



Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 09:38 AM JST

PDB ID : 6LQV
EMDB ID : EMD-0955
Title : Cryo-EM structure of 90S small subunit preribosomes in transition states (State C1)
Authors : Du, Y.; Ye, K.
Deposited on : 2020-01-14
Resolution : 4.80 Å(reported)
Based on initial model : 6LQR

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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

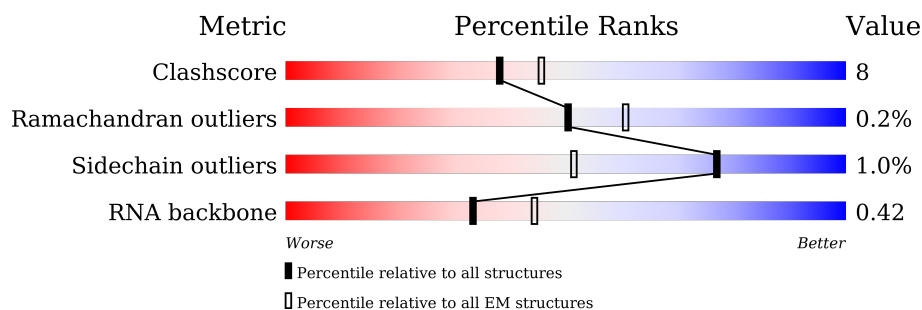
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	3A	333	
2	5A	700	
3	SA	1808	
4	SF	261	
5	SG	225	
6	SH	236	
7	SJ	200	

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Mol	Chain	Length	Quality of chain
8	SK	197	
9	SM	156	
10	SR	143	
11	SY	145	
12	SZ	135	
13	Sd	67	
14	3B	327	
14	3C	327	
15	3D	504	
16	3E	511	
17	3F	573	
18	3G	126	
18	3H	126	
19	A4	776	
20	A5	643	
21	A8	713	
22	A9	575	
23	AE	1769	
24	AF	513	
25	AG	896	
26	B1	923	
27	B2	943	
28	B3	817	
29	B8	594	
30	BE	939	

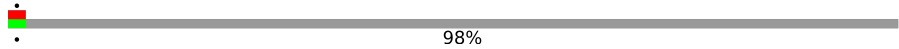
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Mol	Chain	Length	Quality of chain
31	B6	440	
32	5B	214	
33	5C	554	
34	5D	250	
35	5E	593	
36	5F	183	
37	5G	290	
38	5H	610	
39	5I	489	
40	5J	217	
41	5K	189	
42	RA	707	
43	RB	357	
44	RG	252	
44	RH	252	
45	RJ	1183	
46	RK	367	
47	RL	1056	
47	RM	1056	
48	RN	810	
49	RO	552	
50	RP	2493	
51	RQ	899	
52	RS	483	
53	RY	534	

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Mol	Chain	Length	Quality of chain
54	X1	347	 98%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 181752 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 RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3A	175	Total	C	N	O	P	0	0
			3711	1661	648	1227	175		

- Molecule 2 is a RNA chain called 5' ETS.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5A	171	Total	C	N	O	P	0	0
			3668	1637	666	1194	171		

- Molecule 3 is a RNA chain called 18S pre-rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SA	950	Total	C	N	O	P	0	0
			20256	9055	3612	6639	950		

- Molecule 4 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SF	229	Total	C	N	O	S	0	0
			1815	1161	331	320	3		

- Molecule 5 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SG	213	Total	C	N	O	S	0	0
			1669	1045	307	314	3		

- Molecule 6 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SH	167	Total	C	N	O	S	0	0
			1327	834	256	235	2		

- Molecule 7 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SJ	166	Total	C	N	O	S	0	0
			1324	824	262	236	2		

- Molecule 8 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SK	171	Total	C	N	O	S	0	0
			1388	879	268	240	1		

- Molecule 9 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SM	123	Total	C	N	O	S	0	0
			997	641	189	164	3		

- Molecule 10 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	SR	125	Total	C	N	O	0	0
			973	625	174	174		

- Molecule 11 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SY	103	Total	C	N	O	S	0	0
			786	503	144	137	2		

- Molecule 12 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	SZ	102	Total	C	N	O	0	0
			809	517	148	144		

- Molecule 13 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Sd	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 14 is a protein called rRNA 2'-O-methyltransferase fibrillar.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3B	240	Total	C	N	O	S	0	0
			1865	1184	333	338	10		
14	3C	225	Total	C	N	O	S	0	0
			1763	1120	316	317	10		

- Molecule 15 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3D	369	Total	C	N	O	S	0	0
			2848	1811	489	540	8		

- Molecule 16 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3E	431	Total	C	N	O	S	0	0
			3028	1888	543	588	9		

- Molecule 17 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3F	454	Total	C	N	O	S	0	0
			3643	2315	638	680	10		

- Molecule 18 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	3G	121	Total	C	N	O	S	0	0
			916	583	158	171	4		
18	3H	121	Total	C	N	O	S	0	0
			916	583	158	171	4		

- Molecule 19 is a protein called U3 small nucleolar RNA-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A4	662	Total	C	N	O	S	0	0
			5226	3309	910	986	21		

- Molecule 20 is a protein called U3 small nucleolar RNA-associated protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	A5	514	Total	C	N	O	S	0	0
			3976	2520	688	755	13		

- Molecule 21 is a protein called U3 small nucleolar RNA-associated protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A8	532	Total	C	N	O	S	0	0
			3229	2008	592	626	3		

- Molecule 22 is a protein called U3 small nucleolar RNA-associated protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A9	128	Total	C	N	O	S	0	0
			939	594	173	170	2		

- Molecule 23 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AE	1534	Total	C	N	O	S	0	0
			9955	6242	1771	1923	19		

- Molecule 24 is a protein called U3 small nucleolar RNA-associated protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AF	493	Total	C	N	O	S	0	0
			3911	2462	702	735	12		

- Molecule 25 is a protein called NET1-associated nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AG	826	Total	C	N	O	S	0	0
			6570	4181	1111	1259	19		

- Molecule 26 is a protein called Periodic tryptophan protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B1	793	Total	C	N	O	S	0	0
			6331	4046	1085	1182	18		

- Molecule 27 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B2	825	Total	C	N	O	S	0	0
			6502	4156	1096	1223	27		

- Molecule 28 is a protein called U3 small nucleolar RNA-associated protein 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B3	757	Total	C	N	O	S	0	0
			5919	3769	993	1130	27		

- Molecule 29 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B8	477	Total	C	N	O	S	0	0
			3764	2387	662	705	10		

- Molecule 30 is a protein called U3 small nucleolar RNA-associated protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BE	820	Total	C	N	O	S	0	0
			6450	4090	1114	1225	21		

- Molecule 31 is a protein called U3 small nucleolar RNA-associated protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B6	374	Total	C	N	O	S	0	0
			2800	1782	501	505	12		

- Molecule 32 is a protein called Bud site selection protein 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	5B	60	Total	C	N	O	0	0
			495	310	101	84		

- Molecule 33 is a protein called U3 small nucleolar RNA-associated protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	5C	409	Total	C	N	O	S	0	0
			3198	2020	559	608	11		

- Molecule 34 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	5D	167	Total	C	N	O	S	0	0
			1396	862	266	263	5		

- Molecule 35 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	5E	193	Total	C	N	O	S	0	0
			1564	970	280	310	4		

- Molecule 36 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	5F	182	Total	C	N	O	S	0	0
			1530	967	287	269	7		

- Molecule 37 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	5G	219	Total	C	N	O	S	0	0
			1756	1107	325	318	6		

- Molecule 38 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	5H	74	Total	C	N	O		0	0
			596	373	122	101			

- Molecule 39 is a protein called Protein SOF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	5I	461	Total	C	N	O	S	0	0
			3765	2354	686	709	16		

- Molecule 40 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	5J	151	Total	C	N	O	S	0	0
			1280	807	240	228	5		

- Molecule 41 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	5K	175	Total	C	N	O	S	0	0
			1403	896	256	241	10		

- Molecule 42 is a protein called Ribosome biogenesis protein ENP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	RA	338	Total	C	N	O	S	0	0
			2709	1713	463	524	9		

- Molecule 43 is a protein called U3 small nucleolar ribonucleoprotein protein LCP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	RB	134	Total	C	N	O	S	0	0
			1108	664	227	214	3		

- Molecule 44 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	RG	216	Total	C	N	O	S	0	0
			1701	1079	296	315	11		
44	RH	230	Total	C	N	O	S	0	0
			1799	1142	313	333	11		

- Molecule 45 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	RJ	796	Total	C	N	O	S	0	0
			6379	4086	1136	1128	29		

- Molecule 46 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	RK	360	Total	C	N	O	S	0	0
			2781	1781	473	516	11		

- Molecule 47 is a protein called RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	RL	805	Total	C	N	O	S	0	0
			4539	2760	885	887	7		
47	RM	766	Total	C	N	O		0	0
			3779	2247	766	766			

- Molecule 48 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	RN	607	Total	C	N	O	S	0	0
			4529	2861	820	837	11		

- Molecule 49 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	RO	525	Total	C	N	O	S	0	0
			3766	2412	646	696	12		

- Molecule 50 is a protein called U3 small nucleolar RNA-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	RP	1554	Total	C	N	O	S	0	0
			8510	5201	1624	1679	6		

- Molecule 51 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	RQ	138	Total	C	N	O	S	0	0
			974	598	183	192	1		

- Molecule 52 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	RS	251	Total	C	N	O	S	0	0
			2051	1340	349	359	3		

- Molecule 53 is a protein called Protein BFR2.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	RY	37	Total	C	N	O	0	0
			299	191	48	60		

- Molecule 54 is a protein called Unassigned helices.

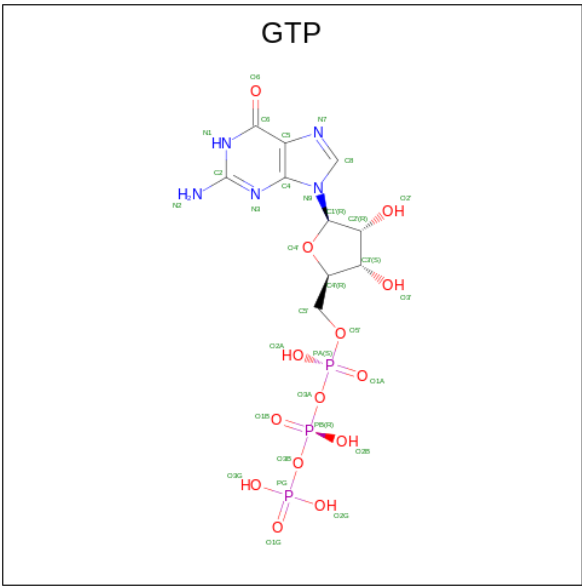
Mol	Chain	Residues	Atoms				AltConf	Trace
54	X1	8	Total	C	N	O	0	0
			40	24	8	8		

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	5K	1	Total	Zn	0
			1	1	

- Molecule 56 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:

C₁₀H₁₆N₅O₁₄P₃).



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

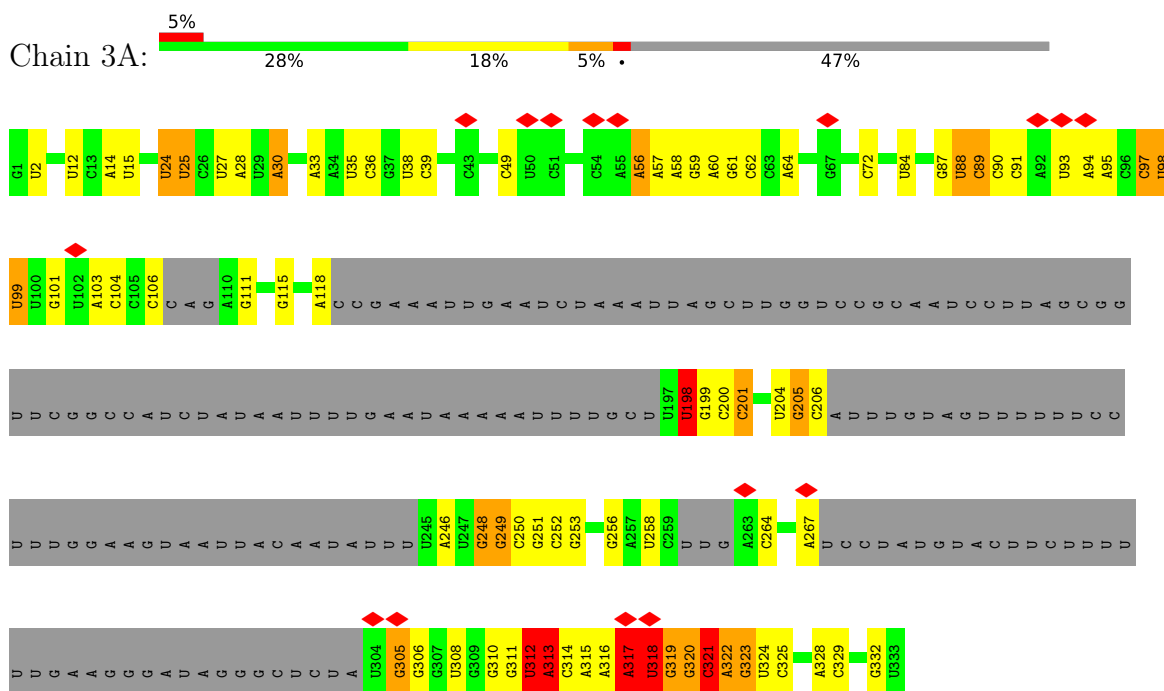
- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	RJ	1	Total	Mg	0
			1	1	

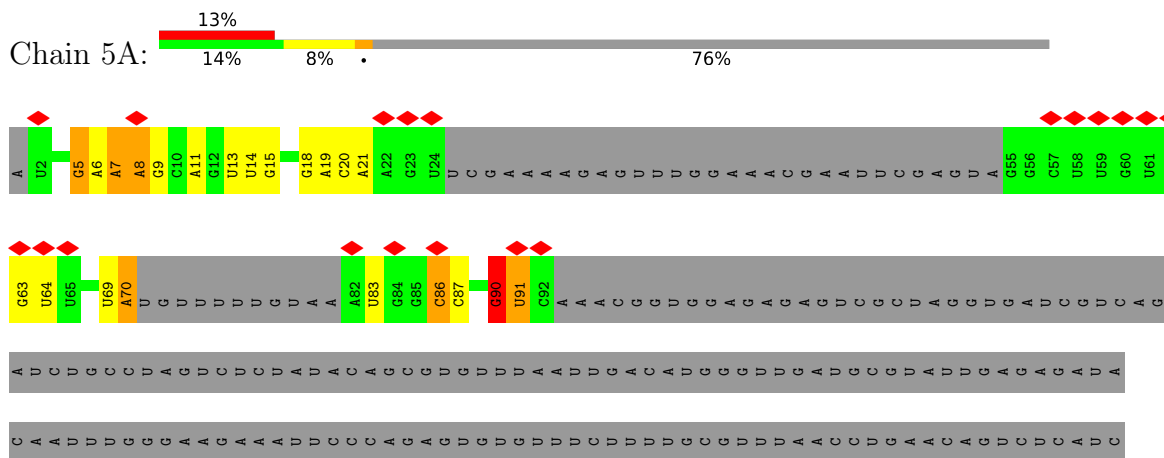
3 Residue-property plots [i](#)

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

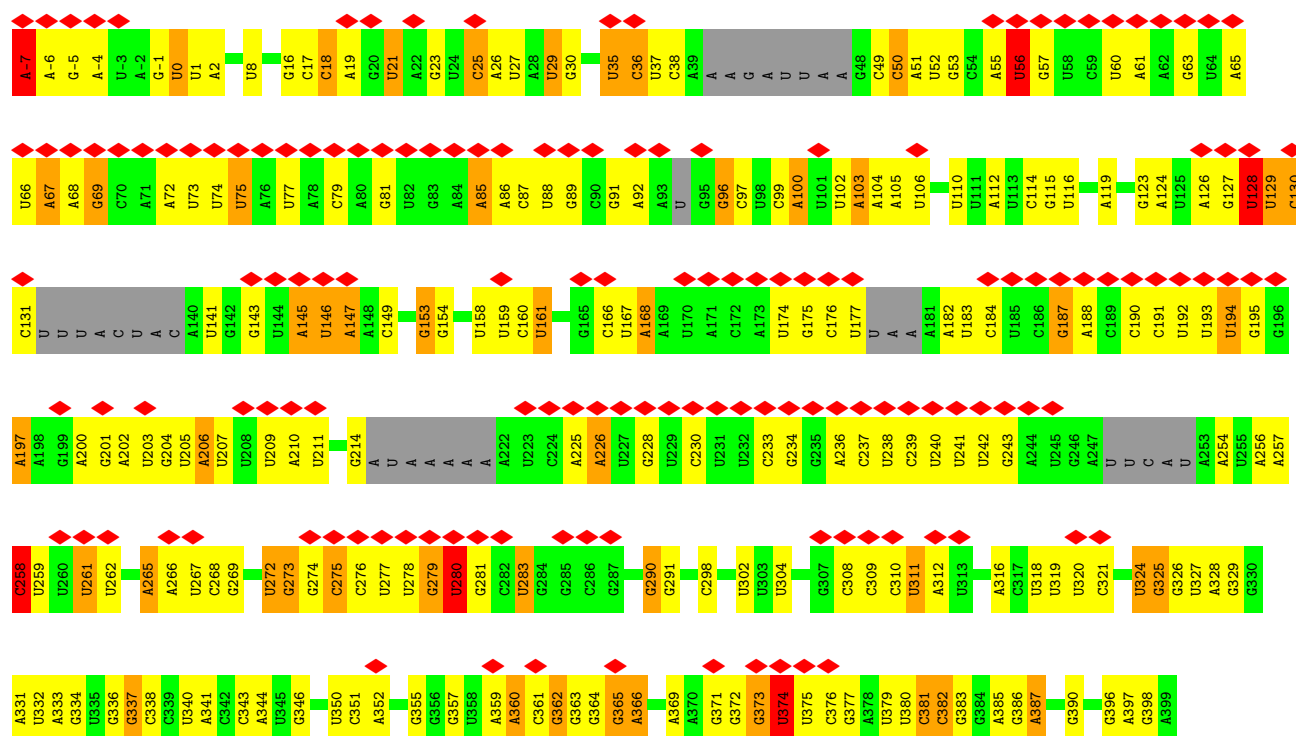
• Molecule 1: U3 snoRNA



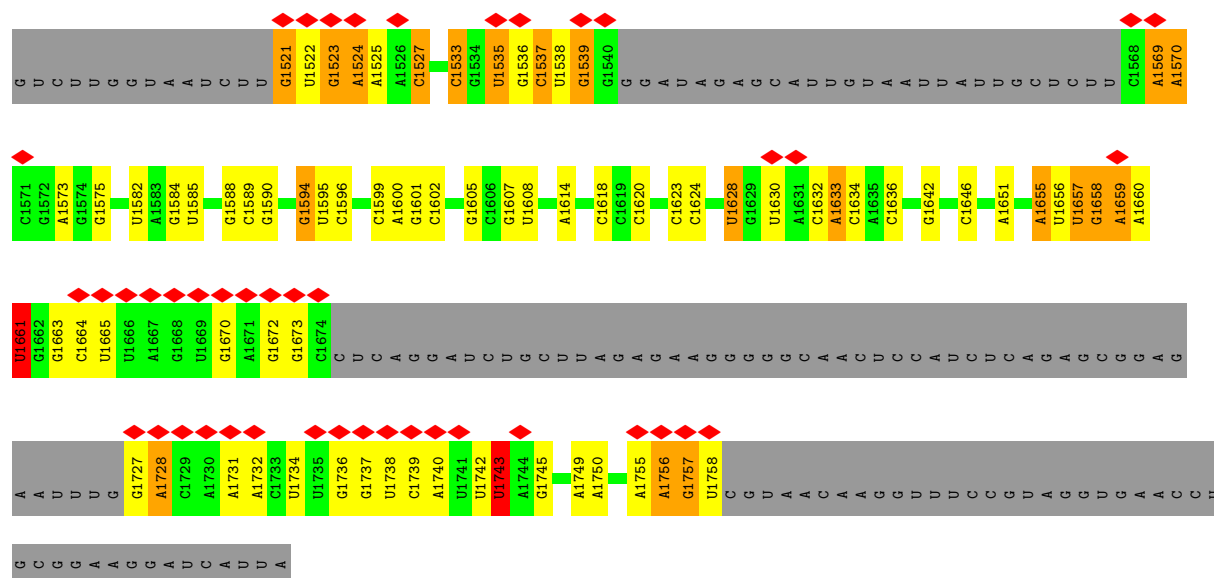
• Molecule 2: 5' ETS



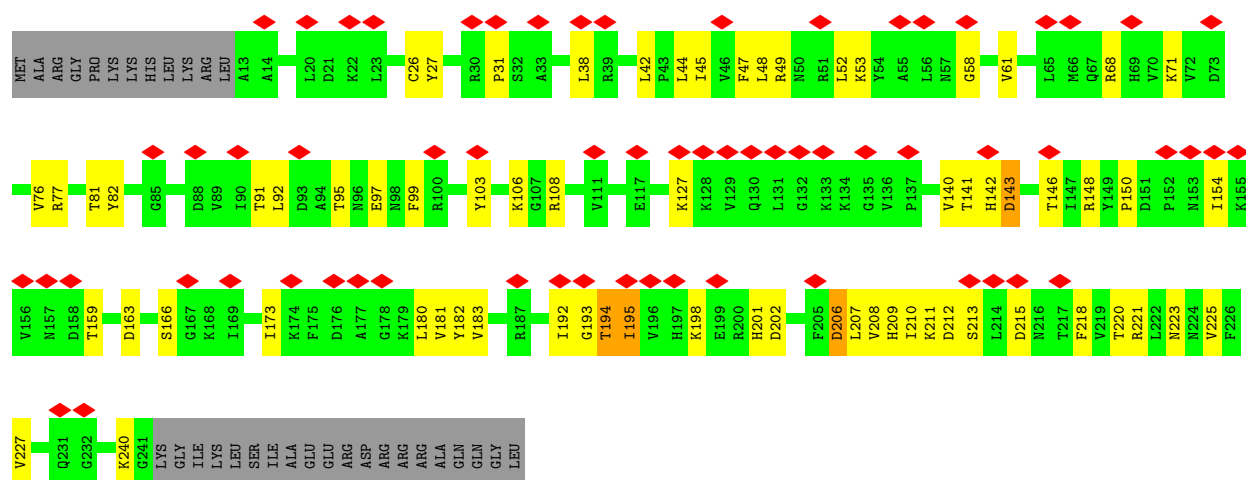
- Molecule 3: 18S pre-rRNA



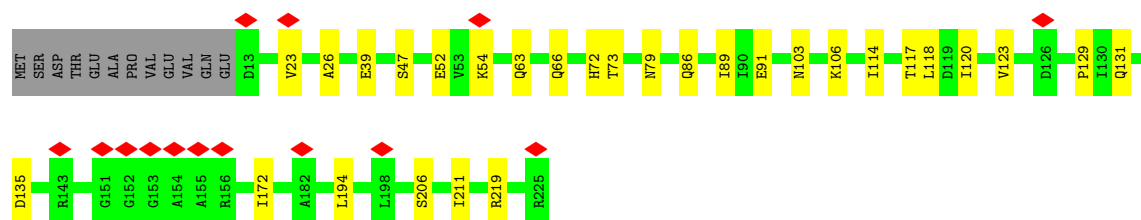
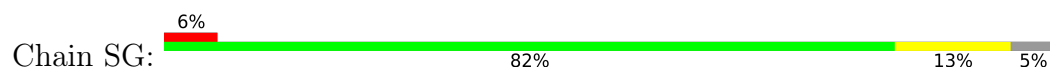




- Molecule 4: 40S ribosomal protein S4-A

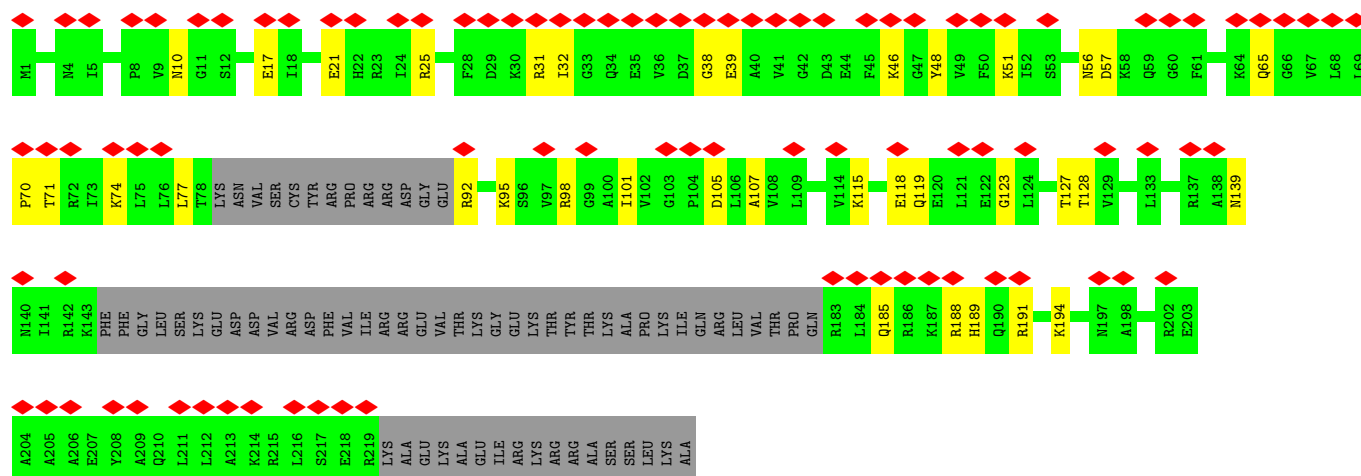


- Molecule 5: 40S ribosomal protein S5

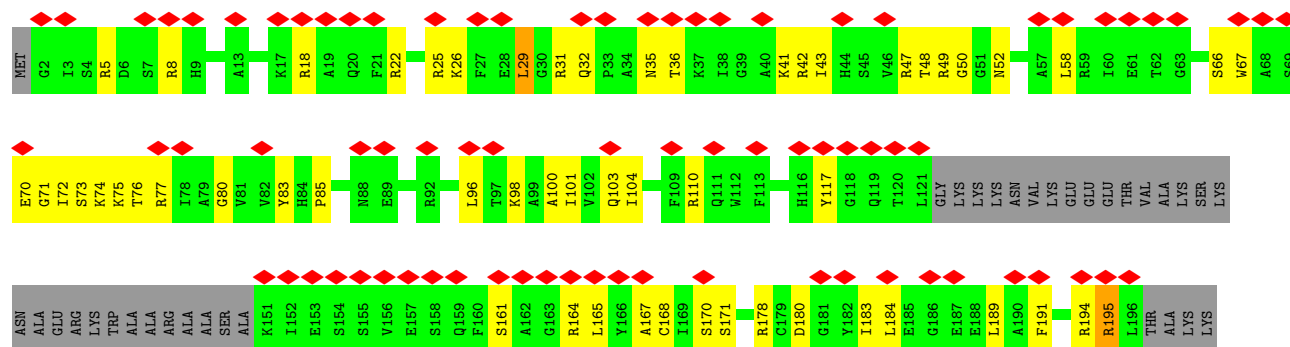


- Molecule 6: 40S ribosomal protein S6-A

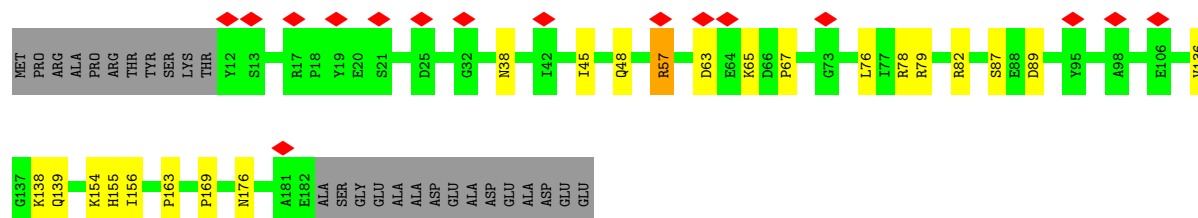
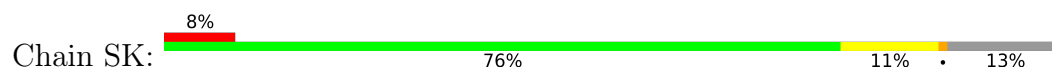




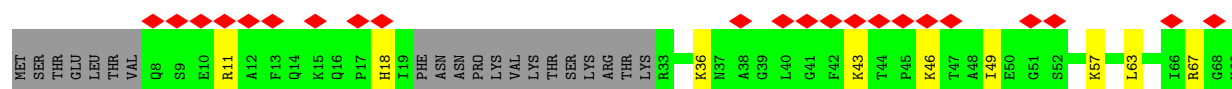
• Molecule 7: 40S ribosomal protein S8-A

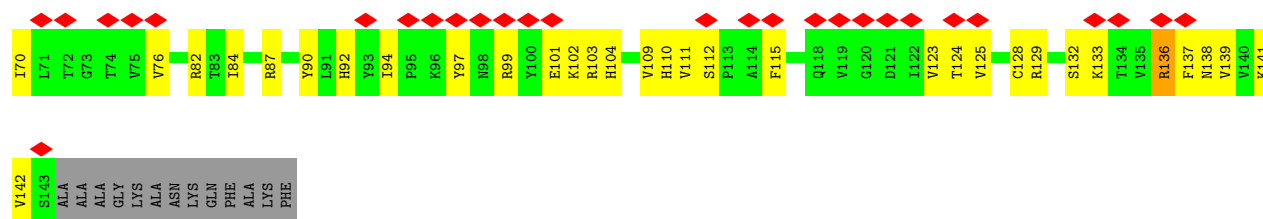


• Molecule 8: 40S ribosomal protein S9-A

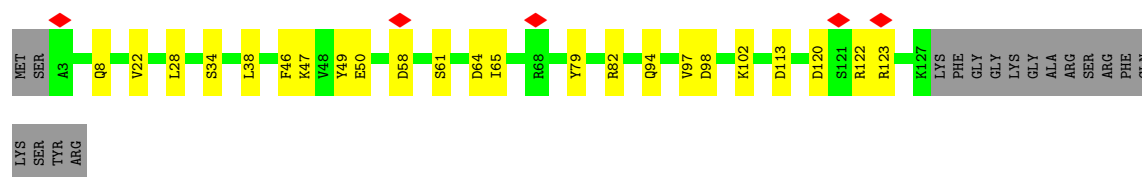


• Molecule 9: 40S ribosomal protein S11-A

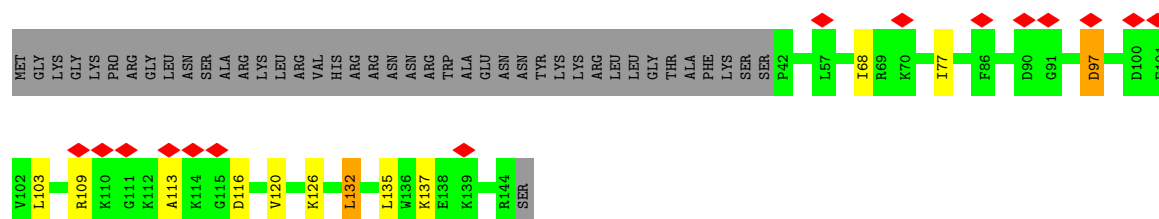




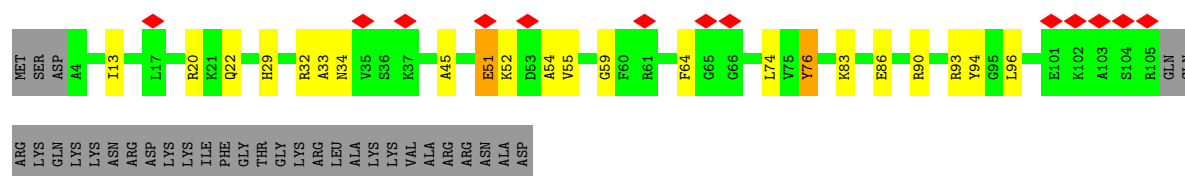
- Molecule 10: 40S ribosomal protein S16-A



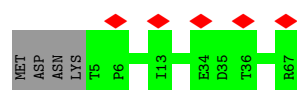
- Molecule 11: 40S ribosomal protein S23-A



- Molecule 12: 40S ribosomal protein S24-A

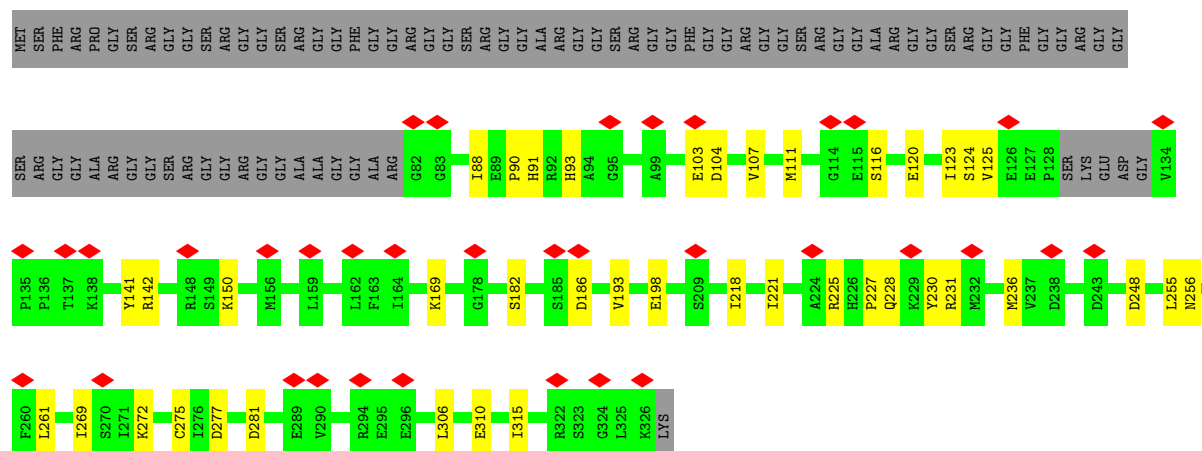


- Molecule 13: 40S ribosomal protein S28-A

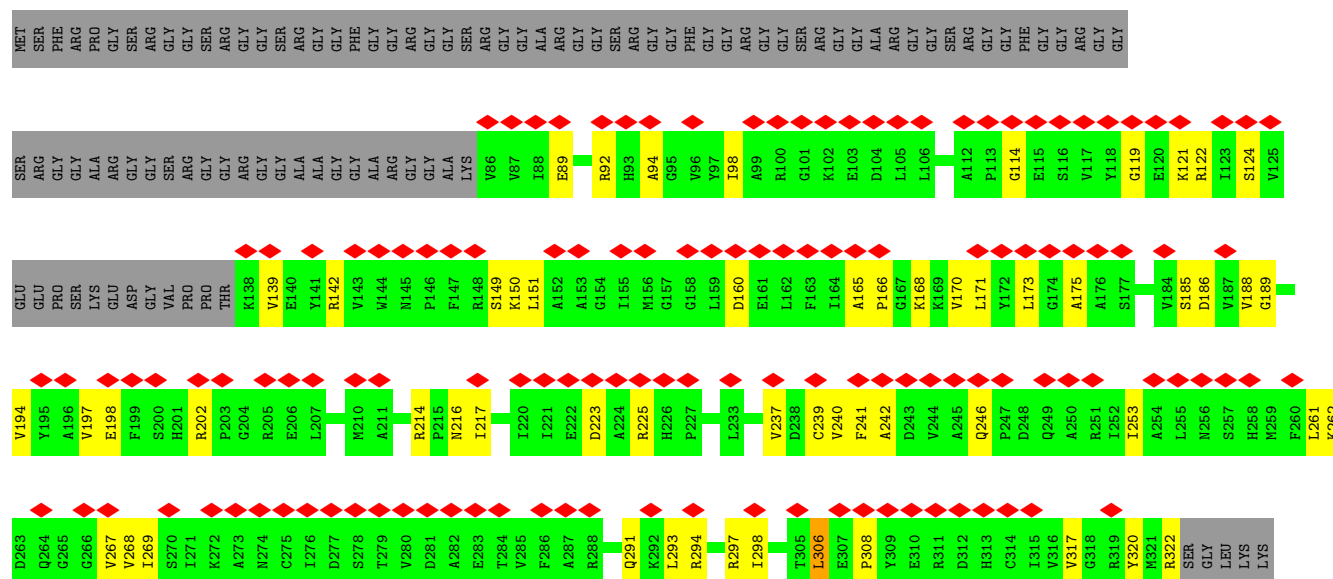
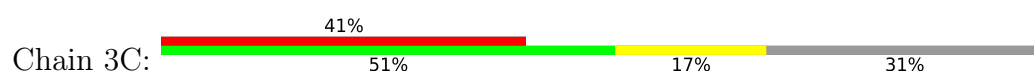


- Molecule 14: rRNA 2'-O-methyltransferase fibrillar

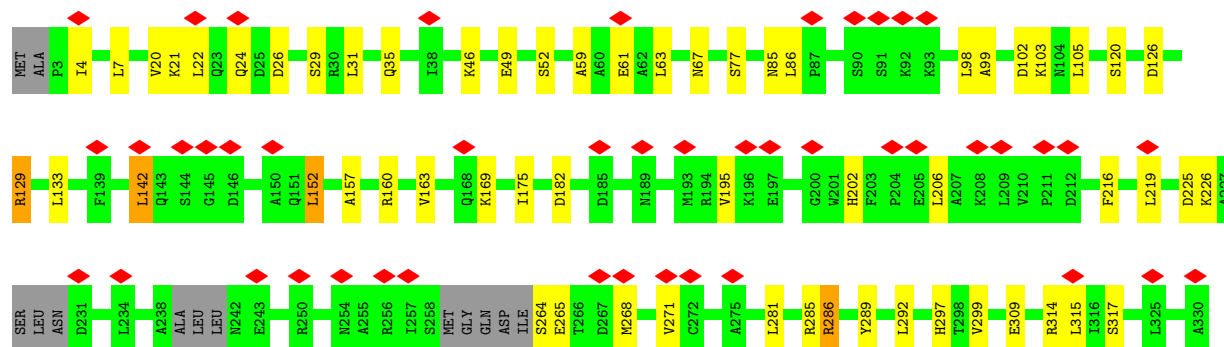




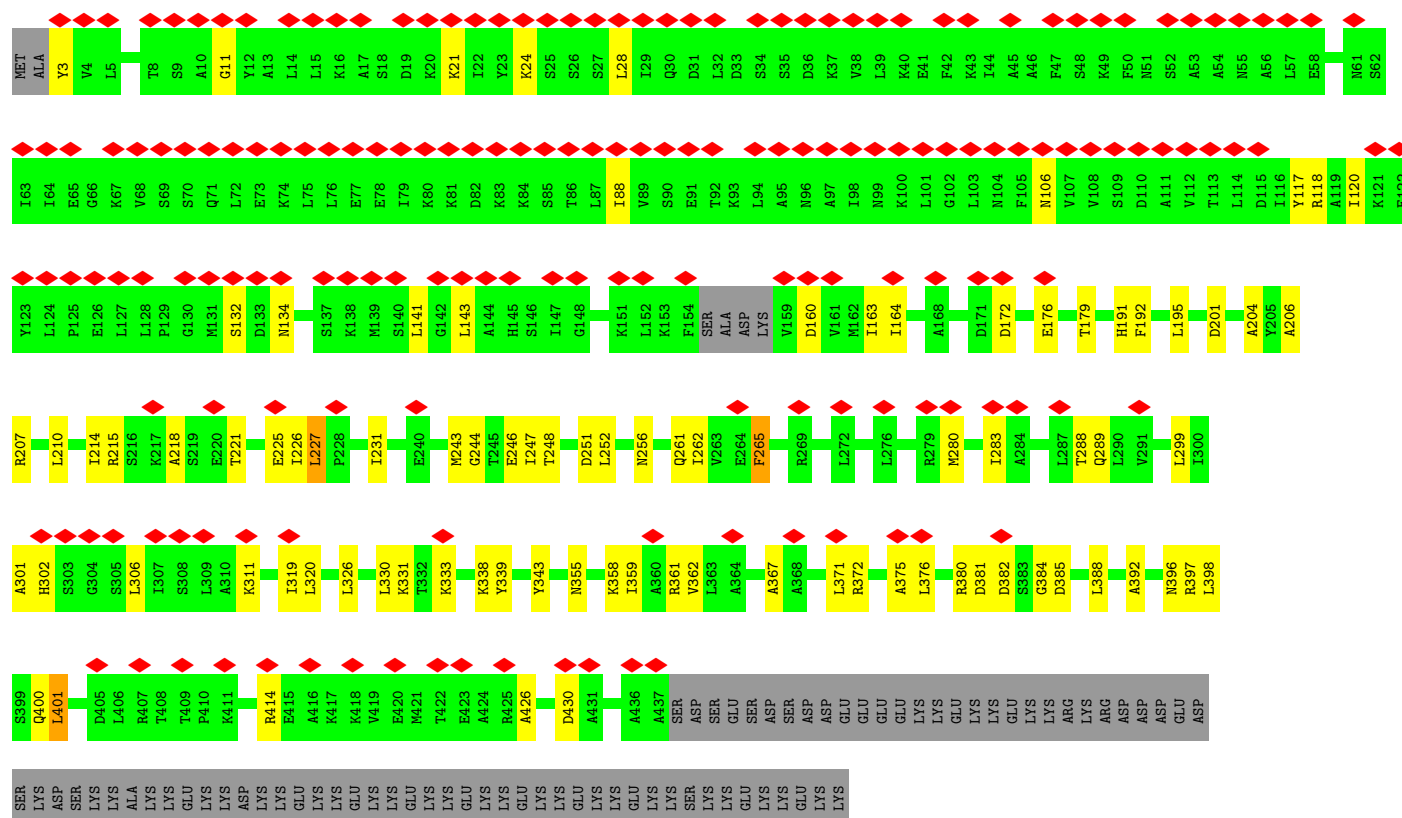
• Molecule 14: rRNA 2'-O-methyltransferase fibrillar



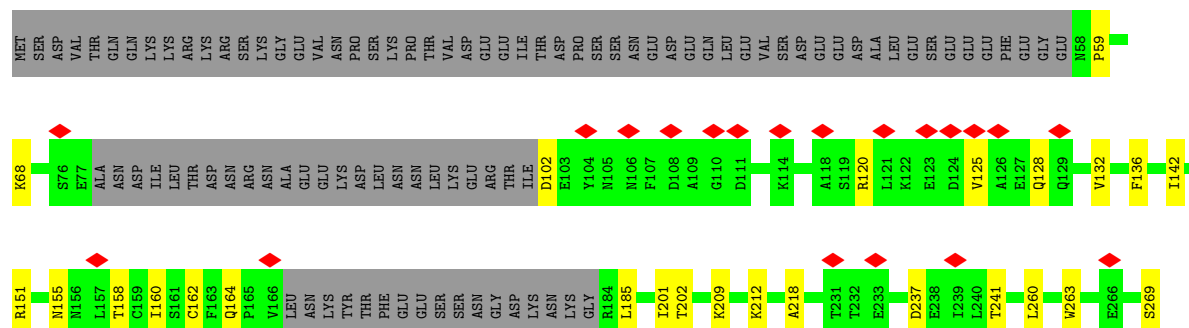
• Molecule 15: Nucleolar protein 56

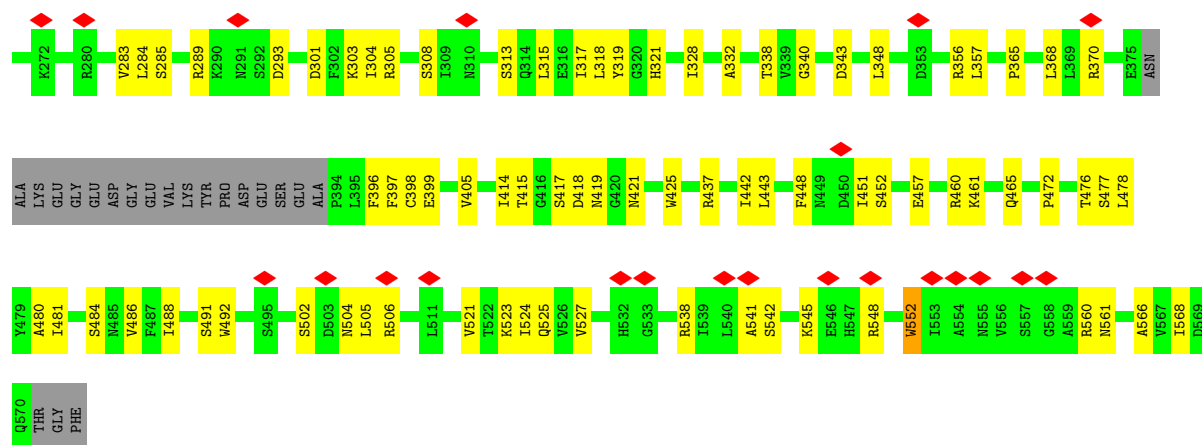


- Molecule 16: Nucleolar protein 58

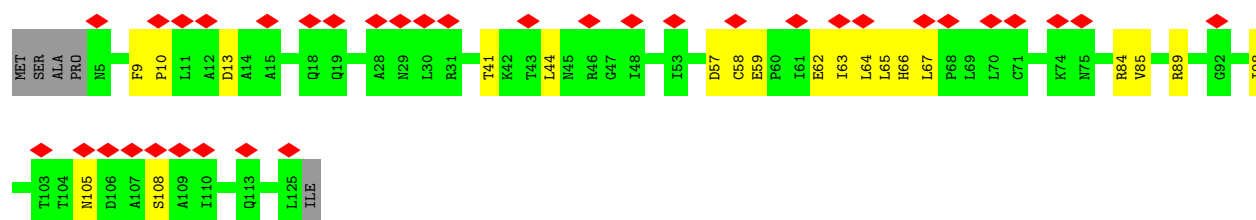
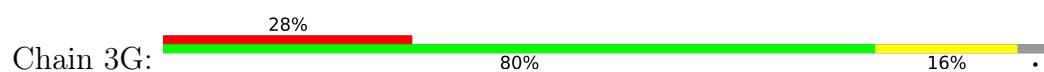


- Molecule 17: Ribosomal RNA-processing protein 9

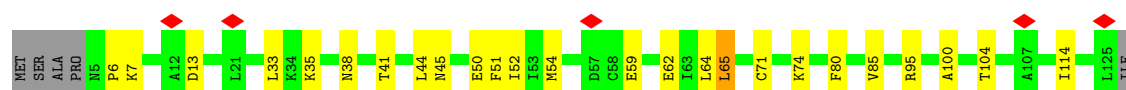
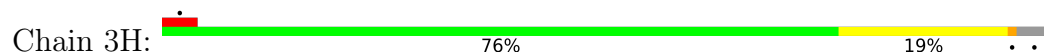




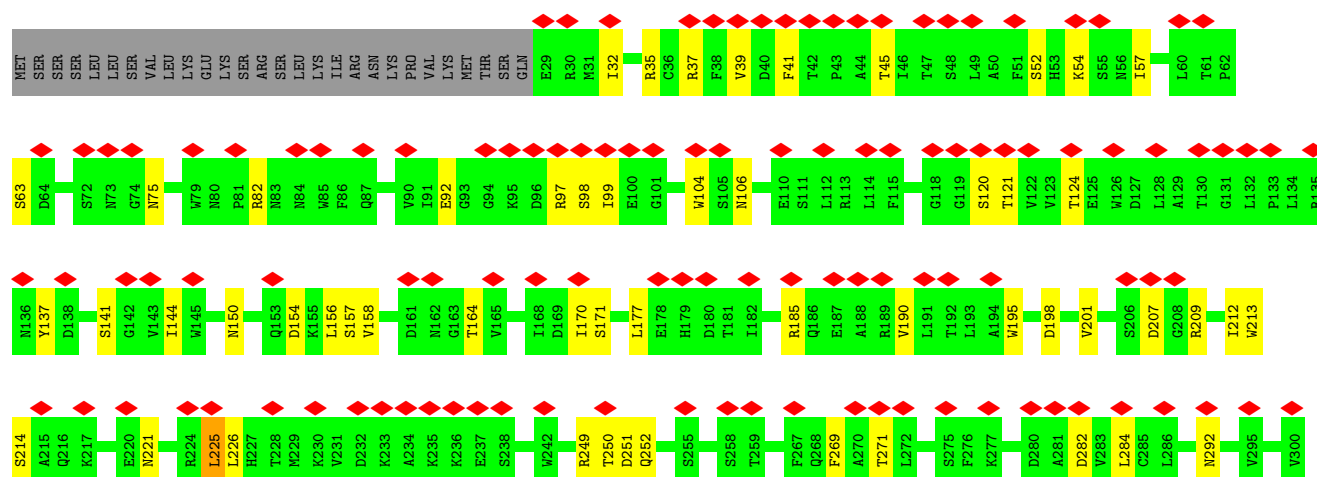
- Molecule 18: 13 kDa ribonucleoprotein-associated protein

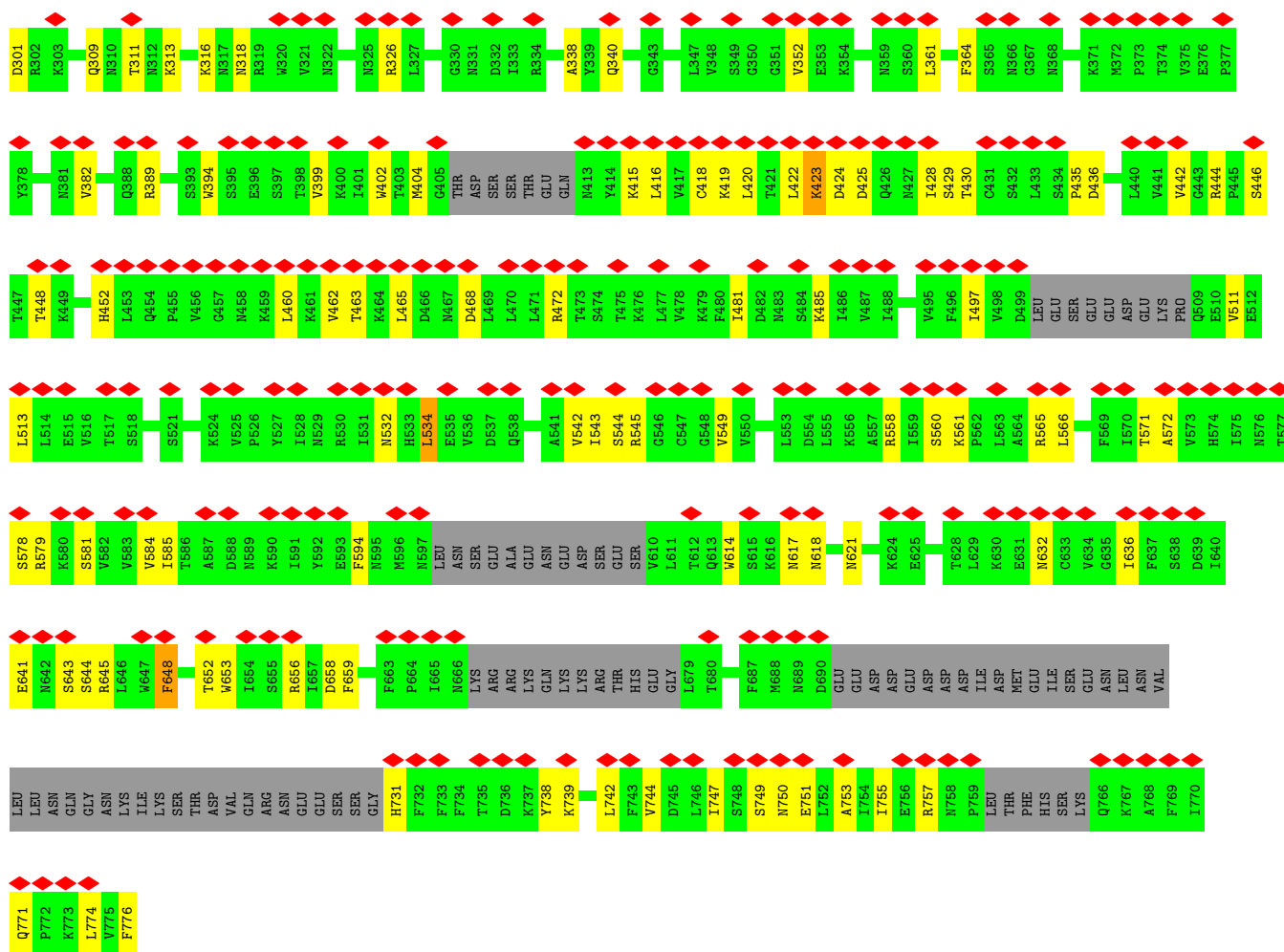


- Molecule 18: 13 kDa ribonucleoprotein-associated protein

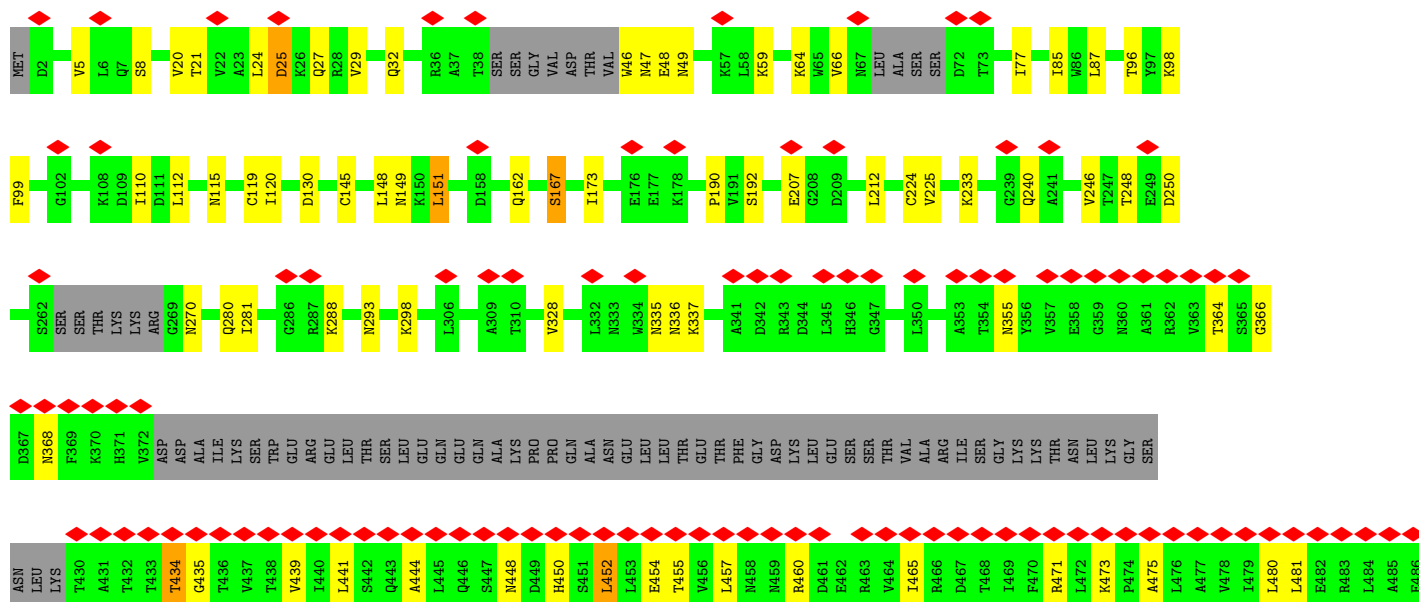


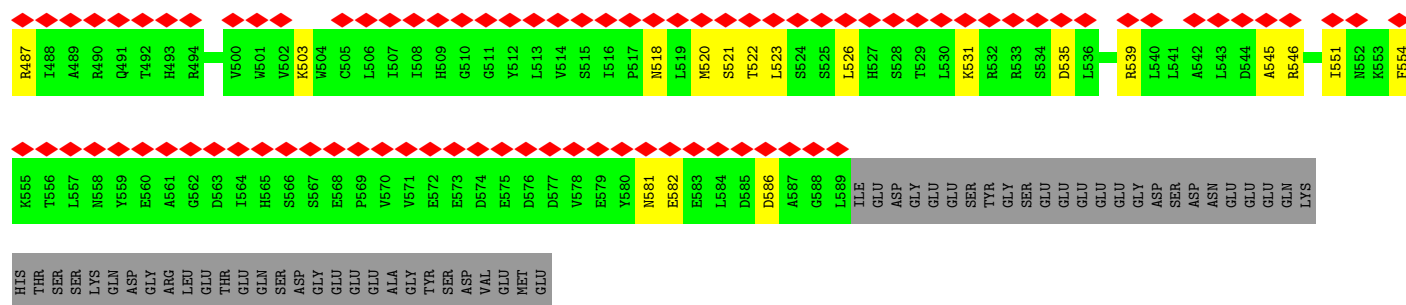
- Molecule 19: U3 small nucleolar RNA-associated protein 4



