



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 06:42 AM UTC

PDB ID : 7R5J / pdb_00007r5j
EMDB ID : EMD-14321
Title : Human nuclear pore complex (dilated)
Authors : Mosalaganti, S.; Obarska-Kosinska, A.; Siggel, M.; Taniguchi, R.; Turonova, B.; Zimmerli, C.E.; Buczak, K.; Schmidt, F.H.; Margiotta, E.; Mackmull, M.T.; Hagen, W.J.H.; Hummer, G.; Kosinski, J.; Beck, M.
Deposited on : 2022-02-10
Resolution : 50.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

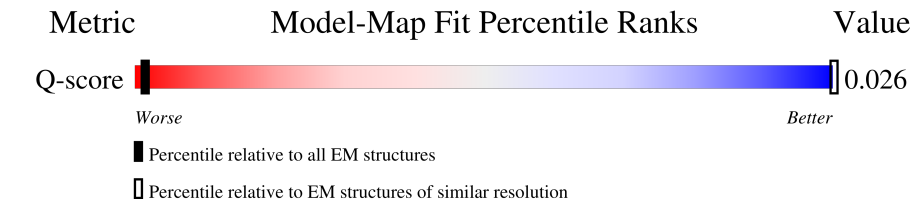
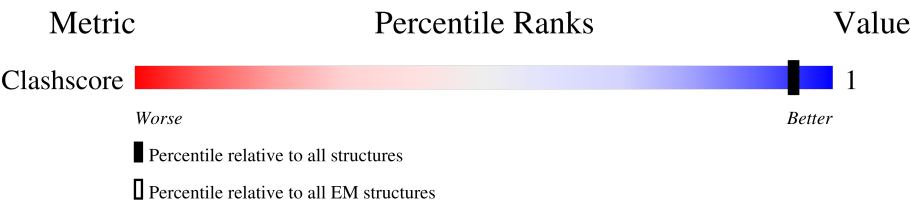
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 50.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	1 (50.00 - 50.00)

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	00	3224	7% 22% 77%
1	01	3224	23% 77%
1	02	3224	23% 77%
1	03	3224	6% 23% 77%
1	04	3224	23% 77%
2	10	1887	73% 94% ...

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Mol	Chain	Length	Quality of chain
2	11	1887	
2	12	1887	
2	13	1887	
2	14	1887	
2	15	1887	
2	16	1887	
2	17	1887	
3	40	546	
3	41	546	
4	A0	819	
4	A1	819	
4	A2	819	
4	A3	819	
4	A4	819	
4	A5	819	
4	A6	819	
5	B0	1749	
5	B1	1749	
6	C0	2012	
6	C1	2012	
6	C2	2012	
6	C3	2012	
6	C4	2012	
7	D0	1391	
7	D1	1391	

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Mol	Chain	Length	Quality of chain
7	D2	1391	
7	D3	1391	
7	D4	1391	
7	D5	1391	
8	E0	674	
8	E1	674	
9	F0	326	
9	F1	326	
9	F2	326	
9	F3	326	
10	H0	507	
10	H1	507	
10	H2	507	
10	H3	507	
11	I0	599	
11	I1	599	
11	I2	599	
11	I3	599	
12	J0	522	
12	J1	522	
12	J2	522	
12	J3	522	
12	J4	522	
13	K0	1156	
13	K1	1156	

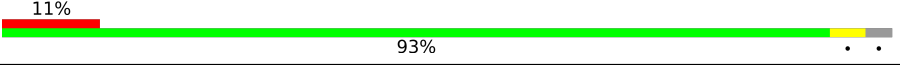
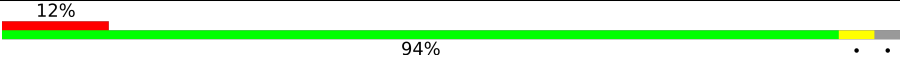
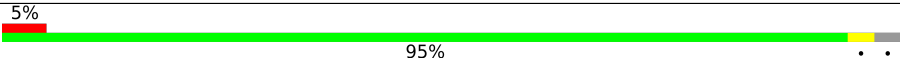
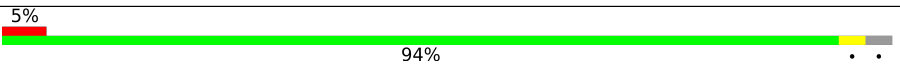
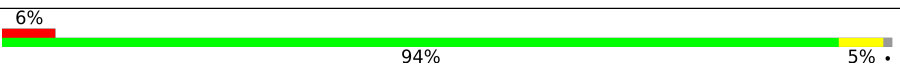
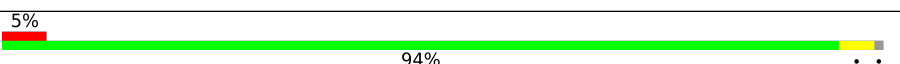
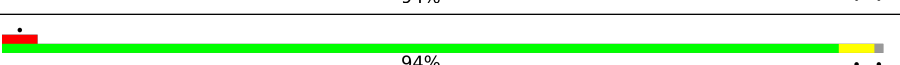
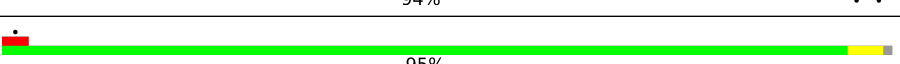
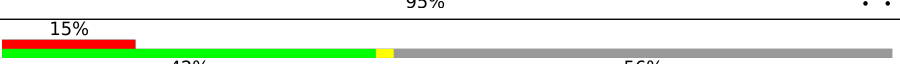
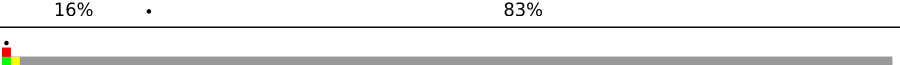
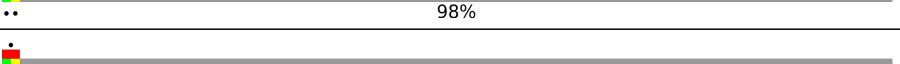
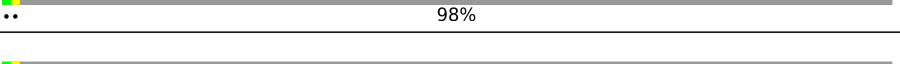
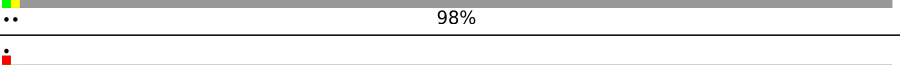
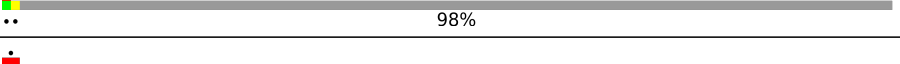
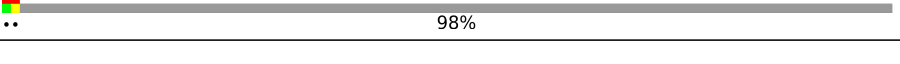
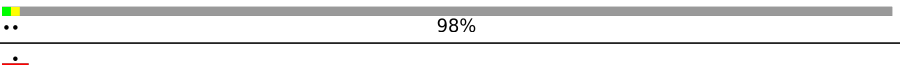
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Mol	Chain	Length	Quality of chain
13	K2	1156	
13	K3	1156	
14	L0	925	
14	L1	925	
14	L2	925	
14	L3	925	
15	M0	937	
15	M1	937	
15	M2	937	
15	M3	937	
16	N0	322	
16	N1	322	
16	N2	322	
16	N3	322	
17	O0	360	
17	O1	360	
17	O2	360	
17	O3	360	
18	P0	656	
18	P1	656	
18	P2	656	
18	P3	656	
19	Q0	380	
19	Q1	380	
19	Q2	380	

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Mol	Chain	Length	Quality of chain
19	Q3	380	
20	R0	1436	
20	R1	1436	
20	R2	1436	
20	R3	1436	
21	S0	326	
21	S1	326	
21	S2	326	
21	S3	326	
22	T0	2266	
22	T1	2266	
23	U0	880	
23	U1	880	
23	U2	880	
23	U3	880	
23	U4	880	
23	U5	880	
23	U6	880	
24	V0	2090	
25	W0	741	

2 Entry composition [i](#)

There are 25 unique types of molecules in this entry. The entry contains 617133 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called E3 SUMO-protein ligase RanBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	00	756	Total	C	N	O	S	0	0
			6085	3866	1045	1147	27		
1	01	756	Total	C	N	O	S	0	0
			6085	3866	1045	1147	27		
1	02	756	Total	C	N	O	S	0	0
			6085	3866	1045	1147	27		
1	03	756	Total	C	N	O	S	0	0
			6085	3866	1045	1147	27		
1	04	756	Total	C	N	O	S	0	0
			6085	3866	1045	1147	27		

- Molecule 2 is a protein called Nuclear pore membrane glycoprotein 210.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	10	1831	Total	C	N	O	S	0	0
			14046	8947	2406	2644	49		
2	11	1831	Total	C	N	O	S	0	0
			14046	8947	2406	2644	49		
2	12	1831	Total	C	N	O	S	0	0
			14046	8947	2406	2644	49		
2	13	1831	Total	C	N	O	S	0	0
			14046	8947	2406	2644	49		
2	14	1831	Total	C	N	O	S	0	0
			14046	8947	2406	2644	49		
2	15	1831	Total	C	N	O	S	0	0
			14046	8947	2406	2644	49		
2	16	1831	Total	C	N	O	S	0	0
			14046	8947	2406	2644	49		
2	17	1831	Total	C	N	O	S	0	0
			14046	8947	2406	2644	49		

- Molecule 3 is a protein called Aladin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	40	383	Total	C	N	O	S	0	0
			2922	1864	509	533	16		
3	41	383	Total	C	N	O	S	0	0
			2922	1864	509	533	16		

- Molecule 4 is a protein called Nuclear pore complex protein Nup93.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A0	818	Total	C	N	O	S	0	0
			6568	4136	1145	1259	28		
4	A1	818	Total	C	N	O	S	0	0
			6568	4136	1145	1259	28		
4	A2	818	Total	C	N	O	S	0	0
			6568	4136	1145	1259	28		
4	A3	818	Total	C	N	O	S	0	0
			6568	4136	1145	1259	28		
4	A4	726	Total	C	N	O	S	0	0
			5860	3705	1018	1109	28		
4	A5	726	Total	C	N	O	S	0	0
			5860	3705	1018	1109	28		
4	A6	726	Total	C	N	O	S	0	0
			5860	3705	1018	1109	28		

- Molecule 5 is a protein called Nucleoporin NUP188 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B0	1748	Total	C	N	O	S	0	0
			13746	8743	2353	2559	91		
5	B1	1748	Total	C	N	O	S	0	0
			13746	8743	2353	2559	91		

- Molecule 6 is a protein called Nuclear pore complex protein Nup205.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C0	2011	Total	C	N	O	S	0	0
			16013	10208	2753	2965	87		
6	C1	2011	Total	C	N	O	S	0	0
			16013	10208	2753	2965	87		
6	C2	2011	Total	C	N	O	S	0	0
			16013	10208	2753	2965	87		
6	C3	2011	Total	C	N	O	S	0	0
			16013	10208	2753	2965	87		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	C4	2011	Total	C	N	O	S	0	0
			16013	10208	2753	2965	87		

- Molecule 7 is a protein called Nuclear pore complex protein Nup155.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D0	1312	Total	C	N	O	S	0	0
			10363	6569	1786	1949	59		
7	D1	1312	Total	C	N	O	S	0	0
			10363	6569	1786	1949	59		
7	D2	1312	Total	C	N	O	S	0	0
			10363	6569	1786	1949	59		
7	D3	1312	Total	C	N	O	S	0	0
			10363	6569	1786	1949	59		
7	D4	1312	Total	C	N	O	S	0	0
			10363	6569	1786	1949	59		
7	D5	1312	Total	C	N	O	S	0	0
			10363	6569	1786	1949	59		

- Molecule 8 is a protein called Nucleoporin NDC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E0	548	Total	C	N	O	S	0	0
			4432	2923	729	758	22		
8	E1	548	Total	C	N	O	S	0	0
			4432	2923	729	758	22		

- Molecule 9 is a protein called Nucleoporin NUP35.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F0	241	Total	C	N	O	S	0	0
			1837	1154	313	359	11		
9	F1	241	Total	C	N	O	S	0	0
			1837	1154	313	359	11		
9	F2	241	Total	C	N	O	S	0	0
			1837	1154	313	359	11		
9	F3	241	Total	C	N	O	S	0	0
			1837	1154	313	359	11		

- Molecule 10 is a protein called Nucleoporin p54.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H0	383	Total	C	N	O	S	0	0
			3066	1921	544	592	9		
10	H1	383	Total	C	N	O	S	0	0
			3066	1921	544	592	9		
10	H2	383	Total	C	N	O	S	0	0
			3066	1921	544	592	9		
10	H3	383	Total	C	N	O	S	0	0
			3066	1921	544	592	9		

- Molecule 11 is a protein called Nucleoporin p58/p45.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I0	173	Total	C	N	O	S	0	0
			1398	881	245	267	5		
11	I1	173	Total	C	N	O	S	0	0
			1398	881	245	267	5		
11	I2	173	Total	C	N	O	S	0	0
			1398	881	245	267	5		
11	I3	173	Total	C	N	O	S	0	0
			1398	881	245	267	5		

- Molecule 12 is a protein called Nuclear pore glycoprotein p62.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J0	171	Total	C	N	O	S	0	0
			1403	872	243	285	3		
12	J1	171	Total	C	N	O	S	0	0
			1403	872	243	285	3		
12	J2	171	Total	C	N	O	S	0	0
			1403	872	243	285	3		
12	J3	171	Total	C	N	O	S	0	0
			1403	872	243	285	3		
12	J4	171	Total	C	N	O	S	0	0
			1403	872	243	285	3		

- Molecule 13 is a protein called Nuclear pore complex protein Nup133.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K0	1086	Total	C	N	O	S	0	0
			8574	5420	1425	1692	37		
13	K1	1086	Total	C	N	O	S	0	0
			8574	5420	1425	1692	37		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	K2	1086	Total	C	N	O	S	0	0
			8574	5420	1425	1692	37		
13	K3	1086	Total	C	N	O	S	0	0
			8574	5420	1425	1692	37		

- Molecule 14 is a protein called Nuclear pore complex protein Nup107.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L0	782	Total	C	N	O	S	0	0
			6383	4064	1079	1208	32		
14	L1	782	Total	C	N	O	S	0	0
			6383	4064	1079	1208	32		
14	L2	782	Total	C	N	O	S	0	0
			6383	4064	1079	1208	32		
14	L3	782	Total	C	N	O	S	0	0
			6383	4064	1079	1208	32		

- Molecule 15 is a protein called Nuclear pore complex protein Nup96.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M0	673	Total	C	N	O	S	0	0
			5461	3467	964	1004	26		
15	M1	673	Total	C	N	O	S	0	0
			5461	3467	964	1004	26		
15	M2	673	Total	C	N	O	S	0	0
			5461	3467	964	1004	26		
15	M3	673	Total	C	N	O	S	0	0
			5461	3467	964	1004	26		

- Molecule 16 is a protein called Protein SEC13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N0	301	Total	C	N	O	S	0	0
			2352	1479	409	452	12		
16	N1	301	Total	C	N	O	S	0	0
			2352	1479	409	452	12		
16	N2	301	Total	C	N	O	S	0	0
			2352	1479	409	452	12		
16	N3	301	Total	C	N	O	S	0	0
			2352	1479	409	452	12		

- Molecule 17 is a protein called Nucleoporin SEH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O0	323	Total	C	N	O	S	0	0
			2528	1584	452	475	17		
17	O1	323	Total	C	N	O	S	0	0
			2528	1584	452	475	17		
17	O2	323	Total	C	N	O	S	0	0
			2528	1584	452	475	17		
17	O3	323	Total	C	N	O	S	0	0
			2528	1584	452	475	17		

- Molecule 18 is a protein called Nuclear pore complex protein Nup85.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P0	655	Total	C	N	O	S	0	0
			5257	3341	898	982	36		
18	P1	655	Total	C	N	O	S	0	0
			5257	3341	898	982	36		
18	P2	655	Total	C	N	O	S	0	0
			5257	3341	898	982	36		
18	P3	655	Total	C	N	O	S	0	0
			5257	3341	898	982	36		

- Molecule 19 is a protein called Nucleoporin Nup43.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q0	345	Total	C	N	O	S	0	0
			2703	1690	474	527	12		
19	Q1	345	Total	C	N	O	S	0	0
			2703	1690	474	527	12		
19	Q2	345	Total	C	N	O	S	0	0
			2703	1690	474	527	12		
19	Q3	345	Total	C	N	O	S	0	0
			2703	1690	474	527	12		

- Molecule 20 is a protein called Nuclear pore complex protein Nup160.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R0	1399	Total	C	N	O	S	0	0
			11132	7093	1878	2088	73		
20	R1	1399	Total	C	N	O	S	0	0
			11132	7093	1878	2088	73		
20	R2	1399	Total	C	N	O	S	0	0
			11132	7093	1878	2088	73		

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Mol	Chain	Residues	Atoms					AltConf	Trace
20	R3	1399	Total	C	N	O	S	0	0
			11132	7093	1878	2088	73		

- Molecule 21 is a protein called Nucleoporin Nup37.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S0	322	Total	C	N	O	S	0	0
			2552	1626	436	475	15		
21	S1	322	Total	C	N	O	S	0	0
			2552	1626	436	475	15		
21	S2	322	Total	C	N	O	S	0	0
			2552	1626	436	475	15		
21	S3	322	Total	C	N	O	S	0	0
			2552	1626	436	475	15		

- Molecule 22 is a protein called Protein ELYS.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T0	1004	Total	C	N	O	S	0	0
			7960	5069	1359	1490	42		
22	T1	1004	Total	C	N	O	S	0	0
			7960	5069	1359	1490	42		

- Molecule 23 is a protein called Nuclear pore complex protein Nup98.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U0	150	Total	C	N	O	S	0	0
			1193	756	205	229	3		
23	U1	19	Total	C	N	O		0	0
			151	98	27	26			
23	U2	19	Total	C	N	O		0	0
			151	98	27	26			
23	U3	19	Total	C	N	O		0	0
			151	98	27	26			
23	U4	19	Total	C	N	O		0	0
			151	98	27	26			
23	U5	19	Total	C	N	O		0	0
			151	98	27	26			
23	U6	19	Total	C	N	O		0	0
			151	98	27	26			

- Molecule 24 is a protein called Nuclear pore complex protein Nup214.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V0	273	Total	C	N	O	S	0	0
			2203	1376	398	423	6		

- Molecule 25 is a protein called Nuclear pore complex protein Nup88.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W0	735	Total	C	N	O	S	0	0
			5836	3714	988	1103	31		



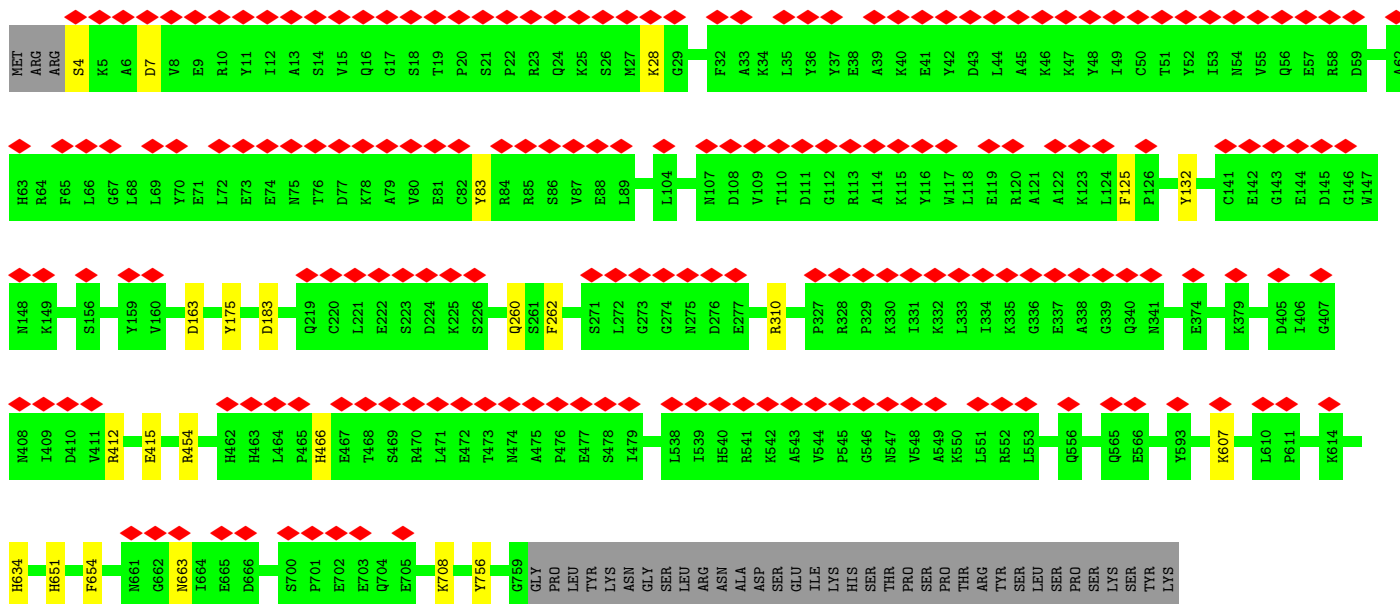






[illegible]

- Molecule 1: E3 SUMO-protein ligase RanBP2





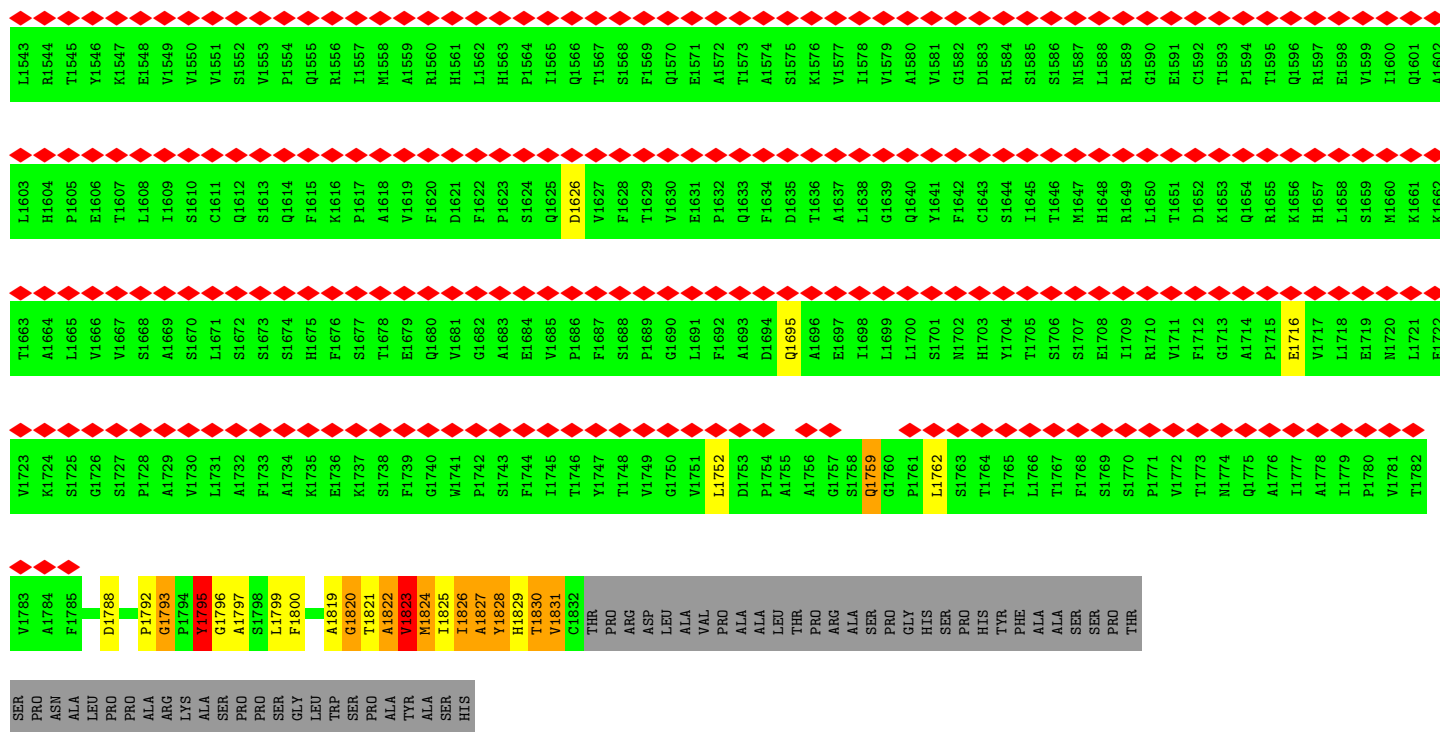
WORLDWIDE
PDB
PROTEIN DATA BANK

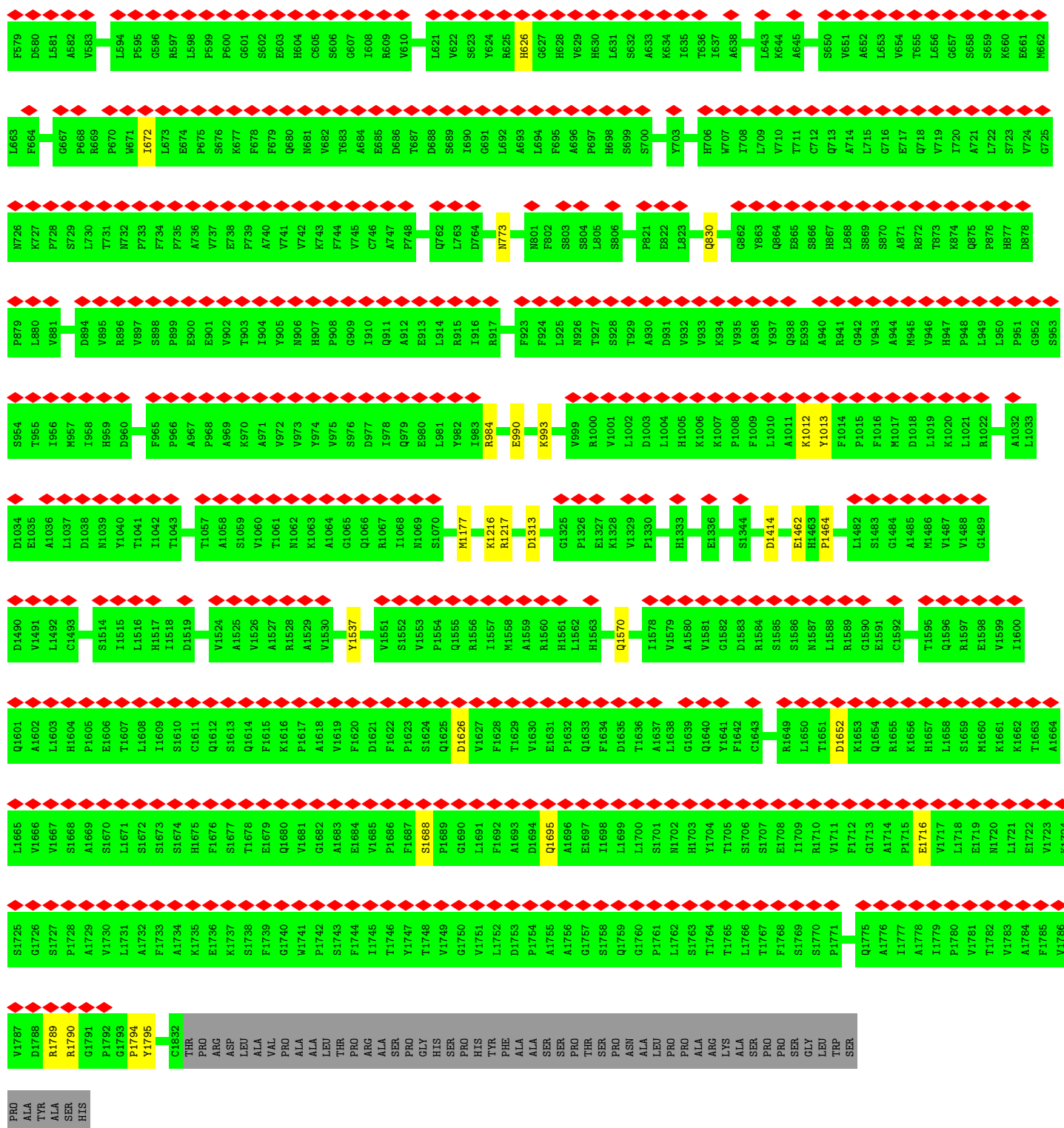
Chain 04:





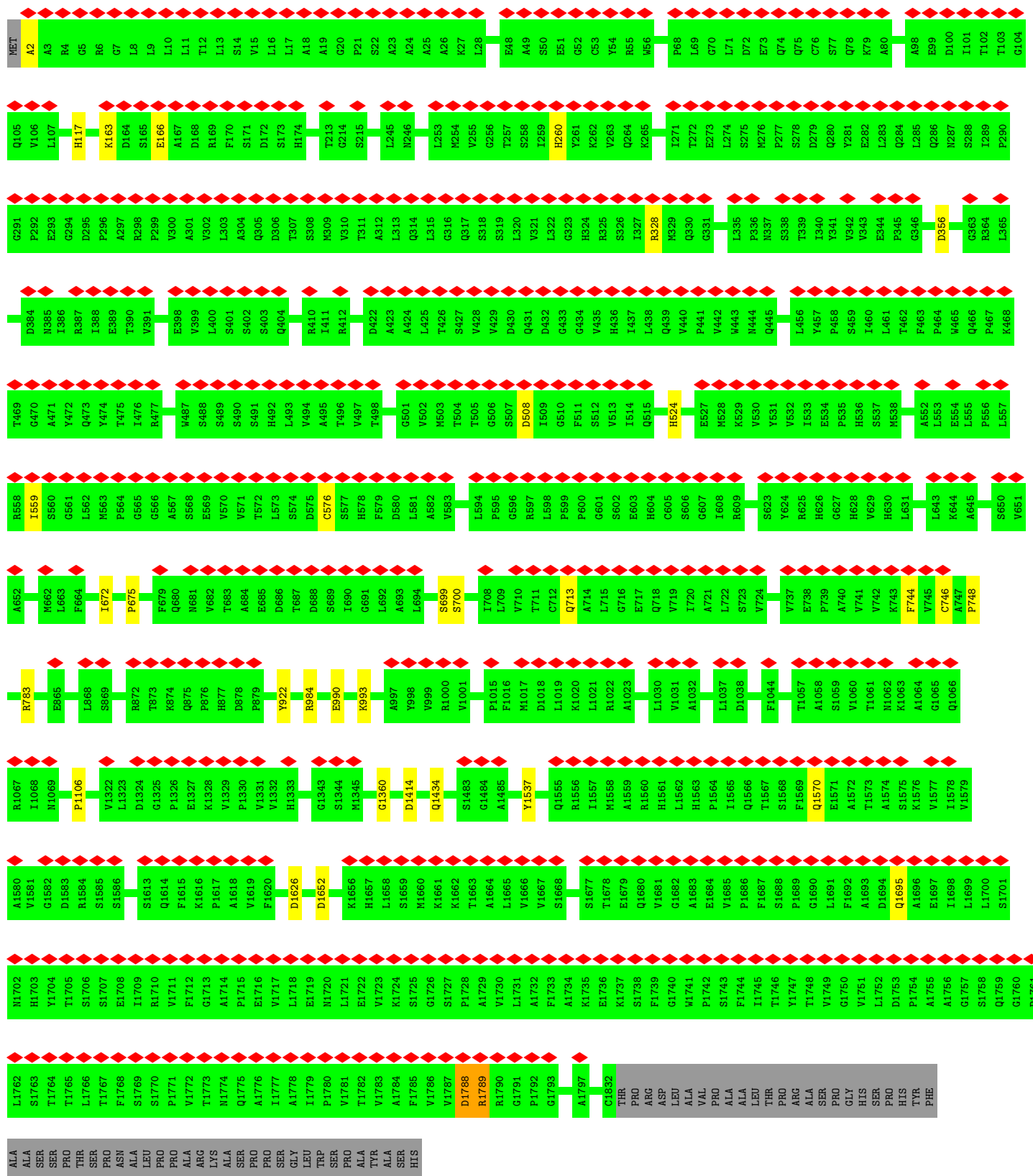
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S1382	P1383	V1384	L1385	H1386	T1387	Q1388	R1312	K1390	E1391	A1392	L1393	V1394	A1395	V1396	P1397	L1398	G1399	M1400	T1401	V1402	T1403	D1414		D1430	D1431	F1432	V1433	Q1434	I1435	G1436	K1437	G1438	P1439	T1440	N1441	N1442	T1443	C1444	V1445	V1446	R1447	T1448	V1449	S1450	V1451	G1452	L1472		P1473	V1474	L1475	Q1476	A1477	T1478	S1479	P1480	E1481	L1482		
Y1305	I1306	K1307	L1308	Q1309	T1310	R1311	R1312	D1313	G1314	A1315	A1316	S1317	L1318	S1319	Y1320	R1321	V1322	L1323	D1324	G1325	P1326	E1327	K1328	V1329	P1330	V1331	V1332	H1333	V1334	D1335	E1336	K1337	G1338	F1339	L1340	A1341	S1342	G1343	S1344	M1345	S1349		T1350	I1351	E1352	V1353	F1359	G1360	A1361	N1362	Q1363	T1364	I1365							
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T873	K874	Q875	P876	H877	D878	P879	L880	V881	P882	L883	S884	A885	S886	L887	E888	L889	T890	L891	V892	E893	D894	V895	R896	V897	S898	P899	E900	E901	V902	T903	I904	Y905	N906	H907	P908	G909	I910	Q911	A912	E913	L914	R915	I916	R917	E918	G919	S920	G921	Y922	P923	F924	L925	N926	T927	S928	T929	D930	A930	V931	H932
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Y624	R625	H626	S632		A633	K634	I635	T636	I637	A638	A639	Y640	L641	P642	L643	K644	A645	V646	P648	S649	S650	V651	A652	L653	V654	T655	L656	G657	S658	P659	K660	E661	M662	L663	F664	E665	Q666	G667	V671	I672	L673	E674	P675	S676	K677	F678	F679	Q680	A684		E685	D686	T687	D688	S689					
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M503	T504	T505	G506	S507	D508	I509	G510	F511	S512	V513	I514	Q515	A516	H517	D518	N521		P522	L523	H524	F525	G526	E527	M528	K529	V530	Y531	V532	I533	E534	P535	H536	S537	M538	E539	F540	A541	P542	C543	Q544	V545	E546	A547	R548	V549	G550	Q551	A552	L553	E554	L555	P556	L557	R558	Y559	S560	G561	L562	M563	





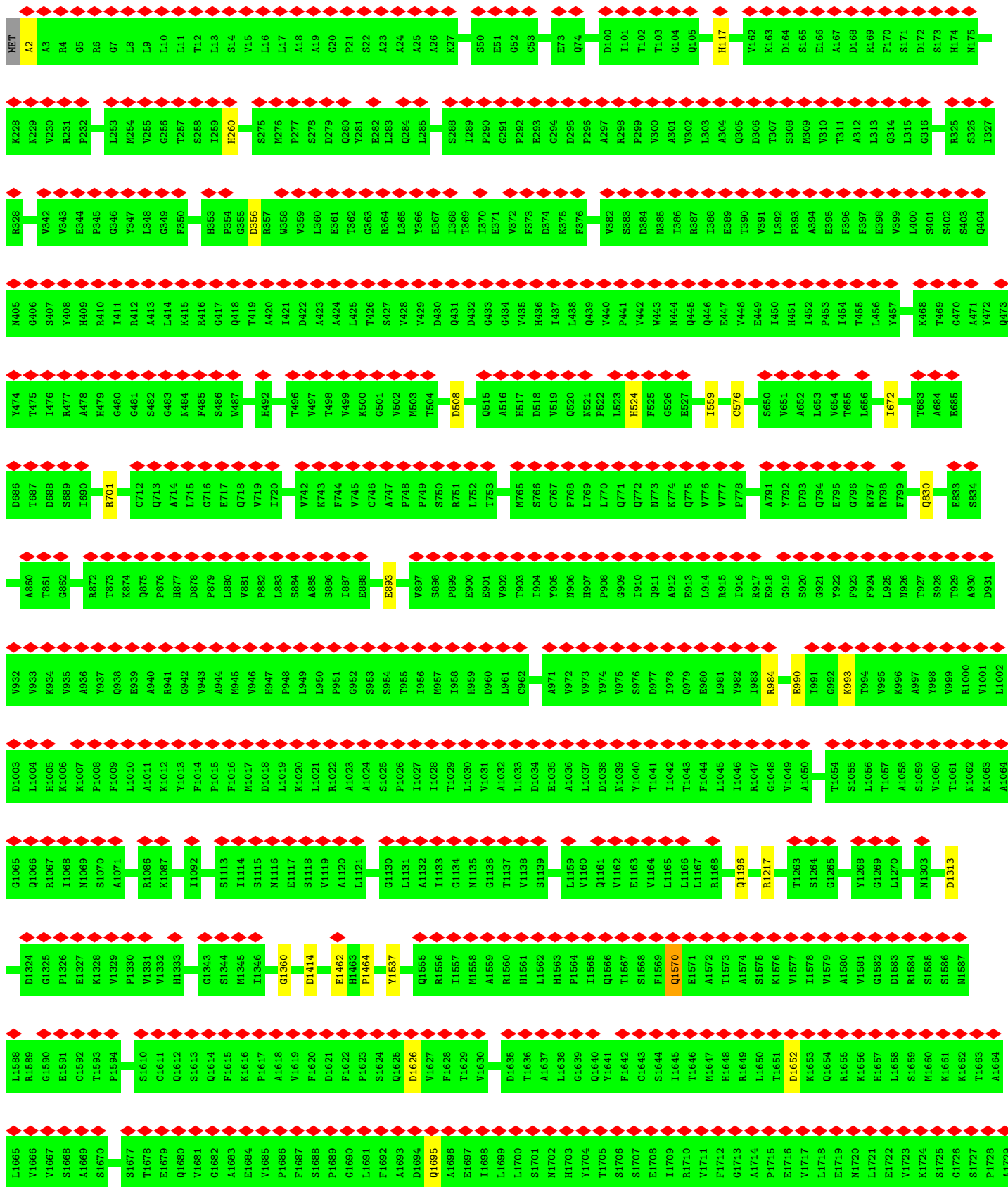
- Molecule 2: Nuclear pore membrane glycoprotein 210

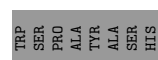
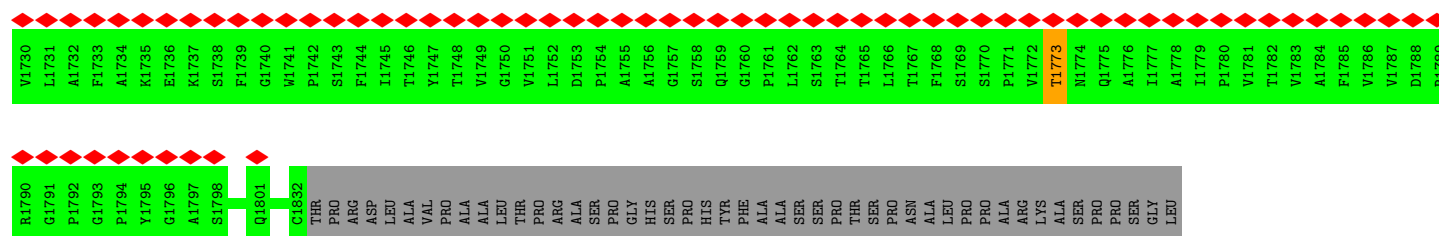




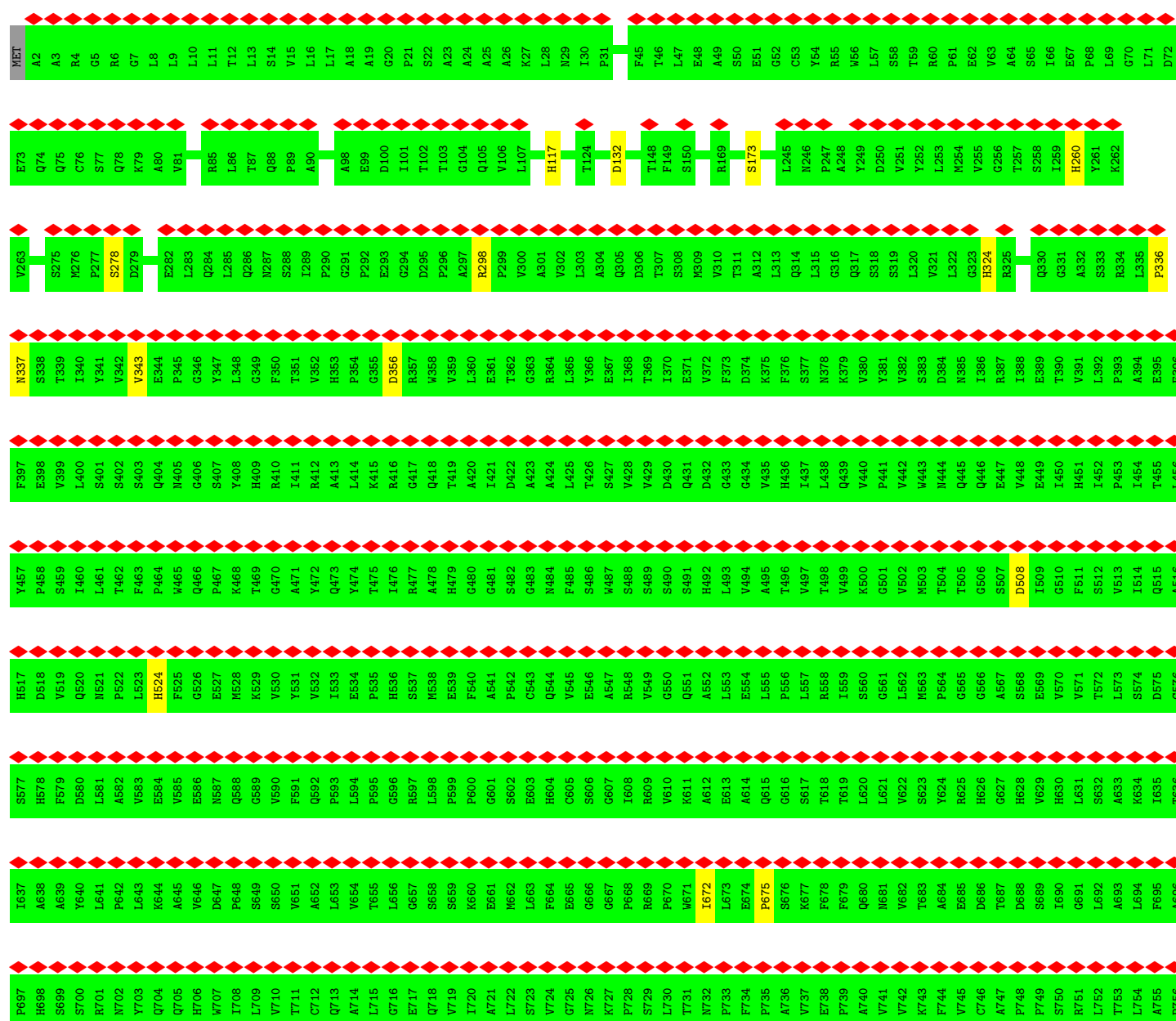
• Molecule 2: Nuclear pore membrane glycoprotein 210





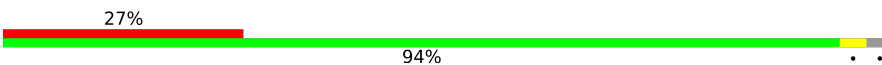


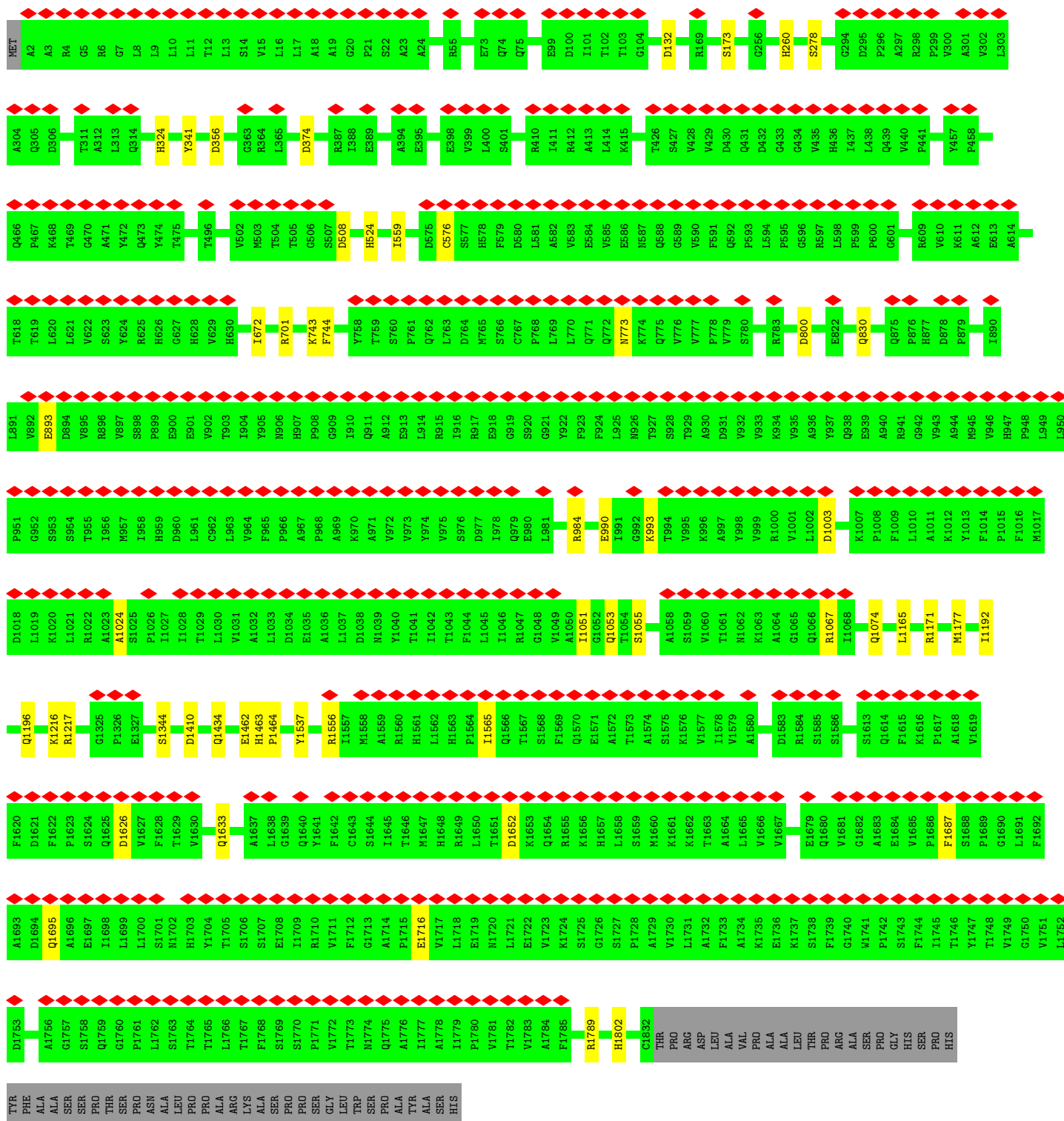
• Molecule 2: Nuclear pore membrane glycoprotein 210



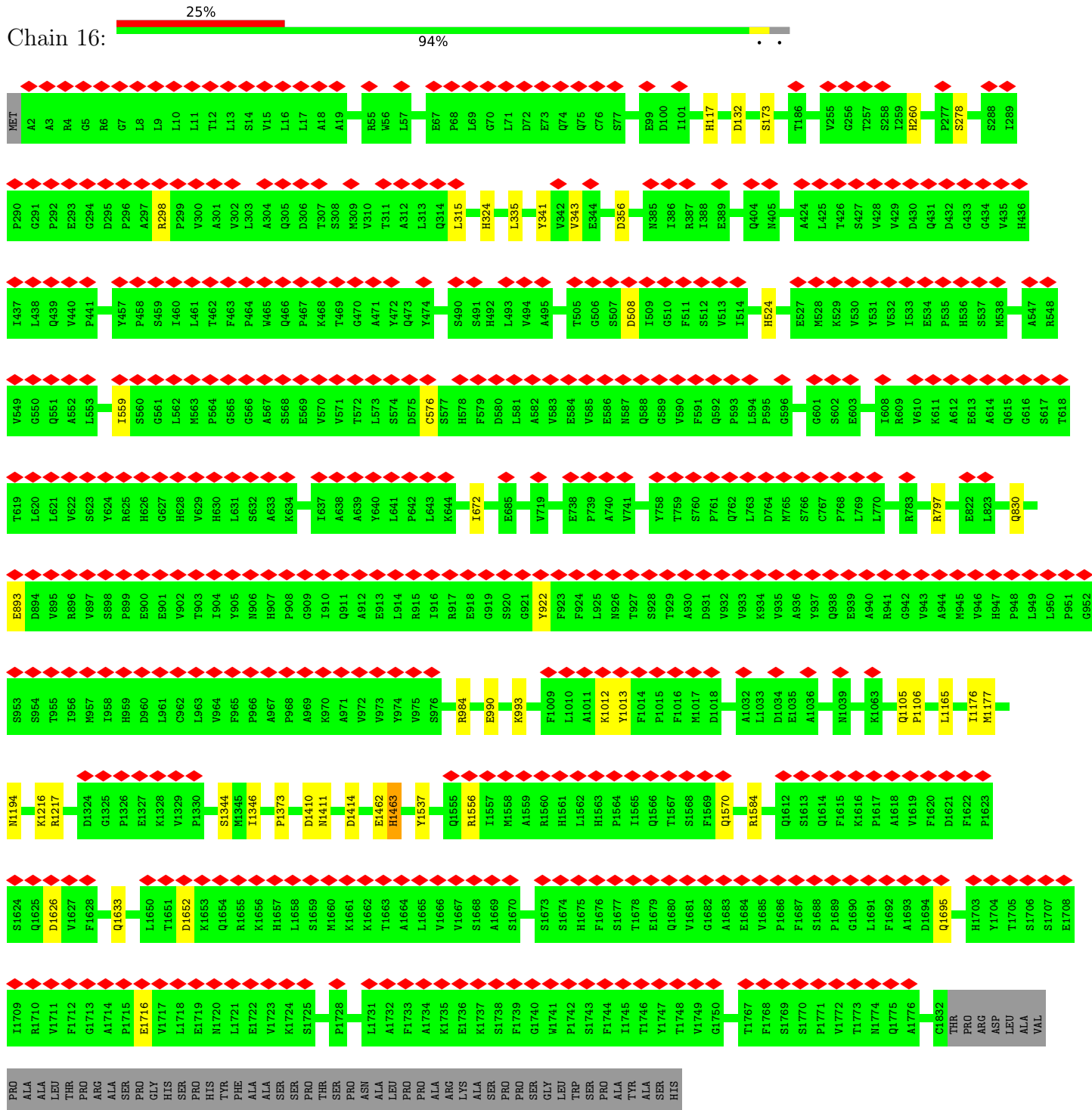
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• Molecule 2: Nuclear pore membrane glycoprotein 210

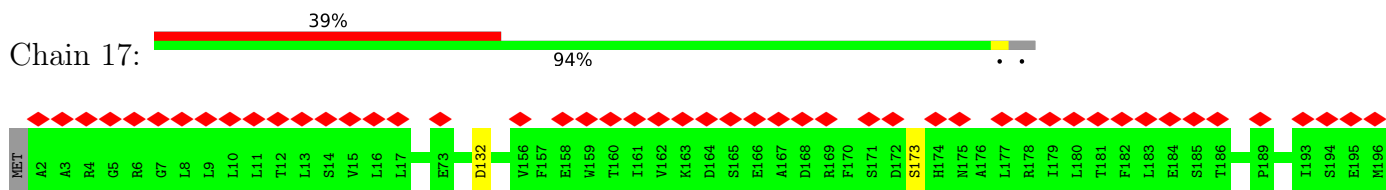
Chain 15:  27% 94%



• Molecule 2: Nuclear pore membrane glycoprotein 210



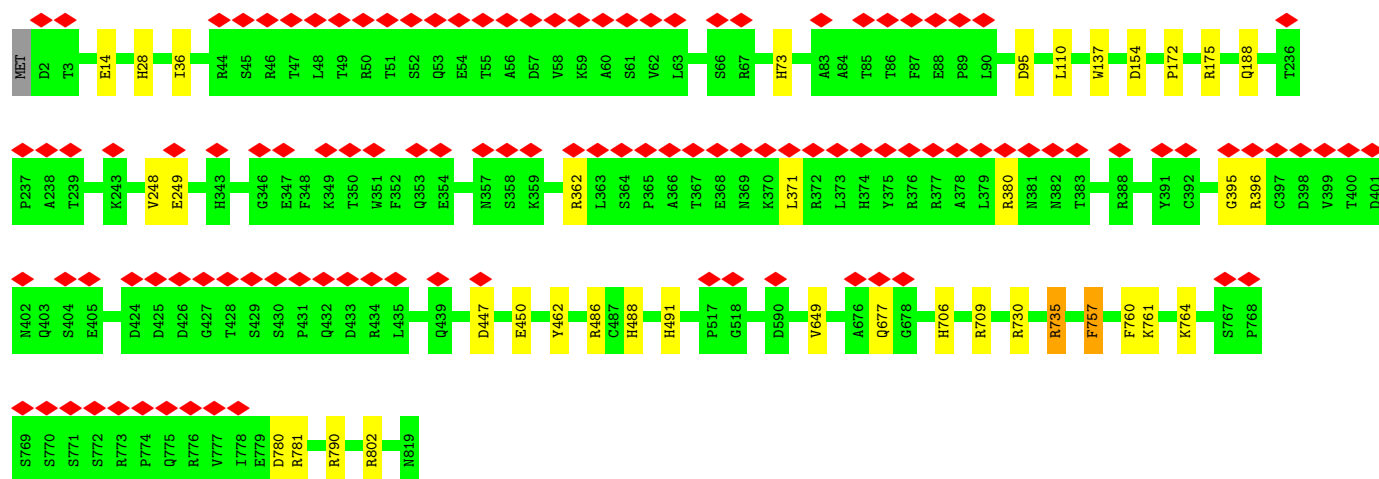
• Molecule 2: Nuclear pore membrane glycoprotein 210



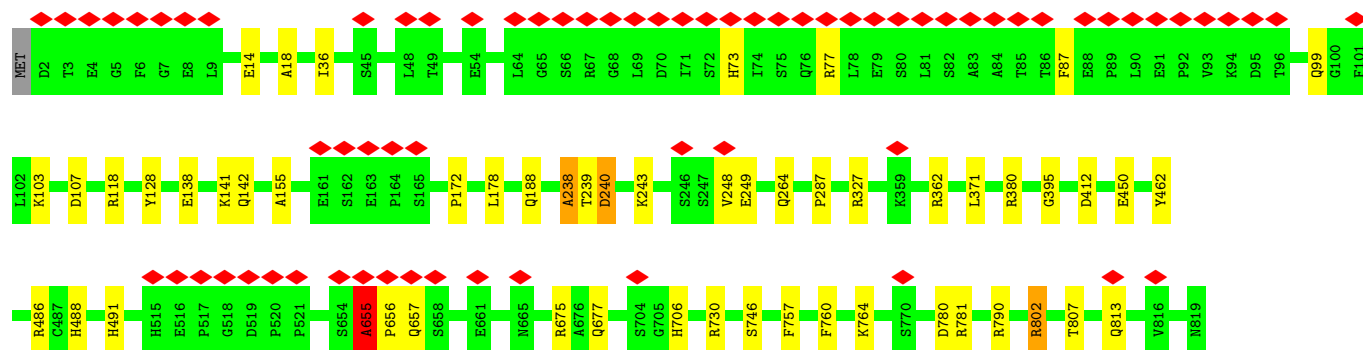




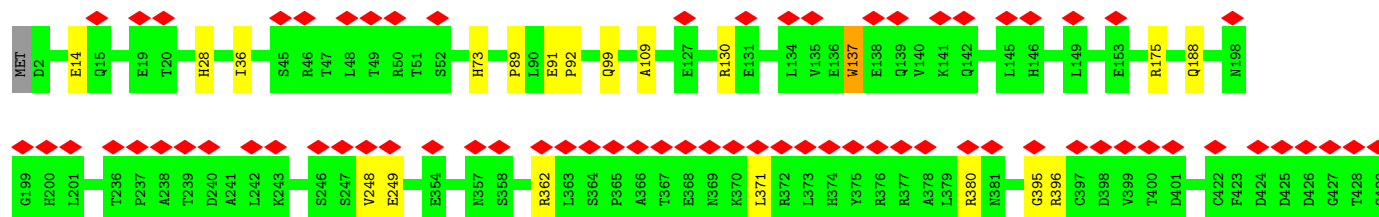
• Molecule 4: Nuclear pore complex protein Nup93

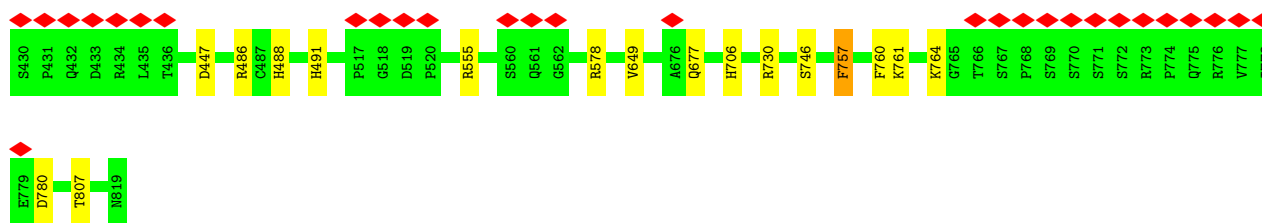


• Molecule 4: Nuclear pore complex protein Nup93

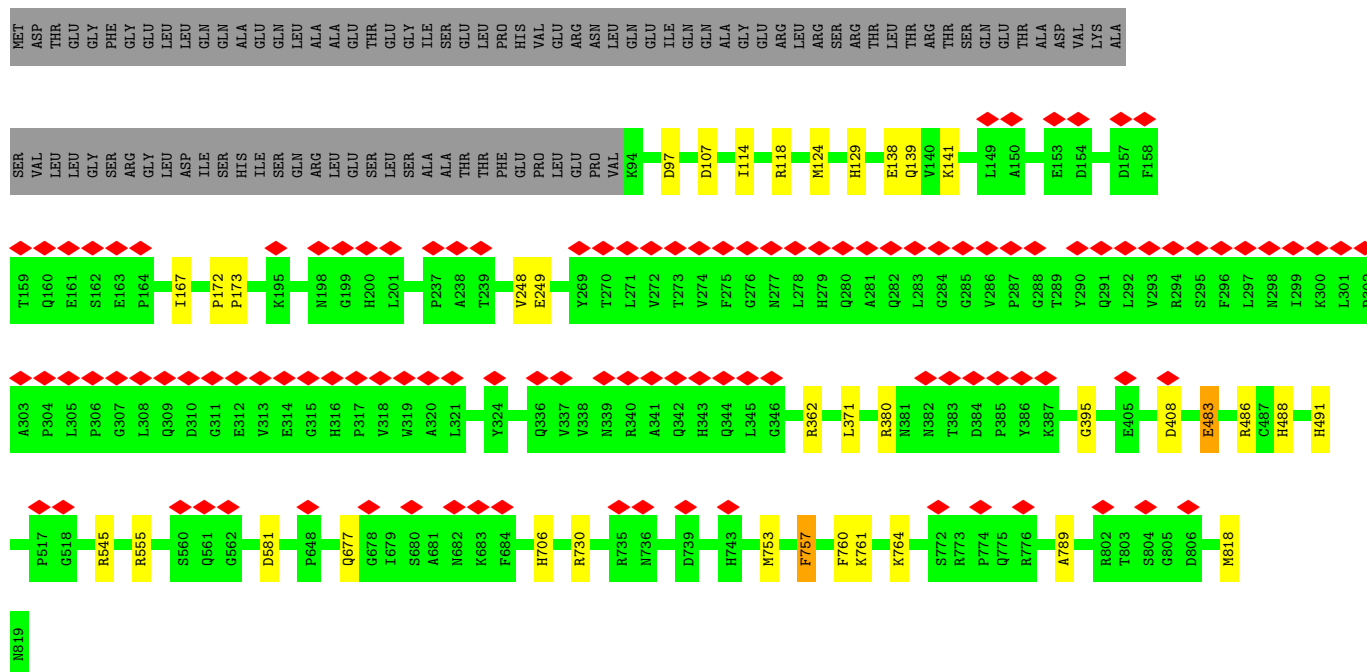
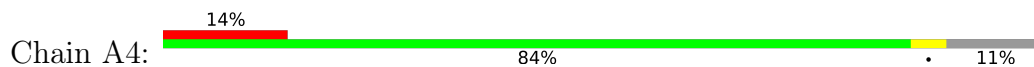


• Molecule 4: Nuclear pore complex protein Nup93

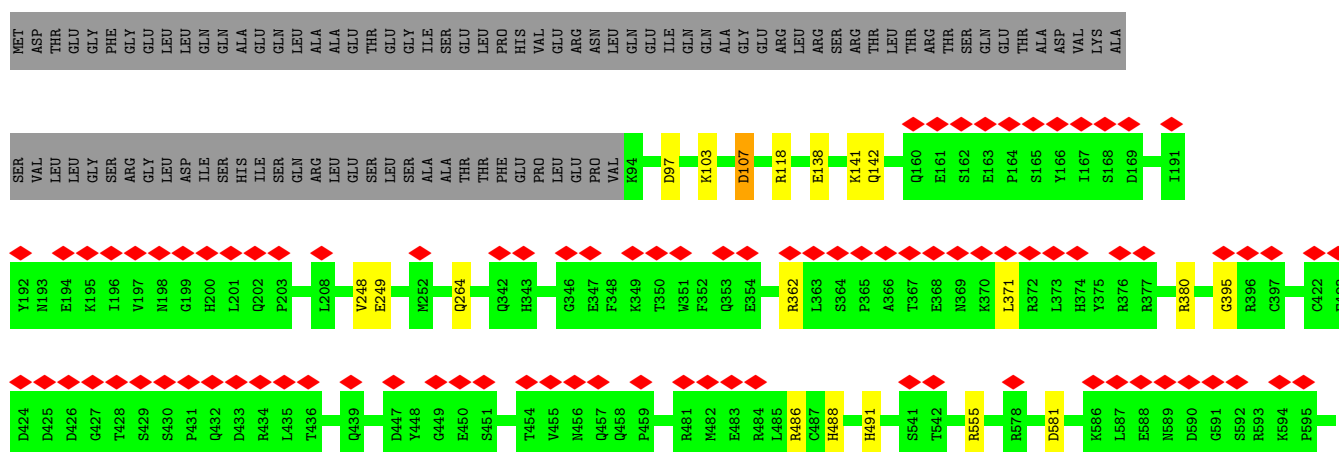
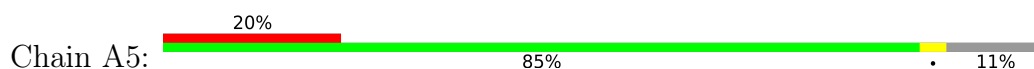


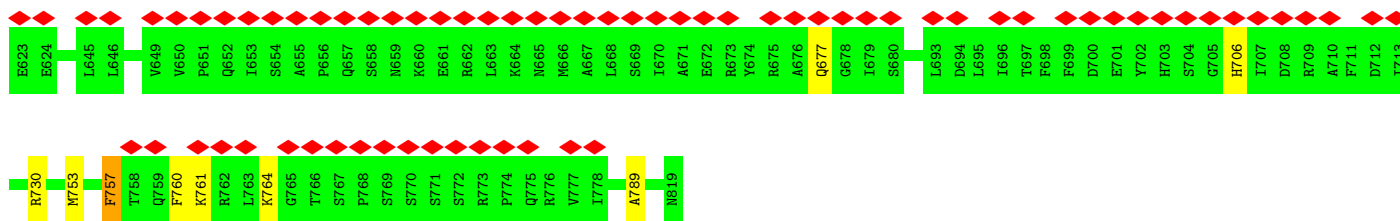


• Molecule 4: Nuclear pore complex protein Nup93



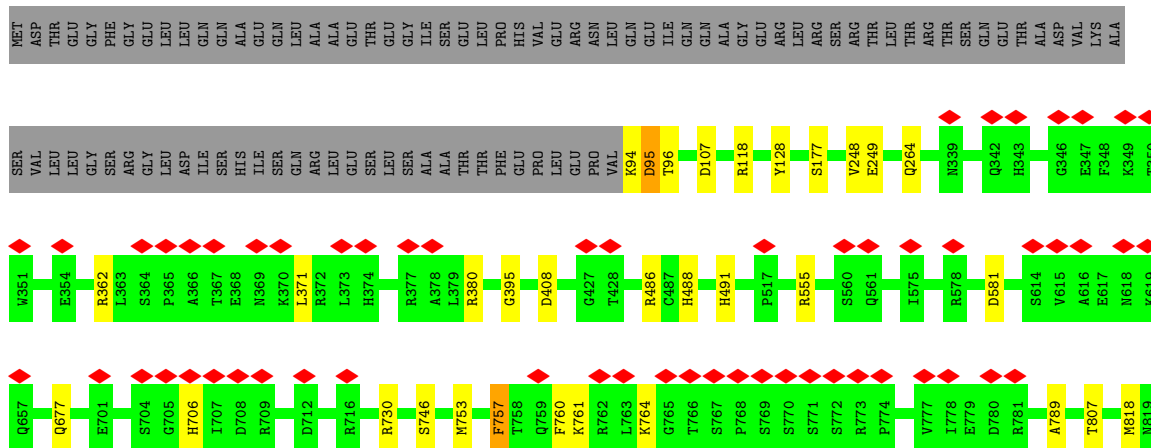
• Molecule 4: Nuclear pore complex protein Nup93





