



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:01 AM UTC

PDB ID : 9IWR / pdb_00009iwr
EMDB ID : EMD-60960
Title : 26S proteasome trimer
Authors : Qu, L.; Tang, X.; Baumeister, W.
Deposited on : 2024-07-25
Resolution : 9.10 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:

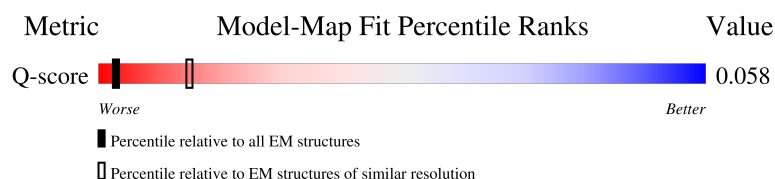
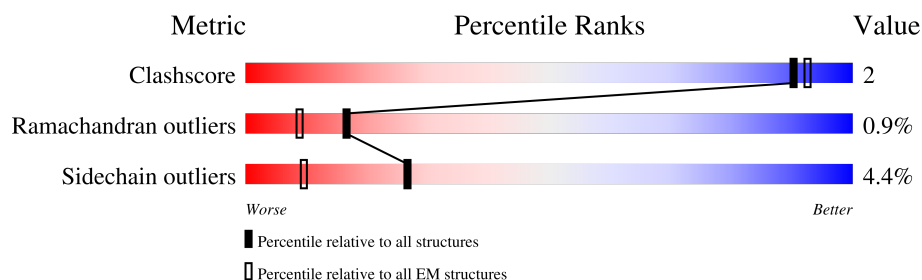
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 9.10 Å.

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



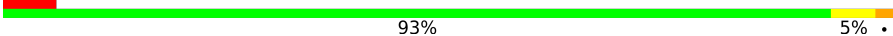
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	244 (8.60 - 9.60)

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	1-1	215	9% 85% 5% • 9%
1	1-h	215	7% 84% 7% 9%
1	2-1	215	85% 5% • 9%
1	2-h	215	85% 6% 9%

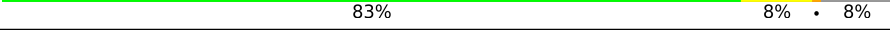
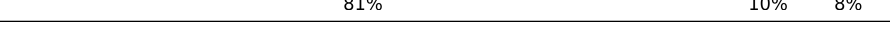
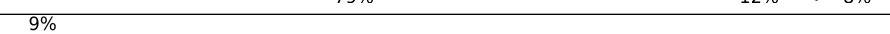
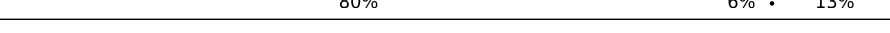
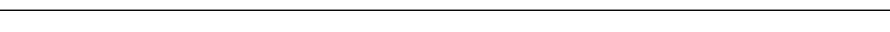
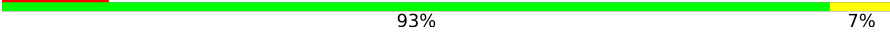
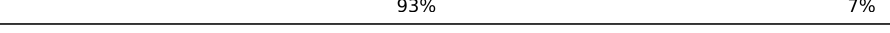
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Mol	Chain	Length	Quality of chain
1	3-1	215	
1	3-h	215	
2	1-2	261	
2	1-i	261	
2	2-2	261	
2	2-i	261	
2	3-2	261	
2	3-i	261	
3	1-3	205	
3	1-j	205	
3	2-3	205	
3	2-j	205	
3	3-3	205	
3	3-j	205	
4	1-4	198	
4	1-k	198	
4	2-4	198	
4	2-k	198	
4	3-4	198	
4	3-k	198	
5	1-5	287	
5	1-l	287	
5	2-5	287	
5	2-l	287	
5	3-5	287	

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Mol	Chain	Length	Quality of chain
5	3-l	287	
6	1-6	241	
6	1-m	241	
6	2-6	241	
6	2-m	241	
6	3-6	241	
6	3-m	241	
7	1-7	266	
7	1-n	266	
7	2-7	266	
7	2-n	266	
7	3-7	266	
7	3-n	266	
8	1-A	252	
8	1-a	252	
8	2-A	252	
8	2-a	252	
8	3-A	252	
8	3-a	252	
9	1-B	250	
9	1-b	250	
9	2-B	250	
9	2-b	250	
9	3-B	250	
9	3-b	250	

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Mol	Chain	Length	Quality of chain
10	1-C	258	
10	1-c	258	
10	2-C	258	
10	2-c	258	
10	3-C	258	
10	3-c	258	
11	1-D	254	
11	1-d	254	
11	2-D	254	
11	2-d	254	
11	3-D	254	
11	3-d	254	
12	1-E	260	
12	1-e	260	
12	2-E	260	
12	2-e	260	
12	3-E	260	
12	3-e	260	
13	1-F	234	
13	1-f	234	
13	2-F	234	
13	2-f	234	
13	3-F	234	
13	3-f	234	
14	1-G	288	

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Mol	Chain	Length	Quality of chain
14	1-g	288	 10% 78% 5% • 16%
14	2-G	288	 77% 6% • 16%
14	2-g	288	 78% 5% • 16%
14	3-G	288	 76% 7% • 16%
14	3-g	288	 76% 7% • 16%
15	1-H	467	 18% 75% 8% • 16%
15	2-H	467	 75% 8% • 16%
15	3-H	467	 72% 11% • 16%
16	1-I	437	 22% 81% 6% • 12%
16	2-I	437	 81% 5% • 12%
16	3-I	437	 79% 7% • 12%
17	1-J	405	 25% 87% 7% • 5%
17	2-J	405	 87% 7% • 5%
17	3-J	405	 84% 9% • 5%
18	1-K	428	 16% 79% 11% 9%
18	2-K	428	 79% 11% 9%
18	3-K	428	 78% 11% • 9%
19	1-L	437	 21% 81% 7% • 11%
19	2-L	437	 80% 7% • 11%
19	3-L	437	 77% 9% • 11%
20	1-M	434	 22% 81% 5% • 12%
20	2-M	434	 82% 5% • 12%
20	3-M	434	 79% 7% • 12%
21	1-N	945	 25% 85% 8% • 6%
21	2-N	945	 86% 8% • 6%

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Mol	Chain	Length	Quality of chain
21	3-N	945	
22	1-O	393	
22	2-O	393	
22	3-O	393	
23	1-P	445	
23	2-P	445	
23	3-P	445	
24	1-Q	434	
24	2-Q	434	
24	3-Q	434	
25	1-R	429	
25	2-R	429	
25	3-R	429	
26	1-S	523	
26	2-S	523	
26	3-S	523	
27	1-T	274	
27	2-T	274	
27	3-T	274	
28	1-U	338	
28	2-U	338	
28	3-U	338	
29	1-V	306	
29	2-V	306	
29	3-V	306	

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Mol	Chain	Length	Quality of chain
30	1-W	268	
30	2-W	268	
30	3-W	268	
31	1-X	156	
31	2-X	156	
31	3-X	156	
32	1-Y	89	
32	2-Y	89	
32	3-Y	89	
33	1-Z	993	
33	2-Z	993	
33	3-Z	993	

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 653142 atoms, of which 327135 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 Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1-1	196	Total	C	H	N	O	S	0	0
			2991	955	1479	250	300	7		
1	2-1	196	Total	C	H	N	O	S	0	0
			2991	955	1479	250	300	7		
1	3-1	196	Total	C	H	N	O	S	0	0
			2991	955	1479	250	300	7		
1	1-h	196	Total	C	H	N	O	S	0	0
			2991	955	1479	250	300	7		
1	2-h	196	Total	C	H	N	O	S	0	0
			2991	955	1479	250	300	7		
1	3-h	196	Total	C	H	N	O	S	0	0
			2991	955	1479	250	300	7		

- Molecule 2 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1-2	226	Total	C	H	N	O	S	0	0
			3436	1082	1717	298	332	7		
2	2-2	226	Total	C	H	N	O	S	0	0
			3436	1082	1717	298	332	7		
2	3-2	226	Total	C	H	N	O	S	0	0
			3436	1082	1717	298	332	7		
2	1-i	226	Total	C	H	N	O	S	0	0
			3436	1082	1717	298	332	7		
2	2-i	226	Total	C	H	N	O	S	0	0
			3436	1082	1717	298	332	7		
2	3-i	226	Total	C	H	N	O	S	0	0
			3436	1082	1717	298	332	7		

- Molecule 3 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	1-3	204	Total	C	H	N	O	S	0	0
			3153	1010	1572	258	305	8		

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Mol	Chain	Residues	Atoms						AltConf	Trace
3	2-3	204	Total	C	H	N	O	S	0	0
			3153	1010	1572	258	305	8		
3	3-3	204	Total	C	H	N	O	S	0	0
			3153	1010	1572	258	305	8		
3	1-j	204	Total	C	H	N	O	S	0	0
			3153	1010	1572	258	305	8		
3	2-j	204	Total	C	H	N	O	S	0	0
			3153	1010	1572	258	305	8		
3	3-j	204	Total	C	H	N	O	S	0	0
			3153	1010	1572	258	305	8		