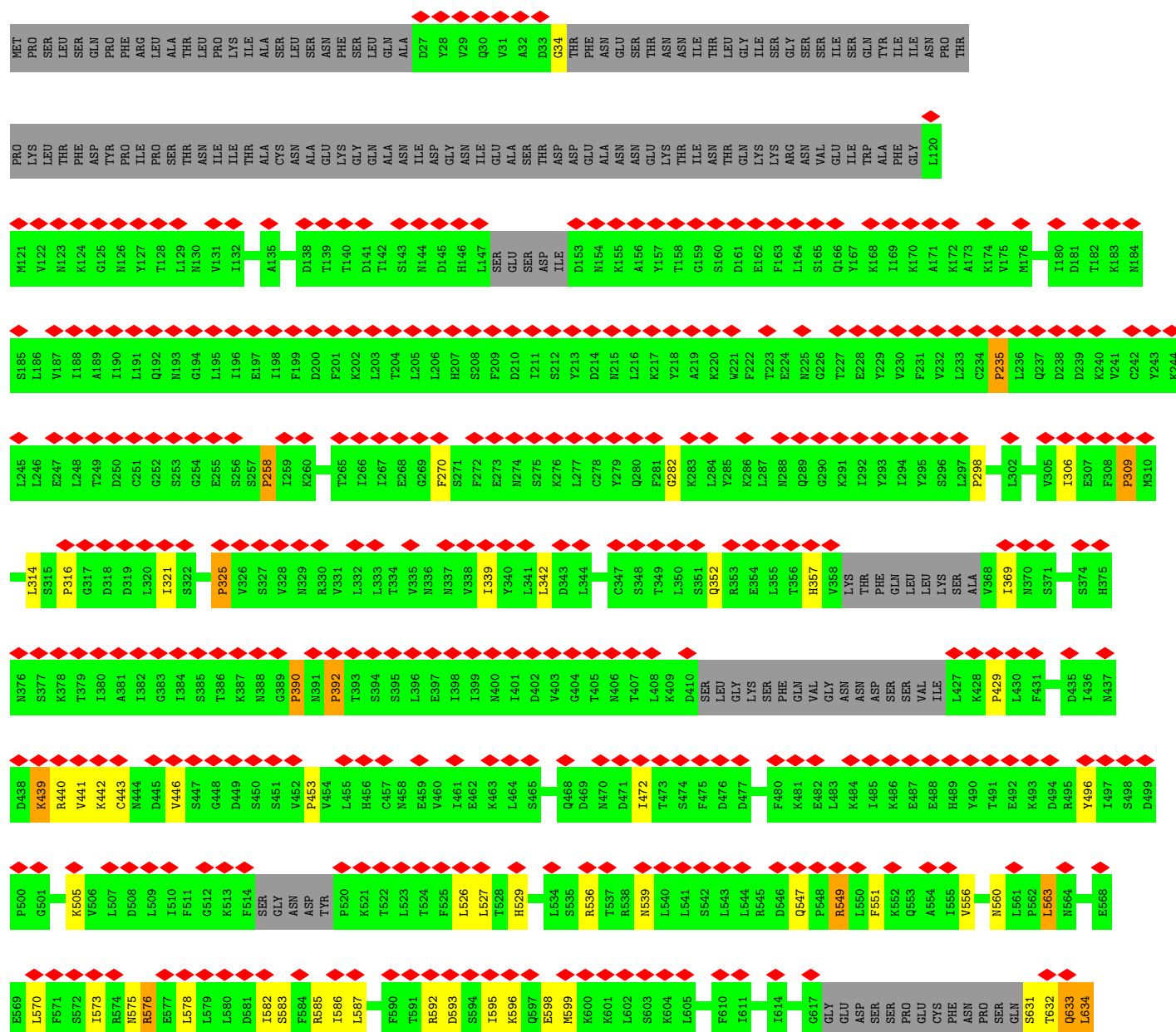


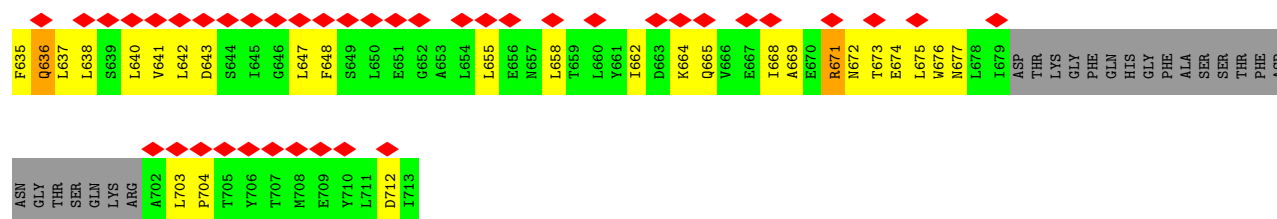
• Molecule 20: U3 small nucleolar RNA-associated protein 5



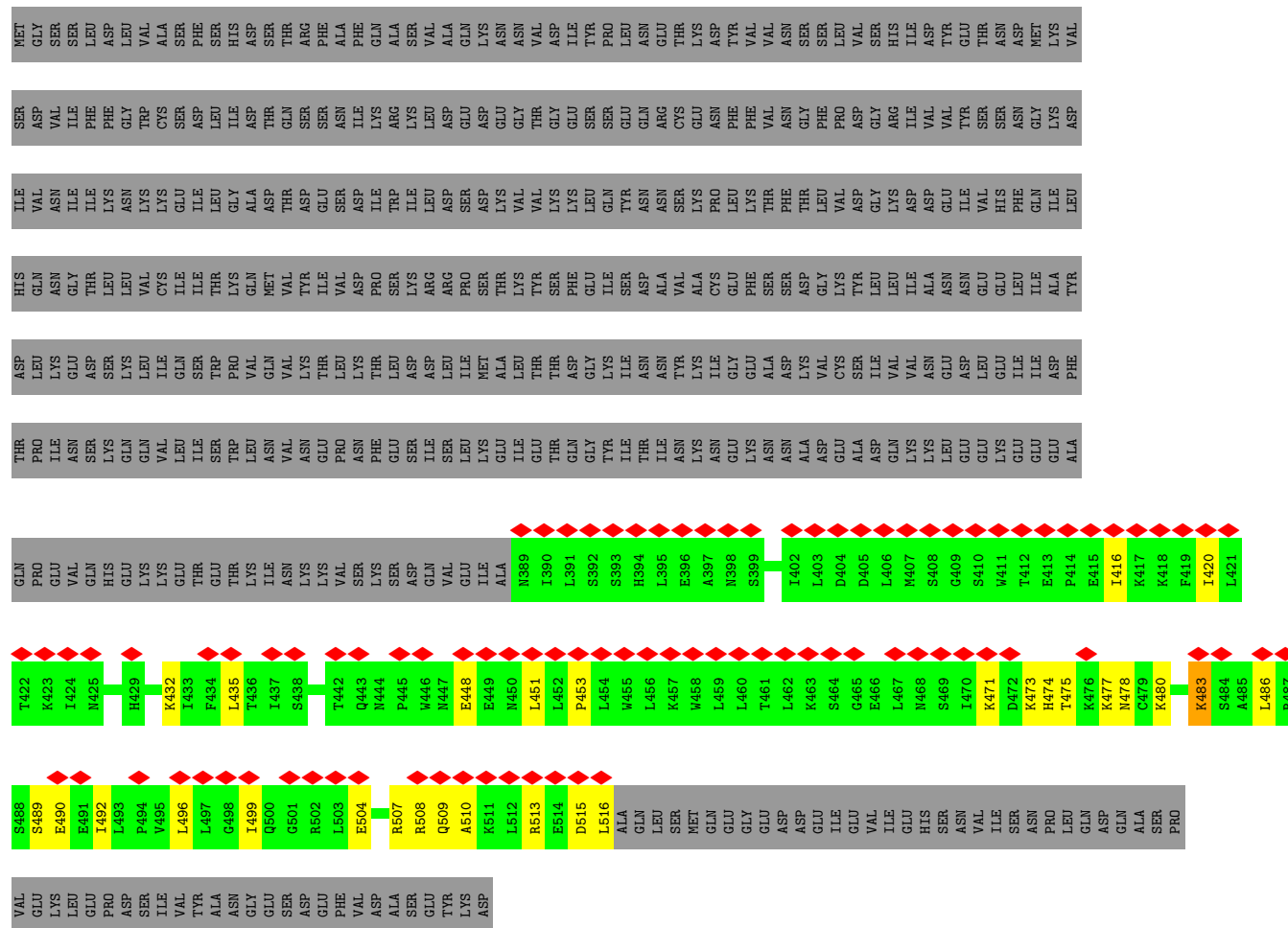


• Molecule 21: U3 small nucleolar RNA-associated protein 8

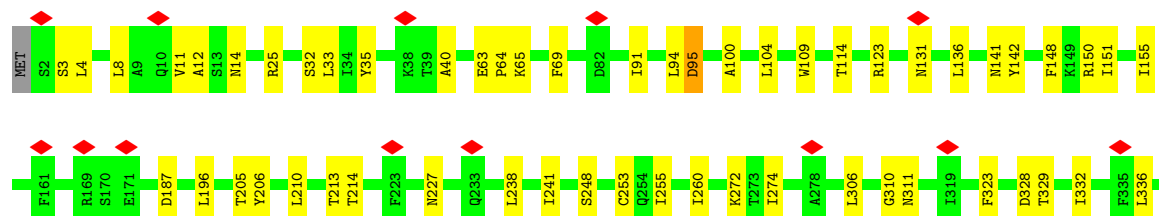
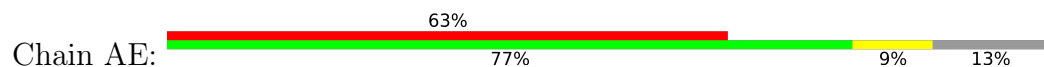




• Molecule 22: U3 small nucleolar RNA-associated protein 9



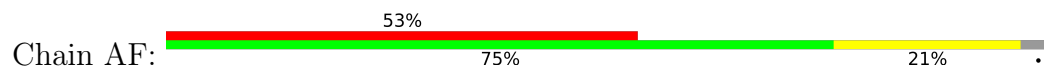
• Molecule 23: U3 small nucleolar RNA-associated protein 10



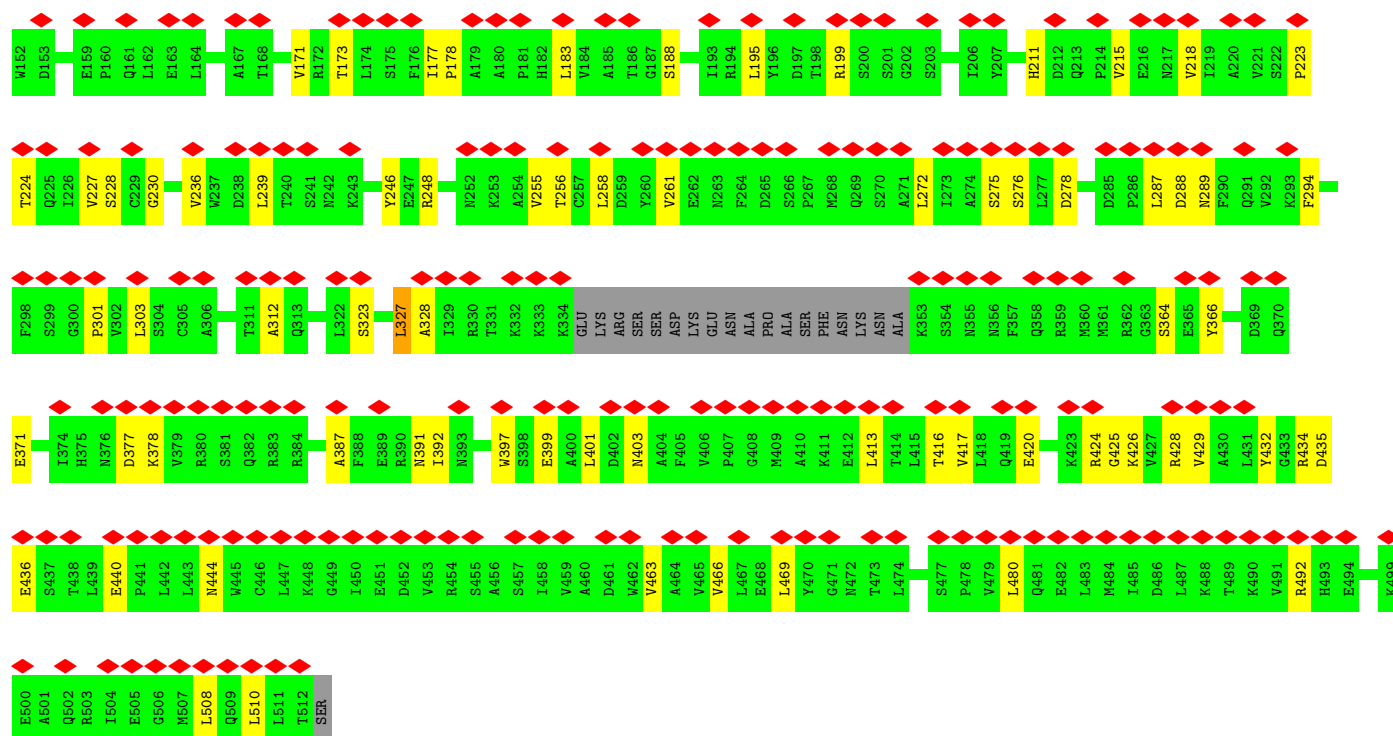


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G1719	E1659	E1599	M1539	S1479	I1419	V1359	E1299	GLN	
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W1722	I1662	D1602	K1542	E1482	V1422	L1362	S1302	V1243	
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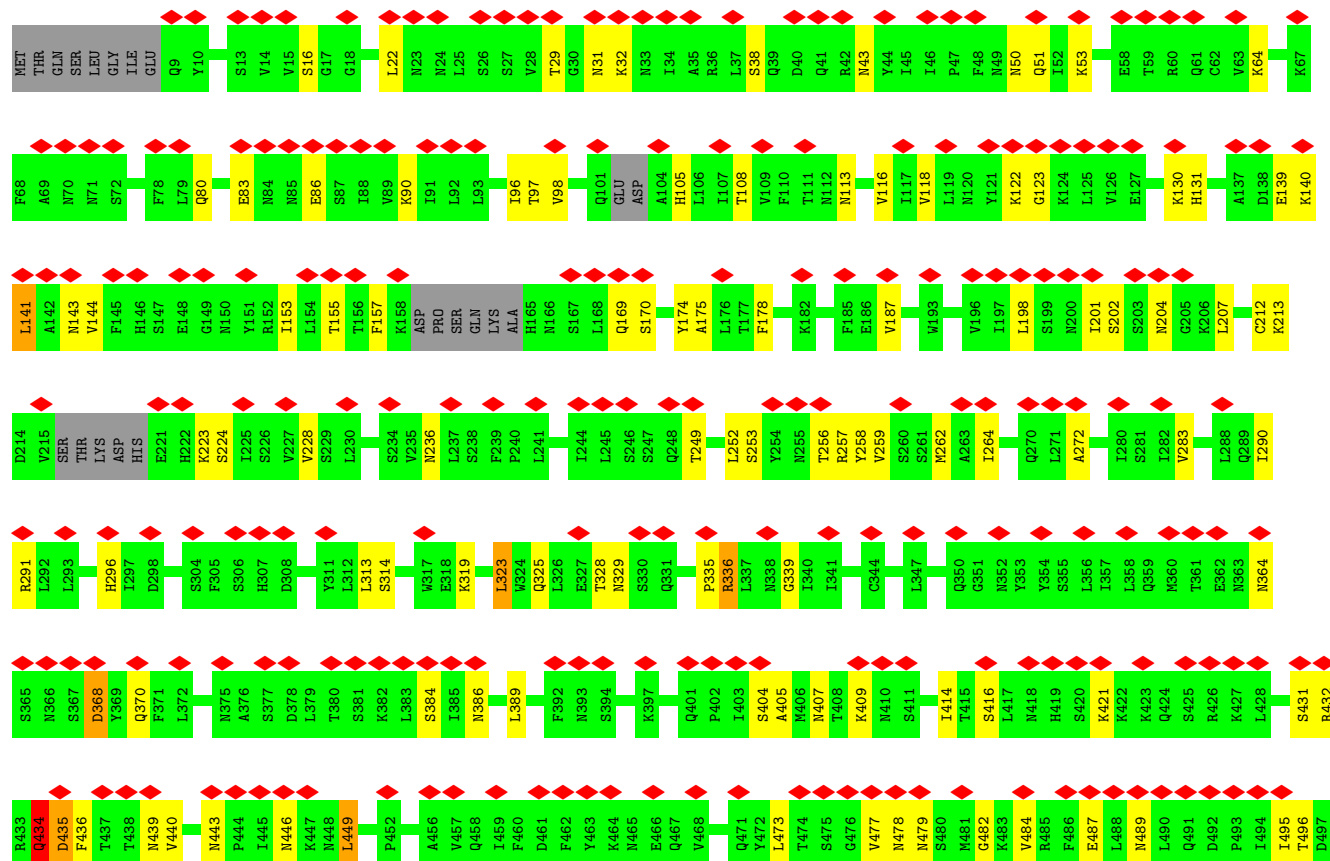
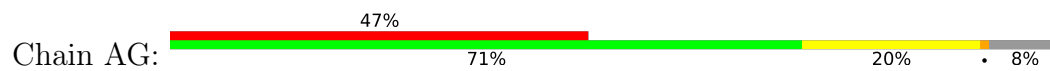
• Molecule 24: U3 small nucleolar RNA-associated protein 15

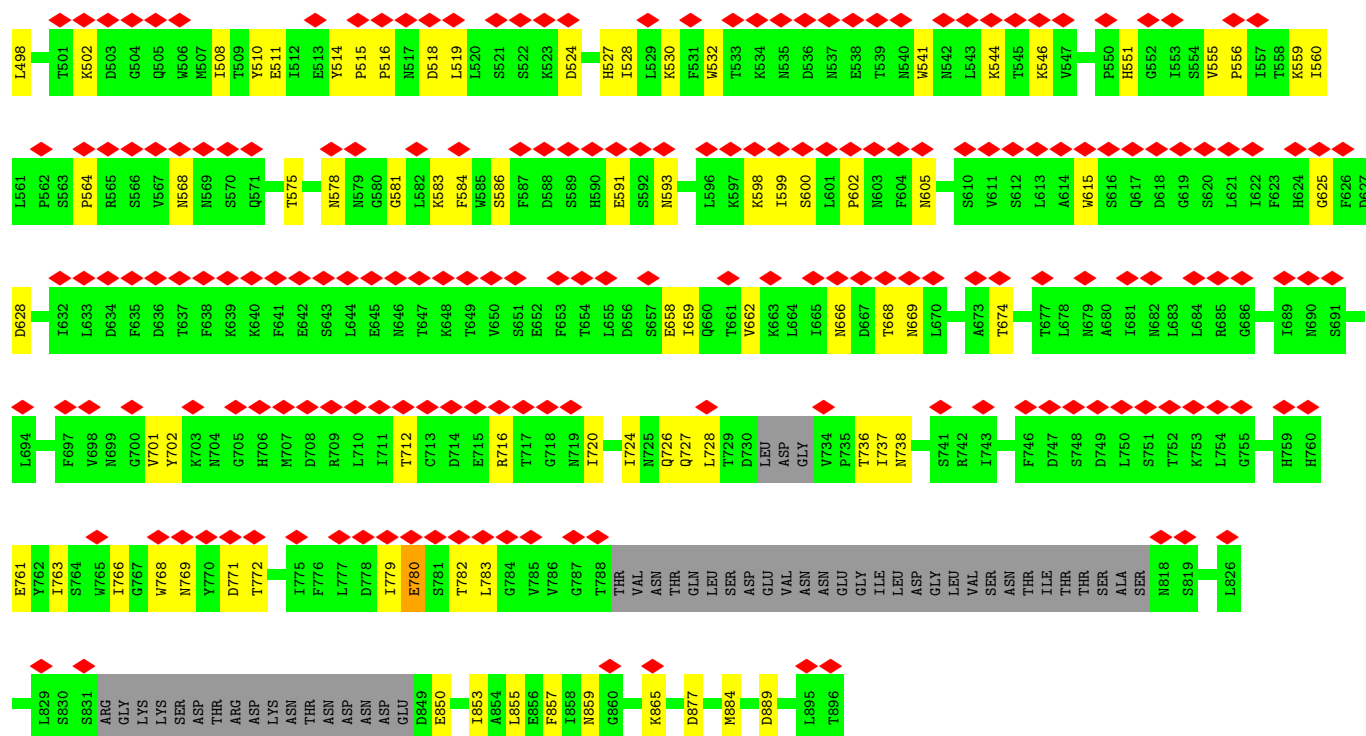


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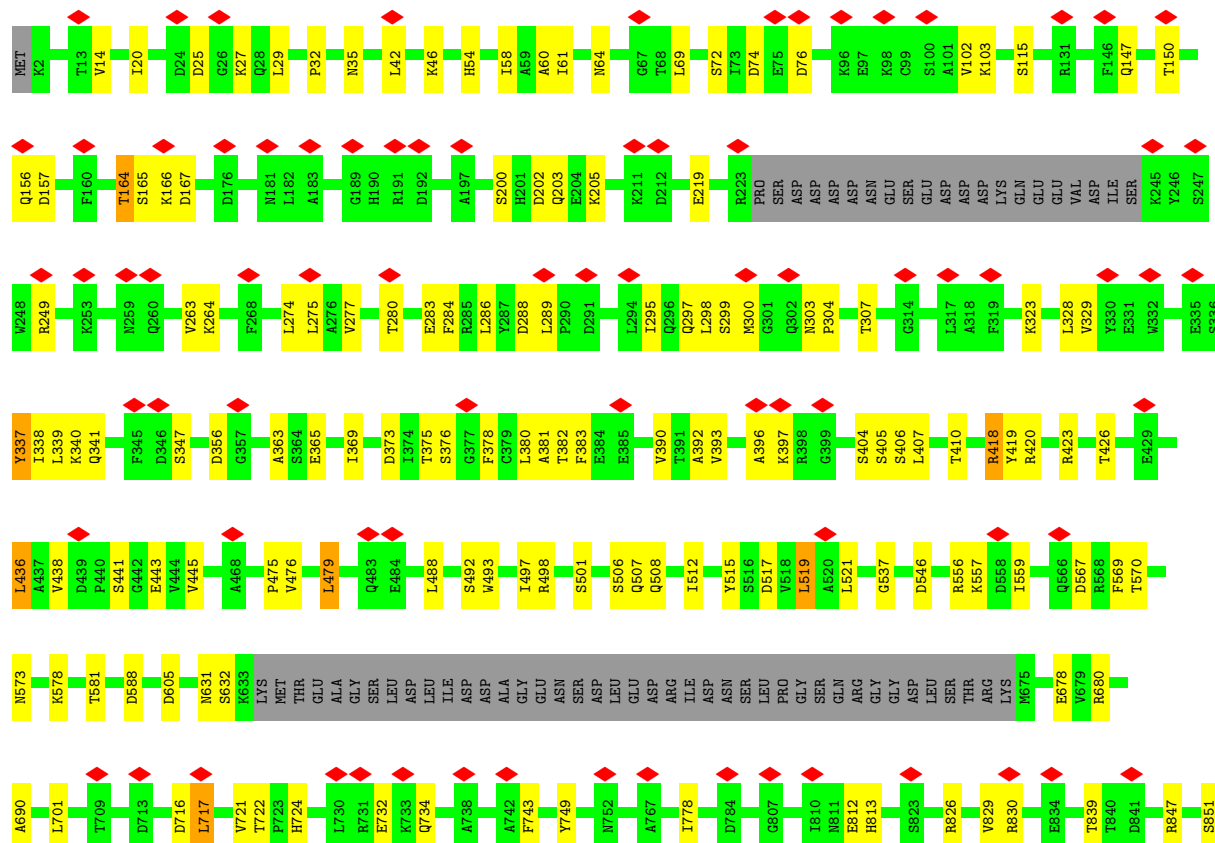
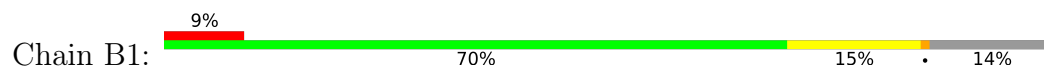


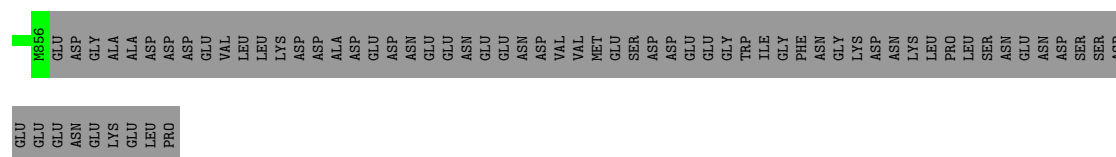
• Molecule 25: NET1-associated nuclear protein 1



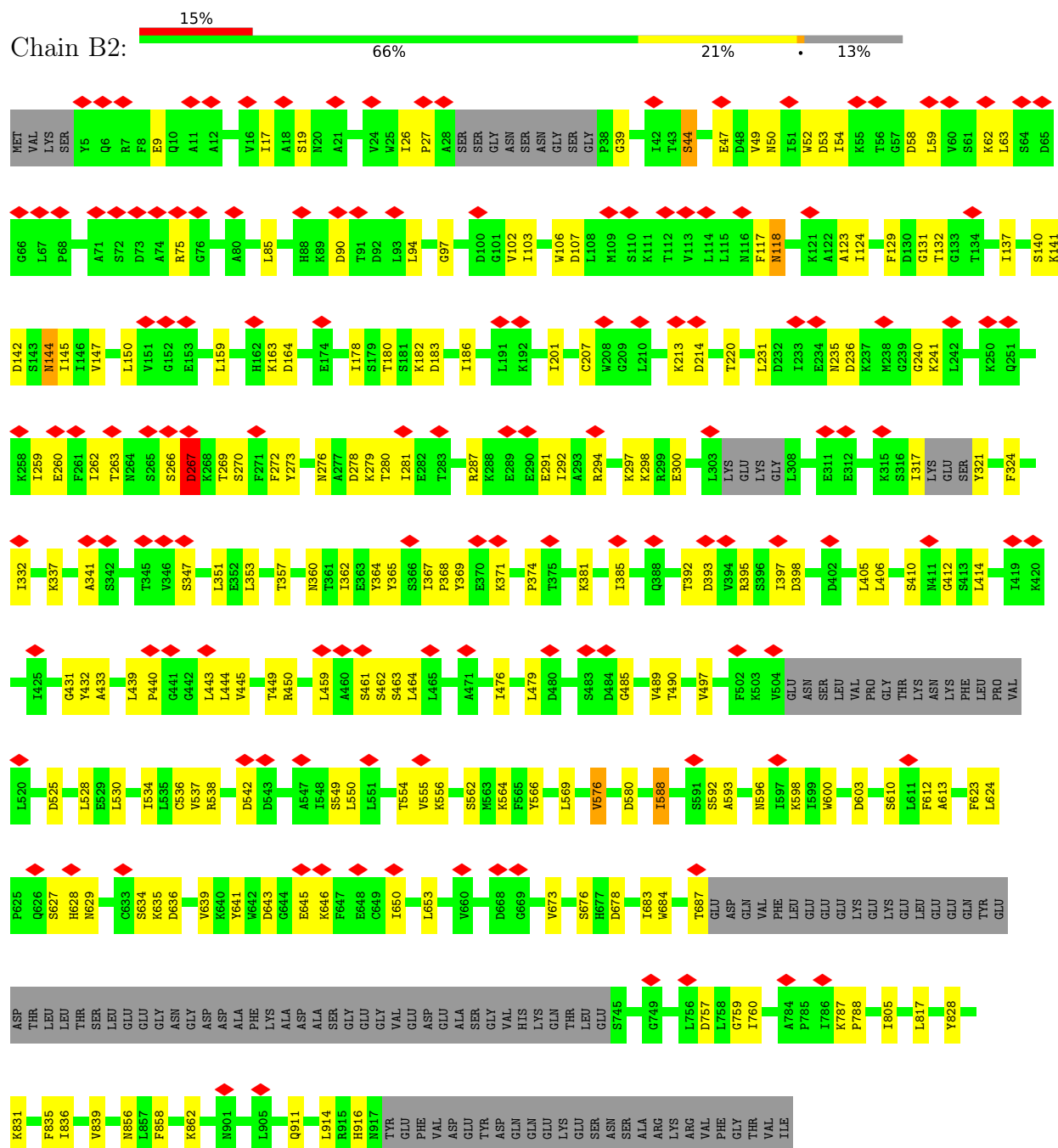


• Molecule 26: Periodic tryptophan protein 2

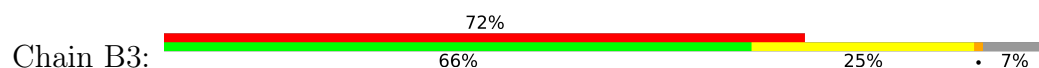


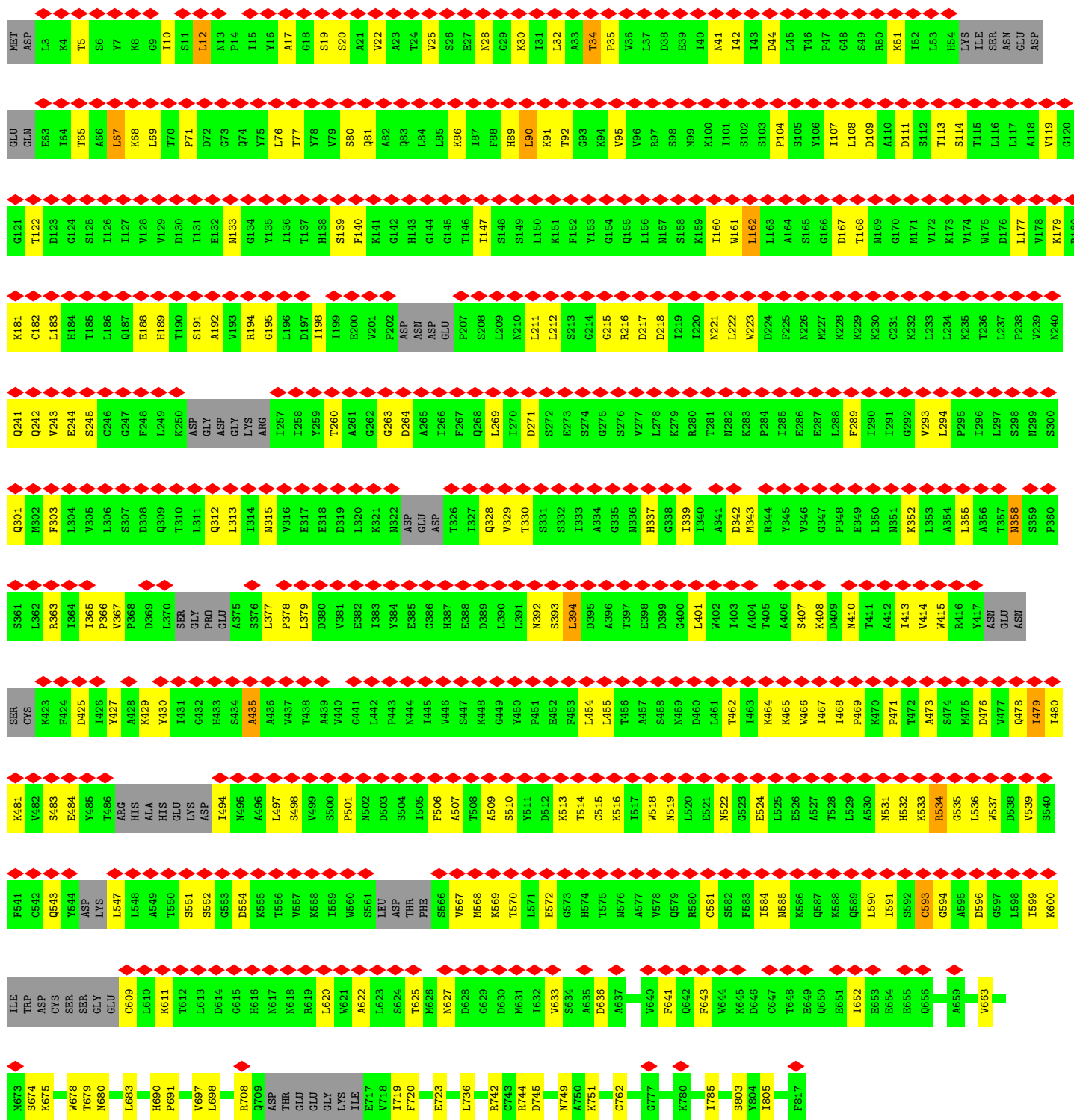


• Molecule 27: U3 small nucleolar RNA-associated protein 12

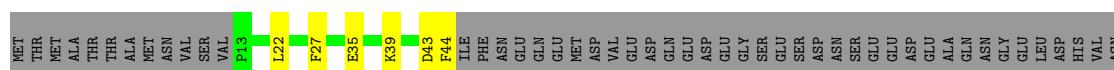


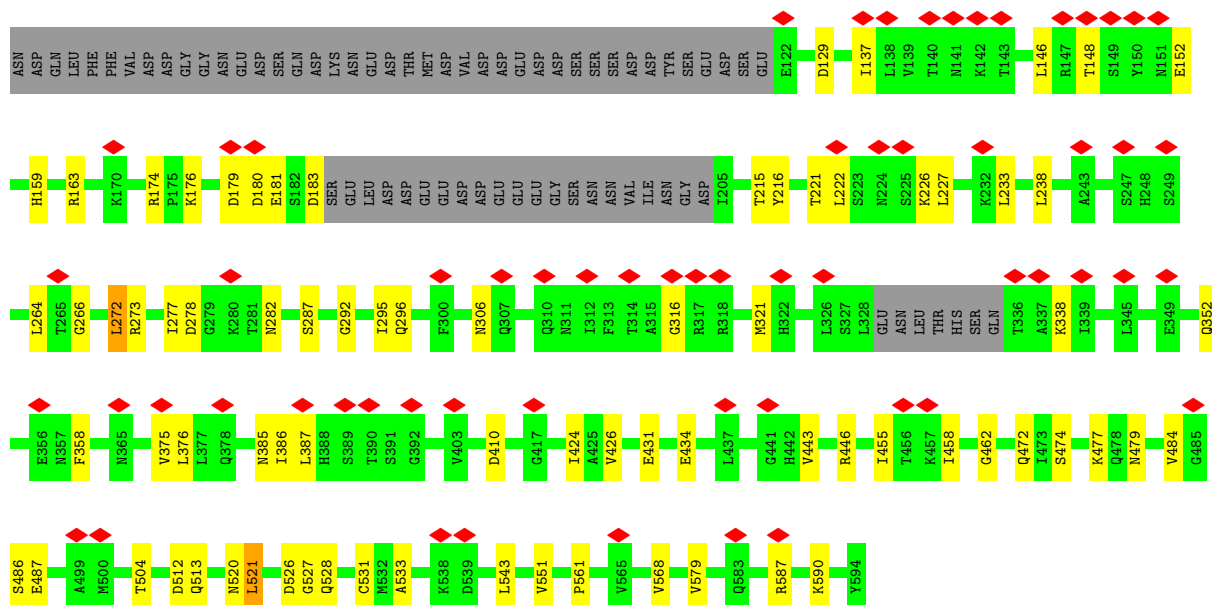
• Molecule 28: U3 small nucleolar RNA-associated protein 13



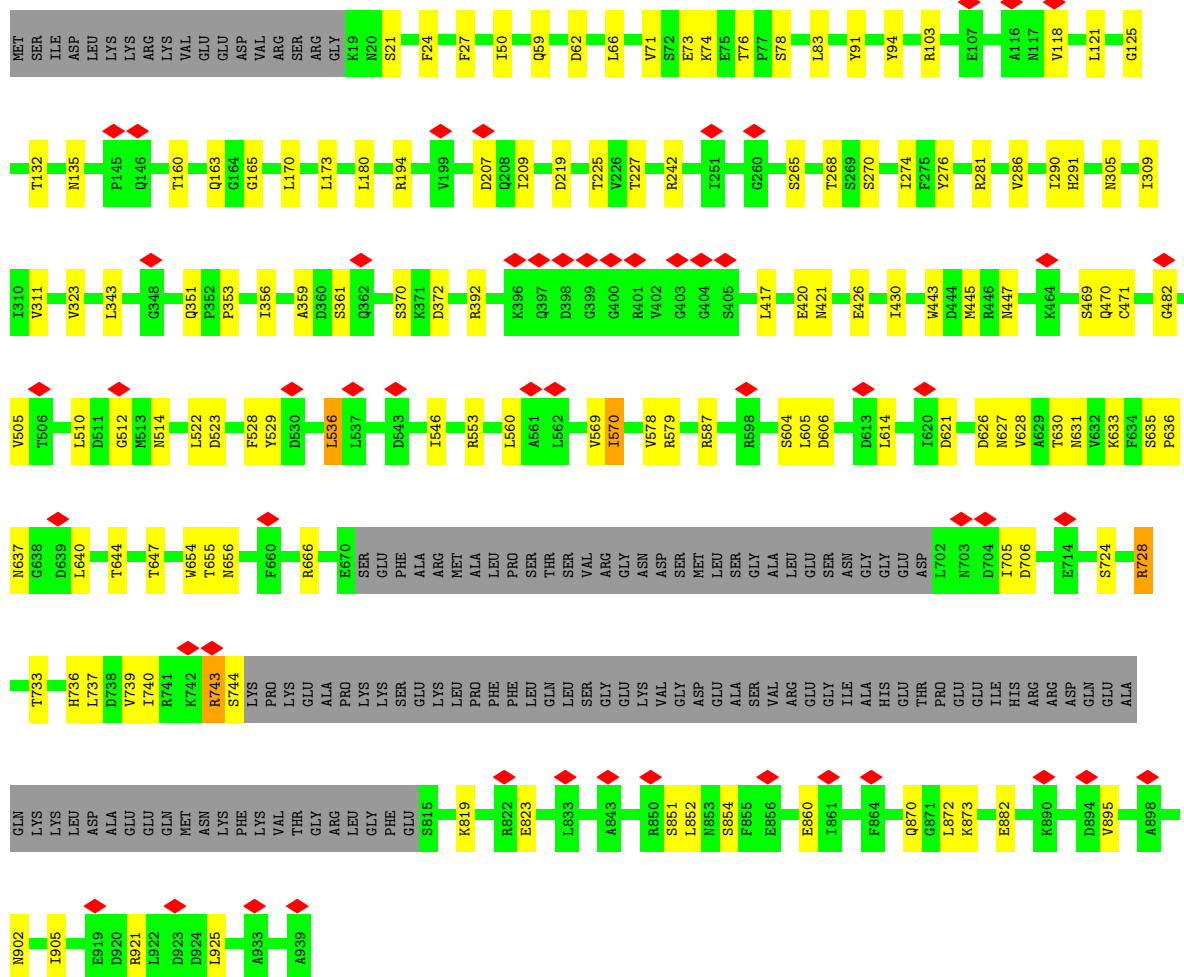
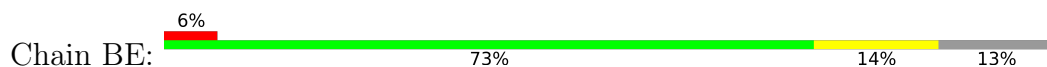


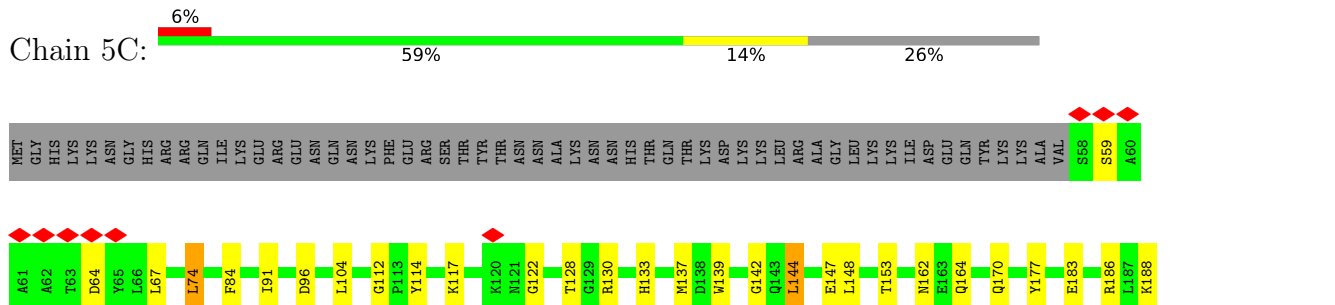
• Molecule 29: U3 small nucleolar RNA-associated protein 18



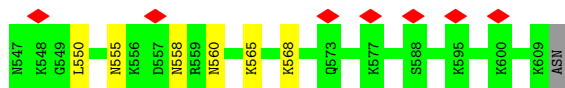


- Molecule 30: U3 small nucleolar RNA-associated protein 21

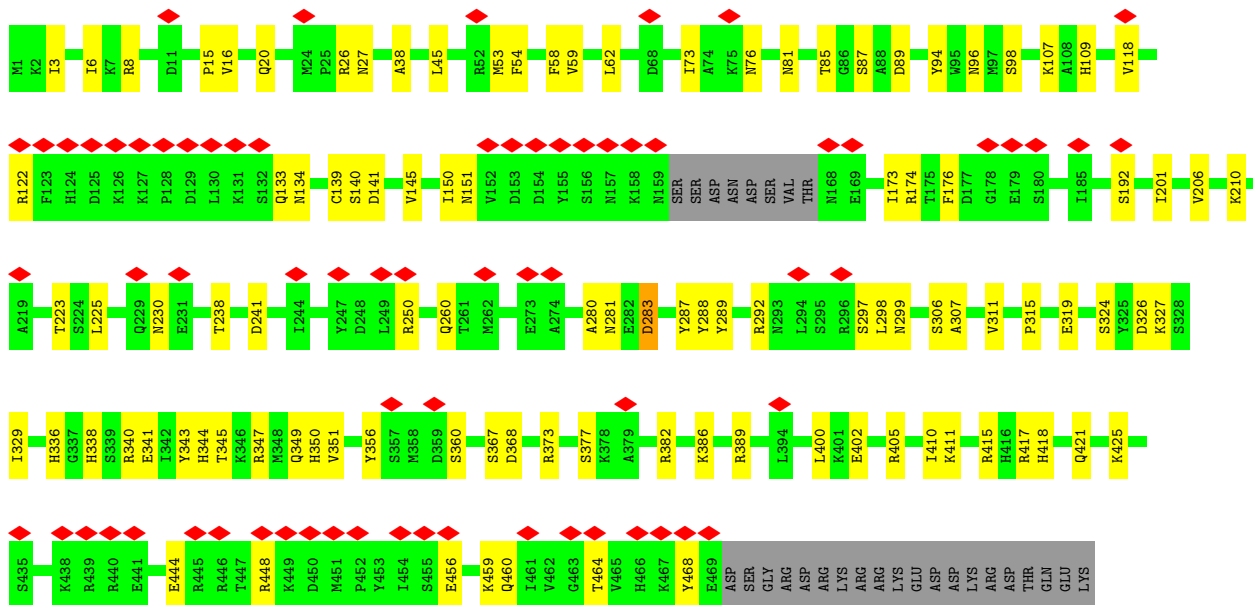




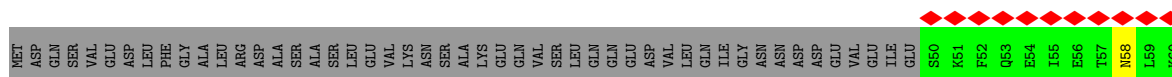
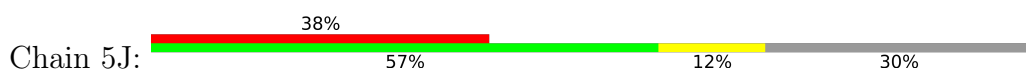


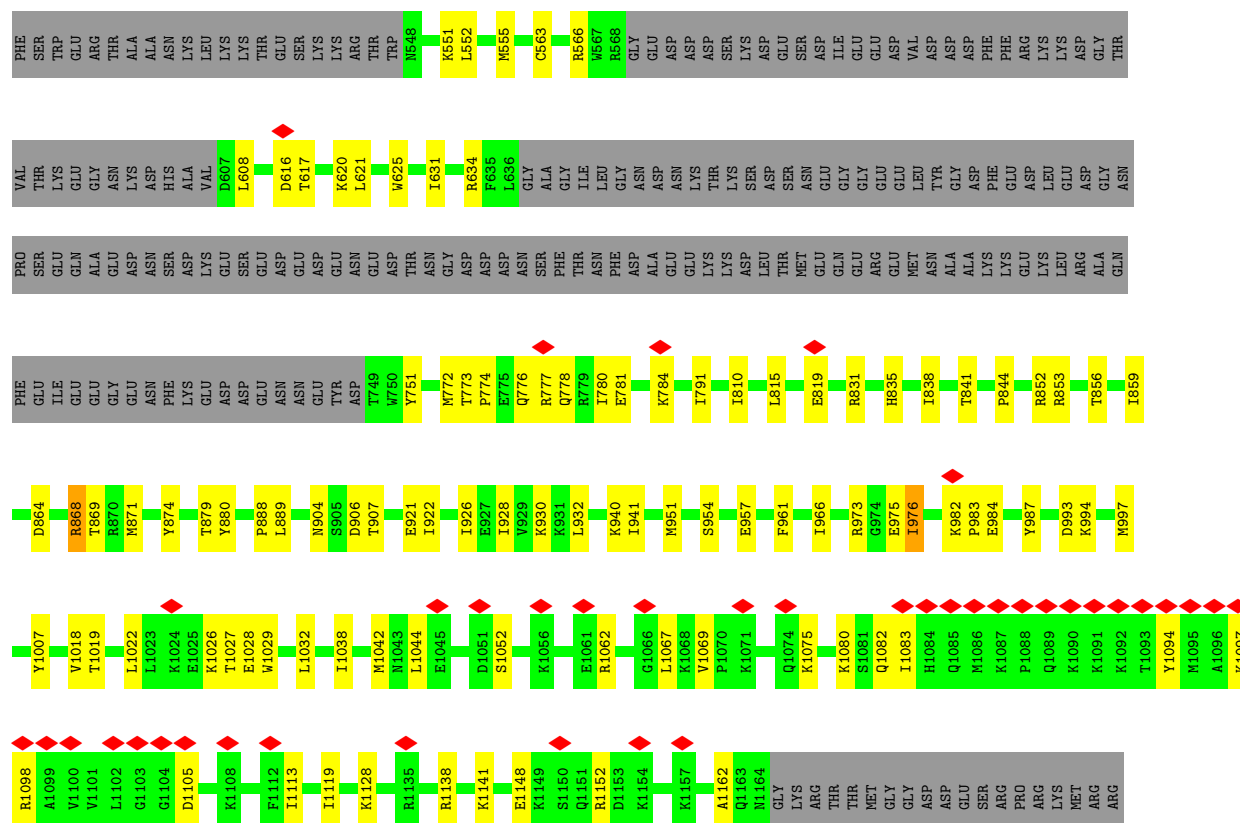


- Molecule 39: Protein SOF1

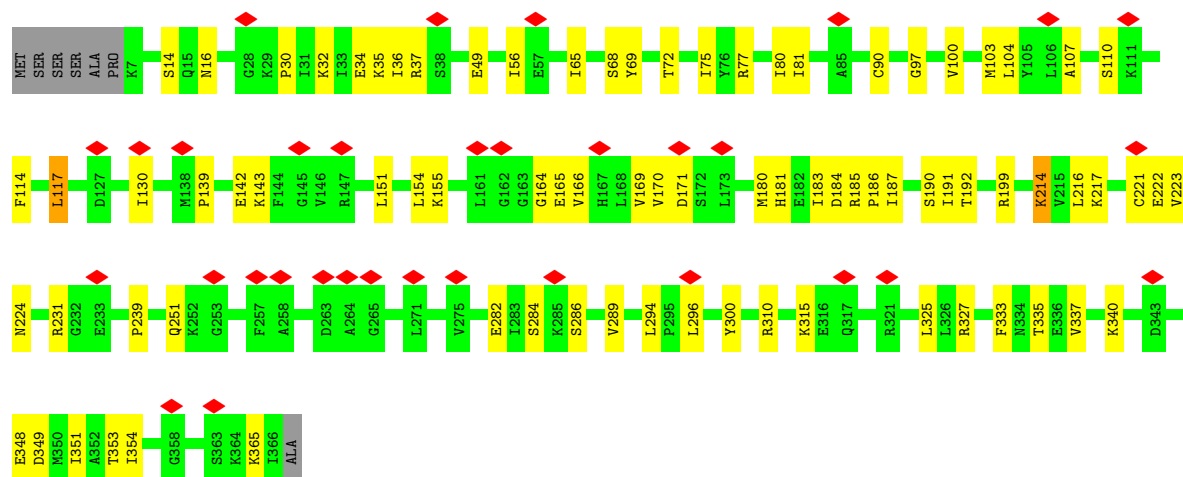
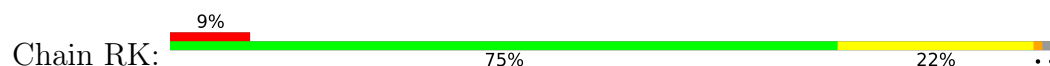


- Molecule 40: rRNA-processing protein FCF2

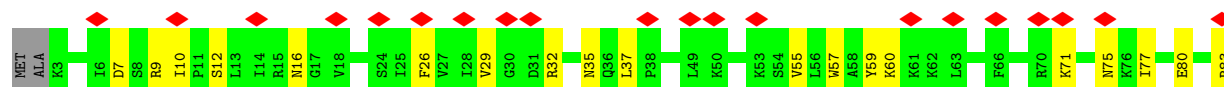
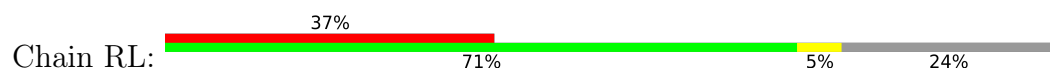




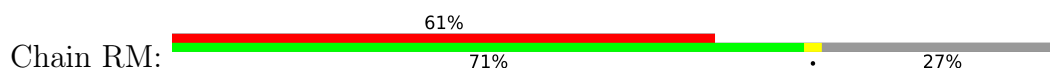
• Molecule 46: RNA 3'-terminal phosphate cyclase-like protein



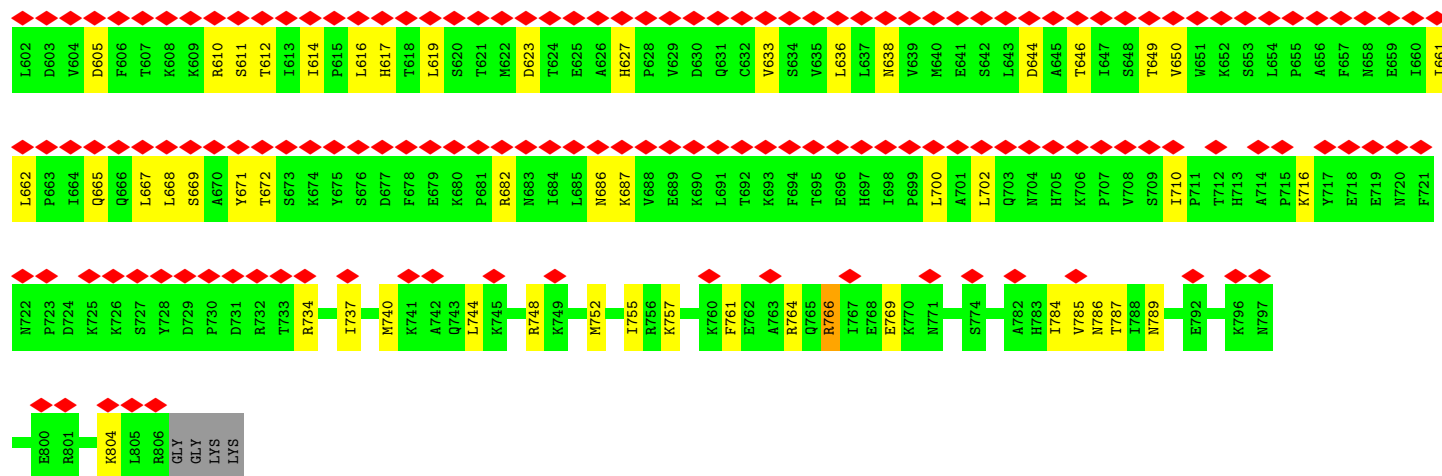
• Molecule 47: RNA cytidine acetyltransferase



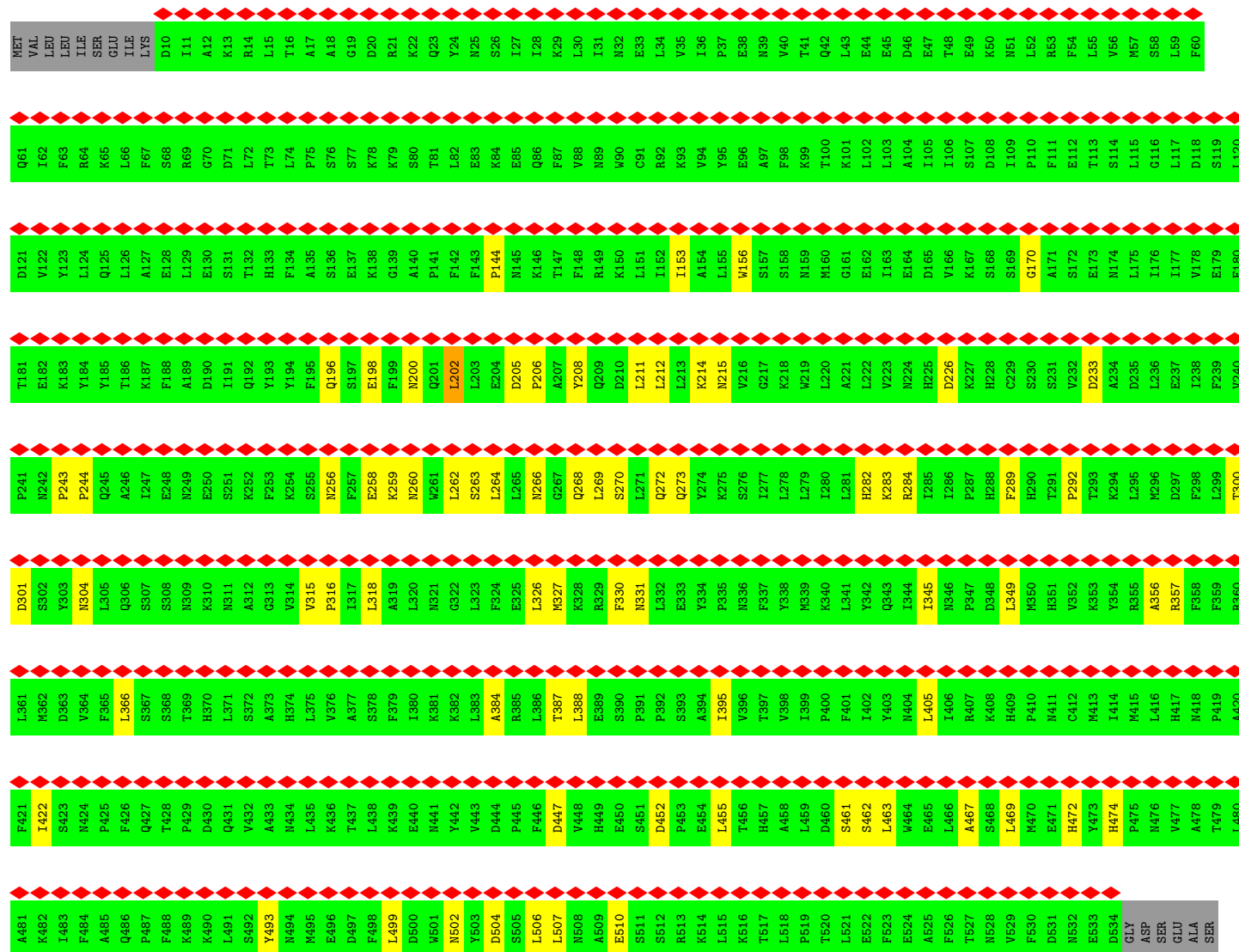
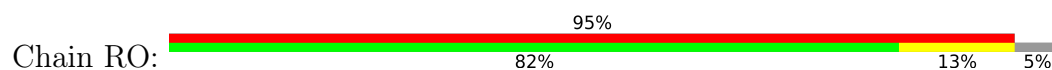