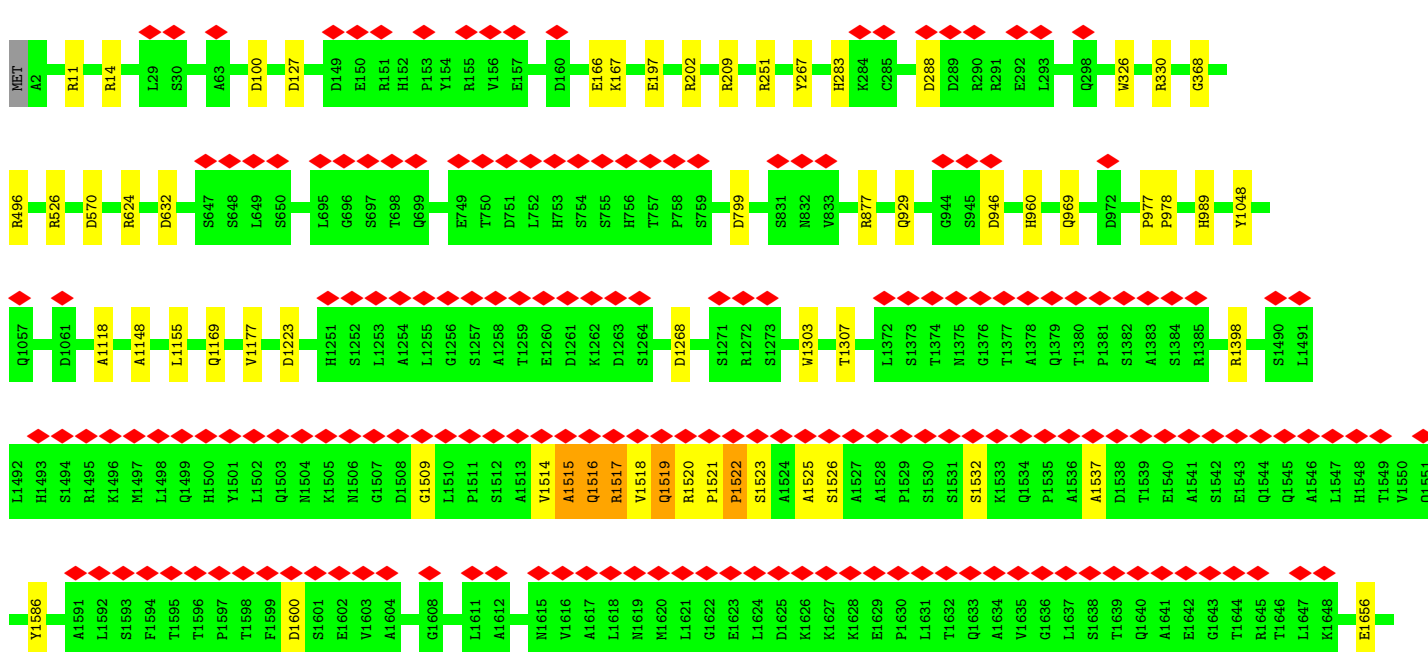
• Molecule 4: Nuclear pore complex protein Nup93

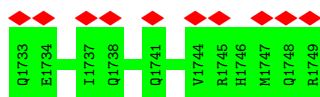
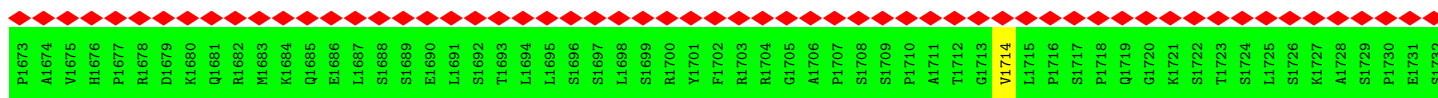
Chain A6: 8% 85% 11%



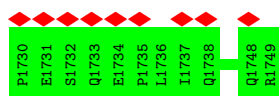
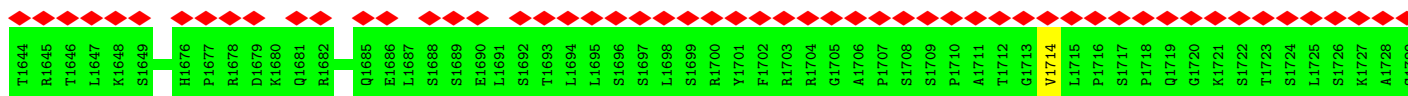
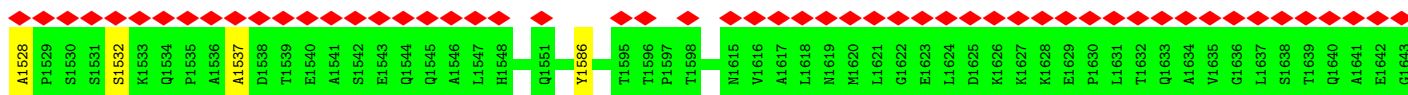
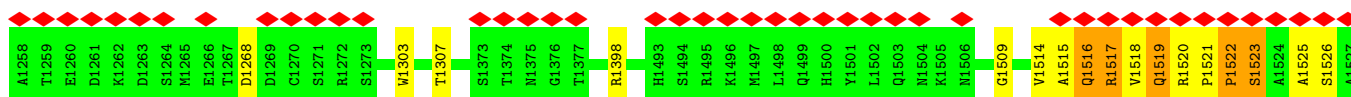
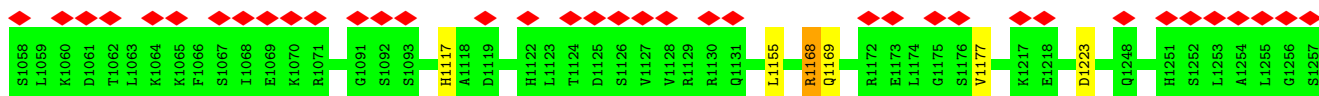
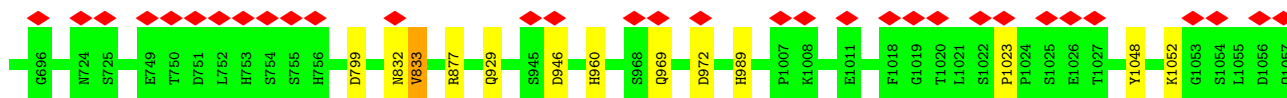
• Molecule 5: Nucleoporin NUP188 homolog

Chain B0: 15% 97%

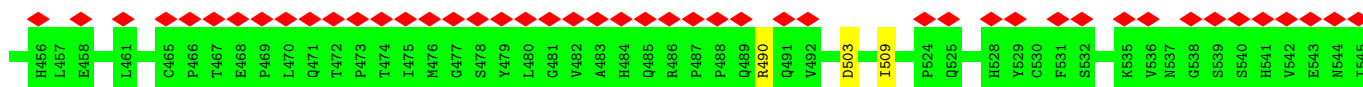
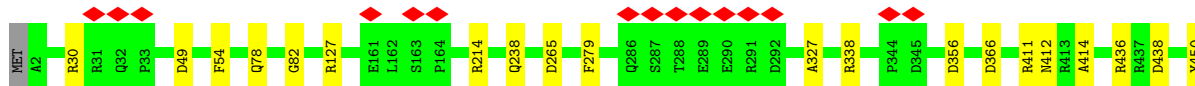


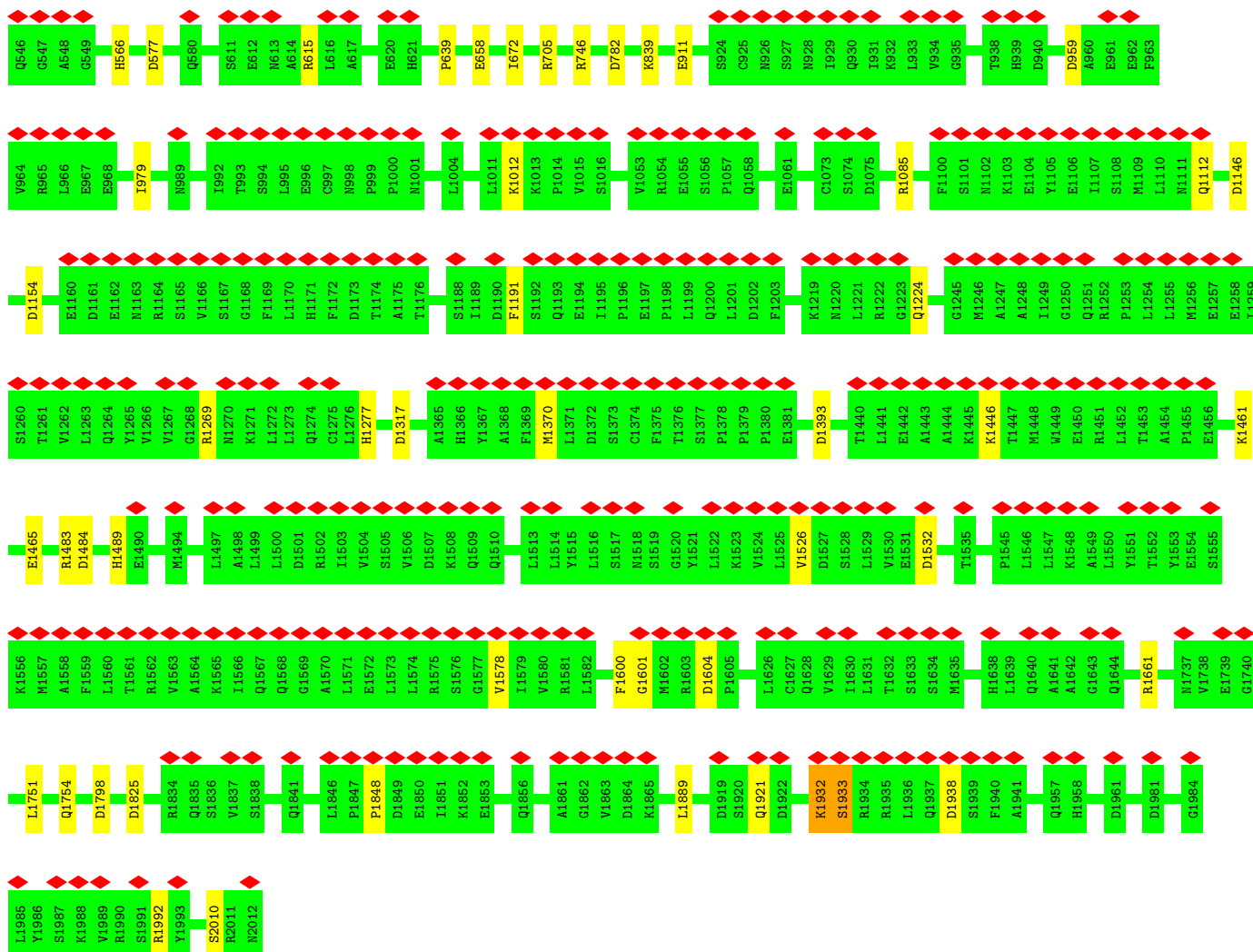


• Molecule 5: Nucleoporin NUP188 homolog

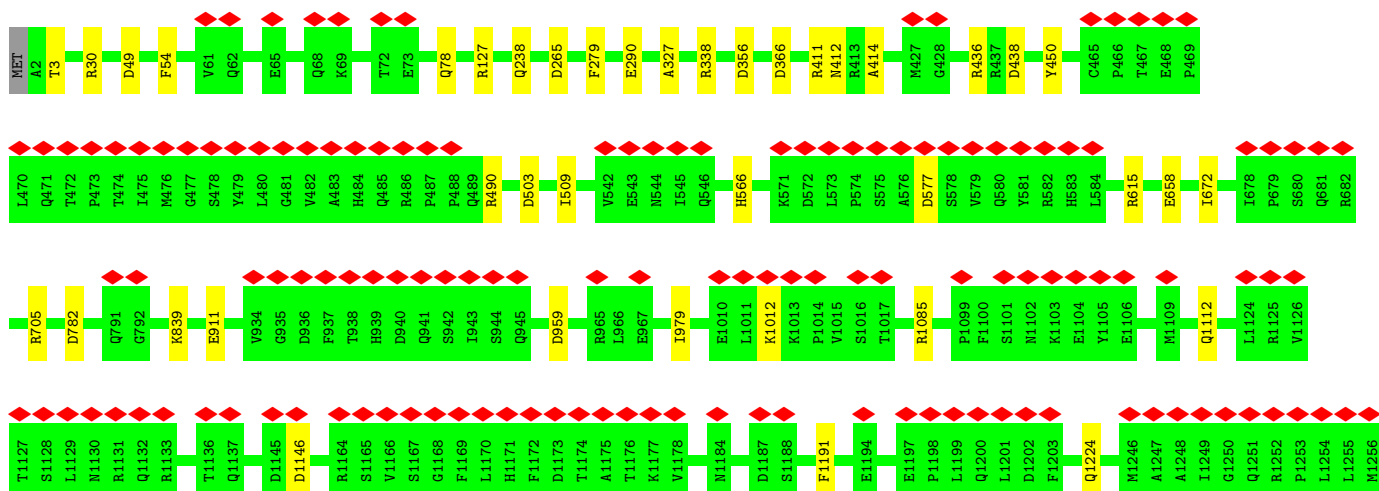


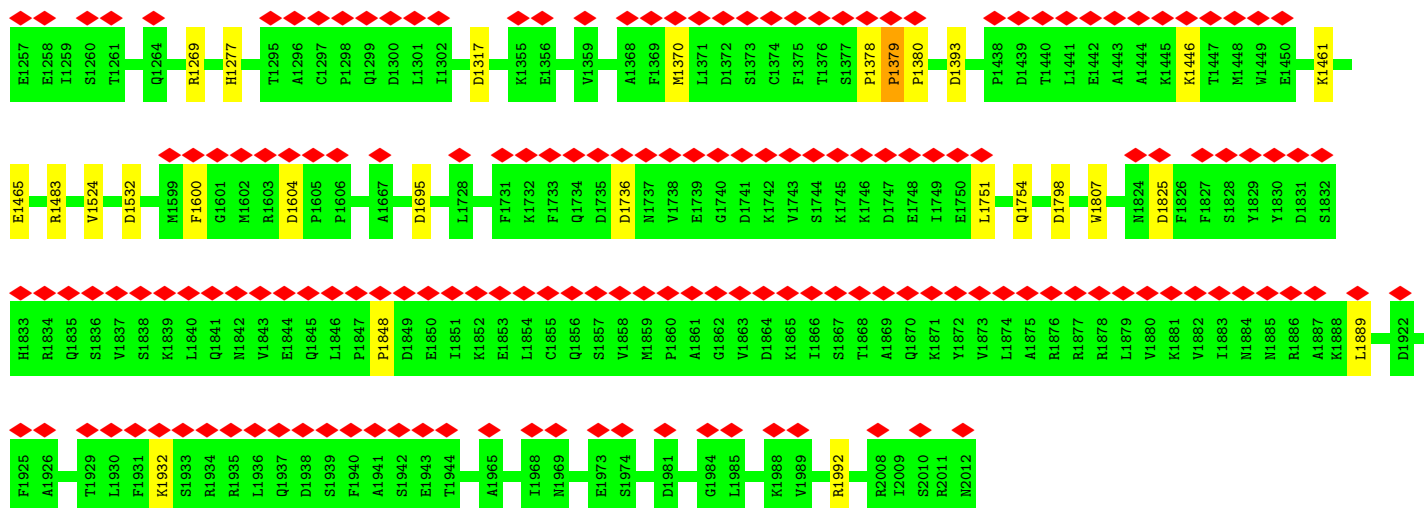
• Molecule 6: Nuclear pore complex protein Nup205



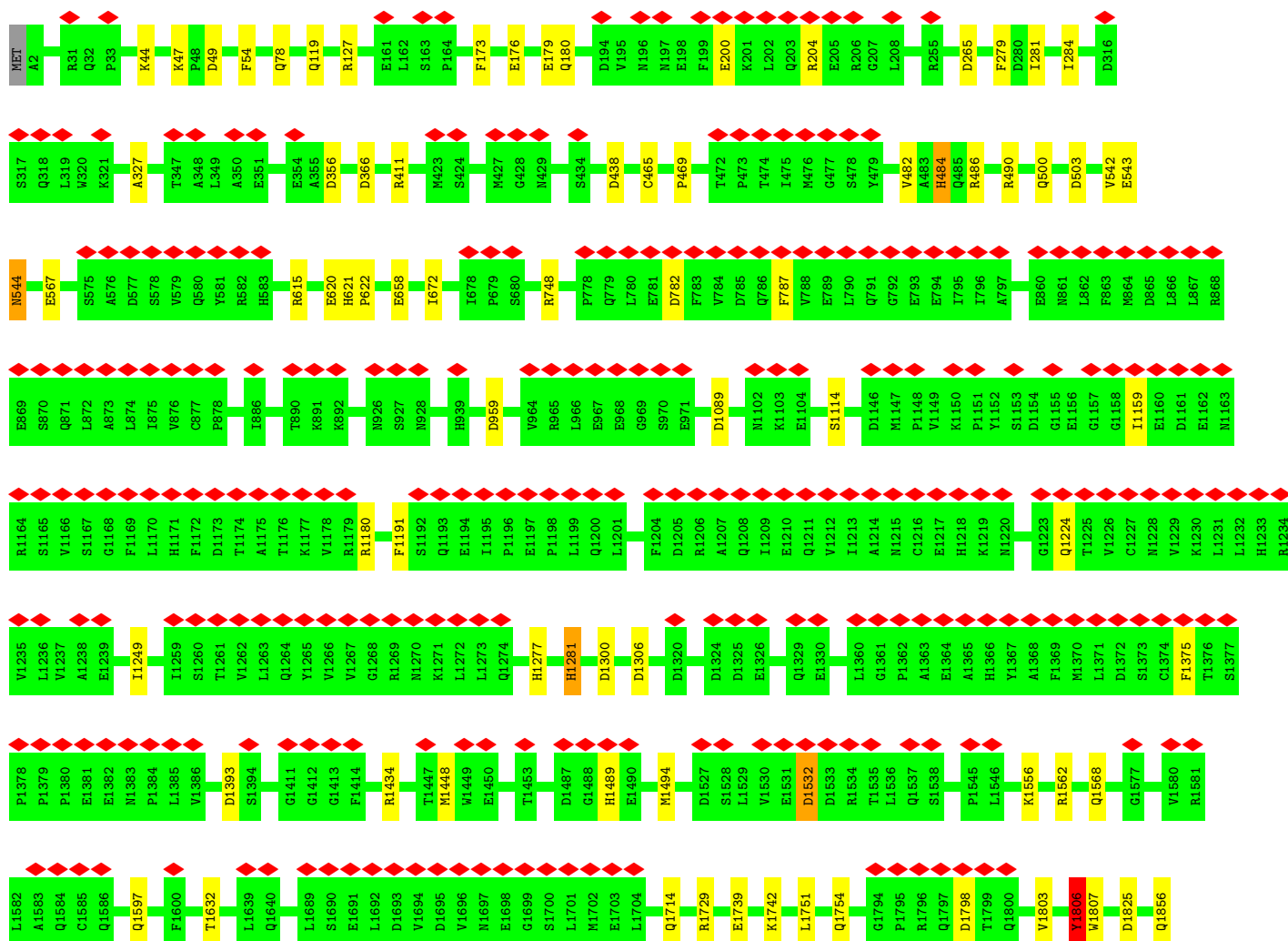


• Molecule 6: Nuclear pore complex protein Nup205





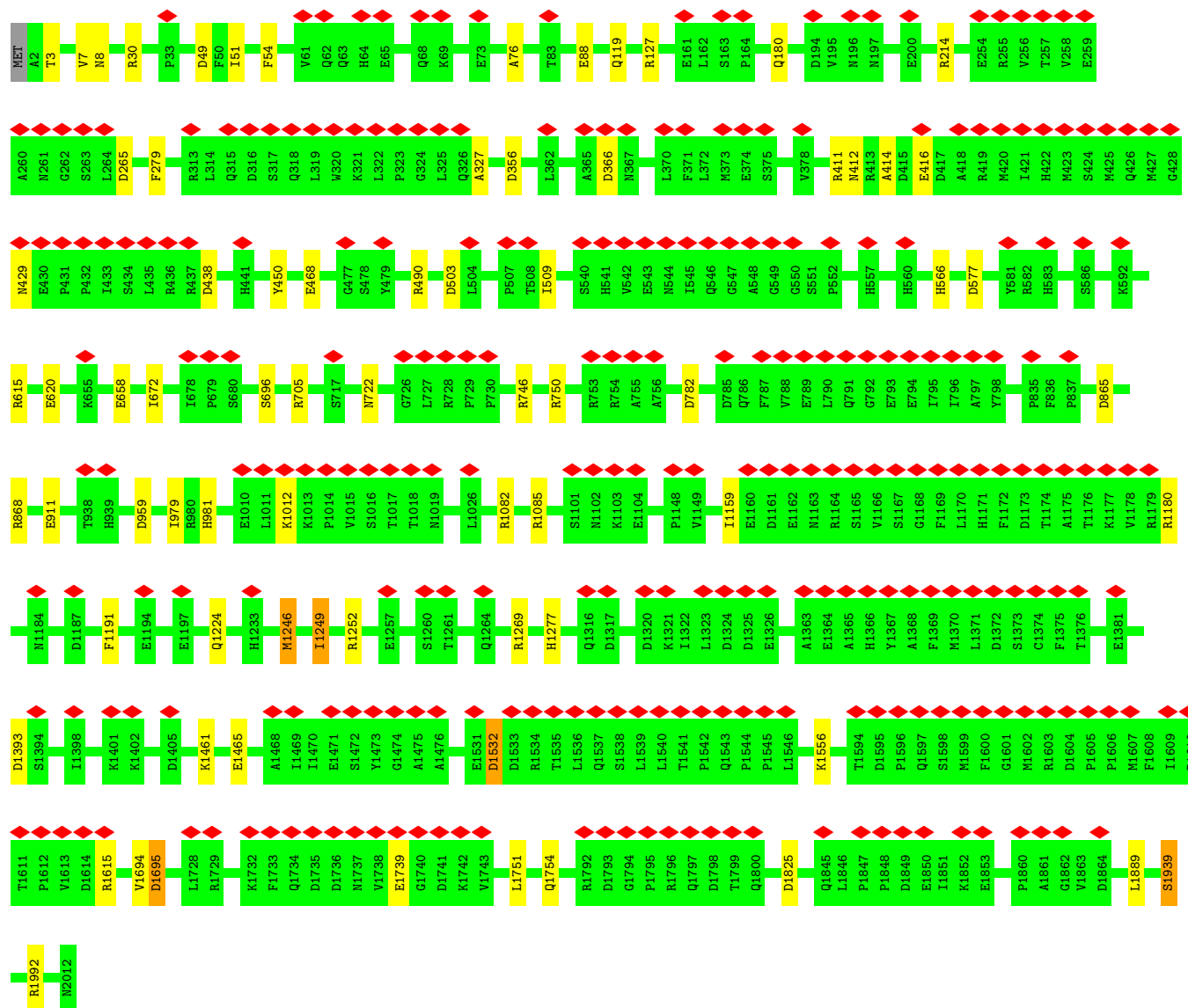
• Molecule 6: Nuclear pore complex protein Nup205





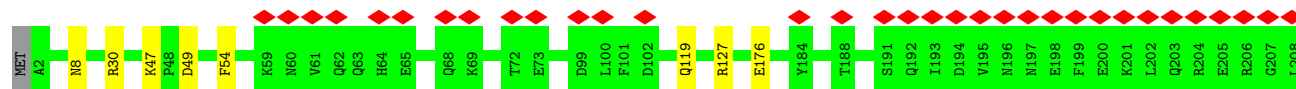
• Molecule 6: Nuclear pore complex protein Nup205

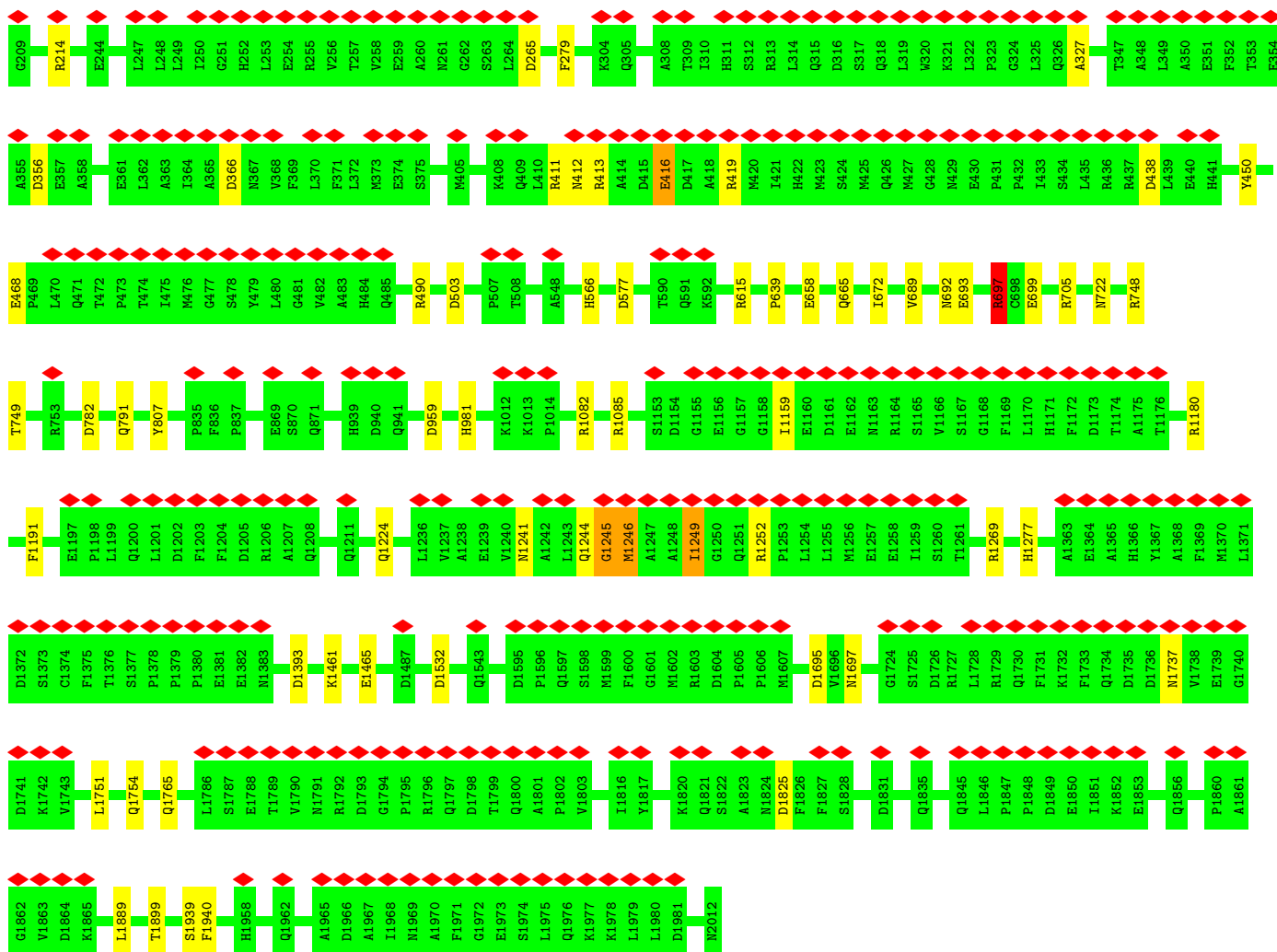
Chain C3: 14% 96%



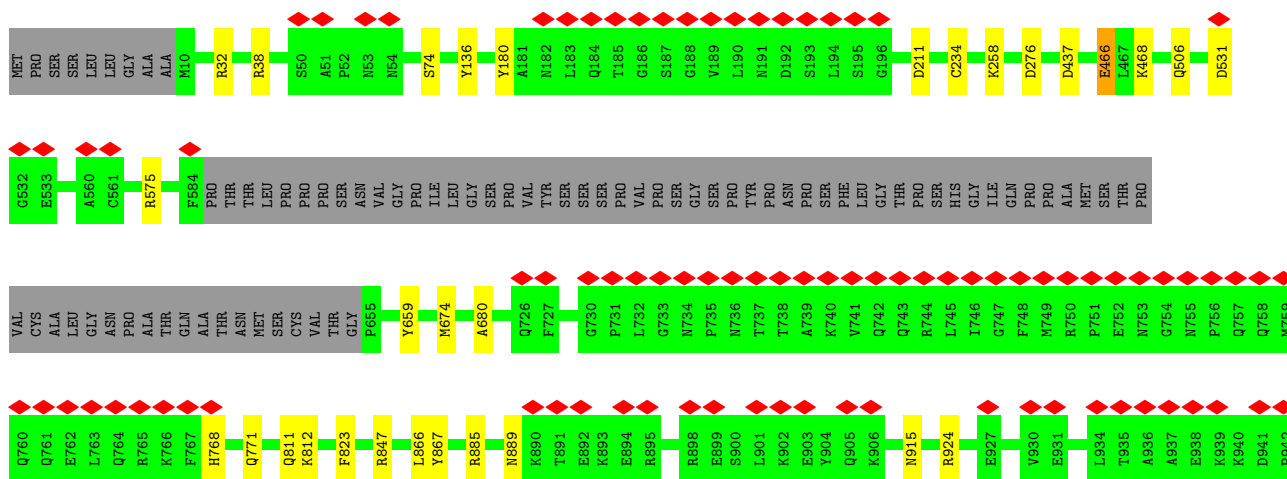
• Molecule 6: Nuclear pore complex protein Nup205

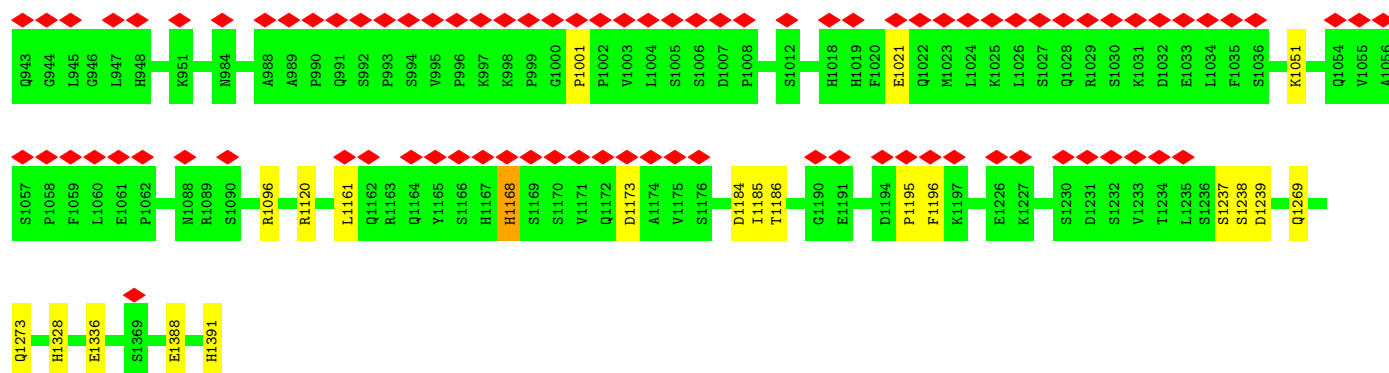
Chain C4: 17% 96%



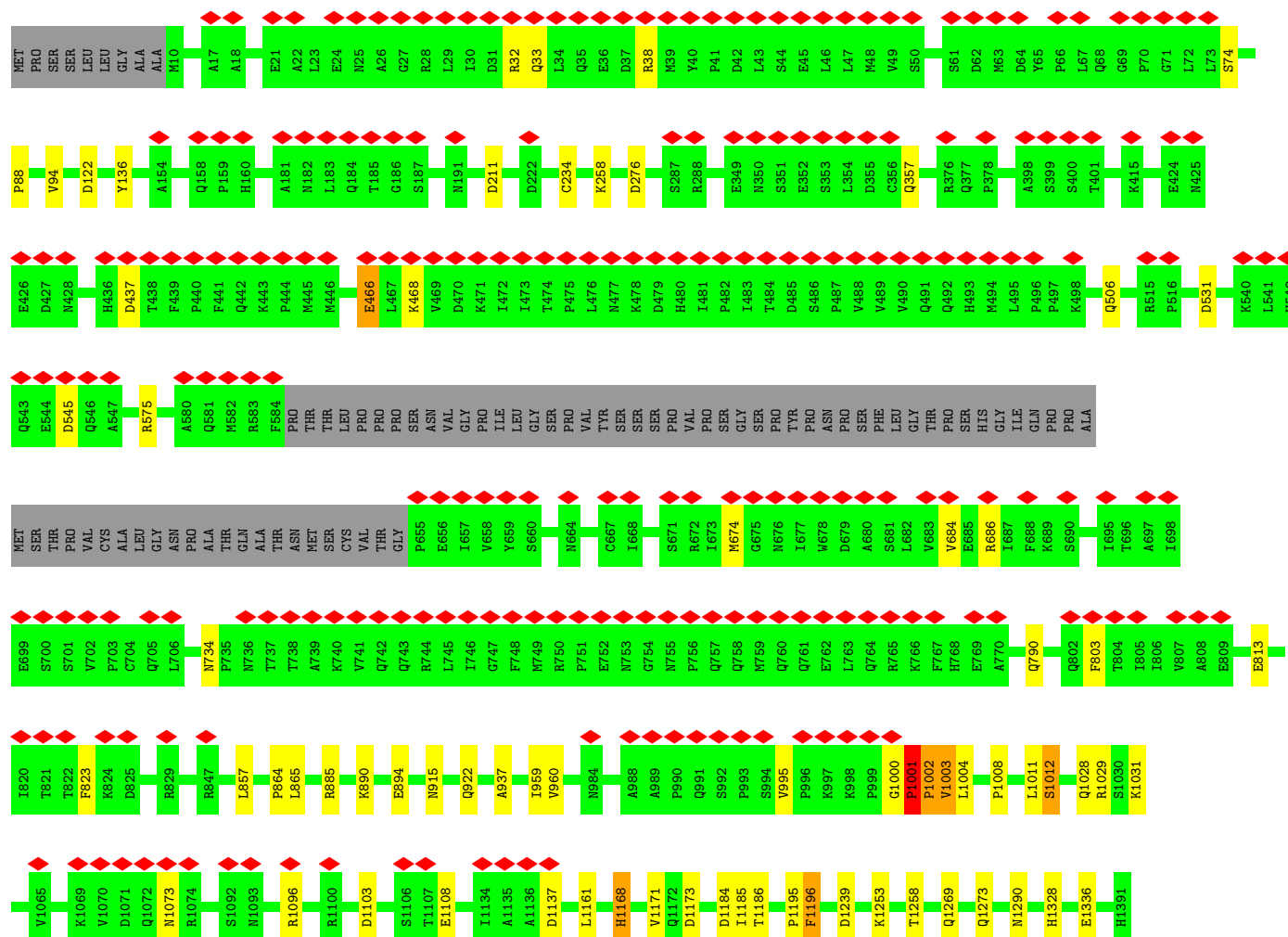
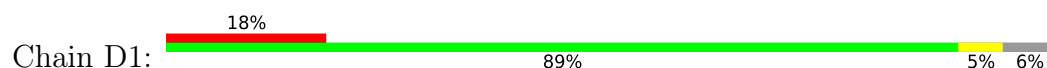


• Molecule 7: Nuclear pore complex protein Nup155



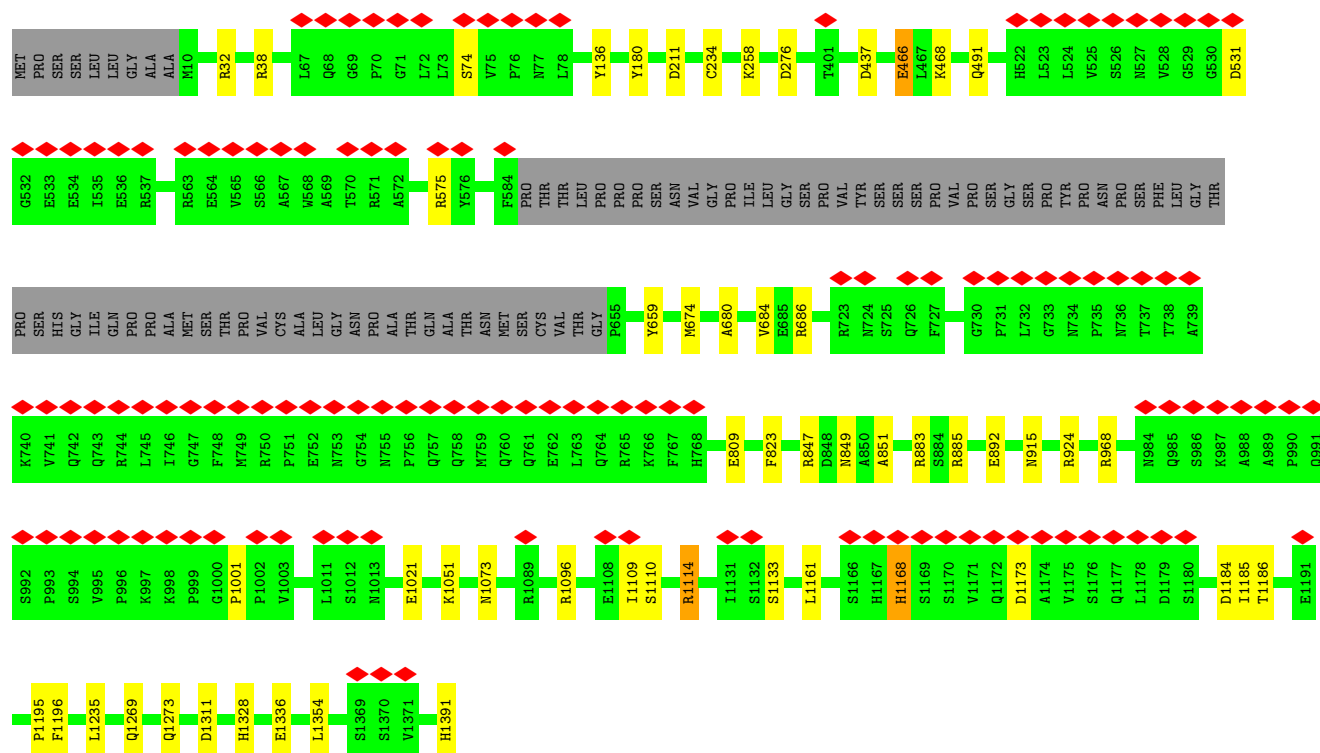


• Molecule 7: Nuclear pore complex protein Nup155

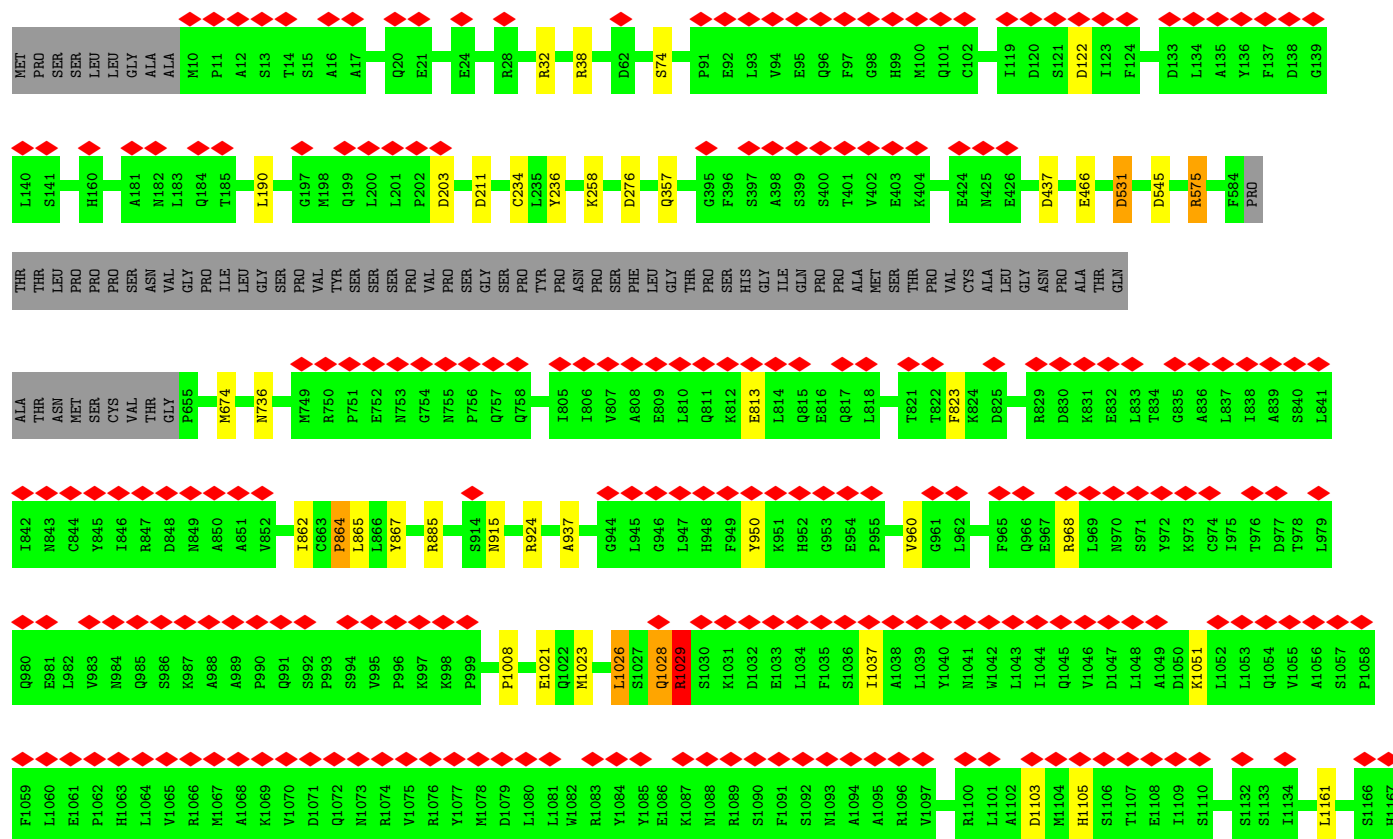
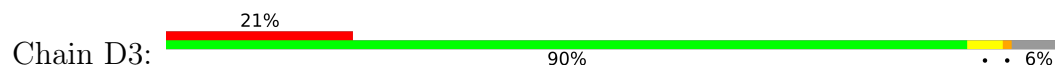


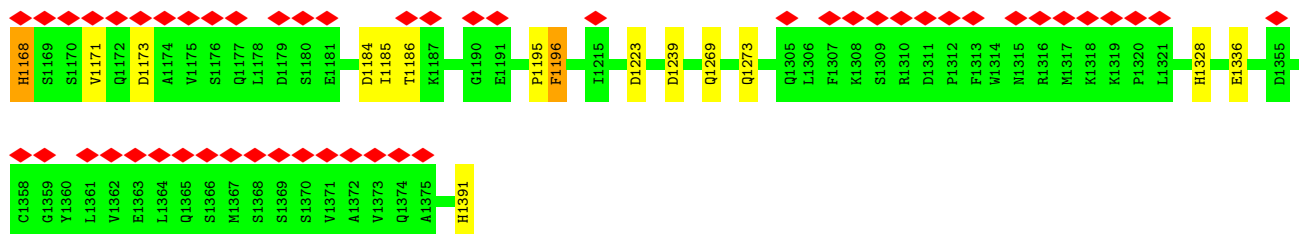
• Molecule 7: Nuclear pore complex protein Nup155



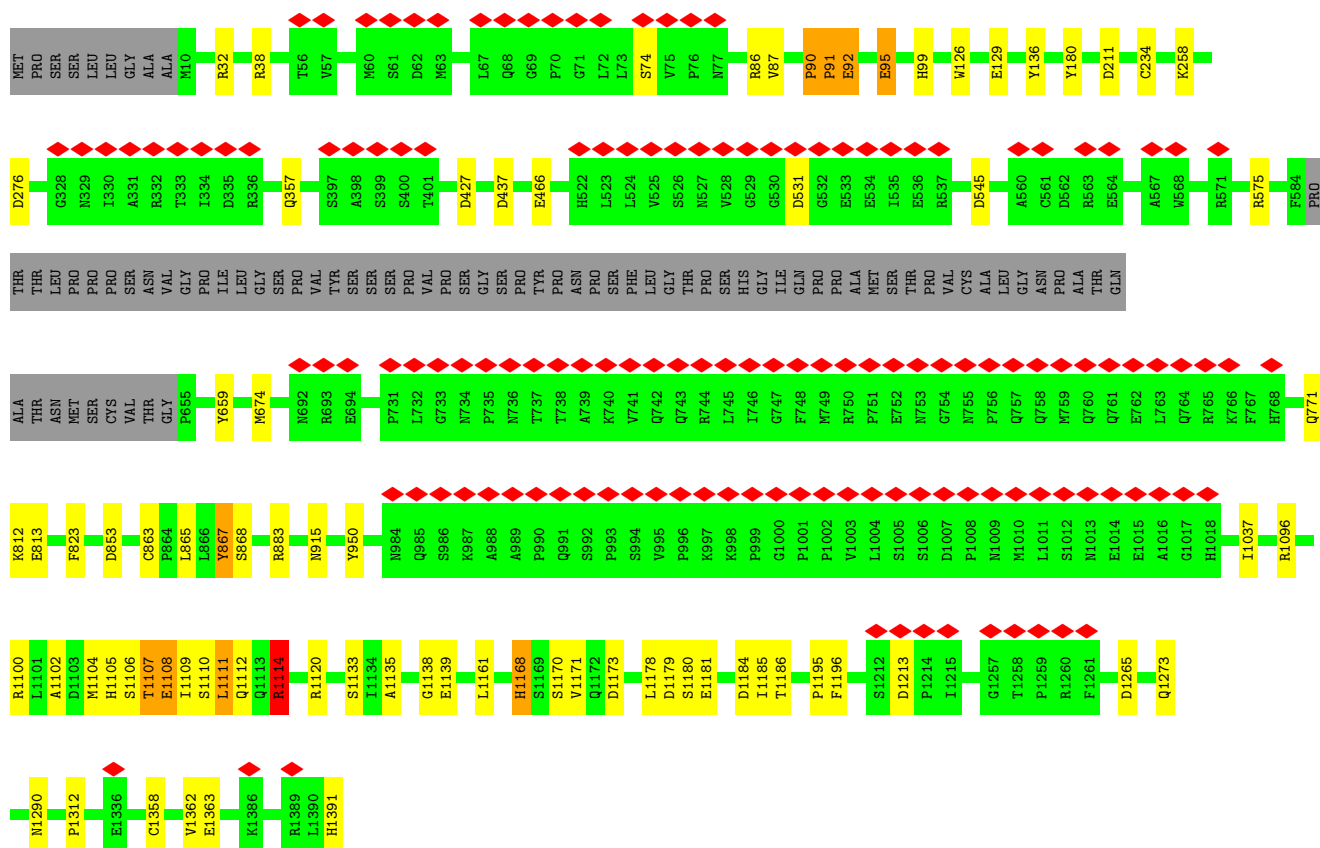
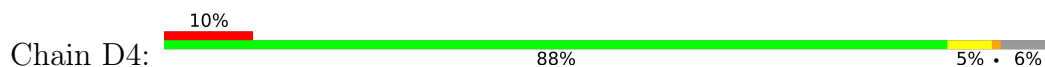


• Molecule 7: Nuclear pore complex protein Nup155



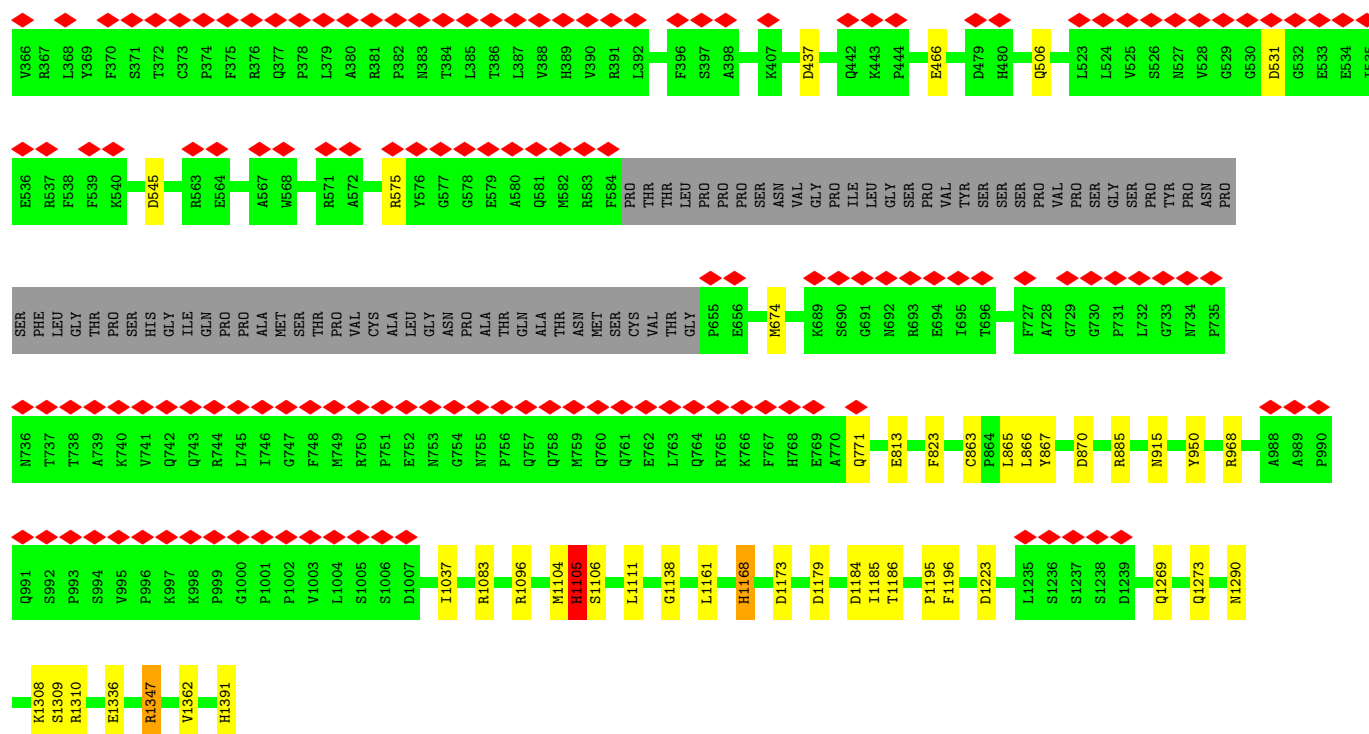


• Molecule 7: Nuclear pore complex protein Nup155

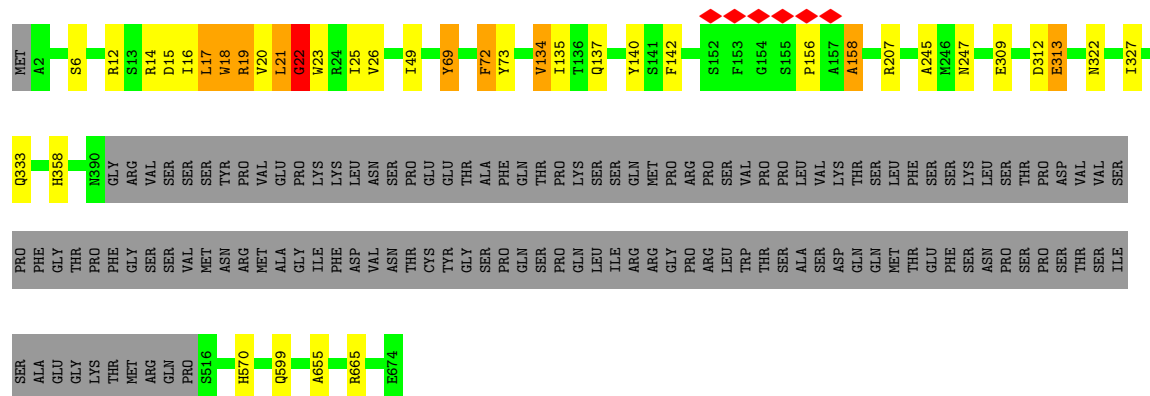
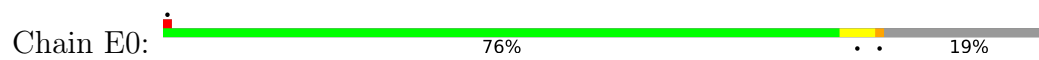


• Molecule 7: Nuclear pore complex protein Nup155

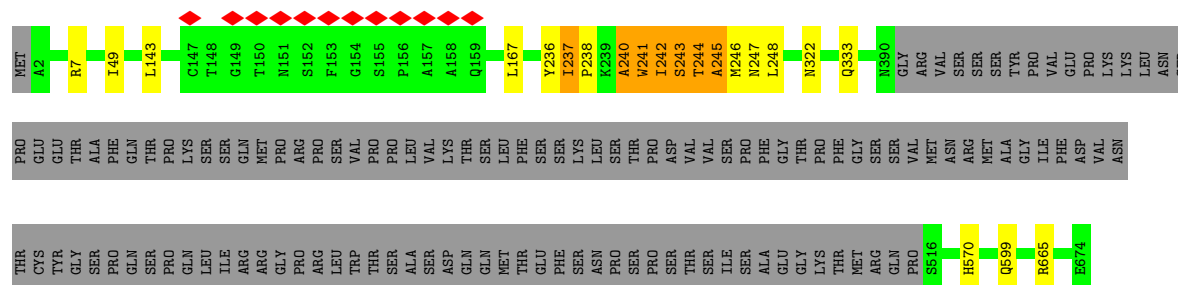
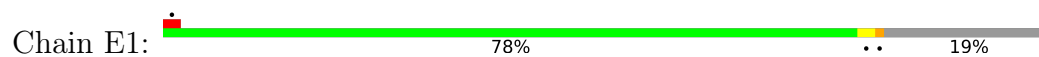




• Molecule 8: Nucleoporin NDC1



• Molecule 8: Nucleoporin NDC1



• Molecule 9: Nucleoporin NUP35



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

VAL MET MET MET ARG SER PRO LEU LEU ALA GLY ALA LEU SER PRO PRO GLN VAL VAL PRO ALA HIS LYS ASP LYS S86 D96 S105 T106 P107 L108 T109 T110 R111 R112 Q113 P114 N115 I116 M119 Q120 S121 P122 L123 V124 G125 V126 G131 T132 G133 Q134 S135 D163 D172

D173 K218 E234 K241 R254 K269 T270 P274 T275 Q301 V302 I303 Q307 T308 P309 K310 W326

• Molecule 9: Nucleoporin NUP35



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

VAL MET MET MET ARG SER PRO LEU LEU ALA GLY ALA LEU SER PRO PRO GLN VAL VAL PRO PRO ALA HIS LYS ASP LYS S86 D96 S109 L103 L108 T109 T110 R111 R112 Q113 P114 M115 I116 S117 V118 M119 Q120 S121 V124 G131 L165 T166 S167 E168 D169 H170 P182

Q183 A184 S185 A186 S187 Y196 M206 T207 K218 L219 R222 E234 S235 L257 S258 S259 P260 S261 L262 A263 F264 T265 P266 I268 K269 T270 L271 Q272 T273 T274 T275 Q276 T277 G278 S279 T280 S284 T285 Y293 K294 A295 S296 Y300 S304 D305 R306 Q307 T308 P309

K310 K311 W326

• Molecule 9: Nucleoporin NUP35

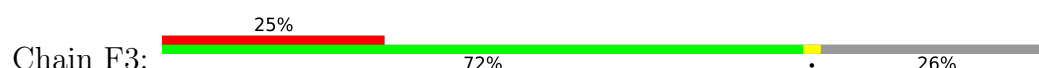


MET ALA ALA PHE MET ARG VAL GLU PRO GLN GLY PRO GLY ALA LEU GLY SER PRO MET MET LEU MET GLY PRO THR SER PRO LYS PRO GLY VAL ASN ALA GLN PHE LEU PRO GLY PHE LEU MET GLY ASP LEU PRO ALA VAL THR PRO GLN ARG PRO ILE SER GLY PRO SER VAL GLY

VAL MET MET MET ARG SER PRO LEU LEU ALA GLY ALA LEU SER PRO PRO GLN VAL VAL PRO PRO ALA HIS LYS ASP LYS S86 G87 A88 D96 G102 L103 G104 S105 T106 P107 L108 T109 S110 R111 R112 Q113 P114 M115 I116 S117 V118 M119 Q120 S121 L123 V124 F137 S138 P139 A140

R146 K147 T148 T149 L150 S151 P152 Q154 L155 D156 D163 S164 L165 T166 S167 E168 D169 H170 D173 Q183 A184 Y196 N206 T207 R230 Q233 E234 K241 K246 E250 R254 T297 S304 T308 W326

• Molecule 9: Nucleoporin NUP35



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



Chain H2:

GLY
LEU
ASN
GLU
THR
ILE
HIS
ILE
ARG
GLY
GLY
VAL
PHE
SER

- Molecule 10: Nucleoporin p54

Chain H3:

L477	I478	S479	I480	I481	K482	D483	D484	L485	E486	D487	I488	K489	L490	V491	E492	H493	GLY	LEU	ASN	GLU	THR	ILE	HIS	ILE	ARG	GLY	GLY	VAL	PHE	SER
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 11: Nucleoporin p58/p45

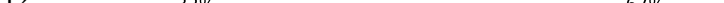
Chain I0:

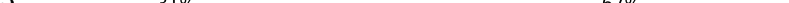
[illegible]



Chain J0:

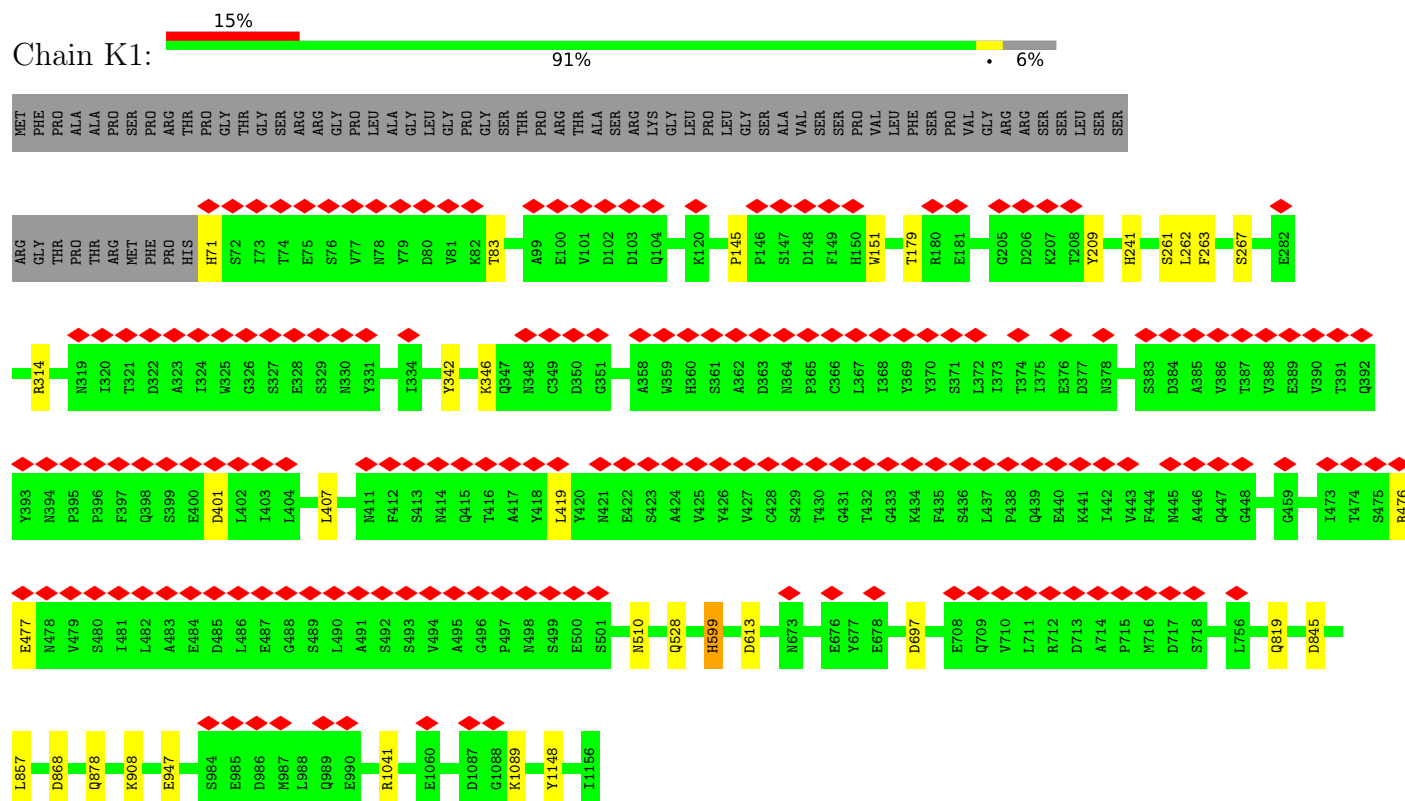


Chain J2: 

Chain J3: 

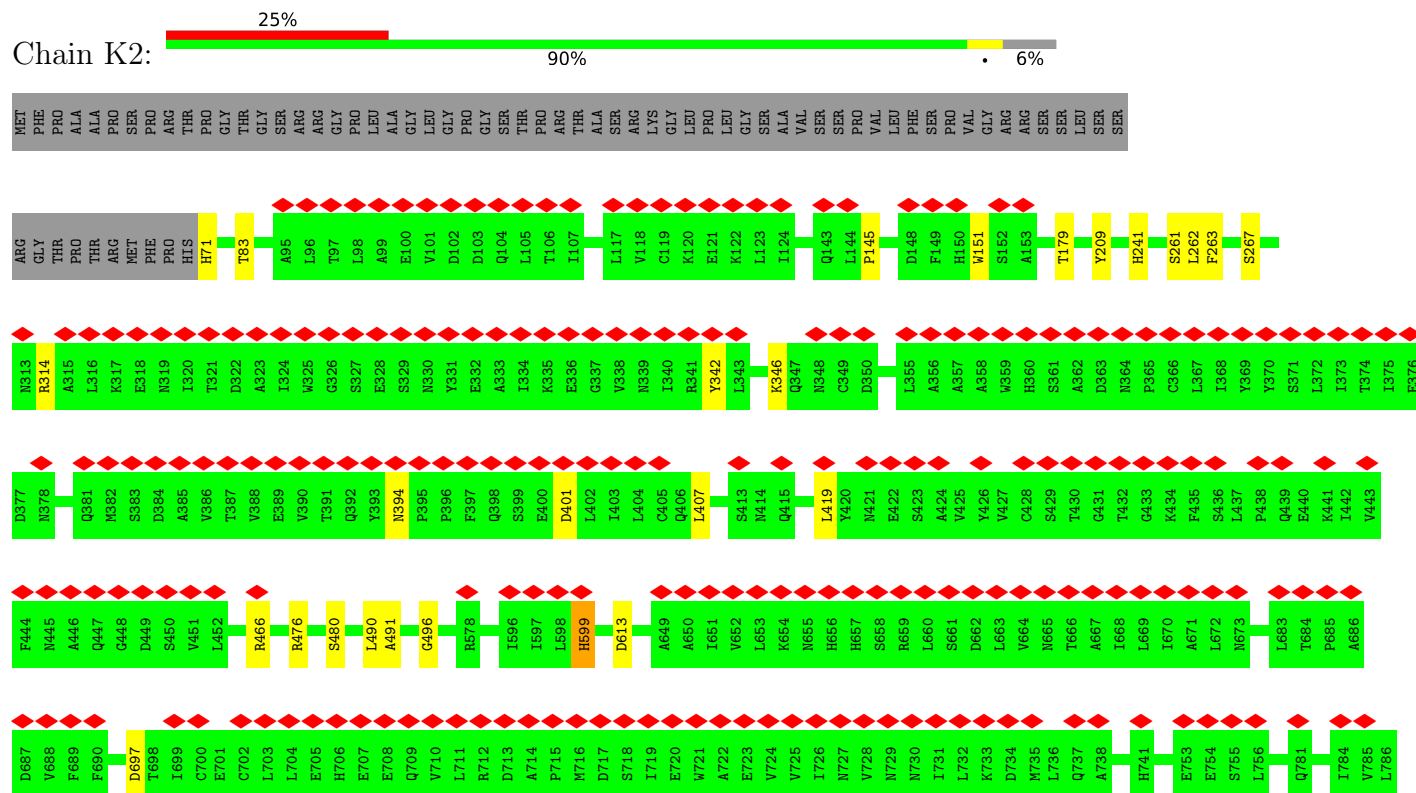
• Molecule 13: Nuclear pore complex protein Nup133

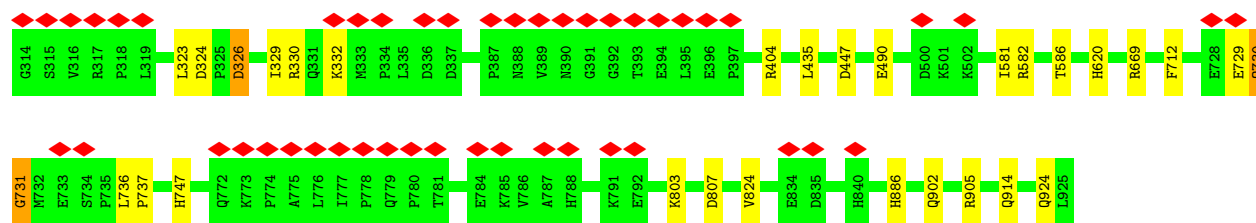
Chain K1:



• Molecule 13: Nuclear pore complex protein Nup133

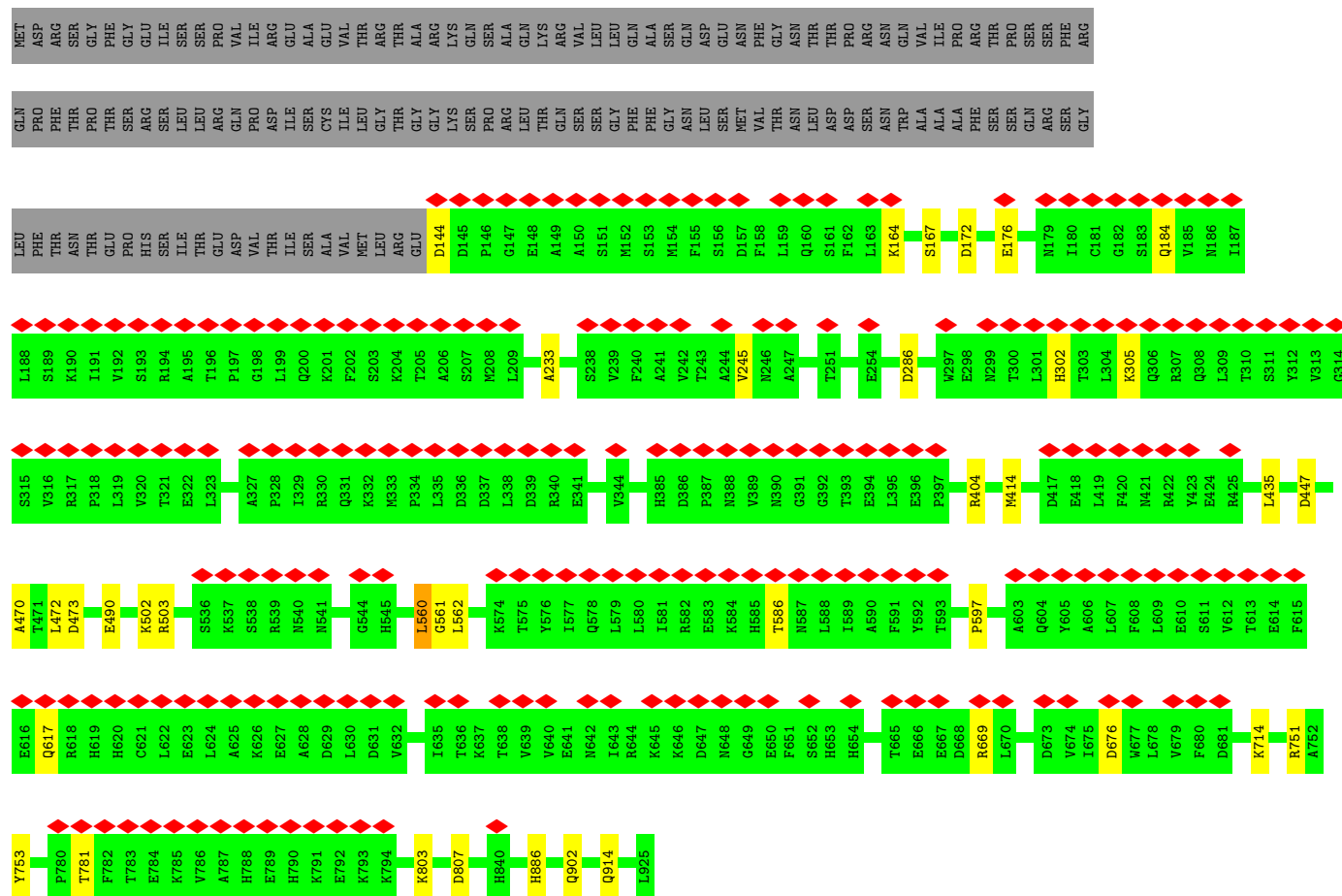
Chain K2:





