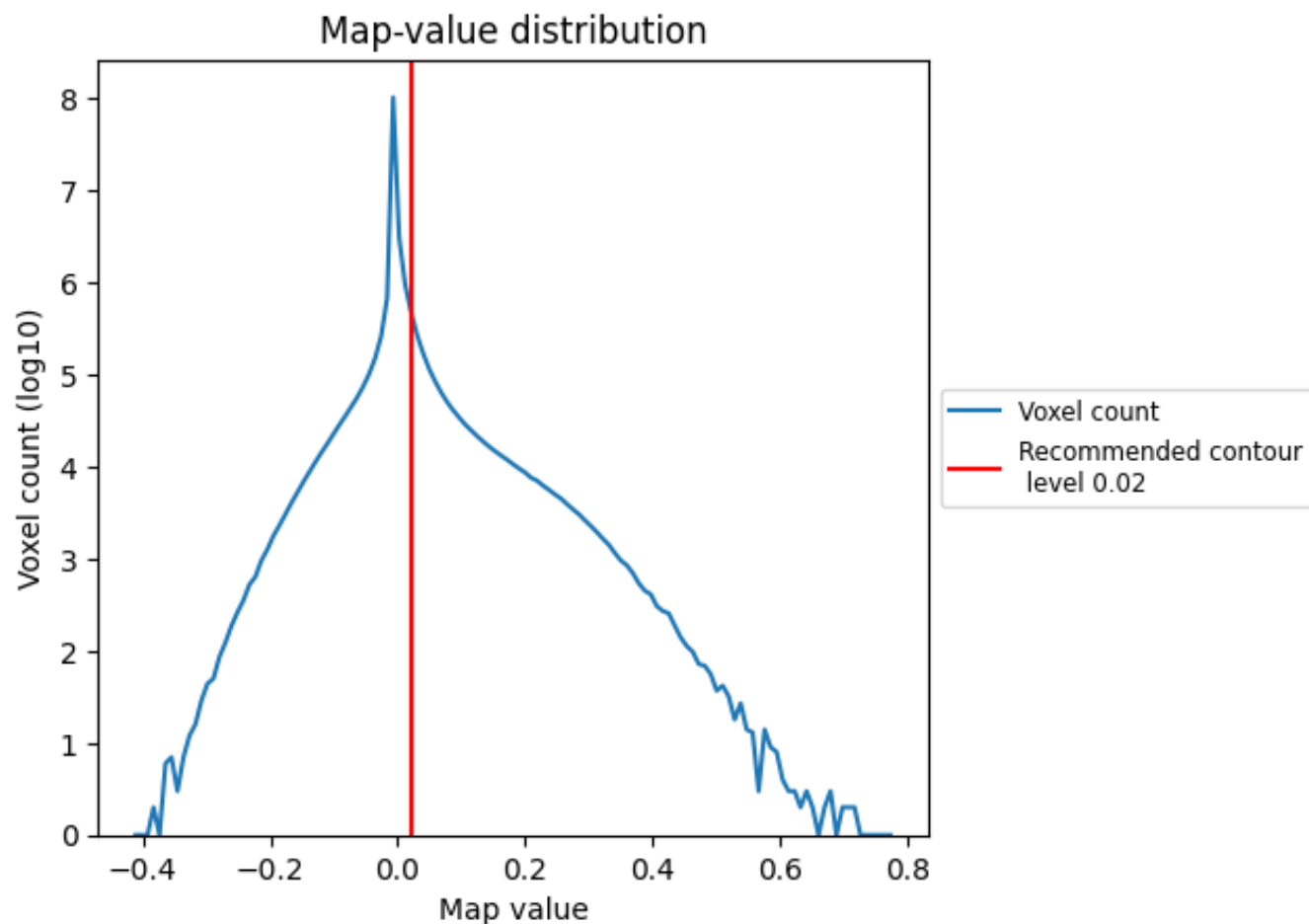
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