MET	K3	K4	A5	I6	D7	S8	R9	I10	P11	S12	I13	I14	R15	I16	G17	V18	I19	T20	K21	Q22	R23	S24	I25	P26	V27	I28	V29	G30	D31	R32	A33	R34	N35	Q36	L37	P38	N39	L40	H41	Y42	L43	M44	M45	S46	A47	D48	L49	K50	M51	N52	K53	S54	V55	L56	K60	K61	K62				
L63	L64	G65	F66	THR	SER	HIS	ARG	LYS	LYS	ASN	LYS	ILE	LYS	GLU	ILE	LYS	ARG	GLY	THR	ARG	GLU	MET	D92	P93	F94	E95	S96	F97	I98	S99	N100	Q101	N102	I103	R104	Y105	Y106	Y107	Y108	K109	E110	S111	E112	K113	I114	L115	G116	M117	T118	Y119	G120	M121	V122								
I123	L124	Q125	D126	F127	E128	A129	T131	P132	M133	L134	L135	A136	R137	T138	I139	E140	V200	T141	V142	E143	G144	G145	G146	I147	V148	V149	I150	L151	K152	L153	S154	M155	S156	K217	L158	K159	Q160	L161	Y162	T163	M164	T165	M166	D167	V168	H169	A170	R171	Y172	ARG	THR	GLU	ALA	HIS	GLY	ASP	V180	V181	A182		
R183	F184	M185	E186	R187	F188	I189	S191	L192	G193	S194	M195	P196	M197	L199	V201	D202	D203	E204	L205	M206	V207	L208	P209	L210	G212	A213	K214	N215	V216	K217	P218	LEU	PRO	PRO	LYS	GLU	D224	D225	E226	L227	P228	P229	V168	K230	Q231	L232	E233	L234	Q235	E236	L237	K238	E239	SER	LEU	GLU	V180	V181	A182		
D243	V244	Q245	P246	A247	G248	S249	L250	V251	S252	L253	S254	K255	T256	V257	N258	Q259	A260	H261	A262	L263	L264	S265	F266	L267	D268	A269	I270	S271	E272	K273	T274	LEU	ASN	PHE	THR	V279	A280	L281	T282	A283	G284	R285	G286	R287	G288	K289	S290	A291	A292	L293	G294	I295	S296	I297	A298	A299	A300	V301	S302		
H303	G304	Y305	S306	N307	I308	F309	V310	T311	S312	P313	S314	P315	E316	N317	L318	K319	T320	L321	F322	L323	F324	I325	F326	K327	G328	F329	D330	A331	L332	G333	Y334	Q335	E336	H337	ILE	ASP	TYR	ASP	ILE	GLN	SER	THR	ASN	PRO	PHE	ALA	I354	V355	R356	V357	D358	I359	K360	ARG	ASP						
HIS	ARG	GLN	THR	ILE	Q368	Y369	I370	V371	P372	Q373	D374	H375	Q376	V377	L378	G379	Q380	A381	E382	L383	V384	V385	I386	E387	E388	A389	A390	A391	I392	PRO	LEU	PRO	I396	V397	K398	N399	L400	L401	G402	P403	Y404	L405	V406	F407	M408	A409	S410	T411	I412	N413	G414	TYR	GLU	GLY	THR	ARG	SER	L422			
S423	L424	K425	L426	I427	Q428	Q429	L430	R431	M432	Q433	ASN	ASN	THR	SER	GLY	ARG	GLU	SER	GLN	THR	ALA	VAL	SER	ARG	ASP	ASN	LYS	GLU	LYS	ASP	SER	HIS	HIS	SER	GLN	SER	ARG	E467	I468	S469	L470	D471	E472	P473	I474	R475	Y476	A477	P478	G479	D480	P481	I482								
E483	K484	W485	L486	N487	K488	L489	L490	C491	Q492	D493	V494	T495	L496	I497	K498	N499	P500	R501	F502	A503	T504	R505	G506	T507	P508	H509	P510	S511	Q512	C513	F516	V517	V518	T522	L523	F524	S525	Y526	H527	P528	V529	S530	E531	N532	F533	L534	E535	K536	M537	M538	A539	Y541	V542	S543	S544						
Y546	K547	N548	S549	P550	N551	D552	L553	Q554	L555	M556	S557	D558	H562	K563	L564	F565	V566	L567	L568	P569	P570	I571	D572	P573	K574	G575	G576	G577	R578	I579	P580	D581	I582	C584	V585	I586	Q587	I588	A589	LEU	GLU	LYS	PHE	THR	ASP	MET	SER	GLU	ASP	VAL	ARG	PRO	LYS	ASP	N601	S602	L603	S604	G605	G606	Q607
R608	I614	L617	I618	Q621	F622	Q623	D624	L630	S631	G632	A633	R634	I635	V636	R637	I638	A639	T640	N641	P642	E643	Y644	A645	G648	Y649	G650	S651	R652	A653	I654	E655	L656	L657	R658	D659	Y660	F661	GLU	GLY	LYS	THR	ASP	MET	SER	GLU	ASP	VAL	ARG	PRO	LYS	ASP	TYR	SER								
ILE	LYS	ARG	VAL	SER	LYS	GLU	ALA	THR	ASN	LEU	LYS	ASP	ASP	VAL	LYS	LEU	ARG	ASP	ALA	PRO	PRO	L708	L709	L710	K711	L712	S713	E714	Q715	P716	P717	H718	A653	L654	E655	L656	L657	R658	D659	Y660	F661	L729	L730	LEU	Q731	S732	L733	H734	K735	MET	V804	T805	E806	S807	S808	Q812	D813	L814	S815	D816	D817



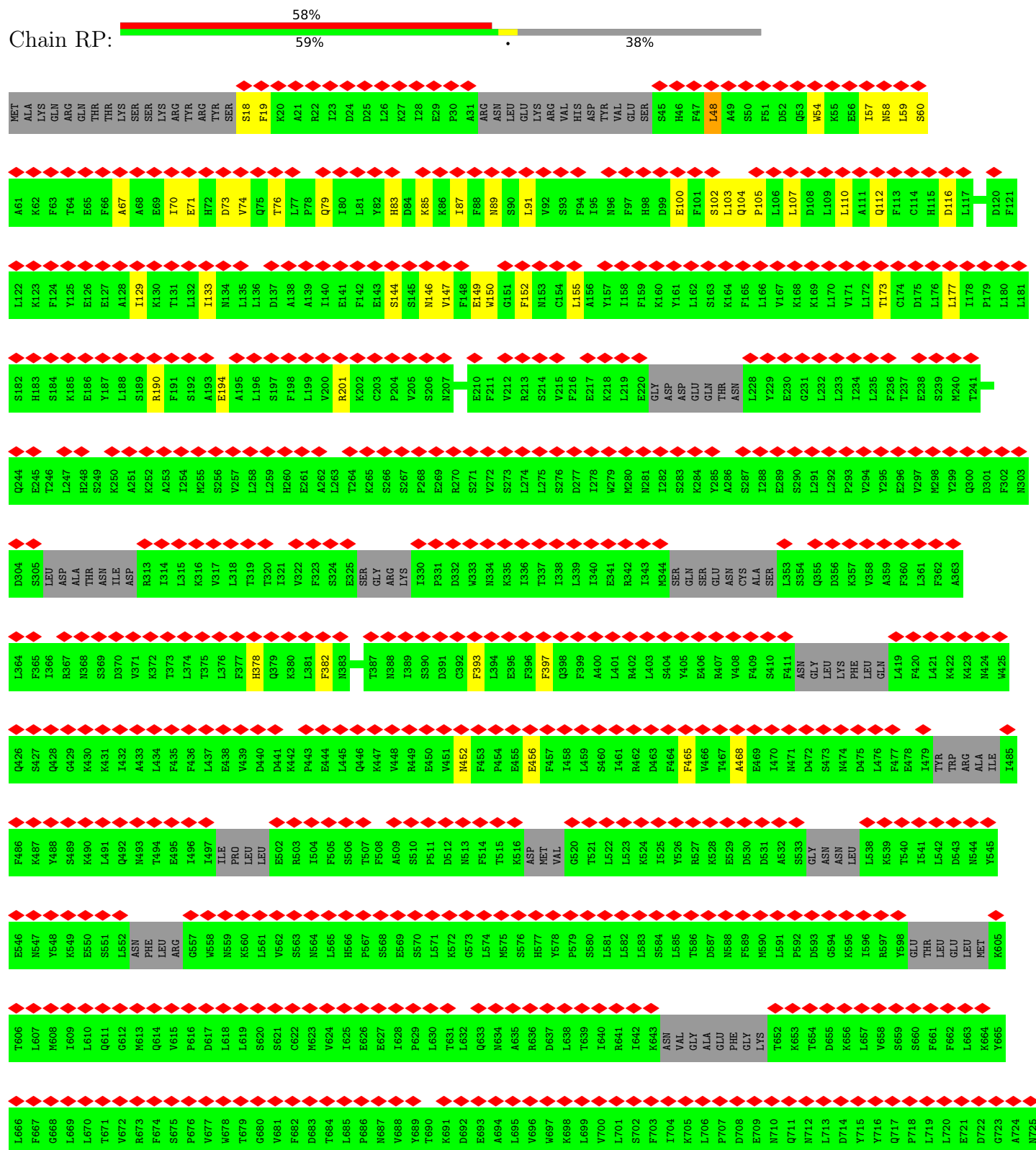
• Molecule 49: Nucleolar complex protein 4



SER
GLN
GLY
ASN
VAL
GLN
THR
LEU
PRO
GLY
VAL
ALA
TRP

● Molecule 50: U3 small nucleolar RNA-associated protein 20

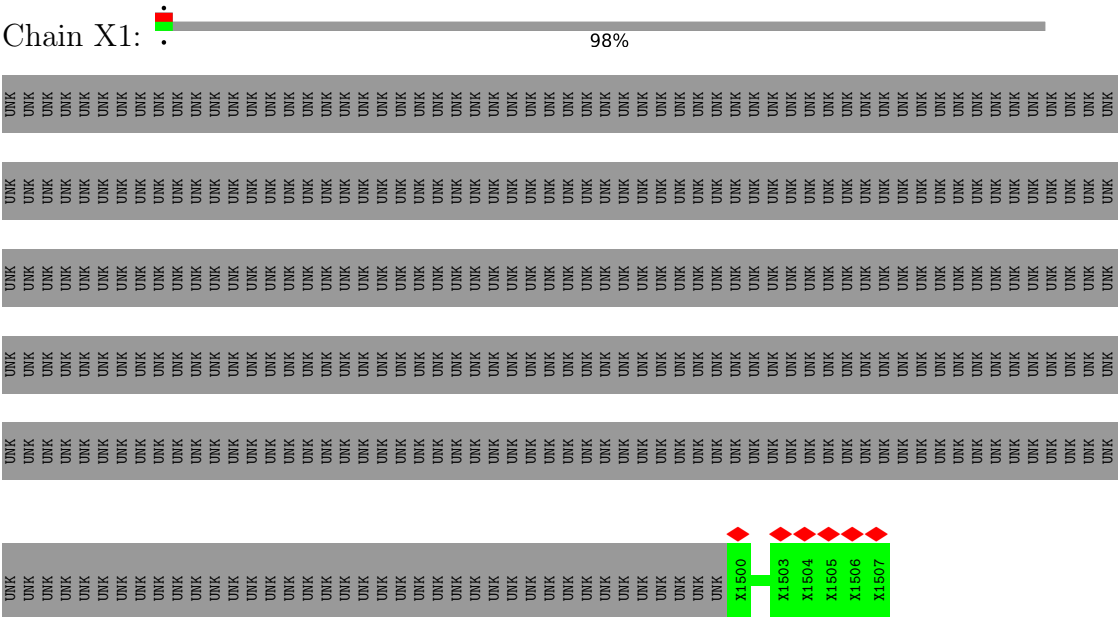
Chain RP:



R1468	L1469	G1470	H1471	H1472	A1473	H1474	Q1475	L1476	K1477	D1478	N1479	S1480	I1481	S1482	H1483	V1484	L1485	I1486	P1487	M1488	I1489	E1490	H1491	V1492	V1493	F1494	S1495	D1496	M1497	A1498	I1499	V1500	N1501	N1502	I1503	G1504	N1505	E1506	T1507	I1508	I1509	PHE	PHE	THR	ASN	ASN	VAL	HIS	ILE	GLN	LEU	HIS	R1461	R1462	Q1463	R1464	N1520	N1521	Q1522	Y1523	K1524	A1525	L1526	L1527
D1408	S1409	L1410	E1411	E1412	V1413	GLN	SER	GLU	TYR	VAL	SER	V1420	L1421	S1422	V1423	M1424	V1425	K1426	N1427	T1428	K1429	Y1430	F1431	T1432	D1433	F1434	E1435	D1436	M1437	A1438	I1439	L1440	L1441	Y1442	N1443	G1444	D1445	E1446	E1447	A1448	D1449	PHE	PHE	THR	ASN	ASN	VAL	HIS	ILE	GLN	LEU	HIS	R1461	R1462	Q1463	R1464	N1520	N1521	Q1522	Y1523	K1467			
F1288	I1289	E1290	L1291	G1292	R1293	K1294	V1295	P1296	E1297	L1298	E1299	S1300	I1301	S1302	K1303	L1304	V1305	A1306	D1307	L1308	N1309	S1310	Y1311	S1312	S1313	S1314	R1315	M1316	H1317	E1318	Y1319	D1320	F1321	P1322	ARG	ILE	LEU	SER	THR	PHE	LYS	GLY	ILE	GLU	ASN	GLY	TRP	LYS	SER	TYR	GLY	LEU	TRP	LEU	PRO	LEU								
L1228	K1229	G1230	K1231	L1232	K1233	K1234	L1235	Q1236	E1237	N1238	D1239	T1240	Q1241	K1242	I1243	L1244	K1245	I1246	L1247	K1248	L1249	I1250	V1251	F1252	N1253	Y1254	N1255	C1256	S1257	W1258	S1259	D1260	I1261	E1262	E1263	L1264	Y1265	T1266	T1267	L1268	G1269	F1270	I1271	ASP	GLY	TRP	LYS	SER	TYR	SER	GLU	LEU	R1278	M1279	L1280	L1284	R1281	V1282	S1283	L1284	T1285	F1286		
V1168	D1169	L1170	V1171	T1172	L1173	I1174	C1175	T1176	S1177	C1178	L1179	K1180	I1181	L1182	P1183	S1184	L1185	Y1186	V1187	K1188	L1189	S1190	D1191	S1192	N1193	S1194	I1195	S1196	T1197	F1198	L1199	M1200	L1201	L1202	V1203	S1204	I1205	T1206	E1207	M1208	G1209	F1210	I1211	Q1212	D1213	D1214	H1215	V1216	R1217	S1218	R1219	L1220	I1221	S1222	S1223	L1224	I1225	S1226						
L1108	F1109	L1110	Y1111	W1112	A1113	H1114	N1115	P1116	S1117	L1118	Y1119	Q1120	F1121	L1122	Y1123	Y1124	D1125	E1126	F1127	A1128	T1129	A1130	T1131	A1132	L1133	M1134	D1135	T1136	I1137	S1138	N1139	Q1140	H1141	V1142	K1143	E1144	A1145	V1146	I1147	P1148	G1148	P1149	I1150	I1151	E1152	A1153	A1154	D1155	S1156	I1157	I1158	R1159	M1160	P1161	V1162	M1163	D1164	D1165	H1166					
L1047	R1048	K1049	M1050	A1051	S1052	N1053	L1054	R1055	Q1056	Q1057	G1058	L1059	K1060	C1061	L1062	S1063	F1066	E1067	F1068	V1069	G1070	N1071	T1072	F1073	D1074	W1075	S1076	T1077	S1078	M1079	E1080	D1081	I1082	Y1083	A1084	V1085	V1086	V1087	K1088	P1089	R1090	I1091	S1092	H1093	F1094	S1095	D1096	E1097	N1098	L1099	Q1100	Q1101	P1102	S1103	S1104	L1105	L1106	R1107						
N980	S981	H982	Q983	I984	N985	S986	S987	K988	A989	T990	L991	K992	T993	I994	R995	R996	M997	T998	G999	F1000	V1004	N1005	S1006	T1007	L1008	Q1009	M1014	L1017	H1018	T1019	N1020	S1021	V1022	L1023	Q1024	I1027	Y1028	S1029	I1030	A1031	M1032	A1033	Y1034	Y1035	V1036	L1037	D1038	T1039	E1040	S1041	T1042	E1043	E1044	V1045	H1046									
N908	G909	S910	Q911	S912	I913	K914	A915	E916	D917	E918	K919	V920	V921	M922	P923	Y924	V925	L926	R927	I928	F929	F930	G931	R932	A933	Q934	V935	P936	P937	T938	S939	G940	Q941	K942	R943	S944	R945	K946	I947	A948	V949	I950	S951	V952	F964	A968	S969	E970	R971	L972	D973	Y974	N975	Y976	F977	F978	G979							
P786	Q787	W788	A789	E790	N791	H792	F793	V794	D795	I796	A797	P798	F799	V800	Y801	N802	D803	F804	K805	T806	Y807	K808	D809	E810	E811	D812	M813	E814	N815	E816	R817	V818	I819	T820	G821	S822	W823	T824	V825	D826	D827	R828	N829	L832	K833	T834	L835	S836	K837	F838	K839	N840	I841	K842	N843	V844	Y845	S846						
A847	T848	E849	L850	H851	D852	H853	L854	M855	V856	L857	L858	G859	S860	R861	N862	T863	D864	V865	Q866	K867	L868	A869	A872	L873	L874	A875	Y876	K877	N878	P879	T880	L881	N882	K883	Y884	R885	D886	N887	L888	K889	N890	L891	L892	D893	D894	T895	L896	F897	K898	D899	E900	I901	T902	T903	F904	L905	T906	E907						
K726	V727	L728	W729	D730	S731	S732	V733	W734	R735	L736	R737	D738	T739	I740	D741	T742	F743	S744	H745	I746	W747	S748	K749	Y750	S751	T752	Q753	N754	T755	S756	I757	I758	W759	T760	T761	I762	E763	R764	R765	T766	N767	T768	T769	Y770	P771	I772	L773	I774	R775	K837	N776	Q777	A778	L779	K780	V781	L782	L783	I785					



● Molecule 54: Unassigned helices



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9421	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.094	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	597.632, 597.632, 597.632	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.334, 1.334, 1.334	Depositor

5 Model quality

5.1 Standard geometry

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

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	3A	0.91	0/4141	1.25	38/6433 (0.6%)
2	5A	0.83	0/4101	1.09	13/6380 (0.2%)
3	SA	0.69	0/22644	1.15	167/35249 (0.5%)
4	SF	0.35	0/1854	0.66	1/2504 (0.0%)
5	SG	0.53	0/1690	0.64	0/2285
6	SH	0.31	0/1341	0.60	0/1789
7	SJ	0.31	0/1347	0.59	1/1801 (0.1%)
8	SK	0.47	0/1410	0.60	0/1888
9	SM	0.31	0/1020	0.58	0/1374
10	SR	0.58	0/990	0.73	1/1335 (0.1%)
11	SY	0.54	0/798	0.67	1/1065 (0.1%)
12	SZ	0.43	0/822	0.64	0/1103
13	Sd	0.54	0/499	0.66	0/670
14	3B	0.59	0/1901	0.66	1/2567 (0.0%)
14	3C	0.44	0/1796	0.62	1/2424 (0.0%)
15	3D	0.44	0/2891	0.63	3/3895 (0.1%)
16	3E	0.41	0/3059	0.62	3/4153 (0.1%)
17	3F	0.42	0/3715	0.64	2/5001 (0.0%)
18	3G	0.52	0/928	0.76	1/1262 (0.1%)
18	3H	0.47	0/928	0.69	2/1262 (0.2%)
19	A4	0.47	0/5321	0.66	5/7207 (0.1%)
20	A5	0.48	0/4044	0.68	5/5493 (0.1%)
21	A8	0.34	0/3249	0.71	10/4454 (0.2%)
22	A9	0.31	0/951	0.58	1/1287 (0.1%)
23	AE	0.37	0/10049	0.56	6/13737 (0.0%)
24	AF	0.53	0/3993	0.67	4/5413 (0.1%)
25	AG	0.47	0/6699	0.65	3/9077 (0.0%)
26	B1	0.64	0/6474	0.68	7/8763 (0.1%)
27	B2	0.43	0/6628	0.67	3/8954 (0.0%)
28	B3	0.39	0/6014	0.69	7/8137 (0.1%)
29	B8	0.58	0/3848	0.66	4/5218 (0.1%)
30	BE	0.58	0/6580	0.66	7/8901 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	B6	0.45	0/2849	0.58	1/3853 (0.0%)
32	5B	0.34	0/499	0.62	0/659
33	5C	0.63	0/3274	0.70	5/4442 (0.1%)
34	5D	0.51	0/1417	0.67	2/1885 (0.1%)
35	5E	0.39	0/1580	0.73	3/2115 (0.1%)
36	5F	0.38	0/1559	0.69	1/2097 (0.0%)
37	5G	0.39	0/1792	0.72	2/2425 (0.1%)
38	5H	0.52	0/601	0.57	0/789
39	5I	0.61	0/3844	0.66	2/5174 (0.0%)
40	5J	0.42	0/1302	0.55	0/1728
41	5K	0.56	0/1426	0.66	1/1917 (0.1%)
42	RA	0.34	0/2769	0.67	1/3753 (0.0%)
43	RB	0.38	0/1121	0.62	0/1487
44	RG	0.39	0/1727	0.68	2/2329 (0.1%)
44	RH	0.42	0/1828	0.61	0/2470
45	RJ	0.50	0/6514	0.61	1/8768 (0.0%)
46	RK	0.44	0/2832	0.65	3/3825 (0.1%)
47	RL	0.29	0/4549	0.50	0/6241
47	RM	0.25	0/3765	0.47	0/5218
48	RN	0.36	0/4591	0.58	2/6187 (0.0%)
49	RO	0.38	0/3849	0.62	5/5261 (0.1%)
50	RP	0.26	0/8541	0.49	2/11805 (0.0%)
51	RQ	0.46	0/985	0.57	0/1339
52	RS	0.33	0/2104	0.67	1/2854 (0.0%)
53	RY	0.29	0/307	0.51	0/415
All	All	0.51	0/187350	0.76	331/260117 (0.1%)

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
4	SF	0	2
7	SJ	0	1
9	SM	0	1
12	SZ	0	1
15	3D	0	3
16	3E	0	1
17	3F	0	1
18	3G	0	2
18	3H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
19	A4	0	1
20	A5	0	1
21	A8	0	2
25	AG	0	2
26	B1	0	2
27	B2	0	8
28	B3	0	11
30	BE	0	1
34	5D	0	1
37	5G	0	2
39	5I	0	2
42	RA	0	2
43	RB	0	1
45	RJ	0	2
46	RK	0	1
47	RL	0	1
47	RM	0	1
48	RN	0	1
49	RO	0	1
50	RP	0	2
All	All	0	58

There are no bond length outliers.

All (331) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3A	321	C	N1-C1'-C2'	-10.80	99.96	114.00
3	SA	376	C	N1-C2-O2	10.43	125.16	118.90
3	SA	1174	C	N1-C2-O2	10.35	125.11	118.90
1	3A	104	C	C5-C6-N1	9.71	125.86	121.00
20	A5	25	ASP	CB-CG-OD1	9.52	126.87	118.30
18	3G	67	LEU	CA-CB-CG	9.36	136.82	115.30
3	SA	1274	C	C6-N1-C2	-9.01	116.70	120.30
2	5A	312	U	P-O3'-C3'	8.94	130.43	119.70
3	SA	1743	U	N1-C2-O2	8.93	129.05	122.80
3	SA	1451	C	N3-C2-O2	-8.87	115.69	121.90
3	SA	1274	C	C2-N1-C1'	8.73	128.40	118.80
3	SA	1174	C	N3-C2-O2	-8.70	115.81	121.90
2	5A	310	U	N3-C2-O2	-8.64	116.15	122.20
1	3A	200	C	C2-N1-C1'	8.62	128.29	118.80
1	3A	104	C	C6-N1-C2	-8.57	116.87	120.30
3	SA	1254	U	N1-C2-O2	8.57	128.80	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AE	95	ASP	CB-CG-OD1	8.49	125.94	118.30
3	SA	376	C	C2-N1-C1'	8.42	128.06	118.80
1	3A	89	C	C2-N1-C1'	8.41	128.05	118.80
3	SA	258	C	N1-C2-O2	8.38	123.93	118.90
3	SA	1451	C	C6-N1-C2	-8.29	116.98	120.30
3	SA	1174	C	C2-N1-C1'	8.29	127.92	118.80
3	SA	1743	U	C2-N1-C1'	8.23	127.58	117.70
3	SA	1274	C	C5-C6-N1	8.22	125.11	121.00
35	5E	448	LEU	CA-CB-CG	8.17	134.10	115.30
3	SA	607	G	N3-C4-C5	-8.17	124.52	128.60
1	3A	200	C	N1-C2-O2	8.15	123.79	118.90
3	SA	275	C	N1-C2-O2	8.10	123.76	118.90
3	SA	607	G	C2-N3-C4	8.05	115.93	111.90
14	3B	306	LEU	CA-CB-CG	8.05	133.82	115.30
3	SA	166	C	N1-C2-O2	7.97	123.68	118.90
3	SA	1254	U	N3-C2-O2	-7.94	116.64	122.20
29	B8	521	LEU	CA-CB-CG	7.91	133.49	115.30
1	3A	89	C	C6-N1-C2	-7.88	117.15	120.30
3	SA	1274	C	N1-C2-O2	7.84	123.61	118.90
3	SA	374	U	C2-N1-C1'	7.83	127.10	117.70
3	SA	258	C	C2-N1-C1'	7.80	127.38	118.80
3	SA	607	G	C4-N9-C1'	7.78	136.62	126.50
42	RA	10	ASP	CB-CG-OD1	7.73	125.26	118.30
3	SA	376	C	N3-C2-O2	-7.72	116.50	121.90
1	3A	201	C	N1-C2-O2	7.70	123.52	118.90
3	SA	374	U	N1-C2-O2	7.67	128.17	122.80
1	3A	89	C	N1-C2-O2	7.66	123.50	118.90
1	3A	89	C	C5-C6-N1	7.59	124.79	121.00
3	SA	1254	U	C2-N1-C1'	7.55	126.76	117.70
2	5A	91	U	C5-C6-N1	7.45	126.42	122.70
19	A4	225	LEU	CA-CB-CG	7.45	132.43	115.30
52	RS	270	LEU	CA-CB-CG	7.36	132.24	115.30
30	BE	536	LEU	CA-CB-CG	7.35	132.21	115.30
1	3A	308	U	N3-C2-O2	-7.30	117.09	122.20
21	A8	258	PRO	N-CA-CB	7.29	112.05	103.30
3	SA	1258	U	C2-N1-C1'	7.28	126.44	117.70
2	5A	310	U	N1-C2-O2	7.28	127.89	122.80
2	5A	90	G	O4'-C1'-N9	7.25	114.00	108.20
3	SA	275	C	C2-N1-C1'	7.25	126.77	118.80
3	SA	1228	G	N3-C4-C5	-7.23	124.99	128.60
3	SA	579	A	P-O3'-C3'	7.14	128.27	119.70
24	AF	469	LEU	CA-CB-CG	7.14	131.73	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	RN	662	LEU	CA-CB-CG	7.13	131.69	115.30
20	A5	24	LEU	CA-CB-CG	7.09	131.62	115.30
2	5A	312	U	C5-C6-N1	-7.09	119.16	122.70
3	SA	311	U	N1-C2-O2	7.09	127.76	122.80
3	SA	272	U	P-O3'-C3'	7.05	128.16	119.70
3	SA	1451	C	N1-C2-O2	7.04	123.13	118.90
33	5C	144	LEU	CA-CB-CG	7.04	131.49	115.30
15	3D	292	LEU	CA-CB-CG	7.00	131.39	115.30
18	3H	65	LEU	CB-CG-CD1	-6.96	99.17	111.00
3	SA	1258	U	N1-C2-O2	6.96	127.67	122.80
1	3A	248	G	O4'-C1'-N9	6.93	113.75	108.20
3	SA	374	U	N3-C2-O2	-6.92	117.35	122.20
3	SA	280	U	N3-C2-O2	-6.92	117.36	122.20
21	A8	325	PRO	N-CA-CB	6.88	111.55	103.30
3	SA	1743	U	C6-N1-C1'	-6.85	111.61	121.20
3	SA	381	C	N3-C2-O2	-6.83	117.12	121.90
1	3A	104	C	C2-N1-C1'	6.82	126.30	118.80
3	SA	209	U	N3-C2-O2	-6.81	117.44	122.20
2	5A	312	U	OP1-P-O3'	6.80	120.17	105.20
1	3A	72	C	C6-N1-C2	-6.79	117.58	120.30
3	SA	258	C	N3-C2-O2	-6.79	117.15	121.90
11	SY	132	LEU	CA-CB-CG	6.75	130.83	115.30
3	SA	311	U	C2-N1-C1'	6.73	125.77	117.70
3	SA	1174	C	C6-N1-C2	-6.71	117.62	120.30
3	SA	56	U	P-O3'-C3'	6.70	127.74	119.70
27	B2	757	ASP	CB-CG-OD1	6.69	124.32	118.30
3	SA	607	G	N3-C4-N9	6.67	130.00	126.00
3	SA	545	A	O4'-C1'-N9	6.67	113.54	108.20
3	SA	1527	C	N1-C2-O2	6.66	122.90	118.90
3	SA	1258	U	N3-C2-O2	-6.65	117.55	122.20
3	SA	1661	U	C5-C6-N1	6.65	126.03	122.70
1	3A	99	U	C4'-C3'-O3'	6.63	126.25	113.00
21	A8	392	PRO	N-CA-CB	6.62	111.25	103.30
3	SA	608	U	C2-N1-C1'	6.60	125.62	117.70
15	3D	142	LEU	CA-CB-CG	6.60	130.47	115.30
31	B6	18	LEU	CA-CB-CG	6.59	130.46	115.30
3	SA	1476	C	C2-N1-C1'	6.55	126.00	118.80
18	3H	65	LEU	CA-CB-CG	6.52	130.30	115.30
3	SA	280	U	N1-C2-O2	6.51	127.36	122.80
3	SA	1175	U	N3-C2-O2	-6.50	117.65	122.20
3	SA	1274	C	N3-C2-O2	-6.49	117.35	121.90
24	AF	327	LEU	CA-CB-CG	6.49	130.24	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	RJ	252	LEU	CA-CB-CG	6.49	130.24	115.30
3	SA	280	U	C2-N1-C1'	6.49	125.48	117.70
3	SA	401	A	P-O3'-C3'	6.49	127.48	119.70
1	3A	318	U	O5'-P-OP2	-6.46	99.88	105.70
26	B1	717	LEU	CA-CB-CG	6.46	130.16	115.30
3	SA	302	U	N3-C2-O2	-6.45	117.68	122.20
3	SA	1535	U	N3-C2-O2	-6.45	117.68	122.20
39	5I	368	ASP	CB-CG-OD1	6.45	124.10	118.30
20	A5	452	LEU	CA-CB-CG	6.44	130.11	115.30
3	SA	166	C	N3-C2-O2	-6.43	117.40	121.90
35	5E	314	LEU	CA-CB-CG	6.42	130.06	115.30
1	3A	250	C	N1-C2-O2	6.40	122.74	118.90
3	SA	1232	U	N1-C2-O2	6.40	127.28	122.80
3	SA	275	C	N3-C2-O2	-6.39	117.43	121.90
3	SA	1228	G	C2-N3-C4	6.39	115.09	111.90
3	SA	1175	U	N1-C2-O2	6.38	127.26	122.80
1	3A	200	C	C6-N1-C1'	-6.36	113.16	120.80
3	SA	1440	C	C6-N1-C2	-6.36	117.75	120.30
1	3A	317	A	C4'-C3'-O3'	6.34	125.68	113.00
3	SA	1594	G	P-O3'-C3'	6.29	127.25	119.70
1	3A	312	U	P-O3'-C3'	6.29	127.24	119.70
24	AF	95	LEU	CA-CB-CG	6.29	129.75	115.30
3	SA	38	C	N1-C2-O2	6.28	122.67	118.90
50	RP	48	LEU	CA-CB-CG	6.28	129.74	115.30
20	A5	457	LEU	CA-CB-CG	6.23	129.63	115.30
21	A8	309	PRO	N-CA-CB	6.21	110.75	103.30
3	SA	1527	C	C2-N1-C1'	6.19	125.61	118.80
2	5A	312	U	C2-N1-C1'	-6.17	110.30	117.70
3	SA	1228	G	C4-N9-C1'	6.16	134.51	126.50
3	SA	1440	C	C5-C6-N1	6.15	124.07	121.00
1	3A	198	U	P-O3'-C3'	6.14	127.07	119.70
3	SA	1441	C	N3-C2-O2	-6.14	117.60	121.90
1	3A	308	U	N1-C2-O2	6.11	127.08	122.80
1	3A	200	C	C5-C6-N1	6.10	124.05	121.00
3	SA	607	G	C8-N9-C1'	-6.10	119.07	127.00
3	SA	209	U	N1-C2-O2	6.09	127.07	122.80
3	SA	273	G	C4-N9-C1'	6.09	134.42	126.50
3	SA	376	C	C6-N1-C2	-6.09	117.86	120.30
49	RO	269	LEU	CA-CB-CG	6.08	129.28	115.30
3	SA	514	G	N7-C8-N9	6.07	116.14	113.10
3	SA	1259	U	C5-C6-N1	6.05	125.72	122.70
3	SA	1476	C	C5-C6-N1	6.04	124.02	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	RK	117	LEU	CA-CB-CG	6.04	129.19	115.30
3	SA	311	U	N3-C2-O2	-6.01	117.99	122.20
3	SA	1439	C	N3-C2-O2	-6.00	117.70	121.90
36	5F	57	LEU	CA-CB-CG	6.00	129.11	115.30
2	5A	492	G	P-O3'-C3'	6.00	126.90	119.70
3	SA	1620	C	N1-C2-O2	6.00	122.50	118.90
26	B1	521	LEU	CA-CB-CG	6.00	129.10	115.30
3	SA	575	C	N1-C2-O2	5.99	122.50	118.90
3	SA	-7	A	P-O3'-C3'	5.99	126.89	119.70
3	SA	1476	C	C6-N1-C2	-5.98	117.91	120.30
1	3A	72	C	C5-C6-N1	5.96	123.98	121.00
7	SJ	29	LEU	CA-CB-CG	5.95	128.99	115.30
21	A8	453	PRO	N-CA-CB	5.94	110.43	103.30
3	SA	1228	G	N3-C4-N9	5.92	129.55	126.00
3	SA	608	U	N1-C2-O2	5.91	126.94	122.80
3	SA	275	C	C6-N1-C2	-5.91	117.94	120.30
3	SA	1232	U	C2-N1-C1'	5.91	124.79	117.70
3	SA	1232	U	N3-C2-O2	-5.91	118.06	122.20
26	B1	479	LEU	CA-CB-CG	5.90	128.87	115.30
3	SA	1216	C	N3-C2-O2	-5.89	117.77	121.90
3	SA	381	C	N1-C2-O2	5.89	122.43	118.90
37	5G	109	LEU	CA-CB-CG	5.88	128.84	115.30
34	5D	28	LEU	CA-CB-CG	5.88	128.82	115.30
3	SA	0	U	P-O3'-C3'	5.87	126.74	119.70
3	SA	1254	U	C5-C6-N1	5.86	125.63	122.70
37	5G	152	LEU	CA-CB-CG	5.86	128.78	115.30
44	RG	96	LEU	CA-CB-CG	5.85	128.76	115.30
3	SA	562	G	O4'-C1'-N9	5.84	112.87	108.20
28	B3	401	LEU	CA-CB-CG	5.83	128.71	115.30
3	SA	542	A	P-O3'-C3'	5.83	126.69	119.70
21	A8	390	PRO	N-CA-CB	5.83	110.29	103.30
26	B1	69	LEU	CA-CB-CG	5.83	128.70	115.30
21	A8	429	PRO	N-CA-CB	5.80	110.27	103.30
21	A8	298	PRO	N-CA-CB	5.79	110.25	103.30
3	SA	411	C	N1-C2-O2	5.79	122.37	118.90
3	SA	1734	U	N3-C2-O2	-5.79	118.15	122.20
3	SA	417	A	P-O3'-C3'	5.78	126.64	119.70
30	BE	522	LEU	CA-CB-CG	5.78	128.60	115.30
33	5C	74	LEU	CA-CB-CG	5.76	128.56	115.30
30	BE	872	LEU	CA-CB-CG	5.75	128.52	115.30
3	SA	194	U	C2-N1-C1'	5.75	124.59	117.70
3	SA	376	C	C5-C6-N1	5.74	123.87	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SA	612	U	C2-N1-C1'	5.74	124.59	117.70
24	AF	195	LEU	CA-CB-CG	5.73	128.47	115.30
30	BE	121	LEU	CA-CB-CG	5.73	128.47	115.30
21	A8	235	PRO	N-CA-CB	5.72	110.16	103.30
3	SA	87	C	C6-N1-C2	-5.72	118.01	120.30
3	SA	1448	G	C5-C6-O6	5.71	132.03	128.60
28	B3	342	ASP	CB-CG-OD1	5.70	123.43	118.30
3	SA	373	G	N3-C4-C5	-5.70	125.75	128.60
3	SA	310	C	C6-N1-C2	-5.70	118.02	120.30
3	SA	1199	G	N3-C4-N9	5.69	129.42	126.00
3	SA	1521	G	P-O3'-C3'	5.69	126.53	119.70
1	3A	201	C	N3-C2-O2	-5.68	117.92	121.90
23	AE	604	LEU	CA-CB-CG	5.68	128.36	115.30
3	SA	376	C	C6-N1-C1'	-5.67	114.00	120.80
29	B8	387	LEU	CA-CB-CG	5.67	128.33	115.30
39	5I	62	LEU	CA-CB-CG	5.66	128.32	115.30
3	SA	569	C	C6-N1-C2	-5.66	118.04	120.30
19	A4	422	LEU	CA-CB-CG	5.65	128.30	115.30
3	SA	1174	C	C5-C6-N1	5.63	123.81	121.00
26	B1	716	ASP	CB-CG-OD1	5.63	123.37	118.30
3	SA	1743	U	N3-C2-O2	-5.63	118.26	122.20
25	AG	449	LEU	CA-CB-CG	5.62	128.23	115.30
1	3A	106	C	C5-C6-N1	5.62	123.81	121.00
3	SA	273	G	N3-C4-N9	5.58	129.35	126.00
19	A4	534	LEU	CA-CB-CG	5.58	128.12	115.30
3	SA	411	C	N3-C2-O2	-5.57	118.00	121.90
3	SA	1441	C	N1-C2-O2	5.56	122.24	118.90
1	3A	313	A	C4-C5-C6	-5.56	114.22	117.00
22	A9	516	LEU	CA-CB-CG	5.55	128.07	115.30
3	SA	273	G	N3-C4-C5	-5.55	125.83	128.60
30	BE	417	LEU	CA-CB-CG	5.54	128.04	115.30
3	SA	38	C	C6-N1-C2	-5.54	118.09	120.30
33	5C	414	LEU	CA-CB-CG	5.53	128.02	115.30
1	3A	313	A	N3-C4-N9	-5.52	122.99	127.40
44	RG	50	LEU	CA-CB-CG	5.51	127.98	115.30
2	5A	90	G	C8-N9-C1'	5.51	134.16	127.00
29	B8	272	LEU	CA-CB-CG	5.51	127.96	115.30
3	SA	87	C	C5-C6-N1	5.50	123.75	121.00
4	SF	42	LEU	CA-CB-CG	5.50	127.96	115.30
3	SA	1585	U	N1-C2-O2	5.50	126.65	122.80
23	AE	526	LEU	CA-CB-CG	5.49	127.93	115.30
3	SA	1161	C	C5-C6-N1	5.48	123.74	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	5K	17	LEU	CA-CB-CG	5.48	127.91	115.30
23	AE	370	LEU	CA-CB-CG	5.48	127.89	115.30
3	SA	1734	U	N1-C2-O2	5.46	126.62	122.80
14	3C	306	LEU	CA-CB-CG	5.45	127.84	115.30
30	BE	614	LEU	CA-CB-CG	5.45	127.84	115.30
3	SA	38	C	C2-N1-C1'	5.45	124.79	118.80
33	5C	416	LEU	CA-CB-CG	5.45	127.83	115.30
28	B3	471	PRO	C-N-CA	5.45	135.31	121.70
3	SA	50	C	C2-N1-C1'	5.44	124.79	118.80
1	3A	89	C	N3-C2-O2	-5.44	118.09	121.90
21	A8	316	PRO	N-CA-CB	5.43	109.82	103.30
3	SA	373	G	C4-N9-C1'	5.43	133.56	126.50
3	SA	1585	U	N3-C2-O2	-5.43	118.40	122.20
46	RK	296	LEU	CA-CB-CG	5.43	127.78	115.30
3	SA	608	U	N3-C2-O2	-5.42	118.40	122.20
3	SA	275	C	C5-C6-N1	5.42	123.71	121.00
3	SA	258	C	C6-N1-C1'	-5.41	114.30	120.80
25	AG	323	LEU	CA-CB-CG	5.41	127.75	115.30
3	SA	258	C	C6-N1-C2	-5.40	118.14	120.30
1	3A	248	G	P-O3'-C3'	5.40	126.18	119.70
3	SA	514	G	C8-N9-C4	-5.40	104.24	106.40
28	B3	736	LEU	CA-CB-CG	5.39	127.71	115.30
3	SA	128	U	C2-N1-C1'	5.38	124.16	117.70
23	AE	547	ILE	CG1-CB-CG2	-5.38	99.55	111.40
3	SA	1448	G	N1-C6-O6	-5.38	116.67	119.90
15	3D	152	LEU	CA-CB-CG	5.37	127.65	115.30
3	SA	1174	C	C6-N1-C1'	-5.37	114.36	120.80
25	AG	889	ASP	CB-CG-OD1	5.37	123.13	118.30
3	SA	311	U	C5-C6-N1	5.36	125.38	122.70
17	3F	315	LEU	CA-CB-CG	5.36	127.63	115.30
3	SA	607	G	C8-N9-C4	-5.36	104.26	106.40
2	5A	312	U	O4'-C1'-N1	5.36	112.49	108.20
3	SA	79	C	N1-C2-O2	5.35	122.11	118.90
3	SA	530	C	N1-C2-O2	5.34	122.11	118.90
16	3E	401	LEU	CA-CB-CG	5.34	127.58	115.30
3	SA	75	U	C2-N1-C1'	5.34	124.10	117.70
28	B3	162	LEU	CB-CG-CD2	-5.33	101.93	111.00
3	SA	1439	C	N1-C2-O2	5.33	122.10	118.90
50	RP	155	LEU	CA-CB-CG	5.33	127.56	115.30
3	SA	38	C	N3-C2-O2	-5.32	118.18	121.90
2	5A	90	G	C4-N9-C1'	-5.32	119.59	126.50
3	SA	1646	C	N1-C2-O2	5.29	122.08	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SA	25	C	C2-N1-C1'	5.29	124.61	118.80
1	3A	104	C	C2-N3-C4	5.27	122.54	119.90
33	5C	148	LEU	CA-CB-CG	5.27	127.43	115.30
3	SA	380	U	N1-C2-O2	5.27	126.49	122.80
3	SA	49	C	C5-C6-N1	5.26	123.63	121.00
3	SA	50	C	C6-N1-C2	-5.26	118.19	120.30
3	SA	443	C	C5-C6-N1	5.26	123.63	121.00
30	BE	536	LEU	CB-CG-CD2	-5.26	102.06	111.00
3	SA	1269	U	N3-C2-O2	-5.26	118.52	122.20
3	SA	1664	C	N3-C2-O2	-5.26	118.22	121.90
49	RO	388	LEU	CA-CB-CG	5.25	127.36	115.30
3	SA	8	U	N3-C2-O2	-5.24	118.53	122.20
16	3E	227	LEU	CA-CB-CG	5.24	127.35	115.30
3	SA	-7	A	OP1-P-O3'	5.23	116.72	105.20
17	3F	348	LEU	CA-CB-CG	5.23	127.33	115.30
28	B3	12	LEU	CA-CB-CG	5.22	127.31	115.30
3	SA	279	G	N3-C4-N9	-5.22	122.87	126.00
23	AE	94	LEU	CA-CB-CG	5.22	127.30	115.30
20	A5	151	LEU	CA-CB-CG	5.21	127.29	115.30
35	5E	449	ASP	CB-CG-OD1	5.20	122.98	118.30
3	SA	373	G	N3-C4-N9	5.20	129.12	126.00
3	SA	1269	U	N1-C2-O2	5.19	126.44	122.80
16	3E	141	LEU	CA-CB-CG	5.19	127.24	115.30
28	B3	394	LEU	CA-CB-CG	5.18	127.23	115.30
1	3A	39	C	C2-N1-C1'	5.18	124.50	118.80
3	SA	612	U	N1-C2-O2	5.18	126.43	122.80
27	B2	267	ASP	C-N-CA	5.18	134.65	121.70
3	SA	380	U	N3-C2-O2	-5.18	118.58	122.20
29	B8	521	LEU	CB-CG-CD1	-5.18	102.20	111.00
1	3A	39	C	C6-N1-C2	-5.17	118.23	120.30
1	3A	205	G	P-O3'-C3'	5.16	125.89	119.70
3	SA	443	C	C6-N1-C2	-5.14	118.24	120.30
49	RO	211	LEU	CA-CB-CG	5.14	127.13	115.30
2	5A	310	U	C6-N1-C2	-5.14	117.92	121.00
3	SA	273	G	C8-N9-C1'	-5.14	120.32	127.00
3	SA	411	C	C6-N1-C2	-5.14	118.25	120.30
46	RK	325	LEU	CA-CB-CG	5.13	127.09	115.30
19	A4	465	LEU	CA-CB-CG	5.09	127.02	115.30
1	3A	249	G	O5'-P-OP1	-5.09	101.12	105.70
3	SA	1492	A	C4-N9-C1'	5.09	135.46	126.30
3	SA	1535	U	C6-N1-C2	-5.09	117.95	121.00
3	SA	35	U	C5-C6-N1	5.09	125.24	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3A	89	C	C6-N1-C1'	-5.08	114.70	120.80
3	SA	130	C	C2-N1-C1'	5.07	124.38	118.80
10	SR	123	ARG	C-N-CD	-5.07	109.46	120.60
1	3A	200	C	C6-N1-C2	-5.06	118.27	120.30
1	3A	198	U	OP1-P-O3'	5.06	116.34	105.20
3	SA	75	U	N3-C2-O2	-5.06	118.66	122.20
3	SA	1664	C	N1-C2-O2	5.05	121.93	118.90
34	5D	91	LEU	CA-CB-CG	5.05	126.91	115.30
49	RO	264	LEU	CA-CB-CG	5.05	126.91	115.30
19	A4	435	PRO	C-N-CA	5.04	134.31	121.70
26	B1	701	LEU	CA-CB-CG	5.04	126.90	115.30
3	SA	1664	C	C2-N1-C1'	5.04	124.34	118.80
27	B2	231	LEU	CA-CB-CG	5.04	126.90	115.30
3	SA	414	C	C5-C6-N1	5.03	123.52	121.00
3	SA	1222	C	C5-C6-N1	5.03	123.52	121.00
3	SA	35	U	N1-C2-O2	5.03	126.32	122.80
26	B1	436	LEU	CA-CB-CG	5.02	126.84	115.30
49	RO	202	LEU	CA-CB-CG	5.01	126.81	115.30
3	SA	1636	C	C5-C6-N1	5.00	123.50	121.00
3	SA	1664	C	C6-N1-C2	-5.00	118.30	120.30
48	RN	744	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (58) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	3D	142	LEU	Peptide
15	3D	202	HIS	Peptide
15	3D	286	ARG	Peptide
16	3E	331	LYS	Peptide
17	3F	237	ASP	Peptide
18	3G	59	GLU	Peptide
18	3G	9	PHE	Peptide
18	3H	59	GLU	Peptide
34	5D	138	ASP	Peptide
37	5G	254	PHE	Peptide
37	5G	74	ASP	Peptide
39	5I	230	ASN	Peptide
39	5I	283	ASP	Peptide
19	A4	54	LYS	Peptide
20	A5	167	SER	Peptide
21	A8	496	TYR	Peptide

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Mol	Chain	Res	Type	Group
21	A8	529	HIS	Peptide
25	AG	178	PHE	Peptide
25	AG	780	GLU	Peptide
26	B1	288	ASP	Peptide
26	B1	690	ALA	Peptide
27	B2	131	GLY	Peptide
27	B2	213	LYS	Peptide
27	B2	266	SER	Peptide
27	B2	267	ASP	Peptide
27	B2	278	ASP	Peptide
27	B2	44	SER	Peptide
27	B2	613	ALA	Peptide
27	B2	916	HIS	Peptide
28	B3	34	THR	Peptide
28	B3	435	ALA	Peptide
28	B3	473	ALA	Peptide
28	B3	479	ILE	Peptide
28	B3	480	ILE	Peptide
28	B3	585	ASN	Peptide
28	B3	593	CYS	Peptide
28	B3	594	GLY	Peptide
28	B3	627	ASN	Peptide
28	B3	89	HIS	Peptide
28	B3	90	LEU	Peptide
30	BE	94	TYR	Peptide
42	RA	111	TRP	Peptide
42	RA	173	LEU	Peptide
43	RB	261	SER	Peptide
45	RJ	1026	LYS	Peptide
45	RJ	868	ARG	Peptide
46	RK	333	PHE	Peptide
47	RL	743	VAL	Peptide
47	RM	743	VAL	Peptide
48	RN	286	SER	Peptide
49	RO	144	PRO	Peptide
50	RP	1746	LYS	Peptide
50	RP	835	LEU	Peptide
4	SF	193	GLY	Peptide
4	SF	195	ILE	Peptide
7	SJ	85	PRO	Peptide
9	SM	128	CYS	Peptide
12	SZ	76	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3A	3711	0	1882	57	0
2	5A	3668	0	1845	35	0
3	SA	20256	0	10219	193	0
4	SF	1815	0	1870	45	0
5	SG	1669	0	1724	18	0
6	SH	1327	0	1403	28	0
7	SJ	1324	0	1344	48	0
8	SK	1388	0	1467	31	0
9	SM	997	0	1048	35	0
10	SR	973	0	1029	19	0
11	SY	786	0	843	8	0
12	SZ	809	0	842	15	0
13	Sd	497	0	535	0	0
14	3B	1865	0	1910	29	0
14	3C	1763	0	1805	42	0
15	3D	2848	0	2815	46	0
16	3E	3028	0	2813	59	0
17	3F	3643	0	3654	79	0
18	3G	916	0	964	11	0
18	3H	916	0	964	24	0
19	A4	5226	0	5199	95	0
20	A5	3976	0	3919	60	0
21	A8	3229	0	2281	130	0
22	A9	939	0	898	45	0
23	AE	9955	0	7968	102	0
24	AF	3911	0	3906	74	0
25	AG	6570	0	6473	140	0
26	B1	6331	0	6236	140	0
27	B2	6502	0	6493	121	0
28	B3	5919	0	6007	134	0
29	B8	3764	0	3757	58	0
30	BE	6450	0	6420	94	0
31	B6	2800	0	2517	32	0
32	5B	495	0	561	12	0
33	5C	3198	0	3157	57	0
34	5D	1396	0	1407	47	0
35	5E	1564	0	1592	165	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	5F	1530	0	1572	79	0
37	5G	1756	0	1765	56	0
38	5H	596	0	661	7	0
39	5I	3765	0	3714	67	0
40	5J	1280	0	1331	23	0
41	5K	1403	0	1484	16	0
42	RA	2709	0	2622	63	0
43	RB	1108	0	1087	25	0
44	RG	1701	0	1767	40	0
44	RH	1799	0	1872	29	0
45	RJ	6379	0	6506	138	0
46	RK	2781	0	2878	49	0
47	RL	4539	0	2874	28	0
47	RM	3779	0	1650	8	0
48	RN	4529	0	4262	82	0
49	RO	3766	0	3269	47	0
50	RP	8510	0	4744	43	0
51	RQ	974	0	802	15	0
52	RS	2051	0	2096	53	0
53	RY	299	0	275	6	0
54	X1	40	0	10	0	0
55	5K	1	0	0	0	0
56	RJ	32	0	12	1	0
57	RJ	1	0	0	0	0
All	All	181752	0	157020	2686	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 8.