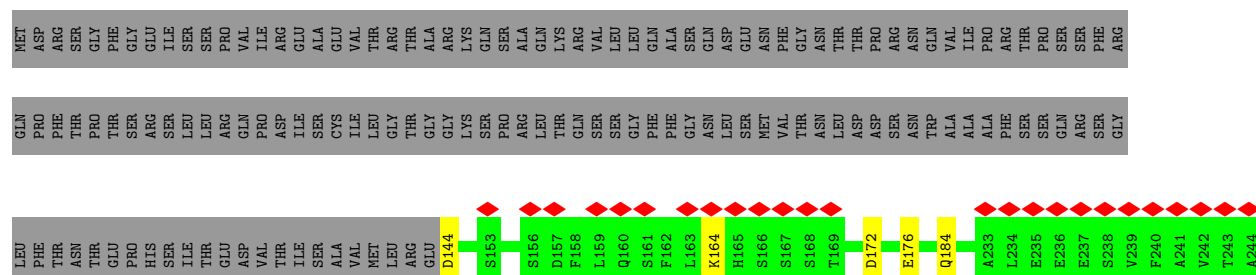
• Molecule 14: Nuclear pore complex protein Nup107

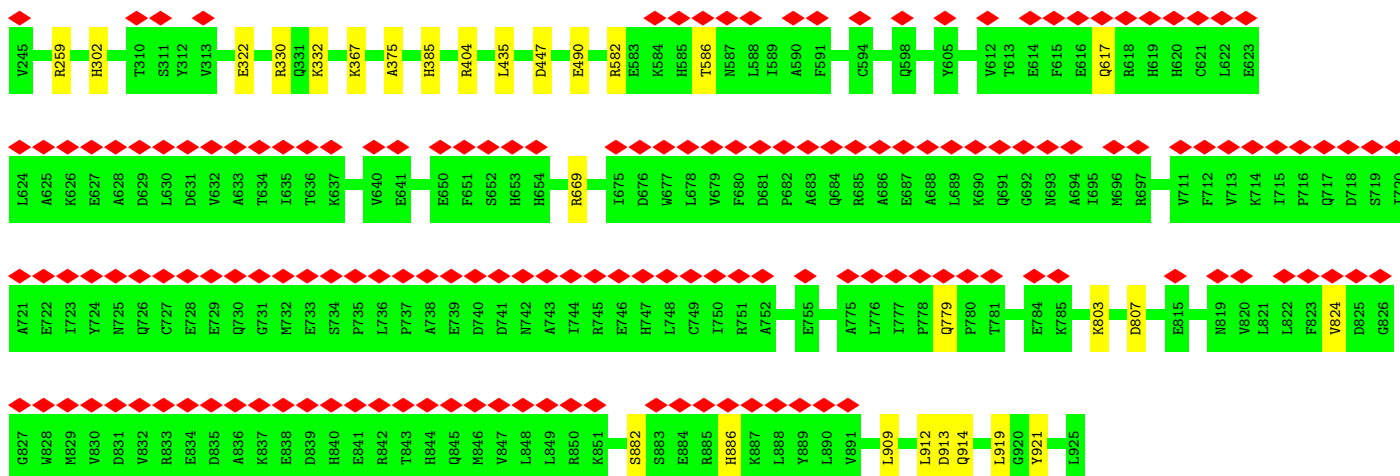
Chain L1: 24% 80% 15%



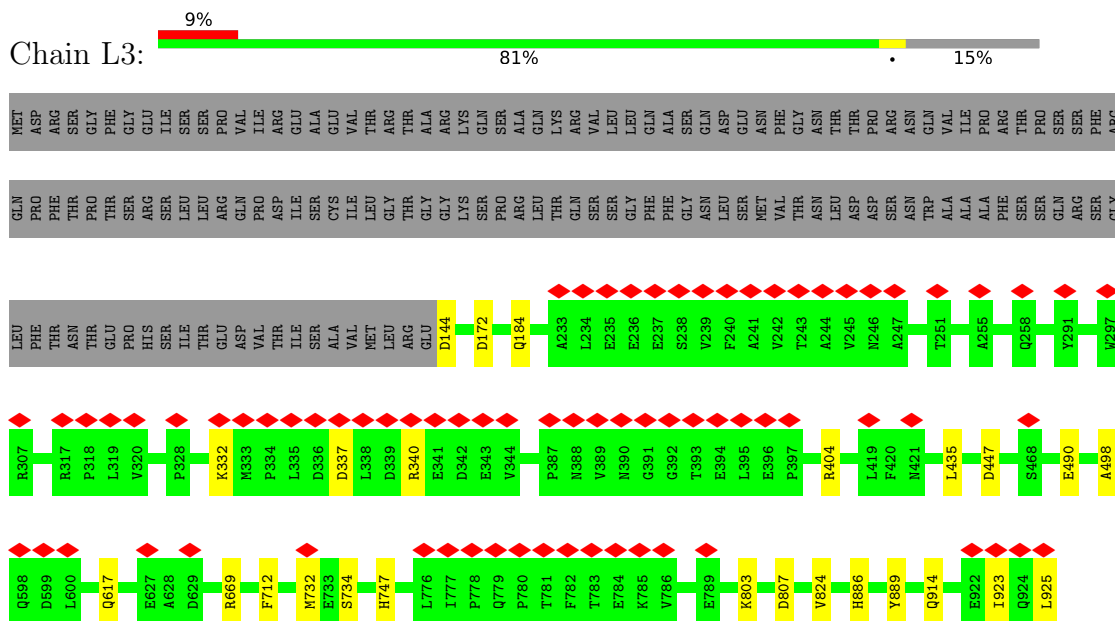
• Molecule 14: Nuclear pore complex protein Nup107

Chain L2: 20% 81% 15%

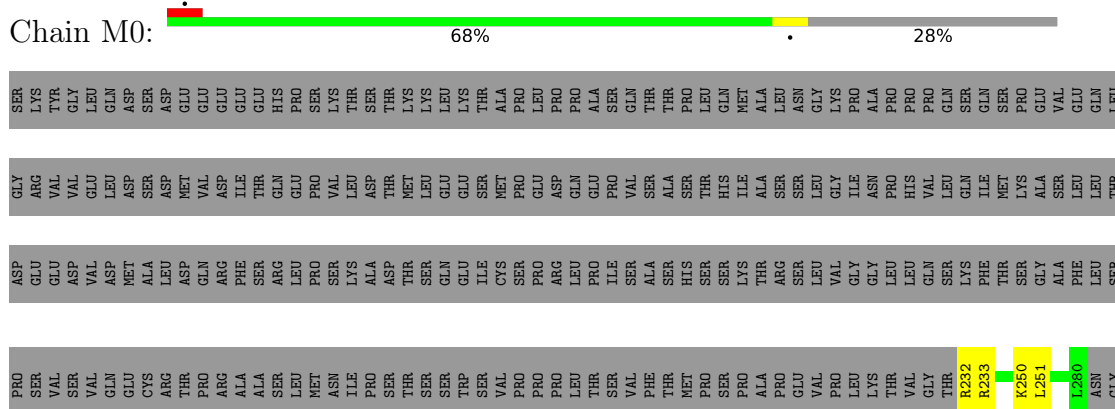


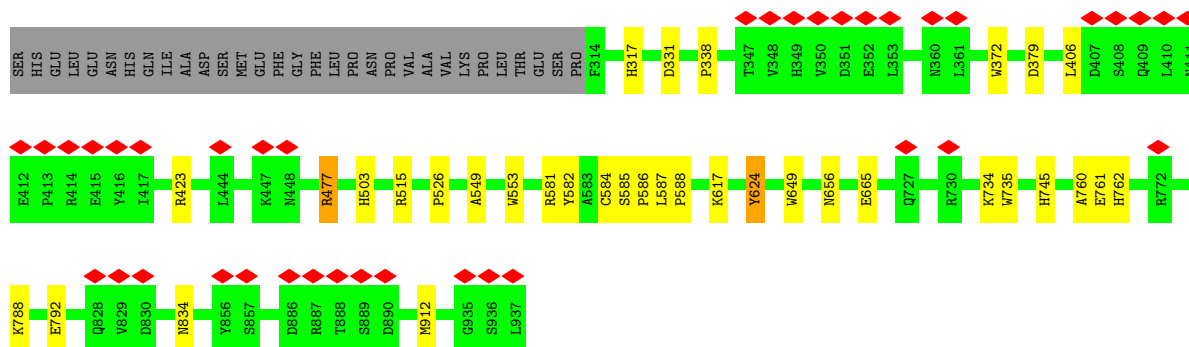


• Molecule 14: Nuclear pore complex protein Nup107

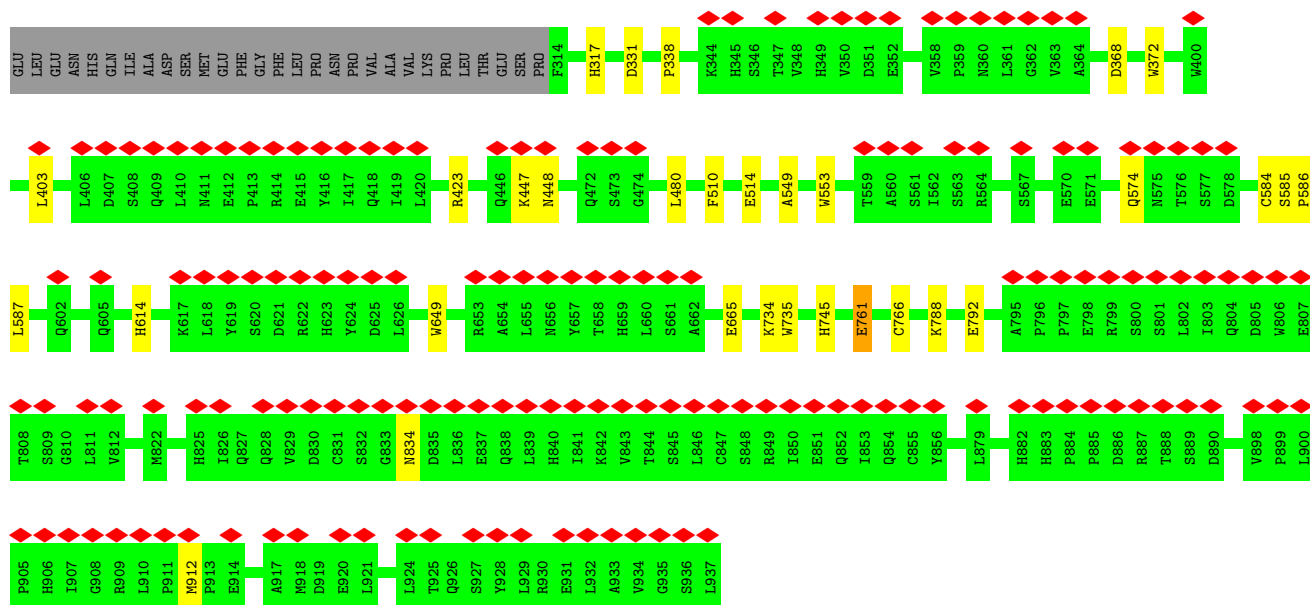
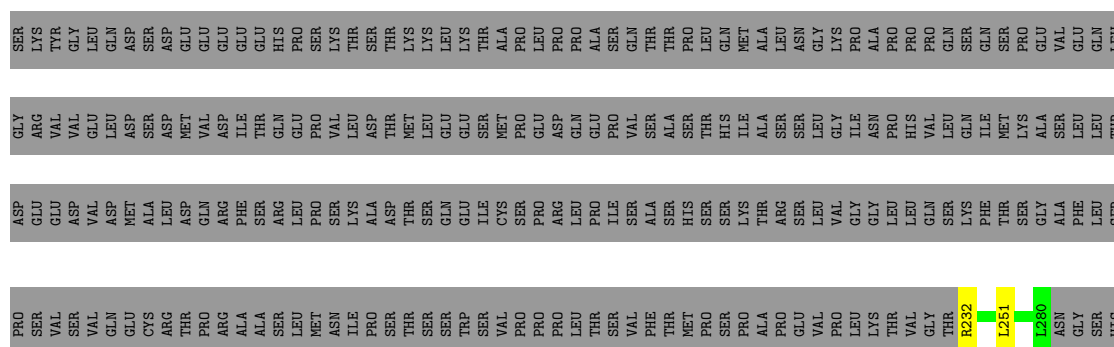


• Molecule 15: Nuclear pore complex protein Nup96

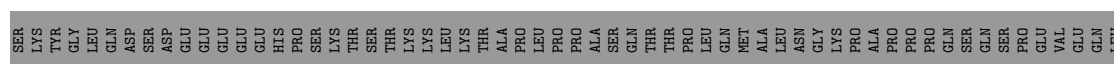


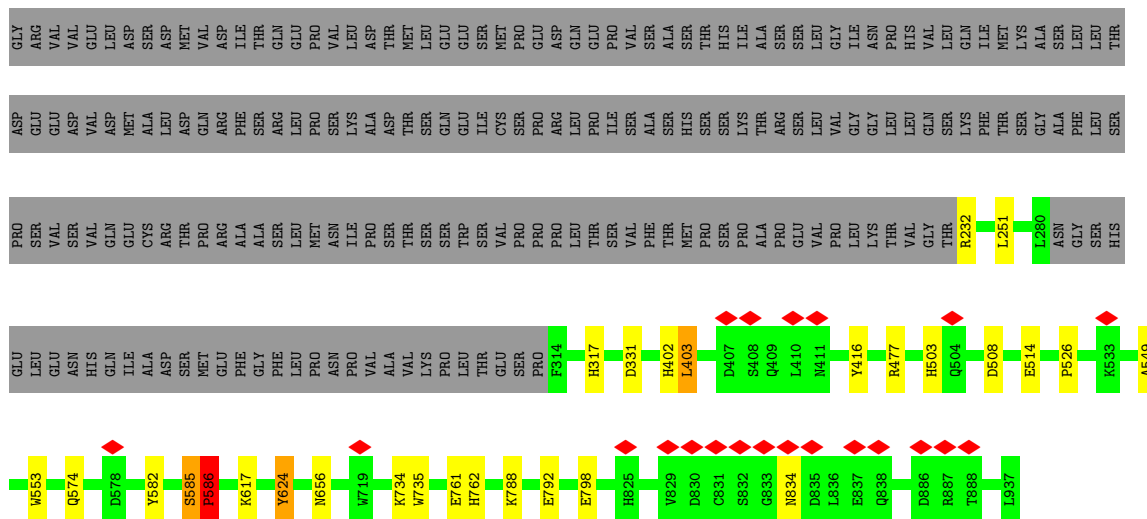


• Molecule 15: Nuclear pore complex protein Nup96

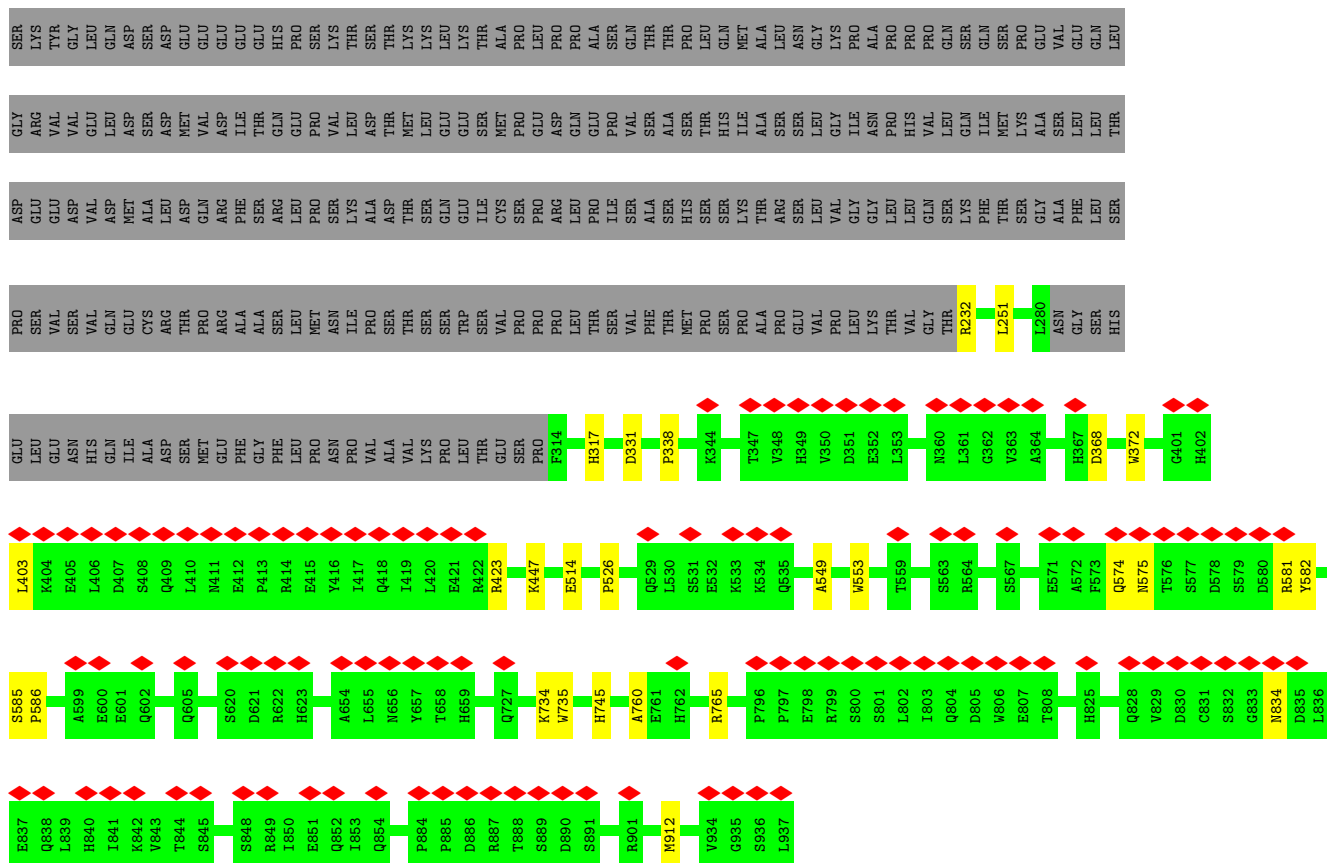


• Molecule 15: Nuclear pore complex protein Nup96

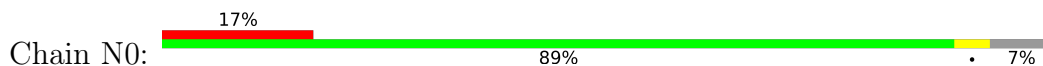




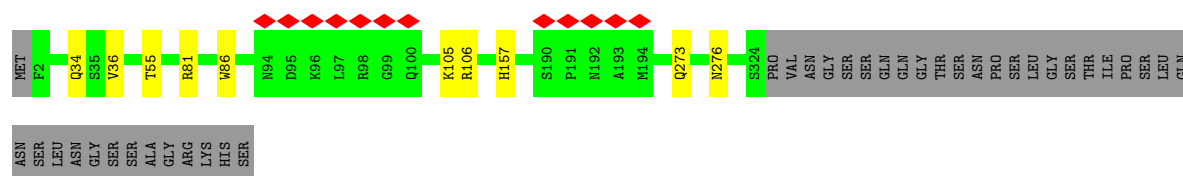
- Molecule 15: Nuclear pore complex protein Nup96



- Molecule 16: Protein SEC13 homolog

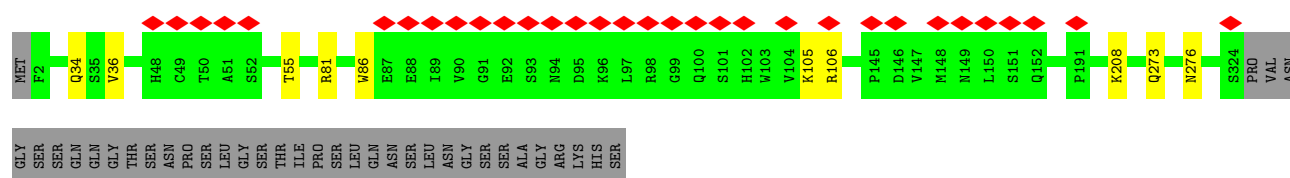


Chain O1:  87% 10%



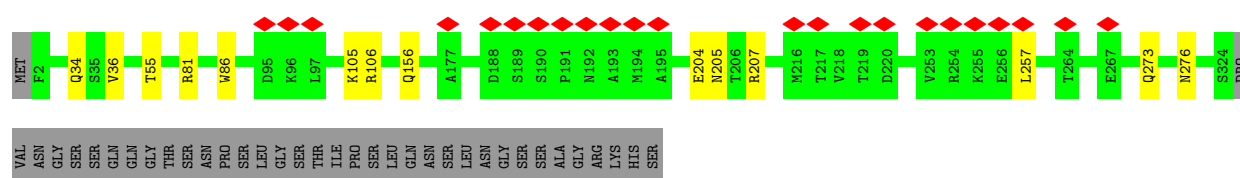
• Molecule 17: Nucleoporin SEH1

Chain O2:  9% 87% 10%



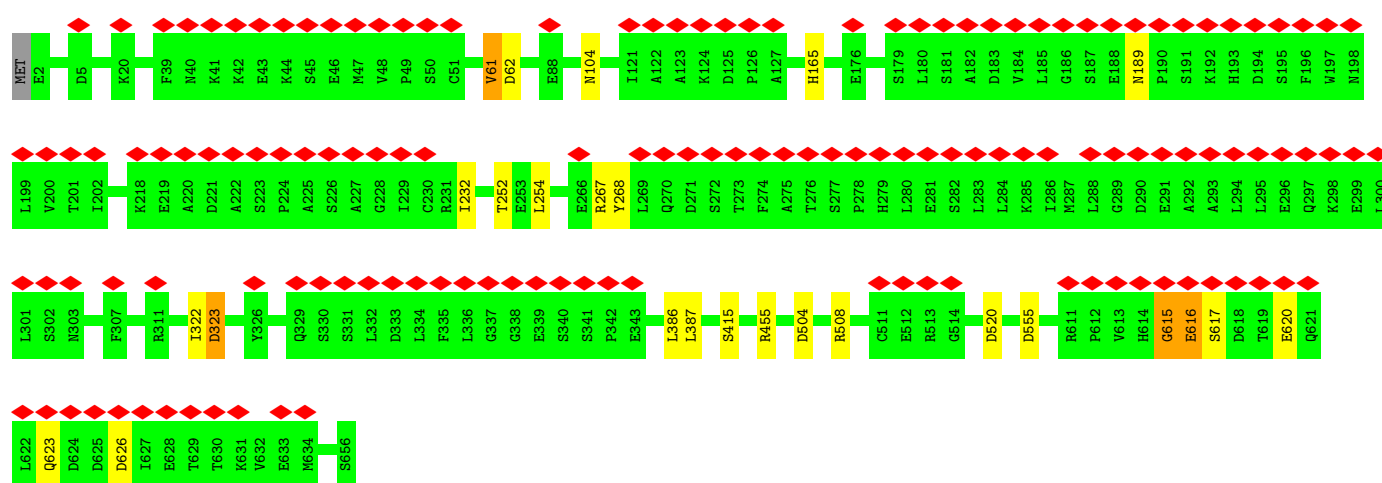
• Molecule 17: Nucleoporin SEH1

Chain O3:  6% 86% 10%



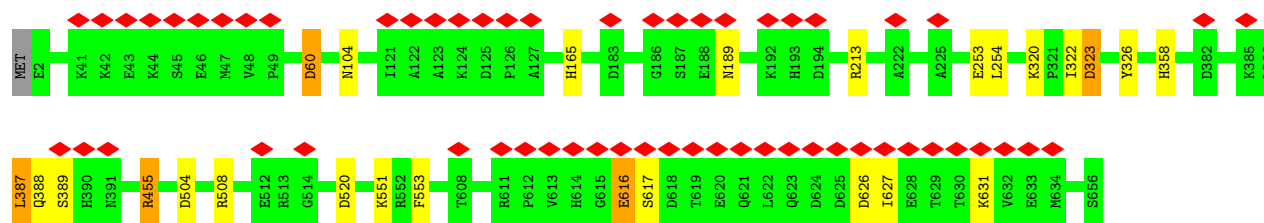
• Molecule 18: Nuclear pore complex protein Nup85

Chain P0:  21% 96%



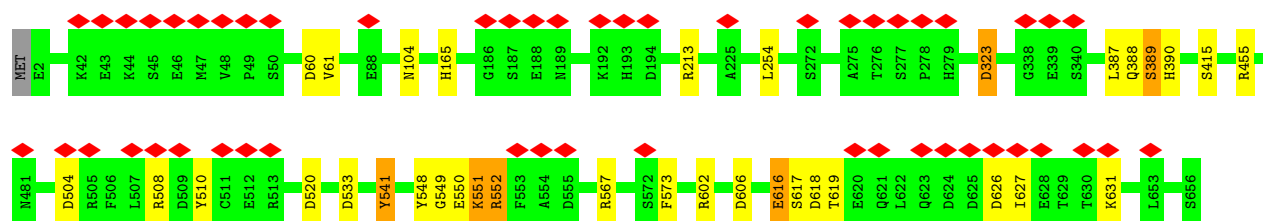
• Molecule 18: Nuclear pore complex protein Nup85

Chain P1:  9% 96%



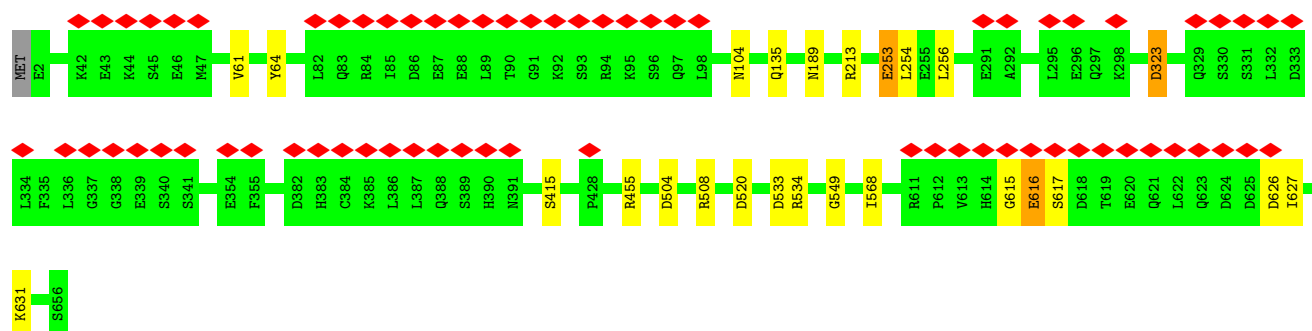
• Molecule 18: Nuclear pore complex protein Nup85

Chain P2: 8% 95%



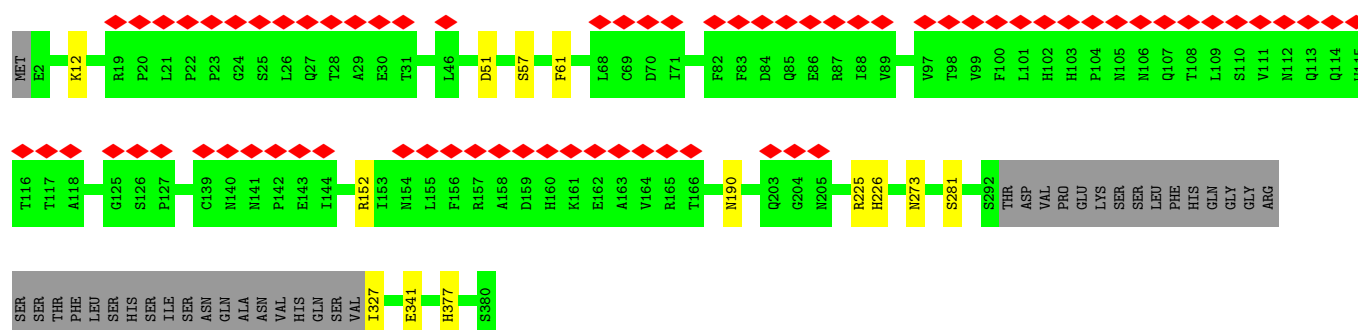
• Molecule 18: Nuclear pore complex protein Nup85

Chain P3: 11% 96%



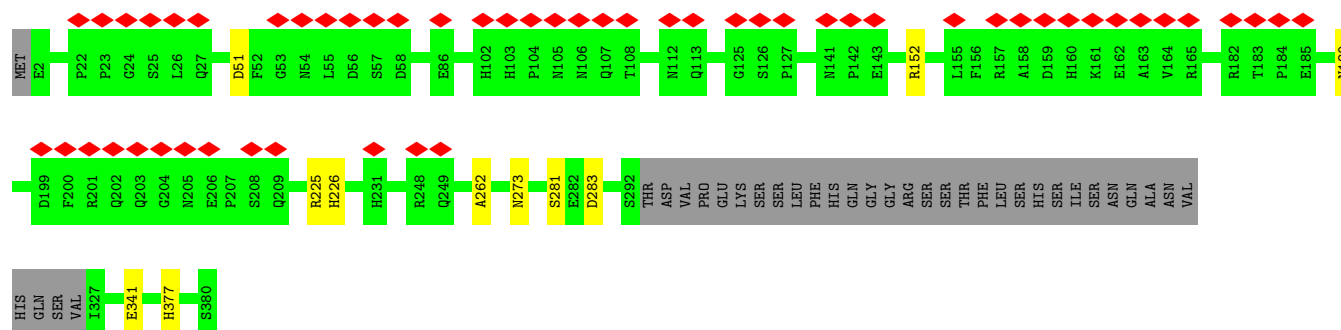
• Molecule 19: Nucleoporin Nup43

Chain Q0: 19% 87% 9%

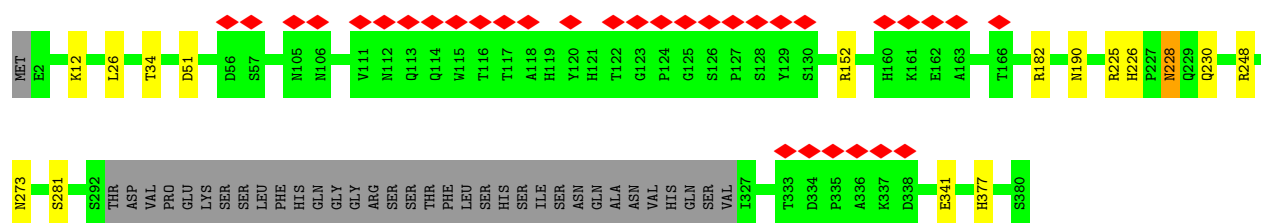
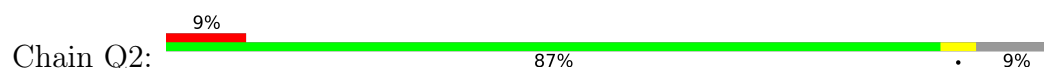


• Molecule 19: Nucleoporin Nup43

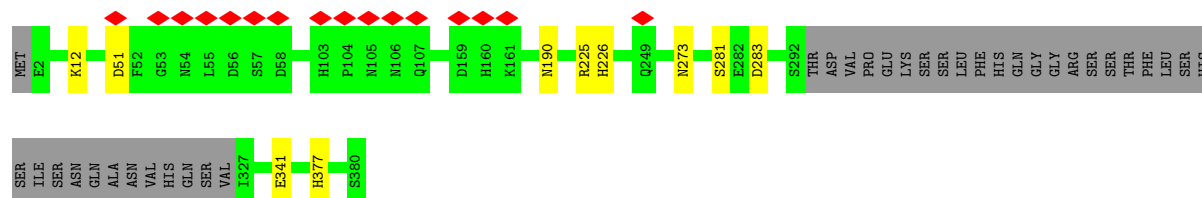
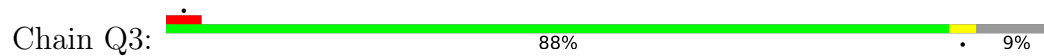
Chain Q1: 14% 88% 9%



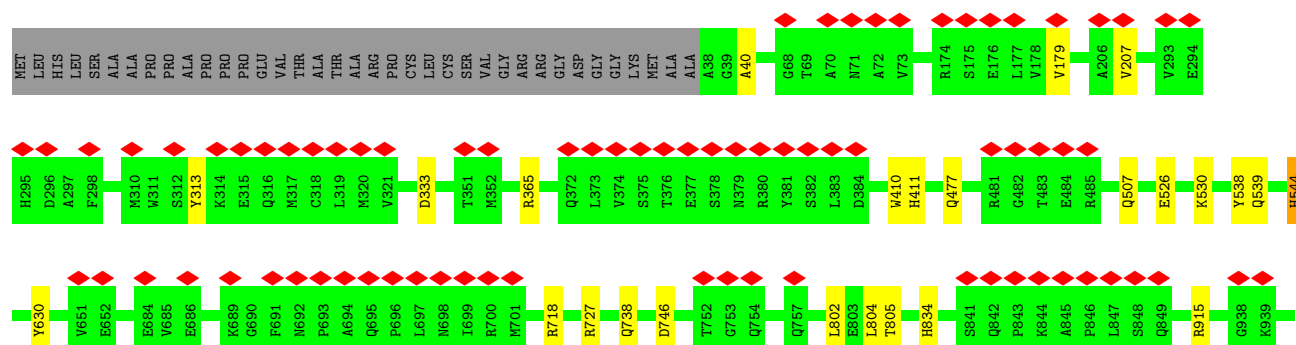
• Molecule 19: Nucleoporin Nup43

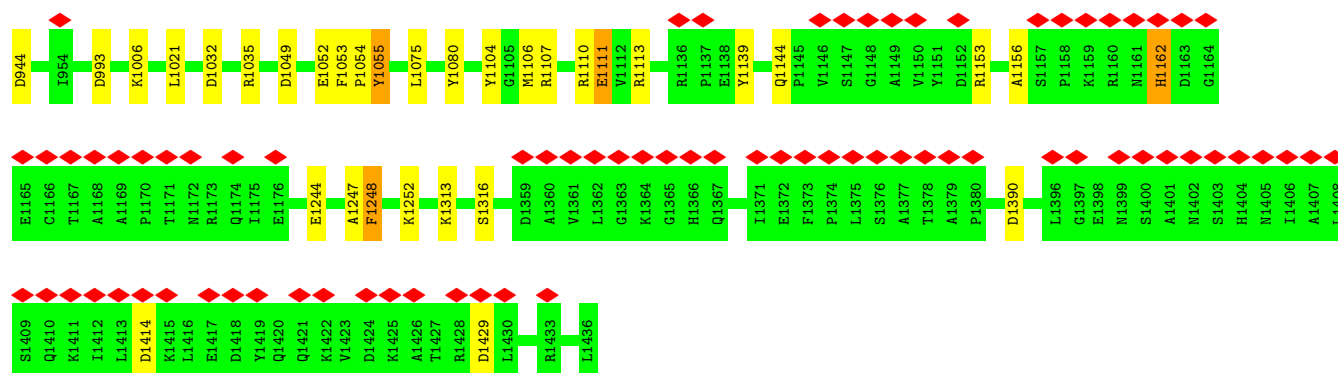


• Molecule 19: Nucleoporin Nup43

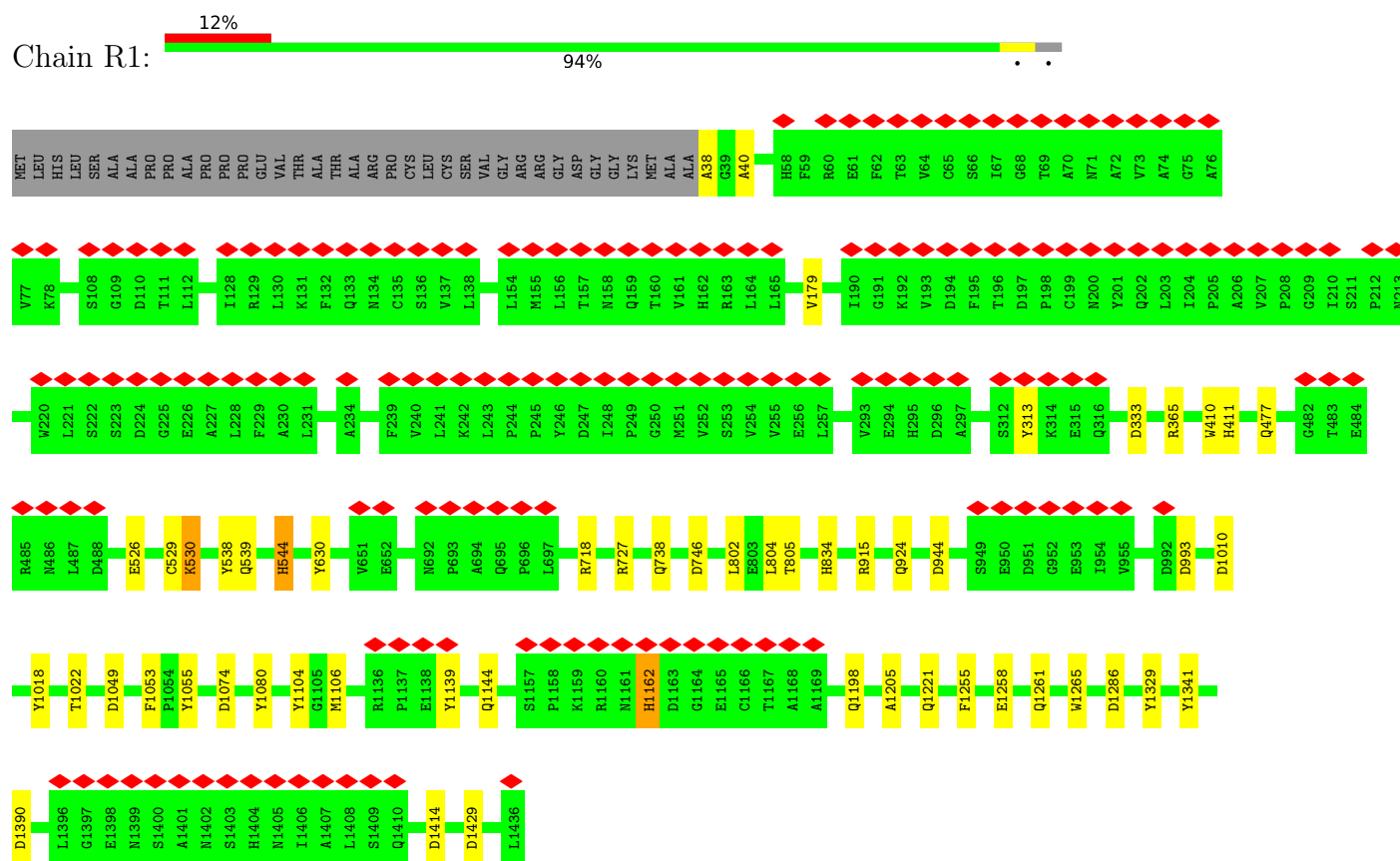


• Molecule 20: Nuclear pore complex protein Nup160

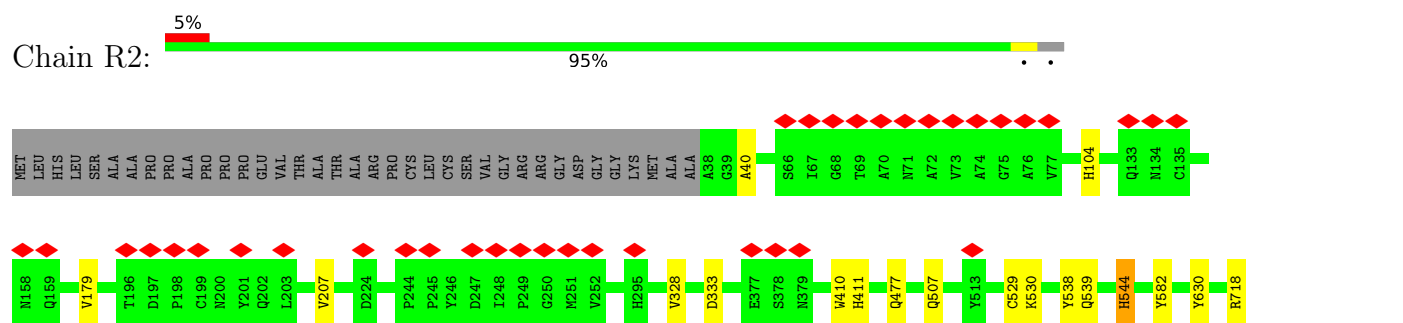


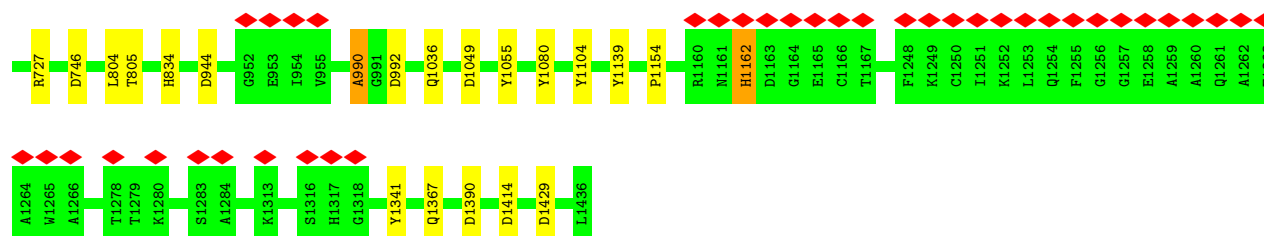


• Molecule 20: Nuclear pore complex protein Nup160

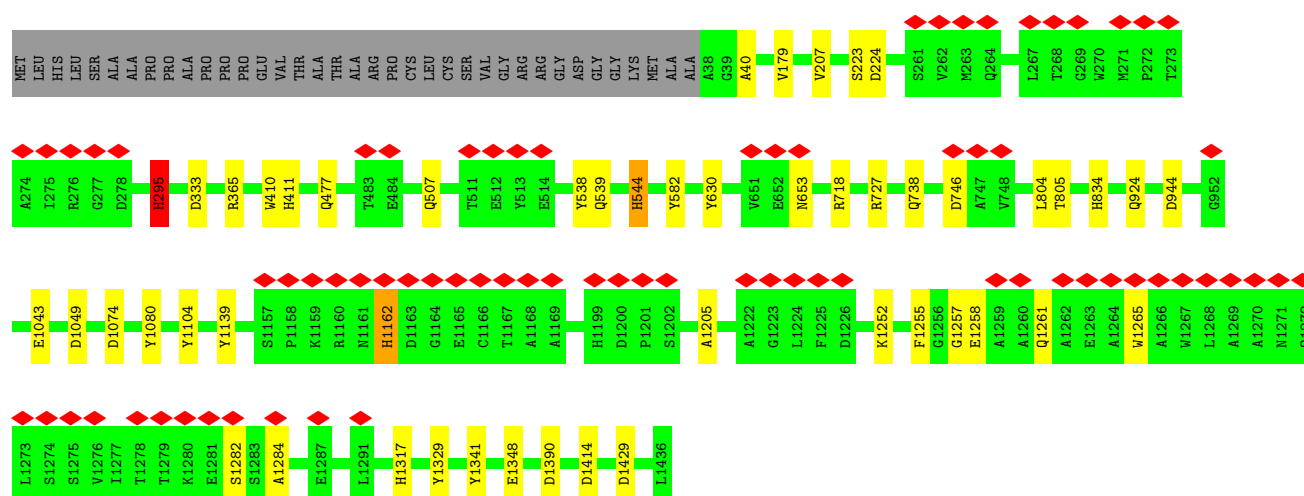


• Molecule 20: Nuclear pore complex protein Nup160

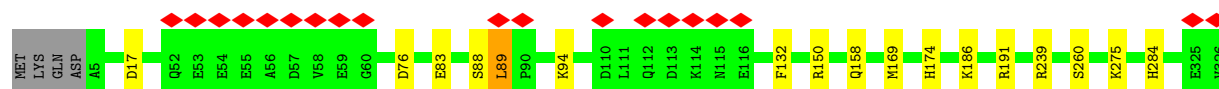




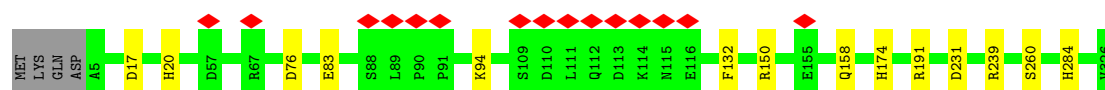
• Molecule 20: Nuclear pore complex protein Nup160



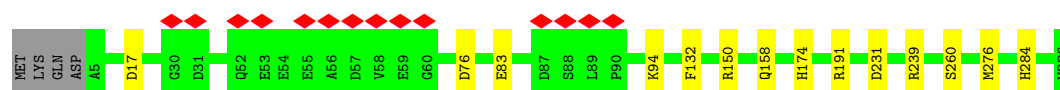
• Molecule 21: Nucleoporin Nup37



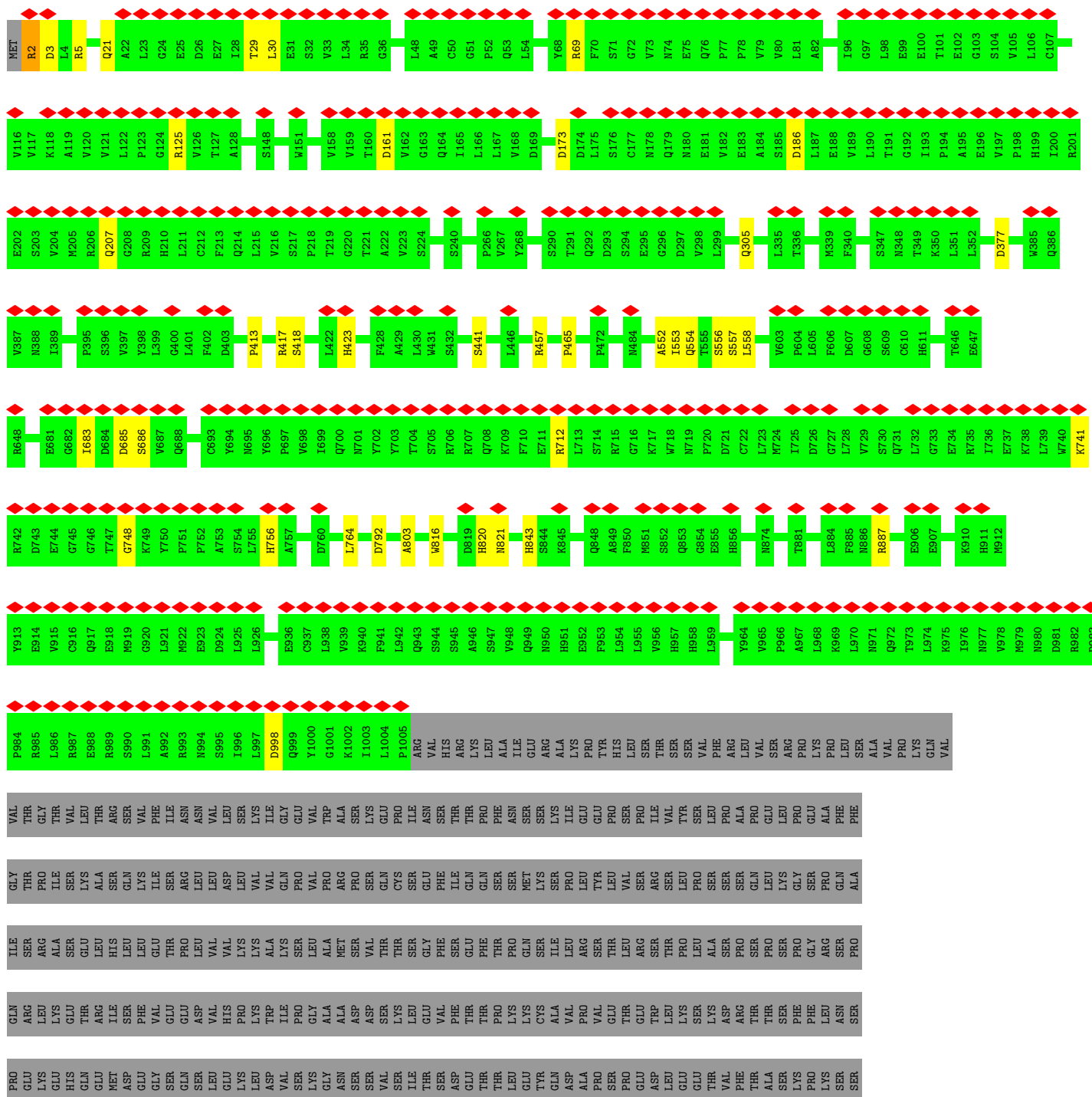
• Molecule 21: Nucleoporin Nup37



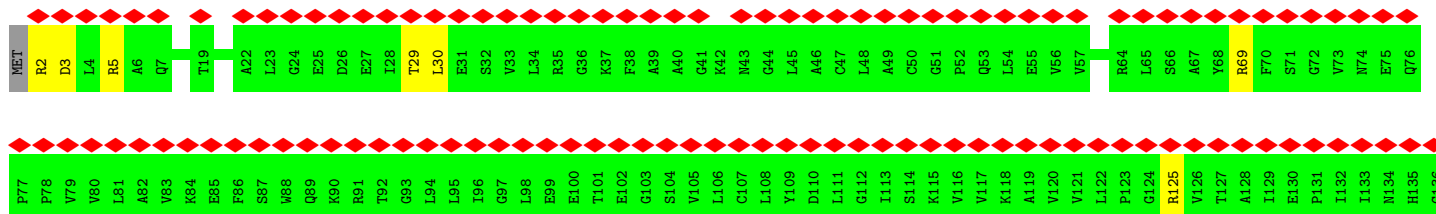
• Molecule 21: Nucleoporin Nup37



• Molecule 21: Nucleoporin Nup37

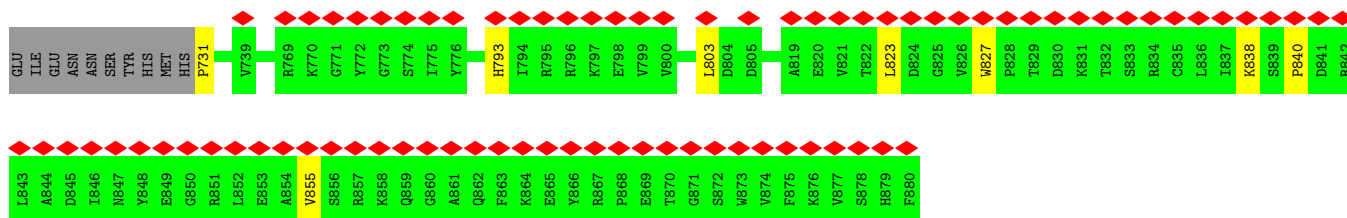
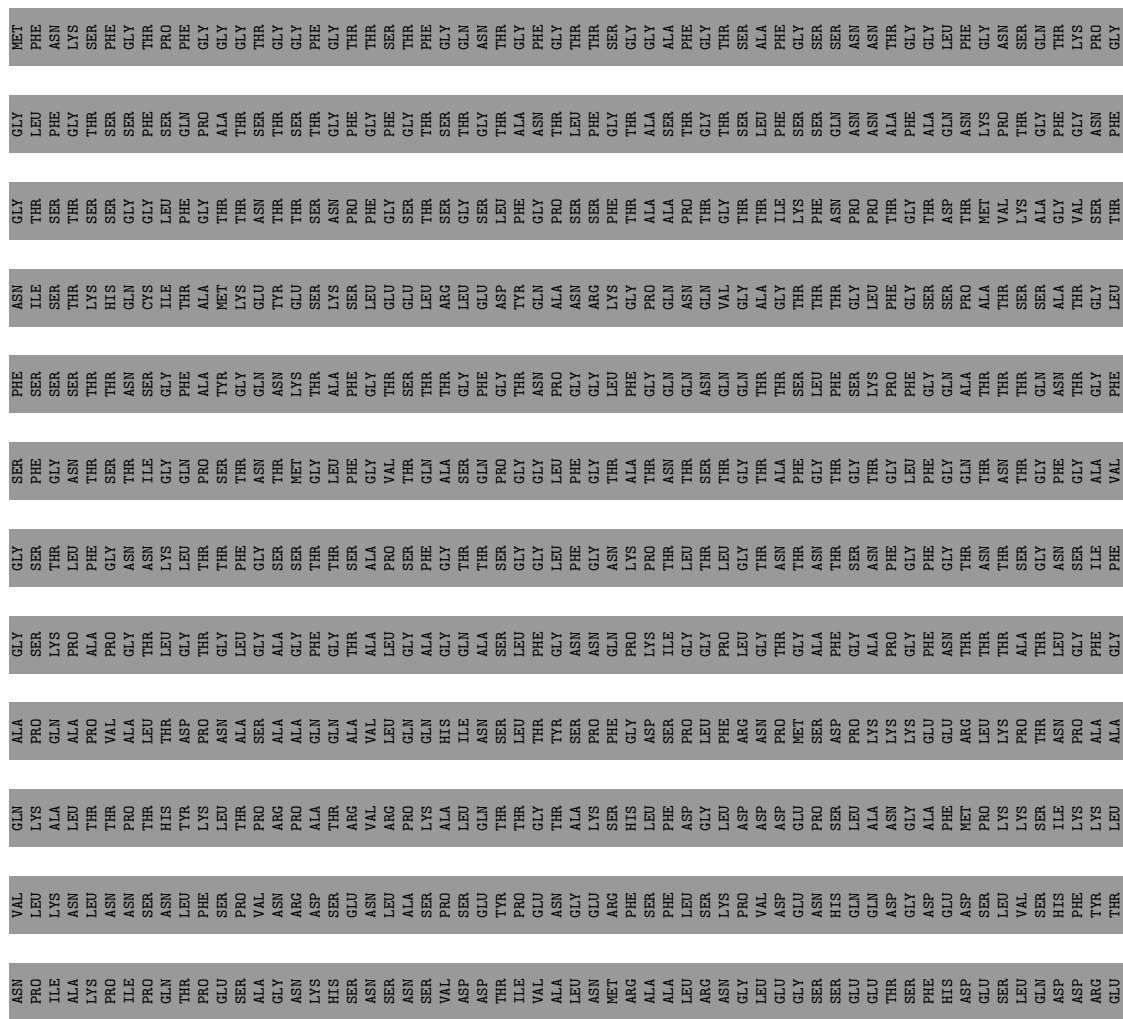


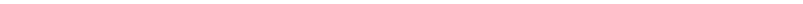
- Molecule 22: Protein ELYS



VAL	T933	A859	I445	D377	G317	Y257	V197	G137
PHE	E934	S872	L446	T378	Q318	I258	P198	A138
ILE	Q935	S873	D447	S379	I319	Q259	H199	S139
ASN	E936	S874	L448	V380	L320	L260	I200	A140
VAL	C937	D875	L449	S381	E321	E261	R201	S141
LEU	L938	D876	V450	S382	E322	S262	E202	T142
SER	V939	D877	L455	F383	G323	G263	S203	Q143
LYS	K940	D878	M456	T384	L324	Q264	V204	H144
ILE	F941	D879	M457	W385	E325	V265	M205	L145
GLY	L942	S786	G458	Q386	Y326	P266	R206	H146
GLU	L943	F787	V459	V387	C327	V267	Q207	P147
TRP	Q943	P788	P460	N388	E328	Y268	G208	S148
ALA	S944	M789	P461	S389	E329	A269	R210	L149
SER	A945	K790	S462	L390	E330	V270	H210	R150
LYS	A946	T791	Y463	Y390	R330	T271	L211	W151
ARG	S947	D792	P465	P395	Y331	T272	C212	L152
THR	V948	A803	P466	S396	T332	F273	F213	F153
ASN	Q949	A804	E467	V397	D334	E274	Q214	G154
LEU	N950	C888	Q468	Y398	L335	P275	L215	V155
ILE	H951	M889	E469	L399	T336	E276	V216	A156
THR	E952	K890	F470	L401	G337	N277	P217	A157
PHE	F953	A892	F471	F402	G338	D278	P218	V158
ASN	L954	W893	M472	D403	M339	P279	T219	V159
SER	L955	L896	N473	I404	F340	R280	G220	T160
LYS	V956	R897	S473	M405	P341	N281	T221	D161
THR	H957	C900	T474	R406	L342	C282	A222	V162
GLU	N958	N901	Y475	W407	R343	C283	V223	G163
LEU	H959	R902	M476	Y408	G344	Y284	S224	Q164
PRO	Q960	L961	F477	H409	Q345	L285	T225	I165
SER	R961	D819	L482	A410	T346	W286	L226	L166
ILE	L962	H820	L483	A411	S347	A287	S227	L167
VAL	N963	N821	M484	Q412	N348	V288	Y228	V168
PHE	E964	D822	L491	M413	T349	Q289	L229	D169
THR	V965	W823	C492	D414	K350	S290	S230	L170
ARG	E966	E824	L493	S415	L351	T291	R231	C171
PRO	L967	S825	C494	L416	L352	Q292	T232	L172
GLU	K968	C826	G494	L417	G353	D293	N233	D173
LEU	H969	L827	F495	S418	C354	S294	Q234	D174
ALA	L970	D828	Q496	S419	Q355	E295	L235	L175
VAL	N971	L829	Q497	E420	S356	G296	A236	S176
GLY	Q972	E913	K498	E421	I357	D297	V237	C177
PHE	T973	V915	E499	Y421	E358	V298	G238	N178
THR	L974	W841	T499	L422	K359	L299	F239	Q179
LYS	A975	D842	L500	H423	F360	S300	S240	N180
ASN	Q976	H843	T501	H424	R361	L301	D241	E181
VAL	E977	S844	F502	C425	S362	H302	G242	V182
THR	N978	K845	L503	S426	H363	L303	Y243	E183
LEU	K979	T846	K504	Y427	G364	L304	L244	A184
VAL	L980	D847	K505	F428	D365	Q305	A245	S185
THR	N981	Q848	S506	A429	R366	L306	L246	D186
ARG	E923	A849	G507	L430	E367	W247	A307	L187
PRO	D924	F850	P508	W431	E368	N248	E188	E188
SER	L925	M851	S509	S432	G369	M249	V189	V189
THR	L926	S852	L510	L433	V370	K250	L190	L190
ALA	K927	Q853	N511	E434	N371	S251	T191	T191
LEU	L928	C854	E512	S435	E372	K312	G192	G192
THR	R929	H773	L513	S441	A373	C313	K253	I193
VAL	P930	R856	L514	G444	L374	L314	R254	P194
SER	T931	Q857	P515		S375	A315	A195	A195
GLN	D932	Q858			P376	S316	Y256	E196

- Molecule 23: Nuclear pore complex protein Nup98



- Chain U1:  98%

[illegible]



[illegible]

- Molecule 23: Nuclear pore complex protein Nup98

Chain U3: 98%

[illegible]

98%

[illegible]

- Molecule 24: Nuclear pore complex protein Nup214

12%

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



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, Not provided	
Number of subtomograms used	150	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	130	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.878	Depositor
Minimum map value	-0.768	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.0891	Depositor
Map size ($\text{\AA}$)	1987.2001, 1987.2001, 1987.2001	wwPDB
Map dimensions	144, 144, 144	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	13.8, 13.8, 13.8	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	00	0.84	0/6212	1.41	17/8405 (0.2%)
1	01	0.83	0/6212	1.40	17/8405 (0.2%)
1	02	0.84	0/6212	1.41	17/8405 (0.2%)
1	03	0.83	0/6212	1.40	11/8405 (0.1%)
1	04	0.84	0/6212	1.40	17/8405 (0.2%)
2	10	1.44	7/14350 (0.0%)	1.32	42/19560 (0.2%)
2	11	0.80	0/14350	1.28	18/19560 (0.1%)
2	12	0.80	1/14350 (0.0%)	1.29	19/19560 (0.1%)
2	13	0.80	0/14350	1.29	20/19560 (0.1%)
2	14	0.81	0/14350	1.31	33/19560 (0.2%)
2	15	0.80	0/14350	1.30	26/19560 (0.1%)
2	16	0.80	0/14350	1.30	29/19560 (0.1%)
2	17	0.85	8/14350 (0.1%)	1.36	51/19560 (0.3%)
3	40	0.85	0/3007	1.30	3/4114 (0.1%)
3	41	0.85	1/3007 (0.0%)	1.30	4/4114 (0.1%)
4	A0	0.84	0/6687	1.39	16/9036 (0.2%)
4	A1	0.83	0/6687	1.39	19/9036 (0.2%)
4	A2	0.84	1/6687 (0.0%)	1.41	28/9036 (0.3%)
4	A3	0.83	0/6687	1.38	20/9036 (0.2%)
4	A4	0.83	0/5972	1.37	13/8068 (0.2%)
4	A5	0.84	0/5972	1.36	13/8068 (0.2%)
4	A6	0.83	0/5972	1.38	14/8068 (0.2%)
5	B0	0.85	1/14018 (0.0%)	1.40	43/19022 (0.2%)
5	B1	0.85	3/14018 (0.0%)	1.40	39/19022 (0.2%)
6	C0	0.85	1/16330 (0.0%)	1.40	39/22131 (0.2%)
6	C1	0.85	1/16330 (0.0%)	1.40	39/22131 (0.2%)
6	C2	1.51	5/16330 (0.0%)	1.38	48/22131 (0.2%)
6	C3	0.85	0/16330	1.39	37/22131 (0.2%)
6	C4	0.85	1/16330 (0.0%)	1.39	36/22131 (0.2%)
7	D0	0.82	0/10568	1.40	22/14320 (0.2%)
7	D1	1.30	5/10568 (0.0%)	1.45	50/14320 (0.3%)
7	D2	0.82	0/10568	1.40	25/14320 (0.2%)
7	D3	0.83	0/10568	1.40	28/14320 (0.2%)
7	D4	1.04	6/10568 (0.1%)	1.42	44/14320 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	D5	0.81	0/10568	1.38	27/14320 (0.2%)
8	E0	1.23	14/4563 (0.3%)	1.48	44/6214 (0.7%)
8	E1	0.97	11/4563 (0.2%)	1.48	27/6214 (0.4%)
9	F0	0.88	0/1882	1.47	13/2556 (0.5%)
9	F1	0.89	0/1882	1.44	7/2556 (0.3%)
9	F2	0.90	0/1882	1.50	14/2556 (0.5%)
9	F3	0.93	0/1882	1.49	5/2556 (0.2%)
10	H0	0.80	1/3114 (0.0%)	1.37	7/4211 (0.2%)
10	H1	0.80	0/3114	1.39	10/4211 (0.2%)
10	H2	0.80	0/3114	1.38	8/4211 (0.2%)
10	H3	0.80	0/3114	1.38	6/4211 (0.1%)
11	I0	0.80	0/1416	1.39	2/1911 (0.1%)
11	I1	0.81	0/1416	1.41	2/1911 (0.1%)
11	I2	0.80	0/1416	1.40	2/1911 (0.1%)
11	I3	0.80	0/1416	1.41	2/1911 (0.1%)
12	J0	0.81	0/1420	1.38	3/1915 (0.2%)
12	J1	0.81	0/1420	1.40	5/1915 (0.3%)
12	J2	0.81	0/1420	1.40	5/1915 (0.3%)
12	J3	0.81	0/1420	1.39	5/1915 (0.3%)
12	J4	0.80	0/1420	1.44	4/1915 (0.2%)
13	K0	0.83	0/8740	1.37	19/11848 (0.2%)
13	K1	0.82	0/8740	1.36	17/11848 (0.1%)
13	K2	0.82	0/8740	1.36	19/11848 (0.2%)
13	K3	0.82	0/8740	1.36	16/11848 (0.1%)
14	L0	0.86	1/6518 (0.0%)	1.42	23/8819 (0.3%)
14	L1	0.84	0/6518	1.39	13/8819 (0.1%)
14	L2	0.85	0/6518	1.39	12/8819 (0.1%)
14	L3	0.85	0/6518	1.39	14/8819 (0.2%)
15	M0	0.86	0/5588	1.42	22/7581 (0.3%)
15	M1	0.87	0/5588	1.41	15/7581 (0.2%)
15	M2	0.86	0/5588	1.41	14/7581 (0.2%)
15	M3	0.86	0/5588	1.40	11/7581 (0.1%)
16	N0	0.85	0/2419	1.37	6/3301 (0.2%)
16	N1	0.85	0/2419	1.37	9/3301 (0.3%)
16	N2	0.85	0/2419	1.37	8/3301 (0.2%)
16	N3	0.85	0/2419	1.37	9/3301 (0.3%)
17	O0	0.84	0/2593	1.35	4/3520 (0.1%)
17	O1	0.85	0/2593	1.35	4/3520 (0.1%)
17	O2	0.84	0/2593	1.35	4/3520 (0.1%)
17	O3	0.85	0/2593	1.36	7/3520 (0.2%)
18	P0	0.85	0/5365	1.40	17/7257 (0.2%)
18	P1	0.85	0/5365	1.38	17/7257 (0.2%)
18	P2	0.85	0/5365	1.42	28/7257 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
18	P3	0.85	0/5365	1.37	13/7257 (0.2%)
19	Q0	0.87	0/2775	1.38	6/3786 (0.2%)
19	Q1	0.87	0/2775	1.38	7/3786 (0.2%)
19	Q2	0.87	0/2775	1.40	11/3786 (0.3%)
19	Q3	0.87	0/2775	1.37	7/3786 (0.2%)
20	R0	0.98	2/11371 (0.0%)	1.39	37/15446 (0.2%)
20	R1	0.84	0/11371	1.37	31/15446 (0.2%)
20	R2	0.84	0/11371	1.37	30/15446 (0.2%)
20	R3	0.84	0/11371	1.37	28/15446 (0.2%)
21	S0	0.85	0/2623	1.34	9/3568 (0.3%)
21	S1	0.85	0/2623	1.33	7/3568 (0.2%)
21	S2	0.85	0/2623	1.33	7/3568 (0.2%)
21	S3	0.85	0/2623	1.33	6/3568 (0.2%)
22	T0	0.84	0/8141	1.38	27/11065 (0.2%)
22	T1	0.84	0/8141	1.38	27/11065 (0.2%)
23	U0	0.85	0/1217	1.35	4/1644 (0.2%)
23	U1	1.41	1/152 (0.7%)	2.13	6/204 (2.9%)
23	U2	1.33	0/152	1.92	4/204 (2.0%)
23	U3	1.38	0/152	2.11	7/204 (3.4%)
23	U4	1.48	1/152 (0.7%)	1.91	3/204 (1.5%)
23	U5	1.41	0/152	2.13	6/204 (2.9%)
23	U6	1.30	0/152	1.90	7/204 (3.4%)
24	V0	0.86	0/2240	1.44	7/3019 (0.2%)
25	W0	0.86	1/5972 (0.0%)	1.37	20/8105 (0.2%)
All	All	0.90	73/630097 (0.0%)	1.38	1720/855041 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	00	0	4
1	01	0	4
1	02	0	3
1	03	0	3
1	04	0	1
2	10	1	9
2	11	0	3
2	12	1	7
2	13	1	3
2	14	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	15	0	7
2	16	0	7
2	17	0	8
3	40	0	5
3	41	0	4
4	A0	0	11
4	A1	0	12
4	A2	0	12
4	A3	0	9
4	A4	0	7
4	A5	0	6
4	A6	1	9
5	B0	0	22
5	B1	0	26
6	C0	1	17
6	C1	1	13
6	C2	1	17
6	C3	1	15
6	C4	1	15
7	D0	0	16
7	D1	0	13
7	D2	0	18
7	D3	0	14
7	D4	1	19
7	D5	0	15
8	E0	0	5
8	E1	0	2
9	F0	0	3
9	F1	0	2
9	F2	0	3
9	F3	0	1
10	H0	0	5
10	H1	0	1
10	H2	0	2
10	H3	0	2
12	J0	0	1
12	J1	0	1
12	J2	0	1
12	J3	0	1
13	K0	0	10
13	K1	0	9
13	K2	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	K3	0	8
14	L0	0	8
14	L1	0	5
14	L2	0	6
14	L3	0	6
15	M0	0	7
15	M1	0	5
15	M2	0	9
15	M3	1	6
16	N0	0	4
16	N1	0	2
16	N2	0	2
16	N3	0	2
17	O0	0	1
17	O1	0	2
17	O2	0	2
17	O3	0	2
18	P0	0	9
18	P1	0	10
18	P2	1	17
18	P3	0	10
19	Q0	0	3
19	Q1	0	3
19	Q2	0	3
19	Q3	0	2
20	R0	0	15
20	R1	0	16
20	R2	0	15
20	R3	0	15
21	S0	0	4
21	S1	0	5
21	S2	0	5
21	S3	0	5
22	T0	2	13
22	T1	2	14
24	V0	0	5
25	W0	0	7
All	All	16	676