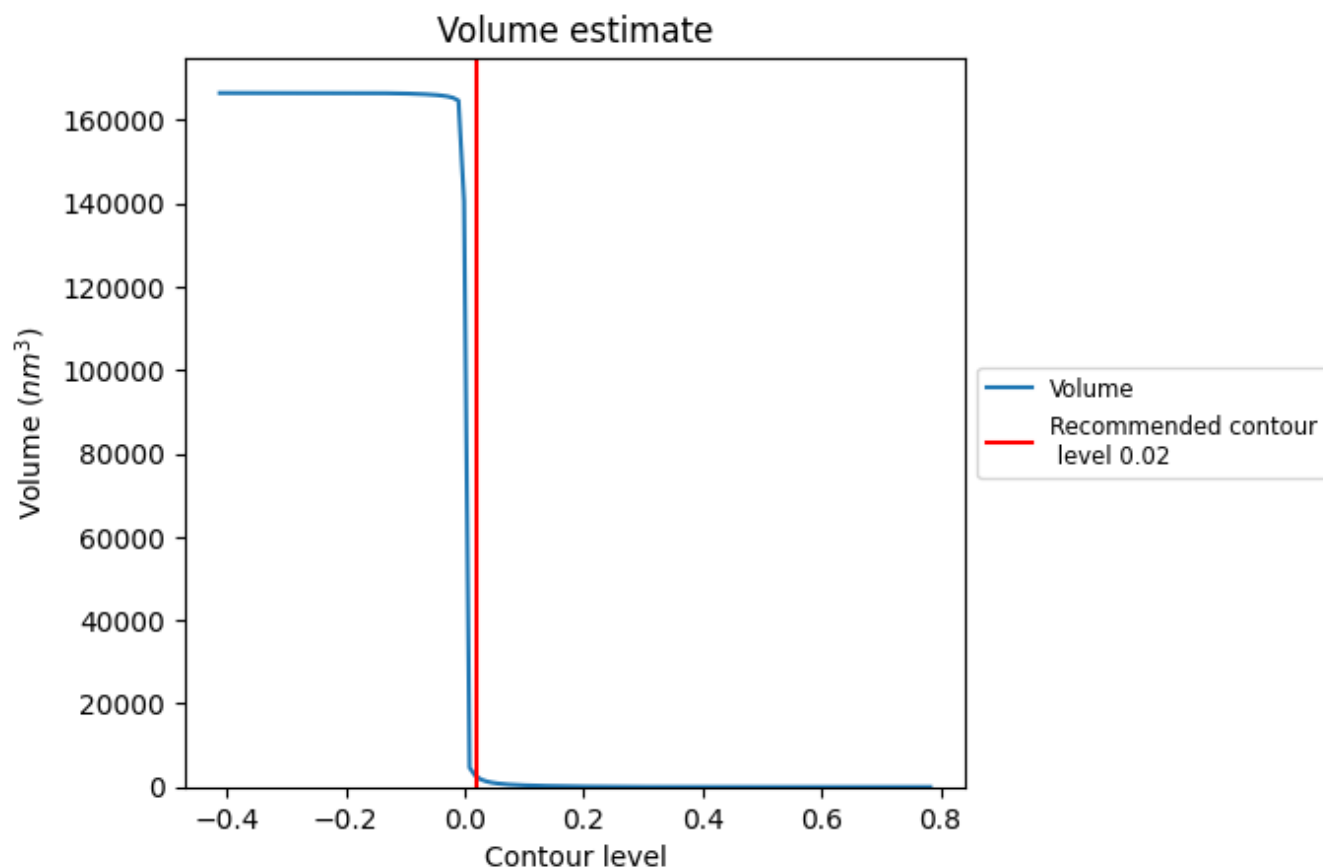
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