All (2686) 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)
21:A8:596:LYS:HE3	21:A8:637:LEU:CD2	1.25	1.58
26:B1:382:THR:O	35:5E:481:PRO:HB3	1.40	1.22
21:A8:596:LYS:HE3	21:A8:637:LEU:HD23	1.23	1.21
35:5E:366:GLU:OE2	37:5G:247:ILE:HG21	1.40	1.19
21:A8:443:CYS:HA	25:AG:728:LEU:HD13	1.25	1.19
21:A8:563:LEU:HB2	21:A8:598:GLU:OE1	1.41	1.17
21:A8:596:LYS:CE	21:A8:637:LEU:CD2	2.21	1.17
21:A8:596:LYS:CE	21:A8:637:LEU:HD22	1.75	1.17
33:5C:430:VAL:HG21	36:5F:3:ARG:HD3	1.25	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:5E:520:LEU:HD11	35:5E:525:LYS:CG	1.74	1.16
21:A8:673:THR:HG22	22:A9:490:GLU:HB2	1.20	1.16
21:A8:633:GLN:O	21:A8:637:LEU:HG	1.44	1.14
34:5D:78:LEU:HB2	45:RJ:1082:GLN:HE21	1.10	1.14
21:A8:673:THR:HG22	22:A9:490:GLU:CB	1.80	1.12
35:5E:520:LEU:CD1	35:5E:525:LYS:HG3	1.80	1.11
36:5F:8:HIS:HA	39:5I:53:MET:HE1	1.29	1.10
35:5E:520:LEU:HD11	35:5E:525:LYS:HG3	1.29	1.10
30:BE:737:LEU:HA	30:BE:740:ILE:CG2	1.82	1.08
21:A8:631:SER:O	21:A8:634:LEU:HG	1.56	1.06
26:B1:298:LEU:HD12	35:5E:476:MET:SD	1.95	1.06
21:A8:443:CYS:N	25:AG:728:LEU:HD22	1.70	1.05
21:A8:443:CYS:CB	25:AG:728:LEU:HB3	1.86	1.05
26:B1:341:GLN:NE2	26:B1:378:PHE:HB3	1.73	1.03
28:B3:690:HIS:CG	35:5E:519:GLU:HB2	1.94	1.03
26:B1:298:LEU:CD1	35:5E:476:MET:SD	2.47	1.02
30:BE:740:ILE:HG13	35:5E:483:TYR:OH	1.58	1.02
36:5F:19:LEU:HG	41:5K:25:LEU:HB3	1.41	1.02
21:A8:592:ARG:HB2	21:A8:596:LYS:HZ1	0.88	1.01
26:B1:418:ARG:HD2	35:5E:489:SER:O	1.59	1.01
27:B2:17:ILE:HG22	27:B2:52:TRP:CZ2	1.94	1.01
48:RN:527:GLN:O	48:RN:531:GLN:HB2	1.60	1.01
21:A8:631:SER:HA	21:A8:634:LEU:HD11	1.43	1.01
21:A8:592:ARG:HB2	21:A8:596:LYS:NZ	1.76	1.00
35:5E:384:ARG:HD2	37:5G:83:ILE:HD12	1.42	1.00
26:B1:337:TYR:OH	35:5E:474:ILE:HD13	1.61	1.00
35:5E:343:GLU:OE2	45:RJ:1007:TYR:HE1	1.43	1.00
3:SA:36:C:H42	3:SA:472:U:H3	1.00	0.99
48:RN:86:ILE:HA	48:RN:89:GLN:HE21	1.26	0.98
33:5C:430:VAL:HG21	36:5F:3:ARG:CD	1.94	0.97
21:A8:593:ASP:HA	21:A8:596:LYS:HD2	1.43	0.97
8:SK:65:LYS:HZ2	17:3F:59:PRO:CD	1.77	0.96
8:SK:65:LYS:HZ2	17:3F:59:PRO:CG	1.78	0.94
1:3A:319:G:H5'	14:3C:121:LYS:NZ	1.82	0.94
21:A8:443:CYS:CA	25:AG:728:LEU:HD22	1.96	0.94
26:B1:54:HIS:HE2	26:B1:72:SER:HG	1.14	0.94
35:5E:319:VAL:HG21	45:RJ:1038:ILE:CG2	1.97	0.93
21:A8:596:LYS:HE2	21:A8:637:LEU:HA	1.48	0.93
30:BE:739:VAL:HG21	35:5E:487:ALA:HB2	1.51	0.92
8:SK:65:LYS:HZ2	17:3F:59:PRO:CB	1.82	0.92
21:A8:443:CYS:HA	25:AG:728:LEU:CD1	2.00	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5A:9:G:H5'	22:A9:483:LYS:NZ	1.85	0.92
26:B1:418:ARG:HH21	26:B1:418:ARG:HG3	1.33	0.91
30:BE:737:LEU:HA	30:BE:740:ILE:HG21	1.50	0.91
21:A8:596:LYS:CE	21:A8:637:LEU:HD23	1.91	0.90
48:RN:86:ILE:HA	48:RN:89:GLN:NE2	1.87	0.90
3:SA:36:C:N4	3:SA:472:U:H3	1.70	0.89
35:5E:343:GLU:OE2	45:RJ:1007:TYR:CE1	2.25	0.89
8:SK:65:LYS:NZ	17:3F:59:PRO:CG	2.35	0.89
1:3A:318:U:H3	14:3C:119:GLY:HA3	1.36	0.88
21:A8:673:THR:HG22	22:A9:490:GLU:CA	2.02	0.88
21:A8:592:ARG:CB	21:A8:596:LYS:HZ1	1.82	0.87
26:B1:418:ARG:CD	35:5E:489:SER:O	2.21	0.87
28:B3:494:ILE:N	28:B3:510:SER:HG	1.71	0.87
35:5E:493:GLN:NE2	35:5E:497:ASN:HB3	1.88	0.86
21:A8:673:THR:CG2	22:A9:490:GLU:CA	2.54	0.86
34:5D:78:LEU:HD22	45:RJ:1082:GLN:CG	2.05	0.86
34:5D:78:LEU:HB2	45:RJ:1082:GLN:NE2	1.91	0.85
8:SK:65:LYS:NZ	17:3F:59:PRO:CD	2.38	0.85
17:3F:415:THR:HG1	17:3F:425:TRP:HE1	1.24	0.85
21:A8:596:LYS:HE3	21:A8:637:LEU:HD22	0.88	0.85
35:5E:384:ARG:HE	37:5G:82:GLY:H	1.22	0.85
33:5C:430:VAL:CG2	36:5F:3:ARG:HD3	2.07	0.85
47:RM:313:PRO:O	47:RM:372:PRO:HA	1.77	0.84
35:5E:319:VAL:HG21	45:RJ:1038:ILE:HG22	1.57	0.84
21:A8:673:THR:CG2	22:A9:490:GLU:HA	2.07	0.84
48:RN:86:ILE:CA	48:RN:89:GLN:HE21	1.89	0.84
21:A8:643:ASP:HA	24:AF:510:LEU:CD1	2.06	0.84
52:RS:424:PHE:O	52:RS:428:TYR:HB2	1.78	0.84
1:3A:24:U:O2	36:5F:13:LEU:HB2	1.77	0.84
45:RJ:871:MET:HE1	45:RJ:930:LYS:CE	2.08	0.84
1:3A:94:A:H61	1:3A:322:A:H61	1.27	0.83
49:RO:502:ASN:O	49:RO:506:LEU:HB2	1.77	0.83
4:SF:213:SER:HG	17:3F:102:ASP:N	1.77	0.83
28:B3:691:PRO:HD2	35:5E:516:SER:HB3	1.60	0.83
26:B1:382:THR:O	35:5E:481:PRO:CB	2.26	0.82
35:5E:384:ARG:HD2	37:5G:83:ILE:CD1	2.10	0.82
30:BE:736:HIS:O	30:BE:740:ILE:HG22	1.78	0.82
35:5E:532:LEU:O	35:5E:536:ARG:HG2	1.78	0.82
35:5E:520:LEU:HD11	35:5E:525:LYS:HG2	1.61	0.82
1:3A:319:G:C5'	14:3C:121:LYS:NZ	2.42	0.82
34:5D:68:HIS:CE1	36:5F:169:THR:HG21	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:5E:384:ARG:HH21	37:5G:81:SER:HB3	1.45	0.81
1:3A:318:U:OP1	1:3A:318:U:H3'	1.80	0.81
51:RQ:346:LEU:O	51:RQ:350:ASN:HA	1.80	0.81
35:5E:384:ARG:CD	37:5G:83:ILE:HD12	2.09	0.81
18:3H:44:LEU:HD22	18:3H:52:ILE:CD1	2.10	0.81
23:AE:151:ILE:O	23:AE:155:ILE:HB	1.81	0.81
34:5D:58:ARG:HD2	36:5F:174:ARG:NH2	1.96	0.81
26:B1:14:VAL:HG21	26:B1:341:GLN:O	1.81	0.80
26:B1:678:GLU:OE2	35:5E:455:HIS:CE1	2.34	0.80
26:B1:298:LEU:HA	35:5E:472:PRO:HB2	1.62	0.80
35:5E:345:LEU:O	35:5E:345:LEU:HD23	1.81	0.80
47:RM:746:TYR:O	47:RM:765:VAL:HA	1.81	0.80
35:5E:533:LYS:HA	35:5E:536:ARG:NE	1.97	0.80
21:A8:596:LYS:HD3	21:A8:640:LEU:HD22	1.62	0.79
30:BE:737:LEU:HA	30:BE:740:ILE:HG22	1.63	0.79
28:B3:690:HIS:CD2	35:5E:519:GLU:HB2	2.18	0.79
21:A8:633:GLN:O	21:A8:637:LEU:CG	2.29	0.79
1:3A:323:G:N3	1:3A:323:G:H2'	1.96	0.79
31:B6:319:TYR:O	31:B6:323:PHE:HB2	1.81	0.79
7:SJ:48:THR:O	7:SJ:52:ASN:HB2	1.83	0.79
35:5E:319:VAL:CG2	45:RJ:1038:ILE:CG2	2.60	0.79
21:A8:631:SER:CA	21:A8:634:LEU:HD21	2.13	0.78
2:5A:9:G:H5'	22:A9:483:LYS:HZ2	1.46	0.78
8:SK:65:LYS:NZ	17:3F:59:PRO:HD3	1.97	0.78
21:A8:672:ASN:HB2	22:A9:489:SER:OG	1.83	0.78
48:RN:86:ILE:O	48:RN:89:GLN:HG3	1.84	0.78
3:SA:1663:G:H1	3:SA:1738:U:H3	1.31	0.78
48:RN:86:ILE:HA	48:RN:89:GLN:HG2	1.66	0.78
21:A8:665:GLN:HB3	22:A9:496:LEU:HD21	1.64	0.78
24:AF:224:THR:O	24:AF:239:LEU:HB2	1.83	0.78
37:5G:239:VAL:HG21	48:RN:13:LEU:HD12	1.65	0.77
35:5E:319:VAL:CG2	45:RJ:1038:ILE:HG21	2.14	0.77
3:SA:153:G:H1	3:SA:161:U:H3	1.33	0.77
21:A8:673:THR:HG21	22:A9:490:GLU:HA	1.66	0.77
21:A8:631:SER:HA	21:A8:634:LEU:HD21	1.66	0.77
35:5E:533:LYS:HA	35:5E:536:ARG:HE	1.47	0.76
21:A8:647:LEU:HB3	22:A9:509:GLN:HE22	1.50	0.76
34:5D:78:LEU:HD22	45:RJ:1082:GLN:HG3	1.68	0.76
36:5F:6:LYS:O	36:5F:9:GLU:HB2	1.85	0.76
26:B1:299:SER:O	35:5E:476:MET:HG2	1.87	0.75
35:5E:319:VAL:HG21	45:RJ:1038:ILE:HG21	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:5D:78:LEU:HD22	45:RJ:1082:GLN:HG2	1.68	0.75
8:SK:138:LYS:H	43:RB:263:GLY:HA3	1.51	0.75
35:5E:493:GLN:HE22	35:5E:497:ASN:ND2	1.84	0.75
3:SA:415:C:H1'	3:SA:419:G:H22	1.50	0.75
36:5F:5:LEU:HB3	36:5F:9:GLU:HB3	1.67	0.75
35:5E:345:LEU:HD22	45:RJ:961:PHE:CZ	2.22	0.74
26:B1:680:ARG:NH1	35:5E:455:HIS:CD2	2.56	0.74
35:5E:533:LYS:HA	35:5E:536:ARG:HG2	1.68	0.74
19:A4:614:TRP:O	19:A4:618:ASN:HB2	1.87	0.74
10:SR:94:GLN:OE1	36:5F:182:PHE:CD1	2.39	0.74
1:3A:319:G:H5'	14:3C:121:LYS:HZ2	1.50	0.74
26:B1:419:TYR:HE2	35:5E:486:ASN:ND2	1.86	0.74
35:5E:384:ARG:CD	37:5G:83:ILE:CD1	2.65	0.74
40:5J:114:ARG:O	40:5J:118:GLN:HB3	1.88	0.74
33:5C:188:LYS:HE2	36:5F:23:GLN:OE1	1.87	0.74
10:SR:94:GLN:OE1	36:5F:182:PHE:HD1	1.69	0.73
1:3A:319:G:C5'	14:3C:121:LYS:HZ2	2.01	0.73
30:BE:737:LEU:CA	30:BE:740:ILE:CG2	2.64	0.73
2:5A:9:G:C5'	22:A9:483:LYS:NZ	2.51	0.72
21:A8:643:ASP:HA	24:AF:510:LEU:HD13	1.69	0.72
21:A8:669:ALA:HA	22:A9:489:SER:HB2	1.69	0.72
35:5E:384:ARG:NE	37:5G:82:GLY:H	1.87	0.72
28:B3:216:ARG:HH11	28:B3:241:GLN:HE22	1.36	0.72
3:SA:1756:A:H5'	35:5E:536:ARG:HB2	1.70	0.72
8:SK:65:LYS:HZ1	17:3F:59:PRO:HD3	1.55	0.72
21:A8:642:LEU:HD12	22:A9:499:ILE:HG23	1.70	0.72
45:RJ:871:MET:CE	45:RJ:930:LYS:NZ	2.53	0.72
26:B1:341:GLN:HE21	26:B1:378:PHE:HB3	1.55	0.72
8:SK:65:LYS:NZ	17:3F:59:PRO:CB	2.52	0.72
21:A8:596:LYS:CG	21:A8:637:LEU:HB3	2.20	0.71
1:3A:318:U:H3'	1:3A:318:U:P	2.30	0.71
3:SA:505:A:H61	3:SA:586:G:H8	1.38	0.71
16:3E:397:ARG:HH21	16:3E:400:GLN:HE21	1.38	0.71
26:B1:298:LEU:HD11	35:5E:476:MET:SD	2.30	0.71
47:RL:29:VAL:HG12	47:RL:152:LEU:HD12	1.72	0.71
35:5E:493:GLN:HE21	35:5E:497:ASN:HB3	1.52	0.71
48:RN:86:ILE:HA	48:RN:89:GLN:CG	2.21	0.71
20:A5:545:ALA:CB	21:A8:674:GLU:HG3	2.20	0.71
21:A8:631:SER:HA	21:A8:634:LEU:CD1	2.18	0.71
25:AG:435:ASP:HB2	25:AG:702:TYR:CD1	2.26	0.71
45:RJ:871:MET:HE2	45:RJ:930:LYS:HZ2	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B3:591:ILE:HG12	28:B3:600:LYS:HZ1	1.56	0.70
36:5F:8:HIS:HA	39:5I:53:MET:CE	2.14	0.70
30:BE:740:ILE:HG13	35:5E:483:TYR:HH	1.52	0.70
35:5E:493:GLN:HE22	35:5E:497:ASN:HD22	1.37	0.70
3:SA:1756:A:N7	35:5E:532:LEU:HB2	2.07	0.70
4:SF:92:LEU:HB2	4:SF:97:GLU:HB2	1.74	0.70
21:A8:596:LYS:CE	21:A8:637:LEU:HA	2.22	0.70
35:5E:340:LEU:HB2	45:RJ:957:GLU:OE2	1.92	0.70
5:SG:206:SER:H	5:SG:211:ILE:HD11	1.55	0.70
1:3A:323:G:OP2	34:5D:116:LYS:HB3	1.92	0.69
26:B1:420:ARG:HH22	35:5E:494:GLU:CD	1.96	0.69
26:B1:337:TYR:CD2	26:B1:340:LYS:HD3	2.27	0.69
26:B1:58:ILE:HA	26:B1:74:ASP:HA	1.74	0.69
35:5E:533:LYS:HA	35:5E:536:ARG:CG	2.22	0.69
48:RN:86:ILE:HG23	48:RN:89:GLN:NE2	2.07	0.69
21:A8:643:ASP:HA	24:AF:510:LEU:HD12	1.75	0.68
12:SZ:29:HIS:HB2	12:SZ:32:ARG:HB2	1.76	0.68
35:5E:517:LYS:NZ	35:5E:517:LYS:HB3	2.09	0.68
8:SK:65:LYS:NZ	17:3F:59:PRO:HB3	2.08	0.68
21:A8:664:LYS:O	21:A8:668:ILE:HG13	1.92	0.68
22:A9:480:LYS:O	22:A9:483:LYS:HG3	1.93	0.68
21:A8:596:LYS:HG3	21:A8:637:LEU:HB3	1.74	0.68
39:5I:345:THR:HG22	39:5I:347:ARG:H	1.58	0.68
21:A8:443:CYS:CB	25:AG:728:LEU:HD22	2.23	0.68
35:5E:315:GLU:HB3	45:RJ:1032:LEU:HD11	1.74	0.68
35:5E:517:LYS:HD2	35:5E:517:LYS:C	2.14	0.68
46:RK:192:THR:HA	46:RK:224:ASN:O	1.92	0.68
23:AE:692:ILE:HA	23:AE:695:TYR:HB3	1.76	0.68
50:RP:173:THR:O	50:RP:177:LEU:HB2	1.94	0.68
24:AF:86:SER:O	24:AF:98:ALA:HA	1.93	0.68
35:5E:366:GLU:OE2	37:5G:247:ILE:CG2	2.33	0.68
24:AF:211:HIS:HD1	24:AF:228:SER:HG	1.41	0.67
27:B2:17:ILE:HG22	27:B2:52:TRP:CH2	2.28	0.67
8:SK:65:LYS:NZ	17:3F:59:PRO:HG3	2.08	0.67
17:3F:443:LEU:HD21	17:3F:492:TRP:HE1	1.59	0.67
48:RN:86:ILE:CB	48:RN:89:GLN:HE21	2.07	0.67
35:5E:520:LEU:CG	35:5E:525:LYS:HG3	2.24	0.67
30:BE:209:ILE:HG22	30:BE:225:THR:HG22	1.76	0.67
35:5E:384:ARG:HH21	37:5G:81:SER:CB	2.08	0.67
35:5E:384:ARG:NH2	37:5G:81:SER:HB3	2.09	0.67
48:RN:85:GLY:O	48:RN:89:GLN:HG2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3F:185:LEU:H	17:3F:202:THR:HB	1.59	0.67
19:A4:645:ARG:HD2	19:A4:656:ARG:HD3	1.76	0.67
21:A8:648:PHE:CE1	22:A9:510:ALA:HA	2.29	0.67
36:5F:11:LYS:HA	36:5F:14:LYS:HE3	1.75	0.67
37:5G:123:VAL:HG12	37:5G:125:PRO:HD2	1.77	0.67
29:B8:513:GLN:HG3	29:B8:551:VAL:HG21	1.76	0.67
35:5E:517:LYS:HB3	35:5E:517:LYS:HZ2	1.60	0.67
27:B2:536:CYS:HB3	27:B2:549:SER:HB3	1.77	0.67
3:SA:187:G:N2	3:SA:197:A:N7	2.43	0.66
12:SZ:51:GLU:HB2	12:SZ:54:ALA:HB3	1.76	0.66
26:B1:20:ILE:H	26:B1:307:THR:HG21	1.58	0.66
35:5E:490:LEU:HD22	35:5E:494:GLU:OE1	1.95	0.66
21:A8:648:PHE:HE1	22:A9:510:ALA:HA	1.59	0.66
25:AG:435:ASP:HB3	25:AG:701:VAL:O	1.96	0.66
30:BE:209:ILE:HA	30:BE:225:THR:HA	1.76	0.66
11:SY:103:LEU:HB3	11:SY:126:LYS:HB2	1.76	0.66
14:3B:103:GLU:HG3	40:5J:134:ARG:HH12	1.60	0.66
9:SM:67:ARG:HH21	9:SM:129:ARG:H	1.44	0.66
26:B1:337:TYR:CD2	30:BE:744:SER:O	2.48	0.66
1:3A:323:G:H5'	34:5D:116:LYS:HG3	1.76	0.66
33:5C:257:SER:HG	33:5C:259:TRP:HE1	1.40	0.66
45:RJ:248:ARG:HB3	45:RJ:272:TYR:HB2	1.78	0.66
25:AG:16:SER:HB2	25:AG:783:LEU:HB2	1.77	0.66
45:RJ:871:MET:HE2	45:RJ:930:LYS:NZ	2.09	0.66
24:AF:52:PRO:HG2	24:AF:312:ALA:HA	1.77	0.65
28:B3:462:THR:HA	28:B3:484:GLU:HG2	1.77	0.65
21:A8:665:GLN:HB3	22:A9:496:LEU:CD2	2.26	0.65
36:5F:5:LEU:HB3	36:5F:9:GLU:CB	2.25	0.65
21:A8:443:CYS:N	25:AG:728:LEU:CD2	2.56	0.65
47:RM:283:ALA:HA	47:RM:411:THR:O	1.96	0.65
3:SA:207:U:H3	3:SA:258:C:H42	1.45	0.65
47:RM:311:THR:O	47:RM:370:ILE:HA	1.97	0.65
21:A8:643:ASP:OD1	24:AF:510:LEU:HA	1.96	0.65
19:A4:497:ILE:HD11	19:A4:511:VAL:HG23	1.78	0.65
27:B2:262:ILE:O	27:B2:270:SER:HA	1.97	0.65
34:5D:61:ASP:O	36:5F:160:TRP:CH2	2.50	0.65
35:5E:345:LEU:HD23	35:5E:345:LEU:C	2.17	0.65
1:3A:84:U:OP2	16:3E:361:ARG:NH2	2.30	0.65
33:5C:170:GLN:NE2	33:5C:177:TYR:OH	2.30	0.64
9:SM:87:ARG:HE	9:SM:104:HIS:HB2	1.62	0.64
17:3F:125:VAL:O	17:3F:128:GLN:NE2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:RG:122:ILE:HA	44:RG:161:LYS:O	1.97	0.64
45:RJ:263:LEU:HD23	45:RJ:267:ARG:HH22	1.63	0.64
49:RO:472:HIS:HD2	49:RO:474:HIS:H	1.46	0.64
1:3A:319:G:C5'	14:3C:121:LYS:HZ1	2.08	0.64
8:SK:57:ARG:HE	41:5K:88:ASP:HB3	1.60	0.64
35:5E:493:GLN:NE2	35:5E:497:ASN:CB	2.61	0.64
2:5A:487:A:H62	51:RQ:876:GLN:HE22	1.45	0.64
3:SA:415:C:H1'	3:SA:419:G:N2	2.12	0.64
3:SA:1727:G:N2	3:SA:1728:A:N7	2.46	0.64
21:A8:576:ARG:HG2	21:A8:578:LEU:H	1.63	0.64
26:B1:438:VAL:HG12	26:B1:445:VAL:HG23	1.79	0.64
27:B2:439:LEU:HB2	27:B2:444:LEU:HB3	1.79	0.64
28:B3:719:ILE:HD11	28:B3:762:CYS:HB3	1.78	0.64
30:BE:631:ASN:HB2	30:BE:644:THR:HB	1.80	0.64
48:RN:86:ILE:HG23	48:RN:89:GLN:HE21	1.63	0.64
11:SY:97:ASP:OD1	11:SY:97:ASP:N	2.31	0.64
26:B1:678:GLU:CD	35:5E:455:HIS:ND1	2.51	0.64
29:B8:521:LEU:HA	29:B8:531:CYS:O	1.98	0.64
21:A8:664:LYS:HD2	22:A9:448:GLU:OE1	1.98	0.64
7:SJ:5:ARG:NH2	7:SJ:29:LEU:O	2.31	0.63
20:A5:145:CYS:HB2	20:A5:148:LEU:HD21	1.80	0.63
49:RO:318:LEU:HA	49:RO:357:ARG:HH12	1.62	0.63
18:3H:44:LEU:HD22	18:3H:52:ILE:HD11	1.80	0.63
34:5D:78:LEU:CB	45:RJ:1082:GLN:HE21	2.01	0.63
35:5E:381:LEU:HB2	37:5G:212:ALA:HA	1.80	0.63
42:RA:18:GLY:HA2	42:RA:339:HIS:HD2	1.62	0.63
35:5E:340:LEU:HD13	45:RJ:957:GLU:OE2	1.98	0.63
3:SA:343:C:H2'	3:SA:344:A:H8	1.63	0.63
7:SJ:42:ARG:HD3	42:RA:57:GLU:HB3	1.80	0.63
12:SZ:20:ARG:HD2	12:SZ:74:LEU:HD12	1.79	0.63
26:B1:298:LEU:HD11	35:5E:476:MET:CE	2.28	0.63
45:RJ:831:ARG:NH2	45:RJ:835:HIS:O	2.30	0.63
3:SA:576:G:H4'	35:5E:327:LYS:HE2	1.81	0.63
35:5E:370:ARG:NH1	48:RN:52:ARG:NH1	2.47	0.63
35:5E:538:LYS:HD3	35:5E:538:LYS:C	2.19	0.63
45:RJ:871:MET:HE1	45:RJ:930:LYS:HD2	1.81	0.63
17:3F:538:ARG:HA	17:3F:566:ALA:O	1.97	0.63
33:5C:386:PHE:O	39:5I:8:ARG:NH2	2.31	0.63
44:RH:192:TYR:HA	44:RH:195:LYS:HD2	1.81	0.63
28:B3:244:GLU:HG2	28:B3:293:VAL:H	1.64	0.63
10:SR:94:GLN:HB2	10:SR:102:LYS:HG3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SK:65:LYS:HZ2	17:3F:59:PRO:HB3	1.64	0.63
19:A4:399:VAL:HG22	19:A4:420:LEU:HB2	1.80	0.63
23:AE:638:SER:HA	23:AE:641:LEU:HD12	1.80	0.63
35:5E:533:LYS:CA	35:5E:536:ARG:HG2	2.29	0.63
42:RA:247:THR:HG23	42:RA:249:ASN:H	1.64	0.63
1:3A:319:G:O5'	14:3C:121:LYS:NZ	2.32	0.62
44:RH:129:ARG:HH11	44:RH:132:ARG:HD3	1.63	0.62
16:3E:384:GLY:O	16:3E:388:LEU:HB2	1.99	0.62
42:RA:287:ASN:HB2	42:RA:302:ARG:HB2	1.80	0.62
45:RJ:932:LEU:HD22	45:RJ:1007:TYR:HB2	1.80	0.62
34:5D:29:GLU:OE2	34:5D:37:ARG:NH1	2.31	0.62
49:RO:300:THR:O	49:RO:304:ASN:ND2	2.32	0.62
52:RS:379:LYS:HD2	52:RS:427:ARG:HE	1.64	0.62
21:A8:672:ASN:CB	22:A9:489:SER:OG	2.46	0.62
28:B3:691:PRO:CD	35:5E:516:SER:HB3	2.29	0.62
31:B6:285:TYR:HD2	31:B6:308:THR:HG22	1.63	0.62
3:SA:146:U:H3	3:SA:168:A:N6	1.97	0.62
48:RN:482:GLN:HG2	49:RO:507:LEU:HD11	1.80	0.62
3:SA:1220:C:H2'	3:SA:1221:A:H8	1.64	0.62
3:SA:1655:A:N6	3:SA:1743:U:O4	2.32	0.62
46:RK:221:CYS:SG	46:RK:222:GLU:N	2.71	0.62
20:A5:120:ILE:HB	20:A5:151:LEU:HD23	1.82	0.62
22:A9:432:LYS:HB3	22:A9:435:LEU:HB3	1.81	0.62
30:BE:733:THR:O	30:BE:737:LEU:HB3	2.00	0.62
36:5F:153:ASN:O	36:5F:153:ASN:ND2	2.32	0.62
45:RJ:871:MET:CE	45:RJ:930:LYS:HD2	2.30	0.62
3:SA:477:A:H5'	38:5H:560:ASN:HD22	1.64	0.62
52:RS:214:TYR:HB3	52:RS:249:THR:HG22	1.80	0.62
21:A8:592:ARG:HH11	25:AG:605:ASN:ND2	1.98	0.61
21:A8:631:SER:C	21:A8:634:LEU:HG	2.19	0.61
26:B1:303:ASN:ND2	26:B1:323:LYS:HD3	2.15	0.61
3:SA:1538:U:H2'	3:SA:1569:A:H61	1.65	0.61
24:AF:440:GLU:O	24:AF:444:ASN:HB2	2.00	0.61
35:5E:345:LEU:CD2	45:RJ:961:PHE:CZ	2.82	0.61
48:RN:95:ARG:HH12	48:RN:757:LYS:HG3	1.64	0.61
18:3H:50:GLU:HG3	18:3H:104:THR:HG22	1.82	0.61
21:A8:631:SER:CA	21:A8:634:LEU:HD11	2.25	0.61
30:BE:471:CYS:SG	30:BE:514:ASN:ND2	2.74	0.61
3:SA:362:G:H22	3:SA:382:C:H1'	1.66	0.61
24:AF:428:ARG:NH2	25:AG:518:ASP:O	2.34	0.61
46:RK:155:LYS:HG2	46:RK:165:GLU:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:RS:423:THR:HA	52:RS:426:GLN:HG2	1.81	0.61
3:SA:521:A:N3	12:SZ:34:ASN:ND2	2.48	0.61
4:SF:95:THR:HG22	50:RP:59:LEU:HB3	1.83	0.61
21:A8:443:CYS:HA	25:AG:728:LEU:CG	2.30	0.61
4:SF:212:ASP:H	4:SF:215:ASP:HA	1.65	0.61
29:B8:424:ILE:HG12	29:B8:434:GLU:HG2	1.83	0.61
20:A5:162:GLN:HA	20:A5:173:ILE:O	2.01	0.61
21:A8:671:ARG:NH2	22:A9:453:PRO:HG2	2.16	0.61
24:AF:51:HIS:O	24:AF:53:HIS:ND1	2.30	0.61
44:RG:36:LYS:HB3	44:RG:172:PRO:HA	1.82	0.61
25:AG:335:PRO:HB2	25:AG:336:ARG:HD3	1.82	0.61
25:AG:769:ASN:ND2	25:AG:771:ASP:OD1	2.33	0.61
31:B6:286:ILE:HG22	31:B6:308:THR:HG21	1.83	0.61
45:RJ:871:MET:HE1	45:RJ:930:LYS:CD	2.31	0.61
35:5E:371:ARG:NH1	35:5E:375:ASP:OD2	2.34	0.61
48:RN:511:SER:HA	48:RN:557:SER:HB2	1.82	0.61
14:3B:142:ARG:NH1	14:3B:186:ASP:OD2	2.34	0.60
17:3F:356:ARG:NH1	43:RB:260:ALA:O	2.34	0.60
20:A5:481:LEU:HD21	20:A5:526:LEU:HD22	1.82	0.60
50:RP:91:LEU:HD21	50:RP:110:LEU:HD12	1.83	0.60
1:3A:319:G:H5'	14:3C:121:LYS:HZ1	1.59	0.60
14:3C:186:ASP:OD1	14:3C:214:ARG:NH1	2.34	0.60
45:RJ:60:ASP:O	45:RJ:239:ASN:ND2	2.34	0.60
3:SA:374:U:H5''	43:RB:331:LYS:HE3	1.83	0.60
26:B1:14:VAL:HG11	26:B1:341:GLN:HB3	1.84	0.60
28:B3:160:ILE:HG22	28:B3:162:LEU:HD13	1.82	0.60
39:5I:260:GLN:NE2	39:5I:289:TYR:OH	2.35	0.60
44:RG:147:LYS:HD3	44:RG:150:ILE:HG22	1.83	0.60
44:RH:156:GLU:HG2	44:RH:157:GLU:HG2	1.81	0.60
49:RO:461:SER:OG	49:RO:462:SER:N	2.33	0.60
34:5D:68:HIS:HE1	36:5F:169:THR:HG21	1.67	0.60
3:SA:435:C:H42	45:RJ:166:ARG:HH12	1.47	0.60
17:3F:328:ILE:HG13	17:3F:338:THR:HG22	1.82	0.60
19:A4:429:SER:HB3	19:A4:444:ARG:HA	1.83	0.60
20:A5:545:ALA:HB2	21:A8:674:GLU:HG3	1.82	0.60
48:RN:548:ARG:NH1	48:RN:638:ASN:OD1	2.34	0.60
49:RO:452:ASP:HB3	49:RO:455:LEU:HB2	1.84	0.60
3:SA:606:A:N3	3:SA:607:G:N1	2.50	0.60
4:SF:194:THR:HG23	4:SF:195:ILE:HG12	1.83	0.60
21:A8:638:LEU:HD21	21:A8:658:LEU:HD11	1.83	0.60
48:RN:649:THR:HG23	48:RN:650:VAL:HG23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SK:65:LYS:HZ2	17:3F:59:PRO:N	1.98	0.60
15:3D:29:SER:O	15:3D:35:GLN:NE2	2.34	0.60
27:B2:54:ILE:HD13	27:B2:364:TYR:HD2	1.66	0.60
28:B3:581:CYS:HA	28:B3:590:LEU:O	2.02	0.60
34:5D:22:ARG:NH1	45:RJ:997:MET:O	2.35	0.60
3:SA:85:A:H2'	3:SA:86:A:H8	1.65	0.60
42:RA:333:ASN:HD21	42:RA:338:MET:HA	1.67	0.60
21:A8:593:ASP:CA	21:A8:596:LYS:HD2	2.26	0.59
23:AE:699:ARG:NH1	23:AE:702:TRP:O	2.35	0.59
24:AF:248:ARG:NH1	24:AF:289:ASN:O	2.35	0.59
36:5F:69:PRO:HA	36:5F:72:ARG:HG2	1.83	0.59
37:5G:239:VAL:HG21	48:RN:13:LEU:CD1	2.30	0.59
46:RK:14:SER:HB2	46:RK:36:ILE:HG23	1.83	0.59
24:AF:301:PRO:HG2	24:AF:323:SER:HB3	1.84	0.59
28:B3:189:HIS:NE2	28:B3:217:ASP:OD1	2.35	0.59
5:SG:131:GLN:NE2	5:SG:135:ASP:OD1	2.35	0.59
6:SH:70:PRO:HB3	6:SH:101:ILE:HB	1.84	0.59
15:3D:382:LYS:HD2	15:3D:404:LEU:HD22	1.83	0.59
24:AF:133:HIS:HD2	24:AF:135:GLN:H	1.50	0.59
45:RJ:871:MET:HE1	45:RJ:930:LYS:HE2	1.83	0.59
25:AG:90:LYS:HG2	25:AG:144:VAL:HG22	1.85	0.59
48:RN:614:ILE:HG22	48:RN:616:LEU:HB2	1.85	0.59
7:SJ:32:GLN:HG2	42:RA:79:PRO:HD2	1.84	0.59
10:SR:122:ARG:NH2	37:5G:133:LYS:HD2	2.17	0.59
30:BE:737:LEU:CA	30:BE:740:ILE:HG22	2.28	0.59
36:5F:109:ARG:NH2	36:5F:155:GLU:OE2	2.36	0.59
50:RP:112:GLN:NE2	50:RP:116:ASP:OD2	2.36	0.59
50:RP:54:TRP:O	50:RP:58:ASN:ND2	2.35	0.59
15:3D:286:ARG:HA	15:3D:289:TYR:HB3	1.85	0.59
16:3E:210:LEU:HD23	16:3E:256:ASN:HD22	1.68	0.59
21:A8:673:THR:CG2	22:A9:490:GLU:CB	2.68	0.59
26:B1:497:ILE:HG23	26:B1:512:ILE:HB	1.84	0.59
31:B6:15:MET:HA	31:B6:18:LEU:HB3	1.85	0.59
48:RN:86:ILE:CG2	48:RN:89:GLN:HE21	2.16	0.59
4:SF:180:LEU:HA	4:SF:194:THR:HG21	1.85	0.59
26:B1:298:LEU:HD11	35:5E:476:MET:HE1	1.84	0.59
35:5E:384:ARG:HE	37:5G:82:GLY:N	1.97	0.59
35:5E:493:GLN:NE2	35:5E:497:ASN:HD22	2.01	0.59
44:RG:125:ASN:ND2	44:RG:127:THR:OG1	2.36	0.59
48:RN:535:ASN:OD1	48:RN:539:ARG:NH1	2.36	0.59
14:3C:114:GLY:O	14:3C:122:ARG:NH1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:5C:190:HIS:HB3	33:5C:207:THR:HG21	1.84	0.58
25:AG:153:ILE:HG22	25:AG:174:TYR:HB2	1.85	0.58
34:5D:58:ARG:NH2	36:5F:174:ARG:NE	2.51	0.58
37:5G:144:GLU:HA	37:5G:149:PRO:HA	1.84	0.58
1:3A:58:A:OP1	36:5F:165:LYS:HE3	2.03	0.58
50:RP:144:SER:HB3	50:RP:147:VAL:HG12	1.86	0.58
19:A4:565:ARG:HD3	23:AE:633:GLU:HB2	1.86	0.58
25:AG:568:ASN:ND2	25:AG:586:SER:OG	2.35	0.58
27:B2:97:GLY:HA3	27:B2:124:ILE:HD11	1.84	0.58
34:5D:113:ILE:HG23	34:5D:117:LYS:HE3	1.86	0.58
36:5F:54:ILE:HD11	36:5F:101:VAL:HG21	1.84	0.58
39:5I:411:LYS:O	39:5I:415:ARG:HB2	2.02	0.58
1:3A:30:A:N6	39:5I:341:GLU:OE2	2.36	0.58
16:3E:11:GLY:HA2	16:3E:143:LEU:HD22	1.86	0.58
34:5D:37:ARG:NH2	45:RJ:994:LYS:O	2.36	0.58
36:5F:9:GLU:HA	36:5F:9:GLU:OE2	2.04	0.58
4:SF:44:LEU:HD13	4:SF:82:TYR:HB3	1.85	0.58
19:A4:269:PHE:O	29:B8:446:ARG:NH2	2.36	0.58
21:A8:631:SER:HA	21:A8:634:LEU:CD2	2.34	0.58
23:AE:248:SER:OG	23:AE:253:CYS:SG	2.62	0.58
25:AG:118:VAL:HB	25:AG:130:LYS:HB2	1.85	0.58
28:B3:494:ILE:N	28:B3:510:SER:OG	2.35	0.58
28:B3:742:ARG:NH1	35:5E:506:GLU:OE1	2.36	0.58
48:RN:86:ILE:CA	48:RN:89:GLN:HG2	2.33	0.58
49:RO:202:LEU:HD22	49:RO:212:LEU:HD22	1.86	0.58
1:3A:251:G:H2'	17:3F:155:ASN:HD21	1.67	0.58
3:SA:126:A:N6	3:SA:291:G:O2'	2.37	0.58
20:A5:546:ARG:NH1	21:A8:677:ASN:O	2.36	0.58
21:A8:632:THR:O	21:A8:636:GLN:HG3	2.04	0.58
25:AG:435:ASP:CB	25:AG:702:TYR:HA	2.34	0.58
27:B2:259:ILE:HA	27:B2:273:TYR:O	2.03	0.58
42:RA:75:GLY:HA3	42:RA:80:GLN:H	1.68	0.58
44:RH:44:VAL:HA	44:RH:113:TYR:O	2.03	0.58
14:3B:236:MET:HG3	15:3D:133:LEU:HA	1.84	0.58
20:A5:545:ALA:HB1	21:A8:674:GLU:HG3	1.86	0.58
25:AG:144:VAL:HG12	25:AG:153:ILE:HG13	1.86	0.58
25:AG:157:PHE:HB2	25:AG:170:SER:HB3	1.86	0.58
26:B1:501:SER:HB2	26:B1:508:GLN:HB2	1.84	0.58
37:5G:183:SER:HB3	37:5G:220:ARG:HD2	1.86	0.58
17:3F:293:ASP:N	17:3F:293:ASP:OD1	2.37	0.57
28:B3:584:ILE:HD11	28:B3:599:ILE:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:RO:270:SER:H	49:RO:273:GLN:HE21	1.50	0.57
1:3A:323:G:OP2	34:5D:116:LYS:CB	2.51	0.57
17:3F:241:THR:HG21	17:3F:285:SER:HA	1.86	0.57
18:3H:44:LEU:HD13	18:3H:52:ILE:HD11	1.86	0.57
23:AE:671:LEU:O	23:AE:675:ASN:HB3	2.04	0.57
24:AF:303:LEU:HD13	24:AF:323:SER:HB2	1.86	0.57
29:B8:221:THR:OG1	29:B8:222:LEU:N	2.38	0.57
30:BE:482:GLY:HA2	30:BE:505:VAL:HG23	1.86	0.57
33:5C:317:THR:HG23	33:5C:334:ARG:HB3	1.86	0.57
45:RJ:773:THR:HA	45:RJ:777:ARG:HH11	1.69	0.57
46:RK:114:PHE:HB2	46:RK:170:VAL:HG22	1.86	0.57
3:SA:1196:A:N3	44:RG:136:ARG:NH2	2.52	0.57
11:SY:109:ARG:NH2	11:SY:120:VAL:O	2.37	0.57
27:B2:365:TYR:HA	27:B2:381:LYS:HA	1.85	0.57
32:5B:194:LYS:HD2	32:5B:199:ILE:HG13	1.86	0.57
35:5E:384:ARG:HE	37:5G:81:SER:HB3	1.69	0.57
44:RH:31:LEU:HD13	44:RH:40:ARG:HE	1.69	0.57
12:SZ:83:LYS:HD2	12:SZ:96:LEU:HD21	1.86	0.57
14:3C:267:VAL:HG21	14:3C:298:ILE:HD12	1.87	0.57
28:B3:744:ARG:HA	28:B3:785:ILE:HG21	1.86	0.57
29:B8:227:LEU:HB2	29:B8:528:GLN:HE22	1.67	0.57
30:BE:359:ALA:O	30:BE:421:ASN:ND2	2.38	0.57
34:5D:113:ILE:CG2	34:5D:117:LYS:HE3	2.34	0.57
1:3A:318:U:H3	14:3C:119:GLY:CA	2.12	0.57
16:3E:339:TYR:HB3	16:3E:343:TYR:HB2	1.85	0.57
23:AE:559:ASN:HA	23:AE:592:ARG:HD3	1.85	0.57
47:RL:29:VAL:HG22	47:RL:202:ASP:HA	1.86	0.57
4:SF:206:ASP:OD1	4:SF:206:ASP:N	2.38	0.57
7:SJ:167:ALA:HB2	7:SJ:183:ILE:HD12	1.87	0.57
20:A5:148:LEU:HD23	20:A5:167:SER:HB3	1.86	0.57
24:AF:24:GLN:O	24:AF:28:ARG:HB3	2.05	0.57
26:B1:264:LYS:HD3	26:B1:280:THR:HG22	1.87	0.57
26:B1:405:SER:HB3	26:B1:436:LEU:HD23	1.85	0.57
28:B3:392:ASN:H	28:B3:407:SER:HA	1.69	0.57
33:5C:430:VAL:HG21	36:5F:3:ARG:NE	2.18	0.57
39:5I:87:SER:OG	39:5I:89:ASP:OD1	2.22	0.57
1:3A:57:A:H5''	36:5F:165:LYS:HG3	1.87	0.57
3:SA:205:U:H2'	3:SA:206:A:H8	1.68	0.57
17:3F:442:ILE:HA	17:3F:472:PRO:HA	1.86	0.57
29:B8:146:LEU:O	29:B8:163:ARG:NH1	2.37	0.57
14:3C:142:ARG:NH1	14:3C:186:ASP:OD2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A8:596:LYS:HG2	21:A8:637:LEU:HB3	1.86	0.57
26:B1:418:ARG:HH21	26:B1:418:ARG:CG	2.09	0.57
42:RA:152:ASP:HA	42:RA:166:ASN:HA	1.86	0.57
45:RJ:1042:MET:HG3	45:RJ:1044:LEU:HD13	1.86	0.57
2:5A:481:U:O2'	31:B6:102:LYS:NZ	2.37	0.57
3:SA:146:U:N3	3:SA:168:A:N6	2.51	0.57
3:SA:559:C:OP1	45:RJ:868:ARG:NH2	2.37	0.57
15:3D:264:SER:OG	15:3D:265:GLU:N	2.37	0.57
17:3F:142:ILE:HA	17:3F:568:ILE:HD11	1.86	0.57
20:A5:434:THR:HG23	49:RO:266:ASN:HD21	1.68	0.57
25:AG:86:GLU:OE1	25:AG:113:ASN:ND2	2.36	0.57
29:B8:129:ASP:OD1	30:BE:194:ARG:NH2	2.36	0.57
39:5I:81:ASN:ND2	39:5I:96:ASN:OD1	2.38	0.57
47:RL:32:ARG:HE	47:RL:35:ASN:HD21	1.53	0.57
3:SA:112:A:O2'	9:SM:67:ARG:NH1	2.37	0.57
30:BE:666:ARG:NH1	30:BE:706:ASP:OD2	2.38	0.57
39:5I:45:LEU:HD13	39:5I:410:ILE:HG22	1.86	0.57
50:RP:54:TRP:HA	50:RP:57:ILE:HG22	1.87	0.57
52:RS:209:LYS:HE3	52:RS:212:LYS:HG3	1.87	0.57
3:SA:1197:C:OP1	44:RG:136:ARG:NH1	2.38	0.56
17:3F:545:LYS:HG2	17:3F:561:ASN:HD21	1.70	0.56
20:A5:212:LEU:HD11	20:A5:246:VAL:HG11	1.87	0.56
21:A8:655:LEU:HD23	22:A9:507:ARG:HB3	1.86	0.56
26:B1:373:ASP:HB2	26:B1:380:LEU:HD21	1.86	0.56
35:5E:310:GLN:HA	35:5E:313:GLN:HG2	1.86	0.56
41:5K:26:LYS:HD3	41:5K:29:GLN:HG3	1.87	0.56
1:3A:94:A:H61	1:3A:322:A:N6	2.01	0.56
25:AG:473:LEU:HB2	25:AG:495:ILE:HD11	1.87	0.56
26:B1:479:LEU:HD12	26:B1:488:LEU:HD11	1.87	0.56
28:B3:690:HIS:ND1	35:5E:519:GLU:HB2	2.20	0.56
39:5I:15:PRO:HB3	39:5I:20:GLN:HE21	1.70	0.56
47:RL:12:SER:O	47:RL:16:ASN:ND2	2.38	0.56
3:SA:439:U:H4'	3:SA:465:G:H22	1.69	0.56
24:AF:147:ARG:NH2	44:RH:16:GLN:O	2.39	0.56
26:B1:298:LEU:HA	35:5E:472:PRO:CB	2.33	0.56
27:B2:598:LYS:NZ	27:B2:610:SER:OG	2.38	0.56
35:5E:507:ILE:HD11	35:5E:528:LEU:HD23	1.86	0.56
42:RA:227:ARG:NH2	42:RA:248:SER:O	2.34	0.56
43:RB:230:ALA:O	43:RB:234:LYS:HB2	2.05	0.56
44:RG:41:MET:HG3	44:RG:202:ILE:HG23	1.88	0.56
3:SA:337:G:N2	3:SA:340:U:OP2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3E:414:ARG:NH1	23:AE:187:ASP:OD2	2.36	0.56
22:A9:473:LYS:O	22:A9:477:LYS:NZ	2.39	0.56
11:SY:132:LEU:HA	11:SY:135:LEU:HB2	1.87	0.56
19:A4:32:ILE:O	19:A4:751:GLU:HA	2.06	0.56
19:A4:37:ARG:NH1	21:A8:704:PRO:O	2.38	0.56
26:B1:329:VAL:HG12	26:B1:339:LEU:HG	1.87	0.56
8:SK:78:ARG:NH2	43:RB:247:GLU:OE1	2.33	0.56
19:A4:301:ASP:O	19:A4:771:GLN:NE2	2.38	0.56
27:B2:145:ILE:HG23	27:B2:159:LEU:HB2	1.88	0.56
27:B2:180:THR:OG1	27:B2:207:CYS:SG	2.62	0.56
47:RL:71:LYS:O	47:RL:75:ASN:ND2	2.38	0.56
2:5A:484:G:OP2	31:B6:3:LYS:NZ	2.39	0.56
19:A4:578:SER:HG	19:A4:643:SER:HG	1.51	0.56
35:5E:474:ILE:HG23	35:5E:476:MET:H	1.71	0.56
49:RO:170:GLY:O	49:RO:272:GLN:NE2	2.32	0.56
2:5A:5:G:N2	2:5A:8:A:OP2	2.39	0.56
14:3C:160:ASP:OD1	14:3C:160:ASP:N	2.37	0.56
20:A5:435:GLY:HA3	49:RO:262:LEU:HD11	1.88	0.56
25:AG:510:TYR:HH	25:AG:527:HIS:HD1	1.52	0.56
26:B1:419:TYR:CE2	35:5E:486:ASN:ND2	2.73	0.56
27:B2:347:SER:O	27:B2:371:LYS:NZ	2.39	0.56
27:B2:461:SER:OG	27:B2:462:SER:N	2.38	0.56
47:RL:7:ASP:HB2	47:RL:10:ILE:HG12	1.88	0.56
3:SA:143:G:OP2	6:SH:139:ASN:ND2	2.38	0.56
3:SA:1657:U:OP1	3:SA:1658:G:O2'	2.23	0.56
7:SJ:104:ILE:O	7:SJ:164:ARG:HA	2.06	0.56
15:3D:389:ILE:HA	18:3H:62:GLU:HB2	1.87	0.56
20:A5:471:ARG:NH2	49:RO:301:ASP:OD2	2.39	0.56
37:5G:76:GLU:OE2	37:5G:201:ARG:NH2	2.36	0.56
41:5K:123:PRO:O	41:5K:126:LYS:NZ	2.39	0.56
23:AE:272:LYS:NZ	23:AE:310:GLY:O	2.39	0.56
39:5I:73:ILE:HG12	39:5I:85:THR:HG22	1.88	0.56
46:RK:34:GLU:HG3	46:RK:35:LYS:HG2	1.88	0.56
46:RK:154:LEU:HB2	46:RK:165:GLU:HG3	1.88	0.56
48:RN:478:ILE:HD13	48:RN:520:PRO:HB2	1.88	0.56
48:RN:512:ASP:OD1	48:RN:512:ASP:N	2.38	0.56
53:RY:487:ASP:N	53:RY:487:ASP:OD1	2.36	0.56
3:SA:1108:G:O2'	3:SA:1109:G:N7	2.37	0.55
3:SA:1490:C:OP1	45:RJ:1062:ARG:NH2	2.38	0.55
14:3C:320:TYR:OH	14:3C:322:ARG:NH2	2.39	0.55
17:3F:417:SER:OG	17:3F:418:ASP:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A5:364:THR:OG1	20:A5:368:ASN:ND2	2.38	0.55
23:AE:95:ASP:HB2	23:AE:131:ASN:HD21	1.71	0.55
25:AG:435:ASP:HB3	25:AG:702:TYR:HA	1.88	0.55
28:B3:12:LEU:HG	28:B3:641:PHE:HB2	1.87	0.55
29:B8:181:GLU:HB3	30:BE:281:ARG:HH12	1.71	0.55
50:RP:67:ALA:O	50:RP:71:GLU:HB2	2.07	0.55
1:3A:94:A:N6	1:3A:322:A:H61	2.00	0.55
3:SA:448:C:OP2	4:SF:49:ARG:NH2	2.38	0.55
6:SH:46:LYS:HB3	6:SH:118:GLU:HG2	1.88	0.55
12:SZ:54:ALA:HB1	12:SZ:76:TYR:HB2	1.88	0.55
18:3H:41:THR:O	18:3H:45:ASN:ND2	2.39	0.55
20:A5:5:VAL:HA	20:A5:21:THR:HG22	1.89	0.55
27:B2:463:SER:OG	27:B2:464:LEU:N	2.39	0.55
27:B2:858:PHE:O	27:B2:862:LYS:HB2	2.06	0.55
40:5J:129:ALA:HB1	45:RJ:1119:ILE:HG22	1.89	0.55
42:RA:101:ASN:HA	42:RA:118:GLN:HA	1.88	0.55
3:SA:128:U:H3	50:RP:906:THR:H	1.53	0.55
26:B1:341:GLN:HG3	26:B1:378:PHE:CD1	2.41	0.55
34:5D:58:ARG:NH2	36:5F:174:ARG:CZ	2.69	0.55
48:RN:86:ILE:O	48:RN:89:GLN:CG	2.54	0.55
3:SA:396:G:O6	7:SJ:26:LYS:NZ	2.37	0.55
7:SJ:195:ARG:NH2	9:SM:11:ARG:O	2.39	0.55
27:B2:124:ILE:HA	27:B2:140:SER:HA	1.89	0.55
27:B2:142:ASP:OD2	27:B2:144:ASN:ND2	2.39	0.55
27:B2:267:ASP:OD1	27:B2:267:ASP:N	2.36	0.55
34:5D:61:ASP:HA	36:5F:160:TRP:HZ3	1.71	0.55
36:5F:4:LYS:O	36:5F:4:LYS:HG2	2.07	0.55
39:5I:26:ARG:NH1	51:RQ:867:GLN:O	2.40	0.55
39:5I:340:ARG:NH2	39:5I:377:SER:O	2.39	0.55
46:RK:139:PRO:HA	46:RK:142:GLU:HB2	1.89	0.55
48:RN:682:ARG:O	48:RN:686:ASN:ND2	2.40	0.55
3:SA:207:U:H3	3:SA:258:C:N4	2.04	0.55
3:SA:444:C:O2	3:SA:460:A:N6	2.39	0.55
3:SA:453:U:O2'	3:SA:455:C:OP2	2.24	0.55
14:3B:225:ARG:NH1	14:3B:248:ASP:OD2	2.38	0.55
14:3C:189:GLY:O	14:3C:216:ASN:ND2	2.39	0.55
14:3C:225:ARG:NH2	14:3C:246:GLN:OE1	2.38	0.55
17:3F:289:ARG:NH2	17:3F:332:ALA:O	2.39	0.55
17:3F:552:TRP:HB3	18:3H:85:VAL:HG13	1.88	0.55
25:AG:262:MET:HA	25:AG:272:ALA:O	2.07	0.55
28:B3:366:PRO:HG2	28:B3:378:PRO:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:5C:162:ASN:HB3	33:5C:164:GLN:H	1.71	0.55
36:5F:13:LEU:CD1	36:5F:16:VAL:HG11	2.37	0.55
39:5I:173:ILE:HG13	39:5I:174:ARG:HG2	1.87	0.55
39:5I:329:ILE:HG12	39:5I:343:TYR:HB2	1.89	0.55
45:RJ:279:PRO:HB3	45:RJ:784:LYS:HA	1.88	0.55
45:RJ:360:ASP:OD1	45:RJ:360:ASP:N	2.35	0.55
45:RJ:608:LEU:HB2	46:RK:16:ASN:HD22	1.72	0.55
45:RJ:921:GLU:HB2	46:RK:365:LYS:HG3	1.88	0.55
7:SJ:41:LYS:HE2	7:SJ:43:ILE:HD11	1.89	0.55
7:SJ:98:LYS:NZ	7:SJ:170:SER:O	2.36	0.55
19:A4:57:ILE:HD13	19:A4:340:GLN:HG2	1.89	0.55
25:AG:583:LYS:HE2	25:AG:599:ILE:HD13	1.88	0.55
29:B8:526:ASP:OD1	29:B8:526:ASP:N	2.38	0.55
29:B8:561:PRO:O	29:B8:587:ARG:NH1	2.39	0.55
31:B6:278:MET:HA	31:B6:312:LEU:HD11	1.89	0.55
43:RB:304:GLU:OE1	43:RB:309:LYS:NZ	2.40	0.55
45:RJ:871:MET:SD	45:RJ:930:LYS:HD2	2.47	0.55
3:SA:365:G:N7	43:RB:231:ARG:NH1	2.55	0.55
3:SA:1232:U:O4	3:SA:1234:A:N6	2.39	0.55
23:AE:1172:ASP:N	23:AE:1236:ASN:O	2.40	0.55
27:B2:163:LYS:HG2	35:5E:522:ARG:HH22	1.71	0.55
27:B2:592:SER:OG	27:B2:593:ALA:N	2.40	0.55
28:B3:179:LYS:O	28:B3:181:LYS:NZ	2.38	0.55
52:RS:445:ARG:NH1	52:RS:445:ARG:O	2.40	0.55
8:SK:139:GLN:NE2	12:SZ:64:PHE:O	2.39	0.55
15:3D:21:LYS:HE2	15:3D:49:GLU:HB2	1.88	0.55
18:3G:57:ASP:O	18:3G:84:ARG:NH1	2.40	0.55
19:A4:641:GLU:OE2	19:A4:645:ARG:NH1	2.40	0.55
21:A8:596:LYS:HE2	21:A8:637:LEU:CA	2.29	0.55
25:AG:51:GLN:HE21	25:AG:53:LYS:HD3	1.72	0.55
26:B1:356:ASP:HB2	26:B1:826:ARG:HG3	1.89	0.55
27:B2:787:LYS:NZ	27:B2:788:PRO:O	2.38	0.55
28:B3:5:THR:O	28:B3:611:LYS:NZ	2.39	0.55
42:RA:166:ASN:ND2	42:RA:168:GLU:O	2.40	0.55
45:RJ:130:ASP:OD2	45:RJ:853:ARG:NH2	2.40	0.55
46:RK:171:ASP:N	46:RK:171:ASP:OD1	2.39	0.55
1:3A:58:A:P	36:5F:165:LYS:HE3	2.47	0.55
3:SA:96:G:N2	3:SA:387:A:N1	2.55	0.55
3:SA:258:C:O2	7:SJ:178:ARG:NH2	2.40	0.55
4:SF:45:ILE:HG13	4:SF:61:VAL:HG11	1.88	0.55
20:A5:454:GLU:OE2	20:A5:487:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AE:196:LEU:HD11	23:AE:213:THR:HG21	1.88	0.55
23:AE:636:ASP:OD1	23:AE:639:ARG:NH1	2.40	0.55
28:B3:107:ILE:HD11	28:B3:147:ILE:HG22	1.88	0.55
46:RK:155:LYS:HG3	46:RK:164:GLY:HA2	1.89	0.55
48:RN:290:LYS:O	52:RS:458:ARG:NH1	2.40	0.55
6:SH:10:ASN:O	6:SH:128:THR:OG1	2.25	0.55
9:SM:125:VAL:HB	9:SM:137:PHE:HB3	1.89	0.55
10:SR:122:ARG:CZ	37:5G:133:LYS:HD2	2.37	0.55
16:3E:280:MET:HG3	16:3E:288:THR:HG22	1.89	0.55
20:A5:531:LYS:O	20:A5:535:ASP:HB2	2.07	0.55
23:AE:12:ALA:HB2	33:5C:142:GLY:HA3	1.89	0.55
23:AE:558:VAL:O	23:AE:592:ARG:NH1	2.40	0.55
38:5H:565:LYS:HA	38:5H:568:LYS:HG2	1.89	0.55
39:5I:349:GLN:O	39:5I:367:SER:OG	2.24	0.55
45:RJ:289:HIS:HB2	45:RJ:815:LEU:HD21	1.89	0.55
45:RJ:871:MET:HE1	45:RJ:930:LYS:NZ	2.18	0.55
3:SA:332:U:OP1	7:SJ:31:ARG:NH2	2.37	0.54
7:SJ:8:ARG:HD2	7:SJ:22:ARG:HH11	1.72	0.54
15:3D:379:LEU:O	15:3D:383:CYS:HB2	2.07	0.54
21:A8:638:LEU:HA	21:A8:641:VAL:HG12	1.89	0.54
24:AF:75:LYS:HD3	24:AF:113:PRO:HD3	1.89	0.54
24:AF:420:GLU:O	24:AF:424:ARG:HB3	2.07	0.54
29:B8:176:LYS:O	29:B8:180:ASP:CB	2.55	0.54
33:5C:96:ASP:OD1	33:5C:96:ASP:N	2.35	0.54
45:RJ:551:LYS:O	45:RJ:555:MET:HB2	2.07	0.54
3:SA:1628:U:OP2	35:5E:534:ARG:NH1	2.40	0.54
25:AG:727:GLN:OE1	25:AG:738:ASN:ND2	2.39	0.54
26:B1:375:THR:OG1	26:B1:376:SER:N	2.41	0.54
29:B8:176:LYS:O	29:B8:180:ASP:HB3	2.07	0.54
31:B6:187:LYS:HE3	40:5J:63:PRO:HB2	1.89	0.54
39:5I:402:GLU:O	39:5I:405:ARG:NH2	2.40	0.54
45:RJ:966:ILE:HD13	45:RJ:976:ILE:HG22	1.88	0.54
49:RO:345:ILE:HA	49:RO:349:LEU:HD13	1.89	0.54
3:SA:562:G:H8	37:5G:283:THR:HB	1.72	0.54
23:AE:205:THR:HB	23:AE:210:LEU:HD21	1.89	0.54
25:AG:850:GLU:HA	25:AG:853:ILE:HD12	1.89	0.54
33:5C:186:ARG:NH1	36:5F:42:GLU:OE2	2.40	0.54
39:5I:133:GLN:NE2	39:5I:151:ASN:OD1	2.40	0.54
43:RB:335:GLU:HA	43:RB:339:SER:HB2	1.89	0.54
46:RK:37:ARG:NH2	46:RK:49:GLU:OE2	2.36	0.54
52:RS:319:LYS:HA	52:RS:323:PHE:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:576:G:C5'	35:5E:327:LYS:HE2	2.37	0.54
10:SR:22:VAL:HG22	10:SR:65:ILE:HG23	1.89	0.54
15:3D:63:LEU:O	15:3D:67:ASN:ND2	2.40	0.54
19:A4:534:LEU:HA	19:A4:542:VAL:O	2.07	0.54
21:A8:527:LEU:HD11	21:A8:549:ARG:HH22	1.72	0.54
26:B1:202:ASP:N	26:B1:202:ASP:OD1	2.40	0.54
28:B3:537:TRP:N	28:B3:551:SER:O	2.37	0.54
33:5C:369:MET:HE1	33:5C:404:PRO:HD2	1.90	0.54
42:RA:78:LYS:O	42:RA:80:GLN:NE2	2.41	0.54
45:RJ:1018:VAL:O	45:RJ:1029:TRP:NE1	2.41	0.54
49:RO:156:TRP:O	49:RO:215:ASN:ND2	2.40	0.54
19:A4:252:GLN:NE2	19:A4:318:ASN:OD1	2.40	0.54
24:AF:215:VAL:HA	24:AF:230:GLY:HA3	1.90	0.54
25:AG:510:TYR:OH	25:AG:527:HIS:ND1	2.35	0.54
28:B3:328:GLN:NE2	28:B3:329:VAL:O	2.41	0.54
29:B8:352:GLN:HE21	29:B8:385:ASN:HD22	1.54	0.54
30:BE:73:GLU:OE2	30:BE:74:LYS:NZ	2.40	0.54
30:BE:626:ASP:N	30:BE:626:ASP:OD1	2.35	0.54
44:RH:114:ILE:HG12	44:RH:122:ILE:HB	1.89	0.54
3:SA:103:A:OP1	7:SJ:18:ARG:NH1	2.40	0.54
15:3D:392:TYR:HB3	18:3H:65:LEU:HD22	1.90	0.54
23:AE:274:ILE:HD11	29:B8:215:THR:HG21	1.90	0.54
45:RJ:73:ALA:HB1	45:RJ:131:ILE:HD12	1.90	0.54
3:SA:511:A:OP2	8:SK:176:ASN:ND2	2.40	0.54
3:SA:1175:U:OP1	48:RN:748:ARG:NH1	2.41	0.54
4:SF:198:LYS:HG3	4:SF:208:VAL:HG23	1.89	0.54
5:SG:26:ALA:HB3	10:SR:28:LEU:HB3	1.89	0.54
10:SR:34:SER:HB2	10:SR:38:LEU:HD12	1.90	0.54
17:3F:398:CYS:O	17:3F:419:ASN:ND2	2.40	0.54
17:3F:414:ILE:HD11	17:3F:480:ALA:HB2	1.90	0.54
18:3G:13:ASP:OD1	18:3G:13:ASP:N	2.39	0.54
26:B1:396:ALA:HB2	26:B1:438:VAL:HG21	1.90	0.54
27:B2:287:ARG:NH1	27:B2:324:PHE:O	2.41	0.54
29:B8:486:SER:OG	29:B8:487:GLU:N	2.41	0.54
35:5E:437:ILE:HD11	36:5F:70:PHE:HE2	1.73	0.54
41:5K:145:VAL:HG23	41:5K:151:TYR:HB2	1.89	0.54
43:RB:310:GLN:O	43:RB:314:ASN:ND2	2.40	0.54
46:RK:347:ASN:ND2	46:RK:349:ASP:OD2	2.40	0.54
48:RN:515:HIS:HB3	48:RN:518:ILE:HG22	1.90	0.54
14:3B:90:PRO:HD3	40:5J:106:LEU:HD12	1.90	0.54
14:3C:268:VAL:HG22	14:3C:317:VAL:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3F:481:ILE:HD12	17:3F:486:VAL:HG13	1.90	0.54
25:AG:325:GLN:NE2	25:AG:328:THR:OG1	2.41	0.54
25:AG:368:ASP:OD1	25:AG:368:ASP:N	2.38	0.54
27:B2:317:ILE:O	27:B2:321:TYR:N	2.41	0.54
28:B3:510:SER:O	28:B3:514:THR:OG1	2.26	0.54
42:RA:64:VAL:HG21	42:RA:323:VAL:HG12	1.90	0.54
42:RA:121:ARG:HH22	53:RY:462:ARG:HD2	1.72	0.54
42:RA:250:GLY:HA2	42:RA:274:ILE:HG23	1.88	0.54
1:3A:258:U:O4	15:3D:377:ARG:NH2	2.41	0.54
3:SA:146:U:O4	3:SA:168:A:N7	2.41	0.54
3:SA:1605:G:OP1	37:5G:119:ARG:NH2	2.40	0.54
14:3B:124:SER:HB3	40:5J:153:ILE:HD11	1.90	0.54
20:A5:20:VAL:HG22	20:A5:29:VAL:HG22	1.89	0.54
21:A8:647:LEU:C	22:A9:509:GLN:NE2	2.62	0.54
23:AE:519:LEU:HD23	23:AE:523:ILE:HD13	1.88	0.54
24:AF:387:ALA:O	24:AF:391:ASN:ND2	2.40	0.54
25:AG:724:ILE:HD11	25:AG:763:ILE:HG22	1.90	0.54
27:B2:260:GLU:O	27:B2:272:PHE:HA	2.08	0.54
30:BE:430:ILE:HB	30:BE:443:TRP:HB2	1.89	0.54
30:BE:604:SER:OG	30:BE:606:ASP:OD1	2.25	0.54
45:RJ:954:SER:HA	45:RJ:984:GLU:HG3	1.89	0.54
3:SA:325:G:H2'	3:SA:326:G:H8	1.73	0.54
3:SA:1539:G:N1	3:SA:1569:A:OP2	2.41	0.54
15:3D:392:TYR:HB2	18:3H:62:GLU:HB3	1.90	0.54
16:3E:380:ARG:NH1	16:3E:382:ASP:OD1	2.40	0.54
17:3F:399:GLU:OE2	17:3F:417:SER:OG	2.26	0.54
18:3H:38:ASN:HA	18:3H:41:THR:HG22	1.90	0.54
19:A4:207:ASP:OD2	19:A4:209:ARG:NH1	2.37	0.54
19:A4:641:GLU:HB3	19:A4:749:SER:HB3	1.90	0.54
28:B3:745:ASP:O	35:5E:512:GLY:O	2.26	0.54
30:BE:160:THR:OG1	30:BE:163:GLN:NE2	2.41	0.54
33:5C:449:ILE:HD11	39:5I:38:ALA:HA	1.89	0.54
45:RJ:1027:THR:HG23	45:RJ:1028:GLU:HG2	1.89	0.54
48:RN:605:ASP:OD1	48:RN:610:ARG:NH1	2.41	0.54
3:SA:1738:U:OP1	27:B2:279:LYS:NZ	2.40	0.53
7:SJ:184:LEU:HD23	7:SJ:189:LEU:HA	1.90	0.53
19:A4:271:THR:HG21	29:B8:443:VAL:HG21	1.91	0.53
25:AG:157:PHE:O	25:AG:169:GLN:NE2	2.40	0.53
27:B2:525:ASP:OD1	27:B2:525:ASP:N	2.41	0.53
36:5F:136:VAL:HA	36:5F:160:TRP:HA	1.90	0.53
39:5I:192:SER:HB2	39:5I:206:VAL:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SK:76:LEU:HB2	43:RB:328:PHE:CE1	2.43	0.53
25:AG:404:SER:OG	25:AG:405:ALA:N	2.40	0.53
30:BE:743:ARG:O	30:BE:743:ARG:HD3	2.08	0.53
44:RH:125:ASN:ND2	44:RH:127:THR:OG1	2.42	0.53
48:RN:96:LYS:HD2	48:RN:761:PHE:HZ	1.73	0.53
1:3A:318:U:N3	14:3C:119:GLY:HA3	2.16	0.53
3:SA:396:G:N7	7:SJ:47:ARG:NH1	2.56	0.53
5:SG:73:THR:OG1	5:SG:91:GLU:OE1	2.27	0.53
19:A4:311:THR:HG22	19:A4:313:LYS:H	1.74	0.53
23:AE:651:LEU:HD21	23:AE:680:TYR:HB2	1.90	0.53
24:AF:173:THR:HG21	24:AF:218:VAL:H	1.74	0.53
26:B1:283:GLU:OE2	26:B1:297:GLN:NE2	2.42	0.53
1:3A:25:U:H5'	36:5F:11:LYS:O	2.07	0.53
14:3B:230:TYR:OH	14:3B:256:ASN:OD1	2.25	0.53
23:AE:626:PHE:HB3	23:AE:629:GLU:HB2	1.90	0.53
26:B1:418:ARG:HG3	26:B1:418:ARG:NH2	2.12	0.53
26:B1:419:TYR:CD2	35:5E:482:LEU:HD12	2.44	0.53
28:B3:596:ASP:OD1	28:B3:596:ASP:N	2.42	0.53
30:BE:737:LEU:O	30:BE:740:ILE:HG23	2.09	0.53
33:5C:312:VAL:HG21	33:5C:353:PRO:HG2	1.90	0.53
17:3F:357:LEU:HD22	43:RB:256:PRO:HB2	1.90	0.53
18:3H:45:ASN:HA	18:3H:74:LYS:HE2	1.90	0.53
25:AG:291:ARG:HD2	25:AG:329:ASN:HD21	1.73	0.53
27:B2:412:GLY:HA2	27:B2:431:GLY:H	1.73	0.53
35:5E:315:GLU:HB3	45:RJ:1032:LEU:CD1	2.37	0.53
6:SH:48:TYR:OH	6:SH:119:GLN:O	2.27	0.53
9:SM:82:ARG:HA	9:SM:111:VAL:HG13	1.91	0.53
25:AG:213:LYS:HA	25:AG:223:LYS:HA	1.91	0.53
44:RG:36:LYS:NZ	44:RG:169:ASP:O	2.40	0.53
46:RK:289:VAL:HG21	46:RK:294:LEU:HD13	1.90	0.53
47:RL:37:LEU:HD13	47:RL:123:ILE:HD13	1.90	0.53
1:3A:98:U:OP2	1:3A:98:U:H6	1.92	0.53
3:SA:513:U:H2'	3:SA:514:G:C8	2.44	0.53
3:SA:1209:C:N3	3:SA:1210:C:N4	2.56	0.53
4:SF:209:HIS:ND1	4:SF:218:PHE:O	2.41	0.53
16:3E:289:GLN:HE21	16:3E:388:LEU:HD13	1.74	0.53
20:A5:46:TRP:HD1	20:A5:48:GLU:HG3	1.74	0.53
25:AG:283:VAL:HG12	25:AG:290:ILE:HG22	1.91	0.53
27:B2:554:THR:OG1	27:B2:556:LYS:NZ	2.39	0.53
44:RG:188:ARG:NH2	44:RH:247:ASP:OD2	2.41	0.53
45:RJ:374:ASP:OD1	45:RJ:374:ASP:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:RS:437:ARG:NH2	52:RS:459:GLU:O	2.42	0.53
19:A4:35:ARG:HH11	19:A4:738:TYR:HD1	1.57	0.53
19:A4:420:LEU:HD23	20:A5:581:ASN:HA	1.91	0.53
22:A9:513:ARG:HH21	22:A9:515:ASP:HA	1.72	0.53
35:5E:322:LYS:HD2	35:5E:327:LYS:HB2	1.90	0.53
42:RA:202:ASN:ND2	42:RA:229:PHE:O	2.41	0.53
44:RG:121:LEU:HD21	44:RG:167:ILE:HG13	1.89	0.53
45:RJ:844:PRO:HA	45:RJ:856:THR:O	2.08	0.53
49:RO:233:ASP:N	49:RO:233:ASP:OD1	2.42	0.53
1:3A:323:G:N3	1:3A:323:G:C2'	2.71	0.53
3:SA:1633:A:O3'	26:B1:418:ARG:NH2	2.38	0.53
15:3D:102:ASP:HB3	15:3D:105:LEU:HB3	1.91	0.53
21:A8:443:CYS:CB	25:AG:728:LEU:CB	2.76	0.53
23:AE:40:ALA:HB1	23:AE:123:ARG:HH12	1.73	0.53
26:B1:284:PHE:HZ	35:5E:476:MET:HE2	1.72	0.53
26:B1:812:GLU:HG3	26:B1:813:HIS:HD2	1.74	0.53
3:SA:1136:U:O2'	27:B2:596:ASN:ND2	2.43	0.52
9:SM:97:TYR:O	9:SM:99:ARG:NH1	2.42	0.52
23:AE:571:LEU:HD11	23:AE:582:VAL:HG11	1.91	0.52
26:B1:418:ARG:NH1	35:5E:492:PRO:HD3	2.24	0.52
29:B8:216:TYR:OH	30:BE:276:TYR:OH	2.27	0.52
35:5E:493:GLN:HE21	35:5E:497:ASN:CB	2.20	0.52
35:5E:500:LYS:O	35:5E:508:ARG:NH2	2.42	0.52
36:5F:123:THR:HG23	36:5F:126:ASP:H	1.74	0.52
42:RA:13:VAL:HG12	42:RA:343:ILE:HG12	1.89	0.52
50:RP:18:SER:OG	50:RP:19:PHE:N	2.42	0.52
1:3A:97:C:O2	1:3A:320:G:C2	2.62	0.52
3:SA:153:G:H2'	3:SA:154:G:H8	1.74	0.52
15:3D:157:ALA:O	31:B6:293:TYR:OH	2.26	0.52
16:3E:251:ASP:OD1	16:3E:251:ASP:N	2.42	0.52
17:3F:162:CYS:SG	17:3F:525:GLN:NE2	2.78	0.52
21:A8:443:CYS:CA	25:AG:728:LEU:CD2	2.79	0.52
21:A8:647:LEU:O	22:A9:509:GLN:NE2	2.41	0.52
24:AF:87:ALA:HA	24:AF:97:CYS:O	2.08	0.52
24:AF:364:SER:O	24:AF:364:SER:OG	2.26	0.52
45:RJ:135:ALA:O	45:RJ:238:ARG:NH2	2.42	0.52
45:RJ:982:LYS:HG3	45:RJ:983:PRO:HD3	1.92	0.52
47:RL:131:THR:OG1	47:RL:133:ASN:ND2	2.42	0.52
3:SA:258:C:H4'	7:SJ:75:LYS:HD2	1.91	0.52
23:AE:502:ILE:HG23	23:AE:542:ILE:HG13	1.90	0.52
45:RJ:90:VAL:HG23	45:RJ:107:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:RK:97:GLY:HA2	46:RK:100:VAL:HG12	1.92	0.52
48:RN:587:ASP:OD1	48:RN:587:ASP:N	2.42	0.52
3:SA:153:G:N2	6:SH:56:ASN:OD1	2.42	0.52
8:SK:67:PRO:HB2	43:RB:334:LEU:HD23	1.91	0.52
19:A4:39:VAL:H	19:A4:755:ILE:HD11	1.75	0.52
19:A4:658:ASP:OD2	19:A4:731:HIS:N	2.42	0.52
20:A5:481:LEU:HD22	20:A5:523:LEU:HD22	1.92	0.52
27:B2:398:ASP:HB2	27:B2:406:LEU:HB3	1.92	0.52
30:BE:470:GLN:NE2	30:BE:512:GLY:O	2.42	0.52
4:SF:53:LYS:O	17:3F:120:ARG:NH2	2.42	0.52
7:SJ:191:PHE:O	7:SJ:195:ARG:NH1	2.41	0.52
28:B3:337:HIS:HD2	28:B3:363:ARG:HD3	1.74	0.52
30:BE:268:THR:HG22	30:BE:270:SER:H	1.75	0.52
35:5E:384:ARG:HD3	37:5G:83:ILE:CD1	2.38	0.52
44:RH:116:THR:HG22	44:RH:118:ARG:H	1.73	0.52
3:SA:494:U:OP1	45:RJ:1138:ARG:NH2	2.32	0.52
3:SA:594:A:OP1	8:SK:38:ASN:ND2	2.43	0.52
14:3B:281:ASP:OD1	14:3B:281:ASP:N	2.41	0.52
15:3D:169:LYS:HA	15:3D:299:VAL:HG22	1.92	0.52
17:3F:284:LEU:O	17:3F:548:ARG:NH2	2.38	0.52
23:AE:556:LYS:O	23:AE:592:ARG:NH2	2.42	0.52
44:RG:169:ASP:N	44:RG:169:ASP:OD1	2.40	0.52
46:RK:30:PRO:HB3	46:RK:77:ARG:HG3	1.90	0.52
50:RP:452:ASN:O	50:RP:456:GLU:N	2.43	0.52
3:SA:331:A:N3	7:SJ:5:ARG:NH1	2.57	0.52
3:SA:1436:A:H1'	52:RS:419:LYS:HD2	1.91	0.52
6:SH:105:ASP:OD1	6:SH:105:ASP:N	2.43	0.52
7:SJ:110:ARG:NH1	7:SJ:161:SER:O	2.43	0.52
22:A9:504:GLU:OE2	22:A9:507:ARG:NH1	2.43	0.52
25:AG:319:LYS:HD2	25:AG:339:GLY:H	1.74	0.52
30:BE:578:VAL:O	30:BE:579:ARG:NH1	2.42	0.52
30:BE:605:LEU:HD23	30:BE:628:VAL:HG11	1.92	0.52
36:5F:66:PRO:O	36:5F:72:ARG:NH2	2.43	0.52
49:RO:258:GLU:HG3	49:RO:289:PHE:HD1	1.74	0.52
52:RS:397:PHE:HD1	52:RS:407:GLU:HG2	1.75	0.52
2:5A:7:A:N7	25:AG:578:ASN:ND2	2.55	0.52
16:3E:426:ALA:HB2	30:BE:305:ASN:HD21	1.75	0.52
25:AG:431:SER:OG	25:AG:432:ARG:N	2.42	0.52
26:B1:678:GLU:OE2	35:5E:455:HIS:ND1	2.43	0.52
28:B3:680:ASN:N	28:B3:680:ASN:OD1	2.42	0.52
30:BE:819:LYS:NZ	30:BE:823:GLU:OE2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:5E:350:THR:OG1	45:RJ:975:GLU:CD	2.48	0.52
40:5J:58:ASN:HA	40:5J:61:LYS:HG2	1.92	0.52
42:RA:147:ASN:ND2	42:RA:154:TYR:OH	2.43	0.52
1:3A:198:U:O4	17:3F:151:ARG:NE	2.38	0.52