- Molecule 4 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	1-4	195	Total	C	H	N	O	S	0	0
			3130	992	1569	264	299	6		
4	2-4	195	Total	C	H	N	O	S	0	0
			3130	992	1569	264	299	6		
4	3-4	195	Total	C	H	N	O	S	0	0
			3130	992	1569	264	299	6		
4	1-k	195	Total	C	H	N	O	S	0	0
			3130	992	1569	264	299	6		
4	2-k	195	Total	C	H	N	O	S	0	0
			3130	992	1569	264	299	6		
4	3-k	195	Total	C	H	N	O	S	0	0
			3130	992	1569	264	299	6		

- Molecule 5 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	1-5	212	Total	C	H	N	O	S	0	0
			3237	1045	1593	280	312	7		
5	2-5	212	Total	C	H	N	O	S	0	0
			3237	1045	1593	280	312	7		
5	3-5	212	Total	C	H	N	O	S	0	0
			3237	1045	1593	280	312	7		
5	1-1	212	Total	C	H	N	O	S	0	0
			3237	1045	1593	280	312	7		
5	2-1	212	Total	C	H	N	O	S	0	0
			3237	1045	1593	280	312	7		
5	3-1	212	Total	C	H	N	O	S	0	0
			3237	1045	1593	280	312	7		

- Molecule 6 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	1-6	222	Total	C	H	N	O	S	0	0
			3466	1115	1709	303	335	4		
6	2-6	222	Total	C	H	N	O	S	0	0
			3466	1115	1709	303	335	4		
6	3-6	222	Total	C	H	N	O	S	0	0
			3466	1115	1709	303	335	4		
6	1-m	222	Total	C	H	N	O	S	0	0
			3466	1115	1709	303	335	4		
6	2-m	222	Total	C	H	N	O	S	0	0
			3466	1115	1709	303	335	4		
6	3-m	222	Total	C	H	N	O	S	0	0
			3466	1115	1709	303	335	4		

- Molecule 7 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	1-7	229	Total	C	H	N	O	S	0	0
			3581	1133	1791	306	344	7		
7	2-7	229	Total	C	H	N	O	S	0	0
			3581	1133	1791	306	344	7		
7	3-7	229	Total	C	H	N	O	S	0	0
			3581	1133	1791	306	344	7		
7	1-n	232	Total	C	H	N	O	S	0	0
			3634	1148	1819	311	349	7		
7	2-n	232	Total	C	H	N	O	S	0	0
			3634	1148	1819	311	349	7		
7	3-n	232	Total	C	H	N	O	S	0	0
			3634	1148	1819	311	349	7		

- Molecule 8 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	1-A	241	Total	C	H	N	O	S	0	0
			3809	1214	1902	320	365	8		
8	2-A	241	Total	C	H	N	O	S	0	0
			3809	1214	1902	320	365	8		
8	3-A	241	Total	C	H	N	O	S	0	0
			3809	1214	1902	320	365	8		
8	1-a	241	Total	C	H	N	O	S	0	0
			3809	1214	1902	320	365	8		
8	2-a	241	Total	C	H	N	O	S	0	0
			3809	1214	1902	320	365	8		

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Mol	Chain	Residues	Atoms						AltConf	Trace
8	3-a	241	Total	C	H	N	O	S	0	0
			3809	1214	1902	320	365	8		

- Molecule 9 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	1-B	250	Total	C	H	N	O	S	0	0
			3844	1219	1929	315	377	4		
9	2-B	250	Total	C	H	N	O	S	0	0
			3844	1219	1929	315	377	4		
9	3-B	250	Total	C	H	N	O	S	0	0
			3844	1219	1929	315	377	4		
9	1-b	250	Total	C	H	N	O	S	0	0
			3844	1219	1929	315	377	4		
9	2-b	250	Total	C	H	N	O	S	0	0
			3844	1219	1929	315	377	4		
9	3-b	250	Total	C	H	N	O	S	0	0
			3844	1219	1929	315	377	4		

- Molecule 10 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	1-C	244	Total	C	H	N	O	S	0	0
			3806	1201	1902	321	379	3		
10	2-C	244	Total	C	H	N	O	S	0	0
			3806	1201	1902	321	379	3		
10	3-C	244	Total	C	H	N	O	S	0	0
			3806	1201	1902	321	379	3		
10	1-c	244	Total	C	H	N	O	S	0	0
			3806	1201	1902	321	379	3		
10	2-c	244	Total	C	H	N	O	S	0	0
			3806	1201	1902	321	379	3		
10	3-c	244	Total	C	H	N	O	S	0	0
			3806	1201	1902	321	379	3		

- Molecule 11 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	1-D	240	Total	C	H	N	O	S	0	0
			3774	1176	1893	329	372	4		
11	2-D	240	Total	C	H	N	O	S	0	0
			3774	1176	1893	329	372	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
11	3-D	240	Total	C	H	N	O	S	0	0
			3774	1176	1893	329	372	4		
11	1-d	240	Total	C	H	N	O	S	0	0
			3774	1176	1893	329	372	4		
11	2-d	240	Total	C	H	N	O	S	0	0
			3774	1176	1893	329	372	4		
11	3-d	240	Total	C	H	N	O	S	0	0
			3774	1176	1893	329	372	4		

- Molecule 12 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	1-E	242	Total 3698	C 1162	H 1837	N 314	O 378	S 7	0	0
12	2-E	242	Total 3698	C 1162	H 1837	N 314	O 378	S 7	0	0
12	3-E	242	Total 3698	C 1162	H 1837	N 314	O 378	S 7	0	0
12	1-e	242	Total 3698	C 1162	H 1837	N 314	O 378	S 7	0	0
12	2-e	242	Total 3698	C 1162	H 1837	N 314	O 378	S 7	0	0
12	3-e	242	Total 3698	C 1162	H 1837	N 314	O 378	S 7	0	0

- Molecule 13 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	1-F	233	Total	C	H	N	O	S	0	0
			3595	1129	1800	312	350	4		
13	2-F	233	Total	C	H	N	O	S	0	0
			3595	1129	1800	312	350	4		
13	3-F	233	Total	C	H	N	O	S	0	0
			3595	1129	1800	312	350	4		
13	1-f	231	Total	C	H	N	O	S	0	0
			3551	1114	1778	307	348	4		
13	2-f	231	Total	C	H	N	O	S	0	0
			3551	1114	1778	307	348	4		
13	3-f	231	Total	C	H	N	O	S	0	0
			3551	1114	1778	307	348	4		

- Molecule 14 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	1-G	243	Total	C	H	N	O	S	0	0
			3777	1203	1885	329	356	4		
14	2-G	243	Total	C	H	N	O	S	0	0
			3777	1203	1885	329	356	4		
14	3-G	243	Total	C	H	N	O	S	0	0
			3777	1203	1885	329	356	4		
14	1-g	243	Total	C	H	N	O	S	0	0
			3776	1203	1884	329	356	4		
14	2-g	243	Total	C	H	N	O	S	0	0
			3776	1203	1884	329	356	4		
14	3-g	243	Total	C	H	N	O	S	0	0
			3776	1203	1884	329	356	4		

- Molecule 15 is a protein called 26S protease regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	1-H	390	Total	C	H	N	O	S	0	0
			6183	1920	3130	546	570	17		
15	2-H	390	Total	C	H	N	O	S	0	0
			6183	1920	3130	546	570	17		
15	3-H	390	Total	C	H	N	O	S	0	0
			6183	1920	3130	546	570	17		

- Molecule 16 is a protein called 26S protease regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	1-I	385	Total	C	H	N	O	S	0	0
			6115	1899	3093	508	598	17		
16	2-I	385	Total	C	H	N	O	S	0	0
			6115	1899	3093	508	598	17		
16	3-I	385	Total	C	H	N	O	S	0	0
			6115	1899	3093	508	598	17		

- Molecule 17 is a protein called 26S protease regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	1-J	386	Total	C	H	N	O	S	0	0
			6190	1906	3157	543	567	17		
17	2-J	386	Total	C	H	N	O	S	0	0
			6190	1906	3157	543	567	17		
17	3-J	386	Total	C	H	N	O	S	0	0
			6190	1906	3157	543	567	17		

- Molecule 18 is a protein called 26S protease regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	1-K	389	Total	C	H	N	O	S	0	0
			6220	1933	3142	540	595	10		
18	2-K	389	Total	C	H	N	O	S	0	0
			6220	1933	3142	540	595	10		
18	3-K	389	Total	C	H	N	O	S	0	0
			6220	1933	3142	540	595	10		

- Molecule 19 is a protein called 26S protease subunit RPT4.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	1-L	388	Total	C	H	N	O	S	0	0
			6240	1942	3158	548	580	12		
19	2-L	388	Total	C	H	N	O	S	0	0
			6240	1942	3158	548	580	12		
19	3-L	388	Total	C	H	N	O	S	0	0
			6240	1942	3158	548	580	12		

- Molecule 20 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	1-M	381	Total	C	H	N	O	S	0	0
			6043	1870	3057	524	580	12		
20	2-M	381	Total	C	H	N	O	S	0	0
			6043	1870	3057	524	580	12		
20	3-M	381	Total	C	H	N	O	S	0	0
			6043	1870	3057	524	580	12		

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	1-N	890	Total	C	H	N	O	S	0	0
			13843	4373	6961	1156	1325	28		
21	2-N	890	Total	C	H	N	O	S	0	0
			13843	4373	6961	1156	1325	28		
21	3-N	890	Total	C	H	N	O	S	0	0
			13843	4373	6961	1156	1325	28		