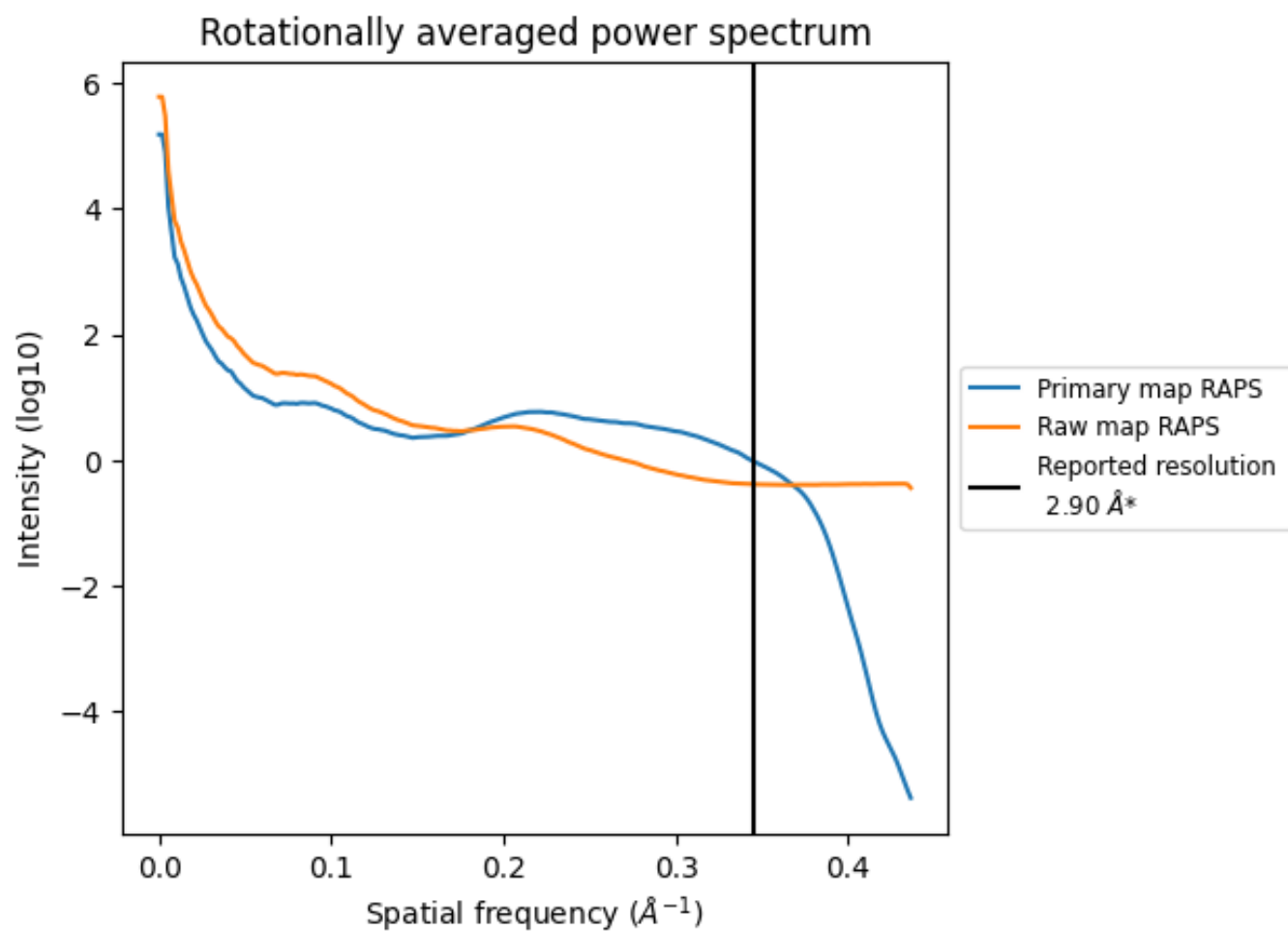
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2523 nm^3 ; this corresponds to an approximate mass of 2279 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 ⓘ