1:3A:312:U:H5''	40:5J:167:LYS:HG2	1.91	0.52
6:SH:39:GLU:HG3	6:SH:46:LYS:HG3	1.91	0.52
14:3C:297:ARG:HD3	14:3C:322:ARG:HA	1.92	0.52
20:A5:503:LYS:HD3	22:A9:508:ARG:HH22	1.75	0.52
21:A8:596:LYS:CD	21:A8:637:LEU:HD22	2.38	0.52
24:AF:256:THR:N	24:AF:275:SER:O	2.39	0.52
26:B1:506:SER:OG	26:B1:507:GLN:N	2.43	0.52
26:B1:678:GLU:OE2	35:5E:455:HIS:HE1	1.92	0.52
27:B2:634:SER:OG	27:B2:635:LYS:N	2.41	0.52
45:RJ:72:VAL:HG22	45:RJ:137:LEU:HB3	1.91	0.52
45:RJ:246:ALA:HB3	45:RJ:810:ILE:HB	1.91	0.52
45:RJ:776:GLN:NE2	45:RJ:781:GLU:OE2	2.40	0.52
49:RO:356:ALA:HA	49:RO:499:LEU:HD22	1.91	0.52
2:5A:9:G:H5'	22:A9:483:LYS:HZ1	1.73	0.52
3:SA:1533:C:OP2	24:AF:114:ARG:NH2	2.43	0.52
16:3E:3:TYR:N	16:3E:21:LYS:O	2.43	0.52
16:3E:359:ILE:HA	16:3E:362:VAL:HG12	1.92	0.52
27:B2:53:ASP:OD2	27:B2:58:ASP:OD1	2.27	0.52
31:B6:296:SER:HB3	31:B6:300:MET:HB2	1.91	0.52
45:RJ:193:ARG:NH2	45:RJ:196:THR:OG1	2.43	0.52
47:RL:589:ALA:HB3	47:RL:593:GLU:H	1.75	0.52
52:RS:360:LEU:HD21	52:RS:393:TYR:HB2	1.92	0.52
5:SG:120:ILE:HA	5:SG:123:VAL:HG12	1.92	0.51
16:3E:385:ASP:OD1	16:3E:385:ASP:N	2.42	0.51
27:B2:54:ILE:CD1	27:B2:364:TYR:CD2	2.93	0.51
33:5C:130:ARG:NH2	33:5C:379:GLU:OE2	2.42	0.51
39:5I:319:GLU:OE2	39:5I:356:TYR:OH	2.27	0.51
39:5I:324:SER:OG	39:5I:326:ASP:OD1	2.23	0.51
49:RO:200:ASN:ND2	49:RO:256:ASN:O	2.43	0.51
2:5A:294:U:OP1	26:B1:631:ASN:ND2	2.43	0.51
3:SA:419:G:H5''	3:SA:419:G:H8	1.75	0.51
3:SA:1599:C:H4'	37:5G:145:HIS:CD2	2.45	0.51
6:SH:74:LYS:HB2	42:RA:88:ASN:HD21	1.75	0.51
14:3B:277:ASP:N	14:3B:277:ASP:OD1	2.43	0.51
18:3H:44:LEU:HD22	18:3H:52:ILE:HD12	1.90	0.51
19:A4:63:SER:HA	19:A4:82:ARG:HH12	1.75	0.51
21:A8:443:CYS:CA	25:AG:728:LEU:HD13	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AE:659:LEU:HD13	23:AE:690:GLU:HB3	1.92	0.51
25:AG:736:THR:HG23	25:AG:738:ASN:H	1.74	0.51
27:B2:281:ILE:HB	27:B2:332:ILE:HG23	1.91	0.51
27:B2:362:ILE:HG12	27:B2:385:ILE:HB	1.92	0.51
33:5C:410:ASN:O	39:5I:27:ASN:ND2	2.43	0.51
37:5G:108:LYS:HD2	37:5G:116:ARG:HB2	1.92	0.51
45:RJ:864:ASP:OD1	45:RJ:864:ASP:N	2.44	0.51
14:3B:120:GLU:OE2	14:3B:142:ARG:NE	2.41	0.51
19:A4:481:ILE:HB	19:A4:485:LYS:HB2	1.91	0.51
21:A8:587:LEU:HD23	21:A8:587:LEU:O	2.10	0.51
25:AG:407:ASN:ND2	25:AG:416:SER:OG	2.44	0.51
27:B2:759:GLY:HA3	27:B2:805:ILE:HD11	1.91	0.51
28:B3:679:THR:HG21	28:B3:723:GLU:HB2	1.93	0.51
37:5G:143:HIS:HB2	37:5G:151:SER:HB2	1.91	0.51
43:RB:348:SER:HB2	50:RP:1728:PHE:HB3	1.93	0.51
45:RJ:616:ASP:HB2	45:RJ:621:LEU:HG	1.90	0.51
49:RO:214:LYS:O	49:RO:268:GLN:NE2	2.43	0.51
4:SF:201:HIS:H	4:SF:206:ASP:HB3	1.75	0.51
7:SJ:171:SER:HB3	7:SJ:180:ASP:H	1.74	0.51
15:3D:126:ASP:HA	15:3D:129:ARG:HG2	1.93	0.51
17:3F:136:PHE:HE1	17:3F:484:SER:HB2	1.74	0.51
21:A8:631:SER:O	21:A8:634:LEU:CG	2.45	0.51
24:AF:59:SER:OG	24:AF:60:SER:N	2.43	0.51
37:5G:185:VAL:O	37:5G:220:ARG:NH1	2.39	0.51
47:RL:117:ASN:O	47:RL:141:THR:OG1	2.26	0.51
50:RP:85:LYS:NZ	50:RP:89:ASN:OD1	2.40	0.51
50:RP:1746:LYS:O	50:RP:1748:ASN:ND2	2.41	0.51
2:5A:473:A:H5"	33:5C:164:GLN:HE22	1.76	0.51
15:3D:26:ASP:OD1	39:5I:98:SER:OG	2.29	0.51
19:A4:402:TRP:HB3	19:A4:416:LEU:HA	1.91	0.51
26:B1:329:VAL:HG13	26:B1:338:ILE:HB	1.92	0.51
30:BE:59:GLN:HG2	30:BE:71:VAL:HG22	1.91	0.51
35:5E:350:THR:HG21	45:RJ:975:GLU:HB2	1.92	0.51
39:5I:329:ILE:HG22	39:5I:351:VAL:HG11	1.93	0.51
44:RG:105:ASN:HD21	44:RG:110:LEU:HD22	1.75	0.51
46:RK:315:LYS:HB2	46:RK:348:GLU:HB3	1.92	0.51
48:RN:661:ILE:HG22	48:RN:665:GLN:HG3	1.92	0.51
5:SG:118:LEU:HG	5:SG:129:PRO:HB2	1.92	0.51
7:SJ:100:ALA:O	7:SJ:168:CYS:HA	2.10	0.51
9:SM:18:HIS:HB2	9:SM:63:LEU:HD21	1.91	0.51
14:3B:91:HIS:HD2	14:3B:93:HIS:H	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A8:712:ASP:OD1	21:A8:712:ASP:N	2.40	0.51
23:AE:558:VAL:HG13	23:AE:615:ASN:HA	1.93	0.51
26:B1:588:ASP:OD1	26:B1:588:ASP:N	2.43	0.51
26:B1:680:ARG:HH11	35:5E:455:HIS:CD2	2.27	0.51
27:B2:180:THR:HG1	27:B2:207:CYS:HG	1.58	0.51
28:B3:501:PRO:HG3	28:B3:543:GLN:HG3	1.91	0.51
30:BE:854:SER:HB2	30:BE:895:VAL:HG21	1.93	0.51
36:5F:6:LYS:HB2	36:5F:9:GLU:HG2	1.91	0.51
39:5I:122:ARG:HB2	39:5I:192:SER:HB3	1.93	0.51
39:5I:327:LYS:HG2	39:5I:350:HIS:H	1.76	0.51
42:RA:101:ASN:HD21	42:RA:116:HIS:HB3	1.76	0.51
52:RS:229:LEU:HD11	52:RS:233:PHE:HD2	1.74	0.51
1:3A:256:G:OP1	15:3D:382:LYS:NZ	2.37	0.51
6:SH:70:PRO:HD3	6:SH:101:ILE:HD12	1.93	0.51
19:A4:420:LEU:HD11	19:A4:462:VAL:HG21	1.92	0.51
25:AG:434:GLN:OE1	25:AG:434:GLN:N	2.43	0.51
26:B1:722:THR:HG22	26:B1:724:HIS:H	1.75	0.51
27:B2:201:ILE:HG13	28:B3:663:VAL:HG11	1.92	0.51
28:B3:497:LEU:HA	28:B3:507:ALA:O	2.11	0.51
52:RS:263:THR:HA	52:RS:266:PHE:HB2	1.93	0.51
7:SJ:67:TRP:NE1	7:SJ:70:GLU:OE1	2.42	0.51
14:3C:94:ALA:HB3	14:3C:166:PRO:HG3	1.92	0.51
21:A8:647:LEU:CB	22:A9:509:GLN:HE22	2.23	0.51
24:AF:258:LEU:HD22	24:AF:272:LEU:HD21	1.93	0.51
26:B1:392:ALA:O	26:B1:404:SER:HA	2.10	0.51
28:B3:414:VAL:HG23	28:B3:427:TYR:HB3	1.92	0.51
33:5C:74:LEU:HD23	33:5C:404:PRO:HG2	1.93	0.51
40:5J:120:ASP:HB2	40:5J:173:ILE:HD12	1.92	0.51
44:RG:150:ILE:HD11	44:RG:160:LEU:HD23	1.92	0.51
47:RL:539:ALA:O	47:RL:543:SER:CB	2.59	0.51
2:5A:293:U:H3	26:B1:632:SER:HB3	1.75	0.51
3:SA:283:U:OP1	6:SH:191:ARG:NH1	2.40	0.51
3:SA:340:U:H2'	3:SA:341:A:H8	1.75	0.51
3:SA:1634:C:P	26:B1:418:ARG:HH22	2.32	0.51
14:3C:171:LEU:HD23	14:3C:240:VAL:HG12	1.92	0.51
21:A8:441:VAL:CA	25:AG:728:LEU:HD21	2.41	0.51
23:AE:522:ARG:HH12	23:AE:561:PHE:HB2	1.76	0.51
25:AG:64:LYS:NZ	25:AG:123:GLY:O	2.39	0.51
28:B3:17:ALA:HB3	28:B3:35:PRO:HA	1.91	0.51
42:RA:282:ASN:HD21	42:RA:325:GLY:H	1.58	0.51
44:RH:178:VAL:HG12	44:RH:223:GLU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3A:59:G:H5'	26:B1:570:THR:HG23	1.92	0.51
1:3A:305:G:H2'	1:3A:306:G:H8	1.75	0.51
3:SA:29:U:H2'	3:SA:30:G:H8	1.74	0.51
3:SA:123:G:OP1	4:SF:77:ARG:NH2	2.40	0.51
7:SJ:104:ILE:HD13	7:SJ:167:ALA:HB3	1.91	0.51
12:SZ:86:GLU:OE2	12:SZ:90:ARG:NH1	2.43	0.51
16:3E:355:ASN:HB2	16:3E:401:LEU:HD13	1.93	0.51
20:A5:8:SER:OG	20:A5:293:ASN:ND2	2.43	0.51
20:A5:439:VAL:HG11	49:RO:300:THR:HG21	1.92	0.51
23:AE:586:LEU:O	23:AE:590:ALA:CB	2.58	0.51
26:B1:732:GLU:HG2	26:B1:734:GLN:HE22	1.76	0.51
30:BE:135:ASN:ND2	30:BE:165:GLY:O	2.42	0.51
35:5E:336:PRO:HB2	35:5E:339:ALA:HB2	1.93	0.51
45:RJ:776:GLN:HA	45:RJ:780:ILE:HG22	1.93	0.51
6:SH:21:GLU:OE2	6:SH:25:ARG:NH2	2.44	0.50
14:3B:142:ARG:NH2	14:3B:182:SER:OG	2.44	0.50
25:AG:668:THR:OG1	25:AG:669:ASN:OD1	2.30	0.50
27:B2:562:SER:HB2	27:B2:564:LYS:HB2	1.93	0.50
27:B2:627:SER:OG	27:B2:628:HIS:N	2.45	0.50
33:5C:91:ILE:HG23	39:5I:3:ILE:HD11	1.92	0.50
34:5D:61:ASP:HB3	36:5F:160:TRP:CZ3	2.46	0.50
44:RG:150:ILE:HG12	44:RG:160:LEU:HB2	1.93	0.50
47:RL:80:GLU:OE2	47:RL:85:THR:OG1	2.29	0.50
3:SA:290:G:H3'	3:SA:291:G:H8	1.76	0.50
3:SA:442:C:O2'	3:SA:525:A:N1	2.35	0.50
20:A5:192:SER:HB3	20:A5:207:GLU:HG3	1.93	0.50
21:A8:34:GLY:HA2	21:A8:352:GLN:HA	1.92	0.50
25:AG:855:LEU:HD23	29:B8:477:LYS:HE3	1.93	0.50
26:B1:328:LEU:HD21	35:5E:476:MET:HG3	1.93	0.50
28:B3:413:ILE:HG22	28:B3:429:LYS:HA	1.92	0.50
39:5I:54:PHE:O	39:5I:382:ARG:NH2	2.44	0.50
3:SA:304:U:OP1	9:SM:136:ARG:NH2	2.45	0.50
3:SA:340:U:H2'	3:SA:341:A:C8	2.47	0.50
3:SA:420:A:H8	3:SA:420:A:H3'	1.76	0.50
14:3C:223:ASP:OD2	14:3C:225:ARG:NH1	2.44	0.50
24:AF:401:LEU:HB3	24:AF:434:ARG:HH22	1.77	0.50
25:AG:207:LEU:HG	25:AG:264:ILE:HD12	1.93	0.50
30:BE:225:THR:OG1	30:BE:227:THR:O	2.29	0.50
30:BE:370:SER:OG	30:BE:372:ASP:OD1	2.20	0.50
31:B6:297:ASP:OD1	31:B6:297:ASP:N	2.44	0.50
36:5F:8:HIS:CA	39:5I:53:MET:HE1	2.21	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:RH:228:SER:OG	44:RH:229:ASN:N	2.44	0.50
1:3A:93:U:OP2	16:3E:302:HIS:ND1	2.42	0.50
1:3A:316:A:H2'	1:3A:317:A:H8	1.76	0.50
3:SA:413:U:H2'	3:SA:414:C:H6	1.77	0.50
22:A9:471:LYS:HZ3	22:A9:474:HIS:H	1.60	0.50
24:AF:224:THR:O	24:AF:239:LEU:CB	2.57	0.50
24:AF:378:LYS:NZ	29:B8:292:GLY:O	2.44	0.50
45:RJ:634:ARG:HD2	46:RK:185:ARG:HH21	1.77	0.50
46:RK:65:ILE:HB	48:RN:112:VAL:HG12	1.94	0.50
46:RK:183:ILE:HG22	46:RK:351:ILE:HD13	1.94	0.50
4:SF:26:CYS:SG	4:SF:27:TYR:N	2.84	0.50
14:3B:111:MET:HB2	14:3B:186:ASP:HB3	1.92	0.50
16:3E:430:ASP:HA	30:BE:125:GLY:HA2	1.93	0.50
19:A4:382:VAL:HG11	19:A4:755:ILE:HG21	1.92	0.50
20:A5:355:ASN:OD1	25:AG:479:ASN:ND2	2.44	0.50
24:AF:399:GLU:O	24:AF:403:ASN:ND2	2.42	0.50
25:AG:249:THR:HG22	25:AG:256:THR:HB	1.93	0.50
35:5E:345:LEU:HD21	45:RJ:961:PHE:CE2	2.46	0.50
44:RH:41:MET:O	44:RH:110:LEU:HA	2.11	0.50
44:RH:41:MET:HG3	44:RH:202:ILE:HG23	1.92	0.50
52:RS:322:LEU:HD21	52:RS:359:LEU:HD11	1.92	0.50
3:SA:420:A:H3'	3:SA:420:A:C8	2.47	0.50
3:SA:1134:C:H1'	27:B2:610:SER:HB2	1.94	0.50
9:SM:109:VAL:HG11	9:SM:139:VAL:HG13	1.94	0.50
14:3C:170:VAL:HG23	14:3C:194:VAL:HG13	1.93	0.50
23:AE:558:VAL:HG22	23:AE:615:ASN:HD22	1.76	0.50
27:B2:102:VAL:HA	27:B2:118:ASN:HA	1.94	0.50
28:B3:182:CYS:SG	28:B3:183:LEU:N	2.84	0.50
32:5B:173:ARG:HE	34:5D:146:PHE:HA	1.76	0.50
2:5A:20:C:H2'	2:5A:21:A:H8	1.77	0.50
3:SA:1192:C:H1'	44:RG:131:PRO:HA	1.92	0.50
3:SA:1194:A:OP2	3:SA:1195:C:N4	2.40	0.50
14:3B:228:GLN:O	14:3B:231:ARG:NH2	2.43	0.50
21:A8:539:ASN:ND2	21:A8:560:ASN:O	2.44	0.50
25:AG:80:GLN:NE2	25:AG:83:GLU:OE1	2.44	0.50
28:B3:407:SER:OG	28:B3:408:LYS:N	2.45	0.50
37:5G:287:LYS:HE2	37:5G:290:LEU:HA	1.94	0.50
46:RK:114:PHE:O	46:RK:169:VAL:HA	2.12	0.50
46:RK:214:LYS:O	46:RK:217:LYS:NZ	2.40	0.50
4:SF:181:VAL:HA	4:SF:227:VAL:HA	1.94	0.50
19:A4:415:LYS:NZ	19:A4:416:LEU:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:AG:139:GLU:HB3	25:AG:155:THR:HB	1.94	0.50
28:B3:455:LEU:HA	28:B3:464:LYS:O	2.12	0.50
35:5E:533:LYS:HA	35:5E:536:ARG:CD	2.42	0.50
44:RG:175:CYS:SG	44:RG:201:SER:OG	2.67	0.50
49:RO:327:MET:O	49:RO:331:ASN:HA	2.11	0.50
52:RS:439:PHE:HA	52:RS:442:GLU:HG3	1.94	0.50
53:RY:472:ILE:HA	53:RY:475:TYR:HB2	1.93	0.50
1:3A:321:C:H2'	1:3A:322:A:C8	2.47	0.50
2:5A:293:U:H2'	26:B1:631:ASN:HA	1.93	0.50
2:5A:484:G:O6	51:RQ:872:ARG:NH1	2.45	0.50
3:SA:1588:G:H1	3:SA:1608:U:H3	1.60	0.50
7:SJ:80:GLY:O	7:SJ:103:GLN:NE2	2.45	0.50
19:A4:156:LEU:HD22	19:A4:170:ILE:HD11	1.93	0.50
19:A4:418:CYS:SG	19:A4:419:LYS:N	2.85	0.50
21:A8:563:LEU:HB2	21:A8:598:GLU:CD	2.27	0.50
24:AF:48:ASN:ND2	24:AF:111:TYR:OH	2.45	0.50
25:AG:370:GLN:NE2	25:AG:384:SER:OG	2.44	0.50
25:AG:877:ASP:N	25:AG:877:ASP:OD1	2.43	0.50
30:BE:587:ARG:HB3	30:BE:605:LEU:HD12	1.92	0.50
32:5B:186:ASP:HA	32:5B:189:THR:HG22	1.94	0.50
34:5D:113:ILE:O	34:5D:117:LYS:HG3	2.12	0.50
45:RJ:852:ARG:HD2	45:RJ:888:PRO:HG3	1.94	0.50
51:RQ:853:ASN:OD1	51:RQ:853:ASN:N	2.45	0.50
9:SM:109:VAL:HG13	9:SM:138:ASN:HA	1.94	0.49
20:A5:115:ASN:ND2	20:A5:130:ASP:OD1	2.45	0.49
21:A8:441:VAL:C	25:AG:728:LEU:HD21	2.33	0.49
23:AE:306:LEU:HD22	23:AE:311:ASN:HA	1.94	0.49
27:B2:828:TYR:HA	27:B2:831:LYS:HG2	1.93	0.49
29:B8:410:ASP:OD1	29:B8:479:ASN:ND2	2.45	0.49
37:5G:202:VAL:HA	37:5G:205:ILE:HG22	1.94	0.49
45:RJ:106:THR:HG23	45:RJ:355:TYR:HB3	1.94	0.49
45:RJ:138:VAL:HB	45:RJ:167:VAL:HG22	1.93	0.49
50:RP:73:ASP:OD2	50:RP:83:HIS:ND1	2.45	0.49
2:5A:485:G:H4'	2:5A:486:U:H5'	1.94	0.49
3:SA:123:G:H21	4:SF:146:THR:HG21	1.76	0.49
3:SA:158:U:H3	3:SA:420:A:HO2'	1.58	0.49
17:3F:365:PRO:HB3	17:3F:397:PHE:HA	1.93	0.49
19:A4:452:HIS:HB3	19:A4:463:THR:HG23	1.94	0.49
19:A4:566:LEU:HD11	19:A4:584:VAL:HG21	1.94	0.49
25:AG:435:ASP:HB2	25:AG:702:TYR:HD1	1.75	0.49
28:B3:65:THR:HA	28:B3:80:SER:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B8:520:ASN:HB2	29:B8:533:ALA:HB3	1.94	0.49
34:5D:67:MET:SD	36:5F:170:LEU:HB3	2.52	0.49
36:5F:96:ASP:HB3	36:5F:100:LYS:HE2	1.94	0.49
42:RA:281:ASP:OD1	42:RA:281:ASP:N	2.45	0.49
45:RJ:1069:VAL:HG11	45:RJ:1083:ILE:HD13	1.93	0.49
3:SA:268:C:H2'	3:SA:269:G:H8	1.76	0.49
21:A8:673:THR:CG2	22:A9:490:GLU:N	2.74	0.49
26:B1:839:THR:HG22	30:BE:882:GLU:HG3	1.95	0.49
27:B2:90:ASP:N	27:B2:90:ASP:OD1	2.39	0.49
27:B2:476:ILE:HD11	27:B2:490:THR:HB	1.93	0.49
28:B3:22:VAL:O	28:B3:68:LYS:NZ	2.45	0.49
28:B3:195:GLY:O	28:B3:245:SER:OG	2.29	0.49
30:BE:118:VAL:HA	30:BE:132:THR:HA	1.94	0.49
33:5C:340:LEU:O	33:5C:368:TYR:N	2.43	0.49
34:5D:149:GLU:HB3	34:5D:153:ASN:HA	1.94	0.49
42:RA:300:TRP:HB3	42:RA:307:ALA:HA	1.95	0.49
45:RJ:1094:TYR:HA	45:RJ:1097:LYS:HG2	1.94	0.49
50:RP:1473:ALA:O	50:RP:1477:LYS:CB	2.61	0.49
23:AE:387:LEU:HD21	23:AE:403:LEU:HD13	1.93	0.49
24:AF:133:HIS:HB2	24:AF:139:ILE:HG13	1.94	0.49
25:AG:584:PHE:HB3	25:AG:598:LYS:HB2	1.94	0.49
33:5C:84:PHE:HA	33:5C:369:MET:HA	1.95	0.49
35:5E:319:VAL:HG23	45:RJ:1038:ILE:HG21	1.91	0.49
42:RA:252:SER:HB2	42:RA:266:LYS:HB3	1.94	0.49
45:RJ:777:ARG:O	45:RJ:778:GLN:NE2	2.46	0.49
45:RJ:951:MET:SD	45:RJ:987:TYR:OH	2.63	0.49
46:RK:107:ALA:HB1	46:RK:170:VAL:HG21	1.94	0.49
48:RN:600:LEU:HD21	48:RN:636:LEU:HD13	1.94	0.49
48:RN:623:ASP:O	48:RN:627:HIS:HB3	2.13	0.49
3:SA:562:G:C8	37:5G:283:THR:HB	2.46	0.49
7:SJ:70:GLU:OE2	7:SJ:117:TYR:OH	2.30	0.49
10:SR:58:ASP:OD1	10:SR:58:ASP:N	2.43	0.49
16:3E:164:ILE:HG12	16:3E:301:ALA:HA	1.93	0.49
18:3H:52:ILE:HG22	18:3H:54:MET:SD	2.52	0.49
21:A8:631:SER:HA	21:A8:634:LEU:CG	2.43	0.49
27:B2:624:LEU:HD12	27:B2:629:ASN:HB2	1.93	0.49
28:B3:513:LYS:HG3	28:B3:532:HIS:HB2	1.95	0.49
33:5C:456:SER:O	33:5C:456:SER:OG	2.28	0.49
39:5I:76:ASN:HA	39:5I:118:VAL:HG21	1.93	0.49
39:5I:140:SER:OG	39:5I:141:ASP:N	2.44	0.49
44:RG:46:ALA:HA	44:RG:115:GLN:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:RK:180:MET:O	46:RK:181:HIS:ND1	2.45	0.49
48:RN:752:MET:HA	48:RN:755:ILE:HG12	1.93	0.49
50:RP:752:THR:O	50:RP:756:SER:CB	2.59	0.49
16:3E:24:LYS:O	16:3E:28:LEU:CB	2.60	0.49
18:3H:7:LYS:HB3	18:3H:65:LEU:HD11	1.95	0.49
18:3H:54:MET:O	18:3H:80:PHE:HA	2.12	0.49
25:AG:96:ILE:HG12	25:AG:108:THR:HG21	1.95	0.49
25:AG:628:ASP:H	25:AG:658:GLU:HA	1.77	0.49
25:AG:736:THR:OG1	25:AG:737:ILE:N	2.45	0.49
26:B1:286:LEU:HD12	26:B1:295:ILE:HB	1.94	0.49
26:B1:406:SER:OG	26:B1:407:LEU:N	2.46	0.49
26:B1:567:ASP:HB3	36:5F:144:ASN:ND2	2.28	0.49
27:B2:549:SER:OG	27:B2:576:VAL:O	2.28	0.49
27:B2:817:LEU:HD11	27:B2:856:ASN:HD21	1.77	0.49
28:B3:466:TRP:HZ3	28:B3:478:GLN:HA	1.77	0.49
31:B6:63:VAL:HG13	31:B6:88:ILE:HD11	1.94	0.49
33:5C:183:GLU:HB3	41:5K:16:THR:HG22	1.94	0.49
34:5D:61:ASP:C	36:5F:160:TRP:CH2	2.86	0.49
43:RB:268:ASN:HB3	43:RB:271:ARG:HB3	1.94	0.49
44:RH:38:THR:O	44:RH:40:ARG:NH1	2.45	0.49
44:RH:69:ASN:HD22	44:RH:72:ASP:HB3	1.77	0.49
45:RJ:176:LEU:HD12	45:RJ:183:LEU:HA	1.94	0.49
1:3A:57:A:N3	36:5F:133:GLN:NE2	2.61	0.49
6:SH:57:ASP:HA	6:SH:107:ALA:H	1.78	0.49
19:A4:338:ALA:HB1	19:A4:361:LEU:HD11	1.95	0.49
21:A8:593:ASP:OD1	21:A8:596:LYS:NZ	2.34	0.49
23:AE:637:ILE:HA	23:AE:640:ILE:HG22	1.94	0.49
26:B1:847:ARG:O	26:B1:851:SER:OG	2.30	0.49
27:B2:397:ILE:HD11	27:B2:405:LEU:HD21	1.94	0.49
27:B2:862:LYS:HE2	28:B3:805:ILE:HD13	1.93	0.49
28:B3:80:SER:OG	28:B3:81:GLN:N	2.46	0.49
29:B8:43:ASP:N	29:B8:43:ASP:OD1	2.40	0.49
34:5D:67:MET:SD	36:5F:170:LEU:CB	3.01	0.49
44:RH:112:VAL:O	44:RH:124:VAL:HB	2.12	0.49
45:RJ:871:MET:CE	45:RJ:930:LYS:CE	2.86	0.49
1:3A:64:A:OP2	30:BE:392:ARG:NH2	2.46	0.49
18:3G:105:ASN:HB3	18:3G:108:SER:HB2	1.94	0.49
21:A8:441:VAL:C	25:AG:728:LEU:CD2	2.80	0.49
24:AF:276:SER:OG	24:AF:278:ASP:OD1	2.30	0.49
25:AG:31:ASN:HD21	25:AG:201:ILE:HB	1.78	0.49
25:AG:116:VAL:O	25:AG:131:HIS:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B1:569:PHE:CZ	36:5F:142:LEU:HD21	2.48	0.49
29:B8:183:ASP:OD1	30:BE:281:ARG:NH2	2.45	0.49
30:BE:528:PHE:HZ	30:BE:570:ILE:HD11	1.78	0.49
39:5I:315:PRO:HG2	39:5I:360:SER:HB3	1.93	0.49
39:5I:421:GLN:HG3	39:5I:425:LYS:HD2	1.95	0.49
41:5K:65:VAL:HG22	41:5K:152:ILE:HB	1.94	0.49
45:RJ:262:GLY:O	45:RJ:264:GLN:NE2	2.44	0.49
48:RN:86:ILE:HA	48:RN:89:GLN:CD	2.33	0.49
48:RN:646:THR:HA	48:RN:649:THR:HG22	1.95	0.49
52:RS:388:ASP:HA	52:RS:391:VAL:HG22	1.93	0.49
4:SF:202:ASP:OD1	4:SF:202:ASP:N	2.41	0.49
14:3B:269:ILE:O	14:3B:315:ILE:HA	2.13	0.49
19:A4:389:ARG:HE	19:A4:404:MET:HB2	1.78	0.49
23:AE:1628:SER:O	23:AE:1632:PHE:CB	2.60	0.49
27:B2:440:PRO:HG3	27:B2:485:GLY:HA3	1.94	0.49
28:B3:198:ILE:HG12	28:B3:211:LEU:HD13	1.95	0.49
29:B8:233:LEU:HD11	29:B8:543:LEU:HD12	1.95	0.49
29:B8:321:MET:HE1	29:B8:375:VAL:HG21	1.94	0.49
30:BE:274:ILE:HG23	30:BE:286:VAL:HG22	1.94	0.49
42:RA:175:PRO:O	42:RA:177:LYS:NZ	2.36	0.49
43:RB:230:ALA:O	43:RB:234:LYS:CB	2.61	0.49
45:RJ:309:PRO:HD2	45:RJ:353:LEU:HD22	1.95	0.49
5:SG:219:ARG:NH2	44:RH:222:ASP:OD2	2.45	0.49
9:SM:109:VAL:HG21	9:SM:125:VAL:HG11	1.95	0.49
15:3D:297:HIS:NE2	15:3D:309:GLU:OE2	2.46	0.49
17:3F:305:ARG:HG2	17:3F:317:ILE:HD13	1.94	0.49
21:A8:635:PHE:HD2	22:A9:492:ILE:CD1	2.26	0.49
26:B1:441:SER:O	26:B1:443:GLU:N	2.43	0.49
28:B3:749:ASN:ND2	35:5E:511:ASN:OD1	2.45	0.49
30:BE:173:LEU:HD13	30:BE:219:ASP:HA	1.95	0.49
30:BE:469:SER:HB3	30:BE:510:LEU:HD23	1.95	0.49
30:BE:902:ASN:HB3	30:BE:905:ILE:HG22	1.95	0.49
39:5I:145:VAL:HB	39:5I:176:PHE:HB2	1.94	0.49
44:RG:197:ASP:OD1	44:RG:197:ASP:N	2.45	0.49
8:SK:82:ARG:NH1	43:RB:323:GLU:OE2	2.46	0.48
16:3E:214:ILE:HD11	16:3E:252:LEU:HD22	1.94	0.48
18:3H:51:PHE:HE1	18:3H:114:ILE:HG23	1.78	0.48
20:A5:280:GLN:HB2	20:A5:288:LYS:HE2	1.95	0.48
24:AF:75:LYS:HD2	24:AF:111:TYR:HA	1.95	0.48
24:AF:428:ARG:HH21	25:AG:518:ASP:HB3	1.76	0.48
26:B1:150:THR:OG1	26:B1:164:THR:OG1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B2:263:THR:HA	27:B2:269:THR:O	2.13	0.48
28:B3:454:LEU:O	28:B3:465:LYS:HA	2.12	0.48
29:B8:462:GLY:HA2	29:B8:527:GLY:HA3	1.95	0.48
34:5D:78:LEU:HD13	45:RJ:1082:GLN:HG2	1.95	0.48
44:RG:190:GLN:HE22	44:RG:247:ASP:HB2	1.78	0.48
48:RN:786:ASN:HA	48:RN:789:ASN:HB2	1.95	0.48
3:SA:129:U:O2'	50:RP:903:THR:O	2.30	0.48
3:SA:1133:A:OP1	46:RK:231:ARG:NE	2.42	0.48
18:3H:54:MET:HB3	18:3H:64:LEU:HD13	1.93	0.48
20:A5:25:ASP:OD2	29:B8:590:LYS:NZ	2.37	0.48
20:A5:149:ASN:HD21	20:A5:190:PRO:HB3	1.77	0.48
25:AG:249:THR:O	25:AG:257:ARG:NH1	2.41	0.48
27:B2:291:GLU:HA	27:B2:294:ARG:HG2	1.94	0.48
32:5B:155:ILE:HD12	32:5B:158:LYS:HE3	1.95	0.48
33:5C:112:GLY:HA3	33:5C:130:ARG:HB3	1.94	0.48
33:5C:284:ARG:NH1	33:5C:408:GLU:OE1	2.39	0.48
39:5I:283:ASP:OD2	39:5I:287:TYR:OH	2.30	0.48
41:5K:149:LYS:HD3	41:5K:170:ILE:HD11	1.95	0.48
50:RP:393:PHE:O	50:RP:397:PHE:CB	2.60	0.48
12:SZ:52:LYS:O	12:SZ:94:TYR:OH	2.23	0.48
15:3D:225:ASP:OD1	15:3D:226:LYS:N	2.46	0.48
17:3F:421:ASN:HD22	17:3F:437:ARG:HA	1.78	0.48
23:AE:8:LEU:HD12	33:5C:144:LEU:HD23	1.96	0.48
23:AE:395:GLU:OE2	23:AE:397:LYS:NZ	2.44	0.48
23:AE:482:SER:HB2	23:AE:484:LEU:HG	1.94	0.48
27:B2:392:THR:HG21	27:B2:410:SER:HB3	1.93	0.48
28:B3:44:ASP:OD1	28:B3:44:ASP:N	2.46	0.48
30:BE:656:ASN:N	30:BE:656:ASN:OD1	2.46	0.48
31:B6:273:ILE:HA	31:B6:276:VAL:HG22	1.95	0.48
37:5G:85:ASP:OD1	37:5G:211:ASN:ND2	2.42	0.48
39:5I:260:GLN:NE2	39:5I:460:GLN:OE1	2.47	0.48
46:RK:103:MET:O	46:RK:107:ALA:HB2	2.13	0.48
9:SM:132:SER:OG	9:SM:133:LYS:N	2.46	0.48
14:3C:170:VAL:HG12	14:3C:239:CYS:HB3	1.96	0.48
21:A8:596:LYS:CE	21:A8:640:LEU:HD13	2.43	0.48
25:AG:771:ASP:OD1	25:AG:771:ASP:N	2.46	0.48
28:B3:536:LEU:HA	28:B3:552:SER:HA	1.96	0.48
28:B3:600:LYS:HA	28:B3:609:CYS:HA	1.95	0.48
41:5K:67:ILE:HD11	41:5K:96:PRO:HB2	1.95	0.48
46:RK:130:ILE:HG23	46:RK:151:LEU:HD23	1.95	0.48
47:RM:716:PRO:O	47:RM:720:LEU:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:RO:447:ASP:OD1	49:RO:447:ASP:N	2.46	0.48
18:3H:13:ASP:OD1	18:3H:13:ASP:N	2.42	0.48
19:A4:150:ASN:ND2	19:A4:198:ASP:OD1	2.37	0.48
21:A8:583:SER:HA	21:A8:586:ILE:HG22	1.94	0.48
21:A8:668:ILE:O	21:A8:671:ARG:HG3	2.14	0.48
26:B1:680:ARG:HH11	35:5E:455:HIS:CG	2.31	0.48
26:B1:717:LEU:HD12	30:BE:578:VAL:HB	1.94	0.48
27:B2:214:ASP:OD1	27:B2:214:ASP:N	2.45	0.48
27:B2:643:ASP:HB3	27:B2:650:ILE:HD11	1.95	0.48
29:B8:148:THR:OG1	29:B8:152:GLU:OE2	2.31	0.48
29:B8:266:GLY:HA3	29:B8:295:ILE:HD11	1.95	0.48
29:B8:458:ILE:HG13	29:B8:484:VAL:HG22	1.95	0.48
30:BE:529:TYR:HA	30:BE:536:LEU:HA	1.95	0.48
30:BE:630:THR:N	30:BE:644:THR:O	2.44	0.48
45:RJ:634:ARG:NH2	46:RK:186:PRO:O	2.42	0.48
1:3A:88:U:OP2	16:3E:338:LYS:NZ	2.41	0.48
3:SA:364:G:N7	3:SA:366:A:N6	2.62	0.48
3:SA:1642:G:OP2	35:5E:530:ARG:NH2	2.47	0.48
4:SF:223:ASN:OD1	4:SF:223:ASN:N	2.47	0.48
7:SJ:72:ILE:HG22	7:SJ:74:LYS:HG2	1.96	0.48
19:A4:424:ASP:N	19:A4:424:ASP:OD1	2.45	0.48
31:B6:426:ASP:O	31:B6:430:TYR:N	2.47	0.48
35:5E:520:LEU:HG	35:5E:525:LYS:HG3	1.96	0.48
9:SM:90:TYR:H	9:SM:103:ARG:HB3	1.79	0.48
12:SZ:20:ARG:NH1	12:SZ:22:GLN:OE1	2.47	0.48
16:3E:225:GLU:HG2	16:3E:226:ILE:HG13	1.96	0.48
17:3F:448:PHE:HA	17:3F:451:ILE:HG22	1.95	0.48
19:A4:171:SER:O	19:A4:171:SER:OG	2.32	0.48
19:A4:579:ARG:NH2	19:A4:644:SER:OG	2.47	0.48
24:AF:420:GLU:O	24:AF:424:ARG:CB	2.61	0.48
25:AG:105:HIS:HB2	25:AG:122:LYS:HG3	1.95	0.48
28:B3:167:ASP:OD1	28:B3:168:THR:N	2.47	0.48
43:RB:237:SER:O	43:RB:237:SER:OG	2.32	0.48
45:RJ:298:VAL:HG23	45:RJ:791:ILE:HG23	1.94	0.48
47:RM:507:THR:H	53:RY:495:ALA:HB3	1.77	0.48
48:RN:734:ARG:HA	48:RN:737:ILE:HG12	1.95	0.48
49:RO:507:LEU:HA	49:RO:510:GLU:HB3	1.95	0.48
10:SR:120:ASP:OD1	10:SR:120:ASP:N	2.40	0.48
23:AE:684:TYR:HB2	23:AE:687:LEU:HD23	1.95	0.48
27:B2:118:ASN:OD1	27:B2:118:ASN:N	2.46	0.48
28:B3:161:TRP:HB3	28:B3:177:LEU:HG	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B8:183:ASP:HB2	30:BE:242:ARG:HA	1.96	0.48
35:5E:517:LYS:NZ	35:5E:518:GLU:HG3	2.29	0.48
42:RA:313:PRO:HG3	42:RA:317:ILE:HD11	1.94	0.48
49:RO:153:ILE:HD13	49:RO:202:LEU:HD21	1.94	0.48
50:RP:48:LEU:HG	50:RP:74:VAL:HG22	1.95	0.48
3:SA:153:G:N2	3:SA:161:U:O2	2.43	0.48
3:SA:464:A:H2'	3:SA:465:G:H8	1.78	0.48
6:SH:31:ARG:HE	42:RA:359:ILE:HD13	1.78	0.48
8:SK:136:VAL:HG12	8:SK:156:ILE:HG12	1.96	0.48
19:A4:560:SER:OG	19:A4:561:LYS:N	2.47	0.48
23:AE:336:LEU:HD22	23:AE:373:ILE:HG21	1.96	0.48
23:AE:484:LEU:HD13	23:AE:663:SER:HB3	1.95	0.48
24:AF:435:ASP:OD1	24:AF:435:ASP:N	2.45	0.48
27:B2:479:LEU:HA	27:B2:489:VAL:O	2.14	0.48
28:B3:271:ASP:OD1	28:B3:271:ASP:N	2.47	0.48
28:B3:301:GLN:HG2	28:B3:315:ASN:HA	1.95	0.48
33:5C:137:MET:HA	33:5C:144:LEU:HA	1.96	0.48
35:5E:384:ARG:NE	37:5G:81:SER:HB3	2.28	0.48
47:RL:55:VAL:HG23	47:RL:121:MET:HB3	1.95	0.48
47:RL:388:GLU:HA	47:RL:410:SER:O	2.14	0.48
50:RP:190:ARG:NH1	50:RP:194:GLU:OE2	2.46	0.48
3:SA:1624:C:H5''	37:5G:185:VAL:HG22	1.96	0.48
15:3D:160:ARG:NH2	16:3E:243:MET:O	2.43	0.48
16:3E:207:ARG:HH11	16:3E:226:ILE:HG12	1.78	0.48
17:3F:523:LYS:O	17:3F:541:ALA:HA	2.13	0.48
21:A8:570:LEU:HD23	21:A8:582:ILE:HD11	1.95	0.48
24:AF:31:THR:OG1	24:AF:32:SER:N	2.46	0.48
25:AG:141:LEU:HD11	25:AG:153:ILE:HD11	1.96	0.48
35:5E:477:GLU:HG2	35:5E:477:GLU:O	2.14	0.48
42:RA:164:ARG:NH2	42:RA:174:ASN:OD1	2.46	0.48
44:RG:173:THR:OG1	44:RG:174:LYS:N	2.47	0.48
50:RP:1709:ASP:HA	50:RP:1758:ALA:HA	1.94	0.48
51:RQ:322:ASN:N	51:RQ:322:ASN:OD1	2.46	0.48
1:3A:94:A:H2'	1:3A:95:A:H8	1.79	0.47
2:5A:90:G:O2'	2:5A:91:U:O4'	2.25	0.47
3:SA:124:A:O2'	4:SF:148:ARG:NH2	2.33	0.47
3:SA:336:G:H1	7:SJ:5:ARG:HB2	1.79	0.47
3:SA:351:C:N3	9:SM:102:LYS:NZ	2.52	0.47
9:SM:124:THR:HG22	9:SM:141:LYS:HB3	1.96	0.47
19:A4:284:LEU:HD21	32:5B:206:LEU:HD21	1.95	0.47
19:A4:747:ILE:HD11	19:A4:753:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A5:335:ASN:O	20:A5:337:LYS:NZ	2.47	0.47
23:AE:329:THR:HG21	23:AE:365:ILE:HG21	1.95	0.47
25:AG:440:VAL:HG11	25:AG:449:LEU:HD12	1.95	0.47
26:B1:205:LYS:HG2	26:B1:219:GLU:HG2	1.96	0.47
28:B3:77:THR:HG22	28:B3:86:LYS:HB3	1.96	0.47
44:RG:232:LEU:HD21	44:RH:103:PRO:HG3	1.96	0.47
45:RJ:1105:ASP:N	45:RJ:1105:ASP:OD1	2.47	0.47
46:RK:282:GLU:O	46:RK:286:SER:HB3	2.14	0.47
47:RL:57:TRP:NE1	47:RL:125:GLN:OE1	2.39	0.47
19:A4:97:ARG:NE	32:5B:191:PRO:O	2.39	0.47
20:A5:460:ARG:HA	20:A5:465:ILE:HD11	1.96	0.47
23:AE:376:GLU:H	23:AE:379:GLU:HG3	1.79	0.47
24:AF:246:TYR:OH	24:AF:289:ASN:ND2	2.44	0.47
27:B2:54:ILE:CD1	27:B2:364:TYR:HD2	2.27	0.47
28:B3:803:SER:O	28:B3:803:SER:OG	2.31	0.47
42:RA:250:GLY:HA3	42:RA:271:GLY:HA2	1.96	0.47
42:RA:273:ASP:O	42:RA:275:LYS:NZ	2.47	0.47
3:SA:1757:G:H2'	35:5E:500:LYS:HD2	1.96	0.47
4:SF:143:ASP:OD1	4:SF:143:ASP:N	2.35	0.47
9:SM:112:SER:HB3	9:SM:139:VAL:HG23	1.95	0.47
19:A4:214:SER:OG	19:A4:221:ASN:O	2.28	0.47
20:A5:473:LYS:HE3	20:A5:475:ALA:HB3	1.96	0.47
24:AF:135:GLN:HE22	24:AF:178:PRO:HA	1.79	0.47
27:B2:137:ILE:HG22	27:B2:147:VAL:HG22	1.97	0.47
27:B2:530:LEU:HD13	27:B2:550:LEU:HD11	1.94	0.47
33:5C:333:SER:HB3	33:5C:381:LEU:HD11	1.95	0.47
34:5D:58:ARG:HH21	36:5F:174:ARG:CZ	2.28	0.47
45:RJ:92:ARG:HH21	45:RJ:221:LEU:HG	1.79	0.47
45:RJ:111:LYS:O	45:RJ:310:THR:OG1	2.32	0.47
1:3A:315:A:H2'	1:3A:316:A:C8	2.49	0.47
3:SA:280:U:H2'	6:SH:188:ARG:HH22	1.80	0.47
8:SK:87:SER:OG	8:SK:89:ASP:OD1	2.33	0.47
25:AG:581:GLY:HA2	25:AG:602:PRO:HD2	1.97	0.47
33:5C:133:HIS:HE1	33:5C:147:GLU:HG3	1.79	0.47
33:5C:450:GLY:O	51:RQ:857:TYR:OH	2.21	0.47
41:5K:152:ILE:HG12	41:5K:171:PRO:HG2	1.95	0.47
47:RL:200:VAL:HG12	47:RL:208:LEU:HD13	1.97	0.47
4:SF:103:TYR:O	4:SF:182:TYR:OH	2.32	0.47
23:AE:141:ASN:ND2	23:AE:206:TYR:OH	2.46	0.47
25:AG:498:LEU:HA	25:AG:508:ILE:O	2.14	0.47
25:AG:855:LEU:O	25:AG:859:ASN:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B2:9:GLU:O	27:B2:684:TRP:HA	2.14	0.47
27:B2:414:LEU:HD11	27:B2:445:VAL:HG11	1.94	0.47
34:5D:58:ARG:HD2	36:5F:174:ARG:CZ	2.45	0.47
43:RB:290:GLU:OE2	43:RB:296:ARG:NH1	2.47	0.47
45:RJ:631:ILE:HG13	45:RJ:634:ARG:HB2	1.97	0.47
49:RO:198:GLU:O	49:RO:202:LEU:HB2	2.13	0.47
50:RP:1278:ARG:O	50:RP:1282:VAL:HA	2.15	0.47
51:RQ:835:VAL:HG13	51:RQ:837:LYS:HG3	1.96	0.47
16:3E:355:ASN:HA	16:3E:358:LYS:HB2	1.97	0.47
19:A4:157:SER:OG	19:A4:195:TRP:NE1	2.47	0.47
19:A4:744:VAL:HA	19:A4:753:ALA:O	2.15	0.47
25:AG:143:ASN:N	25:AG:143:ASN:OD1	2.47	0.47
26:B1:150:THR:N	26:B1:164:THR:O	2.45	0.47
44:RH:153:VAL:HA	48:RN:716:LYS:HB2	1.96	0.47
52:RS:258:VAL:HA	52:RS:261:GLU:HG2	1.97	0.47
3:SA:406:U:H2'	3:SA:407:A:C8	2.50	0.47
6:SH:32:ILE:HD12	6:SH:65:GLN:HA	1.96	0.47
14:3C:173:LEU:HA	14:3C:197:VAL:HG13	1.97	0.47
16:3E:262:ILE:HA	16:3E:265:PHE:HB2	1.96	0.47
19:A4:534:LEU:HB3	19:A4:543:ILE:HG22	1.95	0.47
21:A8:635:PHE:HD2	22:A9:492:ILE:HD12	1.79	0.47
25:AG:175:ALA:O	25:AG:187:VAL:HA	2.15	0.47
26:B1:156:GLN:HB2	26:B1:203:GLN:HE21	1.79	0.47
26:B1:165:SER:OG	26:B1:166:LYS:N	2.48	0.47
26:B1:537:GLY:HA3	26:B1:556:ARG:HB3	1.96	0.47
27:B2:183:ASP:OD1	27:B2:183:ASP:N	2.42	0.47
28:B3:10:ILE:HG23	28:B3:643:PHE:HB2	1.95	0.47
28:B3:108:LEU:HG	28:B3:119:VAL:HG12	1.97	0.47
29:B8:238:LEU:HD11	29:B8:590:LYS:HB2	1.97	0.47
30:BE:207:ASP:N	30:BE:207:ASP:OD1	2.47	0.47
33:5C:257:SER:OG	33:5C:259:TRP:NE1	2.36	0.47
34:5D:52:ARG:NH2	37:5G:270:ASP:OD1	2.43	0.47
36:5F:163:ASN:N	36:5F:183:SER:OG	2.45	0.47
42:RA:80:GLN:HB2	42:RA:82:HIS:HD2	1.78	0.47
45:RJ:879:THR:OG1	45:RJ:880:TYR:N	2.48	0.47
51:RQ:341:LYS:HA	51:RQ:344:GLN:HE21	1.79	0.47
10:SR:50:GLU:OE2	10:SR:82:ARG:NH2	2.47	0.47
12:SZ:59:GLY:O	43:RB:296:ARG:NH2	2.44	0.47
16:3E:176:GLU:HA	16:3E:179:THR:HG22	1.97	0.47
16:3E:191:HIS:HD2	16:3E:246:GLU:HA	1.80	0.47
25:AG:22:LEU:HD12	25:AG:32:LYS:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B2:235:ASN:ND2	27:B2:240:GLY:O	2.40	0.47
27:B2:367:ILE:HD12	27:B2:368:PRO:HD2	1.97	0.47
28:B3:19:SER:OG	28:B3:20:SER:N	2.48	0.47
28:B3:113:THR:OG1	28:B3:114:SER:N	2.48	0.47
28:B3:139:SER:OG	28:B3:140:PHE:N	2.48	0.47
28:B3:339:ILE:HG13	28:B3:358:ASN:HD21	1.80	0.47
28:B3:481:LYS:HE2	28:B3:522:ASN:HA	1.97	0.47
29:B8:568:VAL:HG23	29:B8:579:VAL:HG22	1.96	0.47
31:B6:14:GLU:OE2	31:B6:91:ARG:NH2	2.38	0.47
31:B6:122:ASN:OD1	31:B6:122:ASN:N	2.48	0.47
45:RJ:80:THR:O	56:RJ:1201:GTP:O2B	2.31	0.47
2:5A:69:U:O4	2:5A:70:A:N6	2.48	0.47
3:SA:158:U:N3	3:SA:420:A:O2'	2.46	0.47
18:3G:57:ASP:HB3	18:3G:84:ARG:HG2	1.97	0.47
20:A5:366:GLY:O	25:AG:583:LYS:NZ	2.48	0.47
23:AE:136:LEU:HD21	23:AE:155:ILE:HG12	1.97	0.47
27:B2:393:ASP:OD1	27:B2:393:ASP:N	2.46	0.47
28:B3:245:SER:OG	28:B3:245:SER:O	2.32	0.47
39:5I:201:ILE:HD12	39:5I:225:LEU:HD21	1.97	0.47
45:RJ:347:LEU:O	45:RJ:352:LYS:NZ	2.48	0.47
48:RN:510:THR:HB	48:RN:518:ILE:HD13	1.96	0.47
52:RS:271:THR:OG1	52:RS:274:GLU:OE1	2.31	0.47
2:5A:18:G:H2'	2:5A:19:A:C8	2.50	0.47
2:5A:485:G:H2'	15:3D:22:LEU:HD21	1.97	0.47
19:A4:511:VAL:HA	19:A4:558:ARG:HB3	1.96	0.47
25:AG:443:ASN:ND2	25:AG:446:ASN:OD1	2.48	0.47
26:B1:115:SER:O	26:B1:115:SER:OG	2.33	0.47
26:B1:299:SER:O	35:5E:475:SER:HA	2.15	0.47
27:B2:542:ASP:N	27:B2:542:ASP:OD1	2.45	0.47
27:B2:588:ILE:HG12	27:B2:600:TRP:HB2	1.97	0.47
28:B3:593:CYS:HB2	28:B3:620:LEU:HB3	1.95	0.47
28:B3:622:ALA:HB3	28:B3:636:ASP:H	1.78	0.47
30:BE:170:LEU:HG	30:BE:180:LEU:HD21	1.97	0.47
30:BE:430:ILE:HD11	30:BE:445:MET:HB2	1.97	0.47
36:5F:103:VAL:HA	36:5F:106:ILE:HG22	1.96	0.47
17:3F:477:SER:OG	17:3F:521:VAL:O	2.27	0.46
26:B1:515:TYR:CE2	36:5F:180:PHE:HZ	2.33	0.46
27:B2:360:ASN:OD1	27:B2:360:ASN:N	2.47	0.46
28:B3:352:LYS:HA	28:B3:365:ILE:O	2.15	0.46
28:B3:680:ASN:HA	28:B3:683:LEU:HG	1.96	0.46
28:B3:749:ASN:HB3	28:B3:751:LYS:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:RN:451:THR:O	48:RN:455:LEU:HB2	2.15	0.46
50:RP:1721:ILE:HD11	50:RP:1751:TYR:HB2	1.96	0.46
3:SA:545:A:OP2	38:5H:542:TYR:OH	2.33	0.46
3:SA:1160:A:H2'	3:SA:1161:C:H6	1.80	0.46
4:SF:52:LEU:O	17:3F:120:ARG:NH1	2.48	0.46
4:SF:53:LYS:NZ	43:RB:292:ASP:OD2	2.38	0.46
27:B2:676:SER:OG	27:B2:678:ASP:OD1	2.22	0.46
28:B3:476:ASP:N	28:B3:476:ASP:OD1	2.48	0.46
31:B6:185:TYR:HE2	51:RQ:338:LEU:HD21	1.81	0.46
32:5B:173:ARG:NH2	34:5D:144:ASN:O	2.48	0.46
34:5D:25:TYR:HD1	40:5J:213:ARG:HE	1.62	0.46
35:5E:493:GLN:NE2	35:5E:497:ASN:ND2	2.58	0.46
42:RA:245:CYS:HB3	42:RA:253:TYR:HB2	1.96	0.46
42:RA:251:TYR:HA	42:RA:266:LYS:O	2.16	0.46
43:RB:309:LYS:HB3	43:RB:313:ARG:HH11	1.80	0.46
47:RL:729:LEU:HA	47:RL:764:ASN:HA	1.97	0.46
5:SG:52:GLU:OE2	5:SG:54:LYS:NZ	2.48	0.46
14:3C:194:VAL:HB	14:3C:217:ILE:HD13	1.97	0.46
19:A4:418:CYS:HB2	19:A4:460:LEU:HB2	1.97	0.46
19:A4:742:LEU:HD12	19:A4:757:ARG:HG3	1.96	0.46
23:AE:509:SER:HA	23:AE:512:LEU:HD12	1.98	0.46
25:AG:204:ASN:OD1	25:AG:204:ASN:N	2.47	0.46
25:AG:530:LYS:HG2	25:AG:546:LYS:HB3	1.97	0.46
26:B1:420:ARG:NH2	35:5E:494:GLU:CD	2.66	0.46
27:B2:163:LYS:HG2	35:5E:522:ARG:NH2	2.30	0.46
27:B2:236:ASP:OD1	27:B2:236:ASP:N	2.46	0.46
28:B3:69:LEU:HD13	28:B3:109:ASP:HA	1.96	0.46
35:5E:521:THR:HG23	35:5E:524:ASP:H	1.80	0.46
42:RA:286:GLU:HG3	42:RA:287:ASN:H	1.80	0.46
45:RJ:187:LYS:HE3	45:RJ:187:LYS:HB2	1.75	0.46
46:RK:337:VAL:HG23	46:RK:354:ILE:HG12	1.98	0.46
48:RN:56:ASN:HD21	48:RN:59:GLU:HG3	1.81	0.46
49:RO:202:LEU:HD23	49:RO:208:TYR:HB3	1.98	0.46
12:SZ:45:ALA:HB2	12:SZ:55:VAL:HG11	1.97	0.46
17:3F:417:SER:HB3	17:3F:421:ASN:HB2	1.96	0.46
20:A5:518:ASN:O	20:A5:522:THR:OG1	2.32	0.46
23:AE:374:ARG:NH1	23:AE:375:LEU:O	2.49	0.46
26:B1:32:PRO:HG3	26:B1:61:ILE:HG13	1.97	0.46
28:B3:189:HIS:HD2	28:B3:191:SER:H	1.62	0.46
29:B8:306:ASN:OD1	29:B8:306:ASN:N	2.43	0.46
44:RH:152:SER:OG	44:RH:155:SER:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:RJ:819:GLU:O	45:RJ:852:ARG:NH2	2.47	0.46
45:RJ:1082:GLN:OE1	45:RJ:1082:GLN:HA	2.15	0.46
46:RK:282:GLU:O	46:RK:286:SER:CB	2.64	0.46
49:RO:196:GLN:OE1	49:RO:260:ASN:ND2	2.37	0.46
3:SA:1276:U:H3	3:SA:1434:U:H3	1.64	0.46
14:3C:308:PRO:HG3	34:5D:129:SER:HA	1.96	0.46
19:A4:326:ARG:NH2	19:A4:364:PHE:O	2.49	0.46
20:A5:85:ILE:HB	20:A5:99:PHE:HB2	1.98	0.46
25:AG:212:CYS:HB2	25:AG:224:SER:HB3	1.98	0.46
25:AG:446:ASN:OD1	25:AG:446:ASN:N	2.46	0.46
26:B1:29:LEU:HD22	26:B1:42:LEU:HD11	1.96	0.46
26:B1:557:LYS:NZ	30:BE:426:GLU:OE1	2.44	0.46
26:B1:680:ARG:HH12	35:5E:455:HIS:CD2	2.29	0.46
28:B3:67:LEU:HD23	28:B3:68:LYS:H	1.80	0.46
28:B3:534:ARG:HH11	28:B3:535:GLY:H	1.63	0.46
28:B3:708:ARG:NH2	28:B3:720:PHE:O	2.49	0.46
29:B8:278:ASP:N	29:B8:278:ASP:OD1	2.46	0.46
29:B8:512:ASP:OD1	29:B8:512:ASP:N	2.48	0.46
32:5B:211:LEU:HD13	32:5B:213:LYS:HE3	1.96	0.46
35:5E:384:ARG:HD3	37:5G:83:ILE:HD11	1.97	0.46
35:5E:448:LEU:HD12	36:5F:85:MET:SD	2.55	0.46
36:5F:61:LEU:O	36:5F:71:ARG:NE	2.47	0.46
44:RG:112:VAL:HB	44:RG:124:VAL:HG22	1.97	0.46
45:RJ:360:ASP:HB3	45:RJ:365:LEU:HB2	1.98	0.46
49:RO:462:SER:OG	49:RO:463:LEU:N	2.48	0.46
52:RS:270:LEU:HB3	52:RS:278:PHE:HZ	1.80	0.46
3:SA:328:A:H2'	3:SA:329:G:C8	2.50	0.46
10:SR:113:ASP:N	10:SR:113:ASP:OD1	2.48	0.46
11:SY:113:ALA:HB3	11:SY:116:ASP:HB2	1.96	0.46
21:A8:638:LEU:HD12	21:A8:641:VAL:CG1	2.46	0.46
23:AE:568:ILE:HD11	23:AE:673:ASN:HD21	1.80	0.46
29:B8:472:GLN:NE2	29:B8:474:SER:OG	2.49	0.46
36:5F:115:MET:HG3	36:5F:120:MET:HB3	1.98	0.46
37:5G:119:ARG:HG3	37:5G:122:TYR:HB2	1.98	0.46
39:5I:288:TYR:O	39:5I:298:LEU:N	2.42	0.46
44:RG:55:ILE:O	44:RG:64:LYS:HB2	2.16	0.46
46:RK:104:LEU:O	46:RK:300:TYR:OH	2.33	0.46
50:RP:104:GLN:HG3	50:RP:105:PRO:HD3	1.97	0.46
50:RP:1691:SER:HA	50:RP:1724:ASN:HD21	1.81	0.46
1:3A:56:A:O2'	34:5D:63:TYR:OH	2.34	0.46
2:5A:486:U:H4'	2:5A:487:A:H5''	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:1111:G:C8	45:RJ:1162:ALA:HA	2.51	0.46
6:SH:17:GLU:N	47:RL:604:SER:O	2.47	0.46
7:SJ:48:THR:O	7:SJ:52:ASN:CB	2.58	0.46
19:A4:164:THR:HG22	19:A4:185:ARG:HG2	1.98	0.46
23:AE:583:LYS:HE2	23:AE:627:LEU:HA	1.98	0.46
24:AF:436:GLU:HG2	24:AF:480:LEU:HD23	1.98	0.46
27:B2:63:LEU:HD21	27:B2:106:TRP:CD2	2.50	0.46
27:B2:341:ALA:HB1	27:B2:353:LEU:HD11	1.96	0.46
30:BE:640:LEU:HD23	30:BE:655:THR:HG22	1.98	0.46
34:5D:61:ASP:CA	36:5F:160:TRP:CZ3	2.99	0.46
41:5K:83:VAL:HG12	41:5K:96:PRO:HG3	1.98	0.46
48:RN:547:VAL:HA	48:RN:550:VAL:HG12	1.97	0.46
48:RN:554:GLN:HE21	48:RN:559:ARG:H	1.63	0.46
48:RN:804:LYS:HD3	48:RN:804:LYS:HA	1.75	0.46
49:RO:395:ILE:HG23	49:RO:469:LEU:HD21	1.98	0.46
52:RS:379:LYS:HA	52:RS:379:LYS:HD3	1.72	0.46
52:RS:392:TYR:HA	52:RS:395:MET:HB2	1.96	0.46
52:RS:413:LEU:O	52:RS:418:HIS:NE2	2.49	0.46
7:SJ:32:GLN:HE21	42:RA:78:LYS:HG2	1.81	0.46
15:3D:175:ILE:HD12	15:3D:317:SER:HA	1.98	0.46
15:3D:371:ASN:OD1	15:3D:374:ARG:NH1	2.48	0.46
21:A8:587:LEU:HD23	21:A8:587:LEU:C	2.35	0.46
26:B1:280:THR:HA	26:B1:304:PRO:HB3	1.98	0.46
28:B3:32:LEU:HD12	28:B3:68:LYS:HE2	1.97	0.46
30:BE:323:VAL:HB	30:BE:343:LEU:HD22	1.98	0.46
35:5E:330:VAL:HG21	45:RJ:932:LEU:HD12	1.97	0.46
35:5E:384:ARG:HD2	37:5G:83:ILE:N	2.30	0.46
42:RA:164:ARG:HH12	42:RA:176:PHE:H	1.64	0.46
47:RM:249:SER:O	47:RM:253:LEU:CB	2.63	0.46
2:5A:86:C:N4	25:AG:482:GLY:O	2.45	0.46
3:SA:1273:G:H1	3:SA:1437:U:H2'	1.80	0.46
11:SY:137:LYS:HE2	11:SY:137:LYS:HB3	1.80	0.46
14:3B:261:LEU:O	15:3D:129:ARG:NH1	2.49	0.46
16:3E:392:ALA:O	16:3E:396:ASN:ND2	2.49	0.46
25:AG:253:SER:O	25:AG:256:THR:OG1	2.33	0.46
25:AG:296:HIS:NE2	25:AG:314:SER:OG	2.37	0.46
28:B3:625:THR:HG22	28:B3:633:VAL:HG13	1.97	0.46
32:5B:200:ARG:O	32:5B:204:ARG:HB3	2.15	0.46
39:5I:280:ALA:HB2	39:5I:311:VAL:HB	1.97	0.46
39:5I:281:ASN:ND2	39:5I:283:ASP:OD1	2.49	0.46
42:RA:300:TRP:HA	42:RA:308:TYR:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:RS:280:ASN:ND2	52:RS:320:GLY:O	2.46	0.46
52:RS:359:LEU:HB2	52:RS:372:ILE:HD11	1.97	0.46
3:SA:225:A:H2'	3:SA:226:A:H8	1.79	0.46
19:A4:124:THR:HG21	32:5B:191:PRO:HG3	1.97	0.46
23:AE:495:LEU:HA	23:AE:498:PHE:HB2	1.97	0.46
24:AF:117:LEU:HD12	24:AF:117:LEU:HA	1.79	0.46
33:5C:335:GLY:HA2	33:5C:377:LYS:HG3	1.98	0.46
36:5F:5:LEU:HD23	36:5F:9:GLU:HB3	1.98	0.46
46:RK:199:ARG:HB2	46:RK:239:PRO:HA	1.97	0.46
48:RN:495:ASN:HD22	48:RN:617:HIS:HB2	1.80	0.46
49:RO:366:LEU:HD13	49:RO:405:LEU:HD11	1.96	0.46
7:SJ:83:TYR:HB3	7:SJ:101:ILE:HD11	1.98	0.45
7:SJ:103:GLN:HB3	7:SJ:164:ARG:HG2	1.98	0.45
16:3E:381:ASP:OD1	16:3E:381:ASP:N	2.49	0.45
19:A4:444:ARG:HG3	19:A4:446:SER:H	1.81	0.45
19:A4:545:ARG:HG3	19:A4:549:VAL:HB	1.98	0.45
19:A4:652:THR:HG23	19:A4:653:TRP:HD1	1.81	0.45
35:5E:437:ILE:HD11	36:5F:70:PHE:CE2	2.51	0.45
45:RJ:65:ASP:OD1	45:RJ:65:ASP:N	2.46	0.45
45:RJ:772:MET:HG3	45:RJ:774:PRO:HD2	1.98	0.45
1:3A:36:C:O2'	39:5I:389:ARG:NH1	2.48	0.45
2:5A:485:G:N2	39:5I:386:LYS:O	2.41	0.45
3:SA:381:C:H2'	3:SA:382:C:H4'	1.97	0.45
3:SA:420:A:C8	3:SA:420:A:C3'	2.98	0.45
4:SF:58:GLY:HA2	4:SF:61:VAL:HG12	1.99	0.45
4:SF:127:LYS:HB2	4:SF:140:VAL:HG23	1.99	0.45
9:SM:76:VAL:HG21	9:SM:87:ARG:HH11	1.81	0.45
21:A8:633:GLN:H	21:A8:633:GLN:HG3	1.41	0.45
30:BE:351:GLN:HG3	30:BE:372:ASP:HB3	1.97	0.45
30:BE:420:GLU:HG2	30:BE:470:GLN:HA	1.97	0.45
34:5D:48:LEU:HG	45:RJ:1067:LEU:HD11	1.98	0.45
36:5F:29:ASP:OD2	36:5F:41:ARG:NH1	2.49	0.45
37:5G:100:LEU:HD22	37:5G:144:GLU:HB3	1.97	0.45
39:5I:306:SER:HB3	39:5I:326:ASP:H	1.81	0.45
42:RA:60:ASN:ND2	42:RA:100:GLU:OE2	2.50	0.45
43:RB:229:ASP:HB3	43:RB:232:GLU:HG2	1.97	0.45
3:SA:397:A:H5''	7:SJ:50:GLY:HA2	1.98	0.45
3:SA:1463:C:H4'	48:RN:63:ALA:HB1	1.98	0.45
20:A5:66:VAL:HG12	20:A5:112:LEU:HD21	1.97	0.45
21:A8:631:SER:N	21:A8:634:LEU:HD21	2.31	0.45
23:AE:11:VAL:HA	23:AE:14:ASN:HD22	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AE:255:ILE:HD11	25:AG:884:MET:HB3	1.98	0.45
23:AE:1700:SER:O	23:AE:1703:GLU:N	2.49	0.45
24:AF:69:ARG:HG3	24:AF:70:THR:HG23	1.97	0.45
27:B2:760:ILE:HD11	27:B2:835:PHE:HB2	1.98	0.45
28:B3:343:MET:HB3	28:B3:355:LEU:HD23	1.98	0.45
35:5E:520:LEU:HD11	35:5E:525:LYS:CA	2.45	0.45
36:5F:13:LEU:HG	36:5F:13:LEU:O	2.16	0.45
44:RG:143:GLN:HE22	44:RG:149:SER:HA	1.81	0.45
48:RN:13:LEU:HD22	48:RN:16:ARG:HE	1.81	0.45
50:RP:971:ARG:O	50:RP:975:ASN:HA	2.16	0.45
52:RS:271:THR:H	52:RS:274:GLU:HB2	1.82	0.45
15:3D:379:LEU:HD13	15:3D:408:VAL:HG21	1.98	0.45
19:A4:137:TYR:HB2	19:A4:177:LEU:HD12	1.99	0.45
20:A5:452:LEU:HA	20:A5:455:THR:HG22	1.98	0.45
20:A5:518:ASN:HB2	20:A5:521:SER:HB3	1.98	0.45
20:A5:539:ARG:NH1	25:AG:524:ASP:OD2	2.49	0.45
21:A8:440:ARG:O	25:AG:728:LEU:HD21	2.16	0.45
23:AE:700:SER:O	23:AE:700:SER:OG	2.32	0.45
24:AF:171:VAL:HG22	24:AF:188:SER:HB3	1.99	0.45
27:B2:49:VAL:HG22	27:B2:63:LEU:HD22	1.98	0.45
36:5F:29:ASP:N	36:5F:29:ASP:OD1	2.50	0.45
44:RH:191:ASP:HA	44:RH:194:GLU:HG2	1.98	0.45
48:RN:600:LEU:HD22	48:RN:633:VAL:HG22	1.98	0.45
52:RS:399:ILE:O	52:RS:406:GLY:N	2.50	0.45
3:SA:385:A:OP1	7:SJ:25:ARG:NH2	2.46	0.45
5:SG:117:THR:HG21	5:SG:194:LEU:HD23	1.98	0.45
15:3D:195:VAL:HG12	15:3D:216:PHE:HE2	1.81	0.45
18:3G:58:CYS:HB3	18:3G:98:ILE:HD12	1.99	0.45
19:A4:249:ARG:HB2	19:A4:292:ASN:HD22	1.81	0.45
21:A8:547:GLN:O	21:A8:551:PHE:HB2	2.16	0.45
23:AE:718:ARG:HA	23:AE:721:VAL:HG12	1.99	0.45
25:AG:364:ASN:OD1	25:AG:364:ASN:N	2.42	0.45
26:B1:418:ARG:HD3	35:5E:489:SER:O	2.10	0.45
27:B2:103:ILE:HB	27:B2:117:PHE:HB2	1.99	0.45
27:B2:220:THR:HG22	27:B2:259:ILE:HD11	1.96	0.45
29:B8:264:LEU:HD11	29:B8:272:LEU:HD12	1.97	0.45
31:B6:186:VAL:HG12	31:B6:273:ILE:HG13	1.98	0.45
36:5F:111:LEU:HD13	36:5F:143:ILE:HG21	1.97	0.45
42:RA:21:VAL:HG12	42:RA:46:ARG:HH12	1.81	0.45
44:RH:56:SER:HA	44:RH:63:ASP:HB2	1.99	0.45
2:5A:550:C:H2'	2:5A:551:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:1537:C:N4	44:RH:155:SER:O	2.37	0.45
4:SF:150:PRO:HB2	4:SF:154:ILE:HG13	1.98	0.45
5:SG:39:GLU:OE2	5:SG:47:SER:OG	2.33	0.45
17:3F:164:GLN:HE21	17:3F:527:VAL:HG13	1.81	0.45
17:3F:452:SER:HB3	17:3F:460:ARG:HG2	1.99	0.45
23:AE:864:VAL:O	23:AE:868:LYS:CB	2.65	0.45
25:AG:726:GLN:NE2	25:AG:736:THR:O	2.42	0.45
25:AG:761:GLU:HG3	25:AG:779:ILE:HG22	1.99	0.45
30:BE:851:SER:O	30:BE:851:SER:OG	2.31	0.45
35:5E:325:SER:OG	45:RJ:1007:TYR:CE1	2.69	0.45
42:RA:14:TYR:HE2	42:RA:344:PRO:HG3	1.81	0.45
42:RA:164:ARG:HH12	42:RA:176:PHE:N	2.15	0.45
50:RP:378:HIS:O	50:RP:382:PHE:CB	2.65	0.45
3:SA:67:A:H2'	3:SA:69:G:C8	2.52	0.45
3:SA:420:A:C8	3:SA:420:A:O5'	2.70	0.45
9:SM:92:HIS:HD2	9:SM:94:ILE:HG13	1.82	0.45
15:3D:120:SER:O	15:3D:120:SER:OG	2.33	0.45
19:A4:468:ASP:OD2	19:A4:472:ARG:NH1	2.44	0.45
19:A4:636:ILE:HG23	19:A4:648:PHE:HD2	1.82	0.45
23:AE:583:LYS:HD3	23:AE:631:VAL:HG21	1.99	0.45
25:AG:600:SER:O	25:AG:600:SER:OG	2.33	0.45
27:B2:54:ILE:HD13	27:B2:364:TYR:CD2	2.48	0.45
28:B3:42:ILE:HD11	28:B3:379:LEU:HD13	1.97	0.45
33:5C:104:LEU:HD21	33:5C:139:TRP:HB2	1.99	0.45
47:RL:77:ILE:HD12	47:RL:77:ILE:HA	1.82	0.45
47:RL:846:SER:O	47:RL:850:LEU:CB	2.65	0.45
48:RN:423:GLY:O	48:RN:426:THR:OG1	2.31	0.45
1:3A:316:A:H2'	1:3A:317:A:C8	2.51	0.45
3:SA:145:A:O2'	3:SA:146:U:O5'	2.33	0.45
3:SA:326:G:H4'	9:SM:82:ARG:HD2	1.98	0.45
3:SA:545:A:O2'	3:SA:546:U:O4'	2.22	0.45
4:SF:159:THR:HB	4:SF:173:ILE:HB	1.99	0.45
9:SM:57:LYS:O	9:SM:138:ASN:ND2	2.50	0.45
14:3C:253:ILE:HD11	14:3C:293:LEU:HD21	1.99	0.45
21:A8:635:PHE:CD2	22:A9:492:ILE:HD12	2.51	0.45
23:AE:65:LYS:HB3	23:AE:104:LEU:HD11	1.99	0.45
24:AF:227:VAL:HG22	24:AF:236:VAL:HG12	1.99	0.45
25:AG:38:SER:OG	25:AG:43:ASN:O	2.35	0.45
26:B1:25:ASP:O	26:B1:27:LYS:N	2.49	0.45
26:B1:369:ILE:HD11	26:B1:390:VAL:HG11	1.99	0.45
28:B3:217:ASP:OD1	28:B3:217:ASP:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B3:509:ALA:HB1	28:B3:515:CYS:HA	1.98	0.45
33:5C:311:SER:OG	33:5C:313:GLU:OE2	2.33	0.45
37:5G:104:ALA:HB3	37:5G:116:ARG:HE	1.82	0.45
39:5I:94:TYR:OH	39:5I:134:ASN:ND2	2.41	0.45
42:RA:247:THR:HG21	42:RA:251:TYR:HB2	1.99	0.45
1:3A:12:U:H3	3:SA:1112:G:H1	1.65	0.45
3:SA:265:A:OP2	6:SH:194:LYS:NZ	2.37	0.45
3:SA:1223:A:H2'	3:SA:1224:A:C8	2.52	0.45
14:3B:88:ILE:HD11	14:3B:123:ILE:HG21	1.98	0.45
18:3H:33:LEU:HD23	18:3H:35:LYS:HE3	1.98	0.45
23:AE:348:ILE:HD13	23:AE:348:ILE:HA	1.87	0.45
26:B1:475:PRO:HD2	26:B1:493:TRP:HB2	1.99	0.45
39:5I:297:SER:OG	39:5I:299:ASN:O	2.33	0.45
40:5J:110:ASP:OD1	40:5J:110:ASP:N	2.36	0.45
45:RJ:617:THR:HG23	45:RJ:620:LYS:HE2	1.99	0.45
50:RP:465:PHE:HA	50:RP:468:ALA:HB3	1.98	0.45
52:RS:235:VAL:HG12	52:RS:238:SER:HB3	1.98	0.45
52:RS:429:LYS:HD2	52:RS:437:ARG:HH22	1.82	0.45
3:SA:1634:C:O2	26:B1:397:LYS:NZ	2.50	0.45
14:3C:175:ALA:N	14:3C:198:GLU:OE2	2.48	0.45
20:A5:582:GLU:O	20:A5:586:ASP:N	2.50	0.45
21:A8:633:GLN:O	21:A8:637:LEU:CD2	2.65	0.45
23:AE:659:LEU:HD21	23:AE:691:PHE:HA	1.98	0.45
24:AF:371:GLU:OE2	29:B8:273:ARG:NH2	2.50	0.45
33:5C:214:LEU:HD23	33:5C:228:LEU:HD12	1.99	0.45
33:5C:269:LYS:HB2	51:RQ:830:ILE:HG23	1.98	0.45
33:5C:460:ARG:HB3	51:RQ:847:VAL:HB	1.99	0.45
36:5F:5:LEU:CD2	36:5F:13:LEU:HD21	2.47	0.45
42:RA:231:VAL:HA	42:RA:247:THR:HA	1.98	0.45
46:RK:143:LYS:HE3	46:RK:143:LYS:HB2	1.75	0.45
52:RS:373:LYS:HG3	52:RS:420:ALA:HA	1.99	0.45
9:SM:46:LYS:HD3	9:SM:49:ILE:HD12	1.98	0.44
20:A5:87:LEU:O	20:A5:96:THR:N	2.50	0.44
23:AE:109:TRP:HA	23:AE:114:THR:HG21	2.00	0.44
25:AG:43:ASN:OD1	25:AG:43:ASN:N	2.48	0.44
27:B2:129:PHE:HE1	27:B2:150:LEU:HD11	1.82	0.44
27:B2:292:ILE:HG23	27:B2:324:PHE:HE2	1.83	0.44
27:B2:641:TYR:O	27:B2:650:ILE:N	2.49	0.44
28:B3:498:SER:OG	28:B3:539:VAL:O	2.29	0.44
30:BE:546:ILE:HG21	30:BE:560:LEU:HD22	1.99	0.44
39:5I:210:LYS:HA	39:5I:210:LYS:HD3	1.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:RG:135:LYS:HD3	44:RG:135:LYS:HA	1.87	0.44
45:RJ:1148:GLU:OE2	45:RJ:1152:ARG:NH1	2.49	0.44
50:RP:60:SER:HB3	50:RP:102:SER:HB3	1.99	0.44
3:SA:406:U:H2'	3:SA:407:A:H8	1.82	0.44
9:SM:94:ILE:HD12	9:SM:101:GLU:H	1.81	0.44
14:3B:104:ASP:OD1	14:3B:104:ASP:N	2.38	0.44
26:B1:64:ASN:N	26:B1:64:ASN:OD1	2.49	0.44
45:RJ:889:LEU:HD22	45:RJ:922:ILE:HB	2.00	0.44
47:RL:111:SER:HB3	47:RL:134:LEU:HD12	1.99	0.44
48:RN:737:ILE:HA	48:RN:740:MET:HG2	2.00	0.44
49:RO:282:HIS:CD2	49:RO:283:LYS:HG2	2.52	0.44
16:3E:372:ARG:HG3	18:3G:63:ILE:HA	2.00	0.44
17:3F:405:VAL:HG12	17:3F:415:THR:HG22	2.00	0.44
23:AE:763:LEU:HD12	23:AE:768:LYS:HD3	2.00	0.44
24:AF:51:HIS:O	24:AF:53:HIS:N	2.49	0.44
27:B2:337:LYS:O	27:B2:357:THR:OG1	2.25	0.44
27:B2:566:TYR:OH	27:B2:603:ASP:O	2.33	0.44
27:B2:580:ASP:OD2	27:B2:623:PHE:N	2.40	0.44