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	1-O	388	Total	C	H	N	O	S	0	0
			6400	2051	3214	519	608	8		
22	2-O	388	Total	C	H	N	O	S	0	0
			6400	2051	3214	519	608	8		
22	3-O	388	Total	C	H	N	O	S	0	0
			6400	2051	3214	519	608	8		

- Molecule 23 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	1-P	440	Total	C	H	N	O	S	0	0
			7302	2297	3694	604	697	10		
23	2-P	440	Total	C	H	N	O	S	0	0
			7302	2297	3694	604	697	10		
23	3-P	440	Total	C	H	N	O	S	0	0
			7302	2297	3694	604	697	10		

- Molecule 24 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	1-Q	434	Total	C	H	N	O	S	0	0
			7023	2225	3524	577	681	16		
24	2-Q	434	Total	C	H	N	O	S	0	0
			7023	2225	3524	577	681	16		
24	3-Q	434	Total	C	H	N	O	S	0	0
			7023	2225	3524	577	681	16		

- Molecule 25 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	1-R	381	Total	C	H	N	O	S	0	0
			6145	1955	3085	502	593	10		
25	2-R	381	Total	C	H	N	O	S	0	0
			6145	1955	3085	502	593	10		
25	3-R	381	Total	C	H	N	O	S	0	0
			6145	1955	3085	502	593	10		

- Molecule 26 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	1-S	475	Total	C	H	N	O	S	0	0
			7833	2488	3939	653	738	15		

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Mol	Chain	Residues	Atoms						AltConf	Trace
26	2-S	475	Total	C	H	N	O	S	0	0
			7833	2488	3939	653	738	15		
26	3-S	475	Total	C	H	N	O	S	0	0
			7833	2488	3939	653	738	15		

- Molecule 27 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	1-T	266	Total	C	H	N	O	S	0	0
			4354	1405	2162	349	432	6		
27	2-T	266	Total	C	H	N	O	S	0	0
			4354	1405	2162	349	432	6		
27	3-T	266	Total	C	H	N	O	S	0	0
			4354	1405	2162	349	432	6		

- Molecule 28 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	1-U	298	Total	C	H	N	O	S	0	0
			4776	1496	2403	404	466	7		
28	2-U	298	Total	C	H	N	O	S	0	0
			4776	1496	2403	404	466	7		
28	3-U	298	Total	C	H	N	O	S	0	0
			4776	1496	2403	404	466	7		

- Molecule 29 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	1-V	289	Total	C	H	N	O	S	0	0
			4549	1425	2275	389	446	14		
29	2-V	289	Total	C	H	N	O	S	0	0
			4549	1425	2275	389	446	14		
29	3-V	289	Total	C	H	N	O	S	0	0
			4549	1425	2275	389	446	14		

- Molecule 30 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	1-W	197	Total	C	H	N	O	S	0	0
			3076	962	1542	269	300	3		
30	2-W	197	Total	C	H	N	O	S	0	0
			3076	962	1542	269	300	3		

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Mol	Chain	Residues	Atoms						AltConf	Trace
30	3-W	197	Total	C	H	N	O	S	0	0
			3076	962	1542	269	300	3		

- Molecule 31 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	1-X	127	Total	C	H	N	O	S	0	0
			2050	664	1018	169	195	4		
31	2-X	127	Total	C	H	N	O	S	0	0
			2050	664	1018	169	195	4		
31	3-X	127	Total	C	H	N	O	S	0	0
			2050	664	1018	169	195	4		

- Molecule 32 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	1-Y	51	Total	C	H	N	O	0	0
			831	264	396	69	102		
32	2-Y	51	Total	C	H	N	O	0	0
			831	264	396	69	102		
32	3-Y	51	Total	C	H	N	O	0	0
			831	264	396	69	102		

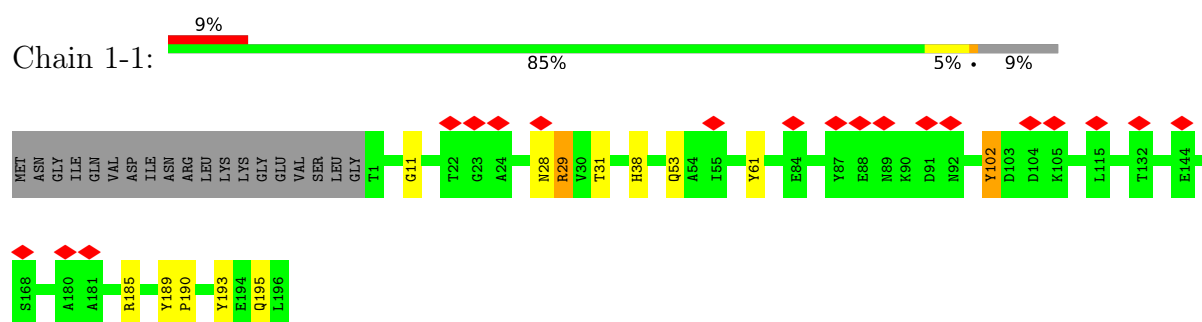
- Molecule 33 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	1-Z	906	Total	C	H	N	O	S	0	0
			13939	4416	6934	1150	1409	30		
33	2-Z	906	Total	C	H	N	O	S	0	0
			13939	4416	6934	1150	1409	30		
33	3-Z	906	Total	C	H	N	O	S	0	0
			13939	4416	6934	1150	1409	30		

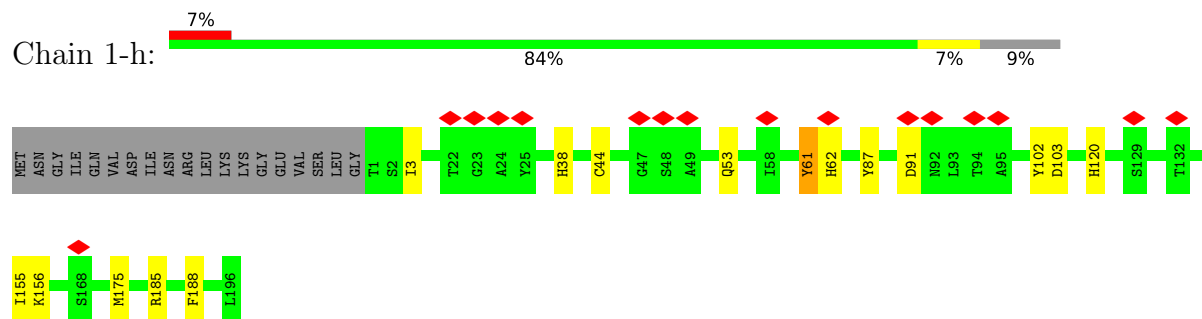
3 Residue-property plots [i](#)

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

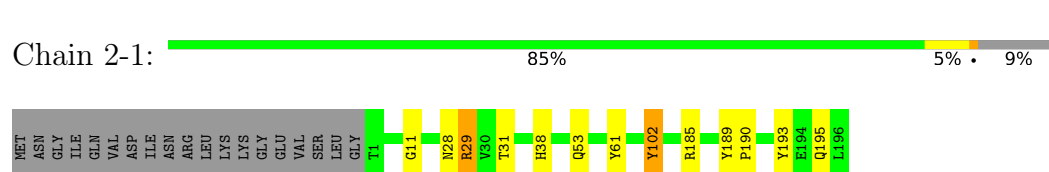
- Molecule 1: Proteasome subunit beta type-1



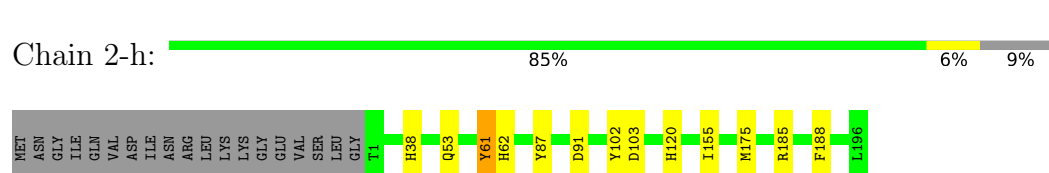
- Molecule 1: Proteasome subunit beta type-1



- Molecule 1: Proteasome subunit beta type-1

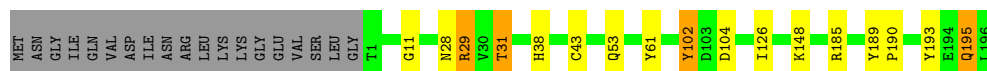


- Molecule 1: Proteasome subunit beta type-1



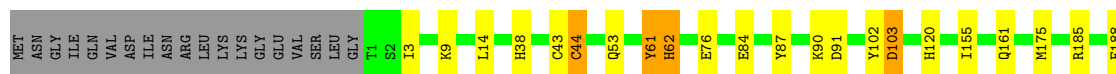
- Molecule 1: Proteasome subunit beta type-1