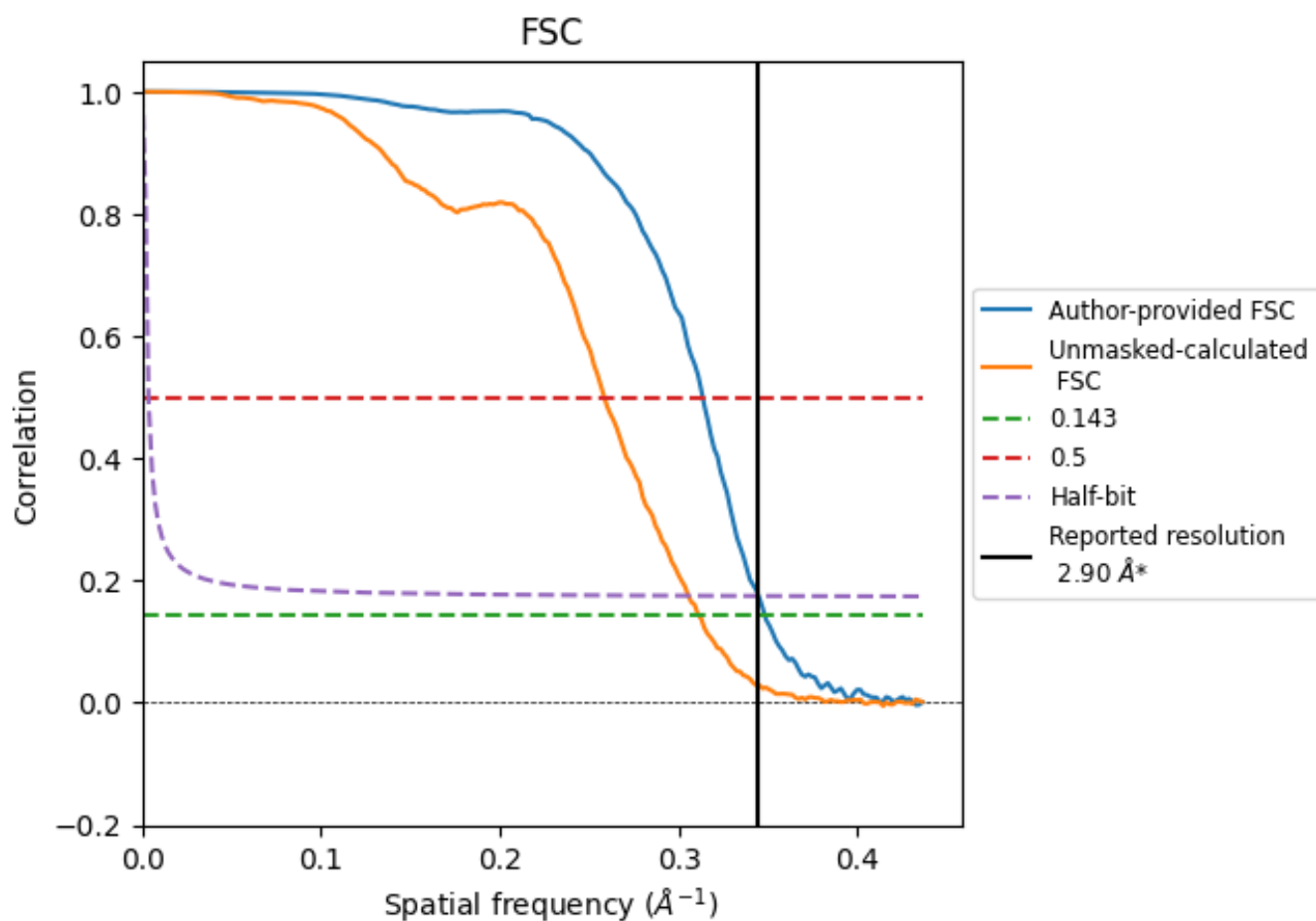


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

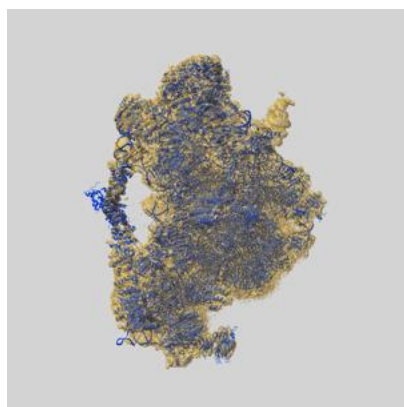
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.87	3.19	2.90
Unmasked-calculated*	3.21	3.87	3.27