28:B3:32:LEU:HD22	28:B3:76:LEU:HD12	2.00	0.44
28:B3:104:PRO:O	28:B3:122:THR:OG1	2.35	0.44
30:BE:921:ARG:O	30:BE:925:LEU:HB2	2.17	0.44
50:RP:107:LEU:HD21	50:RP:150:TRP:HB3	1.98	0.44
3:SA:362:G:H2'	3:SA:363:G:C8	2.52	0.44
3:SA:608:U:O2'	3:SA:609:U:O4'	2.34	0.44
3:SA:1146:G:H2'	3:SA:1147:A:H8	1.83	0.44
3:SA:1660:A:H2'	3:SA:1661:U:C6	2.52	0.44
9:SM:84:ILE:N	9:SM:109:VAL:O	2.47	0.44
15:3D:31:LEU:HD21	39:5I:59:VAL:HG13	1.99	0.44
19:A4:579:ARG:HH12	19:A4:659:PHE:HD1	1.65	0.44
26:B1:157:ASP:N	26:B1:157:ASP:OD1	2.50	0.44
28:B3:430:TYR:HD2	28:B3:454:LEU:HD23	1.82	0.44
28:B3:531:ASN:OD1	28:B3:531:ASN:N	2.49	0.44
35:5E:319:VAL:CG1	45:RJ:1044:LEU:HD22	2.47	0.44
36:5F:43:ASP:HA	36:5F:46:LYS:HG2	1.99	0.44
37:5G:234:ARG:NH1	37:5G:254:PHE:O	2.51	0.44
38:5H:555:ASN:HB3	38:5H:558:ASN:HB2	1.98	0.44
43:RB:302:LYS:HB3	43:RB:306:ARG:HH22	1.81	0.44
46:RK:187:ILE:HB	46:RK:251:GLN:HE22	1.82	0.44
48:RN:65:ASN:OD1	48:RN:65:ASN:N	2.50	0.44
48:RN:443:LYS:HG3	48:RN:448:PHE:HE2	1.81	0.44
2:5A:554:G:H1	2:5A:583:U:H3	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:SG:63:GLN:HE22	5:SG:66:GLN:HB3	1.82	0.44
14:3C:92:ARG:HH12	34:5D:151:PHE:HB2	1.81	0.44
15:3D:281:LEU:HD23	16:3E:261:GLN:HE21	1.82	0.44
19:A4:75:ASN:HB3	19:A4:92:GLU:HA	2.00	0.44
19:A4:201:VAL:HG13	19:A4:213:TRP:HB2	1.99	0.44
23:AE:488:GLY:HA2	23:AE:491:TYR:HB3	1.98	0.44
23:AE:729:LYS:HA	23:AE:733:MET:HG3	2.00	0.44
25:AG:414:ILE:HA	25:AG:414:ILE:HD12	1.80	0.44
26:B1:418:ARG:CZ	35:5E:491:ALA:HA	2.47	0.44
27:B2:443:LEU:HG	27:B2:459:LEU:HD13	2.00	0.44
28:B3:467:ILE:H	28:B3:479:ILE:HD11	1.83	0.44
28:B3:749:ASN:OD1	35:5E:511:ASN:OD1	2.36	0.44
29:B8:358:PHE:HA	29:B8:376:LEU:O	2.17	0.44
30:BE:356:ILE:HG22	30:BE:633:LYS:HG3	2.00	0.44
30:BE:737:LEU:C	30:BE:740:ILE:CG2	2.85	0.44
33:5C:122:GLY:O	33:5C:139:TRP:NE1	2.34	0.44
35:5E:325:SER:OG	45:RJ:1007:TYR:CD1	2.71	0.44
37:5G:138:ASP:N	37:5G:138:ASP:OD1	2.48	0.44
42:RA:60:ASN:HB3	42:RA:74:THR:HB	2.00	0.44
44:RG:242:CYS:O	44:RG:246:GLU:HG3	2.18	0.44
45:RJ:60:ASP:OD2	45:RJ:62:THR:OG1	2.32	0.44
50:RP:70:ILE:HG21	50:RP:87:ILE:HG22	1.98	0.44
2:5A:20:C:H2'	2:5A:21:A:C8	2.52	0.44
3:SA:592:A:O2'	3:SA:596:C:OP1	2.35	0.44
3:SA:1234:A:O2'	3:SA:1236:A:N6	2.50	0.44
5:SG:86:GLN:HE22	26:B1:546:ASP:HB3	1.83	0.44
10:SR:8:GLN:OE1	36:5F:177:ILE:HG23	2.18	0.44
11:SY:77:ILE:HG22	45:RJ:751:TYR:HB2	1.99	0.44
14:3B:125:VAL:HG12	40:5J:150:GLY:HA3	2.00	0.44
14:3B:169:LYS:HA	14:3B:193:VAL:O	2.18	0.44
19:A4:120:SER:OG	19:A4:121:THR:N	2.50	0.44
25:AG:484:VAL:O	25:AG:487:GLU:N	2.51	0.44
26:B1:476:VAL:HA	26:B1:492:SER:HB3	1.98	0.44
26:B1:743:PHE:HZ	26:B1:778:ILE:HD13	1.83	0.44
29:B8:27:PHE:HB3	31:B6:31:LEU:HD23	1.98	0.44
35:5E:447:LYS:HA	35:5E:450:VAL:HG12	1.98	0.44
44:RH:199:ASP:OD1	44:RH:199:ASP:N	2.49	0.44
49:RO:259:LYS:HB3	49:RO:259:LYS:HE2	1.72	0.44
3:SA:398:G:OP2	7:SJ:47:ARG:NH2	2.40	0.44
4:SF:140:VAL:HG12	4:SF:146:THR:HG22	2.00	0.44
8:SK:38:ASN:HA	38:5H:565:LYS:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SM:57:LYS:HG3	9:SM:110:HIS:CE1	2.53	0.44
10:SR:64:ASP:OD1	10:SR:64:ASP:N	2.50	0.44
14:3B:218:ILE:HD11	15:3D:152:LEU:HD22	1.98	0.44
16:3E:227:LEU:HG	16:3E:231:ILE:HB	2.00	0.44
21:A8:675:LEU:CB	22:A9:486:LEU:HD13	2.47	0.44
23:AE:396:ASP:OD1	23:AE:396:ASP:N	2.47	0.44
24:AF:20:THR:HA	24:AF:24:GLN:HE21	1.83	0.44
25:AG:768:TRP:HE1	25:AG:772:THR:HA	1.83	0.44
26:B1:200:SER:OG	26:B1:202:ASP:O	2.29	0.44
28:B3:111:ASP:N	28:B3:111:ASP:OD1	2.48	0.44
39:5I:241:ASP:OD1	39:5I:241:ASP:N	2.39	0.44
42:RA:152:ASP:N	42:RA:152:ASP:OD1	2.51	0.44
45:RJ:841:THR:HB	45:RJ:859:ILE:HA	1.99	0.44
48:RN:314:MET:HA	48:RN:512:ASP:HA	2.00	0.44
50:RP:1183:PRO:O	50:RP:1187:VAL:CB	2.65	0.44
53:RY:489:GLN:O	53:RY:493:PHE:CB	2.66	0.44
7:SJ:66:SER:HA	7:SJ:73:SER:HA	1.99	0.44
15:3D:206:LEU:HD11	15:3D:219:LEU:HD11	2.00	0.44
19:A4:214:SER:HB3	19:A4:226:LEU:HD13	1.99	0.44
23:AE:63:GLU:HA	23:AE:64:PRO:HD3	1.88	0.44
27:B2:107:ASP:OD1	27:B2:107:ASP:N	2.46	0.44
39:5I:444:GLU:OE2	39:5I:448:ARG:NH2	2.37	0.44
42:RA:184:ASN:OD1	42:RA:230:GLN:NE2	2.51	0.44
44:RG:227:LEU:HA	44:RG:227:LEU:HD23	1.79	0.44
3:SA:1599:C:H2'	3:SA:1600:A:C8	2.53	0.44
3:SA:1623:C:O2'	37:5G:184:GLU:HB2	2.18	0.44
6:SH:65:GLN:NE2	42:RA:43:TYR:O	2.51	0.44
7:SJ:67:TRP:HD1	7:SJ:70:GLU:H	1.66	0.44
9:SM:36:LYS:HD2	9:SM:36:LYS:HA	1.74	0.44
19:A4:45:THR:HB	19:A4:352:VAL:HA	1.99	0.44
19:A4:774:LEU:HD12	19:A4:774:LEU:HA	1.83	0.44
21:A8:676:TRP:CE3	21:A8:676:TRP:O	2.70	0.44
23:AE:238:LEU:HA	23:AE:241:ILE:HG22	1.99	0.44
23:AE:538:ALA:HA	23:AE:541:LEU:HB2	2.00	0.44
25:AG:228:VAL:HG23	25:AG:236:ASN:HB3	2.00	0.44
25:AG:510:TYR:HE1	25:AG:527:HIS:HB3	1.83	0.44
25:AG:532:TRP:HB3	25:AG:541:TRP:HB3	1.99	0.44
26:B1:35:ASN:HA	26:B1:58:ILE:HG23	1.99	0.44
26:B1:157:ASP:OD1	26:B1:203:GLN:NE2	2.38	0.44
27:B2:59:LEU:HD21	27:B2:62:LYS:HE2	1.99	0.44
28:B3:188:GLU:O	28:B3:221:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B8:277:ILE:HA	29:B8:282:ASN:HD22	1.83	0.44
30:BE:852:LEU:HD22	30:BE:860:GLU:HG2	2.00	0.44
33:5C:162:ASN:ND2	33:5C:429:GLU:OE1	2.51	0.44
35:5E:384:ARG:CD	37:5G:82:GLY:H	2.30	0.44
35:5E:475:SER:C	35:5E:477:GLU:H	2.21	0.44
44:RH:89:PRO:HG2	44:RH:134:PHE:HZ	1.83	0.44
47:RL:195:ASN:HB3	47:RL:198:CYS:HB3	1.99	0.44
3:SA:257:A:O2'	7:SJ:73:SER:O	2.34	0.43
3:SA:415:C:O2'	3:SA:418:G:O6	2.36	0.43
20:A5:233:LYS:HA	20:A5:233:LYS:HD3	1.82	0.43
20:A5:520:MET:H	20:A5:520:MET:HG3	1.60	0.43
21:A8:573:ILE:HG22	21:A8:575:ASN:H	1.83	0.43
21:A8:634:LEU:HD23	21:A8:634:LEU:H	1.83	0.43
21:A8:642:LEU:HD12	22:A9:499:ILE:CG2	2.44	0.43
23:AE:100:ALA:HB1	29:B8:44:PHE:HZ	1.82	0.43
24:AF:288:ASP:OD1	24:AF:288:ASP:N	2.48	0.43
26:B1:356:ASP:OD1	26:B1:356:ASP:N	2.50	0.43
28:B3:652:ILE:HD12	28:B3:652:ILE:HA	1.92	0.43
30:BE:76:THR:OG1	30:BE:78:SER:O	2.29	0.43
33:5C:228:LEU:HD22	33:5C:264:PRO:HA	1.99	0.43
35:5E:533:LYS:CA	35:5E:536:ARG:HE	2.25	0.43
39:5I:139:CYS:HB3	39:5I:145:VAL:HG22	1.99	0.43
44:RG:177:LYS:HE2	44:RG:177:LYS:HB3	1.68	0.43
45:RJ:203:LYS:HA	45:RJ:203:LYS:HD2	1.78	0.43
50:RP:103:LEU:HD11	50:RP:147:VAL:HG23	1.99	0.43
3:SA:328:A:H2'	3:SA:329:G:H8	1.83	0.43
9:SM:123:VAL:HG12	9:SM:142:VAL:HA	1.99	0.43
14:3B:221:ILE:HD13	15:3D:163:VAL:HB	2.00	0.43
19:A4:212:ILE:O	19:A4:226:LEU:N	2.50	0.43
19:A4:571:THR:HG21	19:A4:632:ASN:HB3	2.00	0.43
20:A5:240:GLN:HE22	20:A5:298:LYS:HB3	1.83	0.43
21:A8:439:LYS:HA	21:A8:442:LYS:CB	2.48	0.43
21:A8:635:PHE:CD2	22:A9:492:ILE:CD1	3.01	0.43
25:AG:712:THR:HG23	25:AG:720:ILE:HD13	1.99	0.43
31:B6:5:ARG:HA	31:B6:5:ARG:HD2	1.80	0.43
45:RJ:625:TRP:HZ2	46:RK:284:SER:HB3	1.83	0.43
47:RM:281:LEU:HA	47:RM:409:ALA:HB3	1.99	0.43
49:RO:292:PRO:HG2	49:RO:330:PHE:HE2	1.82	0.43
49:RO:315:VAL:HG23	49:RO:316:PRO:HD3	1.98	0.43
49:RO:472:HIS:CD2	49:RO:474:HIS:H	2.31	0.43
3:SA:513:U:H2'	3:SA:514:G:H8	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:1146:G:H2'	3:SA:1147:A:C8	2.53	0.43
4:SF:183:VAL:HB	4:SF:225:VAL:HG23	2.00	0.43
4:SF:194:THR:H	4:SF:210:ILE:HG23	1.82	0.43
7:SJ:74:LYS:HD3	7:SJ:74:LYS:HA	1.68	0.43
16:3E:330:LEU:HD13	34:5D:109:THR:HG21	2.00	0.43
19:A4:144:ILE:HD12	19:A4:158:VAL:HB	2.00	0.43
21:A8:633:GLN:HE21	21:A8:633:GLN:HB2	1.55	0.43
25:AG:516:PRO:HG2	25:AG:519:LEU:HD21	2.00	0.43
26:B1:605:ASP:OD1	26:B1:605:ASP:N	2.40	0.43
28:B3:28:ASN:OD1	28:B3:28:ASN:N	2.48	0.43
28:B3:34:THR:HG23	28:B3:68:LYS:HE3	2.00	0.43
34:5D:78:LEU:HA	34:5D:78:LEU:HD12	1.82	0.43
39:5I:306:SER:OG	39:5I:307:ALA:N	2.50	0.43
41:5K:171:PRO:HA	41:5K:184:LYS:HB2	2.00	0.43
49:RO:260:ASN:HA	49:RO:263:SER:HG	1.83	0.43
4:SF:141:THR:OG1	4:SF:142:HIS:N	2.52	0.43
16:3E:206:ALA:HB2	16:3E:262:ILE:HD11	2.00	0.43
19:A4:572:ALA:HB3	19:A4:585:ILE:HD11	2.00	0.43
19:A4:750:ASN:N	19:A4:750:ASN:OD1	2.50	0.43
23:AE:655:ALA:O	23:AE:659:LEU:HB2	2.18	0.43
24:AF:24:GLN:HB2	24:AF:294:PHE:HD1	1.83	0.43
24:AF:115:THR:O	24:AF:115:THR:OG1	2.35	0.43
26:B1:369:ILE:HB	26:B1:383:PHE:HB2	1.99	0.43
28:B3:194:ARG:HD3	28:B3:243:VAL:HG13	1.99	0.43
37:5G:164:GLN:HE21	37:5G:260:GLU:HB3	1.84	0.43
40:5J:207:LYS:HE2	40:5J:207:LYS:HB3	1.88	0.43
45:RJ:904:ASN:HA	45:RJ:907:THR:HB	2.00	0.43
46:RK:68:SER:OG	46:RK:69:TYR:N	2.52	0.43
52:RS:221:LEU:HD22	52:RS:258:VAL:HG11	2.00	0.43
52:RS:373:LYS:HE2	52:RS:373:LYS:HB3	1.84	0.43
2:5A:467:A:N1	2:5A:468:A:N6	2.66	0.43
2:5A:485:G:OP2	15:3D:46:LYS:NZ	2.39	0.43
2:5A:489:G:O6	31:B6:120:ARG:NH1	2.51	0.43
3:SA:18:C:O2'	3:SA:21:U:O4'	2.37	0.43
3:SA:578:U:OP2	45:RJ:874:TYR:OH	2.29	0.43
7:SJ:76:THR:OG1	7:SJ:77:ARG:N	2.52	0.43
8:SK:65:LYS:HZ2	17:3F:59:PRO:CA	2.27	0.43
11:SY:68:ILE:HD12	48:RN:785:VAL:HG23	2.00	0.43
14:3C:185:SER:HB3	14:3C:217:ILE:HD11	2.00	0.43
16:3E:191:HIS:HB2	16:3E:247:ILE:HG23	1.99	0.43
18:3G:62:GLU:HA	18:3G:65:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3H:95:ARG:HD2	18:3H:95:ARG:HA	1.87	0.43
21:A8:443:CYS:CA	25:AG:728:LEU:HB3	2.47	0.43
25:AG:50:ASN:HD21	25:AG:782:THR:HG22	1.84	0.43
25:AG:252:LEU:HD23	25:AG:256:THR:HG21	2.00	0.43
26:B1:829:VAL:HG23	26:B1:830:ARG:HG2	2.01	0.43
27:B2:276:ASN:ND2	27:B2:280:THR:O	2.47	0.43
28:B3:41:ASN:OD1	28:B3:41:ASN:N	2.49	0.43
30:BE:606:ASP:OD1	30:BE:606:ASP:N	2.41	0.43
35:5E:323:LYS:HG2	35:5E:325:SER:H	1.84	0.43
39:5I:8:ARG:HD3	39:5I:8:ARG:HA	1.80	0.43
41:5K:52:PHE:HB3	41:5K:55:TYR:HB3	2.01	0.43
41:5K:161:LYS:HG2	41:5K:172:LEU:HD21	1.99	0.43
50:RP:1610:MET:O	50:RP:1614:GLU:CB	2.67	0.43
52:RS:359:LEU:HD23	52:RS:362:LEU:HD12	2.00	0.43
3:SA:526:A:OP1	12:SZ:93:ARG:NE	2.48	0.43
8:SK:155:HIS:NE2	17:3F:321:HIS:O	2.50	0.43
14:3C:261:LEU:O	16:3E:118:ARG:NH2	2.34	0.43
16:3E:372:ARG:O	16:3E:376:LEU:HB2	2.19	0.43
17:3F:303:LYS:HB3	17:3F:317:ILE:HD11	2.01	0.43
18:3H:52:ILE:HD12	18:3H:71:CYS:SG	2.58	0.43
20:A5:336:ASN:OD1	20:A5:336:ASN:N	2.49	0.43
21:A8:270:PHE:HA	21:A8:282:GLY:HA2	2.00	0.43
21:A8:547:GLN:O	21:A8:551:PHE:CB	2.66	0.43
25:AG:478:ASN:N	25:AG:478:ASN:OD1	2.51	0.43
26:B1:341:GLN:OE1	26:B1:341:GLN:HA	2.19	0.43
27:B2:645:GLU:HG2	27:B2:646:LYS:HG3	1.99	0.43
30:BE:569:VAL:HB	30:BE:579:ARG:HB2	2.01	0.43
35:5E:384:ARG:CZ	37:5G:81:SER:HB3	2.49	0.43
39:5I:6:ILE:HG21	39:5I:8:ARG:HH21	1.84	0.43
42:RA:155:VAL:HG13	42:RA:163:TYR:HB2	2.00	0.43
46:RK:36:ILE:HB	46:RK:72:THR:HA	2.01	0.43
48:RN:590:ASN:OD1	48:RN:590:ASN:N	2.50	0.43
3:SA:532:U:O2'	12:SZ:33:ALA:O	2.27	0.43
5:SG:89:ILE:HD11	5:SG:172:ILE:HD11	2.00	0.43
14:3C:185:SER:HA	14:3C:188:VAL:HG12	2.01	0.43
17:3F:301:ASP:N	17:3F:301:ASP:OD1	2.51	0.43
21:A8:643:ASP:OD1	24:AF:510:LEU:O	2.37	0.43
23:AE:348:ILE:HG21	23:AE:373:ILE:HD11	2.00	0.43
23:AE:715:HIS:HA	23:AE:718:ARG:HG2	2.00	0.43
25:AG:140:LYS:HA	25:AG:140:LYS:HD3	1.78	0.43
28:B3:377:LEU:HA	28:B3:378:PRO:HD3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B3:519:ASN:HD22	28:B3:524:GLU:H	1.67	0.43
28:B3:678:TRP:HE3	28:B3:697:VAL:HG23	1.84	0.43
29:B8:35:GLU:O	29:B8:39:LYS:HB2	2.18	0.43
33:5C:64:ASP:HA	33:5C:67:LEU:HG	1.99	0.43
39:5I:133:GLN:HA	39:5I:150:ILE:O	2.18	0.43
45:RJ:280:LEU:HD12	45:RJ:281:PRO:HD2	2.01	0.43
48:RN:616:LEU:HB3	48:RN:619:LEU:HD13	2.01	0.43
48:RN:644:ASP:OD1	48:RN:687:LYS:NZ	2.51	0.43
4:SF:163:ASP:OD2	4:SF:166:SER:N	2.51	0.43
5:SG:72:HIS:O	10:SR:79:TYR:OH	2.37	0.43
17:3F:209:LYS:HA	17:3F:209:LYS:HD2	1.82	0.43
17:3F:343:ASP:OD1	17:3F:343:ASP:N	2.46	0.43
20:A5:281:ILE:HG12	20:A5:328:VAL:HB	2.01	0.43
22:A9:475:THR:HA	22:A9:478:ASN:HB2	1.99	0.43
24:AF:377:ASP:OD1	24:AF:377:ASP:N	2.51	0.43
24:AF:463:VAL:HA	24:AF:466:VAL:HG12	2.01	0.43
27:B2:596:ASN:HB3	27:B2:612:PHE:HA	1.99	0.43
28:B3:218:ASP:OD1	28:B3:218:ASP:N	2.52	0.43
29:B8:376:LEU:HG	29:B8:386:ILE:HG12	1.99	0.43
30:BE:24:PHE:HB3	30:BE:654:TRP:HB3	2.01	0.43
34:5D:145:GLU:OE1	34:5D:146:PHE:N	2.52	0.43
35:5E:316:ASN:O	35:5E:320:ALA:CB	2.66	0.43
39:5I:344:HIS:NE2	39:5I:418:HIS:O	2.51	0.43
48:RN:700:LEU:HD21	49:RO:467:ALA:HB2	2.00	0.43
53:RY:489:GLN:O	53:RY:493:PHE:HB3	2.19	0.43
1:3A:97:C:C2	1:3A:320:G:N2	2.86	0.43
2:5A:474:A:OP2	33:5C:425:ARG:NH2	2.37	0.43
3:SA:1233:G:H1	3:SA:1253:U:H2'	1.83	0.43
4:SF:182:TYR:CD2	4:SF:192:ILE:HD11	2.54	0.43
5:SG:103:ASN:HA	5:SG:106:LYS:HD2	2.01	0.43
7:SJ:67:TRP:O	7:SJ:71:GLY:HA2	2.18	0.43
15:3D:52:SER:HB2	15:3D:85:ASN:HD21	1.84	0.43
16:3E:218:ALA:HA	16:3E:221:THR:HG22	2.00	0.43
16:3E:319:ILE:HD12	16:3E:326:LEU:HD22	2.01	0.43
17:3F:201:ILE:HG12	17:3F:538:ARG:HD3	2.00	0.43
19:A4:617:ASN:O	19:A4:621:ASN:HB2	2.19	0.43
26:B1:76:ASP:OD1	26:B1:76:ASP:N	2.51	0.43
27:B2:178:ILE:HD11	27:B2:186:ILE:HD11	2.01	0.43
28:B3:192:ALA:HB3	28:B3:216:ARG:HG3	2.00	0.43
29:B8:426:VAL:HG11	29:B8:455:ILE:HG21	2.01	0.43
30:BE:50:ILE:HD13	30:BE:311:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:RJ:831:ARG:HD3	45:RJ:838:ILE:HD12	2.01	0.43
48:RN:484:ARG:HB3	48:RN:492:ALA:HB1	2.01	0.43
48:RN:669:SER:HA	48:RN:672:THR:HG22	2.01	0.43
50:RP:1741:LYS:HD3	50:RP:1741:LYS:HA	1.90	0.43
1:3A:94:A:H2'	1:3A:95:A:C8	2.53	0.43
3:SA:200:A:H2'	3:SA:201:G:H8	1.84	0.43
3:SA:555:A:N6	3:SA:571:G:O2'	2.50	0.43
3:SA:1169:G:N1	3:SA:1575:G:OP2	2.44	0.43
7:SJ:31:ARG:HH12	7:SJ:48:THR:HB	1.84	0.43
19:A4:313:LYS:HA	19:A4:316:LYS:HG2	2.01	0.43
20:A5:110:ILE:HG22	20:A5:119:CYS:HB2	2.00	0.43
20:A5:448:ASN:OD1	20:A5:450:HIS:NE2	2.52	0.43
21:A8:314:LEU:HA	21:A8:321:ILE:HA	2.00	0.43
21:A8:595:ILE:O	21:A8:599:MET:HB2	2.19	0.43
23:AE:586:LEU:O	23:AE:590:ALA:HB2	2.18	0.43
24:AF:413:LEU:HA	24:AF:416:THR:HG22	2.00	0.43
25:AG:202:SER:OG	25:AG:204:ASN:OD1	2.30	0.43
26:B1:493:TRP:HA	26:B1:517:ASP:HB2	2.01	0.43
28:B3:133:ASN:OD1	28:B3:133:ASN:N	2.51	0.43
30:BE:627:ASN:ND2	30:BE:647:THR:OG1	2.52	0.43
30:BE:739:VAL:CG2	35:5E:487:ALA:HB2	2.37	0.43
32:5B:164:LYS:HB3	32:5B:164:LYS:HE3	1.76	0.43
33:5C:268:VAL:HG13	51:RQ:831:ILE:HG12	2.00	0.43
34:5D:102:GLN:HE21	45:RJ:1098:ARG:NH1	2.17	0.43
34:5D:130:SER:O	34:5D:130:SER:OG	2.36	0.43
36:5F:169:THR:HA	36:5F:172:ARG:HG2	2.01	0.43
37:5G:119:ARG:HA	37:5G:122:TYR:HD2	1.84	0.43
41:5K:61:PRO:HB3	41:5K:92:ALA:HB1	2.01	0.43
44:RG:75:GLY:HA2	44:RG:78:LYS:HE3	2.01	0.43
45:RJ:1080:LYS:HA	45:RJ:1080:LYS:HD2	1.80	0.43
48:RN:475:ARG:HH22	48:RN:516:LEU:HB3	1.84	0.43
1:3A:62:C:O2'	30:BE:447:ASN:O	2.35	0.42
3:SA:200:A:O2'	50:RP:1061:CYS:O	2.36	0.42
3:SA:327:U:OP2	9:SM:57:LYS:NZ	2.38	0.42
4:SF:45:ILE:O	4:SF:49:ARG:HB3	2.19	0.42
16:3E:283:ILE:HD13	16:3E:283:ILE:HA	1.88	0.42
17:3F:414:ILE:HG13	17:3F:478:LEU:HD21	2.00	0.42
20:A5:441:LEU:HD11	20:A5:480:LEU:HD13	2.01	0.42
23:AE:476:ILE:HG23	23:AE:515:PHE:HE2	1.84	0.42
27:B2:351:LEU:HB2	27:B2:367:ILE:HG23	2.00	0.42
27:B2:369:TYR:HA	27:B2:374:PRO:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B2:636:ASP:OD1	27:B2:636:ASP:N	2.52	0.42
30:BE:470:GLN:HB3	30:BE:553:ARG:NH1	2.34	0.42
33:5C:230:THR:HG22	33:5C:232:ALA:H	1.83	0.42
42:RA:95:ARG:NH2	42:RA:128:LYS:O	2.51	0.42
42:RA:254:ILE:HD12	42:RA:254:ILE:HA	1.84	0.42
45:RJ:1019:THR:HB	45:RJ:1022:LEU:HD12	2.01	0.42
45:RJ:1075:LYS:HE3	45:RJ:1075:LYS:HB2	1.84	0.42
49:RO:504:ASP:OD1	49:RO:504:ASP:N	2.48	0.42
52:RS:266:PHE:O	52:RS:270:LEU:HB3	2.18	0.42
52:RS:398:ARG:H	52:RS:406:GLY:HA3	1.83	0.42
52:RS:437:ARG:HH21	52:RS:463:GLY:HA3	1.84	0.42
17:3F:160:ILE:HG12	17:3F:542:SER:HB2	2.00	0.42
19:A4:106:ASN:OD1	19:A4:106:ASN:N	2.51	0.42
20:A5:270:ASN:OD1	20:A5:270:ASN:N	2.49	0.42
21:A8:556:VAL:O	21:A8:585:ARG:NH1	2.52	0.42
24:AF:424:ARG:HA	25:AG:477:VAL:HG11	2.01	0.42
25:AG:555:VAL:HA	25:AG:556:PRO:HD3	1.89	0.42
25:AG:857:PHE:HE2	29:B8:226:LYS:HB3	1.84	0.42
27:B2:123:ALA:HB3	27:B2:141:LYS:HD3	2.00	0.42
28:B3:260:THR:HG22	28:B3:269:LEU:HD13	2.01	0.42
30:BE:353:PRO:HA	30:BE:370:SER:HA	2.01	0.42
31:B6:72:LYS:HD2	31:B6:72:LYS:HA	1.78	0.42
38:5H:550:LEU:HD23	38:5H:550:LEU:HA	1.88	0.42
42:RA:217:LYS:HE2	42:RA:217:LYS:HB3	1.87	0.42
42:RA:277:ILE:HA	42:RA:290:VAL:O	2.19	0.42
44:RG:34:LYS:HD3	44:RG:34:LYS:HA	1.84	0.42
49:RO:208:TYR:O	49:RO:212:LEU:HB2	2.19	0.42
52:RS:382:LEU:HD11	52:RS:428:TYR:CG	2.55	0.42
3:SA:274:G:N1	3:SA:283:U:O2'	2.50	0.42
3:SA:1739:C:H2'	3:SA:1740:A:C8	2.53	0.42
14:3B:198:GLU:O	14:3B:221:ILE:HA	2.18	0.42
14:3C:149:SER:OG	14:3C:150:LYS:N	2.52	0.42
16:3E:160:ASP:HB3	16:3E:283:ILE:HG21	2.01	0.42
19:A4:532:ASN:N	19:A4:544:SER:O	2.50	0.42
19:A4:566:LEU:HA	19:A4:566:LEU:HD23	1.83	0.42
23:AE:323:PHE:CZ	23:AE:332:ILE:HD11	2.54	0.42
23:AE:354:SER:O	23:AE:358:TYR:HB2	2.20	0.42
23:AE:422:LEU:HD12	23:AE:422:LEU:HA	1.87	0.42
25:AG:551:HIS:HA	25:AG:583:LYS:HE3	2.00	0.42
26:B1:749:TYR:HE2	30:BE:705:ILE:HG13	1.84	0.42
27:B2:297:LYS:HA	27:B2:300:GLU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B2:673:VAL:HG23	27:B2:683:ILE:HD13	2.01	0.42
28:B3:188:GLU:HB2	28:B3:223:TRP:HZ2	1.83	0.42
28:B3:483:SER:O	28:B3:483:SER:OG	2.35	0.42
28:B3:572:GLU:HG3	28:B3:600:LYS:HD2	2.01	0.42
37:5G:153:THR:HG23	37:5G:164:GLN:HB3	2.02	0.42
42:RA:306:LYS:HA	42:RA:306:LYS:HD2	1.83	0.42
48:RN:86:ILE:HG13	48:RN:89:GLN:NE2	2.34	0.42
3:SA:-7:A:N7	39:5I:292:ARG:NH1	2.68	0.42
6:SH:74:LYS:O	42:RA:88:ASN:ND2	2.52	0.42
8:SK:163:PRO:HB3	8:SK:169:PRO:HA	2.01	0.42
14:3B:272:LYS:HD3	14:3B:275:CYS:HB3	2.01	0.42
21:A8:596:LYS:CE	21:A8:637:LEU:CA	2.95	0.42
21:A8:638:LEU:HA	21:A8:641:VAL:CG1	2.48	0.42
25:AG:780:GLU:O	25:AG:782:THR:N	2.49	0.42
26:B1:515:TYR:HE2	36:5F:180:PHE:HZ	1.67	0.42
27:B2:39:GLY:O	27:B2:54:ILE:HG13	2.20	0.42
27:B2:294:ARG:O	27:B2:298:LYS:NZ	2.44	0.42
27:B2:432:TYR:O	27:B2:450:ARG:N	2.48	0.42
27:B2:497:VAL:HG12	27:B2:528:LEU:HB3	2.01	0.42
33:5C:215:LYS:HG2	33:5C:227:GLU:HG2	2.00	0.42
36:5F:94:ILE:HG23	36:5F:97:LEU:HD12	2.02	0.42
39:5I:456:GLU:HA	39:5I:459:LYS:HE2	2.01	0.42
40:5J:106:LEU:O	40:5J:146:ARG:NH1	2.44	0.42
43:RB:307:LYS:O	43:RB:311:ARG:HB3	2.19	0.42
46:RK:81:ILE:HG22	46:RK:110:SER:HB3	2.01	0.42
47:RL:203:ASP:OD1	47:RL:203:ASP:N	2.52	0.42
48:RN:108:LYS:HA	48:RN:108:LYS:HD2	1.85	0.42
1:3A:58:A:OP2	36:5F:165:LYS:CE	2.68	0.42
3:SA:99:C:H2'	3:SA:100:A:C8	2.54	0.42
3:SA:147:A:N7	3:SA:167:U:O2	2.52	0.42
3:SA:1659:A:H2'	3:SA:1660:A:C8	2.53	0.42
15:3D:4:ILE:HG23	15:3D:20:VAL:HG21	2.01	0.42
26:B1:25:ASP:OD1	26:B1:25:ASP:N	2.50	0.42
26:B1:46:LYS:HE2	26:B1:46:LYS:HB3	1.87	0.42
26:B1:275:LEU:HD22	26:B1:289:LEU:HD13	2.02	0.42
27:B2:534:ILE:HD11	27:B2:537:VAL:HG12	2.01	0.42
27:B2:836:ILE:HA	27:B2:839:VAL:HG12	2.00	0.42
30:BE:27:PHE:HB2	30:BE:655:THR:HG23	2.00	0.42
37:5G:164:GLN:NE2	37:5G:260:GLU:OE1	2.52	0.42
40:5J:216:ARG:HA	40:5J:216:ARG:HD3	1.82	0.42
49:RO:395:ILE:HD12	49:RO:469:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:RS:210:VAL:HG23	52:RS:212:LYS:HG2	2.00	0.42
2:5A:532:A:O2'	51:RQ:332:ASP:OD2	2.37	0.42
4:SF:68:ARG:HH21	4:SF:76:VAL:HG11	1.85	0.42
5:SG:23:VAL:HG23	10:SR:61:SER:HB3	2.00	0.42
15:3D:61:GLU:OE2	15:3D:77:SER:OG	2.36	0.42
25:AG:511:GLU:HG2	25:AG:528:ILE:HB	2.00	0.42
30:BE:21:SER:OG	30:BE:621:ASP:OD2	2.28	0.42
30:BE:523:ASP:OD1	30:BE:523:ASP:N	2.38	0.42
36:5F:124:ILE:H	36:5F:124:ILE:HG13	1.47	0.42
37:5G:154:ILE:O	37:5G:162:THR:HA	2.20	0.42
39:5I:464:THR:HG21	39:5I:468:TYR:HE1	1.85	0.42
45:RJ:217:ASP:O	45:RJ:221:LEU:HB2	2.20	0.42
45:RJ:940:LYS:HB2	45:RJ:940:LYS:HE2	1.73	0.42
46:RK:310:ARG:HB3	46:RK:353:THR:HG22	2.01	0.42
48:RN:501:PHE:HB3	48:RN:549:ILE:HG21	2.02	0.42
52:RS:432:ILE:HG23	52:RS:436:GLN:HB2	2.00	0.42
3:SA:341:A:OP1	42:RA:121:ARG:NH2	2.48	0.42
4:SF:71:LYS:N	4:SF:91:THR:O	2.52	0.42
5:SG:114:ILE:HA	5:SG:117:THR:HG22	2.02	0.42
9:SM:92:HIS:NE2	9:SM:101:GLU:O	2.52	0.42
16:3E:172:ASP:O	16:3E:176:GLU:HG2	2.20	0.42
19:A4:313:LYS:HA	19:A4:316:LYS:HZ3	1.84	0.42
21:A8:596:LYS:HG3	21:A8:637:LEU:HD22	2.00	0.42
23:AE:487:THR:HG22	23:AE:488:GLY:H	1.85	0.42
23:AE:539:LEU:HD12	23:AE:540:LYS:HG3	2.01	0.42
24:AF:119:SER:O	24:AF:119:SER:OG	2.36	0.42
26:B1:60:ALA:HB1	26:B1:102:VAL:HG12	2.02	0.42
28:B3:547:LEU:N	28:B3:569:LYS:HZ1	2.17	0.42
28:B3:674:SER:OG	28:B3:675:LYS:N	2.52	0.42
30:BE:62:ASP:O	30:BE:66:LEU:N	2.48	0.42
35:5E:508:ARG:HG2	35:5E:514:ALA:HB2	2.02	0.42
36:5F:166:ILE:H	36:5F:166:ILE:HG13	1.68	0.42
44:RG:190:GLN:NE2	44:RG:244:GLY:HA2	2.34	0.42
1:3A:118:A:C5	17:3F:218:ALA:HB2	2.55	0.42
7:SJ:67:TRP:O	7:SJ:71:GLY:CA	2.68	0.42
8:SK:45:ILE:HD12	8:SK:48:GLN:HE21	1.84	0.42
9:SM:70:ILE:HA	9:SM:125:VAL:O	2.20	0.42
9:SM:115:PHE:CG	9:SM:142:VAL:HG21	2.55	0.42
14:3C:124:SER:HA	14:3C:139:VAL:O	2.19	0.42
17:3F:560:ARG:HE	17:3F:560:ARG:HB3	1.75	0.42
20:A5:27:GLN:HG3	20:A5:59:LYS:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AE:25:ARG:HH21	39:5I:16:VAL:HG22	1.83	0.42
25:AG:313:LEU:HD23	25:AG:323:LEU:HB3	2.01	0.42
25:AG:559:LYS:HE2	25:AG:559:LYS:HB2	1.79	0.42
28:B3:367:VAL:HG12	28:B3:643:PHE:HE2	1.85	0.42
29:B8:504:THR:O	29:B8:504:THR:OG1	2.35	0.42
30:BE:737:LEU:C	30:BE:740:ILE:HG22	2.41	0.42
46:RK:56:ILE:HD13	46:RK:56:ILE:HA	1.89	0.42
46:RK:216:LEU:HB3	46:RK:223:VAL:HG21	2.01	0.42
47:RL:37:LEU:HD22	47:RL:149:VAL:HG11	2.01	0.42
47:RL:59:TYR:O	47:RL:108:TYR:N	2.53	0.42
52:RS:364:PHE:HE1	52:RS:417:TRP:HE1	1.67	0.42
52:RS:373:LYS:HA	52:RS:376:LEU:HG	2.02	0.42
52:RS:382:LEU:HD21	52:RS:428:TYR:CZ	2.53	0.42
3:SA:565:C:N4	45:RJ:993:ASP:HB3	2.35	0.42
3:SA:1656:U:H3	3:SA:1743:U:H3	1.67	0.42
4:SF:47:PHE:HD2	4:SF:48:LEU:HD12	1.84	0.42
4:SF:220:THR:OG1	4:SF:221:ARG:N	2.53	0.42
20:A5:98:LYS:HE3	20:A5:98:LYS:HB2	1.88	0.42
26:B1:274:LEU:HD11	26:B1:286:LEU:HD13	2.02	0.42
26:B1:284:PHE:CZ	35:5E:476:MET:HE2	2.54	0.42
28:B3:516:LYS:HE2	28:B3:516:LYS:HB2	1.89	0.42
30:BE:361:SER:HA	30:BE:636:PRO:HB2	2.02	0.42
37:5G:157:PHE:O	37:5G:159:HIS:N	2.51	0.42
42:RA:164:ARG:NH2	42:RA:174:ASN:O	2.51	0.42
44:RG:128:VAL:HG22	44:RG:159:LEU:HD22	2.01	0.42
44:RH:176:ARG:NH2	44:RH:192:TYR:OH	2.52	0.42
45:RJ:773:THR:HG23	45:RJ:777:ARG:HD3	2.02	0.42
46:RK:190:SER:OG	46:RK:191:ILE:N	2.51	0.42
48:RN:700:LEU:HD23	48:RN:702:LEU:HG	2.01	0.42
52:RS:437:ARG:HD2	52:RS:460:LEU:HG	2.02	0.42
3:SA:575:C:O2	45:RJ:1052:SER:OG	2.28	0.42
4:SF:31:PRO:HA	4:SF:81:THR:HB	2.01	0.42
6:SH:77:LEU:HD12	6:SH:95:LYS:HD3	2.00	0.42
6:SH:101:ILE:H	6:SH:101:ILE:HG13	1.72	0.42
14:3B:107:VAL:HG13	14:3B:141:TYR:HB3	2.01	0.42
16:3E:117:TYR:HA	16:3E:120:ILE:HG12	2.01	0.42
17:3F:303:LYS:HE3	17:3F:319:TYR:HE2	1.85	0.42
17:3F:415:THR:OG1	17:3F:425:TRP:NE1	2.39	0.42
19:A4:98:SER:OG	19:A4:99:ILE:N	2.53	0.42
19:A4:213:TRP:HA	19:A4:225:LEU:HA	2.02	0.42
20:A5:224:CYS:SG	20:A5:225:VAL:N	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A8:443:CYS:CB	25:AG:728:LEU:CD2	2.97	0.42
23:AE:91:ILE:HD13	23:AE:91:ILE:HA	1.90	0.42
23:AE:420:LYS:HB2	23:AE:420:LYS:HE2	1.91	0.42
25:AG:502:LYS:HD2	25:AG:564:PRO:HA	2.02	0.42
26:B1:147:GLN:HB2	26:B1:167:ASP:H	1.85	0.42
27:B2:26:ILE:HA	27:B2:27:PRO:HD3	1.94	0.42
27:B2:405:LEU:HD11	27:B2:673:VAL:HG21	2.02	0.42
27:B2:555:VAL:HG22	27:B2:569:LEU:HB2	2.02	0.42
28:B3:303:PHE:HA	28:B3:312:GLN:O	2.20	0.42
33:5C:191:ILE:HD13	33:5C:191:ILE:HA	1.87	0.42
40:5J:134:ARG:HD2	40:5J:134:ARG:HA	1.83	0.42
2:5A:490:G:H1'	2:5A:495:G:H5'	2.01	0.41
3:SA:318:U:O2	3:SA:346:G:O6	2.37	0.41
3:SA:576:G:C4'	35:5E:327:LYS:HE2	2.48	0.41
3:SA:1489:U:N3	40:5J:202:ARG:O	2.53	0.41
14:3C:291:GLN:HA	14:3C:294:ARG:HG2	2.01	0.41
16:3E:333:LYS:HD3	34:5D:103:ASP:HB3	2.02	0.41
17:3F:368:LEU:HB3	17:3F:396:PHE:HE2	1.83	0.41
18:3G:44:LEU:HD23	18:3G:44:LEU:HA	1.87	0.41
19:A4:423:LYS:NZ	32:5B:167:ARG:HH11	2.18	0.41
21:A8:662:ILE:HA	21:A8:665:GLN:HB2	2.01	0.41
23:AE:755:ARG:O	23:AE:759:ILE:HG12	2.20	0.41
24:AF:105:VAL:HG21	24:AF:142:THR:HG21	2.02	0.41
39:5I:336:HIS:CE1	39:5I:338:HIS:HB2	2.55	0.41
44:RG:215:ASN:HB2	44:RG:218:ASP:HB2	2.01	0.41
48:RN:611:SER:OG	48:RN:612:THR:N	2.52	0.41
48:RN:616:LEU:HD13	48:RN:619:LEU:HD22	2.01	0.41
50:RP:129:ILE:O	50:RP:133:ILE:HG12	2.20	0.41
2:5A:298:A:OP2	30:BE:103:ARG:NH2	2.45	0.41
3:SA:324:U:OP1	9:SM:133:LYS:NZ	2.41	0.41
15:3D:268:MET:HA	15:3D:271:VAL:HG12	2.02	0.41
17:3F:421:ASN:ND2	17:3F:437:ARG:HA	2.34	0.41
17:3F:476:THR:HG22	17:3F:491:SER:HA	2.02	0.41
23:AE:35:TYR:O	23:AE:150:ARG:NH1	2.53	0.41
23:AE:664:PRO:HB2	23:AE:716:PHE:HE2	1.85	0.41
24:AF:366:TYR:OH	24:AF:371:GLU:OE1	2.23	0.41
25:AG:625:GLY:HA3	25:AG:662:VAL:HG11	2.02	0.41
25:AG:659:ILE:HG22	25:AG:674:THR:HB	2.01	0.41
26:B1:300:MET:HG2	26:B1:328:LEU:HD22	2.02	0.41
26:B1:498:ARG:HH11	26:B1:498:ARG:HD3	1.72	0.41
27:B2:19:SER:HG	27:B2:44:SER:HG	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B2:538:ARG:HD3	27:B2:580:ASP:HA	2.02	0.41
28:B3:506:PHE:CE1	28:B3:518:TRP:HB2	2.55	0.41
28:B3:745:ASP:OD2	35:5E:508:ARG:HD2	2.20	0.41
30:BE:635:SER:OG	30:BE:637:ASN:OD1	2.30	0.41
33:5C:201:TYR:OH	33:5C:415:GLU:OE1	2.29	0.41
35:5E:352:LYS:HE2	48:RN:764:ARG:HE	1.85	0.41
35:5E:533:LYS:HG3	35:5E:536:ARG:HE	1.83	0.41
39:5I:223:THR:HG1	39:5I:238:THR:HG1	1.69	0.41
49:RO:243:PRO:HA	49:RO:244:PRO:HD3	1.81	0.41
50:RP:1756:ILE:HG22	50:RP:1760:ASN:HD21	1.85	0.41
52:RS:255:SER:HB3	52:RS:258:VAL:HG22	2.01	0.41
3:SA:360:A:O2'	3:SA:362:G:N2	2.45	0.41
6:SH:123:GLY:O	6:SH:127:THR:OG1	2.39	0.41
8:SK:154:LYS:HE2	8:SK:154:LYS:HB3	1.88	0.41
14:3B:150:LYS:NZ	14:3B:310:GLU:OE2	2.44	0.41
14:3C:242:ALA:HB3	14:3C:269:ILE:HA	2.01	0.41
15:3D:206:LEU:HB3	15:3D:216:PHE:HE1	1.84	0.41
22:A9:451:LEU:HA	22:A9:451:LEU:HD13	1.83	0.41
23:AE:148:PHE:HA	23:AE:151:ILE:HG12	2.01	0.41
23:AE:480:ASN:HA	23:AE:518:THR:HG21	2.02	0.41
24:AF:177:ILE:HA	24:AF:178:PRO:HD3	1.84	0.41
26:B1:275:LEU:HB2	26:B1:289:LEU:HD22	2.02	0.41
26:B1:363:ALA:HB2	26:B1:393:VAL:HG13	2.01	0.41
26:B1:381:ALA:HA	35:5E:481:PRO:HA	2.01	0.41
26:B1:501:SER:O	26:B1:506:SER:OG	2.38	0.41
26:B1:721:VAL:O	30:BE:579:ARG:NH2	2.53	0.41
31:B6:106:ASP:OD1	31:B6:106:ASP:N	2.38	0.41
36:5F:6:LYS:O	36:5F:10:GLN:N	2.52	0.41
37:5G:73:VAL:HG23	37:5G:208:HIS:HE1	1.85	0.41
46:RK:80:ILE:HD13	46:RK:80:ILE:HA	1.90	0.41
1:3A:49:C:H42	2:5A:467:A:H61	1.67	0.41
1:3A:312:U:O4	1:3A:313:A:N6	2.53	0.41
6:SH:51:LYS:HE2	6:SH:51:LYS:HB3	1.91	0.41
10:SR:97:VAL:HG12	10:SR:98:ASP:H	1.83	0.41
16:3E:388:LEU:HD12	16:3E:388:LEU:HA	1.89	0.41
17:3F:132:VAL:HG21	17:3F:505:LEU:HD21	2.02	0.41
17:3F:260:LEU:HD21	17:3F:283:VAL:HG11	2.02	0.41
17:3F:304:ILE:HB	17:3F:318:LEU:HG	2.03	0.41
18:3G:64:LEU:O	18:3G:66:HIS:N	2.43	0.41
23:AE:559:ASN:HB2	23:AE:614:LEU:HD12	2.02	0.41
23:AE:682:SER:O	23:AE:682:SER:OG	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AF:34:GLN:O	24:AF:328:ALA:HA	2.21	0.41
25:AG:258:TYR:CD1	25:AG:414:ILE:HD11	2.55	0.41
25:AG:386:ASN:HD21	25:AG:389:LEU:HD11	1.86	0.41
26:B1:347:SER:HB2	26:B1:365:GLU:HB3	2.03	0.41
26:B1:559:ILE:HG21	26:B1:578:LYS:HA	2.03	0.41
27:B2:50:ASN:HB3	27:B2:62:LYS:HG3	2.02	0.41
28:B3:195:GLY:HA3	28:B3:245:SER:H	1.85	0.41
28:B3:242:GLN:HA	28:B3:263:GLY:HA3	2.01	0.41
28:B3:264:ASP:HA	28:B3:289:PHE:HB2	2.03	0.41
28:B3:393:SER:OG	28:B3:394:LEU:N	2.53	0.41
28:B3:690:HIS:CE1	35:5E:519:GLU:HB2	2.55	0.41
29:B8:174:ARG:NE	29:B8:179:ASP:OD2	2.44	0.41
29:B8:278:ASP:H	29:B8:282:ASN:HD22	1.67	0.41
29:B8:296:GLN:HB3	29:B8:316:GLY:HA2	2.03	0.41
31:B6:268:ASP:N	31:B6:268:ASP:OD1	2.53	0.41
39:5I:58:PHE:HE1	39:5I:373:ARG:HB3	1.85	0.41
39:5I:107:LYS:NZ	39:5I:109:HIS:O	2.45	0.41
46:RK:32:LYS:HG2	46:RK:75:ILE:HG13	2.02	0.41
47:RL:26:PHE:O	47:RL:149:VAL:HA	2.20	0.41
50:RP:1752:ASP:HA	50:RP:1755:GLU:HG2	2.03	0.41
52:RS:355:ALA:HA	52:RS:358:TYR:CE2	2.55	0.41
4:SF:181:VAL:HG23	4:SF:227:VAL:HG22	2.02	0.41
10:SR:46:PHE:HA	10:SR:49:TYR:HB2	2.02	0.41
14:3C:151:LEU:HD13	14:3C:241:PHE:HE1	1.86	0.41
16:3E:163:ILE:HD13	16:3E:163:ILE:HA	1.86	0.41
17:3F:488:ILE:HG22	17:3F:524:ILE:HD13	2.02	0.41
19:A4:39:VAL:HG12	19:A4:41:PHE:H	1.85	0.41
20:A5:32:GLN:HE22	20:A5:47:ASN:HB3	1.85	0.41
23:AE:526:LEU:HA	23:AE:529:VAL:HG12	2.01	0.41
24:AF:392:ILE:HD11	24:AF:417:VAL:HG23	2.03	0.41
25:AG:97:THR:OG1	25:AG:98:VAL:N	2.54	0.41
25:AG:544:LYS:HD3	25:AG:544:LYS:HA	1.88	0.41
26:B1:14:VAL:CG2	26:B1:341:GLN:O	2.62	0.41
27:B2:433:ALA:HA	27:B2:449:THR:HA	2.03	0.41
36:5F:6:LYS:N	36:5F:9:GLU:HB2	2.36	0.41
42:RA:164:ARG:HB2	42:RA:173:LEU:HB2	2.03	0.41
45:RJ:552:LEU:HD23	45:RJ:552:LEU:HA	1.92	0.41
48:RN:515:HIS:O	48:RN:519:THR:OG1	2.32	0.41
3:SA:88:U:H2'	3:SA:89:G:H8	1.85	0.41
3:SA:110:U:OP1	43:RB:227:ARG:NH1	2.53	0.41
3:SA:1156:C:H2'	3:SA:1157:A:C8	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:1523:G:H1'	3:SA:1524:A:H5'	2.02	0.41
14:3C:89:GLU:HG2	14:3C:98:ILE:HB	2.03	0.41
19:A4:154:ASP:OD1	19:A4:154:ASP:N	2.49	0.41
19:A4:394:TRP:HB3	19:A4:399:VAL:HG12	2.03	0.41
20:A5:551:ILE:HA	20:A5:554:PHE:CE2	2.56	0.41
21:A8:631:SER:C	21:A8:634:LEU:CG	2.86	0.41
23:AE:109:TRP:HB2	23:AE:142:TYR:CZ	2.56	0.41
25:AG:31:ASN:OD1	25:AG:31:ASN:N	2.52	0.41
25:AG:712:THR:HG22	25:AG:766:ILE:HG23	2.01	0.41
26:B1:298:LEU:HD12	35:5E:474:ILE:CG2	2.51	0.41
27:B2:164:ASP:HB3	27:B2:182:LYS:HB3	2.02	0.41
29:B8:137:ILE:HD13	29:B8:137:ILE:HA	1.86	0.41
29:B8:159:HIS:O	29:B8:163:ARG:HG2	2.21	0.41
29:B8:278:ASP:H	29:B8:282:ASN:ND2	2.18	0.41
31:B6:35:LYS:HE3	31:B6:35:LYS:HB3	1.88	0.41
31:B6:311:TYR:O	31:B6:315:GLU:HG2	2.21	0.41
33:5C:59:SER:HG	51:RQ:874:SER:HG	1.60	0.41
33:5C:244:ASN:HB3	33:5C:446:PRO:HG3	2.02	0.41
34:5D:61:ASP:O	36:5F:160:TRP:HH2	2.03	0.41
35:5E:314:LEU:HA	35:5E:317:GLU:HB2	2.03	0.41
35:5E:350:THR:CG2	45:RJ:975:GLU:HB2	2.51	0.41
37:5G:260:GLU:OE2	37:5G:262:ARG:NH2	2.33	0.41
38:5H:542:TYR:CZ	38:5H:546:LYS:HG3	2.56	0.41
44:RH:180:LEU:HD23	44:RH:180:LEU:HA	1.88	0.41
6:SH:70:PRO:O	6:SH:98:ARG:NH2	2.54	0.41
6:SH:115:LYS:HB2	6:SH:115:LYS:HE3	1.76	0.41
9:SM:82:ARG:HD3	9:SM:110:HIS:CD2	2.55	0.41
9:SM:115:PHE:HB2	9:SM:142:VAL:HG11	2.03	0.41
16:3E:132:SER:OG	16:3E:134:ASN:OD1	2.34	0.41
16:3E:192:PHE:CD2	16:3E:195:LEU:HB2	2.56	0.41
17:3F:158:THR:HG23	17:3F:548:ARG:HB2	2.02	0.41
17:3F:308:SER:OG	17:3F:313:SER:OG	2.36	0.41
17:3F:321:HIS:CE1	17:3F:340:GLY:H	2.39	0.41
17:3F:502:SER:OG	17:3F:504:ASN:OD1	2.32	0.41
20:A5:64:LYS:HB3	20:A5:77:ILE:HG13	2.02	0.41
22:A9:416:ILE:O	22:A9:420:ILE:CB	2.69	0.41
23:AE:549:LYS:HD3	23:AE:549:LYS:HA	1.91	0.41
24:AF:255:VAL:HA	24:AF:276:SER:HA	2.03	0.41
26:B1:410:THR:HG22	26:B1:426:THR:HG22	2.01	0.41
28:B3:468:ILE:HA	28:B3:469:PRO:HD3	1.83	0.41
35:5E:522:ARG:HA	35:5E:525:LYS:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:5J:117:VAL:HG11	40:5J:149:ILE:HG13	2.02	0.41
42:RA:94:ASP:N	42:RA:94:ASP:OD1	2.54	0.41
44:RG:232:LEU:HB3	44:RG:236:VAL:HG13	2.02	0.41
48:RN:283:ALA:HA	52:RS:381:ALA:HB1	2.03	0.41
48:RN:784:ILE:HA	48:RN:787:THR:HG22	2.03	0.41
52:RS:264:LYS:HB2	52:RS:264:LYS:HE3	1.81	0.41
3:SA:200:A:H2'	3:SA:201:G:C8	2.56	0.41
7:SJ:35:ASN:HD21	42:RA:119:ASN:HD22	1.69	0.41
7:SJ:58:LEU:HD21	42:RA:77:TYR:HB2	2.02	0.41
8:SK:63:ASP:OD1	8:SK:63:ASP:N	2.46	0.41
15:3D:24:GLN:NE2	15:3D:126:ASP:OD1	2.48	0.41
19:A4:389:ARG:HG2	19:A4:747:ILE:HG21	2.02	0.41
19:A4:428:ILE:HD12	19:A4:444:ARG:HH21	1.85	0.41
20:A5:49:ASN:OD1	20:A5:49:ASN:N	2.49	0.41
20:A5:248:THR:OG1	20:A5:250:ASP:OD1	2.31	0.41
21:A8:563:LEU:H	21:A8:563:LEU:HG	1.51	0.41
21:A8:703:LEU:HA	21:A8:704:PRO:HD3	1.96	0.41
23:AE:32:SER:OG	23:AE:33:LEU:N	2.54	0.41
23:AE:33:LEU:HD11	23:AE:151:ILE:HG22	2.03	0.41
23:AE:69:PHE:HE2	23:AE:104:LEU:HD13	1.85	0.41
23:AE:572:ARG:NH2	23:AE:632:THR:O	2.40	0.41
23:AE:597:HIS:HB3	23:AE:615:ASN:HB3	2.03	0.41
25:AG:439:ASN:ND2	25:AG:496:THR:O	2.54	0.41
25:AG:514:TYR:HA	25:AG:515:PRO:HD3	1.94	0.41
26:B1:419:TYR:HB2	35:5E:482:LEU:CD1	2.50	0.41
28:B3:90:LEU:O	28:B3:92:THR:N	2.54	0.41
30:BE:870:GLN:HA	30:BE:873:LYS:HE3	2.03	0.41
37:5G:260:GLU:HG3	37:5G:276:GLN:HB3	2.03	0.41
42:RA:237:ARG:NE	42:RA:239:ASP:OD2	2.46	0.41
44:RG:40:ARG:O	44:RG:201:SER:HA	2.20	0.41
47:RL:185:ASN:OD1	47:RL:185:ASN:N	2.52	0.41
48:RN:766:ARG:NH2	48:RN:769:GLU:OE2	2.54	0.41
49:RO:226:ASP:OD1	49:RO:284:ARG:NE	2.54	0.41
52:RS:238:SER:O	52:RS:238:SER:OG	2.33	0.41
2:5A:18:G:H2'	2:5A:19:A:H8	1.85	0.41
3:SA:153:G:O6	3:SA:161:U:O4	2.39	0.41
3:SA:1538:U:H1'	3:SA:1570:A:H61	1.84	0.41
5:SG:79:ASN:N	5:SG:79:ASN:OD1	2.54	0.41
6:SH:185:GLN:O	6:SH:189:HIS:ND1	2.44	0.41
7:SJ:36:THR:O	7:SJ:96:LEU:N	2.52	0.41
7:SJ:49:ARG:HA	7:SJ:49:ARG:HD3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:3B:116:SER:OG	14:3B:120:GLU:OE1	2.28	0.41
15:3D:7:LEU:HD12	15:3D:99:ALA:HB3	2.02	0.41
15:3D:157:ALA:HB2	31:B6:292:TYR:CZ	2.56	0.41
16:3E:311:LYS:HB3	16:3E:311:LYS:HE2	1.84	0.41
17:3F:457:GLU:HG3	17:3F:461:LYS:HE2	2.02	0.41
18:3G:85:VAL:O	18:3G:89:ARG:HG2	2.21	0.41
19:A4:52:SER:HA	19:A4:104:TRP:CG	2.56	0.41
19:A4:249:ARG:NH2	19:A4:309:GLN:OE1	2.49	0.41
19:A4:513:LEU:HD12	19:A4:513:LEU:HA	1.89	0.41
19:A4:581:SER:HA	19:A4:594:PHE:O	2.21	0.41
21:A8:342:LEU:HA	21:A8:357:HIS:HA	2.02	0.41
21:A8:443:CYS:HA	25:AG:728:LEU:CD2	2.47	0.41
22:A9:475:THR:HA	22:A9:478:ASN:HD22	1.86	0.41
23:AE:214:THR:HG23	23:AE:260:ILE:HG13	2.03	0.41
23:AE:227:ASN:OD1	23:AE:227:ASN:N	2.53	0.41
24:AF:287:LEU:HD13	24:AF:287:LEU:HA	1.96	0.41
25:AG:591:GLU:O	25:AG:593:ASN:N	2.54	0.41
25:AG:666:ASN:OD1	25:AG:666:ASN:N	2.54	0.41
27:B2:17:ILE:CG2	27:B2:52:TRP:CH2	3.01	0.41
28:B3:567:VAL:HG22	28:B3:568:MET:HG2	2.02	0.41
29:B8:338:LYS:HE3	29:B8:338:LYS:HB2	1.89	0.41
30:BE:724:SER:O	30:BE:728:ARG:NH2	2.39	0.41
33:5C:117:LYS:HD2	33:5C:117:LYS:HA	1.85	0.41
39:5I:400:LEU:HD12	39:5I:400:LEU:HA	1.89	0.41
40:5J:119:ARG:HD3	45:RJ:1113:ILE:HG13	2.02	0.41
42:RA:139:LYS:HA	42:RA:139:LYS:HD2	1.89	0.41
44:RG:31:LEU:HD23	44:RG:31:LEU:HA	1.86	0.41
44:RG:116:THR:HG22	44:RG:118:ARG:H	1.86	0.41
44:RG:123:GLU:HB2	44:RG:161:LYS:HB2	2.03	0.41
44:RG:233:SER:OG	44:RG:234:ALA:N	2.54	0.41
44:RH:177:LYS:HG2	44:RH:203:CYS:HB3	2.03	0.41
45:RJ:43:MET:N	45:RJ:43:MET:SD	2.94	0.41
45:RJ:906:ASP:OD1	45:RJ:906:ASP:N	2.45	0.41
45:RJ:926:ILE:HG12	45:RJ:928:ILE:HG23	2.01	0.41
46:RK:117:LEU:HA	46:RK:166:VAL:O	2.21	0.41
50:RP:76:THR:O	50:RP:79:GLN:N	2.54	0.41
52:RS:288:ARG:O	52:RS:292:GLU:HG2	2.21	0.41
52:RS:407:GLU:HB2	52:RS:411:ARG:HD2	2.03	0.41
3:SA:27:U:H4'	45:RJ:45:ARG:HG3	2.02	0.41
3:SA:1492:A:N6	45:RJ:941:ILE:O	2.46	0.41
3:SA:1655:A:O2'	27:B2:395:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3E:201:ASP:HB3	16:3E:204:ALA:HB3	2.03	0.41
19:A4:425:ASP:OD2	19:A4:444:ARG:NH2	2.53	0.41
24:AF:136:ASP:OD1	24:AF:137:ASN:N	2.54	0.41
24:AF:492:ARG:HD3	24:AF:492:ARG:HA	1.80	0.41
26:B1:263:VAL:HG13	26:B1:277:VAL:HG13	2.03	0.41
27:B2:241:LYS:HB2	27:B2:241:LYS:HE3	1.89	0.41
27:B2:911:GLN:HA	27:B2:914:LEU:HG	2.02	0.41
28:B3:410:ASN:OD1	28:B3:435:ALA:N	2.52	0.41
30:BE:83:LEU:HA	30:BE:91:TYR:O	2.21	0.41
31:B6:26:LYS:HA	31:B6:29:VAL:HG12	2.03	0.41
31:B6:306:LYS:HE3	31:B6:306:LYS:HB2	1.77	0.41
35:5E:533:LYS:O	35:5E:537:SER:HB2	2.21	0.41
36:5F:60:LYS:HZ2	36:5F:63:LEU:HD22	1.86	0.41
39:5I:225:LEU:HA	39:5I:225:LEU:HD23	1.87	0.41
45:RJ:274:TYR:OH	45:RJ:306:ASP:OD1	2.29	0.41
48:RN:668:LEU:HD23	48:RN:671:TYR:HD2	1.86	0.41
50:RP:149:GLU:HA	50:RP:152:PHE:CD2	2.56	0.41
3:SA:304:U:H5''	9:SM:136:ARG:HH21	1.86	0.40
6:SH:38:GLY:N	6:SH:48:TYR:O	2.54	0.40
17:3F:212:LYS:HB2	17:3F:212:LYS:HE3	1.88	0.40
19:A4:250:THR:OG1	19:A4:251:ASP:N	2.53	0.40
22:A9:432:LYS:HA	22:A9:432:LYS:HD3	1.85	0.40
23:AE:688:PHE:HB3	23:AE:730:GLN:HE21	1.86	0.40
24:AF:183:LEU:HD12	24:AF:183:LEU:HA	1.85	0.40
24:AF:397:TRP:CZ3	24:AF:425:GLY:HA3	2.56	0.40
26:B1:519:LEU:HD13	26:B1:581:THR:HG22	2.03	0.40
28:B3:678:TRP:CE3	28:B3:697:VAL:HG23	2.56	0.40
28:B3:745:ASP:OD2	35:5E:508:ARG:CD	2.70	0.40
34:5D:70:ARG:HD3	34:5D:78:LEU:HD11	2.02	0.40
40:5J:77:LYS:HA	40:5J:77:LYS:HD2	1.84	0.40
44:RG:176:ARG:HA	44:RG:176:ARG:HD2	1.91	0.40
46:RK:184:ASP:OD1	46:RK:185:ARG:N	2.53	0.40
48:RN:504:ILE:HA	48:RN:507:LEU:HG	2.03	0.40
3:SA:1525:A:N3	3:SA:1589:C:O2'	2.53	0.40
3:SA:1672:G:H2'	3:SA:1673:G:C8	2.55	0.40
4:SF:97:GLU:HB3	4:SF:99:PHE:CE2	2.56	0.40
14:3B:248:ASP:OD1	14:3B:248:ASP:N	2.37	0.40
14:3C:202:ARG:HA	14:3C:202:ARG:HD2	1.96	0.40
16:3E:88:ILE:HA	16:3E:106:ASN:O	2.22	0.40
18:3G:41:THR:HG21	18:3G:66:HIS:CE1	2.55	0.40
18:3H:33:LEU:HD11	18:3H:100:ALA:HB1	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A4:141:SER:O	19:A4:141:SER:OG	2.34	0.40
23:AE:3:SER:OG	23:AE:4:LEU:N	2.55	0.40
23:AE:328:ASP:N	23:AE:328:ASP:OD1	2.49	0.40
24:AF:57:VAL:HG21	24:AF:327:LEU:HD11	2.04	0.40
24:AF:426:LYS:HB3	24:AF:429:VAL:HB	2.03	0.40
27:B2:639:VAL:HG22	27:B2:653:LEU:HB2	2.03	0.40
28:B3:25:VAL:HG22	28:B3:294:LEU:HD13	2.03	0.40
28:B3:313:LEU:O	28:B3:330:THR:OG1	2.33	0.40
30:BE:265:SER:O	30:BE:265:SER:OG	2.39	0.40
30:BE:290:ILE:HG23	30:BE:291:HIS:CD2	2.56	0.40
31:B6:304:LEU:O	31:B6:308:THR:HG23	2.21	0.40
33:5C:340:LEU:HD22	33:5C:403:VAL:HG11	2.03	0.40
35:5E:362:THR:HA	35:5E:365:LEU:HD23	2.03	0.40
35:5E:445:VAL:HG13	36:5F:81:LYS:HE2	2.03	0.40
40:5J:106:LEU:HD23	40:5J:106:LEU:HA	1.95	0.40
40:5J:195:GLN:O	40:5J:199:THR:HG22	2.22	0.40
49:RO:422:ILE:HD13	49:RO:422:ILE:HA	1.93	0.40
50:RP:100:GLU:OE2	50:RP:146:ASN:ND2	2.54	0.40
52:RS:245:VAL:O	52:RS:249:THR:HG23	2.22	0.40
3:SA:16:G:H4'	41:5K:159:GLY:HA2	2.03	0.40
3:SA:268:C:H2'	3:SA:269:G:C8	2.56	0.40
3:SA:298:C:H5''	4:SF:38:LEU:HG	2.02	0.40
4:SF:106:LYS:HE3	4:SF:106:LYS:HB3	1.88	0.40
8:SK:79:ARG:HE	8:SK:79:ARG:HB3	1.78	0.40
14:3C:165:ALA:HB3	14:3C:168:LYS:HD3	2.04	0.40
15:3D:182:ASP:OD1	15:3D:314:ARG:NH2	2.39	0.40
16:3E:248:THR:OG1	16:3E:251:ASP:OD1	2.29	0.40
16:3E:367:ALA:O	16:3E:371:LEU:HB3	2.22	0.40
17:3F:263:TRP:HA	17:3F:269:SER:O	2.22	0.40
17:3F:465:GLN:HG2	18:3H:6:PRO:HG3	2.03	0.40
19:A4:429:SER:OG	19:A4:430:THR:N	2.52	0.40
25:AG:29:THR:HB	25:AG:198:LEU:HD11	2.03	0.40
25:AG:560:ILE:HG22	25:AG:575:THR:HG22	2.03	0.40
27:B2:687:THR:OG1	27:B2:687:THR:O	2.38	0.40
28:B3:415:TRP:HA	28:B3:425:ASP:O	2.20	0.40
28:B3:690:HIS:CE1	35:5E:519:GLU:HA	2.57	0.40
29:B8:431:GLU:H	29:B8:431:GLU:HG2	1.71	0.40
31:B6:110:TRP:CD2	31:B6:136:LEU:HD13	2.56	0.40
33:5C:114:TYR:HA	33:5C:128:THR:O	2.22	0.40
42:RA:343:ILE:HG22	42:RA:346:LEU:H	1.87	0.40
45:RJ:74:VAL:HG11	45:RJ:82:LYS:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:RJ:563:CYS:SG	46:RK:327:ARG:NH2	2.95	0.40
47:RL:60:LYS:HB3	47:RL:108:TYR:CD2	2.56	0.40
48:RN:424:LYS:O	48:RN:428:VAL:HG23	2.20	0.40
52:RS:446:GLN:HG2	52:RS:447:ARG:HE	1.86	0.40
1:3A:253:G:OP2	18:3H:95:ARG:NH1	2.54	0.40
3:SA:259:U:O2'	3:SA:261:U:OP2	2.32	0.40
3:SA:514:G:H2'	3:SA:515:A:H8	1.87	0.40
3:SA:1463:C:H2'	3:SA:1464:G:O4'	2.22	0.40
3:SA:1464:G:H2'	3:SA:1465:C:C6	2.57	0.40
3:SA:1480:G:H2'	3:SA:1481:C:O4'	2.22	0.40
14:3B:227:PRO:HG2	14:3B:255:LEU:HB3	2.02	0.40
15:3D:86:LEU:HD21	15:3D:98:LEU:HD13	2.03	0.40
15:3D:315:LEU:HD12	15:3D:315:LEU:HA	1.90	0.40
16:3E:215:ARG:NH1	16:3E:244:GLY:O	2.54	0.40
16:3E:299:LEU:HD22	16:3E:320:LEU:HD23	2.03	0.40
16:3E:306:LEU:HG	16:3E:375:ALA:HB2	2.04	0.40
16:3E:359:ILE:HD13	16:3E:398:LEU:HD13	2.03	0.40
19:A4:442:VAL:O	19:A4:448:THR:OG1	2.26	0.40
24:AF:371:GLU:HG3	29:B8:287:SER:OG	2.21	0.40
25:AG:409:LYS:HG2	25:AG:489:ASN:HA	2.03	0.40
26:B1:382:THR:H	35:5E:481:PRO:HB3	1.87	0.40
26:B1:423:ARG:HD3	26:B1:423:ARG:HA	1.88	0.40
28:B3:189:HIS:NE2	28:B3:215:GLY:HA3	2.37	0.40
35:5E:448:LEU:HA	35:5E:451:LEU:HD23	2.02	0.40
36:5F:41:ARG:HA	36:5F:41:ARG:HD2	1.89	0.40
36:5F:102:THR:HG22	36:5F:104:SER:H	1.87	0.40
48:RN:572:LEU:HB3	48:RN:667:LEU:HD13	2.04	0.40
48:RN:710:ILE:HD13	48:RN:710:ILE:HA	1.91	0.40
49:RO:205:ASP:HA	49:RO:206:PRO:HD3	1.89	0.40
49:RO:326:LEU:HA	49:RO:326:LEU:HD12	1.90	0.40
49:RO:384:ALA:HA	49:RO:387:THR:HG22	2.03	0.40
1:3A:59:G:OP1	26:B1:573:ASN:ND2	2.43	0.40
3:SA:56:U:O2	3:SA:91:G:N2	2.54	0.40
7:SJ:191:PHE:HA	7:SJ:194:ARG:HE	1.85	0.40
10:SR:47:LYS:HD2	10:SR:47:LYS:HA	1.93	0.40
12:SZ:13:ILE:HD11	12:SZ:22:GLN:HE21	1.85	0.40
15:3D:59:ALA:HB1	31:B6:292:TYR:HE1	1.87	0.40
17:3F:68:LYS:HE3	17:3F:68:LYS:HB2	1.93	0.40
20:A5:444:ALA:HB2	20:A5:452:LEU:HD12	2.03	0.40
23:AE:677:SER:HA	23:AE:678:PRO:HD3	1.98	0.40
24:AF:178:PRO:HD2	24:AF:223:PRO:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:AG:865:LYS:HE2	25:AG:865:LYS:HB3	1.81	0.40
26:B1:103:LYS:HB3	26:B1:103:LYS:HE3	1.92	0.40
26:B1:298:LEU:HD12	35:5E:474:ILE:HG22	2.04	0.40
27:B2:85:LEU:HD12	27:B2:94:LEU:HD11	2.04	0.40
28:B3:51:LYS:H	28:B3:51:LYS:HG2	1.66	0.40
28:B3:698:LEU:HD23	28:B3:698:LEU:HA	1.92	0.40
33:5C:258:LEU:O	33:5C:267:LEU:N	2.54	0.40
33:5C:307:LYS:HA	33:5C:307:LYS:HD3	1.89	0.40
35:5E:384:ARG:HD2	37:5G:83:ILE:CG1	2.51	0.40
40:5J:121:LEU:HD22	40:5J:141:TRP:HH2	1.87	0.40
45:RJ:286:THR:H	45:RJ:298:VAL:HG12	1.86	0.40
52:RS:258:VAL:O	52:RS:262:ALA:CB	2.69	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	
4	SF	227/261 (87%)	197 (87%)	29 (13%)	1 (0%)	34	72
5	SG	211/225 (94%)	195 (92%)	16 (8%)	0	100	100
6	SH	161/236 (68%)	143 (89%)	18 (11%)	0	100	100
7	SJ	162/200 (81%)	140 (86%)	22 (14%)	0	100	100
8	SK	169/197 (86%)	163 (96%)	6 (4%)	0	100	100
9	SM	119/156 (76%)	103 (87%)	16 (13%)	0	100	100
10	SR	123/143 (86%)	112 (91%)	11 (9%)	0	100	100
11	SY	101/145 (70%)	90 (89%)	11 (11%)	0	100	100
12	SZ	100/135 (74%)	87 (87%)	12 (12%)	1 (1%)	15	53
13	Sd	61/67 (91%)	57 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	3B	236/327 (72%)	222 (94%)	14 (6%)	0	100	100
14	3C	221/327 (68%)	207 (94%)	14 (6%)	0	100	100
15	3D	359/504 (71%)	346 (96%)	13 (4%)	0	100	100
16	3E	427/511 (84%)	387 (91%)	40 (9%)	0	100	100
17	3F	446/573 (78%)	403 (90%)	42 (9%)	1 (0%)	47	81
18	3G	119/126 (94%)	107 (90%)	11 (9%)	1 (1%)	19	59
18	3H	119/126 (94%)	111 (93%)	8 (7%)	0	100	100
19	A4	648/776 (84%)	590 (91%)	58 (9%)	0	100	100
20	A5	504/643 (78%)	465 (92%)	39 (8%)	0	100	100
21	A8	516/713 (72%)	397 (77%)	107 (21%)	12 (2%)	6	36
22	A9	126/575 (22%)	115 (91%)	11 (9%)	0	100	100
23	AE	1496/1769 (85%)	1367 (91%)	129 (9%)	0	100	100
24	AF	489/513 (95%)	442 (90%)	47 (10%)	0	100	100
25	AG	812/896 (91%)	731 (90%)	80 (10%)	1 (0%)	51	85
26	B1	787/923 (85%)	732 (93%)	55 (7%)	0	100	100
27	B2	813/943 (86%)	724 (89%)	87 (11%)	2 (0%)	47	81
28	B3	733/817 (90%)	606 (83%)	125 (17%)	2 (0%)	41	76
29	B8	469/594 (79%)	439 (94%)	30 (6%)	0	100	100
30	BE	814/939 (87%)	765 (94%)	49 (6%)	0	100	100
31	B6	368/440 (84%)	341 (93%)	27 (7%)	0	100	100
32	5B	58/214 (27%)	55 (95%)	3 (5%)	0	100	100
33	5C	407/554 (74%)	377 (93%)	30 (7%)	0	100	100
34	5D	165/250 (66%)	145 (88%)	20 (12%)	0	100	100
35	5E	187/593 (32%)	175 (94%)	10 (5%)	2 (1%)	14	51
36	5F	180/183 (98%)	164 (91%)	16 (9%)	0	100	100
37	5G	217/290 (75%)	203 (94%)	14 (6%)	0	100	100
38	5H	72/610 (12%)	65 (90%)	7 (10%)	0	100	100
39	5I	457/489 (94%)	421 (92%)	36 (8%)	0	100	100
40	5J	147/217 (68%)	136 (92%)	11 (8%)	0	100	100
41	5K	171/189 (90%)	166 (97%)	5 (3%)	0	100	100
42	RA	332/707 (47%)	276 (83%)	56 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	RB	132/357 (37%)	117 (89%)	14 (11%)	1 (1%)	19	59
44	RG	212/252 (84%)	182 (86%)	30 (14%)	0	100	100
44	RH	226/252 (90%)	219 (97%)	7 (3%)	0	100	100
45	RJ	784/1183 (66%)	721 (92%)	62 (8%)	1 (0%)	51	85
46	RK	358/367 (98%)	341 (95%)	17 (5%)	0	100	100
47	RL	781/1056 (74%)	664 (85%)	115 (15%)	2 (0%)	41	76
47	RM	738/1056 (70%)	625 (85%)	109 (15%)	4 (0%)	29	68
48	RN	593/810 (73%)	545 (92%)	47 (8%)	1 (0%)	47	81
49	RO	523/552 (95%)	455 (87%)	68 (13%)	0	100	100
50	RP	1516/2493 (61%)	1336 (88%)	180 (12%)	0	100	100
51	RQ	132/899 (15%)	126 (96%)	6 (4%)	0	100	100
52	RS	247/483 (51%)	225 (91%)	22 (9%)	0	100	100
53	RY	35/534 (7%)	29 (83%)	6 (17%)	0	100	100
All	All	20606/29390 (70%)	18552 (90%)	2022 (10%)	32 (0%)	50	81