Chain 3-1:  83% 6% 9%



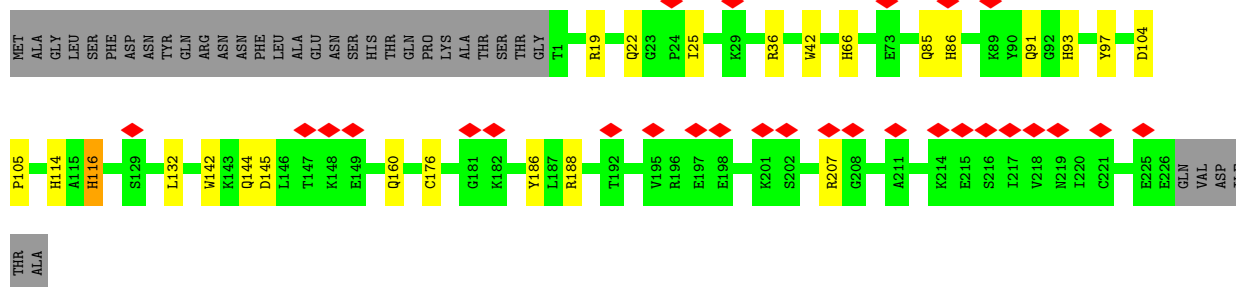
- Molecule 1: Proteasome subunit beta type-1

Chain 3-h:  81% 8% 9%



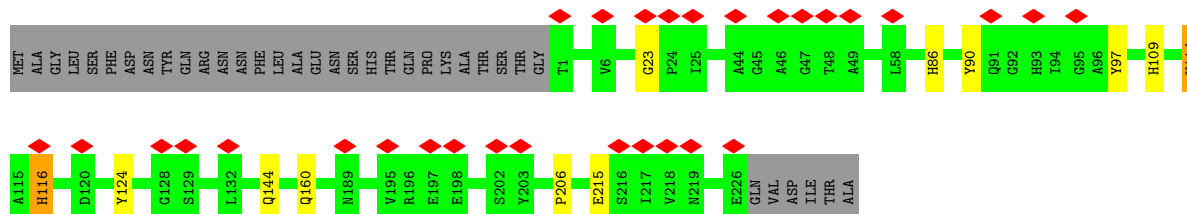
- Molecule 2: Proteasome subunit beta type-2

Chain 1-2:  11% 77% 9% 13%



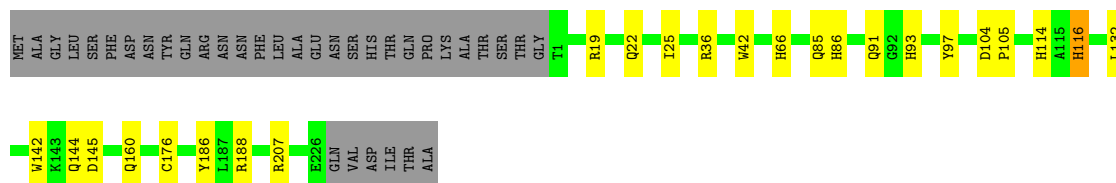
- Molecule 2: Proteasome subunit beta type-2

Chain 1-i:  11% 82% 9% 13%



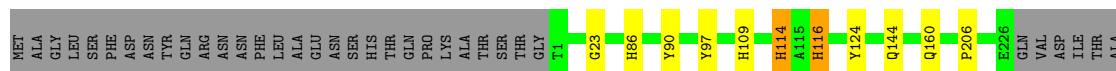
- Molecule 2: Proteasome subunit beta type-2

Chain 2-2:  77% 9% 13%



- Molecule 2: Proteasome subunit beta type-2

Chain 2-i:  82% 13%



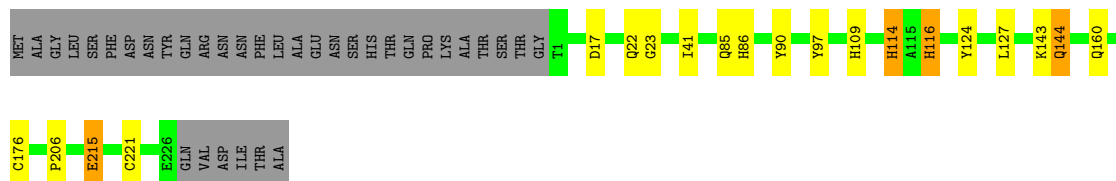
- Molecule 2: Proteasome subunit beta type-2

Chain 3-2:  77% 8% 13%

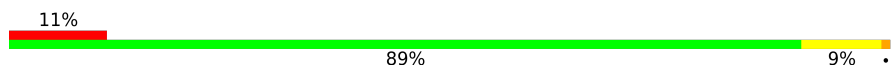


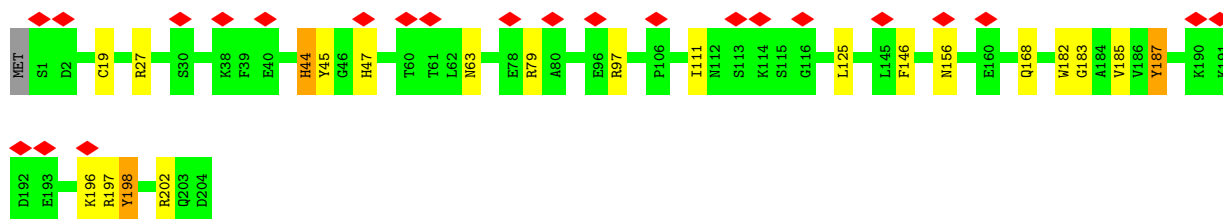
- Molecule 2: Proteasome subunit beta type-2

Chain 3-i:  79% 6% 13%

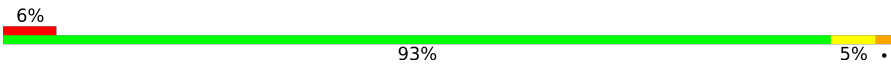


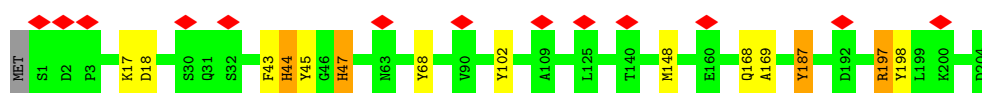
- Molecule 3: Proteasome subunit beta type-3

Chain 1-3:  11% 89% 9%



- Molecule 3: Proteasome subunit beta type-3

Chain 1-j:  6% 93% 5%



- Molecule 3: Proteasome subunit beta type-3

Chain 2-3:  89% 9%



- Molecule 3: Proteasome subunit beta type-3



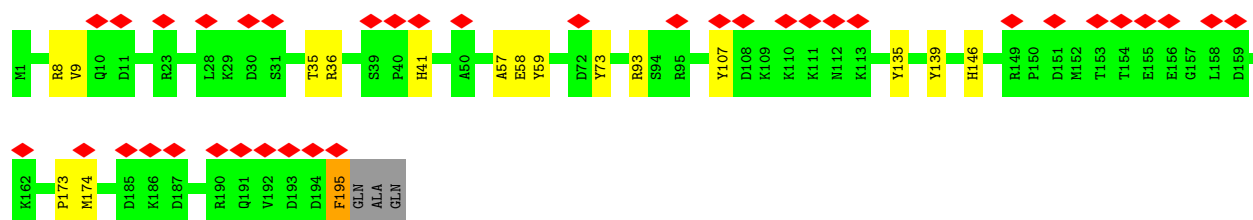
- Molecule 3: Proteasome subunit beta type-3



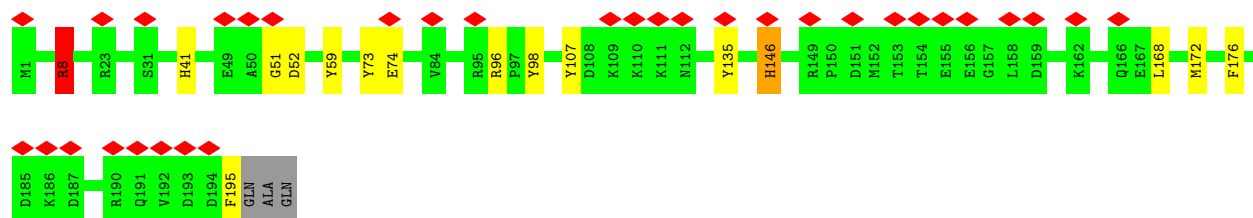
- Molecule 3: Proteasome subunit beta type-3



- Molecule 4: Proteasome subunit beta type-4



- Molecule 4: Proteasome subunit beta type-4



- Molecule 4: Proteasome subunit beta type-4





- Molecule 4: Proteasome subunit beta type-4

Chain 2-k: 90% 7% ..



- Molecule 4: Proteasome subunit beta type-4

Chain 3-4: 87% 11% ..



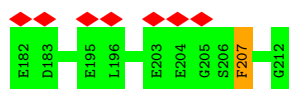
- Molecule 4: Proteasome subunit beta type-4

Chain 3-k: 87% 10% ..