*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 3.21 differs from the reported value 2.9 by more than 10 %

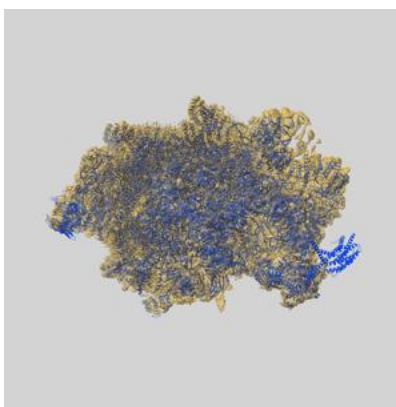
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-66678 and PDB model 9XA8. Per-residue inclusion information can be found in section [3](#) on page [17](#).

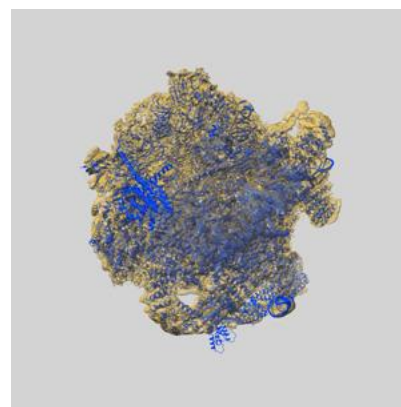
9.1 Map-model overlay [i](#)