All (73) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	10	1824	MET	N-CA	140.20	3.27	1.46
7	D1	1002	PRO	CA-C	103.26	2.99	1.52
6	C2	484	HIS	CD2-NE2	83.30	2.29	1.37
6	C2	484	HIS	CG-ND1	74.67	2.20	1.38
6	C2	484	HIS	ND1-CE1	69.44	2.02	1.32
6	C2	484	HIS	CE1-NE2	68.19	2.00	1.32
6	C2	484	HIS	CG-CD2	60.71	2.02	1.35
20	R0	1111	GLU	CD-OE1	53.48	2.27	1.25
8	E0	18	TRP	NE1-CE2	38.91	1.80	1.37
7	D4	91	PRO	CA-CB	38.16	2.08	1.53
7	D4	91	PRO	N-CA	36.03	1.93	1.47
7	D4	91	PRO	N-CD	30.89	1.91	1.47
8	E0	18	TRP	CD1-NE1	22.68	1.85	1.37
8	E0	18	TRP	CG-CD2	21.25	1.81	1.43
8	E0	18	TRP	CD2-CE2	18.03	1.72	1.41
7	D4	91	PRO	CG-CD	17.73	2.11	1.50
8	E1	244	THR	N-CA	17.69	1.69	1.46
2	10	1824	MET	CA-C	16.97	1.75	1.52
2	17	1788	ASP	CA-C	16.95	1.75	1.52
2	17	1789	ARG	N-CA	14.53	1.65	1.46
8	E1	243	SER	C-N	13.62	1.52	1.33
2	17	1788	ASP	N-CA	12.48	1.62	1.46
7	D4	91	PRO	CB-CG	11.25	2.05	1.49
8	E0	19	ARG	CA-CB	11.04	1.71	1.53
8	E0	18	TRP	CG-CD1	10.91	1.64	1.36
2	17	1789	ARG	CA-C	10.85	1.67	1.52
8	E0	18	TRP	CA-C	10.84	1.67	1.52
2	10	1824	MET	C-N	10.55	1.43	1.33
2	10	1828	TYR	N-CA	10.46	1.59	1.46
2	17	1788	ASP	C-N	10.35	1.48	1.33
2	17	1790	ARG	N-CA	9.98	1.59	1.46
8	E1	244	THR	CA-C	9.56	1.65	1.52
8	E1	243	SER	CA-C	9.49	1.65	1.52
8	E1	245	ALA	CA-C	9.06	1.64	1.52
8	E0	19	ARG	N-CA	9.02	1.56	1.46
7	D1	1000	GLY	C-N	8.98	1.44	1.33
2	10	1827	ALA	C-N	8.81	1.46	1.33
2	17	1790	ARG	CA-CB	8.32	1.67	1.53
2	10	1827	ALA	CA-CB	-7.95	1.40	1.53
8	E0	19	ARG	CA-C	-7.65	1.43	1.52
2	10	1823	VAL	N-CA	7.07	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D1	1002	PRO	CA-CB	6.92	1.63	1.53
8	E1	242	ILE	CA-C	6.43	1.62	1.52
6	C1	1379	PRO	CA-C	6.36	1.55	1.51
8	E0	17	LEU	C-N	-6.33	1.25	1.33
2	17	1787	VAL	C-N	6.27	1.42	1.33
8	E1	241	TRP	CA-C	6.22	1.59	1.52
8	E1	245	ALA	N-CA	6.10	1.54	1.46
5	B1	1521	PRO	CA-C	5.99	1.57	1.52
2	12	748	PRO	CA-C	5.99	1.55	1.51
7	D1	1003	VAL	C-N	5.99	1.42	1.33
5	B0	1521	PRO	CA-C	5.96	1.57	1.52
5	B1	833	VAL	CA-C	-5.94	1.45	1.52
8	E1	242	ILE	N-CA	5.90	1.52	1.46
7	D1	1002	PRO	N-CA	5.89	1.54	1.47
7	D4	91	PRO	CA-C	5.85	1.60	1.52
5	B1	1023	PRO	CA-C	5.71	1.55	1.51
20	R0	1111	GLU	CG-CD	5.70	1.66	1.52
23	U4	610	LEU	N-CA	-5.68	1.38	1.46
8	E0	313	GLU	CA-CB	5.60	1.62	1.53
23	U1	610	LEU	N-CA	-5.48	1.39	1.46
25	W0	503	PRO	CA-C	5.48	1.54	1.51
8	E0	18	TRP	C-N	5.42	1.40	1.33
4	A2	239	THR	N-CA	5.40	1.53	1.46
14	L0	731	GLY	N-CA	5.39	1.53	1.45
8	E1	243	SER	N-CA	5.32	1.52	1.46
8	E1	240	ALA	CA-C	5.24	1.60	1.53
8	E0	18	TRP	N-CA	-5.18	1.40	1.46
8	E0	19	ARG	CG-CD	5.10	1.67	1.52
10	H0	160	PRO	CA-C	5.05	1.54	1.51
6	C0	639	PRO	CA-C	5.02	1.54	1.51
6	C4	639	PRO	CA-C	5.01	1.54	1.51
3	41	10	PRO	CA-C	5.01	1.54	1.51