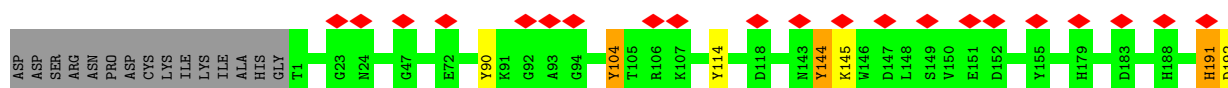
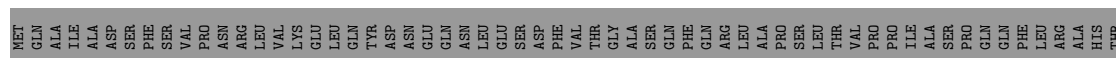
- Molecule 5: Proteasome subunit beta type-5

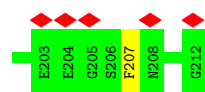
Chain 1-5: 7% 69% 26%



- Molecule 5: Proteasome subunit beta type-5

Chain 1-1: 9% 71% 26%





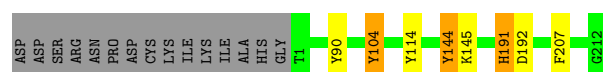
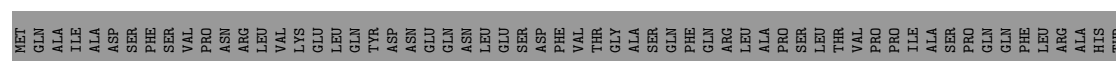
- Molecule 5: Proteasome subunit beta type-5

Chain 2-5: 69% 26%



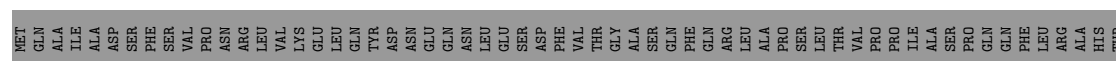
- Molecule 5: Proteasome subunit beta type-5

Chain 2-1: 71% 26%



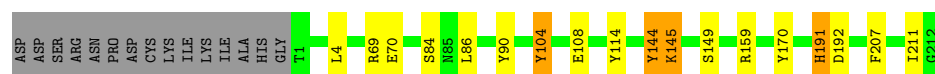
- Molecule 5: Proteasome subunit beta type-5

Chain 3-5: 69% 26%



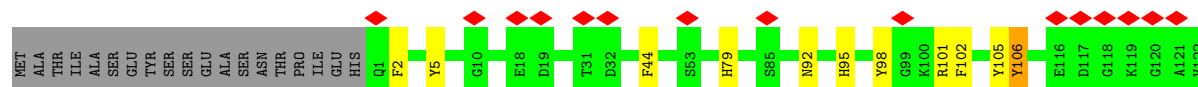
- Molecule 5: Proteasome subunit beta type-5

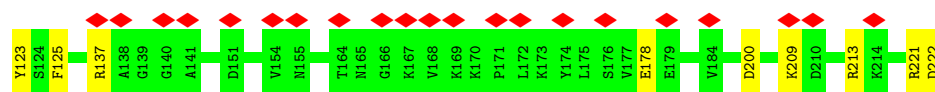
Chain 3-1: 68% 5% 26%



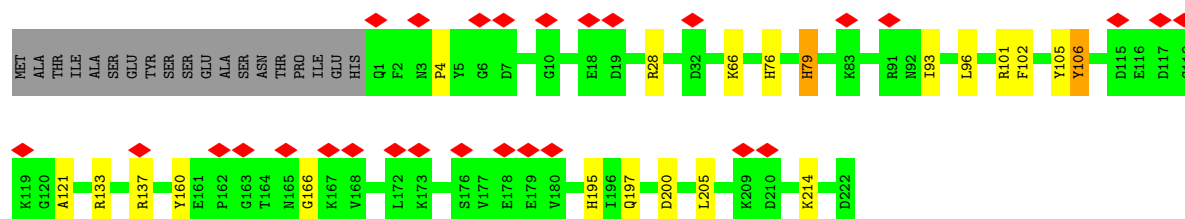
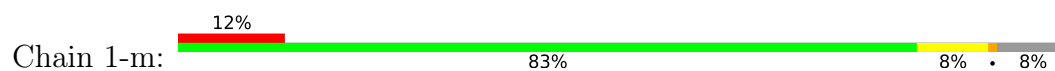
- Molecule 6: Proteasome subunit beta type-6

Chain 1-6: 15% 84% 8% 8%

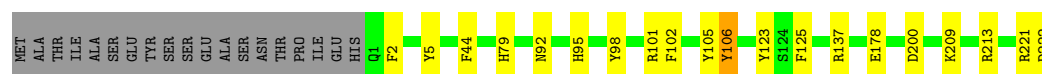
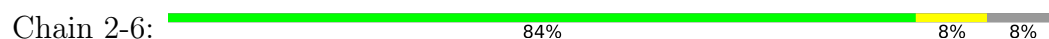




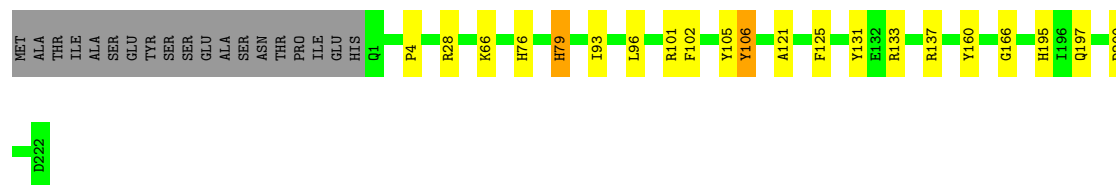
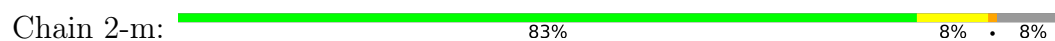
• Molecule 6: Proteasome subunit beta type-6



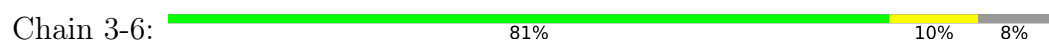
• Molecule 6: Proteasome subunit beta type-6



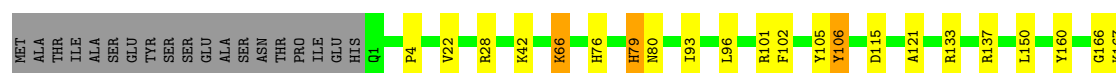
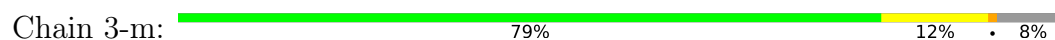
• Molecule 6: Proteasome subunit beta type-6



• Molecule 6: Proteasome subunit beta type-6

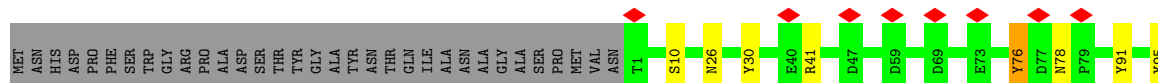
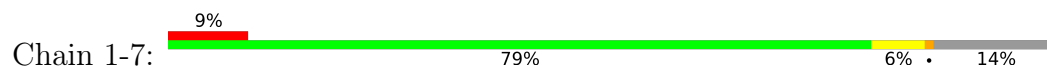


• Molecule 6: Proteasome subunit beta type-6

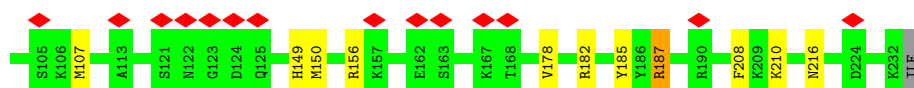
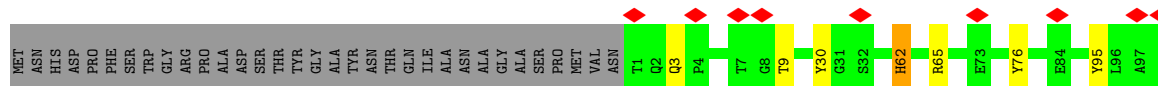
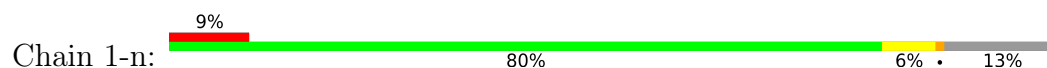




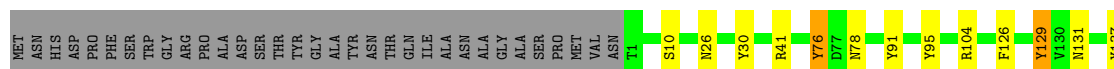
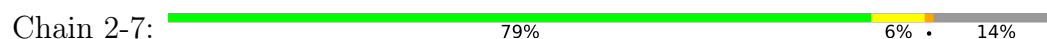
- Molecule 7: Proteasome subunit beta type-7



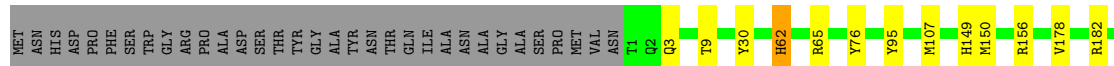
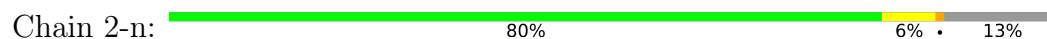
- Molecule 7: Proteasome subunit beta type-7



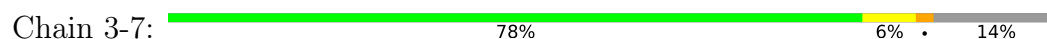
- Molecule 7: Proteasome subunit beta type-7