X



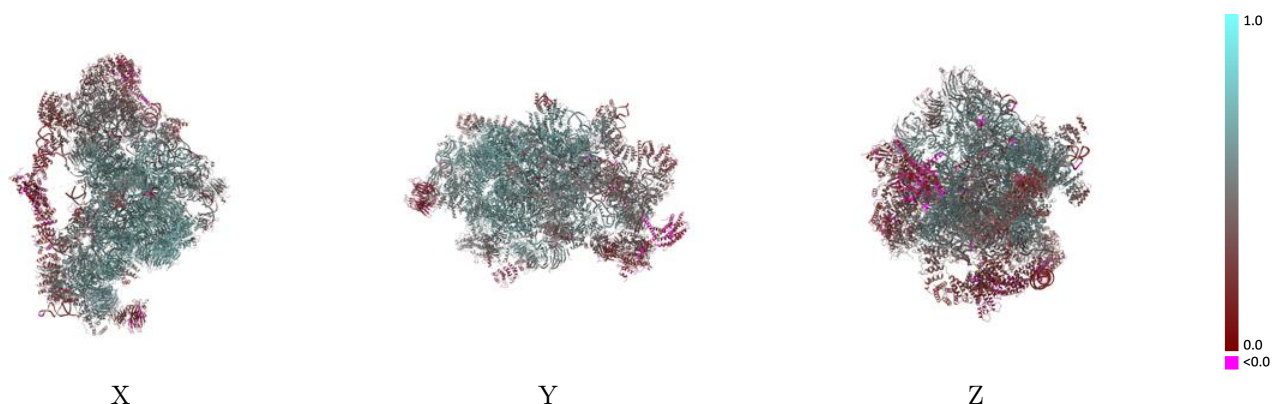
Y



Z

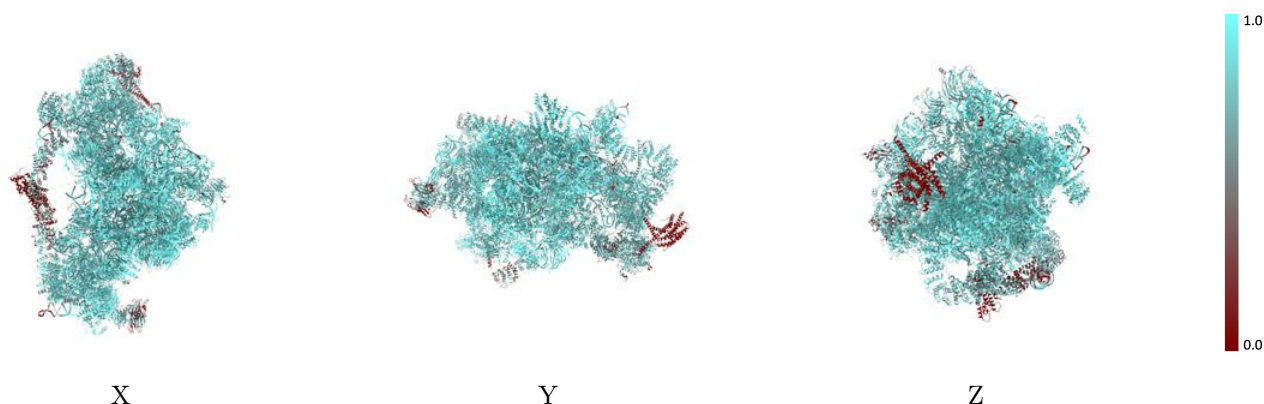
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