All (1720) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E1	243	SER	CA-C-O	-25.86	93.01	120.42
6	C1	1379	PRO	O-C-N	-24.31	110.13	121.31
2	17	1788	ASP	CA-C-N	21.79	163.16	121.54
2	17	1788	ASP	C-N-CA	21.79	163.16	121.54
7	D1	1000	GLY	CA-C-N	16.46	137.34	120.38
7	D1	1000	GLY	C-N-CA	16.46	137.34	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	17	1789	ARG	CA-C-N	16.27	152.61	121.54
2	17	1789	ARG	C-N-CA	16.27	152.61	121.54
2	10	1827	ALA	CA-C-O	-16.21	97.33	120.51
7	D1	1002	PRO	O-C-N	-15.06	102.30	122.64
20	R0	1248	PHE	CA-CB-CG	15.01	128.81	113.80
2	17	1787	VAL	CA-C-N	14.24	148.74	121.54
2	17	1787	VAL	C-N-CA	14.24	148.74	121.54
8	E0	19	ARG	CB-CG-CD	13.72	142.85	111.30
8	E1	243	SER	N-CA-C	13.53	126.11	111.36
8	E0	19	ARG	CA-CB-CG	13.53	141.16	114.10
2	10	1822	ALA	CA-C-N	13.21	137.20	120.56
2	10	1822	ALA	C-N-CA	13.21	137.20	120.56
7	D1	1003	VAL	CA-C-O	-13.08	104.42	120.78
6	C4	1249	ILE	CB-CA-C	13.05	133.30	111.37
2	17	1791	GLY	CA-C-N	12.34	135.26	119.84
2	17	1791	GLY	C-N-CA	12.34	135.26	119.84
8	E1	244	THR	N-CA-C	12.16	136.70	110.80
20	R0	1111	GLU	CG-CD-OE2	-12.11	90.54	118.40
2	17	1788	ASP	N-CA-C	12.02	136.40	110.80
8	E0	18	TRP	CB-CA-C	11.93	130.96	110.68
8	E1	243	SER	CA-C-N	11.78	144.04	121.54
8	E1	243	SER	C-N-CA	11.78	144.04	121.54
2	17	1790	ARG	CA-CB-CG	11.74	137.59	114.10
18	P2	606	ASP	CA-CB-CG	11.59	124.19	112.60
8	E0	18	TRP	CA-C-N	11.40	136.64	120.79
8	E0	18	TRP	C-N-CA	11.40	136.64	120.79
8	E0	19	ARG	CD-NE-CZ	11.37	140.32	124.40
8	E0	312	ASP	CA-C-N	11.37	135.52	120.28
8	E0	312	ASP	C-N-CA	11.37	135.52	120.28
8	E1	242	ILE	CA-C-N	11.34	136.40	120.29
8	E1	242	ILE	C-N-CA	11.34	136.40	120.29
23	U5	610	LEU	CD1-CG-CD2	11.01	135.03	110.80
7	D1	1002	PRO	CB-CA-C	10.90	129.55	111.56
7	D1	1000	GLY	O-C-N	10.77	132.54	121.77
4	A2	238	ALA	O-C-N	-10.76	110.81	122.96
23	U1	610	LEU	CD1-CG-CD2	10.61	134.15	110.80
7	D4	1109	ILE	CB-CA-C	10.49	128.50	111.29
2	10	1827	ALA	CA-C-N	10.40	141.40	121.54
2	10	1827	ALA	C-N-CA	10.40	141.40	121.54
23	U4	610	LEU	CD1-CG-CD2	10.31	133.48	110.80
23	U3	610	LEU	CD1-CG-CD2	10.26	133.38	110.80
7	D4	1111	LEU	N-CA-C	10.19	124.82	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E1	240	ALA	CB-CA-C	10.11	132.09	111.97
9	F0	173	ASP	CA-CB-CG	10.07	122.67	112.60
8	E1	242	ILE	CB-CA-C	10.06	121.85	110.88
23	U1	609	ASN	CA-C-N	-10.02	107.41	120.44
23	U1	609	ASN	C-N-CA	-10.02	107.41	120.44
8	E0	18	TRP	N-CA-CB	-9.98	95.09	110.06
7	D1	1001	PRO	N-CA-C	9.90	122.78	110.70
23	U5	609	ASN	CA-C-N	-9.82	107.67	120.44
23	U5	609	ASN	C-N-CA	-9.82	107.67	120.44
23	U3	609	ASN	CA-C-N	-9.73	107.80	120.44
23	U3	609	ASN	C-N-CA	-9.73	107.80	120.44
2	10	1826	ILE	CA-C-N	-9.69	103.04	121.54
2	10	1826	ILE	C-N-CA	-9.69	103.04	121.54
2	17	1792	PRO	CA-C-N	9.69	137.08	121.87
2	17	1792	PRO	C-N-CA	9.69	137.08	121.87
8	E1	240	ALA	CA-C-N	9.68	135.07	120.17
8	E1	240	ALA	C-N-CA	9.68	135.07	120.17
23	U2	610	LEU	CD1-CG-CD2	9.65	132.02	110.80
18	P2	550	GLU	CA-C-N	9.54	138.88	121.70
18	P2	550	GLU	C-N-CA	9.54	138.88	121.70
5	B0	1525	ALA	CA-C-N	9.30	138.44	121.70
5	B0	1525	ALA	C-N-CA	9.30	138.44	121.70
2	10	1824	MET	N-CA-CB	9.23	126.08	110.49
8	E0	313	GLU	CB-CA-C	-9.15	95.60	110.79
2	14	1106	PRO	CA-C-N	-9.08	108.17	121.24
2	14	1106	PRO	C-N-CA	-9.08	108.17	121.24
5	B0	1525	ALA	O-C-N	-9.03	114.53	123.46
8	E0	18	TRP	CD2-CE2-CZ2	-9.01	113.39	122.40
14	L0	730	GLN	CB-CA-C	8.96	123.44	111.70
23	U6	610	LEU	CD1-CG-CD2	8.90	130.38	110.80
2	10	1827	ALA	O-C-N	8.88	134.40	122.59
8	E1	245	ALA	N-CA-C	8.86	125.17	113.30
2	17	1789	ARG	N-CA-CB	8.86	125.46	110.49
5	B0	1177	VAL	CA-C-N	8.85	132.51	120.38
5	B0	1177	VAL	C-N-CA	8.85	132.51	120.38
25	W0	358	ASP	CA-CB-CG	8.85	121.45	112.60
2	10	1828	TYR	N-CA-C	8.79	129.52	110.80
9	F3	173	ASP	CA-CB-CG	8.68	121.28	112.60
7	D1	1001	PRO	CA-N-CD	-8.66	99.88	112.00
6	C4	1393	ASP	CA-CB-CG	8.65	121.25	112.60
22	T1	556	SER	N-CA-C	8.63	120.06	107.88
18	P0	322	ILE	CA-CB-CG1	8.59	124.99	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B1	1177	VAL	CA-C-N	8.58	132.14	120.38
5	B1	1177	VAL	C-N-CA	8.58	132.14	120.38
7	D3	203	ASP	CA-CB-CG	8.49	121.09	112.60
7	D5	531	ASP	CA-CB-CG	8.45	121.05	112.60
6	C2	542	VAL	CA-C-N	8.45	137.68	121.54
6	C2	542	VAL	C-N-CA	8.45	137.68	121.54
4	A1	154	ASP	CA-CB-CG	8.45	121.05	112.60
14	L2	172	ASP	CA-CB-CG	8.37	120.97	112.60
5	B0	1223	ASP	CA-CB-CG	8.35	120.95	112.60
2	16	1194	ASN	CA-CB-CG	8.34	120.94	112.60
4	A2	240	ASP	CA-C-N	8.32	132.27	120.28
4	A2	240	ASP	C-N-CA	8.32	132.27	120.28
6	C3	1393	ASP	CA-CB-CG	8.32	120.92	112.60
18	P3	323	ASP	CA-CB-CG	8.30	120.91	112.60
2	17	1788	ASP	CA-C-O	-8.25	108.71	120.51
2	16	1176	ILE	O-C-N	-8.25	114.18	123.00
14	L0	731	GLY	CA-C-N	8.25	137.29	121.54
14	L0	731	GLY	C-N-CA	8.25	137.29	121.54
7	D2	1168	HIS	CB-CG-CD2	-8.24	120.48	131.20
5	B1	632	ASP	CA-CB-CG	8.24	120.84	112.60
6	C4	1249	ILE	N-CA-CB	-8.21	98.29	112.08
25	W0	345	ASP	CA-CB-CG	8.17	120.77	112.60
18	P1	323	ASP	CA-CB-CG	8.15	120.75	112.60
6	C2	1393	ASP	CA-CB-CG	8.11	120.71	112.60
8	E1	237	ILE	CA-CB-CG2	-8.10	96.72	110.50
7	D1	1239	ASP	CA-CB-CG	8.09	120.69	112.60
18	P2	323	ASP	CA-CB-CG	8.07	120.67	112.60
7	D0	915	ASN	CA-CB-CG	8.04	120.64	112.60
20	R1	1286	ASP	CA-CB-CG	8.03	120.63	112.60
18	P0	323	ASP	CA-CB-CG	8.03	120.63	112.60
23	U6	611	PHE	CA-C-N	-8.02	109.42	122.26
23	U6	611	PHE	C-N-CA	-8.02	109.42	122.26
14	L3	172	ASP	CA-CB-CG	8.02	120.62	112.60
7	D1	1001	PRO	N-CD-CG	8.00	115.20	103.20
5	B0	632	ASP	CA-CB-CG	7.98	120.58	112.60
6	C2	1159	ILE	CA-C-N	7.97	136.04	121.70
6	C2	1159	ILE	C-N-CA	7.97	136.04	121.70
15	M2	586	PRO	CA-N-CD	-7.96	100.86	112.00
13	K2	910	LYS	CA-C-O	-7.95	113.12	121.55
6	C2	1803	VAL	CB-CA-C	7.94	121.97	111.33
6	C3	1159	ILE	CA-C-N	7.94	135.99	121.70
6	C3	1159	ILE	C-N-CA	7.94	135.99	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C4	1159	ILE	CA-C-N	7.94	135.99	121.70
6	C4	1159	ILE	C-N-CA	7.94	135.99	121.70
23	U2	606	ASN	CA-CB-CG	7.94	120.54	112.60
7	D2	915	ASN	CA-CB-CG	7.90	120.50	112.60
14	L0	172	ASP	CA-CB-CG	7.88	120.48	112.60
4	A3	780	ASP	CA-CB-CG	7.86	120.46	112.60
7	D4	531	ASP	CA-CB-CG	7.85	120.45	112.60
14	L1	172	ASP	CA-CB-CG	7.85	120.45	112.60
8	E1	244	THR	CB-CA-C	-7.83	94.84	110.42
7	D1	531	ASP	CA-CB-CG	7.81	120.41	112.60
4	A1	172	PRO	N-CA-C	7.81	120.22	110.70
7	D3	1239	ASP	CA-CB-CG	7.79	120.39	112.60
5	B1	1223	ASP	CA-CB-CG	7.73	120.33	112.60
18	P0	520	ASP	CA-CB-CG	7.71	120.31	112.60
20	R1	1049	ASP	CA-CB-CG	7.70	120.30	112.60
2	17	1790	ARG	N-CA-CB	7.70	123.50	110.49
14	L3	585	HIS	CA-CB-CG	7.68	121.48	113.80
9	F3	106	THR	CB-CA-C	7.68	116.65	111.20
7	D0	1239	ASP	CA-CB-CG	7.67	120.27	112.60
8	E0	313	GLU	CA-CB-CG	7.65	129.40	114.10
9	F2	156	ASP	CA-CB-CG	7.61	120.21	112.60
23	U4	611	PHE	CA-C-N	-7.58	110.14	122.26
23	U4	611	PHE	C-N-CA	-7.58	110.14	122.26
7	D3	915	ASN	CA-CB-CG	7.57	120.17	112.60
6	C1	1393	ASP	CA-CB-CG	7.54	120.14	112.60
6	C1	1695	ASP	CA-CB-CG	7.54	120.14	112.60
4	A0	543	ASP	CA-CB-CG	7.52	120.12	112.60
6	C0	1393	ASP	CA-CB-CG	7.52	120.12	112.60
6	C0	1932	LYS	O-C-N	-7.52	114.91	123.48
7	D4	1109	ILE	CA-C-N	7.48	135.83	121.54
7	D4	1109	ILE	C-N-CA	7.48	135.83	121.54
14	L0	730	GLN	CA-C-N	7.46	136.04	121.41
14	L0	730	GLN	C-N-CA	7.46	136.04	121.41
20	R0	1111	GLU	CB-CA-C	7.45	120.75	109.13
15	M0	761	GLU	N-CA-C	7.42	120.25	111.71
20	R3	1049	ASP	CA-CB-CG	7.42	120.02	112.60
6	C0	1604	ASP	CA-CB-CG	7.37	119.97	112.60
18	P2	104	ASN	CA-CB-CG	7.35	119.95	112.60
2	17	1795	TYR	N-CA-C	7.34	121.35	110.48
20	R2	1049	ASP	CA-CB-CG	7.33	119.93	112.60
19	Q2	182	ARG	CD-NE-CZ	7.33	134.66	124.40
10	H3	315	ASP	CA-CB-CG	7.28	119.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	17	1791	GLY	C-N-CD	-7.28	95.16	125.00
4	A1	780	ASP	CA-CB-CG	7.27	119.87	112.60
7	D0	1168	HIS	CB-CG-CD2	-7.26	121.76	131.20
1	01	335	LYS	CB-CA-C	7.26	121.69	111.74
6	C2	1306	ASP	CA-CB-CG	7.26	119.86	112.60
1	03	183	ASP	CA-CB-CG	7.25	119.85	112.60
22	T0	557	SER	N-CA-C	7.25	118.08	108.07
8	E0	72	PHE	CB-CA-C	-7.24	99.81	110.96
7	D1	995	VAL	CA-C-N	7.23	128.88	119.84
7	D1	995	VAL	C-N-CA	7.23	128.88	119.84
18	P1	104	ASN	CA-CB-CG	7.23	119.83	112.60
6	C1	1604	ASP	CA-CB-CG	7.21	119.81	112.60
7	D1	915	ASN	CA-CB-CG	7.21	119.81	112.60
2	12	1626	ASP	CA-CB-CG	7.20	119.80	112.60
3	41	390	ASP	CA-CB-CG	7.20	119.80	112.60
13	K0	599	HIS	CB-CG-CD2	-7.17	121.88	131.20
2	10	1626	ASP	CA-CB-CG	7.17	119.77	112.60
20	R0	1049	ASP	CA-CB-CG	7.15	119.75	112.60
5	B1	526	ARG	CD-NE-CZ	7.15	134.41	124.40
6	C0	1933	SER	CB-CA-C	7.15	121.73	109.51
10	H1	315	ASP	CA-CB-CG	7.14	119.74	112.60
4	A0	14	GLU	CA-CB-CG	7.14	128.38	114.10
4	A2	14	GLU	CA-CB-CG	7.14	128.38	114.10
13	K2	697	ASP	CA-CB-CG	7.13	119.73	112.60
8	E0	19	ARG	O-C-N	7.12	129.70	122.08
13	K1	697	ASP	CA-CB-CG	7.12	119.72	112.60
20	R3	295	HIS	CB-CG-CD2	-7.12	121.95	131.20
20	R1	1429	ASP	CA-CB-CG	7.11	119.71	112.60
23	U1	610	LEU	CB-CA-C	7.11	122.04	110.88
13	K3	697	ASP	CA-CB-CG	7.10	119.70	112.60
7	D0	531	ASP	CA-CB-CG	7.09	119.69	112.60
23	U3	610	LEU	CB-CA-C	7.09	122.00	110.88
2	17	1788	ASP	CA-CB-CG	7.08	119.68	112.60
12	J4	450	ASP	CA-CB-CG	7.08	119.68	112.60
2	13	1626	ASP	CA-CB-CG	7.07	119.67	112.60
18	P1	520	ASP	CA-CB-CG	7.06	119.66	112.60
10	H0	315	ASP	CA-CB-CG	7.05	119.65	112.60
7	D0	1168	HIS	CB-CA-C	7.03	122.03	109.38
8	E0	19	ARG	N-CA-C	-7.01	102.47	111.02
6	C0	279	PHE	CA-CB-CG	7.01	120.81	113.80
2	14	1626	ASP	CA-CB-CG	7.00	119.61	112.60
2	11	1626	ASP	CA-CB-CG	7.00	119.60	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C1	279	PHE	CA-CB-CG	7.00	120.80	113.80
7	D3	1029	ARG	CD-NE-CZ	6.99	134.18	124.40
13	K0	697	ASP	CA-CB-CG	6.99	119.59	112.60
15	M2	585	SER	CA-C-N	6.98	128.57	119.84
15	M2	585	SER	C-N-CA	6.98	128.57	119.84
8	E0	158	ALA	CA-C-N	6.97	131.28	120.75
8	E0	158	ALA	C-N-CA	6.97	131.28	120.75
23	U5	611	PHE	CA-CB-CG	-6.96	106.84	113.80
4	A0	780	ASP	CA-CB-CG	6.95	119.55	112.60
2	16	1626	ASP	CA-CB-CG	6.95	119.55	112.60
7	D1	1003	VAL	CA-C-N	-6.94	108.28	121.54
7	D1	1003	VAL	C-N-CA	-6.94	108.28	121.54
6	C0	577	ASP	CA-CB-CG	6.94	119.54	112.60
18	P0	616	GLU	N-CA-C	6.93	120.81	111.24
8	E0	19	ARG	N-CA-CB	6.93	120.35	109.82
18	P2	520	ASP	CA-CB-CG	6.92	119.52	112.60
7	D1	1001	PRO	N-CA-CB	6.91	109.78	103.08
13	K2	599	HIS	CB-CG-CD2	-6.90	122.23	131.20
18	P0	104	ASN	CA-CB-CG	6.90	119.50	112.60
20	R3	1429	ASP	CA-CB-CG	6.90	119.50	112.60
15	M1	584	CYS	CA-C-N	6.88	134.09	121.70
15	M1	584	CYS	C-N-CA	6.88	134.09	121.70
7	D3	531	ASP	CA-CB-CG	6.88	119.48	112.60
18	P3	520	ASP	CA-CB-CG	6.86	119.46	112.60
2	17	1626	ASP	CA-CB-CG	6.85	119.45	112.60
6	C4	279	PHE	CA-CB-CG	6.85	120.65	113.80
14	L3	337	ASP	CA-CB-CG	-6.85	105.75	112.60
17	O3	257	LEU	CA-C-N	6.84	131.85	120.70
17	O3	257	LEU	C-N-CA	6.84	131.85	120.70
18	P3	104	ASN	CA-CB-CG	6.84	119.44	112.60
7	D2	1168	HIS	CB-CA-C	6.84	121.69	109.38
2	16	1410	ASP	CA-CB-CG	6.84	119.44	112.60
23	U2	611	PHE	CA-C-N	-6.83	111.33	122.26
23	U2	611	PHE	C-N-CA	-6.83	111.33	122.26
4	A1	14	GLU	CA-CB-CG	6.83	127.76	114.10
5	B0	526	ARG	CD-NE-CZ	6.83	133.96	124.40
6	C4	1245	GLY	CA-C-N	6.82	134.57	121.54
6	C4	1245	GLY	C-N-CA	6.82	134.57	121.54
4	A3	14	GLU	CA-CB-CG	6.82	127.74	114.10
7	D5	1173	ASP	CA-CB-CG	6.82	119.42	112.60
2	17	1410	ASP	CA-CB-CG	6.82	119.42	112.60
6	C3	279	PHE	CA-CB-CG	6.82	120.61	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E0	19	ARG	CA-C-O	6.82	128.57	121.07
14	L0	324	ASP	CA-CB-CG	6.81	119.41	112.60
2	12	700	SER	CA-C-N	6.80	132.49	122.08
2	12	700	SER	C-N-CA	6.80	132.49	122.08
20	R1	746	ASP	CA-CB-CG	6.80	119.40	112.60
23	U5	610	LEU	CB-CA-C	6.80	121.56	110.88
2	15	1410	ASP	CA-CB-CG	6.79	119.39	112.60
6	C2	1825	ASP	CA-CB-CG	6.78	119.38	112.60
20	R0	746	ASP	CA-CB-CG	6.78	119.38	112.60
5	B0	1520	ARG	CA-C-N	6.76	127.35	120.38
5	B0	1520	ARG	C-N-CA	6.76	127.35	120.38
2	10	1823	VAL	O-C-N	6.76	128.54	121.91
2	15	1626	ASP	CA-CB-CG	6.76	119.36	112.60
3	40	390	ASP	CA-CB-CG	6.75	119.35	112.60
8	E0	19	ARG	CG-CD-NE	6.74	126.83	112.00
17	O3	276	ASN	CA-CB-CG	6.74	119.34	112.60
2	10	1217	ARG	CA-C-N	6.73	129.85	120.29
2	10	1217	ARG	C-N-CA	6.73	129.85	120.29
4	A4	483	GLU	CB-CG-CD	-6.73	101.15	112.60
6	C4	1532	ASP	CA-CB-CG	6.73	119.33	112.60
2	16	1463	HIS	CA-CB-CG	6.72	120.52	113.80
7	D4	1102	ALA	CA-C-N	6.72	132.24	122.77
7	D4	1102	ALA	C-N-CA	6.72	132.24	122.77
6	C1	577	ASP	CA-CB-CG	6.71	119.31	112.60
25	W0	667	LEU	CA-C-N	6.71	124.47	120.24
25	W0	667	LEU	C-N-CA	6.71	124.47	120.24
7	D2	531	ASP	CA-CB-CG	6.71	119.31	112.60
17	O0	276	ASN	CA-CB-CG	6.70	119.30	112.60
18	P0	626	ASP	CA-CB-CG	6.70	119.30	112.60
6	C2	49	ASP	CA-CB-CG	6.69	119.29	112.60
4	A3	137	TRP	N-CA-C	6.69	121.79	107.67
22	T0	186	ASP	CA-CB-CG	6.69	119.29	112.60
2	13	1773	THR	N-CA-C	6.68	118.22	111.07
20	R0	1111	GLU	CG-CD-OE1	6.68	133.77	118.40
8	E1	245	ALA	CA-C-N	6.68	135.36	122.53
8	E1	245	ALA	C-N-CA	6.68	135.36	122.53
17	O1	276	ASN	CA-CB-CG	6.68	119.28	112.60
10	H2	315	ASP	CA-CB-CG	6.67	119.27	112.60
7	D2	1173	ASP	CA-CB-CG	6.67	119.27	112.60
23	U3	611	PHE	CA-CB-CG	-6.66	107.14	113.80
5	B1	1520	ARG	CA-C-N	6.65	127.23	120.38
5	B1	1520	ARG	C-N-CA	6.65	127.23	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	17	1790	ARG	CA-C-N	6.64	132.30	121.87
2	17	1790	ARG	C-N-CA	6.64	132.30	121.87
6	C2	1803	VAL	CA-C-N	6.63	134.39	122.13
6	C2	1803	VAL	C-N-CA	6.63	134.39	122.13
2	14	1410	ASP	CA-CB-CG	6.62	119.22	112.60
7	D4	1114	ARG	CA-CB-CG	6.62	127.33	114.10
6	C3	1532	ASP	CA-CB-CG	6.61	119.21	112.60
2	17	1795	TYR	CA-C-N	6.61	134.37	121.41
2	17	1795	TYR	C-N-CA	6.61	134.37	121.41
13	K1	599	HIS	CB-CG-CD2	-6.61	122.60	131.20
6	C3	54	PHE	CA-CB-CG	6.60	120.40	113.80
7	D4	853	ASP	CA-CB-CG	6.60	119.20	112.60
17	O2	276	ASN	CA-CB-CG	6.60	119.20	112.60
2	12	1788	ASP	CA-CB-CG	-6.59	106.01	112.60
5	B0	288	ASP	CA-CB-CG	6.59	119.19	112.60
7	D4	276	ASP	CA-CB-CG	6.59	119.19	112.60
4	A4	107	ASP	CA-CB-CG	6.58	119.19	112.60
18	P0	61	VAL	CA-C-N	6.58	134.11	121.54
18	P0	61	VAL	C-N-CA	6.58	134.11	121.54
22	T1	186	ASP	CA-CB-CG	6.58	119.18	112.60
8	E1	241	TRP	O-C-N	-6.58	114.08	121.84
7	D3	1173	ASP	CA-CB-CG	6.57	119.17	112.60
7	D4	1173	ASP	CA-CB-CG	6.57	119.17	112.60
20	R0	1429	ASP	CA-CB-CG	6.57	119.17	112.60
6	C0	54	PHE	CA-CB-CG	6.57	120.36	113.80
6	C4	1939	SER	N-CA-C	6.56	120.94	111.56
6	C1	54	PHE	CA-CB-CG	6.54	120.34	113.80
7	D0	1173	ASP	CA-CB-CG	6.54	119.14	112.60
20	R2	333	ASP	CA-CB-CG	6.54	119.14	112.60
1	O2	183	ASP	CA-CB-CG	6.53	119.13	112.60
6	C4	54	PHE	CA-CB-CG	6.53	120.33	113.80
5	B0	1516	GLN	N-CA-C	6.51	118.89	108.41
23	U1	611	PHE	CA-CB-CG	-6.51	107.29	113.80
1	O0	183	ASP	CA-CB-CG	6.50	119.10	112.60
19	Q2	228	ASN	CA-CB-CG	6.48	119.08	112.60
6	C2	2012	ASN	CA-CB-CG	6.48	119.08	112.60
7	D1	1012	SER	CA-C-O	-6.46	111.28	120.51
22	T0	554	GLN	OE1-CD-NE2	-6.45	116.15	122.60
7	D1	1002	PRO	N-CA-CB	-6.45	96.47	103.25
1	O2	140	ASP	CA-CB-CG	6.45	119.05	112.60
20	R0	1053	PHE	CA-CB-CG	6.45	120.25	113.80
7	D0	276	ASP	CA-CB-CG	6.44	119.04	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L1	560	LEU	CA-C-N	6.44	134.03	121.41
14	L1	560	LEU	C-N-CA	6.44	134.03	121.41
6	C2	959	ASP	CA-CB-CG	6.43	119.03	112.60
7	D5	1223	ASP	CA-CB-CG	6.42	119.02	112.60
7	D1	1173	ASP	CA-CB-CG	6.42	119.02	112.60
6	C2	1941	ALA	N-CA-C	6.42	118.42	110.91
2	10	984	ARG	CD-NE-CZ	6.41	133.38	124.40
20	R2	1429	ASP	CA-CB-CG	6.40	119.00	112.60
13	K3	599	HIS	CB-CG-CD2	-6.40	122.88	131.20
4	A6	107	ASP	CA-CB-CG	6.39	119.00	112.60
6	C4	1825	ASP	CA-CB-CG	6.38	118.98	112.60
4	A6	408	ASP	CA-CB-CG	6.37	118.97	112.60
21	S0	17	ASP	CA-CB-CG	6.36	118.96	112.60
5	B1	833	VAL	CA-CB-CG2	-6.36	99.59	110.40
4	A1	757	PHE	CA-CB-CG	6.35	120.15	113.80
6	C2	1936	LEU	CA-C-N	6.35	133.67	121.54
6	C2	1936	LEU	C-N-CA	6.35	133.67	121.54
5	B1	1515	ALA	CA-C-N	6.35	133.67	121.54
5	B1	1515	ALA	C-N-CA	6.35	133.67	121.54
7	D4	1180	SER	N-CA-C	6.35	124.32	110.80
7	D2	276	ASP	CA-CB-CG	6.34	118.94	112.60
5	B1	288	ASP	CA-CB-CG	6.33	118.93	112.60
2	16	984	ARG	CD-NE-CZ	6.33	133.26	124.40
9	F0	301	GLN	OE1-CD-NE2	-6.33	116.27	122.60
8	E0	18	TRP	NE1-CE2-CZ2	6.32	139.59	130.10
18	P2	550	GLU	O-C-N	-6.32	114.18	122.59
12	J4	405	ASP	CA-CB-CG	6.32	118.92	112.60
15	M3	368	ASP	CA-CB-CG	6.32	118.92	112.60
22	T0	552	ALA	CA-C-N	6.31	129.35	121.85
22	T0	552	ALA	C-N-CA	6.31	129.35	121.85
6	C3	1939	SER	N-CA-C	6.30	120.57	111.56
6	C3	577	ASP	CA-CB-CG	6.30	118.90	112.60
8	E0	14	ARG	CA-C-N	6.28	135.30	122.55
8	E0	14	ARG	C-N-CA	6.28	135.30	122.55
2	14	984	ARG	CD-NE-CZ	6.27	133.18	124.40
2	12	984	ARG	CD-NE-CZ	6.27	133.17	124.40
6	C2	1803	VAL	N-CA-CB	6.26	117.77	110.82
6	C3	180	GLN	OE1-CD-NE2	-6.26	116.34	122.60
5	B0	1268	ASP	N-CA-C	6.26	119.81	111.30
7	D3	211	ASP	CA-CB-CG	6.26	118.86	112.60
13	K3	262	LEU	CA-C-N	6.25	132.96	121.70
13	K3	262	LEU	C-N-CA	6.25	132.96	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	H1	111	PRO	CA-N-CD	-6.24	103.26	112.00
18	P0	615	GLY	CA-C-N	6.23	131.83	122.68
18	P0	615	GLY	C-N-CA	6.23	131.83	122.68
7	D4	92	GLU	CB-CA-C	-6.22	100.11	110.68
4	A3	757	PHE	CA-CB-CG	6.21	120.01	113.80
20	R0	1054	PRO	CA-C-N	6.21	133.39	121.54
20	R0	1054	PRO	C-N-CA	6.21	133.39	121.54
6	C0	782	ASP	CA-CB-CG	6.20	118.80	112.60
7	D3	276	ASP	CA-CB-CG	6.20	118.80	112.60
18	P3	616	GLU	N-CA-C	6.20	119.65	111.28
5	B1	1169	GLN	OE1-CD-NE2	-6.19	116.41	122.60
13	K1	262	LEU	CA-C-N	6.19	132.84	121.70
13	K1	262	LEU	C-N-CA	6.19	132.84	121.70
13	K0	262	LEU	CA-C-N	6.19	132.84	121.70
13	K0	262	LEU	C-N-CA	6.19	132.84	121.70
13	K0	401	ASP	CA-CB-CG	6.19	118.79	112.60
21	S0	89	LEU	N-CA-CB	-6.19	103.42	111.09
2	10	1824	MET	O-C-N	-6.18	114.37	122.59
10	H0	415	ASP	CA-CB-CG	6.18	118.78	112.60
7	D4	437	ASP	CA-CB-CG	6.17	118.77	112.60
20	R2	746	ASP	CA-CB-CG	6.17	118.77	112.60
4	A2	178	LEU	CA-C-N	6.17	132.80	121.70
4	A2	178	LEU	C-N-CA	6.17	132.80	121.70
7	D5	870	ASP	CA-C-N	6.16	129.04	120.29
7	D5	870	ASP	C-N-CA	6.16	129.04	120.29
14	L0	447	ASP	CA-CB-CG	6.16	118.76	112.60
15	M0	406	LEU	CA-C-N	6.16	131.01	120.72
15	M0	406	LEU	C-N-CA	6.16	131.01	120.72
13	K2	401	ASP	CA-CB-CG	6.16	118.76	112.60
14	L1	447	ASP	CA-CB-CG	6.16	118.76	112.60
6	C4	959	ASP	CA-CB-CG	6.16	118.76	112.60
13	K3	401	ASP	CA-CB-CG	6.16	118.76	112.60
5	B0	1268	ASP	CA-CB-CG	6.16	118.76	112.60
2	17	984	ARG	CD-NE-CZ	6.15	133.01	124.40
4	A2	87	PHE	CA-CB-CG	6.15	119.95	113.80
7	D5	1105	HIS	CB-CG-CD2	-6.15	123.21	131.20
4	A2	757	PHE	CA-CB-CG	6.15	119.95	113.80
2	17	1688	SER	N-CA-C	6.15	113.75	108.22
8	E0	22	GLY	N-CA-C	6.15	127.75	113.18
13	K2	262	LEU	CA-C-N	6.15	132.76	121.70
13	K2	262	LEU	C-N-CA	6.15	132.76	121.70
15	M2	251	LEU	CA-C-N	6.13	129.34	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	M2	251	LEU	C-N-CA	6.13	129.34	120.38
20	R3	333	ASP	CA-CB-CG	6.13	118.73	112.60
5	B0	1519	GLN	N-CA-C	6.13	123.86	110.80
6	C3	959	ASP	CA-CB-CG	6.12	118.72	112.60
14	L2	447	ASP	CA-CB-CG	6.12	118.72	112.60
8	E0	18	TRP	CB-CG-CD2	-6.12	118.23	126.80
13	K1	401	ASP	CA-CB-CG	6.12	118.72	112.60
7	D4	1107	THR	O-C-N	-6.12	114.16	122.36
18	P1	553	PHE	CA-CB-CG	6.11	119.91	113.80
18	P2	548	TYR	CB-CA-C	6.10	122.56	110.42
7	D4	95	GLU	CB-CA-C	-6.10	101.27	110.90
8	E0	19	ARG	NH1-CZ-NH2	-6.10	111.38	119.30
15	M0	379	ASP	CA-CB-CG	6.09	118.69	112.60
20	R0	1247	ALA	CA-C-N	6.09	129.26	120.79
20	R0	1247	ALA	C-N-CA	6.09	129.26	120.79
2	I1	984	ARG	CD-NE-CZ	6.09	132.93	124.40
22	T0	377	ASP	CA-CB-CG	6.08	118.68	112.60
4	A2	656	PRO	N-CA-CB	6.08	108.60	103.25
7	D4	91	PRO	CB-CA-C	6.08	121.59	111.56
8	E0	599	GLN	OE1-CD-NE2	-6.08	116.52	122.60
6	C4	577	ASP	CA-CB-CG	6.08	118.68	112.60
5	B1	1523	SER	CA-C-N	6.07	132.63	121.70
5	B1	1523	SER	C-N-CA	6.07	132.63	121.70
6	C3	1694	VAL	O-C-N	-6.07	116.33	123.00
14	L3	447	ASP	CA-CB-CG	6.07	118.67	112.60
14	L2	332	LYS	CB-CA-C	6.07	119.99	111.86
22	T1	557	SER	CA-C-N	6.06	133.12	121.54
22	T1	557	SER	C-N-CA	6.06	133.12	121.54
13	K2	613	ASP	CA-CB-CG	6.06	118.66	112.60
15	M1	368	ASP	CA-CB-CG	6.06	118.66	112.60
18	P1	254	LEU	CA-C-N	6.06	128.32	120.44
18	P1	254	LEU	C-N-CA	6.06	128.32	120.44
22	T1	29	THR	CA-C-N	6.06	133.12	121.54
22	T1	29	THR	C-N-CA	6.06	133.12	121.54
7	D5	437	ASP	CA-CB-CG	6.06	118.66	112.60
4	A2	656	PRO	CA-C-N	6.05	133.96	123.91
4	A2	656	PRO	C-N-CA	6.05	133.96	123.91
6	C4	782	ASP	CA-CB-CG	6.05	118.65	112.60
5	B1	1519	GLN	N-CA-C	6.05	123.68	110.80
20	R2	179	VAL	CA-C-N	6.04	129.94	121.24
20	R2	179	VAL	C-N-CA	6.04	129.94	121.24
22	T0	29	THR	CA-C-N	6.04	133.08	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	T0	29	THR	C-N-CA	6.04	133.08	121.54
21	S0	174	HIS	CB-CG-CD2	-6.04	123.35	131.20
14	L0	244	ALA	CA-C-N	6.04	130.94	120.86
14	L0	244	ALA	C-N-CA	6.04	130.94	120.86
2	15	984	ARG	CD-NE-CZ	6.03	132.85	124.40
18	P0	189	ASN	CA-CB-CG	6.03	118.63	112.60
8	E0	18	TRP	CE2-CD2-CE3	-6.03	112.77	118.80
2	13	984	ARG	CD-NE-CZ	6.03	132.84	124.40
9	F2	173	ASP	CA-CB-CG	6.03	118.63	112.60
13	K2	910	LYS	CB-CA-C	6.03	120.41	109.62
24	V0	700	ASP	CA-CB-CG	-6.03	106.57	112.60
20	R1	1390	ASP	CA-CB-CG	6.03	118.63	112.60
2	10	1795	TYR	N-CA-C	6.02	117.05	108.74
4	A5	757	PHE	CA-CB-CG	6.02	119.82	113.80
5	B0	946	ASP	CA-CB-CG	6.02	118.62	112.60
20	R0	1111	GLU	CB-CG-CD	6.02	122.83	112.60
19	Q2	273	ASN	CA-CB-CG	6.01	118.61	112.60
21	S1	174	HIS	CB-CG-CD2	-6.01	123.38	131.20
3	40	138	ASP	CA-CB-CG	6.01	118.61	112.60
19	Q3	273	ASN	CA-CB-CG	6.01	118.61	112.60
7	D1	437	ASP	CA-CB-CG	6.01	118.61	112.60
5	B0	1169	GLN	OE1-CD-NE2	-6.01	116.59	122.60
6	C2	1754	GLN	OE1-CD-NE2	-6.01	116.59	122.60
6	C3	1825	ASP	CA-CB-CG	6.01	118.61	112.60
15	M1	251	LEU	CA-C-N	6.01	129.15	120.38
15	M1	251	LEU	C-N-CA	6.01	129.15	120.38
7	D0	437	ASP	CA-CB-CG	6.00	118.61	112.60
8	E1	599	GLN	OE1-CD-NE2	-6.00	116.60	122.60
7	D0	1001	PRO	N-CA-C	6.00	118.02	110.70
7	D2	437	ASP	CA-CB-CG	6.00	118.60	112.60
6	C1	782	ASP	CA-CB-CG	6.00	118.60	112.60
7	D1	1137	ASP	CA-CB-CG	6.00	118.60	112.60
9	F0	308	THR	N-CA-C	6.00	123.06	109.81
15	M3	251	LEU	CA-C-N	6.00	129.13	120.38
15	M3	251	LEU	C-N-CA	6.00	129.13	120.38
6	C2	1532	ASP	CA-CB-CG	5.99	118.59	112.60
4	A6	248	VAL	CA-C-N	5.99	128.23	120.44
4	A6	248	VAL	C-N-CA	5.99	128.23	120.44
4	A4	248	VAL	CA-C-N	5.99	128.22	120.44
4	A4	248	VAL	C-N-CA	5.99	128.22	120.44
25	W0	185	ASP	CA-CB-CG	5.99	118.59	112.60
6	C2	1300	ASP	CA-CB-CG	5.98	118.58	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	R1	179	VAL	CA-C-N	5.98	129.85	121.24
20	R1	179	VAL	C-N-CA	5.98	129.85	121.24
20	R3	1390	ASP	CA-CB-CG	5.98	118.58	112.60
7	D1	1012	SER	CA-C-N	-5.97	111.23	120.31
7	D1	1012	SER	C-N-CA	-5.97	111.23	120.31
22	T1	554	GLN	OE1-CD-NE2	-5.97	116.62	122.60
19	Q1	273	ASN	CA-CB-CG	5.96	118.56	112.60
4	A2	780	ASP	CA-CB-CG	5.96	118.56	112.60
5	B1	1526	SER	CA-C-N	5.96	132.42	121.70
5	B1	1526	SER	C-N-CA	5.96	132.42	121.70
15	M0	251	LEU	CA-C-N	5.95	129.07	120.38
15	M0	251	LEU	C-N-CA	5.95	129.07	120.38
20	R0	179	VAL	CA-C-N	5.95	129.81	121.24
20	R0	179	VAL	C-N-CA	5.95	129.81	121.24
4	A0	757	PHE	CA-CB-CG	5.95	119.75	113.80
6	C4	1246	MET	CA-C-N	5.95	128.53	120.44
6	C4	1246	MET	C-N-CA	5.95	128.53	120.44
7	D2	1001	PRO	N-CA-C	5.95	117.95	110.70
18	P0	555	ASP	CA-CB-CG	5.94	118.54	112.60
7	D3	32	ARG	CD-NE-CZ	5.94	132.72	124.40
6	C1	1798	ASP	CA-C-N	5.94	129.14	120.71
6	C1	1798	ASP	C-N-CA	5.94	129.14	120.71
19	Q0	273	ASN	CA-CB-CG	5.94	118.54	112.60
8	E0	134	VAL	CB-CA-C	5.93	119.78	112.02
15	M2	403	LEU	N-CA-C	5.93	123.42	110.80
10	H2	415	ASP	CA-CB-CG	5.92	118.53	112.60
5	B0	1518	VAL	N-CA-C	5.92	121.66	109.34
5	B1	946	ASP	CA-CB-CG	5.92	118.52	112.60
12	J1	339	LYS	CG-CD-CE	-5.92	97.68	111.30
21	S3	174	HIS	CB-CG-CD2	-5.92	123.51	131.20
20	R0	1390	ASP	CA-CB-CG	5.91	118.51	112.60
4	A5	706	HIS	CA-C-N	5.91	132.60	121.97
4	A5	706	HIS	C-N-CA	5.91	132.60	121.97
23	U1	610	LEU	CA-CB-CG	-5.90	95.64	116.30
1	04	183	ASP	CA-CB-CG	5.90	118.50	112.60
14	L0	730	GLN	N-CA-CB	-5.89	100.63	111.36
7	D3	437	ASP	CA-CB-CG	5.89	118.49	112.60
20	R2	1390	ASP	CA-CB-CG	5.89	118.49	112.60
21	S2	174	HIS	CB-CG-CD2	-5.89	123.55	131.20
22	T1	377	ASP	CA-CB-CG	5.89	118.49	112.60
13	K1	613	ASP	CA-CB-CG	5.88	118.48	112.60
18	P2	254	LEU	CA-C-N	5.88	128.42	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	P2	254	LEU	C-N-CA	5.88	128.42	120.65
6	C3	782	ASP	CA-CB-CG	5.88	118.48	112.60
5	B1	1526	SER	N-CA-C	5.87	123.31	110.80
2	10	1414	ASP	CA-CB-CG	5.87	118.47	112.60
6	C1	49	ASP	CA-CB-CG	5.87	118.47	112.60
7	D3	545	ASP	CA-CB-CG	5.87	118.47	112.60
4	A1	488	HIS	CB-CG-CD2	-5.87	123.57	131.20
7	D1	32	ARG	CD-NE-CZ	5.87	132.61	124.40
21	S2	17	ASP	CA-CB-CG	5.86	118.46	112.60
9	F2	308	THR	N-CA-C	5.86	122.76	109.81
18	P0	254	LEU	CA-C-N	5.86	128.39	120.65
18	P0	254	LEU	C-N-CA	5.86	128.39	120.65
4	A4	706	HIS	CA-C-N	5.86	132.51	121.97
4	A4	706	HIS	C-N-CA	5.86	132.51	121.97
6	C0	959	ASP	CA-CB-CG	5.86	118.45	112.60
20	R2	992	ASP	CA-C-N	5.86	132.72	121.54
20	R2	992	ASP	C-N-CA	5.86	132.72	121.54
15	M2	586	PRO	N-CA-C	5.85	124.52	112.47
6	C0	1825	ASP	CA-CB-CG	5.85	118.45	112.60
14	L0	326	ASP	CA-CB-CG	5.84	118.44	112.60
4	A6	95	ASP	CA-C-N	5.84	132.22	121.70
4	A6	95	ASP	C-N-CA	5.84	132.22	121.70
6	C0	1532	ASP	CA-CB-CG	5.84	118.44	112.60
2	10	1827	ALA	CB-CA-C	5.84	122.04	110.42
6	C4	697	ARG	CD-NE-CZ	-5.84	116.22	124.40
4	A0	779	GLU	CA-C-N	5.84	128.90	120.38
4	A0	779	GLU	C-N-CA	5.84	128.90	120.38
18	P1	626	ASP	CA-CB-CG	5.83	118.44	112.60
5	B1	609	ASP	CA-CB-CG	5.83	118.43	112.60
6	C1	1825	ASP	CA-CB-CG	5.83	118.43	112.60
9	F0	163	ASP	CA-CB-CG	5.83	118.43	112.60
18	P1	551	LYS	CB-CG-CD	5.83	124.70	111.30
18	P3	61	VAL	CA-C-N	5.82	128.36	120.38
18	P3	61	VAL	C-N-CA	5.82	128.36	120.38
5	B1	1518	VAL	N-CA-C	5.82	121.45	109.34
7	D3	1103	ASP	CA-CB-CG	5.82	118.42	112.60
20	R3	179	VAL	CA-C-N	5.82	129.62	121.24
20	R3	179	VAL	C-N-CA	5.82	129.62	121.24
6	C1	1532	ASP	CA-CB-CG	5.81	118.41	112.60
12	J1	452	LYS	CG-CD-CE	-5.81	97.94	111.30
16	N1	169	ASP	CA-CB-CG	5.81	118.41	112.60
18	P3	626	ASP	CA-CB-CG	5.81	118.41	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A5	248	VAL	CA-C-N	5.80	128.33	120.44
4	A5	248	VAL	C-N-CA	5.80	128.33	120.44
6	C3	1246	MET	CA-C-N	5.80	130.39	120.71
6	C3	1246	MET	C-N-CA	5.80	130.39	120.71
16	N2	169	ASP	CA-CB-CG	5.79	118.39	112.60
18	P0	387	LEU	N-CA-C	5.79	118.03	109.69
18	P3	533	ASP	CA-CB-CG	5.79	118.39	112.60
4	A2	248	VAL	CA-C-N	5.79	127.97	120.44
4	A2	248	VAL	C-N-CA	5.79	127.97	120.44
19	Q2	281	SER	N-CA-C	5.79	117.34	108.42
10	H2	357	ASP	CA-CB-CG	5.79	118.39	112.60
4	A3	447	ASP	CA-CB-CG	5.79	118.39	112.60
5	B1	799	ASP	CA-CB-CG	5.79	118.39	112.60
6	C1	1754	GLN	OE1-CD-NE2	-5.79	116.81	122.60
6	C1	959	ASP	CA-CB-CG	5.78	118.38	112.60
14	L3	184	GLN	OE1-CD-NE2	-5.78	116.82	122.60
6	C0	412	ASN	CA-CB-CG	5.78	118.38	112.60
19	Q1	281	SER	N-CA-C	5.78	117.32	108.42
23	U5	610	LEU	CA-CB-CG	-5.78	96.07	116.30
20	R2	1162	HIS	CB-CG-CD2	-5.78	123.69	131.20
4	A0	488	HIS	CB-CG-CD2	-5.78	123.69	131.20
18	P3	253	GLU	CB-CA-C	-5.78	101.99	110.95
22	T1	792	ASP	CA-CB-CG	5.78	118.38	112.60
6	C0	49	ASP	CA-CB-CG	5.77	118.37	112.60
8	E1	244	THR	CA-CB-OG1	5.77	118.26	109.60
4	A2	488	HIS	CB-CG-CD2	-5.77	123.70	131.20
7	D1	995	VAL	CB-CA-C	5.77	121.86	111.36
2	I3	1652	ASP	CA-CB-CG	-5.77	106.83	112.60
6	C2	544	ASN	CA-CB-CG	-5.77	106.83	112.60
6	C1	412	ASN	CA-CB-CG	5.77	118.37	112.60
6	C4	49	ASP	CA-CB-CG	5.77	118.37	112.60
1	O2	651	HIS	CB-CG-CD2	-5.77	123.70	131.20
18	P2	552	ARG	N-CA-C	5.77	123.08	110.80
6	C2	503	ASP	CA-CB-CG	5.76	118.36	112.60
6	C4	1754	GLN	OE1-CD-NE2	-5.76	116.84	122.60
14	L0	184	GLN	OE1-CD-NE2	-5.76	116.83	122.60
3	41	138	ASP	CA-CB-CG	5.76	118.36	112.60
20	R1	1162	HIS	CB-CG-CD2	-5.76	123.71	131.20
6	C1	438	ASP	CA-CB-CG	5.76	118.36	112.60
6	C3	1754	GLN	OE1-CD-NE2	-5.76	116.84	122.60
1	O4	651	HIS	CB-CG-CD2	-5.75	123.72	131.20
7	D1	211	ASP	CA-CB-CG	5.75	118.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C2	54	PHE	CA-CB-CG	5.75	119.55	113.80
5	B1	1516	GLN	N-CA-C	5.75	123.04	110.80
4	A4	757	PHE	CA-CB-CG	5.75	119.55	113.80
6	C2	1806	TYR	CB-CA-C	5.74	121.85	110.42
20	R2	328	VAL	CA-C-N	5.74	125.87	119.32
20	R2	328	VAL	C-N-CA	5.74	125.87	119.32
4	A2	655	ALA	O-C-N	-5.74	113.22	121.54
6	C0	356	ASP	CA-CB-CG	5.74	118.34	112.60
12	J2	339	LYS	CG-CD-CE	-5.74	98.10	111.30
15	M0	585	SER	CA-C-N	5.74	127.01	119.84
15	M0	585	SER	C-N-CA	5.74	127.01	119.84
8	E0	69	TYR	CA-CB-CG	5.74	124.22	113.90
7	D1	1103	ASP	CA-CB-CG	5.73	118.33	112.60
5	B1	1155	LEU	CA-C-N	5.73	126.30	120.00
5	B1	1155	LEU	C-N-CA	5.73	126.30	120.00
4	A6	757	PHE	CA-CB-CG	5.73	119.53	113.80
5	B0	1523	SER	CA-C-N	5.73	132.01	121.70
5	B0	1523	SER	C-N-CA	5.73	132.01	121.70
16	N3	2	VAL	CA-CB-CG1	5.73	120.13	110.40
20	R3	1162	HIS	CB-CG-CD2	-5.73	123.76	131.20
13	K3	613	ASP	CA-CB-CG	5.72	118.32	112.60
2	14	1695	GLN	OE1-CD-NE2	-5.72	116.88	122.60
4	A1	248	VAL	CA-C-N	5.72	127.87	120.44
4	A1	248	VAL	C-N-CA	5.72	127.87	120.44
4	A6	581	ASP	CA-CB-CG	5.72	118.32	112.60
6	C1	450	TYR	CA-C-N	5.72	129.84	120.63
6	C1	450	TYR	C-N-CA	5.72	129.84	120.63
12	J1	450	ASP	CA-CB-CG	5.71	118.31	112.60
1	04	125	PHE	CA-CB-CG	5.71	119.51	113.80
8	E0	19	ARG	NE-CZ-NH1	5.71	127.21	121.50
19	Q3	281	SER	N-CA-C	5.71	117.21	108.42
2	13	1695	GLN	OE1-CD-NE2	-5.71	116.89	122.60
2	14	1633	GLN	OE1-CD-NE2	-5.71	116.89	122.60
6	C3	356	ASP	CA-CB-CG	5.70	118.30	112.60
20	R2	990	ALA	N-CA-C	5.70	118.20	108.90
12	J3	450	ASP	CA-CB-CG	5.70	118.30	112.60
1	00	651	HIS	CB-CG-CD2	-5.70	123.79	131.20
4	A0	248	VAL	CA-C-N	5.70	127.85	120.44
4	A0	248	VAL	C-N-CA	5.70	127.85	120.44
19	Q0	281	SER	N-CA-C	5.70	117.20	108.42
1	03	651	HIS	CB-CG-CD2	-5.70	123.79	131.20
2	17	1789	ARG	CD-NE-CZ	5.70	132.38	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D3	122	ASP	CA-CB-CG	5.70	118.30	112.60
2	11	1695	GLN	OE1-CD-NE2	-5.70	116.90	122.60
7	D1	545	ASP	CA-CB-CG	5.70	118.30	112.60
2	15	1695	GLN	OE1-CD-NE2	-5.69	116.91	122.60
7	D4	32	ARG	CD-NE-CZ	5.69	132.37	124.40
7	D5	1168	HIS	CB-CG-CD2	-5.69	123.80	131.20
18	P3	254	LEU	CA-C-N	5.69	128.16	120.65
18	P3	254	LEU	C-N-CA	5.69	128.16	120.65
6	C3	450	TYR	CA-C-N	5.69	129.79	120.63
6	C3	450	TYR	C-N-CA	5.69	129.79	120.63
4	A2	656	PRO	CB-CA-C	5.68	118.78	111.56
5	B1	969	GLN	OE1-CD-NE2	-5.68	116.92	122.60
6	C0	1754	GLN	OE1-CD-NE2	-5.68	116.92	122.60
20	R0	333	ASP	CA-CB-CG	5.68	118.28	112.60
6	C1	356	ASP	CA-CB-CG	5.68	118.28	112.60
7	D2	32	ARG	CD-NE-CZ	5.68	132.35	124.40
16	N1	2	VAL	CA-CB-CG1	5.68	120.05	110.40
6	C0	450	TYR	CA-C-N	5.68	129.77	120.63
6	C0	450	TYR	C-N-CA	5.68	129.77	120.63
6	C3	49	ASP	CA-CB-CG	5.67	118.27	112.60
13	K3	819	GLN	OE1-CD-NE2	-5.67	116.93	122.60
2	10	1759	GLN	CB-CA-C	5.67	119.56	110.09
2	15	132	ASP	CA-CB-CG	5.67	118.27	112.60
4	A1	73	HIS	CB-CG-CD2	-5.67	123.83	131.20
18	P1	616	GLU	N-CA-C	5.67	119.46	111.52
18	P3	189	ASN	CA-CB-CG	5.67	118.27	112.60
13	K1	819	GLN	OE1-CD-NE2	-5.67	116.93	122.60
16	N3	284	ASN	CA-CB-CG	5.66	118.26	112.60
20	R2	529	CYS	CA-C-N	5.66	128.44	120.28
20	R2	529	CYS	C-N-CA	5.66	128.44	120.28
21	S0	284	HIS	CB-CG-CD2	-5.66	123.84	131.20
2	17	132	ASP	CA-CB-CG	5.66	118.26	112.60
5	B0	1515	ALA	N-CA-C	5.66	122.85	110.80
18	P1	617	SER	CA-C-N	5.66	131.89	121.70
18	P1	617	SER	C-N-CA	5.66	131.89	121.70
2	13	356	ASP	CA-CB-CG	5.66	118.26	112.60
4	A3	248	VAL	CA-C-N	5.66	127.79	120.44
4	A3	248	VAL	C-N-CA	5.66	127.79	120.44
6	C4	356	ASP	CA-CB-CG	5.66	118.26	112.60
7	D5	211	ASP	CA-CB-CG	5.66	118.26	112.60
13	K2	868	ASP	CA-CB-CG	-5.66	106.94	112.60
7	D5	276	ASP	CA-CB-CG	5.65	118.25	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L0	435	LEU	CA-C-N	5.65	128.42	120.28
14	L0	435	LEU	C-N-CA	5.65	128.42	120.28
6	C2	279	PHE	CA-CB-CG	5.65	119.45	113.80
15	M2	834	ASN	CA-CB-CG	5.65	118.25	112.60
1	04	396	LYS	CA-C-N	5.65	127.85	120.28
1	04	396	LYS	C-N-CA	5.65	127.85	120.28
21	S2	284	HIS	CB-CG-CD2	-5.65	123.86	131.20
2	10	1828	TYR	O-C-N	-5.65	115.08	122.59
20	R0	1162	HIS	CB-CG-CD2	-5.64	123.86	131.20
5	B0	799	ASP	CA-CB-CG	5.64	118.24	112.60
9	F2	234	GLU	CB-CA-C	5.64	120.52	111.66
6	C0	438	ASP	CA-CB-CG	5.64	118.24	112.60
6	C1	1317	ASP	CA-CB-CG	5.64	118.24	112.60
6	C2	1981	ASP	CA-CB-CG	5.64	118.24	112.60
2	17	1695	GLN	OE1-CD-NE2	-5.64	116.96	122.60
22	T0	465	PRO	N-CA-CB	5.64	106.35	103.19
7	D3	1026	LEU	CA-C-N	5.63	127.83	120.28
7	D3	1026	LEU	C-N-CA	5.63	127.83	120.28
11	I1	353	PHE	CA-CB-CG	5.63	119.44	113.80
19	Q2	51	ASP	CA-CB-CG	-5.63	106.97	112.60
16	N2	284	ASN	CA-CB-CG	5.63	118.23	112.60
2	15	1217	ARG	CA-C-N	5.63	130.25	120.68
2	15	1217	ARG	C-N-CA	5.63	130.25	120.68
6	C3	1159	ILE	O-C-N	-5.63	115.53	122.57
18	P2	61	VAL	CA-CB-CG2	5.63	119.97	110.40
1	00	125	PHE	CA-CB-CG	5.62	119.42	113.80
6	C2	1159	ILE	O-C-N	-5.62	115.54	122.57
1	01	183	ASP	CA-CB-CG	5.62	118.22	112.60
4	A2	99	GLN	OE1-CD-NE2	-5.62	116.98	122.60
6	C0	1317	ASP	CA-CB-CG	5.62	118.22	112.60
14	L0	730	GLN	CB-CG-CD	5.62	122.15	112.60
2	10	1824	MET	CA-C-N	5.62	128.98	122.35
2	10	1824	MET	C-N-CA	5.62	128.98	122.35
2	16	1695	GLN	OE1-CD-NE2	-5.62	116.98	122.60
4	A0	188	GLN	OE1-CD-NE2	-5.62	116.98	122.60
4	A2	656	PRO	CA-N-CD	-5.62	104.14	112.00
6	C4	450	TYR	CA-C-N	5.62	129.67	120.63
6	C4	450	TYR	C-N-CA	5.62	129.67	120.63
22	T0	792	ASP	CA-CB-CG	5.62	118.22	112.60
22	T0	843	HIS	CB-CG-CD2	-5.62	123.90	131.20
1	02	125	PHE	CA-CB-CG	5.61	119.41	113.80
16	N1	284	ASN	CA-CB-CG	5.61	118.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	P2	616	GLU	N-CA-C	5.61	119.32	111.74
2	11	356	ASP	CA-CB-CG	5.61	118.21	112.60
22	T1	552	ALA	CA-C-N	5.61	128.44	121.71
22	T1	552	ALA	C-N-CA	5.61	128.44	121.71
16	N0	284	ASN	CA-CB-CG	5.61	118.21	112.60
2	12	356	ASP	CA-CB-CG	5.61	118.21	112.60
20	R3	746	ASP	CA-CB-CG	5.61	118.21	112.60
4	A1	447	ASP	CA-CB-CG	5.61	118.20	112.60
4	A6	706	HIS	CA-C-N	5.61	132.06	121.97
4	A6	706	HIS	C-N-CA	5.61	132.06	121.97
4	A2	188	GLN	OE1-CD-NE2	-5.60	117.00	122.60
2	11	1688	SER	N-CA-C	5.60	113.26	108.22
6	C4	1159	ILE	O-C-N	-5.60	115.57	122.57
6	C3	1012	LYS	CA-C-N	5.60	130.13	122.07
6	C3	1012	LYS	C-N-CA	5.60	130.13	122.07
22	T1	465	PRO	N-CA-CB	5.60	106.33	103.19
17	O1	273	GLN	OE1-CD-NE2	-5.60	117.00	122.60
1	02	83	TYR	CA-C-N	5.59	127.71	120.44
1	02	83	TYR	C-N-CA	5.59	127.71	120.44
19	Q0	51	ASP	CA-CB-CG	-5.59	107.01	112.60
4	A2	155	ALA	N-CA-C	5.59	119.40	112.24
14	L2	617	GLN	OE1-CD-NE2	-5.59	117.01	122.60
6	C2	1249	ILE	CA-C-N	5.58	127.38	120.34
6	C2	1249	ILE	C-N-CA	5.58	127.38	120.34
14	L2	435	LEU	CA-C-N	5.58	128.32	120.28
14	L2	435	LEU	C-N-CA	5.58	128.32	120.28
2	12	1695	GLN	OE1-CD-NE2	-5.58	117.02	122.60
2	17	1217	ARG	CA-C-N	5.58	130.17	120.68
2	17	1217	ARG	C-N-CA	5.58	130.17	120.68
13	K0	819	GLN	OE1-CD-NE2	-5.58	117.02	122.60
20	R1	993	ASP	CA-C-N	5.58	132.21	121.54
20	R1	993	ASP	C-N-CA	5.58	132.21	121.54
1	02	396	LYS	CA-C-N	5.58	127.76	120.28
1	02	396	LYS	C-N-CA	5.58	127.76	120.28
15	M0	834	ASN	CA-CB-CG	5.58	118.18	112.60
20	R1	333	ASP	CA-CB-CG	5.58	118.18	112.60
7	D3	1028	GLN	CA-C-N	5.58	131.57	121.92
7	D3	1028	GLN	C-N-CA	5.58	131.57	121.92
24	V0	884	GLN	CB-CA-C	-5.58	102.12	110.88
5	B0	969	GLN	OE1-CD-NE2	-5.58	117.02	122.60
2	16	1217	ARG	CA-C-N	5.58	130.16	120.68
2	16	1217	ARG	C-N-CA	5.58	130.16	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	R3	1043	GLU	CB-CA-C	5.58	119.98	110.56
20	R3	1074	ASP	CA-C-N	5.58	129.61	120.63
20	R3	1074	ASP	C-N-CA	5.58	129.61	120.63
22	T1	998	ASP	CA-CB-CG	5.58	118.18	112.60
2	14	1217	ARG	CA-C-N	5.57	130.11	120.58
2	14	1217	ARG	C-N-CA	5.57	130.11	120.58
8	E1	322	ASN	CB-CA-C	5.57	115.85	111.00
21	S3	284	HIS	CB-CG-CD2	-5.57	123.95	131.20
22	T0	998	ASP	CA-CB-CG	5.57	118.17	112.60
9	F1	307	GLN	CA-C-N	5.57	128.59	120.51
9	F1	307	GLN	C-N-CA	5.57	128.59	120.51
7	D0	211	ASP	CA-CB-CG	5.57	118.17	112.60
14	L1	184	GLN	OE1-CD-NE2	-5.57	117.03	122.60
4	A1	188	GLN	OE1-CD-NE2	-5.57	117.03	122.60
12	J2	446	ARG	NE-CZ-NH2	5.56	124.21	119.20
2	16	356	ASP	CA-CB-CG	5.56	118.16	112.60
2	17	356	ASP	CA-CB-CG	5.56	118.16	112.60
13	K0	868	ASP	CA-CB-CG	-5.56	107.04	112.60
6	C3	412	ASN	CA-CB-CG	5.55	118.15	112.60
21	S1	284	HIS	CB-CG-CD2	-5.55	123.98	131.20
13	K2	819	GLN	OE1-CD-NE2	-5.55	117.05	122.60
24	V0	839	HIS	CB-CG-CD2	-5.55	123.98	131.20
3	40	190	HIS	CB-CG-CD2	-5.55	123.98	131.20
17	O3	273	GLN	OE1-CD-NE2	-5.55	117.05	122.60
2	15	1652	ASP	CA-CB-CG	-5.55	107.05	112.60
6	C1	566	HIS	CB-CG-CD2	-5.55	123.99	131.20
9	F2	241	LYS	CG-CD-CE	-5.55	98.54	111.30
11	I2	353	PHE	CA-CB-CG	5.55	119.35	113.80
12	J3	339	LYS	CG-CD-CE	-5.54	98.55	111.30
17	O2	273	GLN	OE1-CD-NE2	-5.54	117.06	122.60
2	17	1795	TYR	O-C-N	-5.54	116.69	122.96
6	C0	503	ASP	CA-CB-CG	5.54	118.14	112.60
19	Q2	228	ASN	CB-CA-C	5.54	119.83	111.18
20	R3	582	TYR	N-CA-C	5.54	117.32	111.28
1	03	125	PHE	CA-CB-CG	5.54	119.34	113.80
6	C0	1600	PHE	CA-CB-CG	5.54	119.34	113.80
7	D5	32	ARG	CD-NE-CZ	5.54	132.15	124.40
10	H3	111	PRO	CA-N-CD	-5.54	104.25	112.00
7	D4	1106	SER	N-CA-C	5.54	121.45	114.31
14	L2	184	GLN	OE1-CD-NE2	-5.54	117.06	122.60
8	E0	158	ALA	CB-CA-C	5.53	120.01	110.77
9	F1	96	ASP	CA-CB-CG	5.53	118.13	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D2	211	ASP	CA-CB-CG	5.53	118.13	112.60
13	K1	868	ASP	CA-CB-CG	-5.53	107.07	112.60
16	N2	246	ASP	CA-CB-CG	5.53	118.13	112.60
4	A5	107	ASP	CA-CB-CG	5.53	118.12	112.60
20	R1	529	CYS	CA-C-N	5.53	128.24	120.28
20	R1	529	CYS	C-N-CA	5.53	128.24	120.28
7	D5	545	ASP	CA-CB-CG	5.52	118.12	112.60
9	F1	266	PRO	N-CA-C	5.52	117.44	110.70
7	D0	1269	GLN	OE1-CD-NE2	-5.52	117.08	122.60
10	H0	111	PRO	CA-N-CD	-5.52	104.27	112.00
23	U3	610	LEU	N-CA-CB	5.52	118.02	110.01
14	L1	435	LEU	CA-C-N	5.52	128.23	120.28
14	L1	435	LEU	C-N-CA	5.52	128.23	120.28
1	04	28	LYS	CA-C-N	5.52	126.10	119.98
1	04	28	LYS	C-N-CA	5.52	126.10	119.98
22	T1	30	LEU	N-CA-C	5.52	122.55	110.80
10	H3	493	HIS	CB-CG-CD2	-5.52	124.03	131.20
15	M1	614	HIS	CB-CG-CD2	-5.51	124.03	131.20
22	T0	30	LEU	N-CA-C	5.51	122.55	110.80
2	10	1829	HIS	CA-C-N	5.51	130.12	121.08
2	10	1829	HIS	C-N-CA	5.51	130.12	121.08
18	P1	387	LEU	N-CA-C	5.51	117.01	109.18
1	00	83	TYR	CA-C-N	5.51	127.60	120.44
1	00	83	TYR	C-N-CA	5.51	127.60	120.44
2	10	356	ASP	CA-CB-CG	5.51	118.11	112.60
13	K0	909	GLY	N-CA-C	5.51	119.71	110.56
2	13	1217	ARG	CA-C-N	5.51	130.00	120.58
2	13	1217	ARG	C-N-CA	5.51	130.00	120.58
4	A3	130	ARG	CD-NE-CZ	5.51	132.11	124.40
8	E0	322	ASN	CB-CA-C	5.51	115.79	111.00
22	T1	683	ILE	N-CA-C	5.51	112.10	106.21
17	O0	273	GLN	OE1-CD-NE2	-5.51	117.09	122.60
21	S1	17	ASP	CA-CB-CG	5.50	118.10	112.60
3	41	190	HIS	CB-CG-CD2	-5.50	124.05	131.20
22	T1	843	HIS	CB-CG-CD2	-5.50	124.05	131.20
2	10	930	ALA	CA-C-N	5.50	128.67	120.31
2	10	930	ALA	C-N-CA	5.50	128.67	120.31
11	I0	353	PHE	CA-CB-CG	5.50	119.30	113.80
23	U0	840	PRO	CA-C-N	5.50	127.91	120.65
23	U0	840	PRO	C-N-CA	5.50	127.91	120.65
6	C1	1600	PHE	CA-CB-CG	5.50	119.30	113.80
18	P2	389	SER	CA-C-N	5.50	131.59	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	P2	389	SER	C-N-CA	5.50	131.59	121.70
1	04	83	TYR	CA-C-N	5.49	127.58	120.44
1	04	83	TYR	C-N-CA	5.49	127.58	120.44
2	15	324	HIS	CB-CG-CD2	-5.49	124.06	131.20
23	U3	610	LEU	CA-CB-CG	-5.49	97.09	116.30
19	Q1	51	ASP	CA-CB-CG	-5.49	107.11	112.60
24	V0	884	GLN	CA-CB-CG	5.49	125.07	114.10
14	L3	332	LYS	CB-CA-C	5.48	119.52	111.73
8	E0	69	TYR	N-CA-CB	-5.48	101.78	110.28
20	R1	1074	ASP	CA-C-N	5.48	129.45	120.63
20	R1	1074	ASP	C-N-CA	5.48	129.45	120.63
15	M1	331	ASP	CA-CB-CG	5.48	118.08	112.60
1	00	396	LYS	CA-C-N	5.47	127.62	120.28
1	00	396	LYS	C-N-CA	5.47	127.62	120.28
2	10	1695	GLN	OE1-CD-NE2	-5.47	117.13	122.60
9	F3	249	MET	CA-C-N	5.47	128.16	120.28
9	F3	249	MET	C-N-CA	5.47	128.16	120.28
10	H3	484	ASP	CA-CB-CG	5.47	118.07	112.60
4	A0	73	HIS	CB-CG-CD2	-5.47	124.09	131.20
6	C3	438	ASP	CA-CB-CG	5.47	118.07	112.60
19	Q3	51	ASP	CA-CB-CG	-5.47	107.13	112.60
25	W0	624	ASP	CA-CB-CG	5.47	118.07	112.60
16	N3	169	ASP	CA-CB-CG	5.47	118.07	112.60
2	11	1217	ARG	CA-C-N	5.47	129.93	120.58
2	11	1217	ARG	C-N-CA	5.47	129.93	120.58
14	L0	581	ILE	CB-CA-C	5.47	116.12	110.70
20	R1	365	ARG	CD-NE-CZ	5.47	132.06	124.40
22	T0	557	SER	CA-C-N	5.47	131.99	121.54
22	T0	557	SER	C-N-CA	5.47	131.99	121.54
2	14	278	SER	CA-C-N	5.47	127.55	120.44
2	14	278	SER	C-N-CA	5.47	127.55	120.44
7	D2	1269	GLN	OE1-CD-NE2	-5.47	117.13	122.60
2	14	356	ASP	CA-CB-CG	5.47	118.07	112.60
6	C0	1798	ASP	CA-C-N	5.46	129.00	120.75
6	C0	1798	ASP	C-N-CA	5.46	129.00	120.75
6	C2	782	ASP	CA-CB-CG	5.46	118.06	112.60
20	R1	1198	GLN	OE1-CD-NE2	-5.46	117.14	122.60
6	C4	8	ASN	CA-CB-CG	5.46	118.06	112.60
16	N0	246	ASP	CA-CB-CG	5.46	118.06	112.60
4	A2	172	PRO	N-CA-C	5.46	117.36	110.70
4	A3	488	HIS	CB-CG-CD2	-5.46	124.11	131.20
6	C0	566	HIS	CB-CG-CD2	-5.46	124.11	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C3	8	ASN	CA-CB-CG	5.46	118.06	112.60
7	D4	211	ASP	CA-CB-CG	5.46	118.06	112.60
9	F3	96	ASP	CA-CB-CG	5.46	118.06	112.60
11	I3	353	PHE	CA-CB-CG	5.46	119.25	113.80
21	S0	89	LEU	CB-CA-C	5.46	120.15	111.15
5	B0	570	ASP	CA-CB-CG	5.45	118.05	112.60
2	15	356	ASP	CA-CB-CG	5.45	118.05	112.60
2	16	324	HIS	CB-CG-CD2	-5.45	124.12	131.20
4	A0	99	GLN	OE1-CD-NE2	-5.45	117.15	122.60
4	A5	97	ASP	CA-CB-CG	5.45	118.05	112.60
8	E0	19	ARG	CB-CA-C	-5.45	102.26	110.92
10	H2	111	PRO	CA-N-CD	-5.45	104.37	112.00
15	M3	331	ASP	CA-CB-CG	5.45	118.05	112.60
1	03	83	TYR	CA-C-N	5.45	127.52	120.44
1	03	83	TYR	C-N-CA	5.45	127.52	120.44
2	14	324	HIS	CB-CG-CD2	-5.44	124.12	131.20
5	B1	1517	ARG	N-CA-C	5.44	122.39	110.80
18	P2	618	ASP	CA-C-N	5.44	128.32	120.38
18	P2	618	ASP	C-N-CA	5.44	128.32	120.38
6	C0	1012	LYS	CA-C-N	5.44	129.95	122.06
6	C0	1012	LYS	C-N-CA	5.44	129.95	122.06
22	T0	683	ILE	N-CA-C	5.44	112.03	106.21
7	D4	545	ASP	CA-CB-CG	5.44	118.04	112.60
7	D4	1100	ARG	CA-C-N	5.44	131.21	121.15
7	D4	1100	ARG	C-N-CA	5.44	131.21	121.15
6	C1	503	ASP	CA-CB-CG	5.44	118.04	112.60
6	C2	119	GLN	OE1-CD-NE2	-5.44	117.16	122.60
14	L3	435	LEU	CA-C-N	5.44	128.11	120.28
14	L3	435	LEU	C-N-CA	5.44	128.11	120.28
10	H2	456	ASP	CA-CB-CG	5.43	118.03	112.60
2	17	324	HIS	CB-CG-CD2	-5.43	124.14	131.20
23	U0	793	HIS	CB-CG-CD2	-5.43	124.14	131.20
16	N3	246	ASP	CA-CB-CG	5.43	118.03	112.60
7	D0	32	ARG	CD-NE-CZ	5.43	132.00	124.40
20	R2	582	TYR	N-CA-C	5.43	117.20	111.28
1	01	651	HIS	CB-CG-CD2	-5.43	124.15	131.20
2	17	260	HIS	CB-CG-CD2	-5.43	124.15	131.20
6	C1	1191	PHE	CA-CB-CG	5.42	119.22	113.80
18	P2	626	ASP	CA-CB-CG	5.42	118.02	112.60
4	A3	73	HIS	CB-CG-CD2	-5.42	124.15	131.20
18	P1	358	HIS	CB-CG-CD2	-5.42	124.15	131.20
4	A4	408	ASP	CA-CB-CG	5.42	118.02	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C2	542	VAL	O-C-N	5.42	128.58	122.67
5	B0	1517	ARG	N-CA-C	5.42	122.34	110.80
15	M0	762	HIS	CA-C-N	5.42	131.89	121.54
15	M0	762	HIS	C-N-CA	5.42	131.89	121.54
14	L0	302	HIS	CB-CG-CD2	-5.42	124.16	131.20
2	10	1831	VAL	CA-CB-CG2	5.42	119.61	110.40
10	H1	484	ASP	CA-CB-CG	5.42	118.02	112.60
13	K3	868	ASP	CA-CB-CG	-5.42	107.18	112.60
7	D4	1391	HIS	CB-CG-CD2	-5.42	124.16	131.20
9	F0	96	ASP	CA-CB-CG	5.42	118.02	112.60
2	11	1652	ASP	CA-CB-CG	-5.41	107.19	112.60
5	B0	1526	SER	CA-C-N	5.41	131.44	121.70
5	B0	1526	SER	C-N-CA	5.41	131.44	121.70
7	D5	915	ASN	CA-CB-CG	5.41	118.01	112.60
10	H1	493	HIS	CB-CG-CD2	-5.41	124.16	131.20
7	D3	1168	HIS	CB-CG-CD2	-5.41	124.17	131.20
2	16	260	HIS	CB-CG-CD2	-5.41	124.17	131.20
2	10	1823	VAL	N-CA-CB	5.41	116.87	110.55
2	16	335	LEU	CA-C-N	5.41	126.60	119.84
2	16	335	LEU	C-N-CA	5.41	126.60	119.84
20	R0	365	ARG	CD-NE-CZ	5.41	131.97	124.40
9	F0	241	LYS	CG-CD-CE	-5.40	98.87	111.30
2	16	278	SER	CA-C-N	5.40	127.46	120.44
2	16	278	SER	C-N-CA	5.40	127.46	120.44
6	C0	1191	PHE	CA-CB-CG	5.40	119.20	113.80
7	D3	1105	HIS	CB-CG-CD2	-5.40	124.18	131.20
5	B1	570	ASP	CA-CB-CG	5.40	118.00	112.60
7	D1	1168	HIS	CB-CG-CD2	-5.40	124.19	131.20
7	D3	1223	ASP	CA-CB-CG	5.40	118.00	112.60
20	R0	1055	TYR	N-CA-C	5.40	122.29	110.80
2	12	1652	ASP	CA-CB-CG	-5.39	107.21	112.60
2	16	1633	GLN	OE1-CD-NE2	-5.39	117.20	122.60
25	W0	741	PHE	CA-CB-CG	5.39	119.19	113.80
11	I3	317	GLN	OE1-CD-NE2	-5.39	117.21	122.60
5	B0	1155	LEU	CA-C-N	5.39	125.93	120.00
5	B0	1155	LEU	C-N-CA	5.39	125.93	120.00
10	H2	426	GLN	OE1-CD-NE2	-5.39	117.21	122.60
24	V0	783	ARG	CD-NE-CZ	5.39	131.94	124.40
2	17	1652	ASP	CA-CB-CG	-5.39	107.21	112.60
2	12	1789	ARG	N-CA-C	5.38	116.46	108.60
2	15	260	HIS	CB-CG-CD2	-5.38	124.20	131.20
9	F2	96	ASP	CA-CB-CG	5.38	117.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	R2	1367	GLN	OE1-CD-NE2	-5.38	117.22	122.60
14	L1	617	GLN	OE1-CD-NE2	-5.38	117.22	122.60
20	R2	944	ASP	CA-C-N	5.38	129.69	120.71
20	R2	944	ASP	C-N-CA	5.38	129.69	120.71
25	W0	604	ASP	CA-CB-CG	5.38	117.98	112.60
7	D2	1133	SER	CA-C-N	5.38	127.70	120.50
7	D2	1133	SER	C-N-CA	5.38	127.70	120.50
15	M0	503	HIS	CB-CG-CD2	-5.38	124.21	131.20
2	14	260	HIS	CB-CG-CD2	-5.37	124.21	131.20
6	C2	1281	HIS	CA-CB-CG	5.37	119.17	113.80
6	C4	412	ASN	CA-CB-CG	5.37	117.97	112.60
1	01	83	TYR	CA-C-N	5.37	127.42	120.44
1	01	83	TYR	C-N-CA	5.37	127.42	120.44
5	B1	1268	ASP	CA-CB-CG	5.37	117.97	112.60
16	N3	235	SER	CA-C-N	5.37	129.19	120.60
16	N3	235	SER	C-N-CA	5.37	129.19	120.60
10	H3	388	GLN	OE1-CD-NE2	-5.37	117.23	122.60
10	H1	388	GLN	OE1-CD-NE2	-5.37	117.23	122.60
10	H3	393	GLN	OE1-CD-NE2	-5.37	117.23	122.60
22	T0	821	ASN	CA-CB-CG	5.37	117.97	112.60
1	02	410	ASP	CA-CB-CG	5.36	117.96	112.60
2	14	1414	ASP	CA-CB-CG	5.36	117.96	112.60
6	C2	438	ASP	CA-CB-CG	5.36	117.96	112.60
13	K1	510	ASN	OD1-CG-ND2	-5.36	117.24	122.60
7	D4	86	ARG	CA-C-N	5.36	132.05	122.13
7	D4	86	ARG	C-N-CA	5.36	132.05	122.13
15	M1	834	ASN	CA-CB-CG	5.36	117.96	112.60
4	A2	73	HIS	CB-CG-CD2	-5.36	124.23	131.20
4	A3	188	GLN	OE1-CD-NE2	-5.36	117.24	122.60
4	A4	491	HIS	CA-CB-CG	-5.36	108.44	113.80
9	F0	310	LYS	CA-C-N	5.36	128.48	120.87
9	F0	310	LYS	C-N-CA	5.36	128.48	120.87
7	D4	1181	GLU	N-CA-C	5.36	117.22	109.07
2	16	1652	ASP	CA-CB-CG	-5.36	107.24	112.60
6	C4	503	ASP	CA-CB-CG	5.36	117.96	112.60
10	H2	493	HIS	CB-CG-CD2	-5.36	124.23	131.20
18	P1	617	SER	O-C-N	-5.36	117.63	123.52
21	S0	158	GLN	OE1-CD-NE2	-5.36	117.24	122.60
2	13	1414	ASP	CA-CB-CG	5.35	117.95	112.60
9	F2	241	LYS	CB-CG-CD	5.35	123.61	111.30
18	P2	61	VAL	CB-CA-C	5.35	120.07	111.29
2	12	1414	ASP	CA-CB-CG	5.35	117.95	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C3	503	ASP	CA-CB-CG	5.35	117.95	112.60
1	04	410	ASP	CA-CB-CG	5.35	117.95	112.60
4	A4	581	ASP	CA-CB-CG	5.35	117.95	112.60
7	D3	937	ALA	CA-C-N	5.35	128.84	120.82
7	D3	937	ALA	C-N-CA	5.35	128.84	120.82
7	D4	1168	HIS	CB-CG-CD2	-5.35	124.25	131.20
1	02	28	LYS	CA-C-N	5.35	125.92	119.98
1	02	28	LYS	C-N-CA	5.35	125.92	119.98
20	R1	544	HIS	CB-CG-CD2	-5.35	124.25	131.20
20	R3	544	HIS	CB-CG-CD2	-5.35	124.25	131.20
23	U6	611	PHE	CA-C-O	-5.35	115.27	122.44
7	D5	1290	ASN	CA-CB-CG	5.35	117.95	112.60
2	12	260	HIS	CB-CG-CD2	-5.34	124.25	131.20
2	17	893	GLU	N-CA-CB	-5.34	102.72	110.36
7	D2	1168	HIS	CA-C-N	5.34	127.38	120.44
7	D2	1168	HIS	C-N-CA	5.34	127.38	120.44
12	J0	450	ASP	CA-CB-CG	5.34	117.94	112.60
7	D3	1273	GLN	OE1-CD-NE2	-5.34	117.26	122.60
6	C3	1191	PHE	CA-CB-CG	5.34	119.14	113.80
7	D4	1108	GLU	CA-CB-CG	5.34	124.78	114.10
6	C3	566	HIS	CB-CG-CD2	-5.33	124.26	131.20
7	D3	1269	GLN	OE1-CD-NE2	-5.33	117.27	122.60
20	R2	1414	ASP	CA-CB-CG	5.33	117.94	112.60
21	S3	76	ASP	CA-CB-CG	5.33	117.94	112.60
2	10	260	HIS	CB-CG-CD2	-5.33	124.27	131.20
6	C0	78	GLN	OE1-CD-NE2	-5.33	117.27	122.60
7	D0	1273	GLN	OE1-CD-NE2	-5.33	117.27	122.60
13	K2	145	PRO	N-CA-CB	5.33	105.99	103.22
22	T1	821	ASN	CA-CB-CG	5.33	117.93	112.60
2	15	278	SER	CA-C-N	5.33	127.37	120.44
2	15	278	SER	C-N-CA	5.33	127.37	120.44
7	D4	1290	ASN	CA-CB-CG	5.33	117.93	112.60
7	D5	1391	HIS	CB-CG-CD2	-5.33	124.27	131.20
9	F1	170	HIS	CB-CG-CD2	-5.33	124.27	131.20
5	B0	1520	ARG	N-CA-C	5.33	121.58	109.81
5	B0	1522	PRO	CA-N-CD	-5.33	104.05	111.50
15	M1	587	LEU	CB-CA-C	5.33	120.66	110.17
6	C1	1012	LYS	CA-C-N	5.32	129.78	122.06
6	C1	1012	LYS	C-N-CA	5.32	129.78	122.06
8	E0	140	TYR	CA-C-N	5.32	131.71	121.54
8	E0	140	TYR	C-N-CA	5.32	131.71	121.54
8	E1	242	ILE	N-CA-C	5.32	119.65	113.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	17	748	PRO	N-CA-CB	5.32	105.99	103.22
19	Q0	190	ASN	N-CA-C	5.32	116.36	108.86
1	01	310	ARG	CD-NE-CZ	5.32	131.85	124.40
2	14	1652	ASP	CA-CB-CG	-5.32	107.28	112.60
16	N0	2	VAL	CA-CB-CG1	5.32	119.44	110.40
2	12	713	GLN	OE1-CD-NE2	-5.32	117.28	122.60
2	13	2	ALA	CA-C-N	5.32	131.27	121.70
2	13	2	ALA	C-N-CA	5.32	131.27	121.70
2	13	260	HIS	CB-CG-CD2	-5.32	124.29	131.20
4	A5	488	HIS	CB-CG-CD2	-5.32	124.29	131.20
18	P2	551	LYS	CA-C-N	5.32	131.69	121.54
18	P2	551	LYS	C-N-CA	5.32	131.69	121.54
21	S0	76	ASP	CA-CB-CG	5.32	117.92	112.60
7	D0	1168	HIS	CA-C-N	5.32	127.35	120.44
7	D0	1168	HIS	C-N-CA	5.32	127.35	120.44
7	D1	1269	GLN	OE1-CD-NE2	-5.32	117.28	122.60
17	O2	106	ARG	CD-NE-CZ	5.32	131.84	124.40
2	11	1414	ASP	CA-CB-CG	5.31	117.91	112.60
2	12	508	ASP	CA-CB-CG	5.31	117.91	112.60
10	H0	493	HIS	CB-CG-CD2	-5.31	124.29	131.20
17	O0	106	ARG	CD-NE-CZ	5.31	131.84	124.40
2	11	2	ALA	CA-C-N	5.31	131.26	121.70
2	11	2	ALA	C-N-CA	5.31	131.26	121.70
7	D4	1273	GLN	OE1-CD-NE2	-5.31	117.29	122.60
8	E0	14	ARG	O-C-N	5.31	129.45	122.33
1	00	201	LEU	CA-C-N	5.31	127.34	120.44
1	00	201	LEU	C-N-CA	5.31	127.34	120.44
9	F2	297	THR	CA-C-N	5.31	128.13	120.38
9	F2	297	THR	C-N-CA	5.31	128.13	120.38
19	Q2	190	ASN	N-CA-C	5.31	116.35	108.86
15	M3	317	HIS	CB-CG-CD2	-5.31	124.30	131.20
16	N1	114	HIS	CB-CG-CD2	-5.31	124.30	131.20
7	D1	1273	GLN	OE1-CD-NE2	-5.31	117.29	122.60
5	B0	929	GLN	CA-C-N	5.30	124.49	118.97
5	B0	929	GLN	C-N-CA	5.30	124.49	118.97
2	15	893	GLU	N-CA-CB	-5.30	102.39	110.45
6	C3	1739	GLU	N-CA-C	5.30	116.74	111.07
16	N1	235	SER	CA-C-N	5.30	129.08	120.60
16	N1	235	SER	C-N-CA	5.30	129.08	120.60
20	R3	944	ASP	CA-C-N	5.30	129.56	120.71
20	R3	944	ASP	C-N-CA	5.30	129.56	120.71
2	12	2	ALA	CA-C-N	5.30	131.24	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	12	2	ALA	C-N-CA	5.30	131.24	121.70
2	13	508	ASP	CA-CB-CG	5.30	117.90	112.60
7	D2	1110	SER	CA-C-N	5.30	128.12	120.38
7	D2	1110	SER	C-N-CA	5.30	128.12	120.38
15	M1	317	HIS	CB-CG-CD2	-5.30	124.31	131.20
16	N1	246	ASP	CA-CB-CG	5.30	117.90	112.60
2	16	508	ASP	CA-CB-CG	5.30	117.90	112.60
11	I0	317	GLN	OE1-CD-NE2	-5.30	117.30	122.60
19	Q3	190	ASN	N-CA-C	5.29	116.33	108.86
5	B1	1520	ARG	N-CA-C	5.29	121.51	109.81
7	D2	1273	GLN	OE1-CD-NE2	-5.29	117.31	122.60
13	K0	241	HIS	CB-CG-CD2	-5.29	124.32	131.20
21	S1	158	GLN	OE1-CD-NE2	-5.29	117.31	122.60
2	14	337	ASN	N-CA-C	5.29	117.76	110.35
17	O3	156	GLN	OE1-CD-NE2	-5.29	117.31	122.60
4	A2	142	GLN	OE1-CD-NE2	-5.29	117.31	122.60
6	C2	621	HIS	CA-C-N	5.29	125.10	119.28
6	C2	621	HIS	C-N-CA	5.29	125.10	119.28
15	M0	331	ASP	CA-CB-CG	5.29	117.89	112.60
18	P1	60	ASP	CA-CB-CG	-5.29	107.31	112.60
16	N2	235	SER	CA-C-N	5.29	129.06	120.60
16	N2	235	SER	C-N-CA	5.29	129.06	120.60
15	M1	574	GLN	OE1-CD-NE2	-5.29	117.31	122.60
20	R0	544	HIS	CB-CG-CD2	-5.29	124.33	131.20
4	A6	677	GLN	OE1-CD-NE2	-5.28	117.32	122.60
5	B1	1714	VAL	CA-C-N	5.28	126.35	120.06
5	B1	1714	VAL	C-N-CA	5.28	126.35	120.06
20	R2	544	HIS	CB-CG-CD2	-5.28	124.33	131.20
2	10	508	ASP	CA-CB-CG	5.28	117.88	112.60
20	R1	944	ASP	CA-C-N	5.28	129.52	120.71
20	R1	944	ASP	C-N-CA	5.28	129.52	120.71
13	K0	145	PRO	N-CA-CB	5.27	105.96	103.22
6	C4	438	ASP	CA-CB-CG	5.27	117.87	112.60
13	K2	466	ARG	CD-NE-CZ	5.27	131.78	124.40
2	17	278	SER	CA-C-N	5.27	127.29	120.44
2	17	278	SER	C-N-CA	5.27	127.29	120.44
16	N3	114	HIS	CB-CG-CD2	-5.27	124.35	131.20
21	S1	76	ASP	CA-CB-CG	5.27	117.87	112.60
7	D1	1002	PRO	N-CA-C	5.27	123.33	112.47
12	J2	345	GLU	CA-C-N	5.27	128.79	120.89
12	J2	345	GLU	C-N-CA	5.27	128.79	120.89
14	L2	302	HIS	CB-CG-CD2	-5.27	124.35	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	O3	34	GLN	OE1-CD-NE2	-5.27	117.33	122.60
2	11	508	ASP	CA-CB-CG	5.27	117.87	112.60
13	K2	496	GLY	CA-C-N	5.27	125.26	119.89
13	K2	496	GLY	C-N-CA	5.27	125.26	119.89
2	10	2	ALA	CA-C-N	5.27	131.18	121.70
2	10	2	ALA	C-N-CA	5.27	131.18	121.70
15	M3	834	ASN	CA-CB-CG	5.27	117.87	112.60
16	N0	114	HIS	CB-CG-CD2	-5.26	124.36	131.20
5	B0	1714	VAL	CA-C-N	5.26	126.32	120.06
5	B0	1714	VAL	C-N-CA	5.26	126.32	120.06
2	11	260	HIS	CB-CG-CD2	-5.26	124.36	131.20
2	17	173	SER	CA-C-N	5.26	131.59	121.54
2	17	173	SER	C-N-CA	5.26	131.59	121.54
7	D3	1008	PRO	N-CA-C	5.26	120.44	113.86
15	M2	574	GLN	OE1-CD-NE2	-5.26	117.34	122.60
19	Q1	190	ASN	N-CA-C	5.26	116.28	108.86
1	01	125	PHE	CA-CB-CG	5.26	119.06	113.80
12	J4	359	ASN	CA-CB-CG	5.26	117.86	112.60
2	13	1313	ASP	CA-CB-CG	5.26	117.86	112.60
2	16	173	SER	CA-C-N	5.26	131.58	121.54
2	16	173	SER	C-N-CA	5.26	131.58	121.54
2	16	524	HIS	CB-CG-CD2	-5.26	124.37	131.20
13	K2	241	HIS	CB-CG-CD2	-5.26	124.37	131.20
18	P2	550	GLU	CA-CB-CG	5.26	124.61	114.10
8	E1	243	SER	CA-CB-OG	5.25	121.61	111.10
6	C0	1933	SER	CA-C-N	5.25	130.72	122.21
6	C0	1933	SER	C-N-CA	5.25	130.72	122.21
1	04	706	GLU	CB-CG-CD	5.25	121.53	112.60
7	D3	1391	HIS	CB-CG-CD2	-5.25	124.37	131.20
6	C2	1939	SER	N-CA-C	5.25	121.98	110.80
14	L2	886	HIS	CB-CG-CD2	-5.25	124.38	131.20
25	W0	588	GLN	OE1-CD-NE2	-5.25	117.35	122.60
6	C2	1568	GLN	OE1-CD-NE2	-5.25	117.35	122.60
15	M2	331	ASP	CA-CB-CG	5.25	117.85	112.60
2	12	117	HIS	CB-CG-CD2	-5.25	124.38	131.20
25	W0	439	GLN	OE1-CD-NE2	-5.25	117.36	122.60
16	N3	280	SER	CA-C-N	5.24	125.90	120.60
16	N3	280	SER	C-N-CA	5.24	125.90	120.60
20	R0	805	THR	N-CA-C	5.24	116.87	107.80
4	A5	581	ASP	CA-CB-CG	5.24	117.84	112.60
13	K3	241	HIS	CB-CG-CD2	-5.24	124.39	131.20
2	12	783	ARG	CD-NE-CZ	5.24	131.74	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Q3	377	HIS	CB-CG-CD2	-5.24	124.39	131.20
4	A3	677	GLN	OE1-CD-NE2	-5.24	117.36	122.60
13	K3	845	ASP	CA-CB-CG	5.24	117.84	112.60
7	D5	1347	ARG	CD-NE-CZ	5.24	131.73	124.40
9	F2	233	GLY	CA-C-N	5.24	129.78	122.08
9	F2	233	GLY	C-N-CA	5.24	129.78	122.08
14	L3	886	HIS	CB-CG-CD2	-5.24	124.39	131.20
21	S2	76	ASP	CA-CB-CG	5.24	117.84	112.60
2	I3	1570	GLN	OE1-CD-NE2	-5.23	117.37	122.60
6	C4	1940	PHE	N-CA-C	5.23	118.95	109.32
7	D1	1290	ASN	OD1-CG-ND2	-5.23	117.37	122.60
8	E0	313	GLU	N-CA-CB	5.23	117.81	110.12
20	R0	1111	GLU	OE1-CD-OE2	5.23	135.46	122.90
1	O1	163	ASP	CA-C-N	5.23	131.53	121.54
1	O1	163	ASP	C-N-CA	5.23	131.53	121.54
6	C4	416	GLU	CB-CG-CD	5.23	121.49	112.60
21	S2	158	GLN	OE1-CD-NE2	-5.23	117.37	122.60
4	A5	677	GLN	OE1-CD-NE2	-5.23	117.37	122.60
13	K2	394	ASN	CA-C-N	5.23	123.42	119.66
13	K2	394	ASN	C-N-CA	5.23	123.42	119.66
1	O3	310	ARG	CD-NE-CZ	5.23	131.72	124.40
4	A2	491	HIS	CA-CB-CG	-5.23	108.57	113.80
9	F0	119	MET	CA-C-N	5.23	128.01	120.38
9	F0	119	MET	C-N-CA	5.23	128.01	120.38
22	T1	413	PRO	CA-C-N	5.23	128.25	120.31
22	T1	413	PRO	C-N-CA	5.23	128.25	120.31
2	I4	298	ARG	CD-NE-CZ	5.22	131.72	124.40
16	N2	114	HIS	CB-CG-CD2	-5.22	124.41	131.20
17	O2	34	GLN	OE1-CD-NE2	-5.22	117.38	122.60
20	R0	1414	ASP	CA-CB-CG	5.22	117.82	112.60
4	A4	97	ASP	CA-CB-CG	5.22	117.82	112.60
7	D2	1391	HIS	CB-CG-CD2	-5.22	124.41	131.20
20	R0	944	ASP	CA-C-N	5.22	129.43	120.71
20	R0	944	ASP	C-N-CA	5.22	129.43	120.71
6	C4	1191	PHE	CA-CB-CG	5.22	119.02	113.80
14	L1	886	HIS	CB-CG-CD2	-5.22	124.41	131.20
2	I4	524	HIS	CB-CG-CD2	-5.22	124.42	131.20
6	C1	1378	PRO	CA-C-N	5.22	123.47	119.66
6	C1	1378	PRO	C-N-CA	5.22	123.47	119.66
6	C4	566	HIS	CB-CG-CD2	-5.22	124.42	131.20
13	K0	110	ASP	CA-C-N	5.22	131.50	121.54
13	K0	110	ASP	C-N-CA	5.22	131.50	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L0	914	GLN	OE1-CD-NE2	-5.22	117.38	122.60
21	S3	158	GLN	OE1-CD-NE2	-5.22	117.38	122.60
7	D5	1273	GLN	OE1-CD-NE2	-5.21	117.39	122.60
10	H0	357	ASP	CA-CB-CG	5.21	117.81	112.60
15	M2	317	HIS	CB-CG-CD2	-5.21	124.42	131.20
22	T1	756	HIS	CB-CG-CD2	-5.21	124.42	131.20
10	H1	415	ASP	CA-CB-CG	5.21	117.81	112.60
20	R3	834	HIS	CB-CG-CD2	-5.21	124.42	131.20
2	10	524	HIS	CB-CG-CD2	-5.21	124.43	131.20
2	14	1703	HIS	CB-CG-CD2	-5.21	124.43	131.20
6	C2	1940	PHE	N-CA-C	5.21	121.89	110.80
19	Q2	377	HIS	CB-CG-CD2	-5.21	124.43	131.20
7	D1	122	ASP	CA-CB-CG	5.21	117.81	112.60
15	M3	574	GLN	OE1-CD-NE2	-5.21	117.39	122.60
22	T0	173	ASP	CA-CB-CG	5.21	117.81	112.60
6	C2	544	ASN	CB-CA-C	5.21	119.77	112.07
6	C3	1249	ILE	CB-CA-C	5.21	127.52	110.97
22	T0	161	ASP	CA-CB-CG	5.20	117.80	112.60
5	B1	1522	PRO	CA-N-CD	-5.20	104.22	111.50
8	E0	142	PHE	CA-CB-CG	5.20	119.00	113.80
13	K1	241	HIS	CB-CG-CD2	-5.20	124.44	131.20
2	14	1196	GLN	OE1-CD-NE2	-5.20	117.40	122.60
20	R0	834	HIS	CB-CG-CD2	-5.20	124.44	131.20
2	16	132	ASP	CA-CB-CG	5.20	117.80	112.60
6	C2	465	CYS	N-CA-C	5.20	121.29	109.81
6	C2	1191	PHE	CA-CB-CG	5.20	119.00	113.80
9	F0	303	ILE	N-CA-C	5.20	120.15	109.34
18	P2	551	LYS	CB-CA-C	-5.20	100.23	110.10
2	15	173	SER	CA-C-N	5.19	131.46	121.54
2	15	173	SER	C-N-CA	5.19	131.46	121.54
2	12	524	HIS	CB-CG-CD2	-5.19	124.45	131.20
6	C4	1737	ASN	N-CA-C	5.19	117.73	111.40
2	10	1830	THR	CA-CB-CG2	5.19	119.32	110.50
5	B1	929	GLN	CA-C-N	5.19	124.64	119.24
5	B1	929	GLN	C-N-CA	5.19	124.64	119.24
12	J1	354	GLN	OE1-CD-NE2	-5.19	117.41	122.60
22	T1	686	SER	N-CA-C	5.19	121.86	110.80
6	C2	356	ASP	CA-CB-CG	5.19	117.79	112.60
17	O1	34	GLN	OE1-CD-NE2	-5.19	117.41	122.60
2	14	930	ALA	CA-C-N	5.19	128.19	120.31
2	14	930	ALA	C-N-CA	5.19	128.19	120.31
4	A6	488	HIS	CB-CG-CD2	-5.19	124.46	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	M0	423	ARG	NE-CZ-NH2	5.18	123.87	119.20
18	P2	617	SER	CA-C-N	5.18	131.03	121.70
18	P2	617	SER	C-N-CA	5.18	131.03	121.70
2	14	508	ASP	CA-CB-CG	5.18	117.78	112.60
5	B0	960	HIS	CB-CG-CD2	-5.18	124.47	131.20
19	Q0	226	HIS	CB-CG-CD2	-5.18	124.47	131.20
6	C1	1848	PRO	CA-C-N	5.18	127.64	120.29
6	C1	1848	PRO	C-N-CA	5.18	127.64	120.29
7	D4	357	GLN	OE1-CD-NE2	-5.18	117.42	122.60
14	L0	886	HIS	CB-CG-CD2	-5.18	124.47	131.20
7	D4	771	GLN	OE1-CD-NE2	-5.18	117.42	122.60
11	I1	317	GLN	OE1-CD-NE2	-5.18	117.42	122.60
22	T0	686	SER	N-CA-C	5.18	121.83	110.80
12	J1	486	GLN	OE1-CD-NE2	-5.17	117.43	122.60
25	W0	347	HIS	CB-CG-CD2	-5.17	124.47	131.20
1	04	260	GLN	OE1-CD-NE2	-5.17	117.43	122.60
6	C2	78	GLN	OE1-CD-NE2	-5.17	117.43	122.60
2	17	508	ASP	CA-CB-CG	5.17	117.77	112.60
4	A3	649	VAL	CA-C-N	5.17	125.39	120.43
4	A3	649	VAL	C-N-CA	5.17	125.39	120.43
7	D1	1003	VAL	N-CA-CB	5.17	119.76	111.23
10	H1	111	PRO	N-CA-CB	5.17	108.69	103.00
15	M0	317	HIS	CB-CG-CD2	-5.17	124.48	131.20
22	T0	803	ALA	CA-C-N	5.17	127.43	120.50
22	T0	803	ALA	C-N-CA	5.17	127.43	120.50
22	T1	173	ASP	CA-CB-CG	5.17	117.77	112.60
8	E1	247	ASN	N-CA-C	5.17	121.81	110.80
11	I2	317	GLN	OE1-CD-NE2	-5.17	117.43	122.60
19	Q1	377	HIS	CB-CG-CD2	-5.17	124.48	131.20
22	T0	305	GLN	OE1-CD-NE2	-5.17	117.43	122.60
22	T1	161	ASP	CA-CB-CG	5.17	117.77	112.60
21	S3	260	SER	CA-C-N	5.17	127.92	120.38
21	S3	260	SER	C-N-CA	5.17	127.92	120.38
4	A3	99	GLN	CA-C-N	5.17	125.81	120.03
4	A3	99	GLN	C-N-CA	5.17	125.81	120.03
22	T0	556	SER	N-CA-C	5.17	116.92	109.07
6	C1	78	GLN	OE1-CD-NE2	-5.16	117.44	122.60
12	J3	354	GLN	OE1-CD-NE2	-5.16	117.44	122.60
13	K3	145	PRO	N-CA-CB	5.16	105.91	103.22
20	R1	805	THR	N-CA-C	5.16	116.73	107.80
2	15	508	ASP	CA-CB-CG	5.16	117.76	112.60
4	A2	677	GLN	OE1-CD-NE2	-5.16	117.44	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A3	578	ARG	CD-NE-CZ	5.16	131.62	124.40
4	A1	677	GLN	OE1-CD-NE2	-5.16	117.44	122.60
7	D1	1258	THR	CA-C-N	5.16	125.45	119.47
7	D1	1258	THR	C-N-CA	5.16	125.45	119.47
20	R1	539	GLN	OE1-CD-NE2	-5.16	117.44	122.60
20	R3	365	ARG	CD-NE-CZ	5.16	131.62	124.40
2	17	250	ASP	CA-CB-CG	5.16	117.75	112.60
2	13	893	GLU	N-CA-CB	-5.15	102.62	110.45
7	D4	1265	ASP	CA-CB-CG	5.15	117.75	112.60
20	R1	1010	ASP	CA-CB-CG	5.15	117.75	112.60
2	10	117	HIS	CB-CG-CD2	-5.15	124.50	131.20
2	12	699	SER	O-C-N	-5.15	117.08	123.36
6	C0	265	ASP	CA-CB-CG	5.15	117.75	112.60
20	R2	834	HIS	CB-CG-CD2	-5.15	124.50	131.20
25	W0	687	ASP	CA-CB-CG	5.15	117.75	112.60
4	A5	142	GLN	OE1-CD-NE2	-5.15	117.45	122.60
7	D4	1105	HIS	CB-CG-CD2	-5.15	124.51	131.20
7	D5	771	GLN	OE1-CD-NE2	-5.15	117.45	122.60
12	J3	486	GLN	OE1-CD-NE2	-5.15	117.45	122.60
20	R3	1414	ASP	CA-CB-CG	5.15	117.75	112.60
2	16	298	ARG	CD-NE-CZ	5.14	131.60	124.40
7	D3	357	GLN	OE1-CD-NE2	-5.14	117.45	122.60
20	R3	805	THR	N-CA-C	5.14	116.70	107.80
25	W0	256	GLN	CA-C-N	5.14	132.60	121.64
25	W0	256	GLN	C-N-CA	5.14	132.60	121.64
1	02	262	PHE	CA-CB-CG	5.14	118.94	113.80
2	11	524	HIS	CB-CG-CD2	-5.14	124.52	131.20
2	11	626	HIS	CB-CG-CD2	-5.14	124.52	131.20
10	H0	484	ASP	CA-CB-CG	5.14	117.74	112.60
20	R1	834	HIS	CB-CG-CD2	-5.14	124.52	131.20
20	R2	411	HIS	CB-CG-CD2	-5.14	124.51	131.20
20	R2	805	THR	N-CA-C	5.14	116.70	107.80
25	W0	194	ASP	CA-CB-CG	5.14	117.74	112.60
2	14	173	SER	CA-C-N	5.14	131.36	121.54
2	14	173	SER	C-N-CA	5.14	131.36	121.54
13	K0	517	ASP	CA-CB-CG	5.14	117.74	112.60
13	K0	845	ASP	CA-CB-CG	5.14	117.74	112.60
15	M0	656	ASN	CA-CB-CG	5.14	117.74	112.60
16	N2	280	SER	CA-C-N	5.14	125.79	120.60
16	N2	280	SER	C-N-CA	5.14	125.79	120.60
20	R2	477	GLN	OE1-CD-NE2	-5.14	117.46	122.60
20	R2	539	GLN	OE1-CD-NE2	-5.14	117.46	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	02	260	GLN	OE1-CD-NE2	-5.14	117.46	122.60
12	J4	391	GLN	OE1-CD-NE2	-5.14	117.46	122.60
20	R3	477	GLN	OE1-CD-NE2	-5.14	117.46	122.60
21	S2	260	SER	CA-C-N	5.14	127.88	120.38
21	S2	260	SER	C-N-CA	5.14	127.88	120.38
1	00	260	GLN	OE1-CD-NE2	-5.13	117.47	122.60
2	13	1196	GLN	OE1-CD-NE2	-5.13	117.47	122.60
2	15	1633	GLN	OE1-CD-NE2	-5.13	117.47	122.60
4	A0	677	GLN	OE1-CD-NE2	-5.13	117.47	122.60
20	R3	1257	GLY	O-C-N	-5.13	117.30	122.59
23	U6	605	LEU	CA-C-N	-5.13	115.76	123.00
23	U6	605	LEU	C-N-CA	-5.13	115.76	123.00
1	00	663	ASN	OD1-CG-ND2	-5.13	117.47	122.60
4	A6	491	HIS	CA-CB-CG	-5.13	108.67	113.80
7	D5	1290	ASN	OD1-CG-ND2	-5.13	117.47	122.60
4	A1	735	ARG	NE-CZ-NH2	5.13	123.82	119.20
7	D0	771	GLN	OE1-CD-NE2	-5.13	117.47	122.60
12	J0	345	GLU	CA-C-N	5.13	128.59	120.89
12	J0	345	GLU	C-N-CA	5.13	128.59	120.89
6	C0	1484	ASP	CA-CB-CG	5.13	117.73	112.60
13	K2	932	HIS	CB-CG-CD2	-5.13	124.53	131.20
5	B1	960	HIS	CB-CG-CD2	-5.13	124.53	131.20
7	D0	1328	HIS	CB-CG-CD2	-5.13	124.53	131.20
8	E1	333	GLN	OE1-CD-NE2	-5.13	117.47	122.60
10	H2	484	ASP	CA-CB-CG	5.13	117.73	112.60
20	R0	539	GLN	OE1-CD-NE2	-5.13	117.47	122.60
21	S1	260	SER	CA-C-N	5.13	127.87	120.38
21	S1	260	SER	C-N-CA	5.13	127.87	120.38
2	14	893	GLU	N-CA-CB	-5.13	102.93	110.26
6	C3	265	ASP	CA-CB-CG	5.13	117.73	112.60
14	L2	385	HIS	CB-CG-CD2	-5.13	124.53	131.20
2	17	1633	GLN	OE1-CD-NE2	-5.12	117.47	122.60
22	T1	305	GLN	OE1-CD-NE2	-5.12	117.47	122.60
5	B1	1537	ALA	CA-C-N	5.12	127.65	120.28
5	B1	1537	ALA	C-N-CA	5.12	127.65	120.28
6	C2	265	ASP	CA-CB-CG	5.12	117.72	112.60
7	D4	915	ASN	CA-CB-CG	5.12	117.72	112.60
7	D5	357	GLN	OE1-CD-NE2	-5.12	117.48	122.60
18	P2	389	SER	O-C-N	-5.12	116.72	122.97
20	R3	738	GLN	OE1-CD-NE2	-5.12	117.48	122.60
4	A4	677	GLN	OE1-CD-NE2	-5.12	117.48	122.60
6	C1	839	LYS	CG-CD-CE	-5.12	99.52	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	R1	530	LYS	N-CA-CB	-5.12	102.34	110.22
19	Q2	226	HIS	CB-CG-CD2	-5.12	124.55	131.20
2	16	1414	ASP	CA-CB-CG	5.12	117.72	112.60
6	C2	1856	GLN	OE1-CD-NE2	-5.12	117.48	122.60
7	D1	1328	HIS	CB-CG-CD2	-5.12	124.55	131.20
7	D4	1112	GLN	N-CA-C	5.12	121.81	114.39
14	L3	583	GLU	CA-C-N	5.12	131.31	121.54
14	L3	583	GLU	C-N-CA	5.12	131.31	121.54
14	L3	617	GLN	OE1-CD-NE2	-5.12	117.48	122.60
15	M3	745	HIS	CB-CG-CD2	-5.12	124.55	131.20
20	R1	1414	ASP	CA-CB-CG	5.12	117.72	112.60
1	00	262	PHE	CA-CB-CG	5.11	118.91	113.80
4	A0	491	HIS	CA-CB-CG	-5.11	108.69	113.80
2	10	1820	GLY	CA-C-N	5.11	127.38	120.38
2	10	1820	GLY	C-N-CA	5.11	127.38	120.38
4	A5	491	HIS	CA-CB-CG	-5.11	108.69	113.80
7	D5	1269	GLN	OE1-CD-NE2	-5.11	117.49	122.60
8	E0	72	PHE	N-CA-CB	5.11	117.37	109.91
17	O3	106	ARG	CD-NE-CZ	5.11	131.55	124.40
25	W0	648	HIS	CB-CG-CD2	-5.11	124.56	131.20
2	15	524	HIS	CB-CG-CD2	-5.11	124.56	131.20
2	14	1003	ASP	CA-CB-CG	5.11	117.71	112.60
4	A5	264	GLN	OE1-CD-NE2	-5.11	117.49	122.60
6	C1	265	ASP	CA-CB-CG	5.11	117.71	112.60
10	H0	441	GLN	OE1-CD-NE2	-5.11	117.49	122.60
18	P0	62	ASP	N-CA-C	5.11	121.68	110.80
21	S0	260	SER	CA-C-N	5.11	127.84	120.38
21	S0	260	SER	C-N-CA	5.11	127.84	120.38
4	A1	491	HIS	CA-CB-CG	-5.11	108.69	113.80
13	K1	845	ASP	CA-CB-CG	5.11	117.71	112.60
19	Q1	226	HIS	CB-CG-CD2	-5.11	124.56	131.20
20	R0	477	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	03	28	LYS	CA-C-N	5.10	125.64	119.98
1	03	28	LYS	C-N-CA	5.10	125.64	119.98
4	A6	264	GLN	OE1-CD-NE2	-5.10	117.50	122.60
7	D2	1073	ASN	CA-C-N	5.10	127.37	120.38
7	D2	1073	ASN	C-N-CA	5.10	127.37	120.38
10	H1	348	GLN	OE1-CD-NE2	-5.10	117.50	122.60
13	K1	145	PRO	N-CA-CB	5.10	105.87	103.22
14	L0	902	GLN	OE1-CD-NE2	-5.10	117.50	122.60
6	C0	1489	HIS	CB-CG-CD2	-5.10	124.57	131.20
23	U6	609	ASN	CA-CB-CG	-5.10	107.50	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C3	416	GLU	CB-CG-CD	5.10	121.27	112.60
7	D2	1114	ARG	NE-CZ-NH2	5.10	123.79	119.20
14	L2	914	GLN	OE1-CD-NE2	-5.10	117.50	122.60
2	13	117	HIS	CB-CG-CD2	-5.10	124.57	131.20
6	C1	1112	GLN	OE1-CD-NE2	-5.10	117.50	122.60
7	D5	1138	GLY	CA-C-N	5.10	127.37	120.44
7	D5	1138	GLY	C-N-CA	5.10	127.37	120.44
15	M0	912	MET	CA-C-N	5.10	125.09	119.89
15	M0	912	MET	C-N-CA	5.10	125.09	119.89
20	R0	993	ASP	CA-C-N	5.10	131.28	121.54
20	R0	993	ASP	C-N-CA	5.10	131.28	121.54
2	15	1196	GLN	OE1-CD-NE2	-5.09	117.50	122.60
7	D0	812	LYS	CA-C-N	5.09	127.11	120.28
7	D0	812	LYS	C-N-CA	5.09	127.11	120.28
8	E0	6	SER	N-CA-C	5.09	118.65	111.52
1	00	410	ASP	CA-CB-CG	5.09	117.69	112.60
7	D0	1391	HIS	CB-CG-CD2	-5.09	124.58	131.20
2	14	117	HIS	CB-CG-CD2	-5.09	124.58	131.20
4	A1	28	HIS	CB-CG-CD2	-5.09	124.58	131.20
4	A1	649	VAL	CA-C-N	5.09	125.32	120.43
4	A1	649	VAL	C-N-CA	5.09	125.32	120.43
5	B0	283	HIS	CA-C-N	5.09	127.52	120.29
5	B0	283	HIS	C-N-CA	5.09	127.52	120.29
8	E0	333	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	02	663	ASN	OD1-CG-ND2	-5.09	117.51	122.60
1	04	145	ASP	CA-C-N	5.09	125.59	119.94
1	04	145	ASP	C-N-CA	5.09	125.59	119.94
2	10	1309	GLN	OE1-CD-NE2	-5.09	117.51	122.60
6	C1	1736	ASP	CA-CB-CG	5.09	117.69	112.60
6	C4	119	GLN	OE1-CD-NE2	-5.09	117.51	122.60
15	M2	656	ASN	CA-CB-CG	5.09	117.69	112.60
18	P2	533	ASP	CA-CB-CG	5.09	117.69	112.60
22	T0	756	HIS	CB-CG-CD2	-5.09	124.58	131.20
19	Q0	377	HIS	CB-CG-CD2	-5.09	124.59	131.20
4	A0	142	GLN	OE1-CD-NE2	-5.09	117.51	122.60
14	L0	259	ARG	CD-NE-CZ	5.08	131.52	124.40
20	R0	313	TYR	CA-C-N	5.08	127.36	120.65
20	R0	313	TYR	C-N-CA	5.08	127.36	120.65
2	11	117	HIS	CB-CG-CD2	-5.08	124.59	131.20
2	15	1802	HIS	CB-CG-CD2	-5.08	124.59	131.20
13	K2	845	ASP	CA-CB-CG	5.08	117.68	112.60
14	L1	914	GLN	OE1-CD-NE2	-5.08	117.52	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	00	145	ASP	CA-C-N	5.08	125.58	119.94
1	00	145	ASP	C-N-CA	5.08	125.58	119.94
2	14	892	VAL	CA-C-N	5.08	129.46	120.87
2	14	892	VAL	C-N-CA	5.08	129.46	120.87
2	15	744	PHE	CA-C-N	5.08	129.55	122.23
2	15	744	PHE	C-N-CA	5.08	129.55	122.23
4	A3	89	PRO	N-CA-CB	5.08	105.81	102.25
4	A3	491	HIS	CA-CB-CG	-5.08	108.72	113.80
6	C0	839	LYS	CG-CD-CE	-5.08	99.61	111.30
15	M1	423	ARG	NE-CZ-NH2	5.08	123.77	119.20
20	R2	507	GLN	OE1-CD-NE2	-5.08	117.52	122.60
2	16	797	ARG	CD-NE-CZ	5.08	131.51	124.40
12	J3	452	LYS	CG-CD-CE	-5.08	99.62	111.30
13	K1	908	LYS	N-CA-CB	-5.08	103.37	110.38
1	03	663	ASN	OD1-CG-ND2	-5.08	117.52	122.60
2	15	1003	ASP	CA-CB-CG	5.08	117.68	112.60
4	A1	110	LEU	CA-C-N	5.08	127.40	120.54
4	A1	110	LEU	C-N-CA	5.08	127.40	120.54
6	C2	500	GLN	OE1-CD-NE2	-5.08	117.52	122.60
7	D0	768	HIS	CB-CG-CD2	-5.08	124.60	131.20
7	D1	937	ALA	CA-C-N	5.08	128.44	120.82
7	D1	937	ALA	C-N-CA	5.08	128.44	120.82
12	J2	452	LYS	CG-CD-CE	-5.08	99.62	111.30
1	00	310	ARG	CD-NE-CZ	5.08	131.51	124.40
7	D1	790	GLN	OE1-CD-NE2	-5.08	117.53	122.60
15	M1	745	HIS	CB-CG-CD2	-5.08	124.60	131.20
20	R0	411	HIS	CB-CG-CD2	-5.08	124.60	131.20
20	R3	539	GLN	OE1-CD-NE2	-5.08	117.53	122.60
25	W0	503	PRO	N-CA-CB	5.08	106.03	103.19
2	17	830	GLN	OE1-CD-NE2	-5.07	117.53	122.60
7	D4	1138	GLY	CA-C-N	5.07	127.34	120.44
7	D4	1138	GLY	C-N-CA	5.07	127.34	120.44
9	F0	303	ILE	CA-C-N	5.07	131.23	121.54
9	F0	303	ILE	C-N-CA	5.07	131.23	121.54
13	K0	466	ARG	CD-NE-CZ	5.07	131.50	124.40
1	04	262	PHE	CA-CB-CG	5.07	118.87	113.80
2	11	830	GLN	OE1-CD-NE2	-5.07	117.53	122.60
7	D4	91	PRO	N-CA-CB	5.07	108.58	103.25
14	L1	302	HIS	CB-CG-CD2	-5.07	124.61	131.20
20	R2	530	LYS	N-CA-CB	-5.07	102.41	110.22
20	R3	653	ASN	OD1-CG-ND2	-5.07	117.53	122.60
22	T1	803	ALA	CA-C-N	5.07	127.30	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	T1	803	ALA	C-N-CA	5.07	127.30	120.50
25	W0	532	HIS	CB-CG-CD2	-5.07	124.61	131.20
2	16	893	GLU	N-CA-CB	-5.07	102.74	110.45
4	A2	657	GLN	OE1-CD-NE2	-5.07	117.53	122.60
15	M1	912	MET	CA-C-N	5.07	125.06	119.89
15	M1	912	MET	C-N-CA	5.07	125.06	119.89
4	A4	488	HIS	CB-CG-CD2	-5.07	124.61	131.20
6	C0	238	GLN	OE1-CD-NE2	-5.07	117.53	122.60
7	D2	1328	HIS	CB-CG-CD2	-5.07	124.61	131.20
7	D5	1083	ARG	CD-NE-CZ	5.07	131.50	124.40
22	T0	207	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	01	262	PHE	CA-CB-CG	5.07	118.87	113.80
2	16	830	GLN	OE1-CD-NE2	-5.07	117.53	122.60
15	M2	508	ASP	CA-CB-CG	5.07	117.67	112.60
9	F2	170	HIS	CB-CG-CD2	-5.06	124.62	131.20
6	C1	238	GLN	OE1-CD-NE2	-5.06	117.54	122.60
14	L3	914	GLN	OE1-CD-NE2	-5.06	117.54	122.60
20	R1	411	HIS	CB-CG-CD2	-5.06	124.62	131.20
5	B0	1537	ALA	CA-C-N	5.06	127.56	120.28
5	B0	1537	ALA	C-N-CA	5.06	127.56	120.28
15	M0	745	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	03	262	PHE	CA-CB-CG	5.05	118.85	113.80
6	C2	1489	HIS	CB-CG-CD2	-5.05	124.63	131.20
2	17	1414	ASP	CA-CB-CG	5.05	117.65	112.60
15	M3	912	MET	CA-C-N	5.05	125.04	119.89
15	M3	912	MET	C-N-CA	5.05	125.04	119.89
19	Q2	34	THR	CA-C-N	5.05	125.50	121.61
19	Q2	34	THR	C-N-CA	5.05	125.50	121.61
5	B0	1600	ASP	CA-CB-CG	5.05	117.65	112.60
7	D3	1328	HIS	CB-CG-CD2	-5.05	124.63	131.20
13	K0	932	HIS	CB-CG-CD2	-5.05	124.63	131.20
15	M3	423	ARG	NE-CZ-NH2	5.05	123.75	119.20
2	13	524	HIS	CB-CG-CD2	-5.05	124.64	131.20
7	D1	1073	ASN	CA-C-N	5.05	127.30	120.38
7	D1	1073	ASN	C-N-CA	5.05	127.30	120.38
7	D4	92	GLU	N-CA-CB	5.05	117.63	110.06
1	01	663	ASN	OD1-CG-ND2	-5.05	117.55	122.60
6	C4	265	ASP	CA-CB-CG	5.05	117.65	112.60
6	C0	1848	PRO	CA-C-N	5.05	127.46	120.29
6	C0	1848	PRO	C-N-CA	5.05	127.46	120.29
8	E1	240	ALA	N-CA-CB	-5.05	101.79	111.53
13	K3	1041	ARG	CA-C-N	5.05	129.47	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	K3	1041	ARG	C-N-CA	5.05	129.47	121.44
18	P1	189	ASN	CA-CB-CG	5.05	117.65	112.60
20	R1	313	TYR	CA-C-N	5.05	127.31	120.65
20	R1	313	TYR	C-N-CA	5.05	127.31	120.65
7	D5	867	TYR	N-CA-C	5.04	121.55	110.80
15	M0	584	CYS	CA-C-N	5.04	130.78	121.70
15	M0	584	CYS	C-N-CA	5.04	130.78	121.70
2	16	117	HIS	CB-CG-CD2	-5.04	124.64	131.20
6	C3	1695	ASP	CA-C-N	5.04	128.74	121.18
6	C3	1695	ASP	C-N-CA	5.04	128.74	121.18
9	F2	154	GLN	CA-C-N	5.04	130.10	122.08
9	F2	154	GLN	C-N-CA	5.04	130.10	122.08
22	T0	21	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	04	267	GLN	OE1-CD-NE2	-5.04	117.56	122.60
7	D0	506	GLN	OE1-CD-NE2	-5.04	117.56	122.60
18	P0	165	HIS	CB-CG-CD2	-5.04	124.65	131.20
19	Q3	226	HIS	CB-CG-CD2	-5.04	124.65	131.20
5	B1	972	ASP	CA-CB-CG	5.04	117.64	112.60
7	D2	491	GLN	OE1-CD-NE2	-5.04	117.56	122.60
20	R1	477	GLN	OE1-CD-NE2	-5.04	117.56	122.60
2	17	1802	HIS	CB-CG-CD2	-5.04	124.65	131.20
6	C0	1112	GLN	OE1-CD-NE2	-5.04	117.56	122.60
9	F1	207	THR	CA-C-N	5.04	125.13	120.34
9	F1	207	THR	C-N-CA	5.04	125.13	120.34
20	R0	738	GLN	OE1-CD-NE2	-5.04	117.56	122.60
7	D1	803	PHE	CA-C-N	5.04	127.73	120.38
7	D1	803	PHE	C-N-CA	5.04	127.73	120.38
2	14	132	ASP	CA-CB-CG	5.04	117.64	112.60
4	A0	146	HIS	CB-CG-CD2	-5.04	124.65	131.20
6	C0	1938	ASP	CB-CA-C	5.04	119.47	111.51
17	O1	106	ARG	CD-NE-CZ	5.04	131.45	124.40
1	01	28	LYS	CA-C-N	5.03	125.57	119.98
1	01	28	LYS	C-N-CA	5.03	125.57	119.98
1	02	201	LEU	CA-C-N	5.03	126.98	120.44
1	02	201	LEU	C-N-CA	5.03	126.98	120.44
4	A2	264	GLN	OE1-CD-NE2	-5.03	117.57	122.60
4	A3	28	HIS	CB-CG-CD2	-5.03	124.66	131.20
6	C4	981	HIS	CB-CG-CD2	-5.03	124.66	131.20
7	D2	1311	ASP	CA-CB-CG	5.03	117.63	112.60
8	E1	244	THR	N-CA-CB	5.03	119.00	110.49
15	M0	584	CYS	O-C-N	-5.03	116.91	122.75
22	T1	207	GLN	OE1-CD-NE2	-5.03	117.57	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D1	357	GLN	OE1-CD-NE2	-5.03	117.57	122.60
13	K0	485	ASP	CA-CB-CG	5.03	117.63	112.60
13	K1	878	GLN	OE1-CD-NE2	-5.03	117.57	122.60
7	D5	506	GLN	OE1-CD-NE2	-5.03	117.57	122.60
20	R2	207	VAL	CA-C-O	-5.03	117.33	119.94
23	U0	731	PRO	CA-N-CD	-5.03	104.96	112.00
1	O2	310	ARG	CD-NE-CZ	5.03	131.44	124.40
18	P3	135	GLN	OE1-CD-NE2	-5.03	117.57	122.60
19	Q3	283	ASP	CA-CB-CG	5.03	117.63	112.60
7	D5	33	GLN	OE1-CD-NE2	-5.03	117.58	122.60
20	R0	507	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	O1	267	GLN	OE1-CD-NE2	-5.02	117.58	122.60
13	K3	110	ASP	CA-C-N	5.02	131.14	121.54
13	K3	110	ASP	C-N-CA	5.02	131.14	121.54
8	E1	570	HIS	CB-CG-CD2	-5.02	124.67	131.20
16	N1	280	SER	CA-C-N	5.02	125.67	120.60
16	N1	280	SER	C-N-CA	5.02	125.67	120.60
14	L2	259	ARG	CD-NE-CZ	5.02	131.43	124.40
24	V0	795	LEU	CA-C-N	5.02	127.94	120.31
24	V0	795	LEU	C-N-CA	5.02	127.94	120.31
1	O1	260	GLN	OE1-CD-NE2	-5.02	117.58	122.60
2	11	1313	ASP	CA-CB-CG	5.02	117.62	112.60
2	15	800	ASP	CA-CB-CG	5.02	117.62	112.60
5	B0	1118	ALA	CA-C-N	5.02	127.51	120.28
5	B0	1118	ALA	C-N-CA	5.02	127.51	120.28
6	C1	290	GLU	CA-C-N	5.02	127.31	120.54
6	C1	290	GLU	C-N-CA	5.02	127.31	120.54
20	R1	738	GLN	OE1-CD-NE2	-5.02	117.58	122.60
2	17	1313	ASP	CA-CB-CG	5.02	117.62	112.60
13	K1	1041	ARG	CA-C-N	5.02	129.41	121.44
13	K1	1041	ARG	C-N-CA	5.02	129.41	121.44
2	10	783	ARG	CD-NE-CZ	5.01	131.42	124.40
2	14	800	ASP	CA-CB-CG	5.01	117.61	112.60
2	15	830	GLN	OE1-CD-NE2	-5.01	117.58	122.60
13	K0	1041	ARG	CA-C-N	5.01	129.41	121.44
13	K0	1041	ARG	C-N-CA	5.01	129.41	121.44
16	N0	78	SER	CA-C-N	5.01	127.50	120.28
16	N0	78	SER	C-N-CA	5.01	127.50	120.28
2	13	830	GLN	OE1-CD-NE2	-5.01	117.59	122.60
19	Q1	283	ASP	CA-CB-CG	5.01	117.61	112.60
1	O1	145	ASP	CA-C-N	5.01	125.50	119.94
1	O1	145	ASP	C-N-CA	5.01	125.50	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	04	663	ASN	OD1-CG-ND2	-5.01	117.59	122.60
3	41	400	HIS	CB-CG-CD2	-5.01	124.69	131.20
6	C3	981	HIS	CB-CG-CD2	-5.01	124.69	131.20
14	L3	503	ARG	CD-NE-CZ	5.01	131.42	124.40
15	M2	503	HIS	CB-CG-CD2	-5.01	124.68	131.20
1	03	260	GLN	OE1-CD-NE2	-5.01	117.59	122.60
7	D1	33	GLN	OE1-CD-NE2	-5.01	117.59	122.60
7	D1	506	GLN	OE1-CD-NE2	-5.01	117.59	122.60
7	D4	90	PRO	O-C-N	-5.01	118.80	121.15
17	O0	34	GLN	OE1-CD-NE2	-5.01	117.59	122.60
20	R3	207	VAL	CA-C-O	-5.01	117.33	119.94
20	R3	411	HIS	CB-CG-CD2	-5.01	124.69	131.20
2	17	1793	GLY	CA-C-N	5.01	126.10	119.84
2	17	1793	GLY	C-N-CA	5.01	126.10	119.84
18	P1	165	HIS	CB-CG-CD2	-5.01	124.69	131.20
20	R0	207	VAL	CA-C-O	-5.01	117.34	119.94
25	W0	502	SER	CA-C-N	5.01	123.32	119.66
25	W0	502	SER	C-N-CA	5.01	123.32	119.66
7	D4	812	LYS	CA-C-N	5.01	126.99	120.28
7	D4	812	LYS	C-N-CA	5.01	126.99	120.28
8	E0	570	HIS	CB-CG-CD2	-5.01	124.69	131.20
20	R3	507	GLN	OE1-CD-NE2	-5.01	117.59	122.60
7	D1	276	ASP	CA-CB-CG	5.00	117.61	112.60
14	L0	620	HIS	CB-CG-CD2	-5.00	124.69	131.20
6	C3	119	GLN	OE1-CD-NE2	-5.00	117.60	122.60
10	H1	407	GLU	CA-C-N	5.00	126.95	120.44
10	H1	407	GLU	C-N-CA	5.00	126.95	120.44
13	K3	932	HIS	CB-CG-CD2	-5.00	124.70	131.20
14	L1	503	ARG	CD-NE-CZ	5.00	131.40	124.40
14	L1	902	GLN	OE1-CD-NE2	-5.00	117.60	122.60
18	P2	165	HIS	CB-CG-CD2	-5.00	124.69	131.20
20	R2	104	HIS	CB-CG-CD2	-5.00	124.69	131.20
1	00	267	GLN	OE1-CD-NE2	-5.00	117.60	122.60
13	K1	528	GLN	OE1-CD-NE2	-5.00	117.60	122.60