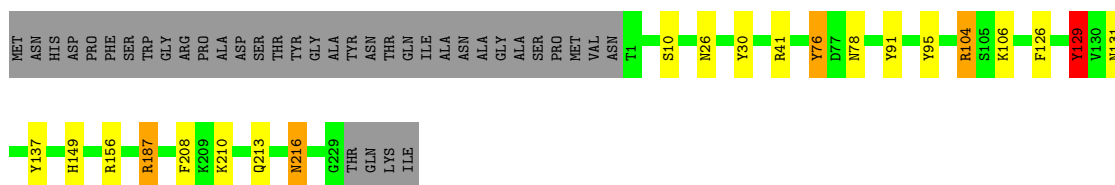


- Molecule 7: Proteasome subunit beta type-7



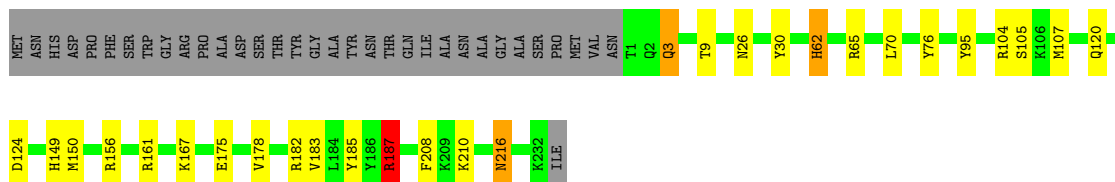
- Molecule 7: Proteasome subunit beta type-7





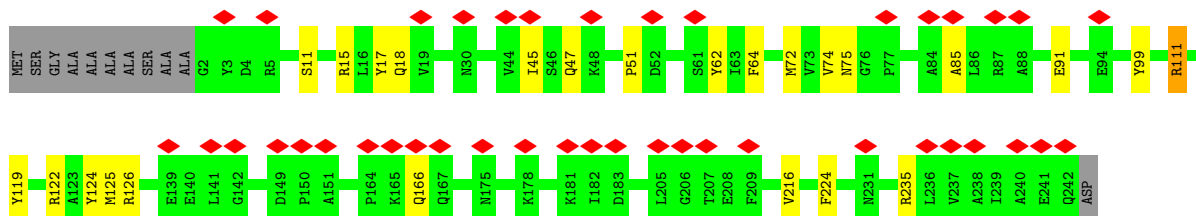
- Molecule 7: Proteasome subunit beta type-7

Chain 3-n: 77% 9% 13%



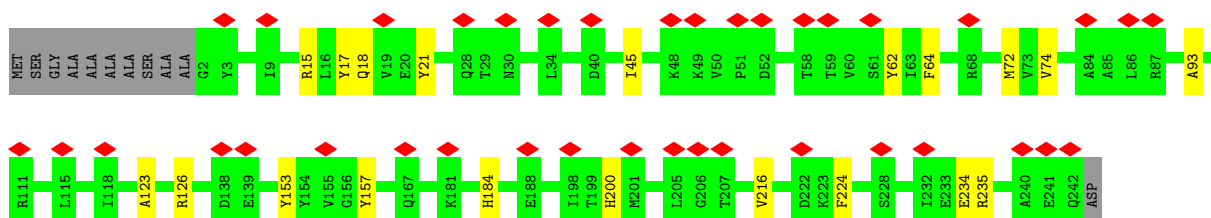
- Molecule 8: Proteasome subunit alpha type-1

Chain 1-A: 16% 86% 10%



- Molecule 8: Proteasome subunit alpha type-1

Chain 1-a: 15% 88% 8%



- Molecule 8: Proteasome subunit alpha type-1

Chain 2-A: 86% 10%



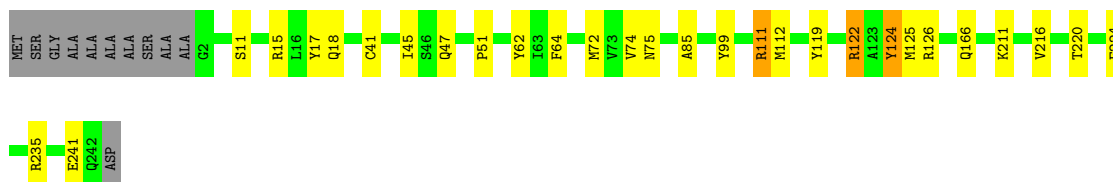
- Molecule 8: Proteasome subunit alpha type-1

Chain 2-a: 88% 8%



- Molecule 8: Proteasome subunit alpha type-1

Chain 3-A: 84% 10% . .



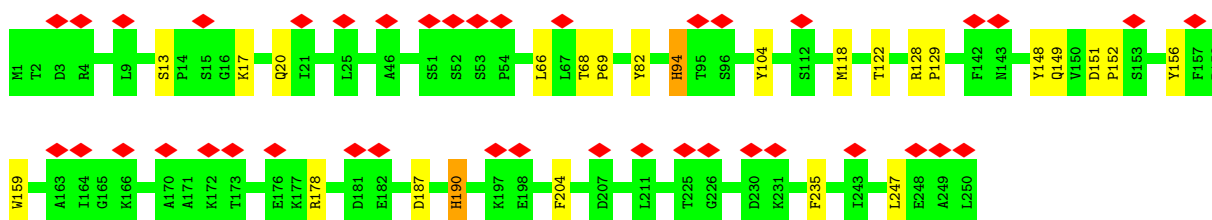
- Molecule 8: Proteasome subunit alpha type-1

Chain 3-a: 83% 12% .



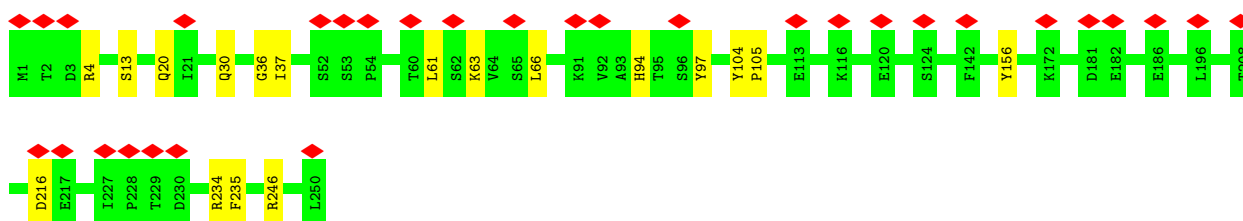
- Molecule 9: Proteasome subunit alpha type-2

Chain 1-B: 16% 90% 9% .



- Molecule 9: Proteasome subunit alpha type-2

Chain 1-b: 12% 93% 7%



- Molecule 9: Proteasome subunit alpha type-2

Chain 2-B: 91% 8% .



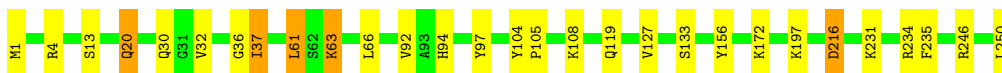
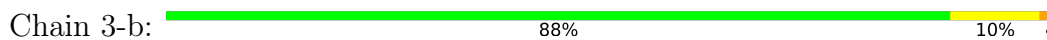
- Molecule 9: Proteasome subunit alpha type-2



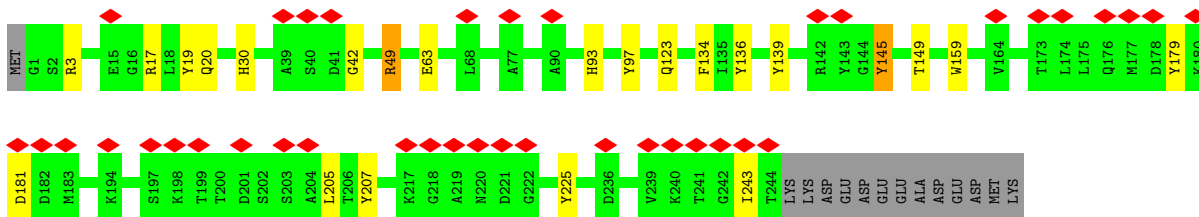
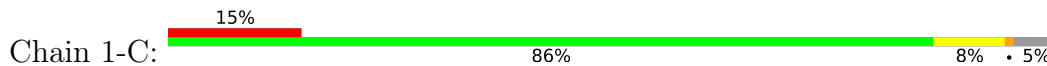
- Molecule 9: Proteasome subunit alpha type-2



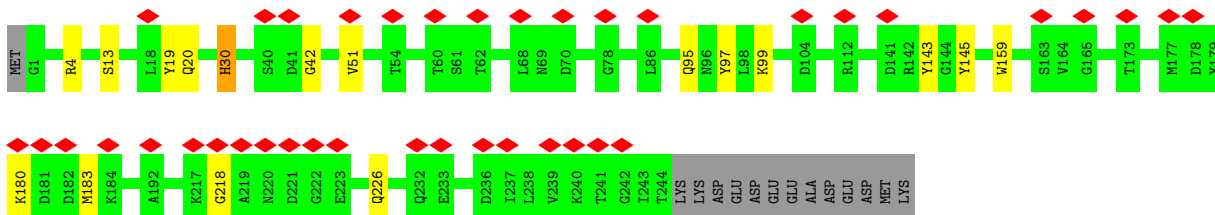
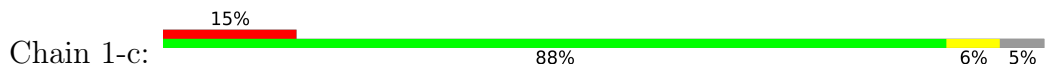
- Molecule 9: Proteasome subunit alpha type-2