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	A8	258	PRO
21	A8	309	PRO
21	A8	325	PRO
21	A8	390	PRO
21	A8	392	PRO
21	A8	446	VAL
21	A8	472	ILE
47	RL	744	PRO
47	RM	744	PRO
47	RM	905	PRO
12	SZ	51	GLU
45	RJ	82	LYS
21	A8	235	PRO
25	AG	434	GLN
27	B2	132	THR
28	B3	91	LYS
47	RM	904	LEU
48	RN	285	PRO
17	3F	552	TRP

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Mol	Chain	Res	Type
21	A8	369	ILE
35	5E	476	MET
4	SF	194	THR
27	B2	118	ASN
35	5E	481	PRO
43	RB	274	ILE
47	RL	743	VAL
47	RM	743	VAL
21	A8	439	LYS
28	B3	71	PRO
18	3G	10	PRO
21	A8	306	ILE
21	A8	339	ILE

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	
4	SF	196/222 (88%)	190 (97%)	6 (3%)	40	62
5	SG	180/191 (94%)	180 (100%)	0	100	100
6	SH	139/201 (69%)	137 (99%)	2 (1%)	67	81
7	SJ	136/161 (84%)	134 (98%)	2 (2%)	65	80
8	SK	147/166 (89%)	146 (99%)	1 (1%)	84	90
9	SM	110/137 (80%)	108 (98%)	2 (2%)	59	77
10	SR	105/119 (88%)	105 (100%)	0	100	100
11	SY	85/120 (71%)	84 (99%)	1 (1%)	71	84
12	SZ	85/113 (75%)	85 (100%)	0	100	100
13	Sd	56/60 (93%)	56 (100%)	0	100	100
14	3B	201/240 (84%)	201 (100%)	0	100	100
14	3C	190/240 (79%)	187 (98%)	3 (2%)	62	79
15	3D	296/435 (68%)	293 (99%)	3 (1%)	76	86
16	3E	262/433 (60%)	261 (100%)	1 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	3F	396/503 (79%)	394 (100%)	2 (0%)	88	93
18	3G	100/104 (96%)	100 (100%)	0	100	100
18	3H	100/104 (96%)	100 (100%)	0	100	100
19	A4	591/713 (83%)	584 (99%)	7 (1%)	71	84
20	A5	433/574 (75%)	432 (100%)	1 (0%)	93	96
21	A8	174/657 (26%)	164 (94%)	10 (6%)	20	47
22	A9	89/533 (17%)	88 (99%)	1 (1%)	73	85
23	AE	708/1633 (43%)	705 (100%)	3 (0%)	91	94
24	AF	437/454 (96%)	433 (99%)	4 (1%)	78	87
25	AG	750/826 (91%)	740 (99%)	10 (1%)	69	82
26	B1	696/812 (86%)	691 (99%)	5 (1%)	84	90
27	B2	712/832 (86%)	707 (99%)	5 (1%)	84	90
28	B3	665/719 (92%)	655 (98%)	10 (2%)	65	80
29	B8	421/529 (80%)	420 (100%)	1 (0%)	93	96
30	BE	718/819 (88%)	714 (99%)	4 (1%)	86	92
31	B6	251/414 (61%)	247 (98%)	4 (2%)	62	79
32	5B	57/196 (29%)	55 (96%)	2 (4%)	36	60
33	5C	349/480 (73%)	347 (99%)	2 (1%)	86	92
34	5D	156/234 (67%)	154 (99%)	2 (1%)	69	82
35	5E	175/535 (33%)	162 (93%)	13 (7%)	13	40
36	5F	171/172 (99%)	169 (99%)	2 (1%)	71	84
37	5G	194/258 (75%)	190 (98%)	4 (2%)	53	72
38	5H	63/538 (12%)	63 (100%)	0	100	100
39	5I	416/443 (94%)	414 (100%)	2 (0%)	88	93
40	5J	140/200 (70%)	140 (100%)	0	100	100
41	5K	157/169 (93%)	157 (100%)	0	100	100
42	RA	303/636 (48%)	300 (99%)	3 (1%)	76	86
43	RB	117/315 (37%)	114 (97%)	3 (3%)	46	67
44	RG	195/222 (88%)	193 (99%)	2 (1%)	76	86
44	RH	206/222 (93%)	204 (99%)	2 (1%)	76	86
45	RJ	683/1039 (66%)	676 (99%)	7 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	RK	307/312 (98%)	303 (99%)	4 (1%)	69	82
47	RL	164/934 (18%)	162 (99%)	2 (1%)	71	84
48	RN	422/732 (58%)	421 (100%)	1 (0%)	93	96
49	RO	329/506 (65%)	328 (100%)	1 (0%)	92	95
50	RP	224/2307 (10%)	222 (99%)	2 (1%)	78	87
51	RQ	81/808 (10%)	80 (99%)	1 (1%)	71	84
52	RS	225/424 (53%)	225 (100%)	0	100	100
53	RY	31/482 (6%)	30 (97%)	1 (3%)	39	61
All	All	14594/25228 (58%)	14450 (99%)	144 (1%)	77	86