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	10	167	ALA	CA
2	12	167	ALA	CA
2	13	1773	THR	CA
4	A6	96	THR	CA

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Mol	Chain	Res	Type	Atom
6	C0	174	THR	CB
6	C1	174	THR	CB
6	C2	174	THR	CB
6	C3	174	THR	CB
6	C4	174	THR	CB
7	D4	1104	MET	CA
15	M3	586	PRO	CA
18	P2	550	GLU	CA
22	T0	856	HIS	CA
22	T0	882	VAL	CA
22	T1	856	HIS	CA
22	T1	882	VAL	CA

All (676) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	00	132	TYR	Sidechain
1	00	161	ARG	Peptide
1	00	175	TYR	Sidechain
1	00	193	ARG	Sidechain
1	01	11	TYR	Sidechain
1	01	161	ARG	Sidechain
1	01	165	VAL	Peptide
1	01	552	ARG	Sidechain
1	02	132	TYR	Sidechain
1	02	175	TYR	Sidechain
1	02	193	ARG	Sidechain
1	03	132	TYR	Sidechain
1	03	163	ASP	Peptide
1	03	175	TYR	Sidechain
1	04	193	ARG	Sidechain
2	10	1537	TYR	Sidechain
2	10	166	GLU	Peptide
2	10	167	ALA	Peptide
2	10	1788	ASP	Peptide
2	10	1792	PRO	Mainchain
2	10	1793	GLY	Peptide
2	10	1795	TYR	Sidechain
2	10	1822	ALA	Mainchain
2	10	1823	VAL	Peptide
2	11	1537	TYR	Sidechain
2	11	1570	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	11	1789	ARG	Peptide
2	12	1537	TYR	Sidechain
2	12	1570	GLN	Peptide
2	12	166	GLU	Peptide
2	12	1788	ASP	Peptide
2	12	1789	ARG	Peptide
2	12	744	PHE	Peptide
2	12	746	CYS	Peptide
2	13	1537	TYR	Sidechain
2	13	1570	GLN	Peptide
2	13	1773	THR	Peptide
2	14	1165	LEU	Peptide
2	14	1537	TYR	Sidechain
2	14	1556	ARG	Sidechain
2	14	1584	ARG	Sidechain
2	14	1787	VAL	Peptide
2	14	1789	ARG	Sidechain
2	14	336	PRO	Peptide
2	14	343	VAL	Peptide
2	15	1165	LEU	Peptide
2	15	1537	TYR	Sidechain
2	15	1556	ARG	Sidechain
2	15	1687	PHE	Peptide
2	15	1789	ARG	Sidechain,Peptide
2	15	743	LYS	Peptide
2	16	1165	LEU	Peptide
2	16	1177	MET	Peptide
2	16	1537	TYR	Sidechain
2	16	1556	ARG	Sidechain
2	16	1570	GLN	Peptide
2	16	1584	ARG	Sidechain
2	16	341	TYR	Sidechain
2	17	1537	TYR	Sidechain
2	17	1556	ARG	Sidechain
2	17	1704	TYR	Sidechain
2	17	1789	ARG	Sidechain,Peptide
2	17	1792	PRO	Peptide,Mainchain
2	17	743	LYS	Peptide
3	40	206	ALA	Peptide
3	40	286	ARG	Peptide
3	40	30	SER	Peptide
3	40	330	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	40	364	GLU	Peptide
3	41	206	ALA	Peptide
3	41	286	ARG	Peptide
3	41	30	SER	Peptide
3	41	364	GLU	Peptide
4	A0	118	ARG	Sidechain
4	A0	128	TYR	Sidechain
4	A0	362	ARG	Sidechain
4	A0	380	ARG	Sidechain
4	A0	481	ARG	Sidechain
4	A0	486	ARG	Sidechain
4	A0	706	HIS	Peptide
4	A0	730	ARG	Sidechain
4	A0	77	ARG	Sidechain
4	A0	781	ARG	Sidechain
4	A0	790	ARG	Sidechain
4	A1	175	ARG	Peptide
4	A1	362	ARG	Sidechain
4	A1	380	ARG	Sidechain
4	A1	396	ARG	Sidechain
4	A1	486	ARG	Sidechain
4	A1	706	HIS	Peptide
4	A1	709	ARG	Sidechain
4	A1	730	ARG	Sidechain
4	A1	781	ARG	Sidechain
4	A1	790	ARG	Sidechain
4	A1	802	ARG	Peptide
4	A1	95	ASP	Peptide
4	A2	118	ARG	Sidechain
4	A2	128	TYR	Sidechain
4	A2	362	ARG	Sidechain
4	A2	380	ARG	Sidechain
4	A2	486	ARG	Sidechain
4	A2	655	ALA	Mainchain
4	A2	706	HIS	Peptide
4	A2	730	ARG	Sidechain
4	A2	77	ARG	Sidechain
4	A2	781	ARG	Sidechain
4	A2	790	ARG	Sidechain
4	A2	802	ARG	Peptide
4	A3	137	TRP	Peptide
4	A3	175	ARG	Peptide

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Mol	Chain	Res	Type	Group
4	A3	362	ARG	Sidechain
4	A3	380	ARG	Sidechain
4	A3	396	ARG	Sidechain
4	A3	486	ARG	Sidechain
4	A3	555	ARG	Sidechain
4	A3	706	HIS	Peptide
4	A3	730	ARG	Sidechain
4	A4	118	ARG	Sidechain
4	A4	362	ARG	Sidechain
4	A4	380	ARG	Sidechain
4	A4	486	ARG	Sidechain
4	A4	545	ARG	Sidechain
4	A4	555	ARG	Sidechain
4	A4	730	ARG	Sidechain
4	A5	118	ARG	Sidechain
4	A5	362	ARG	Sidechain
4	A5	380	ARG	Sidechain
4	A5	486	ARG	Sidechain
4	A5	555	ARG	Sidechain
4	A5	730	ARG	Sidechain
4	A6	118	ARG	Sidechain
4	A6	128	TYR	Sidechain
4	A6	177	SER	Peptide
4	A6	362	ARG	Sidechain
4	A6	380	ARG	Sidechain
4	A6	486	ARG	Sidechain
4	A6	555	ARG	Sidechain
4	A6	730	ARG	Sidechain
4	A6	94	LYS	Peptide
5	B0	1048	TYR	Sidechain
5	B0	11	ARG	Sidechain
5	B0	1398	ARG	Sidechain
5	B0	1509	GLY	Peptide
5	B0	1514	VAL	Peptide
5	B0	1515	ALA	Peptide
5	B0	1516	GLN	Peptide
5	B0	1517	ARG	Peptide,Mainchain
5	B0	1519	GLN	Peptide,Mainchain
5	B0	1522	PRO	Peptide
5	B0	1532	SER	Peptide
5	B0	1586	TYR	Sidechain
5	B0	209	ARG	Sidechain

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Mol	Chain	Res	Type	Group
5	B0	251	ARG	Sidechain
5	B0	267	TYR	Sidechain
5	B0	368	GLY	Peptide
5	B0	496	ARG	Sidechain
5	B0	624	ARG	Sidechain
5	B0	877	ARG	Sidechain
5	B0	989	HIS	Sidechain
5	B1	1048	TYR	Sidechain
5	B1	11	ARG	Sidechain
5	B1	1168	ARG	Sidechain
5	B1	1398	ARG	Sidechain
5	B1	1509	GLY	Peptide
5	B1	1514	VAL	Peptide
5	B1	1516	GLN	Peptide
5	B1	1517	ARG	Peptide,Mainchain
5	B1	1519	GLN	Peptide,Mainchain
5	B1	1522	PRO	Peptide
5	B1	1523	SER	Peptide
5	B1	1525	ALA	Peptide
5	B1	1528	ALA	Peptide
5	B1	1532	SER	Peptide
5	B1	1586	TYR	Sidechain
5	B1	209	ARG	Sidechain
5	B1	251	ARG	Sidechain
5	B1	267	TYR	Sidechain
5	B1	368	GLY	Peptide
5	B1	496	ARG	Sidechain
5	B1	594	TYR	Sidechain
5	B1	624	ARG	Sidechain
5	B1	877	ARG	Sidechain
5	B1	989	HIS	Sidechain
6	C0	1085	ARG	Sidechain
6	C0	1146	ASP	Peptide
6	C0	1269	ARG	Sidechain
6	C0	127	ARG	Sidechain
6	C0	1483	ARG	Sidechain
6	C0	1601	GLY	Peptide
6	C0	2010	SER	Peptide
6	C0	214	ARG	Sidechain
6	C0	30	ARG	Sidechain
6	C0	338	ARG	Sidechain
6	C0	411	ARG	Sidechain

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Mol	Chain	Res	Type	Group
6	C0	436	ARG	Sidechain
6	C0	490	ARG	Sidechain
6	C0	615	ARG	Sidechain
6	C0	672	ILE	Peptide
6	C0	705	ARG	Sidechain
6	C0	746	ARG	Sidechain
6	C1	1085	ARG	Sidechain
6	C1	1146	ASP	Peptide
6	C1	1269	ARG	Sidechain
6	C1	127	ARG	Sidechain
6	C1	1483	ARG	Sidechain
6	C1	30	ARG	Sidechain
6	C1	338	ARG	Sidechain
6	C1	411	ARG	Sidechain
6	C1	436	ARG	Sidechain
6	C1	490	ARG	Sidechain
6	C1	615	ARG	Sidechain
6	C1	672	ILE	Peptide
6	C1	705	ARG	Sidechain
6	C2	1089	ASP	Peptide
6	C2	1180	ARG	Sidechain
6	C2	127	ARG	Sidechain
6	C2	1375	PHE	Peptide
6	C2	1434	ARG	Sidechain
6	C2	1729	ARG	Sidechain
6	C2	1798	ASP	Peptide
6	C2	1806	TYR	Sidechain
6	C2	1878	ARG	Sidechain
6	C2	1927	SER	Peptide
6	C2	1929	THR	Peptide
6	C2	1939	SER	Peptide
6	C2	411	ARG	Sidechain
6	C2	490	ARG	Sidechain
6	C2	615	ARG	Sidechain
6	C2	672	ILE	Peptide
6	C2	748	ARG	Sidechain
6	C3	1082	ARG	Sidechain
6	C3	1085	ARG	Sidechain
6	C3	1180	ARG	Sidechain
6	C3	1269	ARG	Sidechain
6	C3	127	ARG	Sidechain
6	C3	1615	ARG	Sidechain

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Mol	Chain	Res	Type	Group
6	C3	1939	SER	Peptide
6	C3	214	ARG	Sidechain
6	C3	30	ARG	Sidechain
6	C3	411	ARG	Sidechain
6	C3	490	ARG	Sidechain
6	C3	615	ARG	Sidechain
6	C3	672	ILE	Peptide
6	C3	705	ARG	Sidechain
6	C3	746	ARG	Sidechain
6	C4	1082	ARG	Sidechain
6	C4	1085	ARG	Sidechain
6	C4	1180	ARG	Sidechain
6	C4	1269	ARG	Sidechain
6	C4	127	ARG	Sidechain
6	C4	214	ARG	Sidechain
6	C4	30	ARG	Sidechain
6	C4	411	ARG	Sidechain
6	C4	413	ARG	Sidechain
6	C4	490	ARG	Sidechain
6	C4	615	ARG	Sidechain
6	C4	672	ILE	Peptide
6	C4	697	ARG	Sidechain
6	C4	705	ARG	Sidechain
6	C4	748	ARG	Sidechain
7	D0	1096	ARG	Sidechain
7	D0	1120	ARG	Sidechain
7	D0	1168	HIS	Sidechain
7	D0	1336	GLU	Peptide
7	D0	136	TYR	Sidechain
7	D0	180	TYR	Sidechain
7	D0	38	ARG	Sidechain
7	D0	466	GLU	Peptide
7	D0	575	ARG	Sidechain
7	D0	659	TYR	Sidechain
7	D0	680	ALA	Peptide
7	D0	74	SER	Peptide
7	D0	866	LEU	Peptide
7	D0	867	TYR	Peptide
7	D0	885	ARG	Sidechain
7	D0	924	ARG	Sidechain
7	D1	1001	PRO	Peptide
7	D1	1096	ARG	Sidechain

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Mol	Chain	Res	Type	Group
7	D1	1108	GLU	Peptide
7	D1	1196	PHE	Sidechain
7	D1	1336	GLU	Peptide
7	D1	136	TYR	Sidechain
7	D1	38	ARG	Sidechain
7	D1	466	GLU	Peptide
7	D1	575	ARG	Sidechain
7	D1	74	SER	Peptide
7	D1	864	PRO	Peptide
7	D1	865	LEU	Peptide
7	D1	885	ARG	Sidechain
7	D2	1096	ARG	Sidechain
7	D2	1109	ILE	Peptide
7	D2	1114	ARG	Sidechain
7	D2	1168	HIS	Sidechain
7	D2	1336	GLU	Peptide
7	D2	136	TYR	Sidechain
7	D2	180	TYR	Sidechain
7	D2	38	ARG	Sidechain
7	D2	466	GLU	Peptide
7	D2	575	ARG	Sidechain
7	D2	659	TYR	Sidechain
7	D2	680	ALA	Peptide
7	D2	74	SER	Peptide
7	D2	849	ASN	Peptide
7	D2	883	ARG	Sidechain
7	D2	885	ARG	Sidechain
7	D2	924	ARG	Sidechain
7	D2	968	ARG	Sidechain
7	D3	1029	ARG	Sidechain
7	D3	1196	PHE	Sidechain
7	D3	1336	GLU	Peptide
7	D3	236	TYR	Sidechain
7	D3	38	ARG	Sidechain
7	D3	466	GLU	Peptide
7	D3	575	ARG	Sidechain
7	D3	74	SER	Peptide
7	D3	862	ILE	Peptide
7	D3	864	PRO	Peptide
7	D3	867	TYR	Sidechain
7	D3	885	ARG	Sidechain
7	D3	924	ARG	Sidechain

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Mol	Chain	Res	Type	Group
7	D3	968	ARG	Sidechain
7	D4	1096	ARG	Sidechain
7	D4	1104	MET	Peptide
7	D4	1110	SER	Peptide
7	D4	1114	ARG	Sidechain
7	D4	1120	ARG	Sidechain
7	D4	1178	LEU	Peptide
7	D4	1179	ASP	Peptide
7	D4	1213	ASP	Peptide
7	D4	136	TYR	Sidechain
7	D4	180	TYR	Sidechain
7	D4	38	ARG	Sidechain
7	D4	466	GLU	Peptide
7	D4	575	ARG	Sidechain
7	D4	659	TYR	Sidechain
7	D4	74	SER	Peptide
7	D4	863	CYS	Peptide
7	D4	867	TYR	Sidechain
7	D4	868	SER	Peptide
7	D4	883	ARG	Sidechain
7	D5	1096	ARG	Sidechain
7	D5	1104	MET	Peptide
7	D5	1105	HIS	Sidechain
7	D5	1168	HIS	Sidechain
7	D5	1336	GLU	Peptide
7	D5	136	TYR	Sidechain
7	D5	38	ARG	Sidechain
7	D5	466	GLU	Peptide
7	D5	575	ARG	Sidechain
7	D5	74	SER	Peptide
7	D5	863	CYS	Peptide
7	D5	865	LEU	Peptide
7	D5	866	LEU	Peptide
7	D5	885	ARG	Sidechain
7	D5	968	ARG	Sidechain
8	E0	20	VAL	Mainchain
8	E0	21	LEU	Peptide
8	E0	22	GLY	Peptide
8	E0	49	ILE	Peptide
8	E0	665	ARG	Sidechain
8	E1	49	ILE	Peptide
8	E1	665	ARG	Sidechain

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Mol	Chain	Res	Type	Group
9	F0	254	ARG	Sidechain
9	F0	302	VAL	Peptide
9	F0	307	GLN	Peptide
9	F1	170	HIS	Sidechain
9	F1	196	TYR	Sidechain
9	F2	196	TYR	Sidechain
9	F2	230	ARG	Sidechain
9	F2	304	SER	Peptide
9	F3	147	LYS	Peptide
10	H0	178	TYR	Sidechain
10	H0	411	ARG	Sidechain
10	H0	439	ARG	Sidechain
10	H0	454	TYR	Sidechain
10	H0	461	ARG	Sidechain
10	H1	178	TYR	Sidechain
10	H2	178	TYR	Sidechain
10	H2	461	ARG	Sidechain
10	H3	178	TYR	Sidechain
10	H3	411	ARG	Sidechain
12	J0	349	ARG	Sidechain
12	J1	349	ARG	Sidechain
12	J2	349	ARG	Sidechain
12	J3	349	ARG	Sidechain
13	K0	1089	LYS	Peptide
13	K0	1148	TYR	Sidechain
13	K0	209	TYR	Sidechain
13	K0	267	SER	Peptide
13	K0	314	ARG	Sidechain
13	K0	342	TYR	Sidechain
13	K0	586	GLU	Peptide
13	K0	599	HIS	Sidechain
13	K0	903	ARG	Sidechain
13	K0	907	GLU	Peptide
13	K1	1089	LYS	Peptide
13	K1	1148	TYR	Sidechain
13	K1	209	TYR	Sidechain
13	K1	267	SER	Peptide
13	K1	314	ARG	Sidechain
13	K1	342	TYR	Sidechain
13	K1	476	ARG	Sidechain
13	K1	477	GLU	Peptide
13	K1	599	HIS	Sidechain

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Mol	Chain	Res	Type	Group
13	K2	1089	LYS	Peptide
13	K2	1148	TYR	Sidechain
13	K2	209	TYR	Sidechain
13	K2	267	SER	Peptide
13	K2	314	ARG	Sidechain
13	K2	342	TYR	Sidechain
13	K2	476	ARG	Sidechain
13	K2	480	SER	Peptide
13	K2	599	HIS	Sidechain
13	K2	903	ARG	Sidechain
13	K2	911	ARG	Peptide
13	K2	962	ARG	Sidechain
13	K3	1089	LYS	Peptide
13	K3	1148	TYR	Sidechain
13	K3	209	TYR	Sidechain
13	K3	267	SER	Peptide
13	K3	314	ARG	Sidechain
13	K3	342	TYR	Sidechain
13	K3	476	ARG	Sidechain
13	K3	572	TYR	Sidechain
14	L0	144	ASP	Peptide
14	L0	323	LEU	Peptide
14	L0	330	ARG	Sidechain
14	L0	404	ARG	Sidechain
14	L0	582	ARG	Sidechain
14	L0	586	THR	Peptide
14	L0	669	ARG	Sidechain
14	L0	824	VAL	Peptide
14	L1	144	ASP	Peptide
14	L1	404	ARG	Sidechain
14	L1	586	THR	Peptide
14	L1	669	ARG	Sidechain
14	L1	753	TYR	Sidechain
14	L2	144	ASP	Peptide
14	L2	404	ARG	Sidechain
14	L2	582	ARG	Sidechain
14	L2	586	THR	Peptide
14	L2	669	ARG	Sidechain
14	L2	824	VAL	Peptide
14	L3	144	ASP	Peptide
14	L3	404	ARG	Sidechain
14	L3	669	ARG	Sidechain

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Mol	Chain	Res	Type	Group
14	L3	732	MET	Peptide
14	L3	734	SER	Peptide
14	L3	824	VAL	Peptide
15	M0	232	ARG	Peptide
15	M0	477	ARG	Sidechain
15	M0	515	ARG	Sidechain
15	M0	581	ARG	Sidechain
15	M0	586	PRO	Peptide
15	M0	624	TYR	Sidechain
15	M0	760	ALA	Peptide
15	M1	232	ARG	Peptide
15	M1	403	LEU	Peptide
15	M1	585	SER	Peptide
15	M1	586	PRO	Peptide
15	M1	761	GLU	Peptide
15	M2	232	ARG	Peptide
15	M2	402	HIS	Peptide
15	M2	403	LEU	Peptide
15	M2	416	TYR	Sidechain
15	M2	477	ARG	Sidechain
15	M2	586	PRO	Peptide
15	M2	624	TYR	Sidechain
15	M2	761	GLU	Peptide
15	M2	762	HIS	Peptide
15	M3	232	ARG	Peptide
15	M3	403	LEU	Peptide
15	M3	585	SER	Peptide
15	M3	586	PRO	Peptide
15	M3	760	ALA	Peptide
15	M3	765	ARG	Sidechain
16	N0	114	HIS	Sidechain
16	N0	190	LEU	Peptide
16	N0	285	LYS	Peptide
16	N0	55	GLY	Peptide
16	N1	190	LEU	Peptide
16	N1	55	GLY	Peptide
16	N2	190	LEU	Peptide
16	N2	55	GLY	Peptide
16	N3	190	LEU	Peptide
16	N3	55	GLY	Peptide
17	O0	81	ARG	Sidechain
17	O1	157	HIS	Peptide

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Mol	Chain	Res	Type	Group
17	O1	81	ARG	Sidechain
17	O2	208	LYS	Peptide
17	O2	81	ARG	Sidechain
17	O3	207	ARG	Sidechain
17	O3	81	ARG	Sidechain
18	P0	323	ASP	Peptide
18	P0	386	LEU	Peptide
18	P0	455	ARG	Sidechain
18	P0	504	ASP	Peptide
18	P0	508	ARG	Sidechain
18	P0	61	VAL	Peptide
18	P0	615	GLY	Peptide
18	P0	616	GLU	Peptide
18	P0	617	SER	Peptide
18	P1	213	ARG	Sidechain
18	P1	323	ASP	Peptide
18	P1	387	LEU	Peptide
18	P1	388	GLN	Peptide
18	P1	389	SER	Peptide
18	P1	455	ARG	Sidechain
18	P1	504	ASP	Peptide
18	P1	508	ARG	Sidechain
18	P1	60	ASP	Peptide
18	P1	616	GLU	Peptide
18	P2	213	ARG	Sidechain
18	P2	323	ASP	Peptide
18	P2	387	LEU	Peptide
18	P2	388	GLN	Peptide
18	P2	455	ARG	Sidechain
18	P2	504	ASP	Peptide
18	P2	508	ARG	Sidechain
18	P2	510	TYR	Sidechain
18	P2	541	TYR	Sidechain
18	P2	549	GLY	Peptide
18	P2	551	LYS	Peptide
18	P2	552	ARG	Peptide,Mainchain
18	P2	567	ARG	Sidechain
18	P2	60	ASP	Peptide
18	P2	602	ARG	Sidechain
18	P2	616	GLU	Peptide
18	P3	213	ARG	Sidechain
18	P3	323	ASP	Peptide

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Mol	Chain	Res	Type	Group
18	P3	455	ARG	Sidechain
18	P3	504	ASP	Peptide
18	P3	508	ARG	Sidechain
18	P3	549	GLY	Peptide
18	P3	615	GLY	Peptide
18	P3	616	GLU	Peptide
18	P3	617	SER	Peptide
18	P3	64	TYR	Sidechain
19	Q0	152	ARG	Sidechain
19	Q0	225	ARG	Sidechain
19	Q0	341	GLU	Peptide
19	Q1	152	ARG	Sidechain
19	Q1	225	ARG	Sidechain
19	Q1	341	GLU	Peptide
19	Q2	152	ARG	Sidechain
19	Q2	225	ARG	Sidechain
19	Q2	341	GLU	Peptide
19	Q3	225	ARG	Sidechain
19	Q3	341	GLU	Peptide
20	R0	1052	GLU	Peptide
20	R0	1055	TYR	Sidechain
20	R0	1080	TYR	Sidechain
20	R0	1104	TYR	Sidechain
20	R0	1139	TYR	Sidechain
20	R0	1153	ARG	Sidechain
20	R0	1162	HIS	Sidechain
20	R0	40	ALA	Peptide
20	R0	410	TRP	Peptide
20	R0	538	TYR	Sidechain
20	R0	544	HIS	Sidechain
20	R0	630	TYR	Sidechain
20	R0	718	ARG	Sidechain
20	R0	727	ARG	Sidechain
20	R0	804	LEU	Peptide
20	R1	1053	PHE	Peptide
20	R1	1080	TYR	Sidechain
20	R1	1104	TYR	Sidechain
20	R1	1139	TYR	Sidechain
20	R1	1162	HIS	Sidechain
20	R1	1329	TYR	Sidechain
20	R1	1341	TYR	Sidechain
20	R1	38	ALA	Peptide

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Mol	Chain	Res	Type	Group
20	R1	40	ALA	Peptide
20	R1	410	TRP	Peptide
20	R1	538	TYR	Sidechain
20	R1	544	HIS	Sidechain
20	R1	630	TYR	Sidechain
20	R1	718	ARG	Sidechain
20	R1	727	ARG	Sidechain
20	R1	804	LEU	Peptide
20	R2	1055	TYR	Sidechain
20	R2	1080	TYR	Sidechain
20	R2	1104	TYR	Sidechain
20	R2	1139	TYR	Sidechain
20	R2	1162	HIS	Sidechain
20	R2	1341	TYR	Sidechain
20	R2	40	ALA	Peptide
20	R2	410	TRP	Peptide
20	R2	538	TYR	Sidechain
20	R2	544	HIS	Sidechain
20	R2	630	TYR	Sidechain
20	R2	718	ARG	Sidechain
20	R2	727	ARG	Sidechain
20	R2	804	LEU	Peptide
20	R2	990	ALA	Peptide
20	R3	1080	TYR	Sidechain
20	R3	1104	TYR	Sidechain
20	R3	1139	TYR	Sidechain
20	R3	1162	HIS	Sidechain
20	R3	1329	TYR	Sidechain
20	R3	1341	TYR	Sidechain
20	R3	295	HIS	Sidechain
20	R3	40	ALA	Peptide
20	R3	410	TRP	Peptide
20	R3	538	TYR	Sidechain
20	R3	544	HIS	Sidechain
20	R3	630	TYR	Sidechain
20	R3	718	ARG	Sidechain
20	R3	727	ARG	Sidechain
20	R3	804	LEU	Peptide
21	S0	132	PHE	Peptide
21	S0	150	ARG	Sidechain
21	S0	191	ARG	Sidechain
21	S0	239	ARG	Sidechain

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Mol	Chain	Res	Type	Group
21	S1	132	PHE	Peptide
21	S1	150	ARG	Sidechain
21	S1	191	ARG	Sidechain
21	S1	231	ASP	Peptide
21	S1	239	ARG	Sidechain
21	S2	132	PHE	Peptide
21	S2	150	ARG	Sidechain
21	S2	191	ARG	Sidechain
21	S2	231	ASP	Peptide
21	S2	239	ARG	Sidechain
21	S3	132	PHE	Peptide
21	S3	150	ARG	Sidechain
21	S3	191	ARG	Sidechain
21	S3	231	ASP	Peptide
21	S3	239	ARG	Sidechain
22	T0	125	ARG	Sidechain
22	T0	2	ARG	Peptide
22	T0	3	ASP	Peptide
22	T0	441	SER	Peptide
22	T0	457	ARG	Peptide
22	T0	5	ARG	Sidechain
22	T0	553	ILE	Peptide
22	T0	558	LEU	Peptide
22	T0	685	ASP	Peptide
22	T0	69	ARG	Sidechain
22	T0	712	ARG	Sidechain
22	T0	764	LEU	Peptide
22	T0	887	ARG	Sidechain
22	T1	125	ARG	Sidechain
22	T1	2	ARG	Peptide
22	T1	3	ASP	Peptide
22	T1	441	SER	Peptide
22	T1	457	ARG	Peptide
22	T1	5	ARG	Sidechain
22	T1	553	ILE	Peptide
22	T1	554	GLN	Peptide
22	T1	556	SER	Peptide
22	T1	558	LEU	Peptide
22	T1	685	ASP	Peptide
22	T1	69	ARG	Sidechain
22	T1	764	LEU	Peptide
22	T1	887	ARG	Sidechain

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Mol	Chain	Res	Type	Group
24	V0	849	LEU	Peptide
24	V0	851	VAL	Peptide
24	V0	886	ARG	Sidechain
24	V0	906	ILE	Peptide
24	V0	960	ARG	Sidechain
25	W0	224	LEU	Peptide
25	W0	225	ASN	Peptide
25	W0	351	LYS	Peptide
25	W0	36	PRO	Peptide
25	W0	40	GLU	Peptide
25	W0	513	GLU	Peptide
25	W0	539	ARG	Sidechain

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	00	6085	0	6080	35	0
1	01	6085	0	6080	37	0
1	02	6085	0	6080	8	0
1	03	6085	0	6080	10	0
1	04	6085	0	6080	9	0
2	10	14046	0	14194	136	0
2	11	14046	0	14194	24	0
2	12	14046	0	14194	19	0
2	13	14046	0	14194	10	0
2	14	14046	0	14194	28	0
2	15	14046	0	14194	62	0
2	16	14046	0	14194	50	0
2	17	14046	0	14194	84	0
3	40	2922	0	2899	5	0
3	41	2922	0	2899	3	0
4	A0	6568	0	6527	41	0
4	A1	6568	0	6527	9	0
4	A2	6568	0	6527	34	0
4	A3	6568	0	6527	9	0
4	A4	5860	0	5828	30	0
4	A5	5860	0	5828	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A6	5860	0	5828	9	0
5	B0	13746	0	13949	14	0
5	B1	13746	0	13949	17	0
6	C0	16013	0	16224	20	0
6	C1	16013	0	16224	27	0
6	C2	16013	0	16224	73	0
6	C3	16013	0	16224	46	0
6	C4	16013	0	16224	41	0
7	D0	10363	0	10400	65	0
7	D1	10363	0	10400	135	0
7	D2	10363	0	10400	57	0
7	D3	10363	0	10400	84	0
7	D4	10363	0	10400	134	0
7	D5	10363	0	10400	53	0
8	E0	4432	0	4472	140	0
8	E1	4432	0	4472	70	0
9	F0	1837	0	1825	2	0
9	F1	1837	0	1825	15	0
9	F2	1837	0	1825	0	0
9	F3	1837	0	1825	1	0
10	H0	3066	0	3103	5	0
10	H1	3066	0	3103	4	0
10	H2	3066	0	3103	5	0
10	H3	3066	0	3103	2	0
11	I0	1398	0	1431	5	0
11	I1	1398	0	1431	2	0
11	I2	1398	0	1431	5	0
11	I3	1398	0	1431	2	0
12	J0	1403	0	1391	2	0
12	J1	1403	0	1391	2	0
12	J2	1403	0	1391	1	0
12	J3	1403	0	1391	1	0
12	J4	1403	0	1391	2	0
13	K0	8574	0	8438	10	0
13	K1	8574	0	8438	7	0
13	K2	8574	0	8438	49	0
13	K3	8574	0	8438	31	0
14	L0	6383	0	6313	32	0
14	L1	6383	0	6313	63	0
14	L2	6383	0	6313	25	0
14	L3	6383	0	6313	12	0
15	M0	5461	0	5443	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	M1	5461	0	5443	15	0
15	M2	5461	0	5443	10	0
15	M3	5461	0	5443	7	0
16	N0	2352	0	2220	20	0
16	N1	2352	0	2220	1	0
16	N2	2352	0	2220	2	0
16	N3	2352	0	2220	0	0
17	O0	2528	0	2444	7	0
17	O1	2528	0	2444	2	0
17	O2	2528	0	2444	2	0
17	O3	2528	0	2444	5	0
18	P0	5257	0	5249	14	0
18	P1	5257	0	5249	10	0
18	P2	5257	0	5249	5	0
18	P3	5257	0	5249	6	0
19	Q0	2703	0	2555	12	0
19	Q1	2703	0	2555	1	0
19	Q2	2703	0	2555	14	0
19	Q3	2703	0	2555	1	0
20	R0	11132	0	11066	44	0
20	R1	11132	0	11066	17	0
20	R2	11132	0	11066	7	0
20	R3	11132	0	11066	28	0
21	S0	2552	0	2452	5	0
21	S1	2552	0	2452	2	0
21	S2	2552	0	2452	4	0
21	S3	2552	0	2452	2	0
22	T0	7960	0	7896	13	0
22	T1	7960	0	7896	1	0
23	U0	1193	0	1188	4	0
23	U1	151	0	167	61	0
23	U2	151	0	167	36	0
23	U3	151	0	167	48	0
23	U4	151	0	167	38	0
23	U5	151	0	167	48	0
23	U6	151	0	167	37	0
24	V0	2203	0	2226	14	0
25	W0	5836	0	5850	20	0
All	All	617133	0	616873	1526	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 1.