- Molecule 10: Proteasome subunit alpha type-3

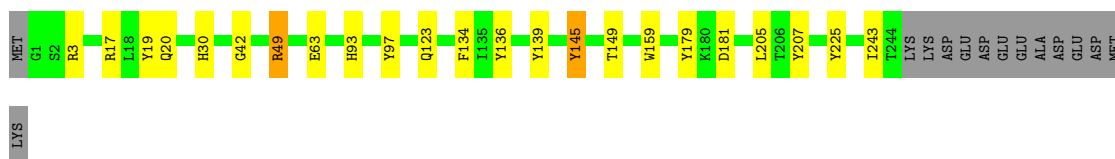


- Molecule 10: Proteasome subunit alpha type-3



- Molecule 10: Proteasome subunit alpha type-3





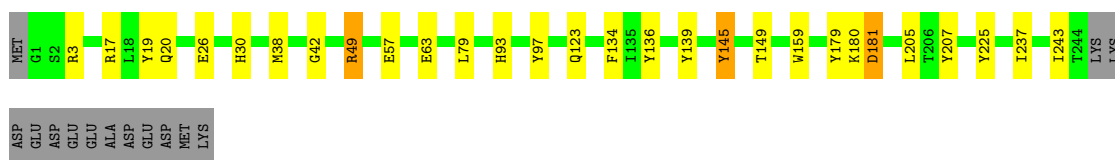
- Molecule 10: Proteasome subunit alpha type-3

Chain 2-c: 88% 6% 5%



- Molecule 10: Proteasome subunit alpha type-3

Chain 3-C: 83% 10% 5%



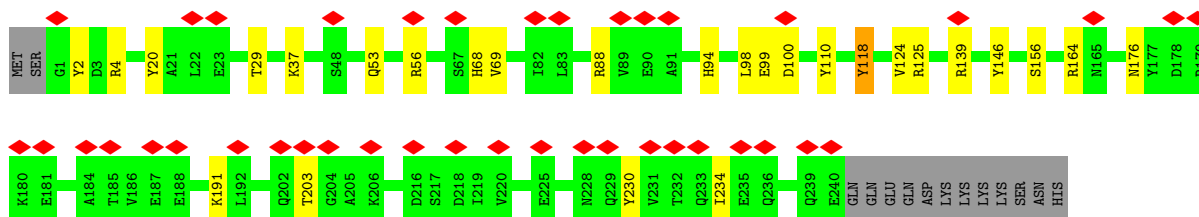
- Molecule 10: Proteasome subunit alpha type-3

Chain 3-c: 86% 7% 5%



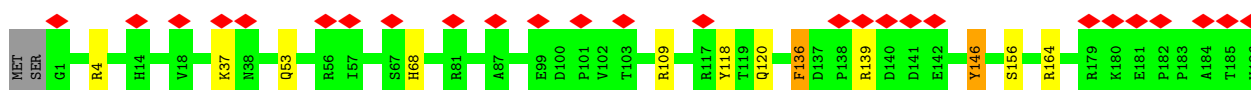
- Molecule 11: Proteasome subunit alpha type-4

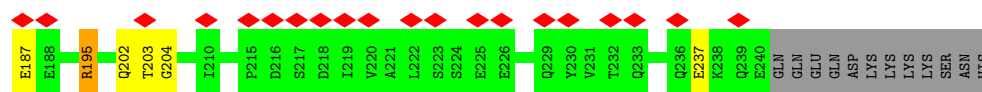
Chain 1-D: 16% 84% 10% 6%



- Molecule 11: Proteasome subunit alpha type-4

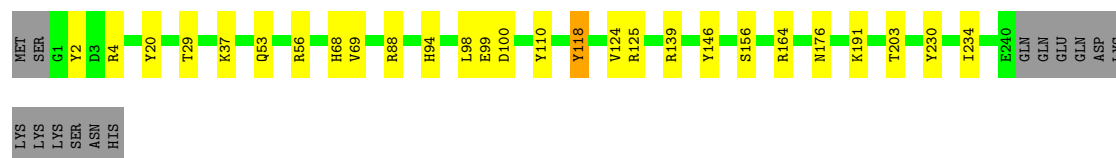
Chain 1-d: 18% 87% 6% 6%





- Molecule 11: Proteasome subunit alpha type-4

Chain 2-D: 84% 10% 6%



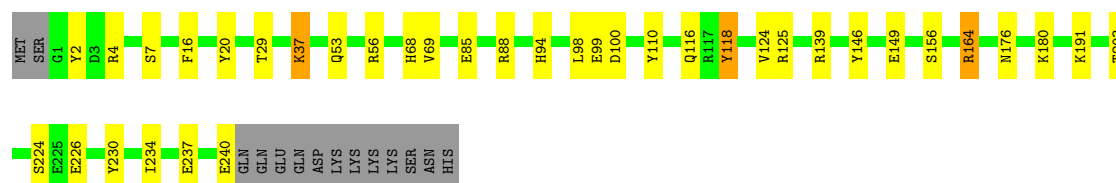
- Molecule 11: Proteasome subunit alpha type-4

Chain 2-d: 87% 6% 6%



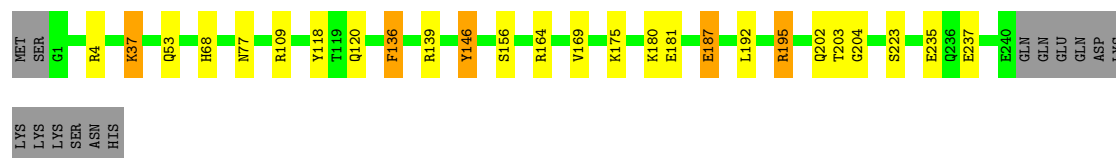
- Molecule 11: Proteasome subunit alpha type-4

Chain 3-D: 80% 13% 6%



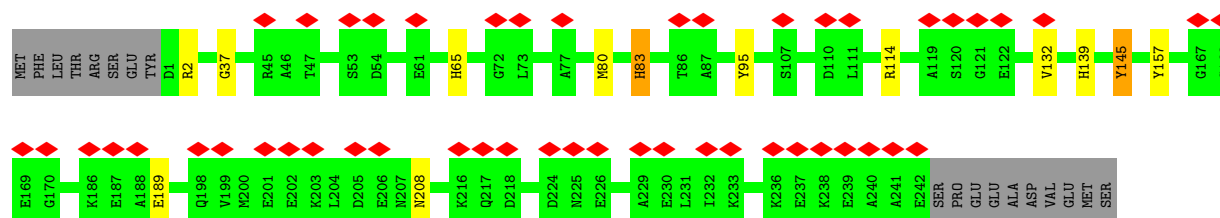
- Molecule 11: Proteasome subunit alpha type-4

Chain 3-d: 84% 8% 6%

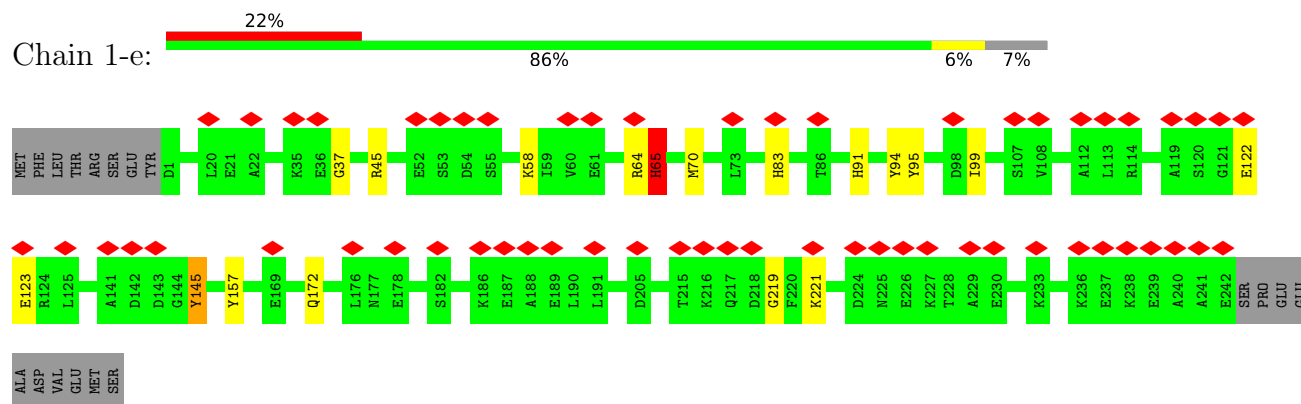


- Molecule 12: Proteasome subunit alpha type-5

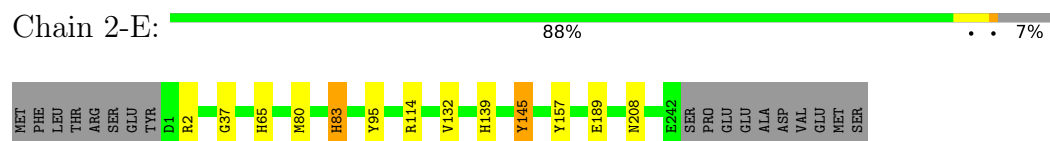
Chain 1-E: 19% 88% 7%



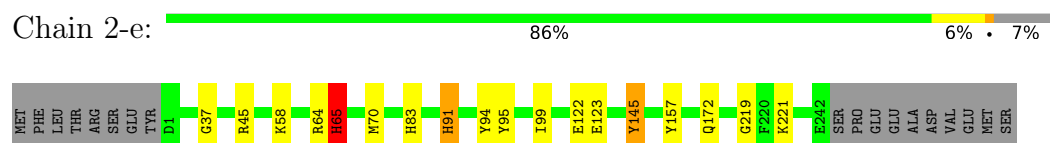
• Molecule 12: Proteasome subunit alpha type-5