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	SF	108	ARG
4	SF	143	ASP
4	SF	206	ASP
4	SF	207	LEU
4	SF	211	LYS
4	SF	240	LYS
6	SH	71	THR
6	SH	92	ARG
7	SJ	165	LEU
7	SJ	195	ARG
8	SK	57	ARG
9	SM	43	LYS
9	SM	136	ARG
11	SY	97	ASP
14	3C	237	VAL
14	3C	262	LYS
14	3C	306	LEU
15	3D	103	LYS
15	3D	129	ARG
15	3D	285	ARG
16	3E	265	PHE
17	3F	370	ARG
17	3F	506	ARG
19	A4	190	VAL
19	A4	282	ASP
19	A4	423	LYS

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Mol	Chain	Res	Type
19	A4	436	ASP
19	A4	648	PHE
19	A4	739	LYS
19	A4	776	PHE
20	A5	434	THR
21	A8	505	LYS
21	A8	526	LEU
21	A8	536	ARG
21	A8	549	ARG
21	A8	563	LEU
21	A8	576	ARG
21	A8	633	GLN
21	A8	634	LEU
21	A8	636	GLN
21	A8	671	ARG
22	A9	483	LYS
23	AE	617	LYS
23	AE	645	ARG
23	AE	699	ARG
24	AF	199	ARG
24	AF	261	VAL
24	AF	432	TYR
24	AF	508	LEU
25	AG	141	LEU
25	AG	259	VAL
25	AG	336	ARG
25	AG	368	ASP
25	AG	421	LYS
25	AG	434	GLN
25	AG	435	ASP
25	AG	436	PHE
25	AG	615	TRP
25	AG	716	ARG
26	B1	164	THR
26	B1	249	ARG
26	B1	337	TYR
26	B1	418	ARG
26	B1	519	LEU
27	B2	47	GLU
27	B2	75	ARG
27	B2	144	ASN
27	B2	576	VAL

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Mol	Chain	Res	Type
27	B2	588	ILE
28	B3	30	LYS
28	B3	67	LEU
28	B3	95	VAL
28	B3	212	LEU
28	B3	222	LEU
28	B3	358	ASN
28	B3	533	LYS
28	B3	534	ARG
28	B3	554	ASP
28	B3	570	THR
29	B8	22	LEU
30	BE	309	ILE
30	BE	570	ILE
30	BE	728	ARG
30	BE	743	ARG
31	B6	4	THR
31	B6	67	ARG
31	B6	106	ASP
31	B6	133	TYR
32	5B	158	LYS
32	5B	211	LEU
33	5C	153	THR
33	5C	392	VAL
34	5D	18	GLN
34	5D	161	ARG
35	5E	302	LYS
35	5E	345	LEU
35	5E	428	GLU
35	5E	448	LEU
35	5E	451	LEU
35	5E	494	GLU
35	5E	515	MET
35	5E	516	SER
35	5E	517	LYS
35	5E	520	LEU
35	5E	522	ARG
35	5E	537	SER
35	5E	538	LYS
36	5F	48	ASN
36	5F	75	GLU
37	5G	211	ASN

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Mol	Chain	Res	Type
37	5G	216	LYS
37	5G	257	ARG
37	5G	282	ARG
39	5I	250	ARG
39	5I	417	ARG
42	RA	76	THR
42	RA	210	ARG
42	RA	227	ARG
43	RB	331	LYS
43	RB	338	THR
43	RB	341	ARG
44	RG	32	THR
44	RG	100	LEU
44	RH	82	ARG
44	RH	197	ASP
45	RJ	214	ARG
45	RJ	566	ARG
45	RJ	869	THR
45	RJ	973	ARG
45	RJ	976	ILE
45	RJ	1128	LYS
45	RJ	1141	LYS
46	RK	90	CYS
46	RK	214	LYS
46	RK	335	THR
46	RK	340	LYS
47	RL	9	ARG
47	RL	83	ARG
48	RN	766	ARG
49	RO	493	TYR
50	RP	201	ARG
50	RP	1749	LYS
51	RQ	330	THR
53	RY	487	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (248) such sidechains are listed below:

Mol	Chain	Res	Type
5	SG	63	GLN
5	SG	169	ASN
5	SG	186	ASN
6	SH	140	ASN

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Mol	Chain	Res	Type
6	SH	201	GLN
7	SJ	32	GLN
7	SJ	84	HIS
7	SJ	103	GLN
7	SJ	159	GLN
9	SM	81	HIS
10	SR	32	ASN
10	SR	74	HIS
14	3B	91	HIS
14	3B	183	HIS
14	3B	258	HIS
15	3D	39	ASN
15	3D	85	ASN
15	3D	168	GLN
15	3D	213	ASN
16	3E	191	HIS
16	3E	256	ASN
16	3E	286	ASN
16	3E	289	GLN
16	3E	400	GLN
17	3F	155	ASN
17	3F	235	HIS
17	3F	525	GLN
17	3F	561	ASN
18	3G	19	GLN
18	3G	29	ASN
18	3G	38	ASN
18	3H	5	ASN
18	3H	18	GLN
18	3H	45	ASN
19	A4	53	HIS
19	A4	179	HIS
19	A4	279	HIS
19	A4	292	ASN
19	A4	317	ASN
19	A4	426	GLN
19	A4	438	GLN
19	A4	452	HIS
19	A4	529	ASN
19	A4	589	ASN
20	A5	32	GLN
20	A5	67	ASN

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Mol	Chain	Res	Type
20	A5	115	ASN
20	A5	293	ASN
20	A5	302	ASN
20	A5	316	ASN
20	A5	324	ASN
20	A5	333	ASN
20	A5	443	GLN
21	A8	588	GLN
22	A9	478	ASN
22	A9	509	GLN
23	AE	14	ASN
23	AE	141	ASN
23	AE	166	ASN
23	AE	219	ASN
23	AE	224	ASN
23	AE	258	HIS
23	AE	477	ASN
23	AE	480	ASN
23	AE	545	ASN
23	AE	673	ASN
23	AE	730	GLN
24	AF	48	ASN
24	AF	64	GLN
24	AF	125	HIS
24	AF	133	HIS
24	AF	156	ASN
24	AF	289	ASN
24	AF	481	GLN
25	AG	50	ASN
25	AG	105	HIS
25	AG	190	GLN
25	AG	266	ASN
25	AG	269	GLN
25	AG	325	GLN
25	AG	332	GLN
25	AG	370	GLN
25	AG	375	ASN
25	AG	393	ASN
25	AG	407	ASN
25	AG	410	ASN
25	AG	453	HIS
25	AG	467	GLN

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Mol	Chain	Res	Type
25	AG	489	ASN
25	AG	568	ASN
25	AG	579	ASN
25	AG	605	ASN
25	AG	669	ASN
25	AG	706	HIS
25	AG	881	ASN
26	B1	92	HIS
26	B1	142	HIS
26	B1	190	HIS
26	B1	201	HIS
26	B1	297	GLN
26	B1	303	ASN
26	B1	349	ASN
26	B1	386	HIS
26	B1	452	ASN
26	B1	456	HIS
26	B1	483	GLN
26	B1	549	GLN
26	B1	552	ASN
26	B1	795	ASN
26	B1	813	HIS
26	B1	837	ASN
26	B1	842	ASN
27	B2	172	GLN
27	B2	390	GLN
27	B2	455	GLN
27	B2	524	HIS
27	B2	596	ASN
27	B2	628	HIS
27	B2	629	ASN
27	B2	657	GLN
27	B2	770	ASN
27	B2	791	ASN
27	B2	856	ASN
27	B2	879	GLN
28	B3	241	GLN
28	B3	337	HIS
28	B3	387	HIS
28	B3	519	ASN
28	B3	667	GLN
28	B3	749	ASN

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Mol	Chain	Res	Type
28	B3	753	HIS
28	B3	767	HIS
28	B3	792	HIS
29	B8	162	ASN
29	B8	167	GLN
29	B8	224	ASN
29	B8	282	ASN
29	B8	311	ASN
29	B8	352	GLN
29	B8	472	GLN
29	B8	492	ASN
29	B8	528	GLN
29	B8	592	ASN
30	BE	163	GLN
30	BE	289	ASN
30	BE	481	ASN
30	BE	501	HIS
30	BE	514	ASN
30	BE	627	ASN
30	BE	708	ASN
30	BE	877	ASN
30	BE	911	ASN
30	BE	916	HIS
31	B6	90	GLN
31	B6	115	ASN
31	B6	166	ASN
31	B6	287	ASN
32	5B	207	ASN
33	5C	101	ASN
33	5C	124	HIS
33	5C	133	HIS
33	5C	151	ASN
33	5C	164	GLN
33	5C	170	GLN
33	5C	371	HIS
33	5C	394	HIS
34	5D	42	HIS
34	5D	68	HIS
34	5D	144	ASN
34	5D	153	ASN
35	5E	303	GLN
35	5E	434	HIS

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Mol	Chain	Res	Type
35	5E	486	ASN
35	5E	493	GLN
36	5F	7	HIS
36	5F	48	ASN
36	5F	144	ASN
36	5F	153	ASN
36	5F	163	ASN
37	5G	118	ASN
37	5G	145	HIS
37	5G	211	ASN
37	5G	235	GLN
38	5H	560	ASN
39	5I	20	GLN
39	5I	46	ASN
39	5I	109	HIS
39	5I	242	ASN
39	5I	260	GLN
39	5I	336	HIS
39	5I	371	ASN
39	5I	406	HIS
39	5I	460	GLN
40	5J	135	HIS
40	5J	184	ASN
41	5K	29	GLN
41	5K	43	ASN
42	RA	82	HIS
42	RA	96	HIS
42	RA	119	ASN
42	RA	147	ASN
42	RA	230	GLN
42	RA	268	GLN
42	RA	282	ASN
42	RA	339	HIS
43	RB	314	ASN
43	RB	318	ASN
44	RG	105	ASN
44	RG	125	ASN
44	RH	69	ASN
44	RH	125	ASN
44	RH	250	ASN
45	RJ	126	ASN
45	RJ	157	ASN

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Mol	Chain	Res	Type
45	RJ	276	HIS
45	RJ	289	HIS
45	RJ	778	GLN
45	RJ	1082	GLN
46	RK	16	ASN
46	RK	334	ASN
47	RL	16	ASN
47	RL	75	ASN
47	RL	133	ASN
48	RN	8	ASN
48	RN	56	ASN
48	RN	89	GLN
48	RN	482	GLN
48	RN	703	GLN
48	RN	771	ASN
48	RN	797	ASN
49	RO	192	GLN
49	RO	266	ASN
49	RO	268	GLN
49	RO	273	GLN
49	RO	304	ASN
49	RO	306	GLN
49	RO	343	GLN
49	RO	434	ASN
49	RO	472	HIS
49	RO	474	HIS
50	RP	58	ASN
50	RP	1686	GLN
50	RP	1702	HIS
50	RP	1707	HIS
51	RQ	344	GLN
51	RQ	839	ASN
51	RQ	867	GLN
51	RQ	876	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3A	169/333 (50%)	55 (32%)	8 (4%)
2	5A	164/700 (23%)	51 (31%)	4 (2%)
3	SA	935/1808 (51%)	373 (39%)	16 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	1268/2841 (44%)	479 (37%)	28 (2%)

All (479) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3A	2	U
1	3A	14	A
1	3A	15	U
1	3A	24	U
1	3A	25	U
1	3A	27	U
1	3A	28	A
1	3A	30	A
1	3A	33	A
1	3A	35	U
1	3A	38	U
1	3A	56	A
1	3A	60	A
1	3A	61	G
1	3A	87	G
1	3A	88	U
1	3A	89	C
1	3A	90	C
1	3A	91	C
1	3A	97	C
1	3A	98	U
1	3A	99	U
1	3A	101	G
1	3A	103	A
1	3A	111	G
1	3A	115	G
1	3A	198	U
1	3A	199	G
1	3A	201	C
1	3A	204	U
1	3A	205	G
1	3A	206	C
1	3A	246	A
1	3A	248	G
1	3A	249	G
1	3A	252	C
1	3A	264	C

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Mol	Chain	Res	Type
1	3A	267	A
1	3A	305	G
1	3A	310	G
1	3A	311	G
1	3A	313	A
1	3A	314	C
1	3A	317	A
1	3A	318	U
1	3A	319	G
1	3A	320	G
1	3A	321	C
1	3A	322	A
1	3A	323	G
1	3A	324	U
1	3A	325	C
1	3A	328	A
1	3A	329	C
1	3A	332	G
2	5A	5	G
2	5A	6	A
2	5A	7	A
2	5A	8	A
2	5A	11	A
2	5A	13	U
2	5A	14	U
2	5A	15	G
2	5A	63	G
2	5A	64	U
2	5A	70	A
2	5A	83	U
2	5A	86	C
2	5A	87	C
2	5A	90	G
2	5A	279	A
2	5A	280	A
2	5A	281	G
2	5A	292	A
2	5A	294	U
2	5A	304	U
2	5A	305	A
2	5A	309	A
2	5A	310	U

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Mol	Chain	Res	Type
2	5A	311	C
2	5A	312	U
2	5A	313	A
2	5A	468	A
2	5A	472	A
2	5A	474	A
2	5A	481	U
2	5A	482	A
2	5A	485	G
2	5A	487	A
2	5A	488	U
2	5A	490	G
2	5A	491	U
2	5A	493	A
2	5A	536	A
2	5A	537	G
2	5A	539	A
2	5A	540	U
2	5A	541	U
2	5A	542	U
2	5A	548	A
2	5A	549	G
2	5A	583	U
2	5A	586	A
2	5A	587	G
2	5A	589	U
2	5A	591	U
3	SA	-6	A
3	SA	-5	G
3	SA	-4	A
3	SA	-1	G
3	SA	0	U
3	SA	1	U
3	SA	2	A
3	SA	17	C
3	SA	18	C
3	SA	19	A
3	SA	21	U
3	SA	23	G
3	SA	25	C
3	SA	26	A
3	SA	29	U

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Mol	Chain	Res	Type
3	SA	35	U
3	SA	36	C
3	SA	37	U
3	SA	50	C
3	SA	51	A
3	SA	52	U
3	SA	53	G
3	SA	55	A
3	SA	56	U
3	SA	57	G
3	SA	60	U
3	SA	61	A
3	SA	63	G
3	SA	65	A
3	SA	66	U
3	SA	67	A
3	SA	68	A
3	SA	69	G
3	SA	72	A
3	SA	73	U
3	SA	74	U
3	SA	75	U
3	SA	77	U
3	SA	81	G
3	SA	85	A
3	SA	92	A
3	SA	96	G
3	SA	97	C
3	SA	100	A
3	SA	102	U
3	SA	103	A
3	SA	104	A
3	SA	105	A
3	SA	106	U
3	SA	114	C
3	SA	115	G
3	SA	116	U
3	SA	119	A
3	SA	127	G
3	SA	128	U
3	SA	129	U
3	SA	130	C

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Mol	Chain	Res	Type
3	SA	131	C
3	SA	141	U
3	SA	145	A
3	SA	146	U
3	SA	147	A
3	SA	149	C
3	SA	153	G
3	SA	159	U
3	SA	160	C
3	SA	161	U
3	SA	168	A
3	SA	174	U
3	SA	175	G
3	SA	176	C
3	SA	177	U
3	SA	182	A
3	SA	183	U
3	SA	184	C
3	SA	187	G
3	SA	188	A
3	SA	190	C
3	SA	191	C
3	SA	192	U
3	SA	193	U
3	SA	194	U
3	SA	195	G
3	SA	197	A
3	SA	202	A
3	SA	203	U
3	SA	204	G
3	SA	206	A
3	SA	210	A
3	SA	211	U
3	SA	214	G
3	SA	226	A
3	SA	228	G
3	SA	230	C
3	SA	233	C
3	SA	234	G
3	SA	236	A
3	SA	237	C
3	SA	238	U

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Mol	Chain	Res	Type
3	SA	239	C
3	SA	240	U
3	SA	241	U
3	SA	242	U
3	SA	243	G
3	SA	254	A
3	SA	256	A
3	SA	258	C
3	SA	261	U
3	SA	262	U
3	SA	265	A
3	SA	266	A
3	SA	267	U
3	SA	272	U
3	SA	273	G
3	SA	275	C
3	SA	276	C
3	SA	277	U
3	SA	278	U
3	SA	279	G
3	SA	280	U
3	SA	281	G
3	SA	283	U
3	SA	290	G
3	SA	308	C
3	SA	309	C
3	SA	311	U
3	SA	312	A
3	SA	316	A
3	SA	319	U
3	SA	320	U
3	SA	321	C
3	SA	324	U
3	SA	325	G
3	SA	333	A
3	SA	334	G
3	SA	337	G
3	SA	338	C
3	SA	350	U
3	SA	352	A
3	SA	355	G
3	SA	357	G

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Mol	Chain	Res	Type
3	SA	359	A
3	SA	360	A
3	SA	361	C
3	SA	362	G
3	SA	365	G
3	SA	366	A
3	SA	369	A
3	SA	371	G
3	SA	373	G
3	SA	374	U
3	SA	375	U
3	SA	377	G
3	SA	379	U
3	SA	382	C
3	SA	383	G
3	SA	386	G
3	SA	387	A
3	SA	390	G
3	SA	400	A
3	SA	401	A
3	SA	402	C
3	SA	403	G
3	SA	411	C
3	SA	416	A
3	SA	417	A
3	SA	418	G
3	SA	419	G
3	SA	421	A
3	SA	422	G
3	SA	423	G
3	SA	424	C
3	SA	425	A
3	SA	426	G
3	SA	429	G
3	SA	436	A
3	SA	437	A
3	SA	439	U
3	SA	440	U
3	SA	441	A
3	SA	444	C
3	SA	445	A
3	SA	448	C

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Mol	Chain	Res	Type
3	SA	454	U
3	SA	455	C
3	SA	456	A
3	SA	457	G
3	SA	468	A
3	SA	469	C
3	SA	470	A
3	SA	471	A
3	SA	473	A
3	SA	477	A
3	SA	480	G
3	SA	486	G
3	SA	487	G
3	SA	496	G
3	SA	501	U
3	SA	502	U
3	SA	505	A
3	SA	506	A
3	SA	514	G
3	SA	520	A
3	SA	534	A
3	SA	538	A
3	SA	539	G
3	SA	541	A
3	SA	542	A
3	SA	543	C
3	SA	545	A
3	SA	557	G
3	SA	558	U
3	SA	563	U
3	SA	564	G
3	SA	565	C
3	SA	570	A
3	SA	572	C
3	SA	574	G
3	SA	575	C
3	SA	578	U
3	SA	579	A
3	SA	580	A
3	SA	583	C
3	SA	584	C
3	SA	585	A

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Mol	Chain	Res	Type
3	SA	586	G
3	SA	587	C
3	SA	594	A
3	SA	595	G
3	SA	602	U
3	SA	603	U
3	SA	604	A
3	SA	606	A
3	SA	608	U
3	SA	609	U
3	SA	610	G
3	SA	611	U
3	SA	612	U
3	SA	613	G
3	SA	614	C
3	SA	615	A
3	SA	616	G
3	SA	1106	U
3	SA	1107	G
3	SA	1108	G
3	SA	1109	G
3	SA	1110	G
3	SA	1111	G
3	SA	1114	G
3	SA	1118	G
3	SA	1119	G
3	SA	1122	G
3	SA	1125	A
3	SA	1126	G
3	SA	1127	G
3	SA	1128	C
3	SA	1129	U
3	SA	1131	A
3	SA	1132	A
3	SA	1145	U
3	SA	1146	G
3	SA	1158	C
3	SA	1164	G
3	SA	1178	G
3	SA	1191	U
3	SA	1192	C
3	SA	1193	A

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Mol	Chain	Res	Type
3	SA	1195	C
3	SA	1196	A
3	SA	1197	C
3	SA	1198	G
3	SA	1199	G
3	SA	1200	G
3	SA	1201	G
3	SA	1202	A
3	SA	1205	C
3	SA	1206	U
3	SA	1208	A
3	SA	1210	C
3	SA	1213	G
3	SA	1217	A
3	SA	1218	G
3	SA	1219	A
3	SA	1220	C
3	SA	1223	A
3	SA	1227	A
3	SA	1228	G
3	SA	1229	G
3	SA	1230	A
3	SA	1232	U
3	SA	1233	G
3	SA	1235	C
3	SA	1236	A
3	SA	1252	C
3	SA	1253	U
3	SA	1254	U
3	SA	1255	G
3	SA	1258	U
3	SA	1263	G
3	SA	1266	U
3	SA	1268	G
3	SA	1271	G
3	SA	1272	U
3	SA	1273	G
3	SA	1275	A
3	SA	1276	U
3	SA	1436	A
3	SA	1440	C
3	SA	1441	C

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Mol	Chain	Res	Type
3	SA	1442	U
3	SA	1443	U
3	SA	1449	U
3	SA	1450	U
3	SA	1453	G
3	SA	1457	C
3	SA	1461	C
3	SA	1469	A
3	SA	1472	C
3	SA	1473	U
3	SA	1474	G
3	SA	1475	A
3	SA	1476	C
3	SA	1482	C
3	SA	1488	G
3	SA	1492	A
3	SA	1522	U
3	SA	1523	G
3	SA	1524	A
3	SA	1527	C
3	SA	1533	C
3	SA	1535	U
3	SA	1536	G
3	SA	1537	C
3	SA	1539	G
3	SA	1569	A
3	SA	1570	A
3	SA	1573	A
3	SA	1582	U
3	SA	1584	G
3	SA	1590	G
3	SA	1594	G
3	SA	1595	U
3	SA	1596	C
3	SA	1601	G
3	SA	1602	C
3	SA	1607	G
3	SA	1614	A
3	SA	1618	C
3	SA	1628	U
3	SA	1630	U
3	SA	1633	A

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Mol	Chain	Res	Type
3	SA	1651	A
3	SA	1655	A
3	SA	1657	U
3	SA	1658	G
3	SA	1659	A
3	SA	1661	U
3	SA	1665	U
3	SA	1670	G
3	SA	1728	A
3	SA	1731	A
3	SA	1732	A
3	SA	1736	G
3	SA	1737	G
3	SA	1742	U
3	SA	1743	U
3	SA	1745	G
3	SA	1749	A
3	SA	1750	A
3	SA	1755	A
3	SA	1756	A
3	SA	1757	G
3	SA	1758	U

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	3A	97	C
1	3A	98	U
1	3A	198	U
1	3A	248	G
1	3A	312	U
1	3A	318	U
1	3A	322	A
1	3A	323	G
2	5A	312	U
2	5A	487	A
2	5A	492	G
2	5A	536	A
3	SA	-7	A
3	SA	0	U
3	SA	56	U
3	SA	68	A

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Mol	Chain	Res	Type
3	SA	272	U
3	SA	372	G
3	SA	401	A
3	SA	417	A
3	SA	538	A
3	SA	542	A
3	SA	579	A
3	SA	602	U
3	SA	1197	C
3	SA	1521	G
3	SA	1594	G
3	SA	1632	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
56	GTP	RJ	1201	57	26,34,34	0.94	2 (7%)	32,54,54	0.92	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
56	GTP	RJ	1201	57	-	3/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	RJ	1201	GTP	C5-C6	-2.47	1.42	1.47
56	RJ	1201	GTP	C8-N7	-2.05	1.31	1.35

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

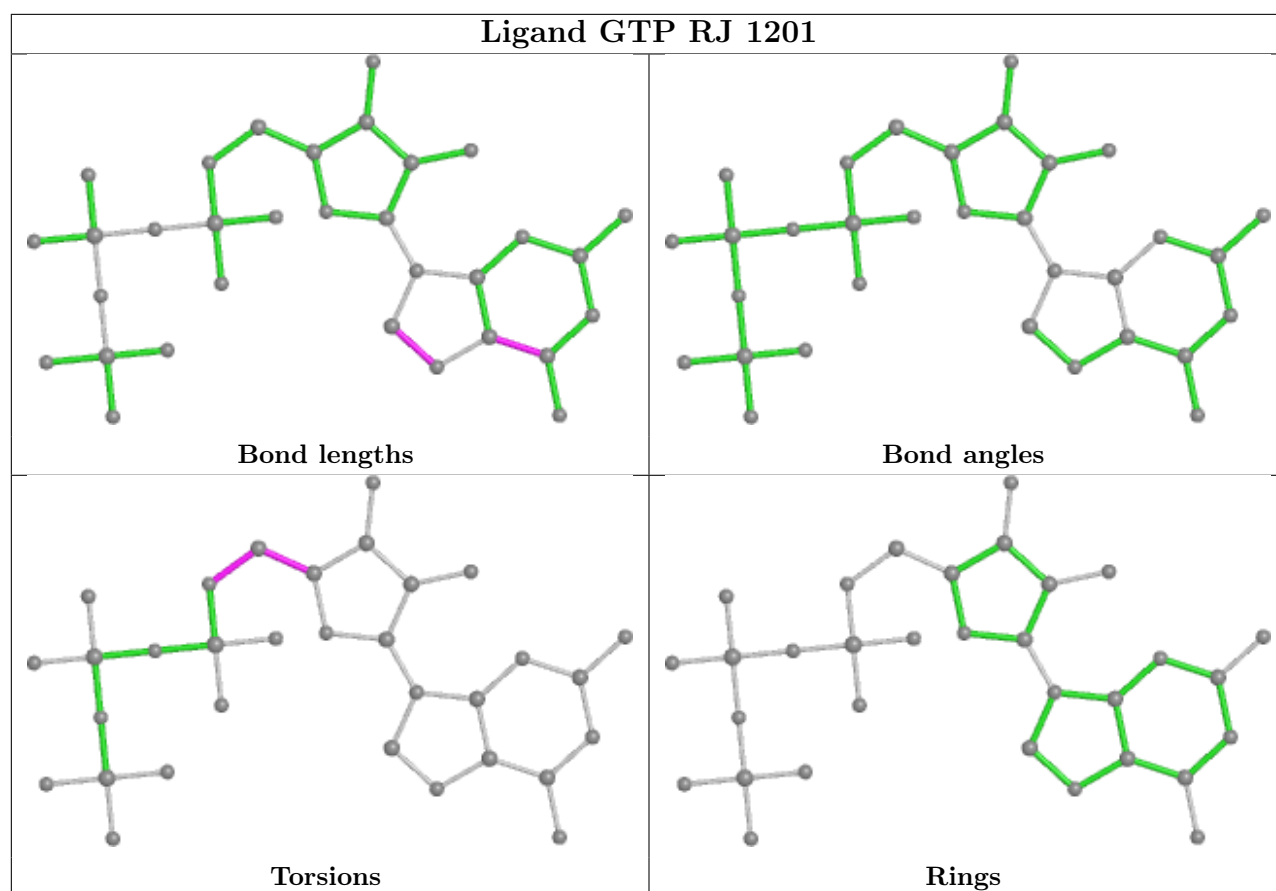
Mol	Chain	Res	Type	Atoms
56	RJ	1201	GTP	O4'-C4'-C5'-O5'
56	RJ	1201	GTP	C3'-C4'-C5'-O5'
56	RJ	1201	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	RJ	1201	GTP	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 [i](#)

There are no chain breaks in this entry.

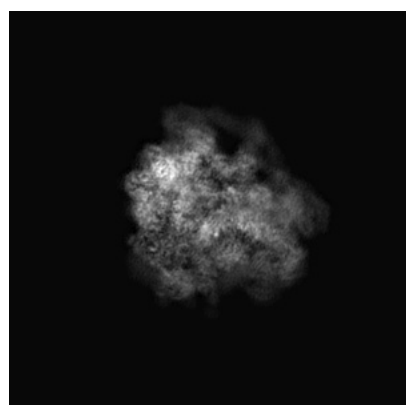
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0955. These allow visual inspection of the internal detail of the map and identification of artifacts.

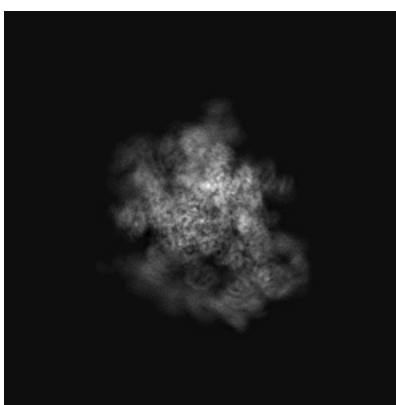
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

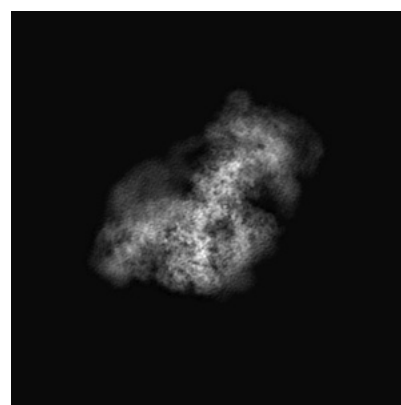
6.1.1 Primary map



X



Y

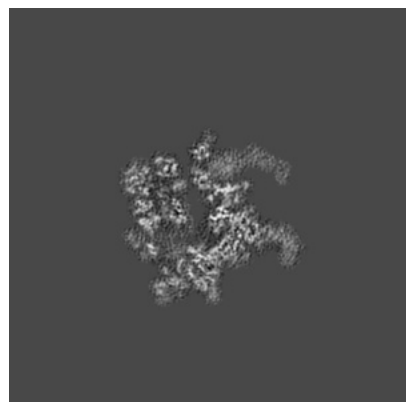


Z

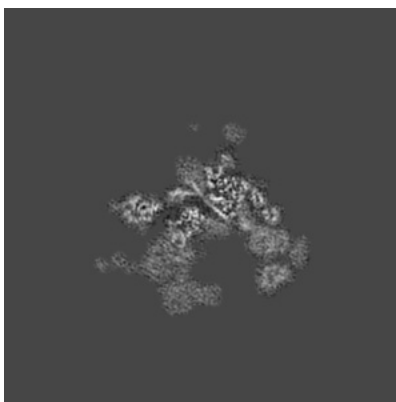
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

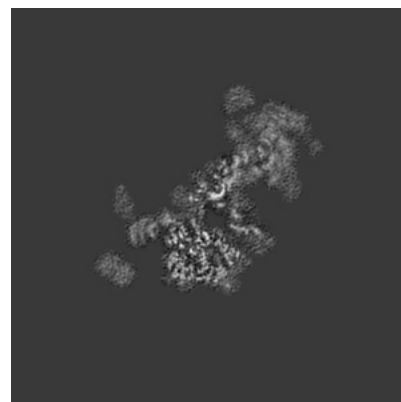
6.2.1 Primary map



X Index: 224



Y Index: 224



Z Index: 224

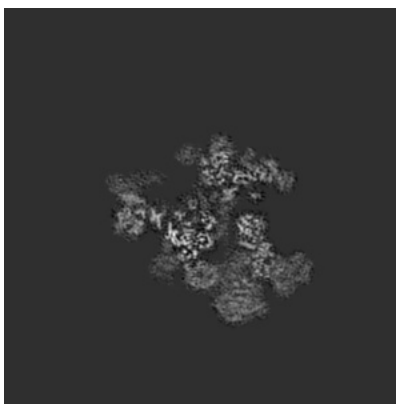
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

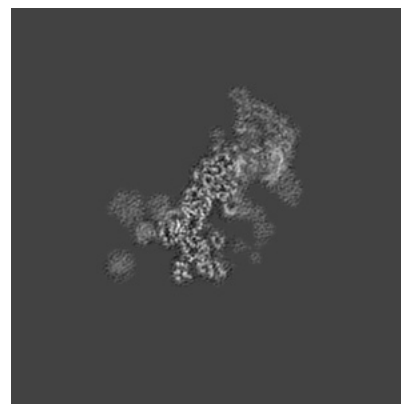
6.3.1 Primary map



X Index: 212



Y Index: 197



Z Index: 206

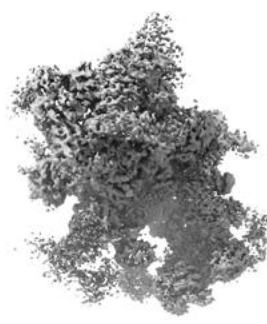
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

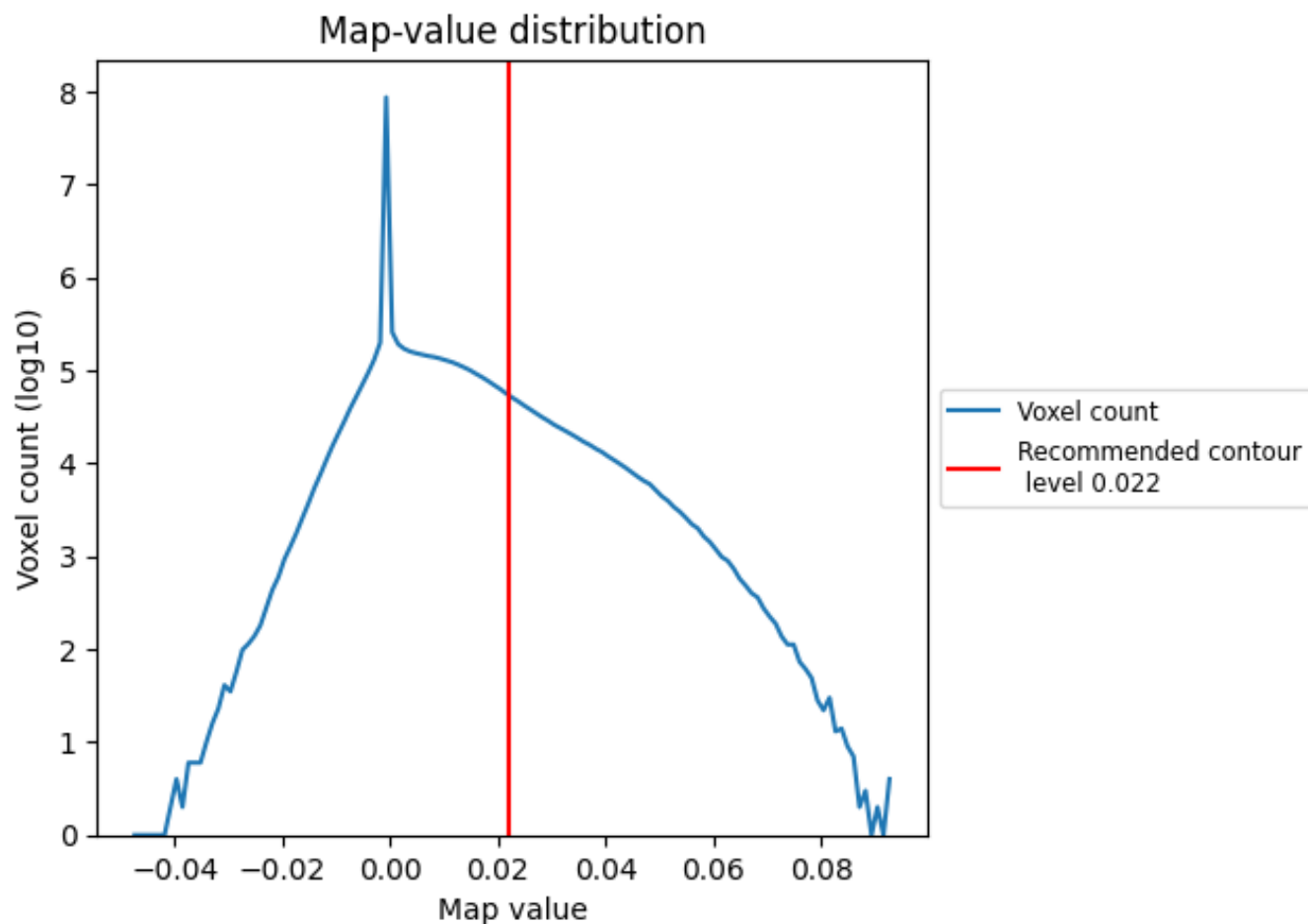
6.5 Mask visualisation

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

7 Map analysis [i](#)

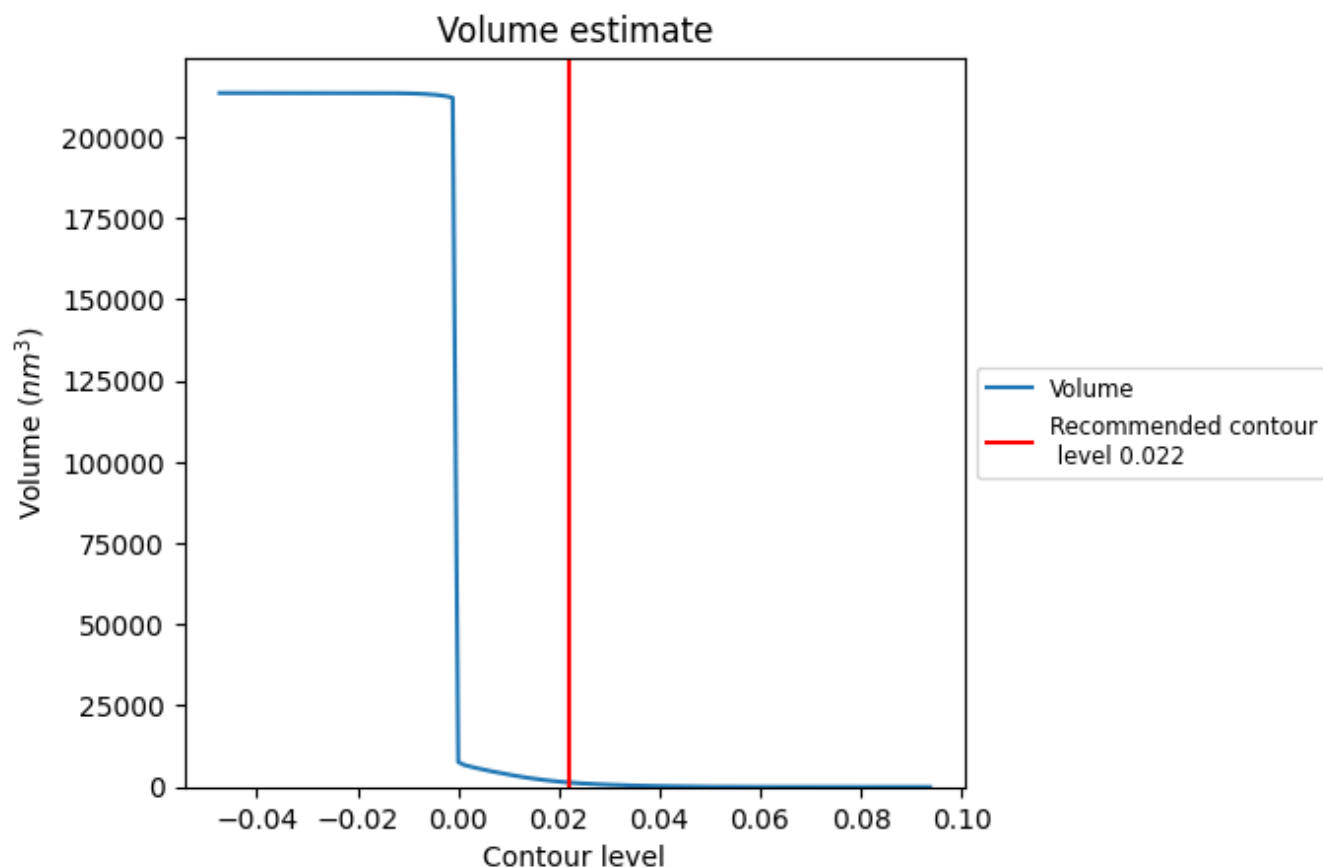
This section contains the results of statistical analysis of the map.

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.

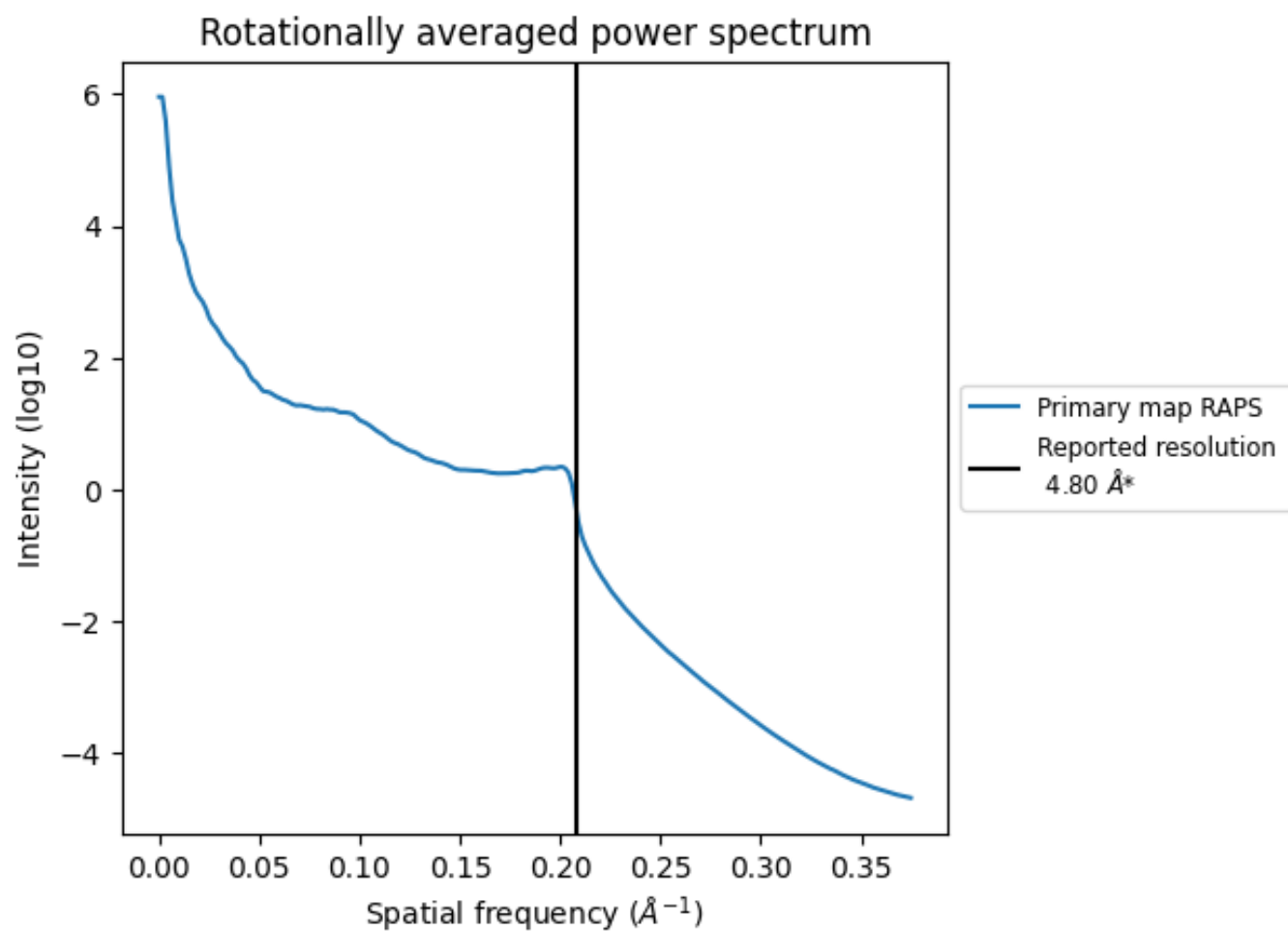
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1377 nm^3 ; this corresponds to an approximate mass of 1244 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 0.208 Å⁻¹

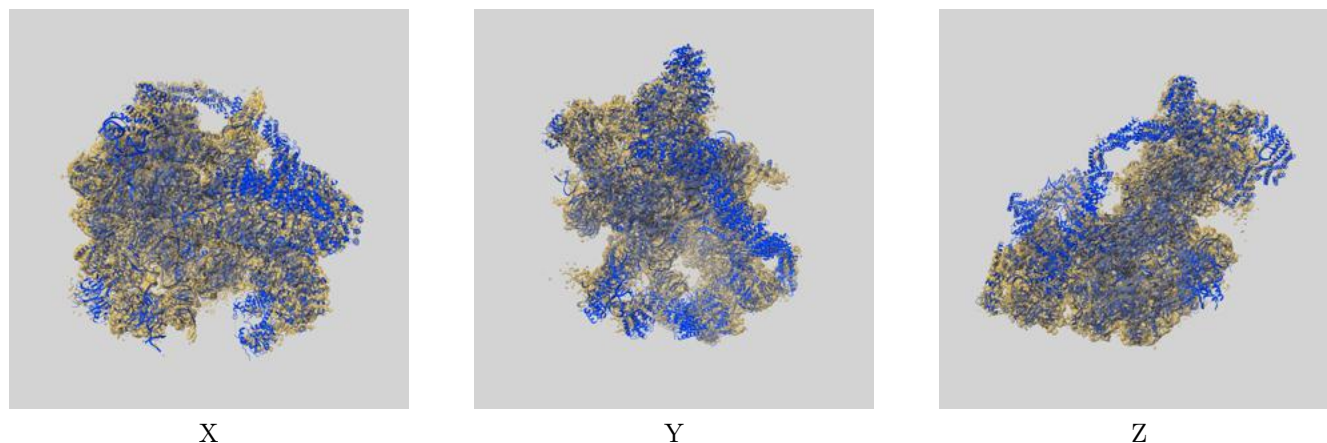
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

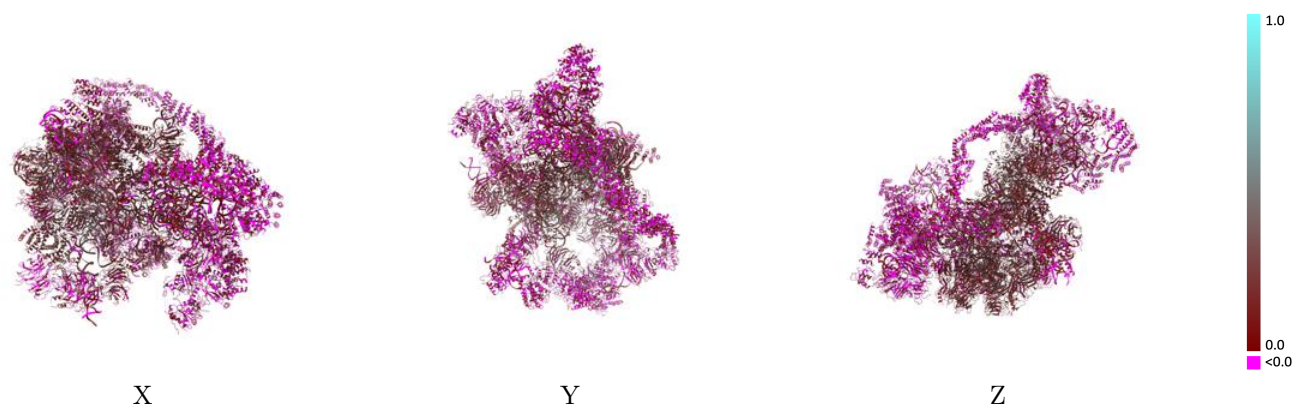
This section contains information regarding the fit between EMDB map EMD-0955 and PDB model 6LQV. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



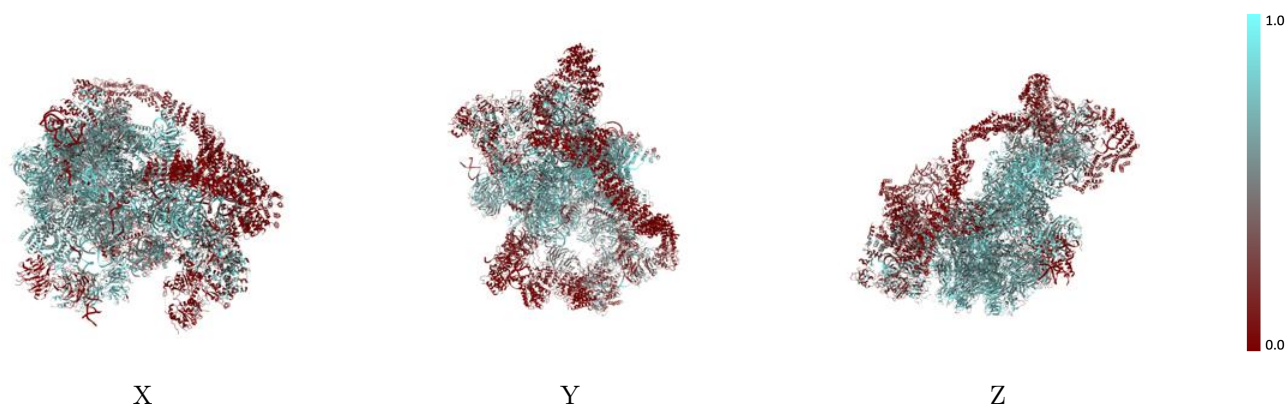
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



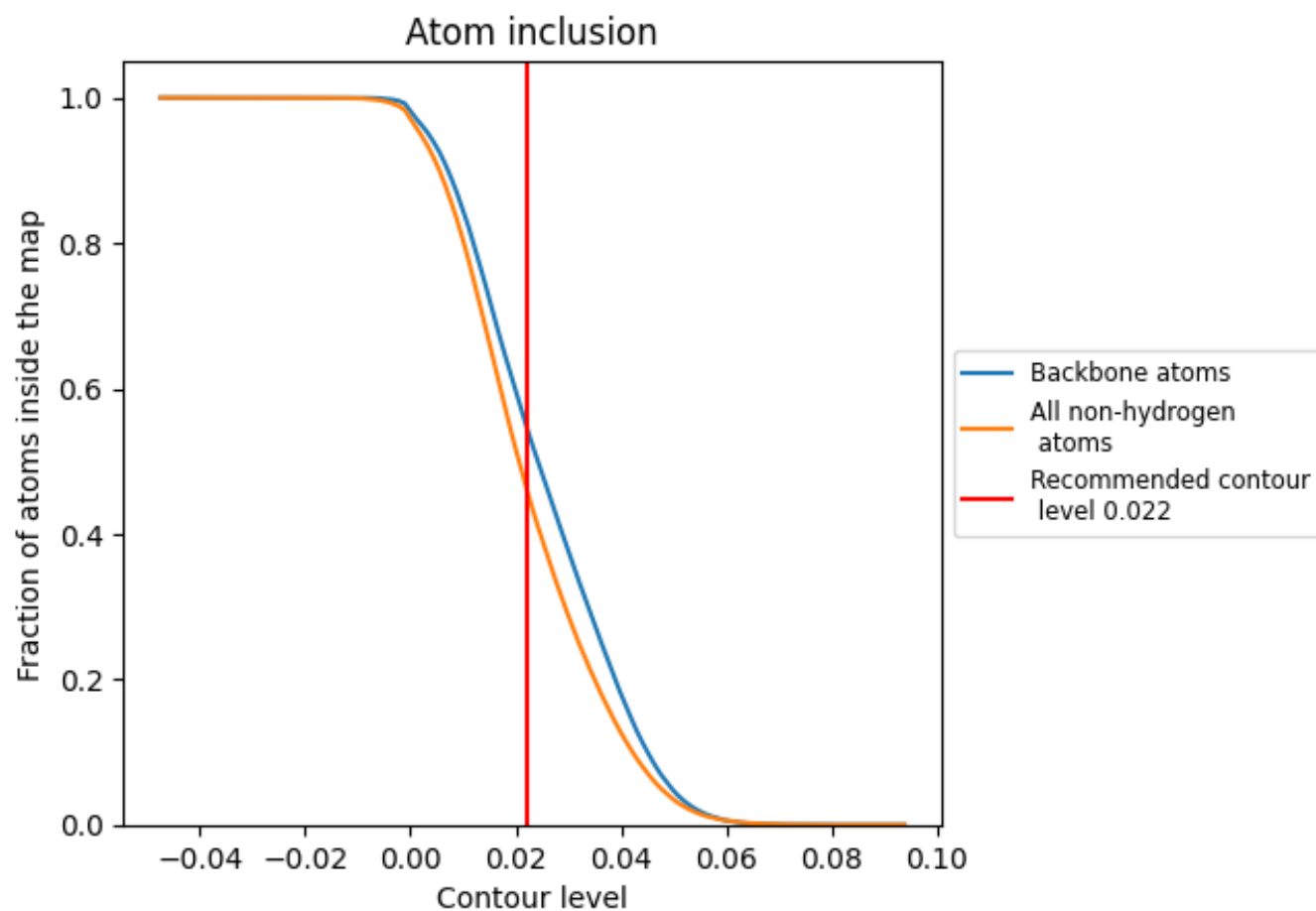
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 46% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4643	0.1300
3A	0.7750	0.2060
3B	0.6394	0.2150
3C	0.3494	0.0730
3D	0.6490	0.2060
3E	0.5025	0.1390
3F	0.6876	0.2280
3G	0.5763	0.1250
3H	0.6748	0.2540
5A	0.4032	0.0860
5B	0.0604	0.0360
5C	0.6715	0.2430
5D	0.2858	0.0990
5E	0.6220	0.2160
5F	0.6691	0.2490
5G	0.6532	0.2350
5H	0.6661	0.2450
5I	0.6427	0.2000
5J	0.3574	0.1150
5K	0.5968	0.2210
A4	0.4141	0.0400
A5	0.4856	0.1360
A8	0.2722	0.0490
A9	0.2527	0.0090
AE	0.2431	0.0890
AF	0.3846	0.0850
AG	0.4179	0.0280
B1	0.6838	0.2210
B2	0.6528	0.1650
B3	0.2008	0.0520
B6	0.5891	0.1660
B8	0.6508	0.1760
BE	0.7130	0.2240
RA	0.3973	0.0330
RB	0.4760	0.1580



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Chain	Atom inclusion	Q-score
RG	 0.1070	 0.0470
RH	 0.1615	 0.0610
RJ	 0.6610	 0.2200
RK	 0.6831	 0.2240
RL	 0.4771	 0.1490
RM	 0.1667	 0.0470
RN	 0.1121	 0.0520
RO	 0.0072	 0.0120
RP	 0.0918	 0.0270
RQ	 0.1561	 0.0700
RS	 0.0529	 0.0280
RY	 0.1297	 -0.0200
SA	 0.5862	 0.1420
SF	 0.5527	 0.1410
SG	 0.6652	 0.2440
SH	 0.3659	 0.0530
SJ	 0.4498	 0.0380
SK	 0.6562	 0.2280
SM	 0.4845	 0.0430
SR	 0.6908	 0.2420
SY	 0.6245	 0.2260
SZ	 0.6201	 0.2110
Sd	 0.6960	 0.2790
X1	 0.4250	 0.1700