All (1526) 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)
8:E0:18:TRP:CD2	8:E0:18:TRP:CG	1.82	1.64
2:10:1824:MET:C	2:10:1824:MET:CA	1.75	1.59
2:17:1788:ASP:C	2:17:1788:ASP:CA	1.75	1.54
8:E1:244:THR:N	8:E1:244:THR:CA	1.69	1.52
8:E0:18:TRP:NE1	8:E0:18:TRP:CE2	1.80	1.49
6:C2:484:HIS:CD2	6:C2:484:HIS:CG	2.02	1.46
7:D4:1168:HIS:NE2	23:U1:611:PHE:HA	1.31	1.45
2:14:1653:LYS:HD2	2:15:1565:ILE:CD1	1.45	1.43
7:D1:1168:HIS:NE2	23:U3:611:PHE:HA	1.31	1.42
7:D3:1168:HIS:NE2	23:U5:611:PHE:HA	1.35	1.41
8:E0:18:TRP:NE1	8:E0:18:TRP:CD1	1.85	1.41
2:15:1024:ALA:CB	2:16:1346:ILE:HD12	1.46	1.40
2:10:1825:ILE:HD11	8:E0:23:TRP:CH2	1.57	1.38
7:D0:889:ASN:ND2	9:F1:103:LEU:HD23	1.38	1.36
7:D5:1347:ARG:CD	20:R2:1154:PRO:HB3	1.55	1.36
2:16:1106:PRO:HB3	2:17:1178:ARG:NH2	1.38	1.35
7:D4:91:PRO:N	7:D4:91:PRO:CD	1.91	1.34
7:D4:91:PRO:CG	7:D4:91:PRO:CB	2.05	1.33
7:D4:91:PRO:N	7:D4:91:PRO:CA	1.93	1.31
7:D4:91:PRO:CB	7:D4:91:PRO:CA	2.08	1.30
6:C2:484:HIS:CE1	6:C2:484:HIS:NE2	2.00	1.29
7:D4:91:PRO:CD	7:D4:91:PRO:CG	2.11	1.29
6:C2:484:HIS:CE1	6:C2:484:HIS:ND1	2.02	1.28
1:00:92:THR:CG2	14:L0:262:LEU:HD22	1.64	1.27
7:D4:1184:ASP:CB	23:U1:597:ILE:HG23	1.64	1.25
2:10:1824:MET:HA	8:E0:18:TRP:CG	1.72	1.25
4:A4:172:PRO:CB	6:C3:3:THR:HG21	1.63	1.25
6:C2:484:HIS:CD2	20:R0:1111:GLU:CD	2.15	1.25
1:00:92:THR:HG21	14:L0:262:LEU:CD2	1.68	1.23
2:10:1824:MET:CA	8:E0:18:TRP:CD1	2.20	1.23
6:C2:484:HIS:CG	20:R0:1111:GLU:CD	2.16	1.22
2:10:1824:MET:CA	8:E0:18:TRP:CG	2.21	1.22
7:D0:1184:ASP:CB	23:U2:597:ILE:HG23	1.68	1.21
4:A4:167:ILE:HD13	6:C3:76:ALA:CB	1.71	1.21
6:C2:484:HIS:CE1	20:R0:1111:GLU:CD	2.18	1.21
7:D1:1002:PRO:HA	7:D4:91:PRO:N	1.53	1.20
2:10:1824:MET:CA	8:E0:18:TRP:CE2	2.23	1.20
2:16:1106:PRO:CB	2:17:1178:ARG:HH21	1.54	1.19
13:K2:1142:PHE:CD1	13:K3:577:PRO:HG2	1.76	1.19
2:10:1824:MET:CA	8:E0:18:TRP:CD2	2.26	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D1:1002:PRO:HA	7:D4:91:PRO:CA	1.73	1.18
2:15:1024:ALA:HB1	2:16:1346:ILE:HB	1.18	1.18
7:D4:1186:THR:CG2	23:U1:601:VAL:HB	1.73	1.18
4:A0:773:ARG:NH2	7:D1:88:PRO:HB3	1.58	1.17
14:L1:502:LYS:HD3	16:N0:175:LYS:CE	1.75	1.16
4:A0:773:ARG:HH21	7:D1:88:PRO:CB	1.57	1.15
7:D5:1184:ASP:CB	23:U6:597:ILE:HG23	1.75	1.15
7:D1:1002:PRO:CA	7:D4:91:PRO:CA	2.25	1.15
7:D1:1002:PRO:CA	7:D4:91:PRO:CG	2.26	1.14
1:01:553:LEU:CD1	14:L1:233:ALA:HB1	1.77	1.14
7:D0:1184:ASP:CB	23:U2:597:ILE:CG2	2.24	1.14
7:D3:1184:ASP:HB2	23:U5:597:ILE:HG23	1.25	1.14
1:01:553:LEU:HD13	14:L1:233:ALA:CB	1.78	1.13
2:15:1024:ALA:CB	2:16:1346:ILE:CD1	2.25	1.12
4:A4:172:PRO:HB3	6:C3:3:THR:CG2	1.79	1.12
7:D1:1002:PRO:CA	7:D4:91:PRO:CB	2.28	1.12
1:01:553:LEU:HD13	14:L1:233:ALA:HB1	1.19	1.12
7:D2:1354:LEU:HD13	7:D3:960:VAL:HG21	1.27	1.12
7:D4:1184:ASP:CB	23:U1:597:ILE:CG2	2.27	1.12
6:C4:468:GLU:OE1	20:R3:1205:ALA:HB1	1.49	1.12
7:D5:1184:ASP:HB2	23:U6:597:ILE:HG23	1.12	1.11
2:11:1177:MET:CG	2:12:1106:PRO:HB2	1.80	1.11
6:C4:1697:ASN:OD1	18:P3:256:LEU:HD21	1.49	1.11
1:00:729:LEU:HD23	14:L1:781:THR:HG22	1.24	1.10
7:D0:1184:ASP:HB3	23:U2:597:ILE:HG22	1.28	1.10
7:D1:1002:PRO:C	7:D4:91:PRO:CD	2.25	1.10
7:D5:1184:ASP:CB	23:U6:597:ILE:CG2	2.30	1.10
7:D5:1186:THR:HG23	23:U6:601:VAL:H	1.13	1.10
4:A4:172:PRO:HG3	6:C3:3:THR:OG1	1.49	1.09
7:D1:1002:PRO:C	7:D4:91:PRO:CB	2.25	1.09
14:L1:502:LYS:HD3	16:N0:175:LYS:HE2	1.31	1.09
6:C2:484:HIS:CG	6:C2:484:HIS:ND1	2.20	1.09
6:C2:484:HIS:CD2	20:R0:1111:GLU:OE1	2.06	1.09
7:D0:1186:THR:HG23	23:U2:601:VAL:N	1.66	1.09
7:D1:1184:ASP:HB2	23:U3:597:ILE:HG23	1.22	1.09
7:D4:1186:THR:HG21	23:U1:601:VAL:HB	1.26	1.08
2:10:1824:MET:N	8:E0:18:TRP:CD1	2.21	1.08
7:D0:1186:THR:HG23	23:U2:601:VAL:H	1.14	1.08
7:D2:1354:LEU:HD22	7:D3:960:VAL:HG22	1.35	1.07
7:D5:1347:ARG:HD2	20:R2:1154:PRO:HB3	1.37	1.07
2:10:1824:MET:CA	8:E0:18:TRP:NE1	2.17	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C2:484:HIS:CG	20:R0:1111:GLU:OE1	2.07	1.07
7:D1:1002:PRO:CA	7:D4:91:PRO:CD	2.32	1.07
2:15:1024:ALA:HB1	2:16:1346:ILE:CB	1.83	1.06
2:14:1653:LYS:HD2	2:15:1565:ILE:HD13	1.29	1.06
7:D1:1002:PRO:C	7:D4:91:PRO:CA	2.28	1.06
7:D3:1186:THR:HG23	23:U5:601:VAL:H	1.15	1.06
2:11:1177:MET:HG2	2:12:1106:PRO:HB2	1.06	1.05
2:14:1653:LYS:HD2	2:15:1565:ILE:HD11	1.10	1.05
6:C2:484:HIS:CE1	20:R0:1111:GLU:OE1	2.09	1.05
8:E1:244:THR:N	8:E1:244:THR:HA	1.64	1.05
13:K2:966:LYS:HG3	14:L2:919:LEU:HD12	1.31	1.05
7:D5:1347:ARG:HD3	20:R2:1154:PRO:HB3	1.13	1.05
14:L1:502:LYS:HZ2	16:N0:175:LYS:HG2	1.22	1.05
2:10:1824:MET:N	8:E0:18:TRP:CD2	2.23	1.05
7:D1:1186:THR:HG23	23:U3:601:VAL:H	1.19	1.05
7:D2:1184:ASP:HB2	23:U4:597:ILE:HG23	1.37	1.05
7:D0:1184:ASP:HB3	23:U2:597:ILE:CG2	1.83	1.04
7:D4:1184:ASP:HB3	23:U1:597:ILE:CG2	1.86	1.04
1:00:34:LYS:HE3	14:L0:243:THR:OG1	1.56	1.04
2:10:1824:MET:N	8:E0:18:TRP:CE2	2.25	1.04
7:D1:1002:PRO:C	7:D4:91:PRO:CG	2.30	1.04
7:D1:1184:ASP:CB	23:U3:597:ILE:HG23	1.87	1.04
7:D4:1184:ASP:HB2	23:U1:597:ILE:HG23	1.09	1.04
6:C3:468:GLU:OE1	20:R1:1205:ALA:HB1	1.56	1.04
7:D4:1184:ASP:HB3	23:U1:597:ILE:HG22	1.39	1.04
7:D2:1354:LEU:HD13	7:D3:960:VAL:CG2	1.88	1.03
2:10:1824:MET:N	8:E0:18:TRP:CG	2.25	1.03
7:D4:1186:THR:HG23	23:U1:601:VAL:H	1.23	1.03
4:A4:167:ILE:HD13	6:C3:76:ALA:HB3	1.33	1.03
7:D0:1184:ASP:HB2	23:U2:597:ILE:HG23	1.07	1.03
7:D3:1184:ASP:CB	23:U5:597:ILE:HG23	1.89	1.03
7:D5:1184:ASP:HB3	23:U6:597:ILE:HG22	1.37	1.03
13:K2:1142:PHE:CE1	13:K3:578:ARG:HG3	1.94	1.03
13:K2:1142:PHE:HD1	13:K3:577:PRO:HG2	1.21	1.02
2:17:1829:HIS:CD2	8:E1:7:ARG:NH2	2.27	1.02
6:C2:484:HIS:NE2	20:R0:1111:GLU:CD	2.17	1.02
7:D3:1186:THR:HG23	23:U5:601:VAL:N	1.74	1.02
7:D4:1186:THR:HG23	23:U1:601:VAL:N	1.74	1.02
1:01:553:LEU:CD1	14:L1:233:ALA:CB	2.35	1.02
18:P0:267:ARG:CD	24:V0:734:SER:HB2	1.88	1.02
18:P0:267:ARG:HD2	24:V0:734:SER:HB2	1.02	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D2:1186:THR:HG23	23:U4:601:VAL:H	1.22	1.01
7:D5:1186:THR:HG23	23:U6:601:VAL:N	1.75	1.01
2:10:1821:THR:HG22	8:E0:26:VAL:HG21	1.40	1.01
13:K2:794:ASP:OD2	14:L2:779:GLN:HG2	1.61	1.00
6:C2:484:HIS:CD2	6:C2:484:HIS:NE2	2.29	1.00
6:C2:484:HIS:ND1	20:R0:1111:GLU:CD	2.20	1.00
1:04:92:THR:HG21	14:L1:751:ARG:NH2	1.76	0.99
2:15:1024:ALA:HB2	2:16:1346:ILE:CD1	1.89	0.99
7:D1:1168:HIS:NE2	23:U3:611:PHE:CA	2.26	0.99
2:14:1653:LYS:CD	2:15:1565:ILE:CD1	2.40	0.99
7:D1:1168:HIS:CE1	23:U3:611:PHE:HA	1.97	0.99
1:01:541:ARG:HH12	14:L1:597:PRO:HB3	1.28	0.98
7:D4:1168:HIS:NE2	23:U1:611:PHE:CA	2.26	0.98
2:10:1825:ILE:HD11	8:E0:23:TRP:CZ2	1.98	0.98
7:D1:1184:ASP:CB	23:U3:597:ILE:CG2	2.43	0.97
18:P0:267:ARG:HD2	24:V0:734:SER:CB	1.93	0.97
2:14:1109:ASN:CG	2:15:1171:ARG:HH12	1.73	0.97
4:A0:277:ASN:OD1	7:D2:892:GLU:HG2	1.64	0.96
7:D1:1184:ASP:HB3	23:U3:597:ILE:HG22	1.46	0.96
7:D1:1002:PRO:CA	7:D4:91:PRO:N	2.28	0.96
7:D3:1184:ASP:HB3	23:U5:597:ILE:HG22	1.47	0.95
2:10:1825:ILE:CD1	8:E0:23:TRP:CH2	2.50	0.95
2:17:1789:ARG:H	8:E1:243:SER:C	1.73	0.95
7:D1:1186:THR:HG23	23:U3:601:VAL:N	1.82	0.94
2:11:1216:LYS:NZ	2:12:1434:GLN:HE21	1.63	0.94
13:K2:1142:PHE:CZ	13:K3:578:ARG:HG3	2.02	0.94
6:C2:44:LYS:HE2	7:D4:1139:GLU:OE2	1.67	0.94
7:D1:1002:PRO:HB2	7:D4:91:PRO:HB3	1.50	0.94
13:K2:912:GLY:CA	14:L2:909:LEU:HD13	1.98	0.94
7:D0:1388:GLU:CD	7:D1:959:ILE:HD12	1.93	0.93
2:17:1788:ASP:HA	8:E1:243:SER:O	1.67	0.93
13:K2:912:GLY:HA2	14:L2:909:LEU:HD13	1.50	0.93
7:D3:1184:ASP:CB	23:U5:597:ILE:CG2	2.45	0.93
2:15:1024:ALA:HB2	2:16:1346:ILE:HD12	0.93	0.93
2:17:1791:GLY:C	8:E1:240:ALA:HB1	1.93	0.92
2:12:922:TYR:CE2	2:13:701:ARG:NH2	2.38	0.92
7:D2:1186:THR:HG23	23:U4:601:VAL:N	1.83	0.92
2:16:1106:PRO:CB	2:17:1178:ARG:NH2	2.21	0.92
7:D5:1184:ASP:HB2	23:U6:597:ILE:CG2	1.95	0.92
19:Q0:57:SER:HB3	25:W0:702:PRO:HB2	1.48	0.92
2:11:1177:MET:HG2	2:12:1106:PRO:CB	1.98	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L1:502:LYS:HZ2	16:N0:175:LYS:CG	1.81	0.92
2:10:1824:MET:N	8:E0:18:TRP:NE1	2.18	0.92
7:D1:1002:PRO:C	7:D4:91:PRO:N	2.28	0.91
2:15:1434:GLN:HE21	2:16:1216:LYS:HE2	1.33	0.91
7:D5:1184:ASP:HB3	23:U6:597:ILE:CG2	1.96	0.91
6:C3:696:SER:HB3	19:Q0:327:ILE:CG1	1.99	0.91
6:C3:696:SER:HB3	19:Q0:327:ILE:HG12	1.51	0.91
7:D3:1168:HIS:CE1	23:U5:611:PHE:HA	2.06	0.91
2:14:1653:LYS:CD	2:15:1565:ILE:HD11	2.00	0.91
1:01:541:ARG:HH12	14:L1:597:PRO:CB	1.83	0.90
7:D5:1347:ARG:HD3	20:R2:1154:PRO:CB	2.00	0.90
1:01:24:GLN:NE2	14:L1:473:ASP:H	1.70	0.90
7:D5:1186:THR:HG21	23:U6:601:VAL:HB	1.53	0.90
7:D3:1186:THR:HG21	23:U5:601:VAL:HB	1.54	0.90
2:10:1824:MET:HA	8:E0:18:TRP:CD2	2.04	0.89
7:D3:1168:HIS:NE2	23:U5:611:PHE:CA	2.30	0.89
6:C4:807:TYR:OH	19:Q2:26:LEU:HD11	1.71	0.89
7:D1:1184:ASP:HB3	23:U3:597:ILE:CG2	2.02	0.89
7:D3:1184:ASP:HB3	23:U5:597:ILE:CG2	2.01	0.89
18:P1:320:LYS:HE2	25:W0:659:ARG:NH2	1.86	0.89
6:C2:1448:MET:HE1	6:C3:88:GLU:OE2	1.73	0.88
14:L1:502:LYS:CD	16:N0:175:LYS:CE	2.51	0.88
2:14:1653:LYS:CD	2:15:1565:ILE:HD13	2.01	0.88
7:D0:889:ASN:ND2	9:F1:103:LEU:CD2	2.33	0.88
6:C2:469:PRO:HG3	20:R0:1113:ARG:NH1	1.88	0.88
4:A0:773:ARG:HH21	7:D1:88:PRO:HB3	0.73	0.88
13:K2:966:LYS:CG	14:L2:919:LEU:HD12	2.02	0.88
2:10:1825:ILE:HD11	8:E0:23:TRP:HH2	1.35	0.88
2:15:1055:SER:OG	2:16:1346:ILE:HD11	1.73	0.88
2:10:1825:ILE:CD1	8:E0:23:TRP:CZ2	2.57	0.87
7:D3:1186:THR:CG2	23:U5:601:VAL:HB	2.04	0.87
14:L1:502:LYS:NZ	16:N0:175:LYS:CG	2.36	0.87
6:C2:484:HIS:ND1	20:R0:1111:GLU:OE1	2.08	0.87
7:D4:1168:HIS:CE1	23:U1:611:PHE:HA	2.08	0.87
2:10:1823:VAL:C	8:E0:18:TRP:CD1	2.52	0.87
6:C2:484:HIS:NE2	20:R0:1111:GLU:OE1	2.07	0.87
7:D0:1186:THR:CG2	23:U2:601:VAL:HB	2.05	0.87
7:D0:889:ASN:HB2	9:F1:103:LEU:HG	1.56	0.87
7:D2:1184:ASP:CB	23:U4:597:ILE:HG23	2.04	0.87
2:17:1790:ARG:H	8:E1:243:SER:N	1.72	0.87
7:D0:889:ASN:HD22	9:F1:103:LEU:HD23	0.99	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:17:1790:ARG:HB2	8:E1:242:ILE:H	1.40	0.86
7:D0:1186:THR:CG2	23:U2:601:VAL:H	1.88	0.86
7:D5:1310:ARG:HB2	21:S2:276:MET:HE3	1.57	0.86
7:D4:1186:THR:CG2	23:U1:601:VAL:CB	2.53	0.86
4:A0:770:SER:O	7:D1:94:VAL:CG1	2.23	0.86
2:10:1824:MET:C	8:E0:18:TRP:CD1	2.54	0.86
2:17:1790:ARG:CG	8:E1:243:SER:H	1.89	0.85
7:D2:1354:LEU:CD1	7:D3:960:VAL:HG21	2.05	0.85
6:C3:468:GLU:OE1	20:R1:1205:ALA:CB	2.24	0.85
7:D5:1186:THR:CG2	23:U6:601:VAL:HB	2.06	0.85
2:10:1824:MET:CB	8:E0:18:TRP:CE2	2.60	0.84
2:16:1106:PRO:HB3	2:17:1178:ARG:HH21	0.70	0.84
2:15:701:ARG:NH2	2:16:922:TYR:HE2	1.75	0.84
2:17:1788:ASP:C	2:17:1788:ASP:HA	2.01	0.84
6:C2:1597:GLN:HE21	25:W0:287:PRO:HG2	1.41	0.84
2:17:1790:ARG:HA	8:E1:243:SER:CA	2.08	0.84
2:15:1053:GLN:OE1	2:16:1411:ASN:HB2	1.78	0.84
2:10:1825:ILE:HG12	8:E0:23:TRP:CZ2	2.12	0.84
2:10:1827:ALA:HB3	8:E0:18:TRP:CA	2.07	0.84
13:K2:966:LYS:HG3	14:L2:919:LEU:CD1	2.07	0.83
4:A4:167:ILE:CD1	6:C3:76:ALA:CB	2.54	0.83
2:10:1752:LEU:HD21	2:11:1790:ARG:HH21	1.43	0.83
2:10:1824:MET:HG3	8:E0:22:GLY:HA3	1.60	0.83
1:01:18:SER:O	14:L1:472:LEU:HD11	1.78	0.83
2:10:1828:TYR:HA	8:E0:19:ARG:CB	2.08	0.83
2:15:1055:SER:OG	2:16:1346:ILE:CD1	2.27	0.83
2:11:1216:LYS:HZ2	2:12:1434:GLN:HE21	1.24	0.82
7:D2:1184:ASP:HB3	23:U4:597:ILE:HG22	1.60	0.82
7:D0:1186:THR:HG21	23:U2:601:VAL:HB	1.59	0.82
2:10:1825:ILE:CG1	8:E0:23:TRP:CZ2	2.62	0.82
7:D1:1186:THR:HG21	23:U3:601:VAL:HB	1.62	0.82
4:A0:239:THR:HG22	7:D1:1029:ARG:HG2	1.60	0.82
7:D2:1196:PHE:CD2	23:U4:610:LEU:HD11	2.15	0.82
1:00:543:ALA:HB3	14:L0:168:SER:CB	2.09	0.82
15:M1:447:LYS:HG2	18:P0:623:GLN:OE1	1.80	0.82
2:15:1024:ALA:HB1	2:16:1346:ILE:CD1	2.10	0.81
7:D4:1186:THR:HG23	23:U1:601:VAL:CA	2.10	0.81
2:17:1788:ASP:N	8:E1:244:THR:HA	1.94	0.81
2:17:1790:ARG:HG3	8:E1:243:SER:H	1.43	0.81
4:A0:606:LYS:HE3	7:D1:857:LEU:HD13	1.62	0.81
7:D2:1184:ASP:CB	23:U4:597:ILE:CG2	2.58	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D0:1237:SER:HB2	7:D1:734:ASN:HD21	1.45	0.81
7:D1:1186:THR:CG2	23:U3:601:VAL:HB	2.11	0.81
13:K2:1142:PHE:CE1	13:K3:577:PRO:HG2	2.15	0.81
2:15:1434:GLN:HE21	2:16:1216:LYS:CE	1.95	0.80
2:11:1795:TYR:HD2	8:E0:247:ASN:HD21	1.25	0.80
2:10:1828:TYR:N	8:E0:19:ARG:HA	1.97	0.80
2:10:1821:THR:HG22	8:E0:26:VAL:CG2	2.10	0.80
4:A4:172:PRO:HB3	6:C3:3:THR:HG21	0.83	0.80
7:D4:1185:ILE:CG2	23:U1:600:LEU:HB2	2.11	0.80
1:00:92:THR:HG21	14:L0:262:LEU:HD22	0.82	0.79
6:C3:620:GLU:HB3	20:R1:1221:GLN:OE1	1.82	0.79
1:00:543:ALA:HB3	14:L0:168:SER:HB3	1.62	0.79
2:10:1828:TYR:HA	8:E0:19:ARG:CG	2.13	0.79
2:10:1827:ALA:HB3	8:E0:18:TRP:N	1.98	0.78
7:D1:1002:PRO:CB	7:D4:91:PRO:HB3	2.13	0.78
14:L1:502:LYS:CD	16:N0:175:LYS:HE2	2.10	0.78
2:15:1074:GLN:OE1	2:16:1373:PRO:HB2	1.82	0.78
1:00:34:LYS:CE	14:L0:243:THR:OG1	2.30	0.78
4:A0:773:ARG:NH2	7:D1:88:PRO:CB	2.30	0.78
4:A0:558:LYS:HG3	7:D1:1031:LYS:HZ2	1.49	0.78
13:K2:912:GLY:HA2	14:L2:909:LEU:CD1	2.14	0.78
13:K2:1150:TYR:CE1	13:K3:596:ILE:CD1	2.67	0.78
4:A0:770:SER:O	7:D1:94:VAL:HG12	1.82	0.78
20:R3:223:SER:HB2	22:T0:417:ARG:NE	1.97	0.78
1:01:28:LYS:HE2	14:L1:470:ALA:HB1	1.66	0.77
7:D5:1308:LYS:O	21:S2:276:MET:HE1	1.84	0.77
1:01:541:ARG:NH1	14:L1:597:PRO:HB3	1.99	0.77
7:D0:1186:THR:CG2	23:U2:601:VAL:N	2.45	0.77
4:A4:167:ILE:HD13	6:C3:76:ALA:HB1	1.65	0.77
2:12:922:TYR:HE2	2:13:701:ARG:NH2	1.83	0.77
7:D1:1001:PRO:C	7:D4:91:PRO:HD3	2.10	0.77
20:R0:1111:GLU:CD	20:R0:1111:GLU:OE1	2.27	0.77
7:D1:1002:PRO:CB	7:D4:91:PRO:CB	2.62	0.77
4:A0:606:LYS:HZ1	7:D1:857:LEU:HD11	1.48	0.76
4:A4:173:PRO:HG2	6:C3:7:VAL:CG2	2.15	0.76
7:D5:1347:ARG:CD	20:R2:1154:PRO:CB	2.51	0.76
20:R3:224:ASP:OD2	22:T0:417:ARG:HB3	1.85	0.76
2:17:1829:HIS:HD2	8:E1:7:ARG:NH2	1.84	0.76
4:A0:558:LYS:HG3	7:D1:1031:LYS:NZ	2.01	0.76
7:D5:1196:PHE:CD2	23:U6:610:LEU:HD11	2.19	0.76
15:M1:447:LYS:CG	18:P0:623:GLN:OE1	2.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A4:173:PRO:HG2	6:C3:7:VAL:HG22	1.68	0.76
6:C0:82:GLY:HA3	12:J1:421:ILE:HD13	1.67	0.76
7:D0:1237:SER:HB2	7:D1:734:ASN:ND2	2.01	0.75
7:D2:1354:LEU:HD22	7:D3:960:VAL:CG2	2.14	0.75
2:15:1074:GLN:NE2	2:16:1373:PRO:HB2	2.01	0.75
13:K2:963:TYR:CZ	14:L2:921:TYR:HB3	2.20	0.75
6:C3:750:ARG:HG2	19:Q0:327:ILE:N	2.02	0.75
6:C2:484:HIS:CD2	20:R0:1111:GLU:CG	2.69	0.75
1:01:475:ALA:CB	14:L1:167:SER:OG	2.34	0.75
7:D0:889:ASN:HD22	9:F1:103:LEU:CD2	1.92	0.75
6:C2:1448:MET:CE	6:C3:88:GLU:OE2	2.35	0.74
7:D1:1008:PRO:HG3	7:D4:99:HIS:HE1	1.52	0.74
7:D1:1196:PHE:CE2	23:U3:610:LEU:HD13	2.22	0.74
7:D1:1196:PHE:CZ	23:U3:610:LEU:CD2	2.70	0.74
14:L1:502:LYS:NZ	16:N0:175:LYS:HG3	2.02	0.74
2:10:1825:ILE:N	8:E0:18:TRP:CD1	2.56	0.74
1:00:334:ILE:HA	14:L0:730:GLN:HB3	1.70	0.74
4:A4:167:ILE:CD1	6:C3:76:ALA:HB1	2.18	0.74
4:A4:141:LYS:HE3	6:C2:1992:ARG:HH11	1.53	0.74
2:10:1824:MET:HA	8:E0:18:TRP:HA	1.70	0.74
2:17:1788:ASP:CA	8:E1:244:THR:HA	2.18	0.74
6:C4:699:GLU:OE1	19:Q2:248:ARG:NH2	2.20	0.74
7:D0:1184:ASP:HB2	23:U2:597:ILE:CG2	1.94	0.74
2:14:1067:ARG:NH1	2:15:1344:SER:OG	2.21	0.74
2:17:1829:HIS:HD2	8:E1:7:ARG:HH22	1.36	0.74
7:D2:1184:ASP:HB3	23:U4:597:ILE:CG2	2.18	0.73
1:00:729:LEU:HD23	14:L1:781:THR:CG2	2.13	0.73
7:D0:847:ARG:HD2	9:F1:124:VAL:CG2	2.18	0.73
7:D0:1388:GLU:CD	7:D1:959:ILE:CD1	2.61	0.73
8:E0:358:HIS:CE1	9:F1:115:ASN:HD22	2.06	0.73
1:01:553:LEU:CD1	14:L1:233:ALA:HB3	2.19	0.73
6:C2:469:PRO:HG3	20:R0:1113:ARG:HH12	1.49	0.73
7:D2:1186:THR:HG21	23:U4:601:VAL:HB	1.70	0.73
2:10:1824:MET:CG	8:E0:22:GLY:HA3	2.18	0.73
7:D2:1186:THR:CG2	23:U4:601:VAL:H	2.01	0.73
13:K2:963:TYR:CE2	14:L2:921:TYR:CB	2.71	0.73
14:L1:502:LYS:CD	16:N0:175:LYS:HE3	2.17	0.73
7:D0:1196:PHE:CD2	23:U2:610:LEU:HD11	2.22	0.73
7:D3:1196:PHE:CE2	23:U5:610:LEU:HD13	2.23	0.73
7:D2:1186:THR:CG2	23:U4:601:VAL:HB	2.18	0.72
7:D4:1186:THR:HG23	23:U1:601:VAL:CB	2.17	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C2:469:PRO:CG	20:R0:1113:ARG:NH1	2.51	0.72
7:D1:1184:ASP:HB2	23:U3:597:ILE:CG2	2.06	0.72
7:D3:1196:PHE:CZ	23:U5:610:LEU:CD2	2.71	0.72
8:E1:236:TYR:O	8:E1:240:ALA:HB3	1.89	0.72
14:L3:498:ALA:HB1	15:M2:798:GLU:HG2	1.70	0.72
7:D5:1196:PHE:CG	23:U6:610:LEU:HD11	2.25	0.72
2:10:1828:TYR:O	8:E0:19:ARG:HG3	1.88	0.72
13:K2:1150:TYR:HE1	13:K3:596:ILE:HD12	1.54	0.72
2:15:1024:ALA:CB	2:16:1346:ILE:HB	2.10	0.71
13:K2:963:TYR:CE2	14:L2:921:TYR:HB3	2.24	0.71
2:10:1820:GLY:C	8:E0:18:TRP:CZ2	2.68	0.71
18:P1:320:LYS:HE2	25:W0:659:ARG:HH21	1.55	0.71
7:D4:1186:THR:HG23	23:U1:601:VAL:HB	1.72	0.71
7:D0:1196:PHE:CG	23:U2:610:LEU:HD11	2.26	0.71
7:D5:1184:ASP:CB	23:U6:597:ILE:HG22	2.08	0.71
2:10:1824:MET:HG2	8:E0:18:TRP:CZ2	2.25	0.71
6:C2:469:PRO:HB3	20:R0:1113:ARG:HD2	1.72	0.71
4:A0:606:LYS:HE3	7:D1:857:LEU:CD1	2.20	0.71
19:Q0:61:PHE:HE2	24:V0:905:SER:HB2	1.54	0.71
4:A4:172:PRO:HG3	6:C3:3:THR:CB	2.21	0.71
18:P0:232:ILE:HG23	24:V0:738:LYS:NZ	2.06	0.71
1:04:92:THR:HG21	14:L1:751:ARG:HH21	1.55	0.71
4:A2:243:LYS:NZ	7:D3:1029:ARG:HA	2.05	0.71
7:D2:1196:PHE:CG	23:U4:610:LEU:HD11	2.25	0.71
7:D3:1186:THR:CG2	23:U5:601:VAL:H	1.97	0.70
2:15:1074:GLN:CD	2:16:1373:PRO:HB2	2.15	0.70
6:C2:622:PRO:HA	20:R0:1316:SER:HB2	1.71	0.70
2:10:1831:VAL:HB	8:E0:19:ARG:HG2	1.73	0.70
7:D0:1186:THR:HA	23:U2:600:LEU:HD12	1.72	0.70
2:15:701:ARG:NH1	2:16:922:TYR:CE2	2.60	0.70
2:17:1829:HIS:CD2	8:E1:7:ARG:HH22	2.08	0.70
2:10:1824:MET:HG3	8:E0:22:GLY:CA	2.20	0.70
7:D0:889:ASN:CG	9:F1:103:LEU:HD23	2.16	0.70
7:D4:1196:PHE:CE1	23:U1:610:LEU:HD21	2.27	0.70
1:01:541:ARG:HH22	14:L1:597:PRO:HB3	1.57	0.70
7:D0:1238:SER:H	7:D1:734:ASN:HD22	1.39	0.70
7:D4:1108:GLU:HA	7:D4:1114:ARG:HB2	1.74	0.70
14:L1:502:LYS:CG	16:N0:175:LYS:HE3	2.22	0.70
2:17:1788:ASP:C	2:17:1788:ASP:CB	2.64	0.70
7:D1:1002:PRO:N	7:D4:91:PRO:CD	2.54	0.70
23:U5:603:LYS:HE2	23:U5:606:ASN:ND2	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:15:1024:ALA:HB1	2:16:1346:ILE:CG1	2.22	0.69
2:15:701:ARG:HH22	2:16:922:TYR:HE2	1.36	0.69
2:10:1824:MET:HA	8:E0:18:TRP:CA	2.22	0.69
2:10:1827:ALA:C	8:E0:19:ARG:CA	2.65	0.69
6:C2:469:PRO:HB3	20:R0:1113:ARG:NH1	2.06	0.69
7:D1:1002:PRO:HA	7:D4:91:PRO:HA	1.73	0.69
2:15:1053:GLN:OE1	2:16:1411:ASN:CB	2.39	0.69
7:D0:1186:THR:CG2	23:U2:601:VAL:CB	2.70	0.69
7:D1:1196:PHE:CE1	23:U3:610:LEU:HD22	2.28	0.69
2:15:1434:GLN:NE2	2:16:1216:LYS:HE2	2.06	0.69
7:D2:1196:PHE:CE2	23:U4:610:LEU:HD11	2.27	0.69
20:R3:223:SER:HB2	22:T0:417:ARG:HE	1.57	0.69
23:U3:603:LYS:HE2	23:U3:606:ASN:ND2	2.08	0.69
2:10:1827:ALA:CB	8:E0:19:ARG:H	2.06	0.69
23:U6:603:LYS:HE2	23:U6:606:ASN:ND2	2.08	0.69
2:10:1827:ALA:HB2	8:E0:15:ASP:HA	1.75	0.68
2:15:1074:GLN:HE22	2:16:1373:PRO:HB2	1.58	0.68
13:K2:910:LYS:HA	14:L2:913:ASP:CG	2.18	0.68
23:U4:603:LYS:HE2	23:U4:606:ASN:ND2	2.07	0.68
23:U1:603:LYS:HE2	23:U1:606:ASN:ND2	2.08	0.68
2:10:1824:MET:SD	8:E0:18:TRP:CE3	2.86	0.68
2:17:1788:ASP:C	8:E1:244:THR:C	2.60	0.68
7:D2:1354:LEU:CD2	7:D3:960:VAL:HG22	2.19	0.68
2:16:1106:PRO:HB3	2:17:1178:ARG:CZ	2.18	0.68
1:03:7:ASP:HB3	15:M1:448:ASN:OD1	1.94	0.68
2:17:1790:ARG:HB2	8:E1:242:ILE:N	2.09	0.68
2:17:1790:ARG:HB3	8:E1:240:ALA:HA	1.76	0.68
14:L3:498:ALA:CB	15:M2:798:GLU:HG2	2.23	0.68
1:01:475:ALA:HB2	14:L1:167:SER:OG	1.94	0.68
2:10:1820:GLY:O	8:E0:18:TRP:CE2	2.47	0.67
7:D1:1161:LEU:HD22	7:D1:1196:PHE:CZ	2.28	0.67
7:D4:1196:PHE:CZ	23:U1:610:LEU:HD21	2.29	0.67
14:L3:580:LEU:HD22	14:L3:585:HIS:CE1	2.29	0.67
7:D3:1196:PHE:CZ	23:U5:610:LEU:HD21	2.29	0.67
7:D5:1347:ARG:HD2	20:R2:1154:PRO:CB	2.18	0.67
7:D1:1002:PRO:O	7:D4:91:PRO:CG	2.41	0.67
7:D4:1196:PHE:CE2	23:U1:610:LEU:HD13	2.29	0.67
7:D3:1161:LEU:HD22	7:D3:1196:PHE:CZ	2.29	0.67
18:P0:232:ILE:HG23	24:V0:738:LYS:HZ3	1.60	0.67
7:D4:1186:THR:HA	23:U1:600:LEU:HD12	1.77	0.67
7:D4:1196:PHE:CE1	23:U1:610:LEU:CD2	2.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D1:1195:PRO:O	23:U3:611:PHE:CE2	2.47	0.67
7:D4:1185:ILE:HG22	23:U1:600:LEU:HB2	1.76	0.67
23:U6:606:ASN:H	23:U6:606:ASN:HD22	1.43	0.67
13:K2:912:GLY:HA3	14:L2:909:LEU:HD13	1.75	0.66
2:17:1790:ARG:CB	8:E1:243:SER:H	2.07	0.66
7:D5:1186:THR:HA	23:U6:600:LEU:HD12	1.77	0.66
2:13:1360:GLY:HA3	2:16:1105:GLN:OE1	1.95	0.66
7:D3:1186:THR:CG2	23:U5:601:VAL:N	2.57	0.66
7:D3:1196:PHE:CE1	23:U5:610:LEU:CD2	2.79	0.66
6:C4:1246:MET:HA	20:R3:1265:TRP:CZ2	2.29	0.66
13:K2:1150:TYR:CE1	13:K3:596:ILE:HD12	2.30	0.66
23:U3:610:LEU:C	23:U3:610:LEU:HD23	2.21	0.66
2:10:1759:GLN:CB	8:E0:158:ALA:HB3	2.25	0.66
4:A0:606:LYS:CE	7:D1:857:LEU:HD13	2.26	0.66
5:B0:197:GLU:CD	6:C0:1154:ASP:OD1	2.39	0.66
4:A0:606:LYS:CE	7:D1:857:LEU:CD1	2.74	0.66
19:Q0:61:PHE:CE2	24:V0:905:SER:HB2	2.31	0.66
23:U1:606:ASN:H	23:U1:606:ASN:HD22	1.44	0.66
7:D4:1196:PHE:CZ	23:U1:610:LEU:CD2	2.79	0.66
2:10:1827:ALA:C	8:E0:19:ARG:HE	2.04	0.66
23:U5:606:ASN:H	23:U5:606:ASN:HD22	1.44	0.65
6:C2:484:HIS:NE2	20:R0:1111:GLU:HG3	2.10	0.65
17:O0:86:TRP:CZ2	17:O0:105:LYS:HE2	2.31	0.65
7:D4:1196:PHE:CE2	23:U1:610:LEU:CD1	2.79	0.65
2:14:1109:ASN:CG	2:15:1171:ARG:NH1	2.53	0.65
4:A0:656:PRO:HG2	6:C1:1932:LYS:NZ	2.12	0.65
6:C2:484:HIS:NE2	20:R0:1111:GLU:CG	2.59	0.65
8:E1:238:PRO:C	8:E1:240:ALA:H	2.05	0.65
6:C2:1597:GLN:NE2	25:W0:287:PRO:HG2	2.11	0.65
18:P0:268:TYR:OH	24:V0:738:LYS:HD2	1.97	0.65
2:17:1788:ASP:CA	2:17:1788:ASP:O	2.42	0.65
7:D3:1196:PHE:CE2	23:U5:610:LEU:CD1	2.80	0.65
7:D4:1185:ILE:CG2	23:U1:600:LEU:HD13	2.26	0.65
2:17:1790:ARG:HA	8:E1:243:SER:C	2.20	0.65
7:D1:1003:VAL:N	7:D4:91:PRO:CA	2.60	0.65
13:K2:1142:PHE:CZ	13:K3:576:ASP:OD1	2.50	0.65
23:U4:606:ASN:HD22	23:U4:606:ASN:H	1.44	0.65
2:10:1824:MET:C	2:10:1824:MET:CB	2.67	0.64
7:D4:1185:ILE:O	23:U1:600:LEU:CD1	2.45	0.64
2:17:1790:ARG:H	8:E1:242:ILE:C	2.04	0.64
6:C4:1244:GLN:NE2	17:O3:205:ASN:OD1	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O2:86:TRP:CZ2	17:O2:105:LYS:HE2	2.32	0.64
2:11:1216:LYS:NZ	2:12:1434:GLN:NE2	2.42	0.64
7:D4:1185:ILE:HG22	23:U1:600:LEU:CB	2.27	0.64
1:00:548:VAL:HG11	14:L0:168:SER:O	1.98	0.64
7:D0:1388:GLU:OE2	7:D1:959:ILE:CD1	2.46	0.64
4:A0:770:SER:O	7:D1:94:VAL:HG11	1.96	0.64
6:C4:699:GLU:CG	19:Q2:248:ARG:HH12	2.11	0.64
7:D0:1196:PHE:CE1	23:U2:610:LEU:HD11	2.33	0.64
6:C3:750:ARG:CG	19:Q0:327:ILE:N	2.61	0.64
7:D1:1002:PRO:N	7:D4:91:PRO:HD3	2.13	0.64
2:11:1795:TYR:HD2	8:E0:247:ASN:ND2	1.94	0.64
7:D1:1196:PHE:CE1	23:U3:610:LEU:CD2	2.80	0.64
23:U3:606:ASN:HD22	23:U3:606:ASN:H	1.44	0.64
2:17:1788:ASP:CA	8:E1:243:SER:O	2.43	0.63
8:E0:18:TRP:CD2	8:E0:18:TRP:CD1	2.83	0.63
6:C2:622:PRO:CA	20:R0:1316:SER:HB2	2.27	0.63
7:D5:1196:PHE:CE2	23:U6:610:LEU:HD11	2.33	0.63
2:17:1790:ARG:HH12	8:E1:143:LEU:HD11	1.63	0.63
7:D1:1196:PHE:CZ	23:U3:610:LEU:HD21	2.34	0.63
13:K2:1150:TYR:CE1	13:K3:596:ILE:HD11	2.33	0.63
17:O3:86:TRP:CZ2	17:O3:105:LYS:HE2	2.34	0.63
5:B0:1148:ALA:HB1	23:U3:599:LYS:CE	2.29	0.63
23:U5:610:LEU:C	23:U5:610:LEU:HD23	2.24	0.63
7:D1:1196:PHE:CE2	23:U3:610:LEU:CD1	2.82	0.63
7:D3:1196:PHE:CE1	23:U5:610:LEU:HD22	2.34	0.63
8:E0:16:ILE:HG22	8:E0:327:ILE:HD13	1.80	0.63
17:O1:86:TRP:CZ2	17:O1:105:LYS:HE2	2.33	0.63
23:U4:603:LYS:HE2	23:U4:606:ASN:HD21	1.64	0.63
7:D3:1195:PRO:O	23:U5:611:PHE:CE2	2.51	0.63
23:U5:603:LYS:HE2	23:U5:606:ASN:HD21	1.64	0.63
2:10:1752:LEU:HD21	2:11:1790:ARG:NH2	2.12	0.63
7:D0:1388:GLU:O	7:D1:960:VAL:CG2	2.47	0.62
7:D3:1186:THR:CG2	23:U5:601:VAL:CB	2.75	0.62
6:C2:1597:GLN:NE2	25:W0:287:PRO:CG	2.62	0.62
7:D2:1161:LEU:HD21	7:D2:1196:PHE:CG	2.35	0.62
20:R3:224:ASP:OD2	22:T0:417:ARG:C	2.42	0.62
2:10:1823:VAL:C	8:E0:18:TRP:CG	2.76	0.62
14:L1:502:LYS:HG2	16:N0:175:LYS:HE3	1.80	0.62
2:17:747:ALA:HB1	2:17:748:PRO:HD2	1.80	0.62
2:10:1830:THR:H	8:E0:19:ARG:HD3	1.62	0.62
7:D0:1196:PHE:CD1	23:U2:610:LEU:HD11	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D0:1196:PHE:CE2	23:U2:610:LEU:HD11	2.34	0.62
7:D2:1184:ASP:HB2	23:U4:597:ILE:CG2	2.18	0.62
2:10:1799:LEU:HA	8:E0:72:PHE:CD2	2.35	0.62
5:B1:833:VAL:HG21	6:C1:1380:PRO:HD2	1.81	0.62
7:D0:1161:LEU:HD21	7:D0:1196:PHE:CG	2.34	0.62
7:D1:1011:LEU:HD12	7:D1:1012:SER:H	1.64	0.62
23:U6:603:LYS:HE2	23:U6:606:ASN:HD21	1.64	0.62
4:A2:675:ARG:HH21	7:D3:190:LEU:CD1	2.13	0.62
7:D0:811:GLN:OE1	9:F1:131:GLY:CA	2.47	0.62
7:D2:1196:PHE:CD1	23:U4:610:LEU:HD21	2.34	0.62
6:C4:468:GLU:OE1	20:R3:1205:ALA:CB	2.38	0.62
7:D2:1196:PHE:CE1	23:U4:610:LEU:HD11	2.35	0.62
1:01:24:GLN:HE22	14:L1:473:ASP:H	1.44	0.61
23:U1:603:LYS:HE2	23:U1:606:ASN:HD21	1.65	0.61
2:11:773:ASN:O	2:12:675:PRO:HG3	2.00	0.61
2:14:675:PRO:HG2	2:15:773:ASN:O	2.00	0.61
13:K2:963:TYR:CE2	14:L2:921:TYR:HB2	2.35	0.61
2:11:1795:TYR:CD2	8:E0:247:ASN:ND2	2.69	0.61
2:14:1071:ALA:CB	2:15:1463:HIS:CD2	2.83	0.61
2:15:701:ARG:CZ	2:16:922:TYR:HE2	2.14	0.61
23:U3:603:LYS:HE2	23:U3:606:ASN:HD21	1.65	0.61
2:10:1827:ALA:O	8:E0:19:ARG:CG	2.48	0.61
4:A2:238:ALA:HB1	7:D3:1029:ARG:HH22	1.65	0.61
2:15:1074:GLN:OE1	2:16:1373:PRO:CB	2.48	0.61
7:D4:1358:CYS:SG	20:R0:1035:ARG:NH1	2.73	0.61
6:C2:469:PRO:CB	20:R0:1113:ARG:NH1	2.63	0.61
7:D0:1388:GLU:OE2	7:D1:959:ILE:HD12	1.99	0.61
6:C3:696:SER:HB3	19:Q0:327:ILE:HG13	1.81	0.61
7:D4:1184:ASP:HB2	23:U1:597:ILE:CG2	2.00	0.61
2:10:1828:TYR:HA	8:E0:19:ARG:HG3	1.82	0.60
2:12:163:LYS:HE2	2:12:328:ARG:HH22	1.66	0.60
2:10:1799:LEU:HA	8:E0:72:PHE:CG	2.36	0.60
2:17:1790:ARG:C	8:E1:240:ALA:HA	2.25	0.60
13:K2:911:ARG:HD2	14:L2:912:LEU:HB3	1.82	0.60
1:01:553:LEU:HD13	14:L1:233:ALA:HB3	1.74	0.60
7:D1:1002:PRO:N	7:D4:91:PRO:CG	2.63	0.60
7:D5:1196:PHE:CE1	23:U6:610:LEU:HD11	2.35	0.60
2:17:1789:ARG:N	8:E1:243:SER:C	2.53	0.60
2:17:1789:ARG:HB3	8:E1:245:ALA:H	1.66	0.60
2:11:1216:LYS:HZ3	2:12:1434:GLN:HE21	1.45	0.60
2:17:1789:ARG:N	8:E1:244:THR:N	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D5:1196:PHE:CD1	23:U6:610:LEU:HD11	2.36	0.60
6:C4:699:GLU:HG3	19:Q2:248:ARG:NH1	2.15	0.60
7:D5:1161:LEU:HD21	7:D5:1196:PHE:CG	2.36	0.60
8:E0:18:TRP:CG	8:E0:18:TRP:CE2	2.87	0.60
7:D4:87:VAL:HG11	7:D4:129:GLU:C	2.26	0.60
4:A4:172:PRO:CB	6:C3:3:THR:CG2	2.56	0.60
7:D0:1237:SER:CB	7:D1:734:ASN:HD21	2.14	0.60
7:D4:1185:ILE:HG23	23:U1:600:LEU:HD13	1.84	0.60
2:17:1787:VAL:O	8:E1:243:SER:C	2.45	0.59
1:01:553:LEU:HD11	14:L1:233:ALA:CB	2.29	0.59
7:D2:1161:LEU:HD21	7:D2:1196:PHE:CD2	2.37	0.59
7:D2:1354:LEU:CD1	7:D3:960:VAL:CG2	2.71	0.59
2:10:1824:MET:SD	8:E0:18:TRP:CD2	2.96	0.59
2:14:1071:ALA:HB2	2:15:1463:HIS:CD2	2.37	0.59
14:L1:502:LYS:NZ	16:N0:175:LYS:HG2	2.00	0.59
2:14:1434:GLN:HE22	2:15:1216:LYS:CE	2.14	0.59
5:B0:197:GLU:OE2	6:C0:1154:ASP:OD1	2.20	0.59
2:10:1827:ALA:C	8:E0:19:ARG:CB	2.75	0.59
2:11:1216:LYS:HZ2	2:12:1434:GLN:NE2	1.98	0.59
4:A0:773:ARG:NH2	7:D1:88:PRO:CG	2.66	0.59
7:D1:1186:THR:HA	23:U3:600:LEU:HD12	1.84	0.59
7:D2:1354:LEU:HB3	7:D3:960:VAL:CG2	2.33	0.59
7:D0:811:GLN:OE1	9:F1:131:GLY:HA3	2.03	0.59
1:00:38:GLU:OE2	14:L0:242:VAL:HG13	2.02	0.59
2:17:1791:GLY:N	8:E1:240:ALA:HA	2.17	0.59
4:A4:129:HIS:HA	6:C2:1632:THR:HG21	1.85	0.59
5:B0:1148:ALA:HB1	23:U3:599:LYS:HE2	1.84	0.59
7:D3:1023:MET:HA	7:D3:1026:LEU:HD12	1.83	0.59
2:10:1762:LEU:HD13	8:E0:156:PRO:CG	2.32	0.59
2:17:1790:ARG:N	8:E1:244:THR:N	2.51	0.59
4:A2:287:PRO:HB2	8:E0:655:ALA:CB	2.32	0.59
4:A2:675:ARG:HH21	7:D3:190:LEU:HD11	1.68	0.59
7:D2:1196:PHE:CZ	23:U4:610:LEU:HD11	2.37	0.59
7:D4:1161:LEU:HD22	7:D4:1196:PHE:CE1	2.38	0.59
2:11:1794:PRO:HG2	8:E0:247:ASN:OD1	2.03	0.58
4:A2:655:ALA:HB2	6:C0:1932:LYS:HA	1.85	0.58
13:K2:1142:PHE:CE1	13:K3:576:ASP:OD1	2.56	0.58
2:14:1071:ALA:HB2	2:15:1463:HIS:HD2	1.67	0.58
4:A0:239:THR:HG22	7:D1:1029:ARG:CG	2.30	0.58
2:10:1830:THR:C	8:E0:313:GLU:HG3	2.29	0.58
6:C4:791:GLN:HA	20:R3:1348:GLU:OE2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K2:1142:PHE:CZ	13:K3:578:ARG:CG	2.82	0.58
2:10:1759:GLN:HB2	8:E0:158:ALA:HB3	1.85	0.58
3:40:184:ILE:HD13	7:D5:95:GLU:OE2	2.03	0.58
13:K2:1150:TYR:HE1	13:K3:596:ILE:CD1	2.10	0.58
1:00:34:LYS:HE3	14:L0:243:THR:HG1	1.68	0.58
2:10:1827:ALA:CB	8:E0:18:TRP:HB3	2.33	0.58
4:A0:656:PRO:HG2	6:C1:1932:LYS:HZ2	1.68	0.58
2:15:1434:GLN:NE2	2:16:1216:LYS:CE	2.63	0.58
7:D4:1161:LEU:HD22	7:D4:1196:PHE:CZ	2.38	0.58
7:D4:1186:THR:HG22	23:U1:601:VAL:O	2.04	0.58
4:A0:606:LYS:NZ	7:D1:857:LEU:HD11	2.18	0.58
4:A2:675:ARG:NH2	7:D3:190:LEU:HD12	2.18	0.58
7:D5:1161:LEU:HD21	7:D5:1196:PHE:CD2	2.38	0.58
13:K2:911:ARG:HB2	14:L2:909:LEU:HD22	1.86	0.58
2:16:1106:PRO:CA	2:17:1178:ARG:NH2	2.66	0.58
7:D0:1196:PHE:CD1	23:U2:610:LEU:HD21	2.39	0.58
7:D1:1011:LEU:HD13	7:D4:95:GLU:HG3	1.85	0.58
7:D4:1312:PRO:HG3	21:S0:275:LYS:HD2	1.85	0.58
7:D5:1105:HIS:CG	7:D5:1106:SER:H	2.22	0.58
2:10:1827:ALA:HB3	8:E0:19:ARG:H	1.68	0.57
4:A2:287:PRO:HB2	8:E0:655:ALA:HB3	1.85	0.57
7:D3:1196:PHE:CE1	23:U5:610:LEU:HD21	2.39	0.57
7:D0:1238:SER:H	7:D1:734:ASN:ND2	2.02	0.57
7:D2:1196:PHE:CD1	23:U4:610:LEU:HD11	2.38	0.57
7:D4:1161:LEU:HD21	7:D4:1196:PHE:CD2	2.39	0.57
19:Q0:61:PHE:HE2	24:V0:905:SER:CB	2.17	0.57
23:U1:610:LEU:C	23:U1:610:LEU:HD23	2.28	0.57
2:10:1828:TYR:CA	8:E0:19:ARG:HA	2.33	0.57
8:E0:18:TRP:CE2	8:E0:18:TRP:CD1	2.93	0.57
6:C4:722:ASN:HD21	20:R3:1255:PHE:HE1	1.51	0.57
2:12:922:TYR:HE2	2:13:701:ARG:HH22	1.38	0.57
2:17:1790:ARG:HH11	8:E1:167:LEU:HD22	1.68	0.57
4:A2:238:ALA:HB1	7:D3:1029:ARG:NH2	2.18	0.57
2:10:1796:GLY:H	8:E0:69:TYR:HB3	1.70	0.57
13:K3:947:GLU:CD	13:K3:947:GLU:H	2.13	0.57
4:A0:773:ARG:HH22	7:D1:88:PRO:HG3	1.69	0.57
17:O0:200:PHE:CZ	17:O0:211:LYS:HE2	2.40	0.57
7:D0:1196:PHE:CZ	23:U2:610:LEU:HD11	2.39	0.57
13:K2:490:LEU:HD13	13:K2:491:ALA:H	1.70	0.57
2:10:1827:ALA:O	8:E0:19:ARG:CB	2.53	0.57
2:10:1831:VAL:HG21	8:E0:16:ILE:HG23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A4:172:PRO:CG	6:C3:3:THR:HG21	2.32	0.57
6:C2:469:PRO:HB3	20:R0:1113:ARG:HH11	1.69	0.57
7:D1:1002:PRO:HA	7:D4:91:PRO:CD	2.32	0.57
7:D2:1235:LEU:CD2	7:D3:736:ASN:HD21	2.18	0.57
1:00:543:ALA:HB3	14:L0:168:SER:HB2	1.87	0.56
7:D1:1168:HIS:CE1	23:U3:611:PHE:CA	2.82	0.56
1:01:475:ALA:HB2	14:L1:167:SER:CB	2.34	0.56
4:A2:243:LYS:NZ	7:D3:1028:GLN:O	2.38	0.56
7:D1:1168:HIS:CD2	23:U3:611:PHE:CD1	2.93	0.56
13:K2:1142:PHE:CE1	13:K3:577:PRO:HD2	2.40	0.56
20:R1:1022:THR:HG22	20:R1:1055:TYR:CD1	2.40	0.56
1:00:454:ARG:HE	1:00:466:HIS:CE1	2.24	0.56
1:01:454:ARG:HE	1:01:466:HIS:CE1	2.24	0.56
1:03:454:ARG:HE	1:03:466:HIS:CE1	2.24	0.56
2:10:1824:MET:HG2	8:E0:18:TRP:CH2	2.39	0.56
2:10:1827:ALA:HB3	8:E0:19:ARG:N	2.21	0.56
2:15:701:ARG:CZ	2:16:922:TYR:CE2	2.88	0.56
2:17:1789:ARG:CB	8:E1:245:ALA:H	2.19	0.56
6:C3:429:ASN:HB3	21:S0:89:LEU:HD13	1.87	0.56
7:D0:1161:LEU:HD21	7:D0:1196:PHE:CD2	2.41	0.56
14:L1:502:LYS:NZ	16:N0:175:LYS:CE	2.69	0.56
2:10:1827:ALA:O	8:E0:19:ARG:CD	2.53	0.56
4:A2:802:ARG:HH22	6:C1:1524:VAL:HG22	1.70	0.56
6:C0:1661:ARG:NH2	6:C1:1807:TRP:HE1	2.03	0.56
1:01:541:ARG:NH2	14:L1:597:PRO:HB3	2.19	0.56
6:C2:484:HIS:ND1	20:R0:1111:GLU:OE2	2.39	0.56
7:D1:1008:PRO:CG	7:D4:99:HIS:HE1	2.18	0.56
5:B0:1148:ALA:CB	23:U3:599:LYS:HE2	2.35	0.56
7:D5:1186:THR:CG2	23:U6:601:VAL:CB	2.80	0.56
7:D2:1186:THR:CG2	23:U4:601:VAL:N	2.63	0.56
7:D5:1196:PHE:CD1	23:U6:610:LEU:HD21	2.41	0.56
13:K2:1142:PHE:CD1	13:K3:577:PRO:CG	2.70	0.56
1:02:454:ARG:HE	1:02:466:HIS:CE1	2.24	0.56
6:C2:543:GLU:OE2	16:N0:49:LEU:HD13	2.06	0.56
6:C4:1244:GLN:OE1	17:O3:205:ASN:HA	2.05	0.56
6:C4:1695:ASP:CG	18:P3:253:GLU:HG3	2.31	0.56
7:D4:1171:VAL:HG22	7:D4:1196:PHE:CZ	2.40	0.56
1:00:334:ILE:HB	1:00:337:GLU:CD	2.31	0.55
7:D3:1161:LEU:HD21	7:D3:1196:PHE:CD2	2.41	0.55
2:15:1074:GLN:HE22	2:16:1373:PRO:CB	2.19	0.55
4:A4:167:ILE:CD1	6:C3:76:ALA:HB3	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D3:1186:THR:HG22	23:U5:601:VAL:O	2.07	0.55
7:D5:1196:PHE:CZ	23:U6:610:LEU:HD11	2.41	0.55
13:K2:911:ARG:CB	14:L2:909:LEU:HD22	2.37	0.55
20:R1:1022:THR:HG22	20:R1:1055:TYR:CE1	2.41	0.55
8:E0:18:TRP:CD2	8:E0:18:TRP:CB	2.76	0.55
7:D1:1168:HIS:HE1	23:U3:612:SER:H	1.55	0.55
7:D4:1185:ILE:O	23:U1:600:LEU:HD13	2.05	0.55
2:10:1824:MET:C	8:E0:18:TRP:NE1	2.65	0.55
4:A0:36:ILE:CG2	11:I0:392:ILE:HD11	2.37	0.55
7:D1:1161:LEU:HD21	7:D1:1196:PHE:CD2	2.42	0.55
2:10:1828:TYR:N	8:E0:19:ARG:CA	2.70	0.55
4:A4:483:GLU:OE2	6:C3:51:ILE:HG23	2.07	0.55
1:00:35:LEU:HD21	14:L0:245:VAL:HG22	1.89	0.55
2:14:1105:GLN:HA	2:14:1106:PRO:C	2.32	0.55
14:L1:502:LYS:HZ3	16:N0:175:LYS:HG3	1.71	0.55
7:D2:1354:LEU:HB3	7:D3:960:VAL:HG21	1.89	0.55
18:P1:322:ILE:HG23	25:W0:663:LYS:HZ1	1.72	0.55
1:04:454:ARG:HE	1:04:466:HIS:CE1	2.25	0.54
7:D2:1354:LEU:HD13	7:D3:960:VAL:CG1	2.36	0.54
7:D3:1186:THR:HA	23:U5:600:LEU:HD12	1.88	0.54
8:E1:238:PRO:C	8:E1:240:ALA:N	2.64	0.54
2:10:1827:ALA:HB3	8:E0:18:TRP:CB	2.37	0.54
4:A2:243:LYS:HZ3	7:D3:1029:ARG:HA	1.72	0.54
7:D2:1186:THR:HA	23:U4:600:LEU:HD12	1.88	0.54
20:R3:224:ASP:OD2	22:T0:417:ARG:CB	2.54	0.54
4:A1:36:ILE:CG2	11:I1:392:ILE:HD11	2.37	0.54
4:A1:371:LEU:HD22	4:A1:395:GLY:HA3	1.89	0.54
21:S0:88:SER:C	21:S0:89:LEU:HG	2.32	0.54
25:W0:613:LYS:HE2	25:W0:617:GLU:CD	2.32	0.54
1:00:541:ARG:HD3	14:L0:166:SER:HB3	1.90	0.54
2:10:1762:LEU:HD13	8:E0:156:PRO:HG3	1.90	0.54
2:10:1824:MET:CB	8:E0:18:TRP:CD2	2.87	0.54
2:17:1793:GLY:CA	8:E1:237:ILE:HG23	2.37	0.54
4:A3:36:ILE:CG2	11:I3:392:ILE:HD11	2.38	0.54
7:D1:1002:PRO:O	7:D4:91:PRO:HG2	2.06	0.54
7:D5:1161:LEU:CD2	7:D5:1196:PHE:CG	2.91	0.54
6:C3:1246:MET:HG2	20:R1:1265:TRP:CH2	2.43	0.54
7:D4:1186:THR:HG21	23:U1:601:VAL:CB	2.17	0.54
1:03:634:HIS:HD2	14:L1:286:ASP:OD2	1.90	0.54
2:17:1789:ARG:HB2	8:E1:246:MET:N	2.23	0.54
4:A0:371:LEU:HD22	4:A0:395:GLY:HA3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B0:197:GLU:OE1	6:C0:1154:ASP:OD1	2.25	0.54
7:D2:674:MET:HE2	7:D2:823:PHE:CE2	2.43	0.54
23:U1:606:ASN:HD22	23:U1:606:ASN:N	2.06	0.54
2:10:1820:GLY:O	8:E0:18:TRP:CZ2	2.61	0.54
6:C4:1252:ARG:CZ	20:R3:1258:GLU:HB2	2.38	0.54
7:D3:1161:LEU:HD22	7:D3:1196:PHE:CE2	2.42	0.54
7:D4:1168:HIS:HE1	23:U1:612:SER:H	1.56	0.54
13:K0:947:GLU:H	13:K0:947:GLU:CD	2.16	0.54
14:L3:340:ARG:NH2	16:N2:198:GLU:O	2.41	0.54
1:03:454:ARG:HH21	1:03:466:HIS:CG	2.26	0.54
2:10:1831:VAL:HA	8:E0:313:GLU:HA	1.90	0.54
2:17:1790:ARG:HG3	8:E1:243:SER:N	2.17	0.54
4:A2:36:ILE:CG2	11:I2:392:ILE:HD11	2.38	0.54
6:C4:699:GLU:HG3	19:Q2:248:ARG:HH12	1.71	0.54
7:D3:864:PRO:HB2	7:D3:865:LEU:HD22	1.89	0.54
24:V0:715:LYS:HE2	24:V0:719:GLU:CD	2.33	0.54
2:10:1828:TYR:C	8:E0:19:ARG:HG3	2.32	0.54
2:10:1831:VAL:CB	8:E0:19:ARG:HG2	2.38	0.54
2:14:1150:GLY:O	2:15:1192:ILE:O	2.25	0.54
2:15:701:ARG:NH2	2:16:922:TYR:CE2	2.67	0.54
2:17:1790:ARG:HB3	8:E1:240:ALA:CA	2.38	0.54
7:D3:1021:GLU:CD	7:D3:1051:LYS:HZ2	2.15	0.54
13:K1:947:GLU:CD	13:K1:947:GLU:H	2.15	0.54
14:L1:305:LYS:HE2	15:M1:510:PHE:CE1	2.42	0.54
2:10:1824:MET:CG	8:E0:18:TRP:CD2	2.91	0.53
7:D1:1008:PRO:CB	7:D4:99:HIS:CE1	2.91	0.53
7:D2:1354:LEU:HD13	7:D3:960:VAL:HG11	1.90	0.53
13:K2:1142:PHE:CE1	13:K3:577:PRO:CG	2.88	0.53
2:14:1716:GLU:H	2:14:1716:GLU:CD	2.16	0.53
7:D4:1185:ILE:HG22	23:U1:600:LEU:CD1	2.39	0.53
13:K3:979:LEU:HD13	14:L3:889:TYR:CD2	2.43	0.53
4:A5:371:LEU:HD22	4:A5:395:GLY:HA3	1.91	0.53
7:D0:1238:SER:N	7:D1:734:ASN:HD22	2.05	0.53
7:D1:1168:HIS:CD2	23:U3:611:PHE:HD1	2.26	0.53
6:C2:544:ASN:HD21	16:N0:49:LEU:H	1.55	0.53
6:C2:1597:GLN:HE21	25:W0:287:PRO:CG	2.14	0.53
8:E1:243:SER:HB2	8:E1:248:LEU:O	2.08	0.53
15:M3:447:LYS:O	18:P2:619:THR:HG21	2.08	0.53
2:10:1716:GLU:CD	2:10:1716:GLU:H	2.17	0.53
2:10:1759:GLN:HB3	8:E0:158:ALA:HB3	1.90	0.53
4:A0:773:ARG:NH2	7:D1:88:PRO:HG3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:01:475:ALA:HB3	14:L1:167:SER:OG	2.09	0.53
2:10:1821:THR:C	8:E0:18:TRP:HE1	2.17	0.53
7:D0:674:MET:HE2	7:D0:823:PHE:CE2	2.44	0.53
7:D1:1186:THR:CG2	23:U3:601:VAL:CB	2.85	0.53
7:D4:1186:THR:CG2	23:U1:601:VAL:O	2.57	0.53
2:10:1827:ALA:HB3	8:E0:18:TRP:C	2.33	0.53
4:A3:371:LEU:HD22	4:A3:395:GLY:HA3	1.90	0.53
7:D3:1186:THR:HG21	23:U5:601:VAL:CB	2.34	0.53
4:A0:141:LYS:HE3	6:C0:1992:ARG:HH11	1.73	0.53
4:A2:746:SER:HB2	4:A2:807:THR:HG21	1.90	0.53
6:C4:699:GLU:HG2	19:Q2:248:ARG:HH12	1.73	0.53
7:D1:1002:PRO:CA	7:D4:91:PRO:HG3	2.34	0.53
7:D2:1161:LEU:CD2	7:D2:1196:PHE:CG	2.92	0.53
4:A6:95:ASP:H	4:A6:96:THR:HA	1.73	0.53
7:D1:1003:VAL:N	7:D4:92:GLU:H	2.07	0.53
7:D3:1161:LEU:HD22	7:D3:1196:PHE:CE1	2.43	0.53
23:U5:606:ASN:HD22	23:U5:606:ASN:N	2.06	0.53
4:A2:243:LYS:HZ3	7:D3:1029:ARG:CA	2.22	0.52
6:C4:692:ASN:O	19:Q2:230:GLN:OE1	2.28	0.52
7:D0:1021:GLU:CD	7:D0:1051:LYS:HZ2	2.17	0.52
4:A2:371:LEU:HD22	4:A2:395:GLY:HA3	1.89	0.52
7:D1:1011:LEU:HD12	7:D1:1012:SER:N	2.24	0.52
7:D1:1161:LEU:HD22	7:D1:1196:PHE:CE1	2.44	0.52
7:D1:1196:PHE:CZ	23:U3:610:LEU:HD22	2.42	0.52
1:00:334:ILE:CA	14:L0:730:GLN:HB3	2.38	0.52
2:10:1795:TYR:CE2	8:E0:137:GLN:HG2	2.44	0.52
2:10:1825:ILE:HG12	8:E0:23:TRP:CE2	2.44	0.52
2:10:1827:ALA:HB3	8:E0:18:TRP:HB3	1.90	0.52
2:16:1716:GLU:CD	2:16:1716:GLU:H	2.17	0.52
7:D4:1196:PHE:CE1	23:U1:610:LEU:HD22	2.44	0.52
17:O0:200:PHE:CE1	17:O0:211:LYS:HE2	2.43	0.52
21:S2:83:GLU:CD	21:S2:94:LYS:HZ2	2.17	0.52
21:S3:83:GLU:CD	21:S3:94:LYS:HZ3	2.17	0.52
23:U2:599:LYS:HD3	23:U2:600:LEU:N	2.25	0.52
1:00:454:ARG:HH21	1:00:466:HIS:CG	2.28	0.52
2:15:341:TYR:CZ	2:15:374:ASP:HB3	2.44	0.52
2:17:1716:GLU:H	2:17:1716:GLU:CD	2.18	0.52
2:17:1790:ARG:CA	8:E1:243:SER:N	2.73	0.52
7:D4:1195:PRO:O	23:U1:611:PHE:CE2	2.62	0.52
7:D1:1002:PRO:N	7:D4:91:PRO:HG3	2.24	0.52
7:D1:1003:VAL:N	7:D4:91:PRO:N	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U3:599:LYS:HD3	23:U3:600:LEU:N	2.25	0.52
2:17:1789:ARG:H	8:E1:244:THR:N	2.04	0.52
6:C4:1245:GLY:HA2	20:R3:1282:SER:O	2.10	0.52
21:S0:83:GLU:CD	21:S0:94:LYS:HZ2	2.17	0.52
4:A4:371:LEU:HD22	4:A4:395:GLY:HA3	1.92	0.52
5:B1:833:VAL:HG21	6:C1:1380:PRO:CD	2.40	0.52
13:K1:71:HIS:N	13:K1:83:THR:HG1	2.08	0.52
17:O0:204:GLU:H	17:O0:204:GLU:CD	2.17	0.52
18:P0:252:THR:CG2	25:W0:7:PRO:HD3	2.40	0.52
19:Q0:57:SER:HB2	25:W0:703:THR:O	2.10	0.52
1:01:708:LYS:HE2	1:01:756:TYR:CG	2.45	0.52
2:11:1716:GLU:CD	2:11:1716:GLU:H	2.18	0.52
2:17:1788:ASP:C	8:E1:244:THR:CA	2.83	0.52
13:K3:71:HIS:N	13:K3:83:THR:HG1	2.08	0.52
2:17:1791:GLY:O	8:E1:240:ALA:HB1	2.10	0.52
7:D2:1021:GLU:CD	7:D2:1051:LYS:HZ2	2.18	0.52
1:00:38:GLU:OE2	14:L0:242:VAL:CG1	2.57	0.52
1:01:454:ARG:HH21	1:01:466:HIS:CG	2.28	0.52
2:10:1824:MET:HA	8:E0:18:TRP:CB	2.31	0.52
8:E0:358:HIS:CE1	9:F1:115:ASN:ND2	2.76	0.52
23:U1:599:LYS:HD3	23:U1:600:LEU:N	2.25	0.52
1:02:454:ARG:HH21	1:02:466:HIS:CG	2.28	0.51
2:15:1055:SER:HG	2:16:1346:ILE:HD11	1.73	0.51
6:C4:1249:ILE:CG2	20:R3:1261:GLN:C	2.83	0.51
13:K2:947:GLU:CD	13:K2:947:GLU:H	2.17	0.51
23:U5:599:LYS:HD3	23:U5:600:LEU:N	2.25	0.51
10:H1:111:PRO:HD2	10:H2:250:ASN:O	2.10	0.51
23:U6:599:LYS:HD3	23:U6:600:LEU:N	2.25	0.51
1:03:708:LYS:HE2	1:03:756:TYR:CG	2.45	0.51
4:A2:675:ARG:NH2	7:D3:190:LEU:CD1	2.72	0.51
5:B1:833:VAL:HG22	6:C1:1379:PRO:CB	2.40	0.51
7:D1:1161:LEU:HD22	7:D1:1196:PHE:CE2	2.44	0.51
4:A6:371:LEU:HD22	4:A6:395:GLY:HA3	1.92	0.51
1:04:454:ARG:HH21	1:04:466:HIS:CG	2.29	0.51
7:D1:1002:PRO:CA	7:D4:91:PRO:HA	2.27	0.51
7:D1:1171:VAL:HG22	7:D1:1196:PHE:CE1	2.46	0.51
7:D3:1168:HIS:HE1	23:U5:612:SER:H	1.57	0.51
14:L0:729:GLU:HB3	14:L0:730:GLN:HG3	1.93	0.51
21:S1:83:GLU:CD	21:S1:94:LYS:HZ2	2.17	0.51
23:U4:599:LYS:HD3	23:U4:600:LEU:N	2.25	0.51
2:16:315:LEU:HD22	2:16:343:VAL:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A2:802:ARG:HH22	6:C1:1524:VAL:CG2	2.24	0.51
4:A2:760:PHE:CE1	4:A2:764:LYS:HE3	2.46	0.51
4:A4:760:PHE:CE1	4:A4:764:LYS:HE3	2.46	0.51
7:D2:1354:LEU:CB	7:D3:960:VAL:HG21	2.41	0.51
1:O1:475:ALA:HB2	14:L1:167:SER:HB2	1.93	0.51
1:O1:553:LEU:HD11	14:L1:233:ALA:HB3	1.88	0.51
2:14:1653:LYS:HB2	2:15:1565:ILE:HG21	1.92	0.51
2:17:1792:PRO:HA	8:E1:240:ALA:O	2.11	0.51
7:D1:1003:VAL:H	7:D4:92:GLU:H	1.58	0.51
7:D3:1171:VAL:HG22	7:D3:1196:PHE:CZ	2.46	0.51
13:K0:904:TRP:CH2	13:K0:908:LYS:HE3	2.46	0.51
23:U4:603:LYS:CE	23:U4:606:ASN:HD21	2.24	0.51
10:H1:185:LYS:HE2	10:H1:287:GLU:OE1	2.10	0.51
13:K2:1142:PHE:CE1	13:K3:577:PRO:CD	2.94	0.51
23:U4:606:ASN:HD22	23:U4:606:ASN:N	2.06	0.51
2:15:1074:GLN:OE1	2:16:1373:PRO:CG	2.60	0.51
6:C3:327:ALA:HB2	6:C3:366:ASP:HB2	1.93	0.51
7:D3:1171:VAL:HG22	7:D3:1196:PHE:CE1	2.46	0.51
2:14:1109:ASN:ND2	2:15:1171:ARG:HH12	2.08	0.50
4:A6:760:PHE:CE1	4:A6:764:LYS:HE3	2.46	0.50
20:R0:1244:GLU:CD	20:R0:1313:LYS:HZ3	2.18	0.50
2:10:1827:ALA:CB	8:E0:18:TRP:N	2.73	0.50
7:D0:1161:LEU:CD2	7:D0:1196:PHE:CG	2.94	0.50
2:17:1790:ARG:N	8:E1:243:SER:N	2.50	0.50
7:D2:1186:THR:CG2	23:U4:601:VAL:CB	2.88	0.50
7:D4:1108:GLU:HG2	7:D4:1114:ARG:H	1.76	0.50
13:K2:911:ARG:HD2	14:L2:912:LEU:CB	2.42	0.50
13:K2:976:LEU:HD11	14:L2:882:SER:HB3	1.94	0.50
14:L2:909:LEU:O	14:L2:913:ASP:CG	2.54	0.50
1:O0:202:GLU:CD	1:O0:202:GLU:H	2.20	0.50
2:10:1828:TYR:N	8:E0:19:ARG:HE	2.10	0.50
7:D3:674:MET:HE2	7:D3:823:PHE:CE2	2.47	0.50
14:L2:322:GLU:CD	14:L2:330:ARG:HH21	2.19	0.50
6:C2:1806:TYR:CD2	25:W0:259:LYS:HE3	2.46	0.50
7:D4:674:MET:HE2	7:D4:823:PHE:CE2	2.46	0.50
7:D0:1186:THR:HG21	23:U2:601:VAL:CB	2.31	0.50
7:D4:1185:ILE:HG22	23:U1:600:LEU:HD13	1.92	0.50
23:U3:603:LYS:CE	23:U3:606:ASN:HD21	2.25	0.50
2:17:1789:ARG:N	8:E1:244:THR:CA	2.75	0.50
6:C1:1751:LEU:HA	6:C1:1889:LEU:HD21	1.94	0.50
6:C3:722:ASN:HD21	20:R1:1255:PHE:HE1	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C3:1751:LEU:HA	6:C3:1889:LEU:HD21	1.94	0.50
7:D4:1168:HIS:CD2	23:U1:611:PHE:CD1	3.00	0.50
15:M0:788:LYS:HE3	15:M0:792:GLU:HG3	1.94	0.50
18:P1:322:ILE:HG23	25:W0:663:LYS:NZ	2.26	0.50
20:R3:224:ASP:OD2	22:T0:418:SER:N	2.44	0.50
23:U0:855:VAL:HG11	25:W0:233:SER:HA	1.93	0.50
6:C0:1370:MET:SD	6:C0:1446:LYS:HE3	2.52	0.50
6:C1:327:ALA:HB2	6:C1:366:ASP:HB2	1.94	0.50
7:D1:1008:PRO:HB3	7:D4:99:HIS:NE2	2.26	0.50
13:K2:1142:PHE:CE2	13:K3:578:ARG:HD3	2.47	0.50
1:00:708:LYS:HE2	1:00:756:TYR:CG	2.47	0.49
2:10:1828:TYR:HA	8:E0:19:ARG:HA	1.94	0.49
6:C4:1246:MET:HA	20:R3:1265:TRP:CE2	2.47	0.49
7:D5:1186:THR:HG23	23:U6:601:VAL:CA	2.40	0.49
2:10:1828:TYR:CA	8:E0:19:ARG:CG	2.88	0.49
3:41:346:THR:HG21	3:41:399:ALA:HB3	1.94	0.49
7:D0:889:ASN:CB	9:F1:103:LEU:HG	2.35	0.49
7:D4:1161:LEU:CD2	7:D4:1196:PHE:CG	2.95	0.49
7:D4:1358:CYS:HB3	20:R0:1035:ARG:HH11	1.77	0.49
23:U6:614:VAL:HG12	23:U6:615:ASN:N	2.27	0.49
4:A0:606:LYS:CE	7:D1:857:LEU:HD11	2.42	0.49
6:C2:567:GLU:OE1	15:M0:233:ARG:NH2	2.44	0.49
23:U5:603:LYS:CE	23:U5:606:ASN:HD21	2.24	0.49
23:U6:603:LYS:CE	23:U6:606:ASN:HD21	2.24	0.49
1:02:708:LYS:HE2	1:02:756:TYR:CG	2.47	0.49
5:B0:1303:TRP:CZ2	5:B0:1307:THR:HG21	2.47	0.49
7:D1:1168:HIS:HE1	23:U3:612:SER:N	2.10	0.49
7:D4:1168:HIS:HE1	23:U1:612:SER:N	2.10	0.49
15:M1:734:LYS:HE3	15:M1:735:TRP:CE2	2.47	0.49
23:U1:614:VAL:HG12	23:U1:615:ASN:N	2.28	0.49
1:00:334:ILE:HG12	14:L0:731:GLY:C	2.37	0.49
2:15:1716:GLU:CD	2:15:1716:GLU:H	2.19	0.49
6:C0:327:ALA:HB2	6:C0:366:ASP:HB2	1.94	0.49
6:C4:1695:ASP:CG	18:P3:253:GLU:CG	2.85	0.49
6:C4:1751:LEU:HA	6:C4:1889:LEU:HD21	1.94	0.49
7:D5:1105:HIS:CD2	7:D5:1106:SER:H	2.31	0.49
23:U2:614:VAL:HG12	23:U2:615:ASN:N	2.27	0.49
4:A0:558:LYS:HD2	7:D1:1031:LYS:HD3	1.94	0.49
4:A2:813:GLN:NE2	6:C0:1921:GLN:OE1	2.45	0.49
6:C0:1751:LEU:HA	6:C0:1889:LEU:HD21	1.94	0.49
6:C1:658:GLU:H	6:C1:658:GLU:CD	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C4:665:GLN:OE1	20:R3:1317:HIS:O	2.30	0.49
7:D2:1235:LEU:HD22	7:D3:736:ASN:HD21	1.76	0.49
23:U3:614:VAL:HG12	23:U3:615:ASN:N	2.27	0.49
2:10:1828:TYR:HA	8:E0:19:ARG:CA	2.43	0.49
4:A0:239:THR:HG21	7:D1:1028:GLN:C	2.38	0.49
6:C0:658:GLU:CD	6:C0:658:GLU:H	2.21	0.49
6:C1:1370:MET:SD	6:C1:1446:LYS:HE3	2.52	0.49
7:D2:1196:PHE:CG	23:U4:610:LEU:CD1	2.95	0.49
2:17:1788:ASP:CB	2:17:1788:ASP:O	2.61	0.49
4:A5:249:GLU:CD	4:A5:249:GLU:H	2.21	0.49
6:C4:327:ALA:HB2	6:C4:366:ASP:HB2	1.94	0.49
7:D1:1171:VAL:HG22	7:D1:1196:PHE:CZ	2.47	0.49
7:D3:1168:HIS:CD2	23:U5:611:PHE:CD1	3.00	0.49
23:U3:606:ASN:HD22	23:U3:606:ASN:N	2.06	0.49
7:D1:1011:LEU:HD13	7:D4:95:GLU:N	2.27	0.49
20:R3:224:ASP:CG	22:T0:417:ARG:HB3	2.38	0.49
1:00:729:LEU:HB3	14:L1:781:THR:HG21	1.95	0.49
4:A6:249:GLU:H	4:A6:249:GLU:CD	2.21	0.49
6:C4:749:THR:HG21	19:Q2:228:ASN:HB2	1.95	0.49
6:C4:1241:ASN:HA	20:R3:1258:GLU:HG2	1.95	0.49
13:K0:71:HIS:N	13:K0:83:THR:HG1	2.11	0.49
1:01:541:ARG:HH12	14:L1:597:PRO:CG	2.26	0.48
2:10:1824:MET:HB2	8:E0:18:TRP:CE2	2.47	0.48
2:17:1790:ARG:CB	8:E1:242:ILE:H	2.17	0.48
4:A0:760:PHE:CE1	4:A0:764:LYS:HE3	2.48	0.48
7:D4:1362:VAL:CG2	20:R0:1032:ASP:HB3	2.43	0.48
2:10:1826:ILE:O	2:10:1827:ALA:C	2.41	0.48
2:17:1790:ARG:CA	8:E1:244:THR:H	2.26	0.48
13:K3:908:LYS:HE2	14:L3:923:ILE:HG21	1.95	0.48
23:U5:614:VAL:HG12	23:U5:615:ASN:N	2.28	0.48
6:C0:1224:GLN:HE21	6:C0:1277:HIS:CG	2.31	0.48
5:B1:833:VAL:HG21	6:C1:1380:PRO:N	2.28	0.48
7:D1:674:MET:HE2	7:D1:823:PHE:CE2	2.48	0.48
7:D4:1185:ILE:HG21	23:U1:600:LEU:HB2	1.91	0.48
7:D5:1195:PRO:HB2	23:U6:610:LEU:HD13	1.95	0.48
1:01:475:ALA:CB	14:L1:167:SER:CB	2.91	0.48
2:15:1067:ARG:NH1	2:16:1344:SER:OG	2.36	0.48
4:A5:760:PHE:CE1	4:A5:764:LYS:HE3	2.48	0.48
6:C1:1224:GLN:HE21	6:C1:1277:HIS:CG	2.31	0.48
10:H1:198:LYS:HE2	10:H1:236:ASP:CG	2.38	0.48
17:O3:204:GLU:CD	17:O3:204:GLU:H	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C2:327:ALA:HB2	6:C2:366:ASP:HB2	1.96	0.48
13:K2:71:HIS:N	13:K2:83:THR:HG1	2.11	0.48
1:04:708:LYS:HE2	1:04:756:TYR:CG	2.48	0.48
2:10:1762:LEU:C	2:10:1762:LEU:HD12	2.38	0.48
6:C3:658:GLU:CD	6:C3:658:GLU:H	2.22	0.48
7:D0:1185:ILE:CG2	23:U2:600:LEU:HB2	2.43	0.48
7:D3:1185:ILE:CG2	23:U5:600:LEU:HD13	2.43	0.48
14:L0:736:LEU:HD13	14:L0:737:PRO:HD2	1.96	0.48
15:M1:447:LYS:HB3	18:P0:623:GLN:OE1	2.12	0.48
15:M2:788:LYS:HE3	15:M2:792:GLU:HG3	1.95	0.48
2:10:1827:ALA:HB2	8:E0:15:ASP:CA	2.41	0.48
14:L1:490:GLU:CD	14:L1:490:GLU:H	2.22	0.48
15:M1:788:LYS:HE3	15:M1:792:GLU:HG3	1.96	0.48
23:U4:614:VAL:HG12	23:U4:615:ASN:N	2.28	0.48
1:01:552:ARG:NH1	14:L1:561:GLY:HA3	2.28	0.48
2:12:1360:GLY:HA3	2:15:1051:ILE:HG21	1.96	0.48
4:A3:91:GLU:H	4:A3:92:PRO:CD	2.27	0.48
6:C2:484:HIS:CG	20:R0:1111:GLU:OE2	2.62	0.48
6:C3:1532:ASP:CG	6:C3:1556:LYS:HZ2	2.22	0.48
15:M3:575:ASN:CG	15:M3:581:ARG:HH21	2.22	0.48
2:13:559:ILE:HD12	2:13:576:CYS:SG	2.54	0.48
5:B0:166:GLU:OE2	5:B0:167:LYS:HE3	2.14	0.48
6:C2:176:GLU:OE1	7:D4:1135:ALA:HA	2.14	0.48
23:U0:823:LEU:HD12	25:W0:230:TYR:CE1	2.49	0.48
2:10:1827:ALA:C	8:E0:19:ARG:N	2.72	0.47
2:14:990:GLU:CD	2:14:993:LYS:HE3	2.39	0.47
2:14:1434:GLN:HE22	2:15:1216:LYS:HE3	1.79	0.47
12:J4:429:GLU:OE2	18:P1:326:TYR:CZ	2.67	0.47
15:M0:734:LYS:HE3	15:M0:735:TRP:CE2	2.49	0.47
1:02:607:LYS:HE3	1:02:654:PHE:CE1	2.48	0.47
2:10:990:GLU:CD	2:10:993:LYS:HE3	2.39	0.47
4:A3:760:PHE:CE1	4:A3:764:LYS:HE3	2.49	0.47
6:C2:47:LYS:HD3	7:D4:1135:ALA:H	1.79	0.47
6:C4:1224:GLN:HE21	6:C4:1277:HIS:CG	2.32	0.47
7:D1:1196:PHE:CE1	23:U3:610:LEU:HD21	2.48	0.47
2:10:1825:ILE:H	8:E0:18:TRP:CD1	2.31	0.47
6:C4:699:GLU:CD	19:Q2:248:ARG:HH22	2.23	0.47
7:D4:1161:LEU:HD22	7:D4:1196:PHE:CE2	2.49	0.47
15:M3:734:LYS:HE3	15:M3:735:TRP:CE2	2.49	0.47
2:10:1824:MET:SD	8:E0:25:ILE:HD12	2.55	0.47
2:14:1109:ASN:ND2	2:15:1171:ARG:NH1	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:17:1790:ARG:N	8:E1:243:SER:C	2.73	0.47
3:40:228:SER:HB3	7:D5:99:HIS:CE1	2.50	0.47
5:B0:1303:TRP:CH2	5:B0:1307:THR:HG21	2.50	0.47
13:K2:1142:PHE:HZ	13:K3:576:ASP:OD1	1.94	0.47
15:M2:734:LYS:HE3	15:M2:735:TRP:CE2	2.50	0.47
1:01:541:ARG:CZ	14:L1:597:PRO:HB3	2.44	0.47
1:03:607:LYS:HE3	1:03:654:PHE:CE1	2.50	0.47
2:17:559:ILE:HD12	2:17:576:CYS:SG	2.55	0.47
6:C2:1224:GLN:HE21	6:C2:1277:HIS:CD2	2.33	0.47
7:D3:1185:ILE:CG2	23:U5:600:LEU:HB2	2.45	0.47
14:L2:490:GLU:H	14:L2:490:GLU:CD	2.22	0.47
15:M0:617:LYS:HE2	15:M0:624:TYR:CD1	2.49	0.47
15:M1:549:ALA:HB1	15:M1:553:TRP:CZ3	2.49	0.47
23:U1:603:LYS:CE	23:U1:606:ASN:HD21	2.25	0.47
2:14:1109:ASN:OD1	2:15:1171:ARG:NH1	2.48	0.47
2:17:1789:ARG:N	8:E1:245:ALA:N	2.62	0.47
8:E0:12:ARG:HA	8:E0:15:ASP:HB2	1.97	0.47
1:02:202:GLU:CD	1:02:202:GLU:H	2.22	0.47
1:04:607:LYS:HE3	1:04:654:PHE:CE1	2.49	0.47
2:10:559:ILE:HD12	2:10:576:CYS:SG	2.55	0.47
2:10:1762:LEU:HD13	8:E0:156:PRO:CB	2.45	0.47
7:D0:1186:THR:HG22	23:U2:601:VAL:O	2.15	0.47
7:D2:1161:LEU:HD22	7:D2:1196:PHE:CD1	2.49	0.47
7:D2:1196:PHE:CD2	23:U4:610:LEU:CD1	2.95	0.47
7:D5:674:MET:HE2	7:D5:823:PHE:CE2	2.50	0.47
14:L3:490:GLU:H	14:L3:490:GLU:CD	2.22	0.47
2:12:922:TYR:CZ	2:13:701:ARG:NH2	2.81	0.47
2:16:559:ILE:HD12	2:16:576:CYS:SG	2.54	0.47
6:C2:1114:SER:HB3	6:C2:1281:HIS:CD2	2.49	0.47
6:C4:658:GLU:CD	6:C4:658:GLU:H	2.22	0.47
6:C4:1246:MET:SD	20:R3:1265:TRP:CZ3	3.08	0.47
7:D3:1161:LEU:CD2	7:D3:1196:PHE:CE2	2.98	0.47
2:11:1795:TYR:OH	8:E0:245:ALA:HA	2.15	0.47
2:17:340:ILE:HD13	2:17:340:ILE:H	1.80	0.47
5:B1:833:VAL:CG2	6:C1:1379:PRO:HA	2.45	0.47
6:C2:1714:GLN:HG2	6:C2:1806:TYR:CD2	2.50	0.47
7:D0:1195:PRO:C	23:U2:610:LEU:HD13	2.39	0.47
10:H3:198:LYS:HE2	10:H3:236:ASP:CG	2.40	0.47
24:V0:894:TRP:CG	24:V0:895:SER:H	2.33	0.47
1:00:378:ASN:ND2	13:K1:857:LEU:HD13	2.30	0.46
2:17:1794:PRO:C	8:E1:237:ILE:HG21	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A0:757:PHE:CE1	4:A0:761:LYS:HE3	2.51	0.46
7:D0:1186:THR:CG2	23:U2:601:VAL:CA	2.93	0.46
7:D3:1185:ILE:HG23	23:U5:600:LEU:HD13	1.96	0.46
7:D4:1196:PHE:CD1	23:U1:610:LEU:HD22	2.50	0.46
15:M2:549:ALA:HB1	15:M2:553:TRP:CZ3	2.50	0.46
18:P1:320:LYS:CE	25:W0:659:ARG:NH2	2.68	0.46
1:04:92:THR:CG2	14:L1:751:ARG:NH2	2.64	0.46
2:14:672:ILE:H	2:14:672:ILE:HD12	1.80	0.46
7:D0:1196:PHE:CG	23:U2:610:LEU:CD1	2.98	0.46
7:D3:531:ASP:HB2	7:D3:575:ARG:CZ	2.46	0.46
7:D4:1168:HIS:CE1	23:U1:611:PHE:CA	2.90	0.46
10:H0:470:GLN:HE22	11:J0:392:ILE:HG22	1.80	0.46
14:L0:490:GLU:CD	14:L0:490:GLU:H	2.22	0.46
2:10:672:ILE:H	2:10:672:ILE:HD12	1.80	0.46
4:A4:757:PHE:CE1	4:A4:761:LYS:HE3	2.50	0.46
6:C4:468:GLU:CD	20:R3:1205:ALA:HB1	2.35	0.46
7:D2:1161:LEU:CD2	7:D2:1196:PHE:CD1	2.99	0.46
7:D4:1185:ILE:HG22	23:U1:600:LEU:CA	2.44	0.46
7:D4:1358:CYS:CB	20:R0:1035:ARG:HH11	2.29	0.46
7:D5:1195:PRO:C	23:U6:610:LEU:HD13	2.39	0.46
22:T1:741:LYS:HE3	22:T1:748:GLY:HA3	1.97	0.46
2:11:559:ILE:HD12	2:11:576:CYS:SG	2.55	0.46
2:12:672:ILE:HD12	2:12:672:ILE:H	1.80	0.46
5:B1:833:VAL:HG21	6:C1:1379:PRO:HA	1.97	0.46
6:C3:1224:GLN:HE21	6:C3:1277:HIS:CG	2.32	0.46
7:D4:1161:LEU:HD21	7:D4:1196:PHE:CG	2.51	0.46
8:E0:21:LEU:HG	8:E0:21:LEU:O	2.15	0.46
20:R3:1258:GLU:CD	20:R3:1258:GLU:H	2.23	0.46
1:00:607:LYS:HE3	1:00:654:PHE:CE1	2.49	0.46
1:01:24:GLN:NE2	14:L1:473:ASP:N	2.52	0.46
1:01:24:GLN:HE21	14:L1:473:ASP:H	1.57	0.46
2:11:672:ILE:HD12	2:11:672:ILE:H	1.80	0.46
2:17:1788:ASP:C	8:E1:243:SER:O	2.59	0.46
6:C4:1765:GLN:HE21	6:C4:1899:THR:HG23	1.81	0.46
7:D0:234:CYS:SG	7:D0:258:LYS:HE3	2.55	0.46
7:D3:1196:PHE:CZ	23:U5:610:LEU:HD22	2.49	0.46
20:R0:1248:PHE:CD1	20:R0:1313:LYS:HE3	2.51	0.46
23:U5:614:VAL:HG12	23:U5:615:ASN:O	2.16	0.46
1:01:24:GLN:HE22	14:L1:473:ASP:N	2.11	0.46
2:10:1830:THR:C	8:E0:19:ARG:HD3	2.41	0.46
2:13:672:ILE:HD12	2:13:672:ILE:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A0:371:LEU:C	4:A0:371:LEU:HD23	2.41	0.46
4:A2:243:LYS:HZ1	7:D3:1029:ARG:HA	1.77	0.46
4:A4:249:GLU:CD	4:A4:249:GLU:H	2.23	0.46
4:A4:753:MET:HE1	4:A4:789:ALA:HB1	1.97	0.46
6:C2:47:LYS:HD2	7:D4:1135:ALA:HB2	1.98	0.46
6:C3:722:ASN:ND2	20:R1:1255:PHE:CE1	2.81	0.46
7:D2:234:CYS:SG	7:D2:258:LYS:HE3	2.55	0.46
7:D4:813:GLU:CD	7:D4:813:GLU:H	2.24	0.46
23:U0:827:TRP:CE3	23:U0:838:LYS:HE2	2.51	0.46
1:00:334:ILE:HB	1:00:337:GLU:OE2	2.16	0.46
2:12:559:ILE:HD12	2:12:576:CYS:SG	2.55	0.46
2:15:559:ILE:HD12	2:15:576:CYS:SG	2.56	0.46
2:16:990:GLU:CD	2:16:993:LYS:HE3	2.41	0.46
4:A1:760:PHE:CE1	4:A1:764:LYS:HE3	2.50	0.46
4:A3:757:PHE:CE1	4:A3:761:LYS:HE3	2.50	0.46
4:A6:757:PHE:CE1	4:A6:761:LYS:HE3	2.51	0.46
7:D0:1161:LEU:CD2	7:D0:1196:PHE:CD1	2.98	0.46
7:D2:1161:LEU:HD22	7:D2:1196:PHE:CE1	2.51	0.46
7:D3:1161:LEU:CD2	7:D3:1196:PHE:CG	2.98	0.46
7:D5:1161:LEU:HD22	7:D5:1196:PHE:CD1	2.51	0.46
23:U4:614:VAL:HG12	23:U4:615:ASN:O	2.16	0.46
2:16:1012:LYS:HE3	2:16:1013:TYR:CE1	2.51	0.46
4:A2:240:ASP:HB3	7:D3:1029:ARG:HH11	1.80	0.46
6:C2:787:PHE:N	17:O0:256:GLU:OE2	2.49	0.46
7:D0:1161:LEU:HD22	7:D0:1196:PHE:CD1	2.51	0.46
2:10:1012:LYS:HE3	2:10:1013:TYR:CE1	2.50	0.46
2:12:990:GLU:CD	2:12:993:LYS:HE3	2.41	0.46
2:16:672:ILE:HD12	2:16:672:ILE:H	1.81	0.46
2:17:672:ILE:HD12	2:17:672:ILE:H	1.81	0.46
4:A1:371:LEU:C	4:A1:371:LEU:HD23	2.41	0.46
4:A2:103:LYS:HE2	4:A2:107:ASP:OD2	2.16	0.46
5:B1:188:TRP:HH2	6:C1:3:THR:HG23	1.81	0.46
7:D3:1168:HIS:CD2	23:U5:611:PHE:HD1	2.34	0.46
23:U5:611:PHE:O	23:U5:612:SER:HB2	2.16	0.46
2:15:672:ILE:HD12	2:15:672:ILE:H	1.81	0.46
2:17:1012:LYS:HE3	2:17:1013:TYR:CE1	2.50	0.46
4:A3:371:LEU:HD23	4:A3:371:LEU:C	2.41	0.46
7:D2:1186:THR:HG22	23:U4:601:VAL:O	2.16	0.46
7:D4:1185:ILE:HG22	23:U1:600:LEU:HA	1.97	0.46
15:M3:549:ALA:HB1	15:M3:553:TRP:CZ3	2.50	0.46
20:R0:1021:LEU:C	20:R0:1021:LEU:HD23	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R3:295:HIS:NE2	22:T0:413:PRO:HA	2.30	0.46
22:T0:741:LYS:HE3	22:T0:748:GLY:HA3	1.97	0.46
2:10:1824:MET:CG	8:E0:18:TRP:CZ2	2.98	0.45
4:A0:138:GLU:HA	6:C0:1992:ARG:NH1	2.31	0.45
4:A2:371:LEU:C	4:A2:371:LEU:HD23	2.41	0.45
6:C3:722:ASN:ND2	20:R1:1255:PHE:HE1	2.14	0.45
7:D1:1002:PRO:C	7:D4:91:PRO:HB2	2.34	0.45
7:D1:1196:PHE:CD1	23:U3:610:LEU:HD22	2.51	0.45
7:D5:1161:LEU:CD2	7:D5:1196:PHE:CD1	2.99	0.45
13:K3:346:LYS:HE2	13:K3:407:LEU:O	2.17	0.45
23:U1:611:PHE:O	23:U1:612:SER:HB2	2.16	0.45
2:10:1830:THR:HG22	8:E0:309:GLU:O	2.16	0.45
4:A5:141:LYS:HE3	6:C3:1992:ARG:HH11	1.80	0.45
7:D4:1195:PRO:O	23:U1:611:PHE:HE2	1.99	0.45
13:K0:346:LYS:HE2	13:K0:407:LEU:O	2.16	0.45
13:K0:506:THR:HG23	13:K0:509:LYS:HE3	1.98	0.45
13:K1:346:LYS:HE2	13:K1:407:LEU:O	2.16	0.45
15:M0:549:ALA:HB1	15:M0:553:TRP:CZ3	2.51	0.45
20:R0:802:LEU:HD11	20:R0:915:ARG:HH21	1.80	0.45
23:U1:614:VAL:HG12	23:U1:615:ASN:O	2.16	0.45
7:D1:1161:LEU:CD2	7:D1:1196:PHE:CE2	2.99	0.45
7:D5:813:GLU:CD	7:D5:813:GLU:H	2.25	0.45
15:M2:526:PRO:HB2	15:M2:582:TYR:CE1	2.51	0.45
2:10:1824:MET:HB3	8:E0:22:GLY:HA3	1.99	0.45
3:40:346:THR:HG21	3:40:399:ALA:HB3	1.98	0.45
6:C4:658:GLU:HB3	20:R3:1252:LYS:HE2	1.99	0.45
7:D1:1002:PRO:CB	7:D4:91:PRO:CA	2.94	0.45
2:11:1012:LYS:HE3	2:11:1013:TYR:CE1	2.52	0.45
7:D3:1196:PHE:CD1	23:U5:610:LEU:HD22	2.51	0.45
7:D5:1161:LEU:HD22	7:D5:1196:PHE:CE1	2.52	0.45
14:L0:326:ASP:N	15:M0:477:ARG:HE	2.14	0.45
15:M1:447:LYS:CB	18:P0:623:GLN:OE1	2.64	0.45
15:M2:617:LYS:HE2	15:M2:624:TYR:CD1	2.52	0.45
18:P3:415:SER:HB2	19:Q3:12:LYS:HE3	1.99	0.45
18:P3:534:ARG:HE	18:P3:568:ILE:HG23	1.81	0.45
23:U6:614:VAL:HG12	23:U6:615:ASN:O	2.17	0.45
24:V0:735:GLU:CD	24:V0:735:GLU:N	2.74	0.45
2:10:1796:GLY:H	8:E0:69:TYR:CB	2.28	0.45
5:B1:166:GLU:OE2	5:B1:167:LYS:HE3	2.16	0.45
7:D1:1004:LEU:H	7:D4:91:PRO:HB2	1.80	0.45
7:D4:1168:HIS:CD2	23:U1:611:PHE:HD1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K2:1142:PHE:CZ	13:K3:578:ARG:CD	3.00	0.45
13:K3:908:LYS:HD3	14:L3:925:LEU:HD11	1.98	0.45
15:M2:514:GLU:CD	15:M2:514:GLU:H	2.25	0.45
1:00:708:LYS:HE2	1:00:756:TYR:CD1	2.52	0.45
1:04:708:LYS:HE2	1:04:756:TYR:CD1	2.52	0.45
4:A5:757:PHE:CE1	4:A5:761:LYS:HE3	2.52	0.45
7:D1:1001:PRO:HG2	7:D1:1002:PRO:HD3	1.98	0.45
11:I0:312:LYS:HZ1	12:J0:392:GLU:CD	2.24	0.45
18:P0:415:SER:HB2	19:Q0:12:LYS:HE3	1.99	0.45
23:U3:614:VAL:HG12	23:U3:615:ASN:O	2.16	0.45
1:01:708:LYS:HE2	1:01:756:TYR:CD1	2.51	0.45
6:C2:469:PRO:CB	20:R0:1113:ARG:HH11	2.27	0.45
7:D0:1195:PRO:HB2	23:U2:610:LEU:HD13	1.97	0.45
4:A2:138:GLU:HA	6:C1:1992:ARG:NH1	2.32	0.45
4:A6:753:MET:HE1	4:A6:789:ALA:HB1	1.97	0.45
6:C2:1532:ASP:CG	6:C2:1556:LYS:HZ2	2.25	0.45
14:L2:164:LYS:HZ2	14:L2:176:GLU:CD	2.25	0.45
17:O1:36:VAL:HG23	17:O1:55:THR:HG21	1.99	0.45
23:U6:606:ASN:HD22	23:U6:606:ASN:N	2.06	0.45
3:41:315:GLU:CD	3:41:361:ARG:HH22	2.24	0.44
4:A0:249:GLU:CD	4:A0:249:GLU:H	2.26	0.44
6:C2:1807:TRP:CZ2	25:W0:259:LYS:HD3	2.52	0.44
10:H2:198:LYS:HE2	10:H2:236:ASP:CG	2.42	0.44
18:P2:541:TYR:CE1	18:P2:573:PHE:CZ	3.05	0.44
24:V0:780:GLU:CD	24:V0:783:ARG:HE	2.25	0.44
1:02:708:LYS:HE2	1:02:756:TYR:CD1	2.52	0.44
2:10:1827:ALA:HB1	8:E0:16:ILE:C	2.42	0.44
16:N0:237:ASP:O	16:N0:260:LYS:HE2	2.17	0.44
17:O3:36:VAL:HG23	17:O3:55:THR:HG21	1.99	0.44
18:P3:627:ILE:HG22	18:P3:631:LYS:HE3	1.99	0.44
20:R3:1265:TRP:CZ2	20:R3:1284:ALA:HA	2.53	0.44
23:U6:606:ASN:C	23:U6:607:ASN:HD22	2.26	0.44
1:03:708:LYS:HE2	1:03:756:TYR:CD1	2.52	0.44
6:C1:1461:LYS:HE2	6:C1:1465:GLU:OE1	2.17	0.44
7:D2:1195:PRO:C	23:U4:610:LEU:HD13	2.42	0.44
7:D4:1171:VAL:HG22	7:D4:1196:PHE:CE1	2.52	0.44
17:O2:36:VAL:HG23	17:O2:55:THR:HG21	1.99	0.44
23:U2:614:VAL:HG12	23:U2:615:ASN:O	2.16	0.44
1:03:634:HIS:CD2	14:L1:286:ASP:OD2	2.70	0.44
4:A0:558:LYS:HD2	7:D1:1031:LYS:CD	2.48	0.44
4:A4:371:LEU:C	4:A4:371:LEU:HD23	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C1:1461:LYS:HE2	6:C1:1465:GLU:CD	2.42	0.44
7:D4:1161:LEU:HD22	7:D4:1196:PHE:CD1	2.52	0.44
7:D4:1168:HIS:CE1	23:U1:612:SER:N	2.85	0.44
23:U3:611:PHE:O	23:U3:612:SER:HB2	2.17	0.44
4:A2:243:LYS:CE	7:D3:1028:GLN:O	2.66	0.44
4:A5:371:LEU:C	4:A5:371:LEU:HD23	2.42	0.44
7:D3:1168:HIS:HE1	23:U5:612:SER:N	2.16	0.44
7:D4:90:PRO:HD3	7:D4:126:TRP:CD1	2.52	0.44
7:D5:1196:PHE:CG	23:U6:610:LEU:CD1	2.99	0.44
2:10:1824:MET:HE3	8:E0:17:LEU:O	2.18	0.44
4:A0:558:LYS:CG	7:D1:1031:LYS:NZ	2.78	0.44
4:A2:249:GLU:H	4:A2:249:GLU:CD	2.25	0.44
7:D2:1354:LEU:CG	7:D3:960:VAL:HG21	2.47	0.44
13:K2:1142:PHE:HE1	13:K3:577:PRO:CD	2.30	0.44
4:A3:249:GLU:CD	4:A3:249:GLU:H	2.26	0.44
6:C0:1461:LYS:HE2	6:C0:1465:GLU:CD	2.42	0.44
7:D4:1107:THR:HB	7:D4:1108:GLU:O	2.17	0.44
7:D4:1161:LEU:CD2	7:D4:1196:PHE:CE2	3.01	0.44
7:D5:234:CYS:SG	7:D5:258:LYS:HE3	2.58	0.44
18:P2:389:SER:HA	18:P2:390:HIS:C	2.43	0.44
2:10:1824:MET:CB	8:E0:18:TRP:CZ2	2.99	0.44
4:A2:18:ALA:CB	11:I2:303:ARG:HE	2.30	0.44
4:A5:103:LYS:HE2	4:A5:107:ASP:OD2	2.18	0.44
4:A6:371:LEU:C	4:A6:371:LEU:HD23	2.43	0.44
7:D3:1168:HIS:CE1	23:U5:611:PHE:CA	2.91	0.44
7:D4:1108:GLU:O	7:D4:1111:LEU:HA	2.18	0.44
1:00:332:LYS:HB3	14:L0:731:GLY:H	1.83	0.44
2:10:1819:ALA:O	2:10:1820:GLY:O	2.36	0.44
2:10:1825:ILE:N	8:E0:18:TRP:NE1	2.66	0.44
2:11:1177:MET:H	2:12:1106:PRO:HB3	1.82	0.44
2:17:1790:ARG:H	8:E1:243:SER:CA	2.29	0.44
7:D1:1161:LEU:CD2	7:D1:1196:PHE:CG	3.01	0.44
7:D4:1108:GLU:CA	7:D4:1114:ARG:HB2	2.46	0.44
14:L0:729:GLU:C	14:L0:730:GLN:CG	2.91	0.44
1:01:607:LYS:HE3	1:01:654:PHE:CE1	2.52	0.43
2:13:1360:GLY:CA	2:16:1105:GLN:OE1	2.66	0.43
2:17:990:GLU:CD	2:17:993:LYS:HE3	2.43	0.43
2:17:1790:ARG:HA	8:E1:243:SER:N	2.33	0.43
6:C2:47:LYS:NZ	6:C2:173:PHE:CD2	2.83	0.43
6:C2:482:VAL:HG12	20:R0:1111:GLU:O	2.18	0.43
6:C2:486:ARG:HH22	20:R0:1156:ALA:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D2:809:GLU:CD	7:D2:847:ARG:HH12	2.26	0.43
15:M2:585:SER:N	15:M2:586:PRO:HD2	2.33	0.43
20:R1:1018:TYR:O	20:R1:1022:THR:HG23	2.18	0.43
6:C2:484:HIS:CG	20:R0:1107:ARG:HH21	2.36	0.43
7:D0:1161:LEU:HD22	7:D0:1196:PHE:CE1	2.52	0.43
20:R0:1106:MET:HE3	20:R0:1144:GLN:HE22	1.82	0.43
20:R1:802:LEU:HD11	20:R1:915:ARG:HH21	1.83	0.43
4:A0:18:ALA:CB	11:I0:303:ARG:HE	2.31	0.43
7:D0:889:ASN:HB2	9:F1:103:LEU:CG	2.38	0.43
7:D4:1161:LEU:CD2	7:D4:1196:PHE:CD2	3.01	0.43
14:L1:502:LYS:CE	16:N0:175:LYS:HE2	2.48	0.43
23:U4:606:ASN:C	23:U4:607:ASN:HD22	2.26	0.43
1:01:541:ARG:NH1	14:L1:597:PRO:CB	2.65	0.43
2:10:1827:ALA:HB1	8:E0:16:ILE:N	2.33	0.43
2:17:1790:ARG:CB	8:E1:242:ILE:N	2.79	0.43
4:A0:450:GLU:HG2	4:A0:462:TYR:CE2	2.54	0.43
4:A1:249:GLU:CD	4:A1:249:GLU:H	2.26	0.43
4:A4:124:MET:HE1	6:C2:1562:ARG:NH1	2.34	0.43
5:B1:832:ASN:C	5:B1:833:VAL:HG23	2.43	0.43
7:D4:950:TYR:CE2	7:D4:1037:ILE:HD13	2.54	0.43
13:K2:346:LYS:HE2	13:K2:407:LEU:O	2.17	0.43
1:03:4:SER:HB3	18:P0:620:GLU:OE1	2.19	0.43
2:14:1106:PRO:CA	2:15:1177:MET:HG3	2.49	0.43
4:A3:746:SER:HB2	4:A3:807:THR:HG21	2.00	0.43
6:C4:697:ARG:HA	19:Q2:248:ARG:HD3	1.99	0.43
7:D1:234:CYS:SG	7:D1:258:LYS:HE3	2.58	0.43
14:L1:502:LYS:HZ3	16:N0:175:LYS:HE3	1.82	0.43
17:O0:36:VAL:HG23	17:O0:55:THR:HG21	2.00	0.43
20:R3:295:HIS:CE1	22:T0:413:PRO:HA	2.53	0.43
2:10:1752:LEU:CD2	2:11:1790:ARG:HH21	2.24	0.43
5:B1:833:VAL:HG21	6:C1:1379:PRO:CA	2.48	0.43
6:C2:787:PHE:O	17:O0:256:GLU:OE2	2.36	0.43
7:D2:1195:PRO:HB2	23:U4:610:LEU:HD13	2.00	0.43
2:17:1789:ARG:N	8:E1:246:MET:H	2.17	0.43
2:17:1795:TYR:N	8:E1:237:ILE:HG21	2.34	0.43
7:D4:865:LEU:C	7:D4:867:TYR:H	2.27	0.43
10:H3:458:ASP:CG	10:H3:461:ARG:HH21	2.26	0.43
13:K2:151:TRP:CH2	13:K2:179:THR:HB	2.54	0.43
15:M3:526:PRO:HB2	15:M3:582:TYR:CE1	2.53	0.43
1:00:334:ILE:C	14:L0:730:GLN:HB3	2.43	0.43
10:H2:470:GLN:HE22	11:I2:392:ILE:HG22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L1:803:LYS:HE2	14:L1:807:ASP:OD2	2.19	0.43
2:10:1830:THR:HG23	8:E0:19:ARG:NH1	2.34	0.43
2:17:1788:ASP:O	8:E1:246:MET:N	2.52	0.43
4:A1:757:PHE:CE1	4:A1:761:LYS:HE3	2.54	0.43
6:C0:911:GLU:HG2	6:C0:979:ILE:HD13	2.01	0.43
8:E0:73:TYR:CE2	8:E0:134:VAL:HG11	2.54	0.43
23:U4:610:LEU:O	23:U4:612:SER:N	2.51	0.43
1:02:161:ARG:C	1:02:163:ASP:H	2.27	0.43
2:17:1790:ARG:C	8:E1:240:ALA:C	2.87	0.43
6:C4:749:THR:CB	19:Q2:228:ASN:HB2	2.49	0.43
10:H0:470:GLN:NE2	11:I0:392:ILE:HG22	2.33	0.43
2:10:1824:MET:HE2	8:E0:25:ILE:HD12	2.00	0.42
2:13:990:GLU:CD	2:13:993:LYS:HE3	2.43	0.42
7:D3:813:GLU:H	7:D3:813:GLU:CD	2.27	0.42
9:F0:234:GLU:N	9:F0:234:GLU:CD	2.77	0.42
6:C2:658:GLU:H	6:C2:658:GLU:CD	2.27	0.42
7:D1:890:LYS:HE2	7:D1:894:GLU:OE2	2.19	0.42
7:D4:1363:GLU:CD	20:R0:1006:LYS:HE3	2.43	0.42
9:F1:234:GLU:N	9:F1:234:GLU:CD	2.77	0.42
18:P1:627:ILE:HG22	18:P1:631:LYS:HE3	2.01	0.42
20:R1:526:GLU:CD	20:R1:530:LYS:HZ2	2.27	0.42
1:01:11:TYR:HE2	14:L1:245:VAL:HG13	1.83	0.42
6:C2:1739:GLU:HA	6:C2:1742:LYS:HE3	2.02	0.42
7:D1:1003:VAL:CG1	7:D4:92:GLU:HB2	2.50	0.42
14:L1:560:LEU:C	14:L1:562:LEU:H	2.26	0.42
15:M1:338:PRO:HG3	15:M1:372:TRP:CH2	2.54	0.42
2:17:1790:ARG:HG3	8:E1:243:SER:CB	2.50	0.42
5:B0:14:ARG:HH22	5:B0:100:ASP:CG	2.28	0.42
6:C2:180:GLN:NE2	6:C2:180:GLN:HA	2.34	0.42
7:D0:811:GLN:OE1	9:F1:131:GLY:HA2	2.18	0.42
7:D1:1185:ILE:HG23	23:U3:600:LEU:HD13	2.02	0.42
12:J4:381:LYS:HE2	12:J4:385:ASP:OD2	2.20	0.42
15:M0:526:PRO:HB2	15:M0:582:TYR:CE1	2.54	0.42
15:M3:338:PRO:HG3	15:M3:372:TRP:CH2	2.55	0.42
18:P1:322:ILE:O	25:W0:663:LYS:HE2	2.19	0.42
18:P2:415:SER:HB2	19:Q2:12:LYS:HE3	2.00	0.42
20:R1:1258:GLU:CD	20:R1:1258:GLU:H	2.28	0.42
1:01:476:PRO:HD2	1:01:552:ARG:NH2	2.35	0.42
2:10:1825:ILE:H	8:E0:18:TRP:NE1	2.16	0.42
3:40:315:GLU:CD	3:40:361:ARG:HH22	2.27	0.42
6:C1:911:GLU:HG2	6:C1:979:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C2:281:ILE:HG23	6:C2:284:ILE:HD12	2.01	0.42
10:H0:185:LYS:HE2	10:H0:287:GLU:OE2	2.19	0.42
10:H2:470:GLN:NE2	11:I2:392:ILE:HG22	2.34	0.42
12:J2:339:LYS:CE	12:J2:343:GLU:OE1	2.68	0.42
13:K2:1146:ALA:HA	13:K3:595:LEU:HD13	2.01	0.42
20:R3:924:GLN:HE22	21:S3:20:HIS:CE1	2.37	0.42
1:00:334:ILE:HA	14:L0:730:GLN:CB	2.45	0.42
6:C2:620:GLU:OE1	20:R0:1252:LYS:HE3	2.19	0.42
7:D1:1161:LEU:HD21	7:D1:1196:PHE:CG	2.54	0.42
21:S0:169:MET:SD	21:S0:186:LYS:HE3	2.59	0.42
23:U3:606:ASN:C	23:U3:607:ASN:HD22	2.27	0.42
23:U5:606:ASN:C	23:U5:607:ASN:HD22	2.26	0.42
2:17:1792:PRO:HD3	8:E1:244:THR:CG2	2.50	0.42
2:17:1795:TYR:O	8:E1:237:ILE:HG22	2.19	0.42
2:17:1829:HIS:CD2	8:E1:7:ARG:HH21	2.27	0.42
4:A1:735:ARG:NH2	7:D1:1253:LYS:HZ1	2.18	0.42
4:A5:138:GLU:HA	6:C3:1992:ARG:NH1	2.34	0.42
7:D3:1161:LEU:CD2	7:D3:1196:PHE:CD2	3.02	0.42
13:K3:979:LEU:CD1	14:L3:889:TYR:CD2	3.03	0.42
18:P0:252:THR:HG21	25:W0:7:PRO:HD3	2.00	0.42
4:A2:655:ALA:HA	6:C0:1933:SER:H	1.85	0.42
4:A6:746:SER:HB2	4:A6:807:THR:HG21	2.02	0.42
6:C1:414:ALA:HB1	6:C1:509:ILE:HD11	2.02	0.42
6:C2:620:GLU:CD	20:R0:1252:LYS:HE3	2.45	0.42
7:D1:684:VAL:HG23	7:D1:686:ARG:HE	1.84	0.42
7:D5:1105:HIS:CG	7:D5:1106:SER:N	2.88	0.42
1:00:547:ASN:HD21	14:L0:234:LEU:HD22	1.85	0.42
2:10:1793:GLY:C	2:10:1795:TYR:H	2.27	0.42
2:10:1795:TYR:C	2:10:1797:ALA:H	2.28	0.42
2:11:990:GLU:CD	2:11:993:LYS:HE3	2.44	0.42
2:15:990:GLU:CD	2:15:993:LYS:HE3	2.45	0.42
2:17:1789:ARG:N	8:E1:244:THR:C	2.77	0.42
4:A5:753:MET:HE1	4:A5:789:ALA:HB1	2.01	0.42
5:B1:326:TRP:CZ2	5:B1:330:ARG:HD3	2.55	0.42
5:B1:1303:TRP:CZ2	5:B1:1307:THR:HG21	2.54	0.42
6:C3:1249:ILE:CG2	20:R1:1261:GLN:C	2.93	0.42
10:H0:198:LYS:HE2	10:H0:236:ASP:CG	2.44	0.42
18:P2:627:ILE:HG22	18:P2:631:LYS:HE3	2.01	0.42
23:U1:606:ASN:C	23:U1:607:ASN:HD22	2.27	0.42
4:A0:103:LYS:HE2	4:A0:107:ASP:OD2	2.20	0.42
4:A2:243:LYS:NZ	7:D3:1029:ARG:CA	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C4:1461:LYS:HE2	6:C4:1465:GLU:OE2	2.19	0.42
7:D1:1003:VAL:N	7:D4:92:GLU:N	2.67	0.42
7:D3:1161:LEU:HD21	7:D3:1196:PHE:CG	2.55	0.42
7:D5:1309:SER:O	21:S2:276:MET:SD	2.78	0.42
12:J0:339:LYS:CE	12:J0:343:GLU:OE1	2.68	0.42
14:L1:414:MET:SD	15:M1:480:LEU:HD11	2.59	0.42
14:L3:803:LYS:HE2	14:L3:807:ASP:OD2	2.19	0.42
15:M1:514:GLU:CD	15:M1:514:GLU:H	2.27	0.42
1:00:334:ILE:HB	1:00:337:GLU:OE1	2.20	0.41
2:10:1825:ILE:O	2:10:1828:TYR:HB2	2.20	0.41
7:D1:922:GLN:HE22	7:D4:427:ASP:HB3	1.84	0.41
7:D1:1004:LEU:N	7:D4:91:PRO:HB2	2.35	0.41
7:D5:950:TYR:CE2	7:D5:1037:ILE:HD13	2.54	0.41
11:I1:392:ILE:HD12	12:J1:478:LEU:HD22	2.02	0.41
14:L0:329:ILE:O	14:L0:332:LYS:HE2	2.20	0.41
20:R1:924:GLN:HE22	21:S1:20:HIS:CE1	2.38	0.41
2:10:1823:VAL:O	8:E0:18:TRP:CD1	2.71	0.41
4:A0:302:PRO:O	7:D2:851:ALA:CB	2.69	0.41
4:A4:141:LYS:CE	6:C2:1992:ARG:HH11	2.27	0.41
6:C2:1751:LEU:HA	6:C2:1889:LEU:HD21	2.02	0.41
6:C4:689:VAL:HG13	6:C4:693:GLU:CD	2.45	0.41
7:D4:234:CYS:SG	7:D4:258:LYS:HE3	2.59	0.41
13:K1:261:SER:C	13:K1:263:PHE:HA	2.45	0.41
14:L1:164:LYS:HZ2	14:L1:176:GLU:CD	2.27	0.41
15:M3:514:GLU:H	15:M3:514:GLU:CD	2.28	0.41
19:Q0:61:PHE:CE2	24:V0:905:SER:CB	2.98	0.41
2:15:1434:GLN:NE2	2:16:1216:LYS:HD3	2.35	0.41
6:C4:47:LYS:HZ2	6:C4:176:GLU:CD	2.28	0.41
7:D0:1388:GLU:CG	7:D1:959:ILE:HD12	2.50	0.41
13:K0:942:ASN:OD1	14:L0:905:ARG:NH1	2.54	0.41
13:K3:261:SER:C	13:K3:263:PHE:HA	2.46	0.41
14:L0:712:PHE:CE2	14:L0:747:HIS:CE1	3.08	0.41
14:L3:498:ALA:HB2	15:M2:798:GLU:HG2	2.01	0.41
15:M0:250:LYS:HE2	16:N0:236:GLN:CG	2.50	0.41
16:N2:237:ASP:O	16:N2:260:LYS:HE2	2.20	0.41
2:15:1434:GLN:HE22	2:16:1216:LYS:HD3	1.84	0.41
4:A4:760:PHE:CZ	4:A4:818:MET:HA	2.55	0.41
6:C0:1526:VAL:HG13	6:C0:1578:VAL:HA	2.02	0.41
6:C2:179:GLU:OE2	7:D4:1133:SER:HB2	2.21	0.41
7:D3:1186:THR:CG2	23:U5:601:VAL:CA	2.98	0.41
9:F0:172:ASP:OD2	9:F0:218:LYS:HE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K3:151:TRP:CH2	13:K3:179:THR:HB	2.55	0.41
14:L0:803:LYS:HE2	14:L0:807:ASP:OD2	2.20	0.41
14:L2:803:LYS:HE2	14:L2:807:ASP:OD2	2.21	0.41
2:10:1795:TYR:OH	8:E0:135:ILE:HA	2.21	0.41
2:17:1462:GLU:C	2:17:1464:PRO:HD3	2.46	0.41
3:40:280:VAL:HG13	8:E0:207:ARG:HH12	1.86	0.41
6:C0:911:GLU:CG	6:C0:979:ILE:HD13	2.50	0.41
7:D5:1186:THR:HG22	23:U6:601:VAL:O	2.20	0.41
7:D5:1362:VAL:HG11	20:R2:1036:GLN:OE1	2.19	0.41
13:K0:261:SER:C	13:K0:263:PHE:HA	2.45	0.41
15:M1:761:GLU:CD	15:M1:766:CYS:HB3	2.45	0.41
20:R3:1258:GLU:CD	20:R3:1258:GLU:N	2.78	0.41
2:10:1823:VAL:O	8:E0:18:TRP:CG	2.73	0.41
2:10:1827:ALA:C	8:E0:19:ARG:CG	2.94	0.41
4:A2:141:LYS:HE3	6:C1:1992:ARG:HH11	1.85	0.41
5:B0:326:TRP:CZ2	5:B0:330:ARG:HD3	2.55	0.41
6:C1:911:GLU:CG	6:C1:979:ILE:HD13	2.50	0.41
7:D0:1184:ASP:HB3	23:U2:597:ILE:N	2.34	0.41
13:K0:962:ARG:NH2	14:L0:924:GLN:OE1	2.54	0.41
13:K2:911:ARG:CD	14:L2:912:LEU:HB3	2.48	0.41
14:L3:712:PHE:CE2	14:L3:747:HIS:CE1	3.09	0.41
20:R0:526:GLU:CD	20:R0:530:LYS:HZ2	2.27	0.41
23:U0:803:LEU:HD12	23:U0:803:LEU:N	2.36	0.41
1:02:454:ARG:HH21	1:02:466:HIS:CD2	2.39	0.41
2:10:1827:ALA:C	8:E0:19:ARG:HA	2.37	0.41
2:15:1462:GLU:C	2:15:1464:PRO:HD3	2.45	0.41
2:16:1462:GLU:HB2	2:16:1463:HIS:CD2	2.56	0.41
2:17:1790:ARG:HB2	8:E1:241:TRP:N	2.36	0.41
2:17:1790:ARG:C	8:E1:244:THR:H	2.29	0.41
6:C3:327:ALA:HB2	6:C3:366:ASP:CB	2.51	0.41
6:C3:1461:LYS:HE2	6:C3:1465:GLU:OE2	2.20	0.41
7:D3:234:CYS:SG	7:D3:258:LYS:HE3	2.60	0.41
7:D5:1184:ASP:HB3	23:U6:597:ILE:N	2.35	0.41
12:J3:339:LYS:CE	12:J3:343:GLU:OE1	2.68	0.41
13:K1:151:TRP:CH2	13:K1:179:THR:HB	2.56	0.41
23:U2:610:LEU:HA	23:U2:610:LEU:HD12	1.86	0.41
2:10:1825:ILE:O	2:10:1828:TYR:CB	2.69	0.41
2:10:1830:THR:N	8:E0:19:ARG:HD3	2.33	0.41
2:14:1012:LYS:HE3	2:14:1013:TYR:CE1	2.56	0.41
5:B0:977:PRO:HA	5:B0:978:PRO:HD3	1.97	0.41
5:B1:1052:LYS:HE2	5:B1:1117:HIS:HD1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C0:414:ALA:HB1	6:C0:509:ILE:HD11	2.02	0.41
7:D1:813:GLU:CD	7:D1:813:GLU:H	2.29	0.41
2:10:1795:TYR:CD1	8:E0:69:TYR:CD2	3.09	0.41
2:10:1795:TYR:CE1	8:E0:69:TYR:CD2	3.09	0.41
2:10:1799:LEU:HD22	2:10:1800:PHE:CD2	2.56	0.41
2:10:1827:ALA:CB	8:E0:19:ARG:N	2.77	0.41
2:11:1462:GLU:C	2:11:1464:PRO:HD3	2.46	0.41
2:14:783:ARG:HH22	2:14:894:ASP:CG	2.28	0.41
4:A1:450:GLU:HG2	4:A1:462:TYR:CE2	2.56	0.41
4:A2:287:PRO:HB2	8:E0:655:ALA:HB1	2.01	0.41
4:A2:327:ARG:HE	4:A2:412:ASP:CG	2.29	0.41
4:A4:114:ILE:CD1	6:C2:1494:MET:HE3	2.51	0.41
4:A4:138:GLU:HA	6:C2:1992:ARG:NH1	2.36	0.41
4:A6:760:PHE:CZ	4:A6:818:MET:HA	2.55	0.41
5:B0:127:ASP:CG	5:B0:202:ARG:HH22	2.29	0.41
5:B1:833:VAL:HG22	6:C1:1379:PRO:HB3	2.02	0.41
6:C3:865:ASP:CG	6:C3:868:ARG:HH21	2.29	0.41
6:C3:1695:ASP:HB2	18:P1:253:GLU:CD	2.46	0.41
6:C4:699:GLU:CG	19:Q2:248:ARG:NH1	2.77	0.41
9:F3:234:GLU:CD	9:F3:234:GLU:N	2.79	0.41
13:K0:908:LYS:HE2	13:K0:908:LYS:O	2.20	0.41
14:L1:305:LYS:HE2	15:M1:510:PHE:CD1	2.56	0.41
15:M0:649:TRP:HE1	15:M0:665:GLU:CD	2.29	0.41
20:R1:1106:MET:HE3	20:R1:1144:GLN:HE22	1.86	0.41
22:T0:816:TRP:CZ2	22:T0:820:HIS:CD2	3.09	0.41
2:17:1105:GLN:HA	2:17:1106:PRO:C	2.46	0.41
5:B1:14:ARG:HH22	5:B1:100:ASP:CG	2.28	0.41
7:D1:1002:PRO:C	7:D4:91:PRO:HD2	2.34	0.41
7:D1:1168:HIS:CE1	23:U3:612:SER:N	2.89	0.41
7:D1:1185:ILE:CG2	23:U3:600:LEU:HD13	2.51	0.41
7:D5:1111:LEU:H	7:D5:1179:ASP:CG	2.29	0.41
13:K1:419:LEU:C	13:K1:419:LEU:HD23	2.46	0.41
20:R3:295:HIS:NE2	22:T0:413:PRO:CB	2.84	0.41
2:16:1105:GLN:HA	2:16:1106:PRO:C	2.46	0.40
4:A1:137:TRP:CZ2	5:B0:1656:GLU:HB3	2.57	0.40
4:A3:109:ALA:HA	5:B1:1168:ARG:HD2	2.03	0.40
4:A4:139:GLN:C	6:C2:1992:ARG:HH22	2.29	0.40
10:H2:417:ILE:HG23	11:I2:357:LEU:HD11	2.04	0.40
13:K0:151:TRP:CH2	13:K0:179:THR:HB	2.56	0.40
13:K2:419:LEU:C	13:K2:419:LEU:HD23	2.46	0.40
14:L0:803:LYS:HE3	14:L0:807:ASP:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L1:676:ASP:CG	14:L1:714:LYS:HZ2	2.29	0.40
16:N1:237:ASP:O	16:N1:260:LYS:HE2	2.21	0.40
2:14:831:ASP:OD1	2:14:837:LYS:HE3	2.21	0.40
6:C4:807:TYR:OH	19:Q2:26:LEU:CD1	2.57	0.40
7:D1:466:GLU:OE1	7:D1:468:LYS:HE2	2.22	0.40
7:D1:1186:THR:HG22	23:U3:601:VAL:O	2.21	0.40
7:D2:1185:ILE:CG2	23:U4:600:LEU:HD13	2.51	0.40
10:H1:468:LYS:HE2	10:H1:472:GLU:CD	2.46	0.40
13:K2:261:SER:C	13:K2:263:PHE:HA	2.45	0.40
15:M0:338:PRO:HG3	15:M0:372:TRP:CH2	2.56	0.40
20:R0:1110:ARG:C	20:R0:1111:GLU:HG2	2.46	0.40
22:T0:2:ARG:HA	22:T0:423:HIS:O	2.21	0.40
2:13:1462:GLU:C	2:13:1464:PRO:HD3	2.47	0.40
2:17:1789:ARG:HB2	8:E1:246:MET:H	1.86	0.40
2:17:1790:ARG:CB	8:E1:243:SER:N	2.80	0.40
5:B1:1303:TRP:CH2	5:B1:1307:THR:HG21	2.56	0.40
6:C1:327:ALA:HB2	6:C1:366:ASP:CB	2.51	0.40
6:C3:414:ALA:HB1	6:C3:509:ILE:HD11	2.03	0.40
6:C4:416:GLU:HG2	6:C4:419:ARG:CZ	2.51	0.40
7:D2:684:VAL:HG23	7:D2:686:ARG:HE	1.86	0.40
7:D3:950:TYR:CE2	7:D3:1037:ILE:HD13	2.56	0.40
7:D4:1170:SER:OG	23:U1:610:LEU:O	2.38	0.40
14:L2:367:LYS:HE3	14:L2:375:ALA:HB1	2.02	0.40
23:U2:614:VAL:CG1	23:U2:615:ASN:N	2.85	0.40
23:U6:609:ASN:HD22	23:U6:609:ASN:HA	1.62	0.40
25:W0:592:LYS:HE2	25:W0:596:ASP:OD2	2.21	0.40
1:03:412:ARG:HH21	1:03:415:GLU:CD	2.30	0.40
1:04:454:ARG:HH21	1:04:466:HIS:CD2	2.39	0.40
2:10:1824:MET:HB3	8:E0:22:GLY:C	2.47	0.40
4:A2:450:GLU:HG2	4:A2:462:TYR:CE2	2.57	0.40
6:C3:911:GLU:CG	6:C3:979:ILE:HD13	2.51	0.40
7:D1:1002:PRO:CB	7:D4:91:PRO:HA	2.51	0.40
7:D5:1185:ILE:CG2	23:U6:600:LEU:HB2	2.51	0.40
1:00:454:ARG:HH21	1:00:466:HIS:CD2	2.39	0.40
2:10:1827:ALA:CA	8:E0:19:ARG:H	2.34	0.40
3:41:143:PHE:CE1	3:41:291:THR:HG21	2.56	0.40
4:A0:277:ASN:OD1	7:D2:892:GLU:CG	2.53	0.40
6:C2:200:GLU:CD	6:C2:204:ARG:HH21	2.29	0.40
6:C2:484:HIS:HD2	20:R0:1075:LEU:HD11	1.86	0.40
6:C3:1252:ARG:CZ	20:R1:1258:GLU:HB2	2.52	0.40
7:D0:466:GLU:OE1	7:D0:468:LYS:HE2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D0:1185:ILE:HG22	23:U2:600:LEU:HB2	2.03	0.40
7:D0:1186:THR:HG22	23:U2:601:VAL:HB	1.97	0.40
7:D2:466:GLU:OE1	7:D2:468:LYS:HE2	2.22	0.40
10:H0:198:LYS:CE	10:H0:236:ASP:CG	2.95	0.40
11:I3:310:LYS:HE2	11:I3:314:GLU:OE1	2.22	0.40
13:K2:490:LEU:CD1	13:K2:491:ALA:H	2.32	0.40
15:M0:587:LEU:HB3	15:M0:588:PRO:CD	2.52	0.40
15:M1:649:TRP:HE1	15:M1:665:GLU:CD	2.30	0.40
18:P1:455:ARG:NH2	19:Q1:262:ALA:HB2	2.37	0.40
23:U4:609:ASN:HD22	23:U4:609:ASN:HA	1.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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-14321. 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](#)