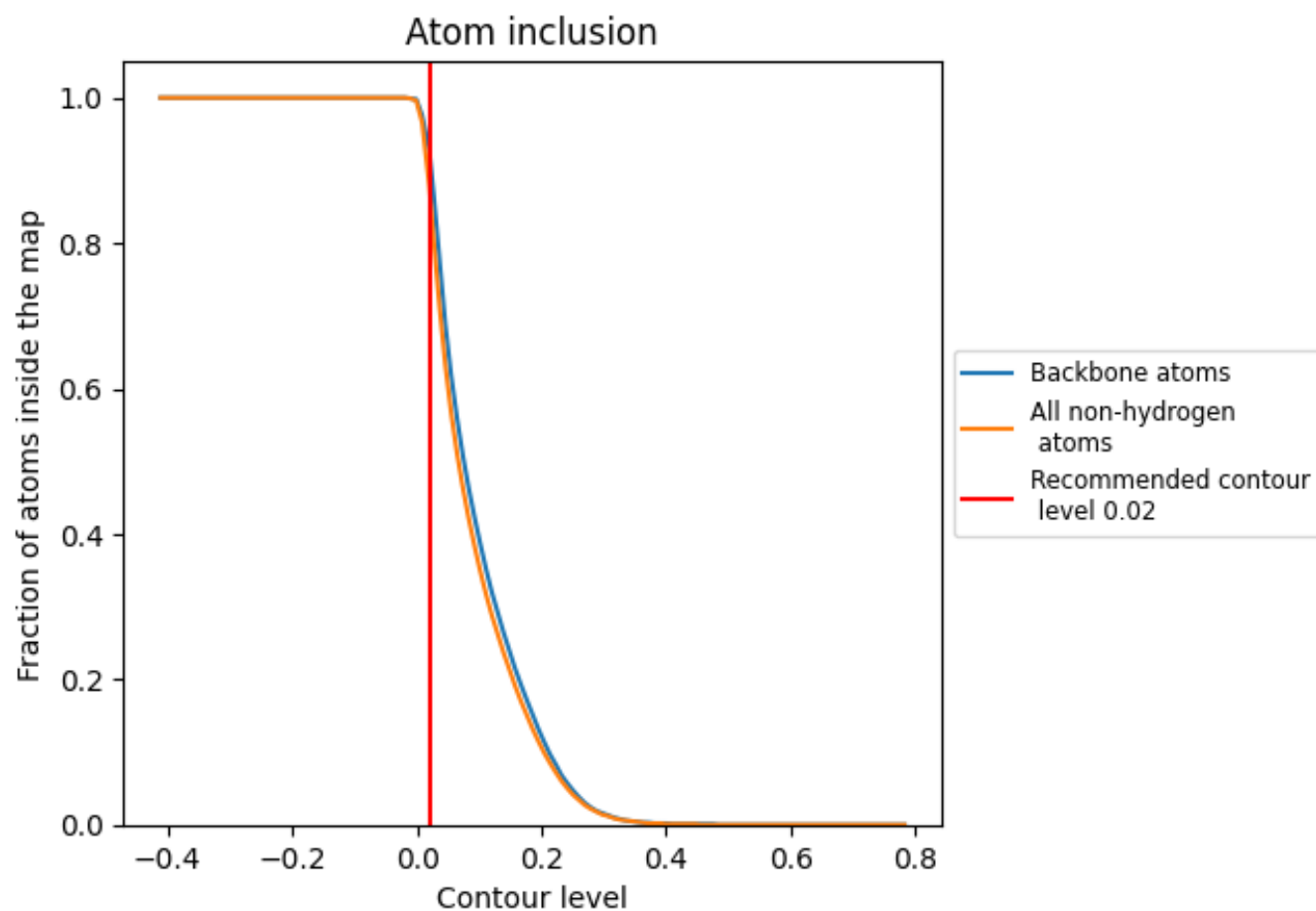
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 88% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8780	 0.4920
C1	 0.9490	 0.5220
C2	 0.8960	 0.4800
CA	 0.9850	 0.6460
CB	 0.8940	 0.5060
CC	 0.9490	 0.5460
CD	 0.8920	 0.5110
CE	 0.9800	 0.6270
CF	 0.9750	 0.5840
CG	 0.9440	 0.5200
CH	 0.9700	 0.5910
CI	 0.9580	 0.5920
CJ	 0.9980	 0.6830
CK	 0.9930	 0.6590
CL	 0.7040	 0.4730
CM	 0.9900	 0.6520
CN	 0.9530	 0.5650
CO	 0.8690	 0.4430
CP	 0.9230	 0.5240
CQ	 0.9260	 0.4880
CR	 0.8250	 0.3980
CS	 0.7060	 0.2820
CT	 0.9720	 0.6190
CU	 0.9340	 0.5680
CW	 0.8800	 0.4580
CX	 0.3920	 0.1320
CY	 0.4100	 0.2510
CZ	 0.1350	 0.1160
Ca	 0.9220	 0.5130
Cb	 0.8690	 0.4200
Cc	 0.9850	 0.6390
Cd	 0.9290	 0.4980
Ce	 0.8880	 0.4450
Cf	 0.9030	 0.4480
Cg	 0.9920	 0.6190



Continued on next page...

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Chain	Atom inclusion	Q-score
Ch	 0.8010	 0.3720
Ci	 0.9560	 0.5470
Cj	 0.9950	 0.6690
Ck	 0.8770	 0.4040
Cl	 0.8660	 0.4530
Cm	 0.9570	 0.5830
Cn	 0.9880	 0.6490
Co	 0.8730	 0.4240
Cp	 0.9930	 0.6270
UA	 0.9930	 0.6630
UB	 0.8860	 0.4640
UC	 0.3740	 0.2980
UD	 0.9730	 0.5820
UE	 0.9490	 0.5370
UF	 0.9370	 0.5220
UG	 0.9830	 0.6460
UH	 0.6640	 0.3150
UI	 0.9140	 0.4590
UJ	 0.6710	 0.3120
UK	 0.9660	 0.6190
UL	 0.9630	 0.5520
UM	 0.8210	 0.4540
UN	 0.9550	 0.5890
UO	 0.9840	 0.6110
UP	 0.9480	 0.5490
UQ	 0.9700	 0.5880
UR	 0.9860	 0.6500
US	 0.9070	 0.4560
UT	 0.8300	 0.3520
UU	 0.9870	 0.6480
UX	 0.9800	 0.6290
UZ	 0.9360	 0.5030