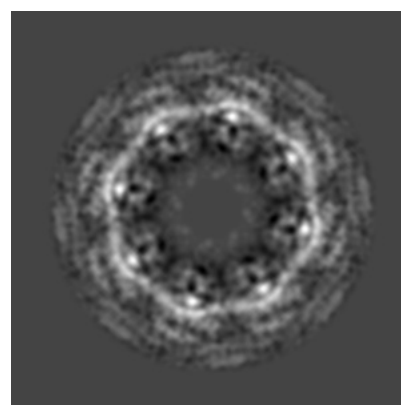
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

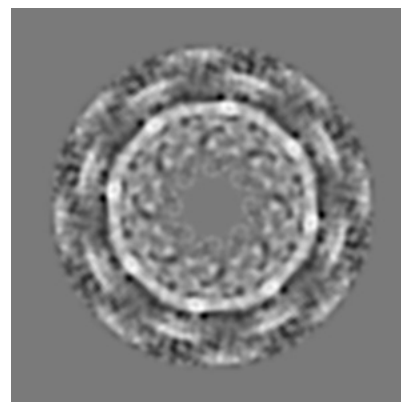
6.2.1 Primary map



X Index: 72



Y Index: 72



Z Index: 72

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

6.3 Largest variance slices [i](#)

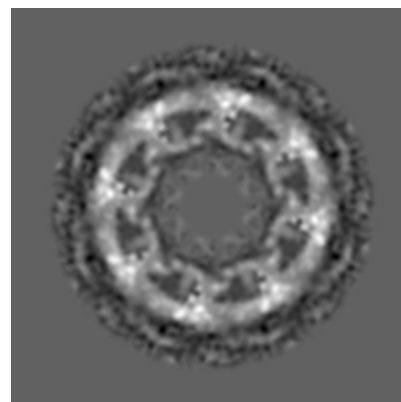
6.3.1 Primary map



X Index: 36



Y Index: 36

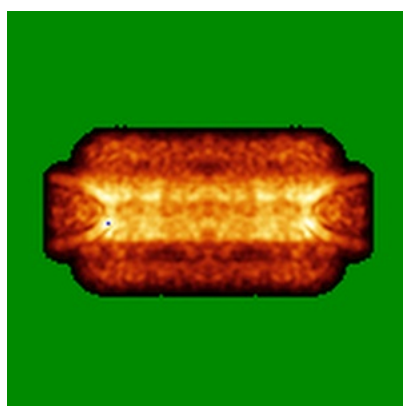


Z Index: 77

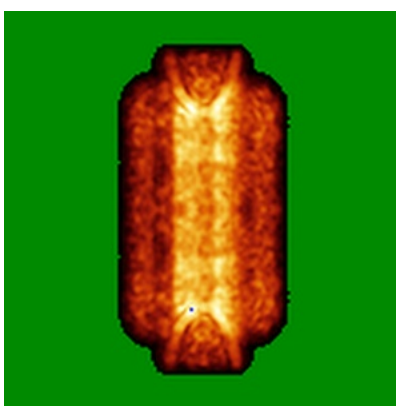
The images above show the largest variance slices of the map in three orthogonal directions.

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

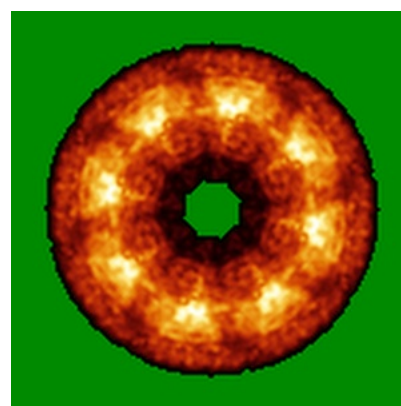
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0891. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

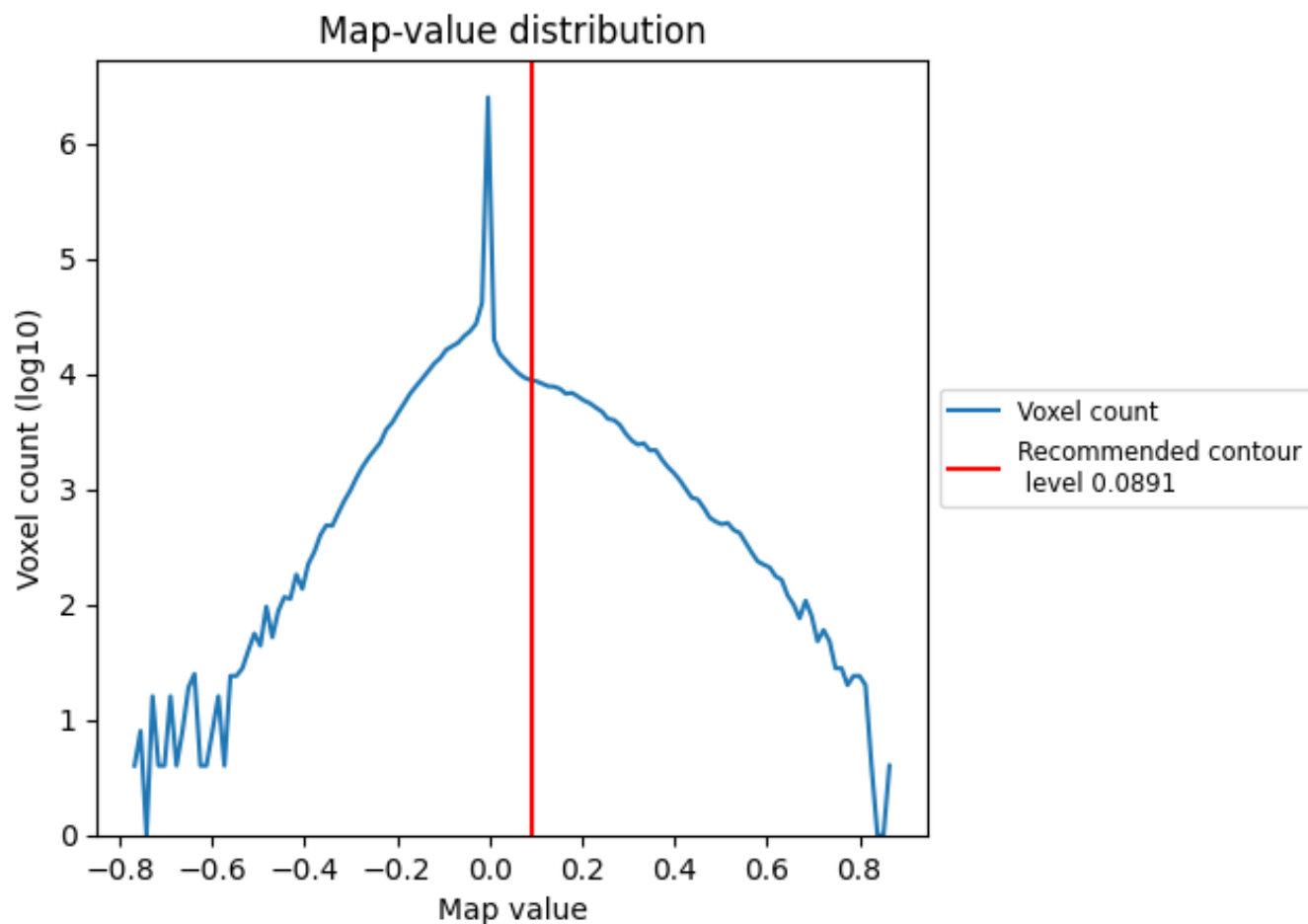
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

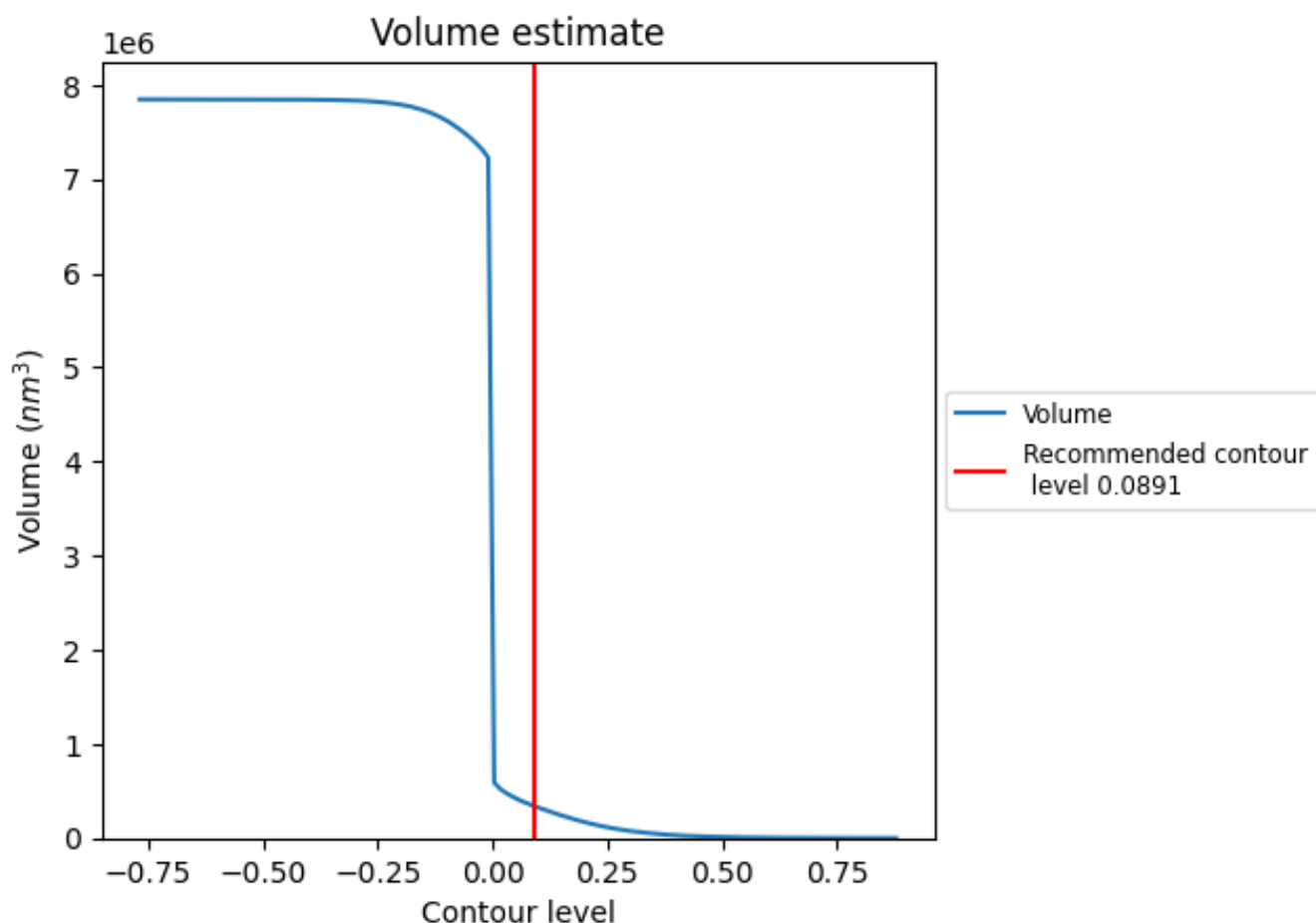
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

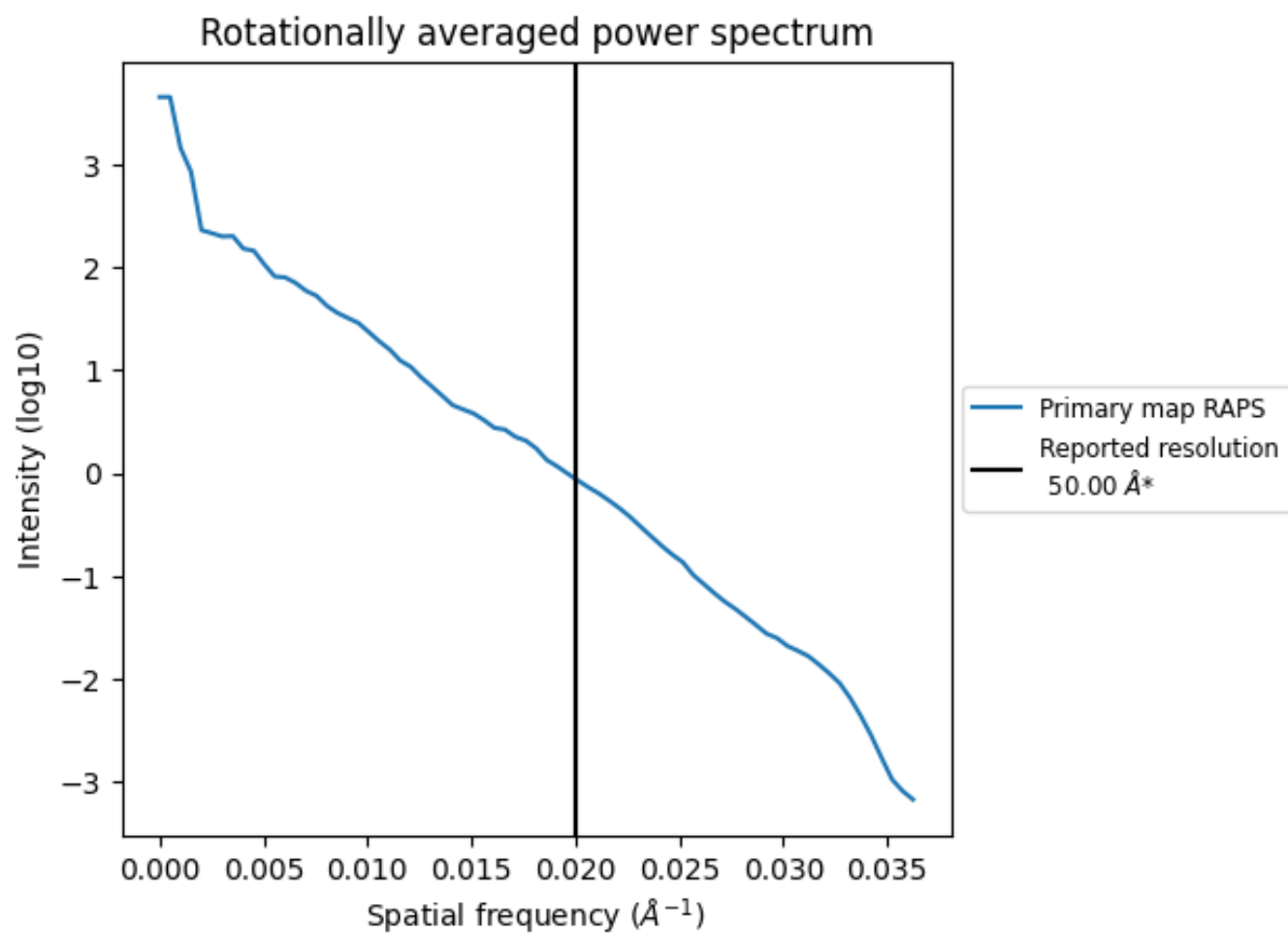
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 342613 nm³; this corresponds to an approximate mass of 309491 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 0.020 Å⁻¹

8 Fourier-Shell correlation

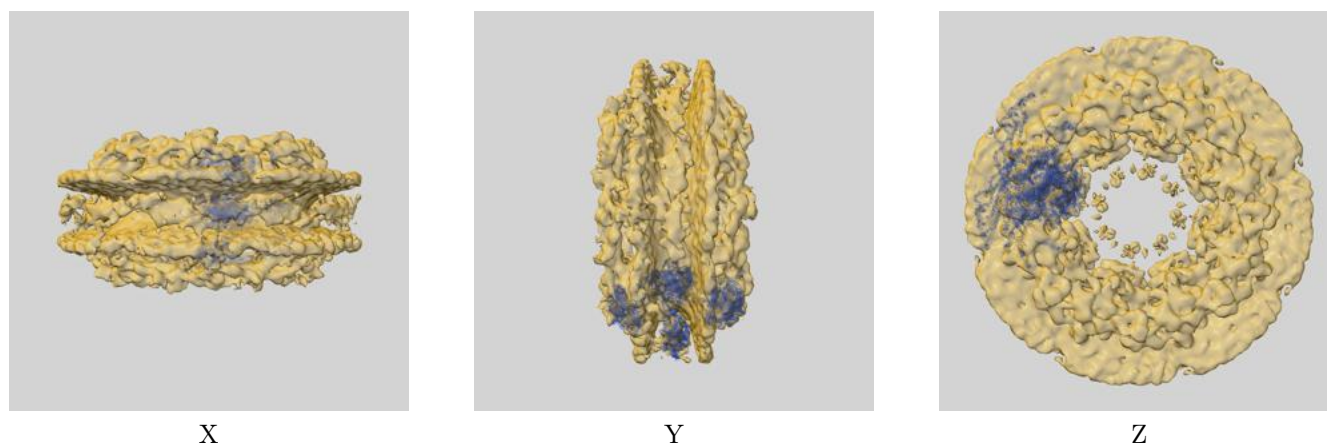
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

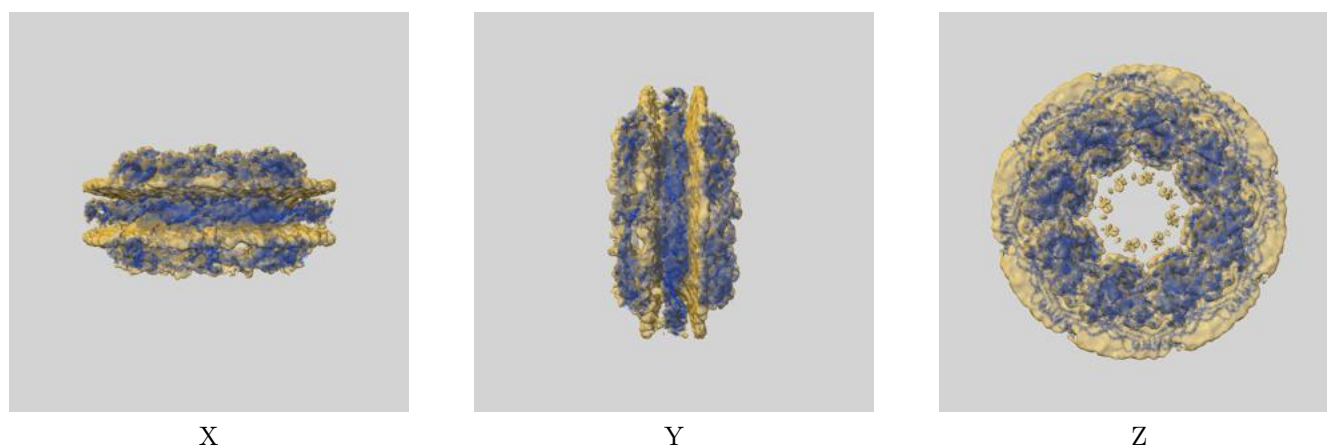
This section contains information regarding the fit between EMDB map EMD-14321 and PDB model 7R5J. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

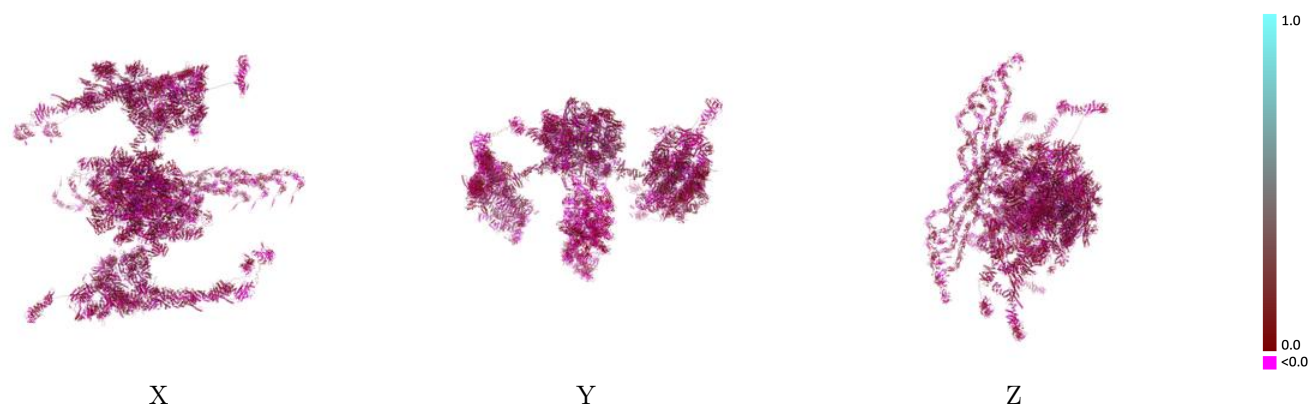


9.1.2 Map-model assembly overlay [i](#)



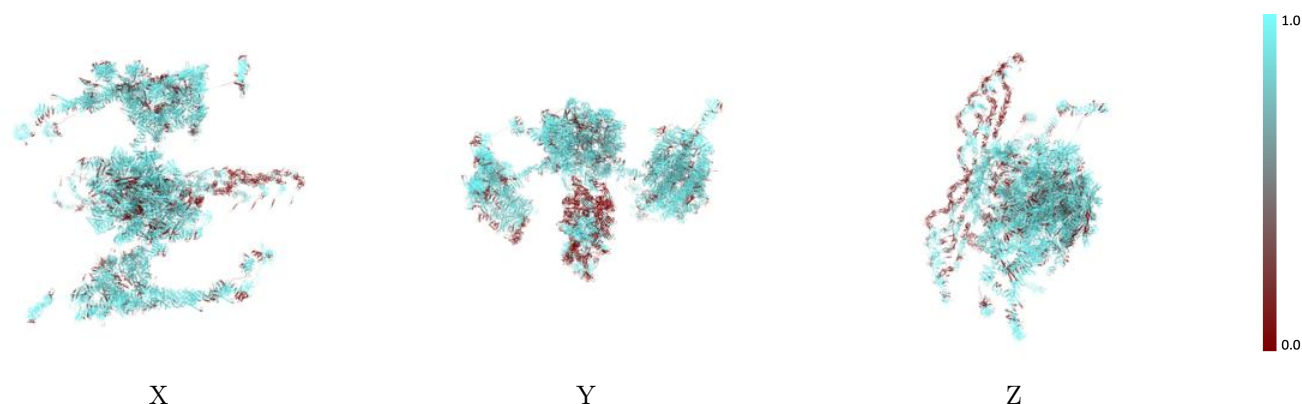
The images above show the 3D surface view of the map at the recommended contour level 0.0891 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



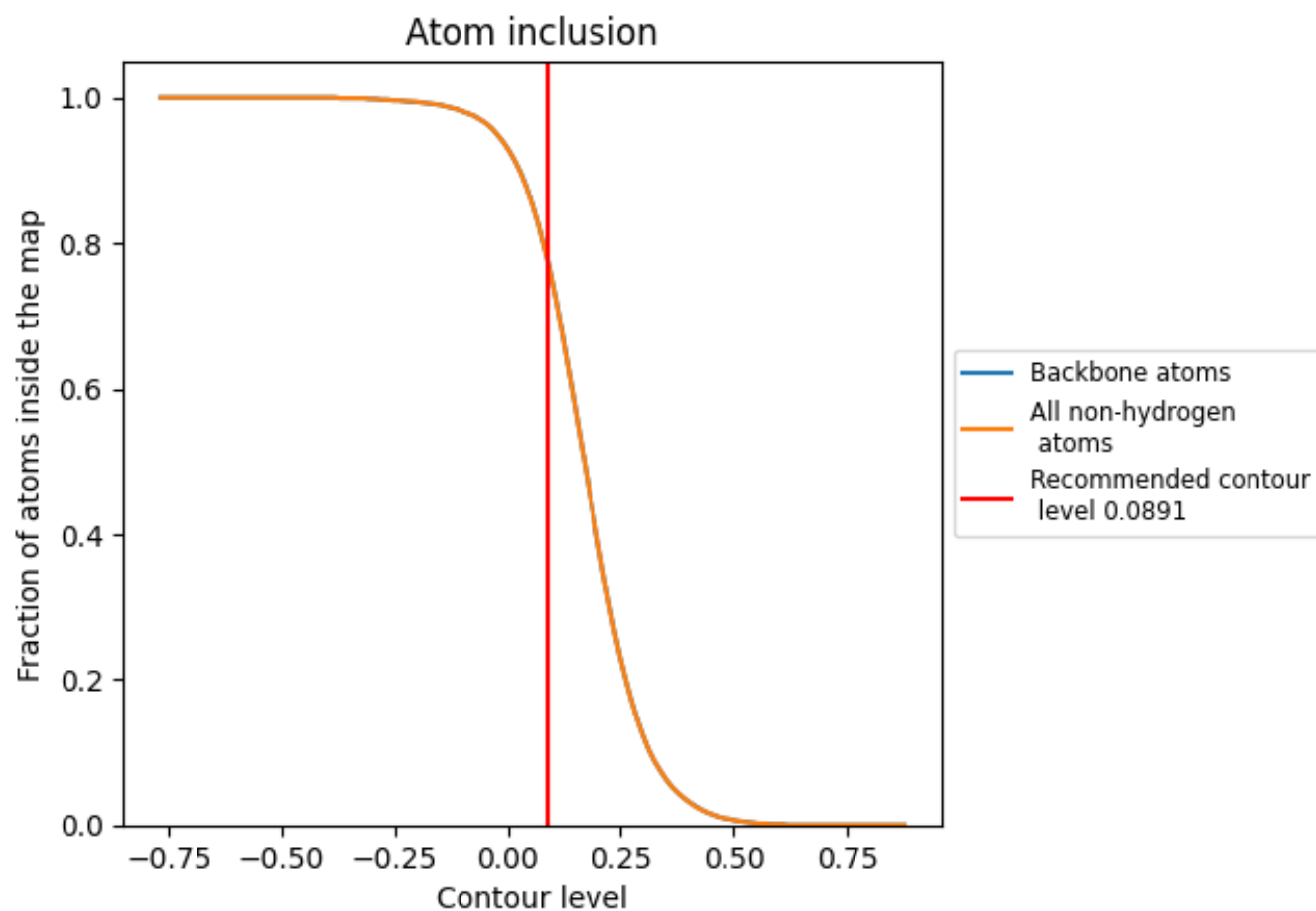
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0891).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 77% 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 (0.0891) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7740	 0.0260
00	 0.6940	 0.0260
01	 0.8320	 0.0420
02	 0.8560	 0.0400
03	 0.7250	 0.0330
04	 0.8890	 0.0470
10	 0.2440	 0.0150
11	 0.4850	 0.0150
12	 0.6710	 0.0220
13	 0.5790	 0.0240
14	 0.2910	 0.0000
15	 0.7150	 0.0220
16	 0.7300	 0.0210
17	 0.5870	 0.0250
40	 0.9960	 0.0240
41	 0.9990	 0.0270
A0	 0.9250	 0.0230
A1	 0.8520	 0.0330
A2	 0.9070	 0.0210
A3	 0.8760	 0.0420
A4	 0.8380	 0.0390
A5	 0.7590	 0.0160
A6	 0.9110	 0.0340
B0	 0.8480	 0.0340
B1	 0.8550	 0.0320
C0	 0.8060	 0.0240
C1	 0.8360	 0.0180
C2	 0.8300	 0.0340
C3	 0.8520	 0.0170
C4	 0.8220	 0.0280
D0	 0.8470	 0.0270
D1	 0.8020	 0.0260
D2	 0.8970	 0.0310
D3	 0.7720	 0.0200
D4	 0.8920	 0.0340



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Chain	Atom inclusion	Q-score
D5	 0.8260	 0.0310
E0	 0.9900	 0.0160
E1	 0.9800	 0.0070
F0	 0.8740	 0.0280
F1	 0.7040	 0.0170
F2	 0.7790	 0.0280
F3	 0.6710	 0.0170
H0	 0.7580	 0.0260
H1	 0.7630	 0.0350
H2	 0.7230	 0.0180
H3	 0.8260	 0.0390
I0	 0.5810	 0.0190
I1	 0.6700	 0.0260
I2	 0.7210	 0.0430
I3	 0.6500	 0.0200
J0	 0.6840	 0.0250
J1	 0.5620	 0.0110
J2	 0.7980	 0.0440
J3	 0.5780	 0.0030
J4	 0.8320	 0.0220
K0	 0.7780	 0.0190
K1	 0.8210	 0.0400
K2	 0.7120	 0.0140
K3	 0.7450	 0.0420
L0	 0.9130	 0.0390
L1	 0.7030	 0.0100
L2	 0.7540	 0.0260
L3	 0.8890	 0.0300
M0	 0.9300	 0.0410
M1	 0.7500	 0.0420
M2	 0.9600	 0.0380
M3	 0.8000	 0.0360
N0	 0.7930	 0.0160
N1	 0.9130	 0.0390
N2	 0.9890	 0.0250
N3	 0.9200	 0.0370
O0	 0.8330	 0.0330
O1	 0.9650	 0.0360
O2	 0.8840	 0.0290
O3	 0.9170	 0.0230
P0	 0.7830	 0.0380
P1	 0.9050	 0.0250

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Chain	Atom inclusion	Q-score
P2	 0.9040	 0.0330
P3	 0.8850	 0.0300
Q0	 0.7680	 0.0330
Q1	 0.8240	 0.0380
Q2	 0.8960	 0.0260
Q3	 0.9450	 0.0330
R0	 0.8850	 0.0290
R1	 0.8770	 0.0250
R2	 0.9450	 0.0280
R3	 0.9440	 0.0240
S0	 0.9310	 0.0410
S1	 0.9470	 0.0360
S2	 0.9460	 0.0200
S3	 0.9570	 0.0410
T0	 0.6370	 -0.0040
T1	 0.1820	 -0.0130
U0	 0.4430	 0.0070
U1	 0.5560	 0.0070
U2	 0.2650	 0.0290
U3	 0.9200	 0.0140
U4	 0.3840	 0.0040
U5	 0.1990	 0.0090
U6	 0.7880	 0.0380
V0	 0.7210	 0.0220
W0	 0.8030	 0.0250