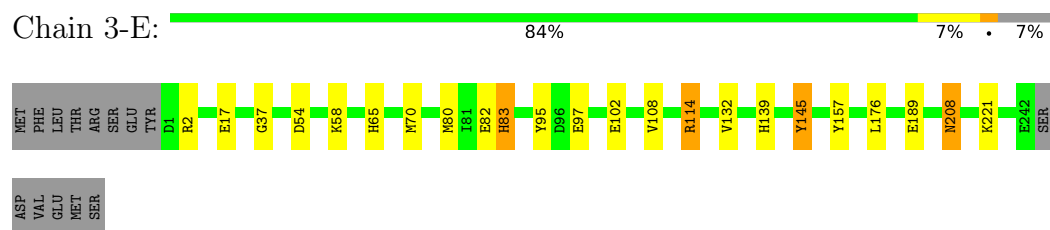
• Molecule 12: Proteasome subunit alpha type-5



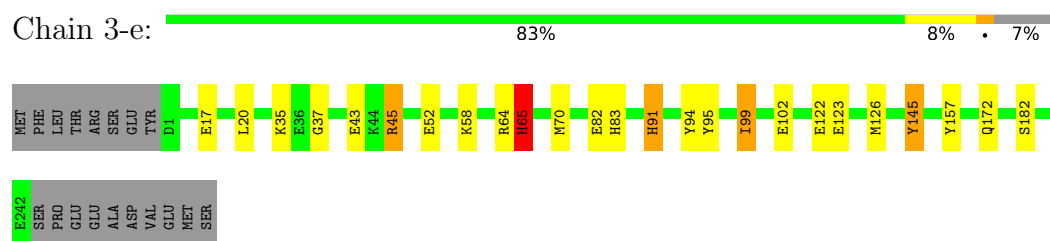
• Molecule 12: Proteasome subunit alpha type-5



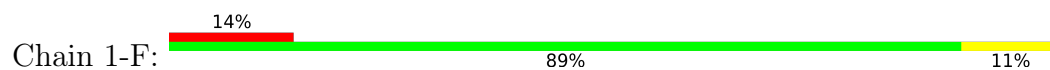
• Molecule 12: Proteasome subunit alpha type-5

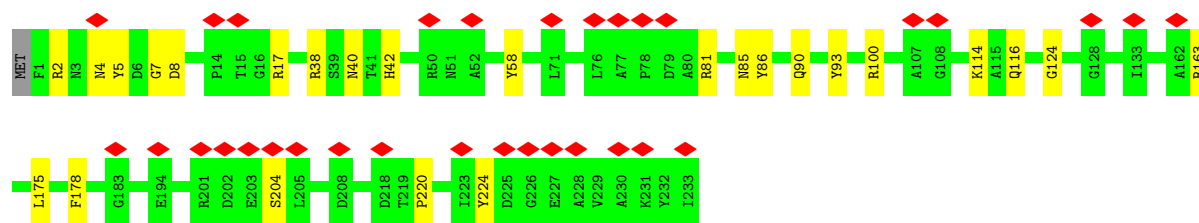


• Molecule 12: Proteasome subunit alpha type-5

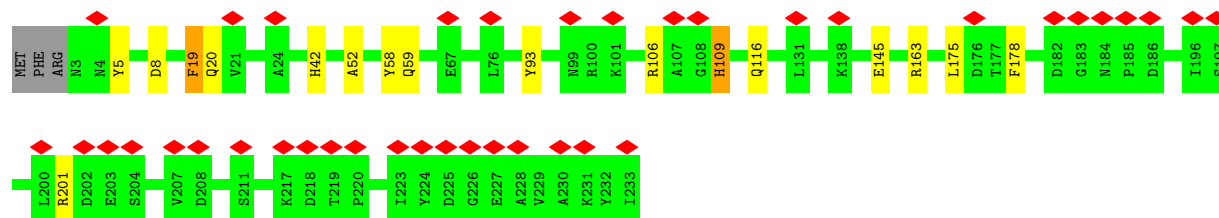


• Molecule 13: Proteasome subunit alpha type-6

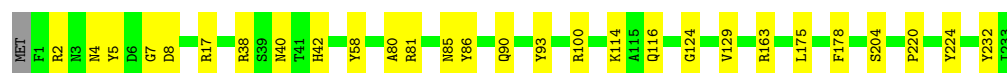




- Molecule 13: Proteasome subunit alpha type-6



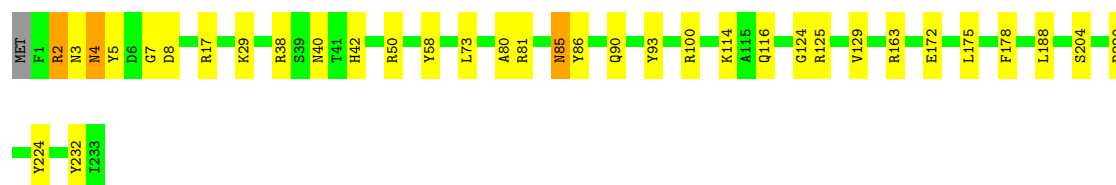
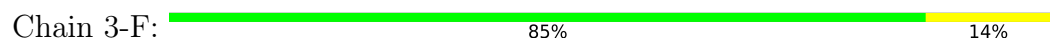
- Molecule 13: Proteasome subunit alpha type-6



- Molecule 13: Proteasome subunit alpha type-6



- Molecule 13: Proteasome subunit alpha type-6



- Molecule 13: Proteasome subunit alpha type-6



- | MET |
|------|
| TMR |
| IIE |
| GLY |
| T2 |
| G3 |
| Y4 |
| D6 |
| F11 |
| K59 |
| Y74 |
| L77 |
| G81 |
| R82 |
| H83 |
| R87 |
| G88 |
| R89 |
| R111 |
| L121 |
| Y122 |
| F134 |
| V137 |
| D138 |
| K139 |
| Y145 |
| E148 |
| Q166 |
| H178 |
| H179 |
| G182 |
| C215 |
| Q240 |
| N244 |
| GLY |
| ASP |
| ASP |
| ASP |
| GLU |
| ASP |
| GLU |

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

- Molecule 14: Probable proteasome subunit alpha type-7

Chain 3-g:  76% 7% 16%

MET THR SER ILE GLY T2 G3 Y4 F11 S12 P13 R16 K48 T51 Y74 H83 R87 E91 R111 Y115 Y122 N140 M146 S150 L172 L175 H179 I195 E205 C215 E219 H224 Y244 GLY ASP ASP ASP

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

- Molecule 15: 26S protease regulatory subunit 7 homolog

Chain 1-H:  18% 75% 8% 16%

MET PRO PRO LYS GLU ASP TRP GLU LYS TYR LYS ALA PRO LEU GLU ASP ASP LYS LYS PRO ASP ASP ASP LYS ILE VAL PRO LEU LYS SER ASP THR GLY ASP ILE GLN VAL LYS SER TYR GLY A42 A43 P44 Y45 A46 A47 K48 L49 K50 Q51 T52 E53 N54 D55 L56 K57 D58 A61

R62 R66 V69 K70 E71 S72 D73 A77 P78 S79 H80 L81 W82 D83 R83 K107 GLY ASN GLY GLU SER LEU THR THR THR ASP ASN ASN ASN SER GLY ASN SER SER SER ASN GLN SER THR ASP ALA ASP ASP ASP ASP ASP F144 Y145

L149 K150 Q151 I152 A153 K154 F155 L159 G160 E161 R162 V163 T166 D167 I168 S179 K180 Y181 E184 L185 P186 D192 P193 S194 E201 E202 D205 V206 T207 D210 C214 E223 V224 L227 L230 S231 P232 E233 R234 T237 L238 Q239 I240 D241 P242 P243

I246 L247 F271 V274 E278 L279 V280 R289 M290 P297 K301 K302 A303 C304 I305 E310 I311 D312 A313 V314 G315 G316 A317 D320 D321 G322 A323 G324 E335 L336 P345 K350 V351 M352 F353 N356 R357 T360 R373 F389 H392 R400

R420 R434 K441 L444 K445 Y454 Y466 W467

- Molecule 15: 26S protease regulatory subunit 7 homolog

Chain 2-H:  75% 8% 16%

MET PRO PRO LYS GLU ASP TRP GLU LYS TYR LYS ALA PRO LEU GLU ASP ASP LYS LYS PRO ASP ASP ASP LYS ILE VAL PRO LEU LYS SER TYR GLY A42 Y45 R62 R66 A77 P78 S79 H80 K107 GLY ASN GLY GLY SER

ASP GLU THR THR ASP ASN ASN ASN GLY SER SER ASN SER SER ASN GLN GLN SER THR ASP ALA ASP ASP GLU ASP ASP S179 K180 Y181 P186 D192 P193 E223 V224 L227 E233 R234 P242 I246 F271 V274

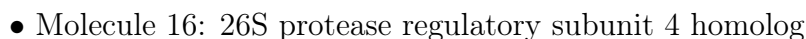
L279 V280 R289 M290 A303 E310 I311 G315 G324 P352 F353 N356 R357 R373 F389 H392 R420 R434 Y454 Y466 W467

- Molecule 15: 26S protease regulatory subunit 7 homolog

72% 11% 16%



Frequency	Percentage
Daily	81%
Weekly	22%
Monthly	6%
Other	12%



81% 5% 12%



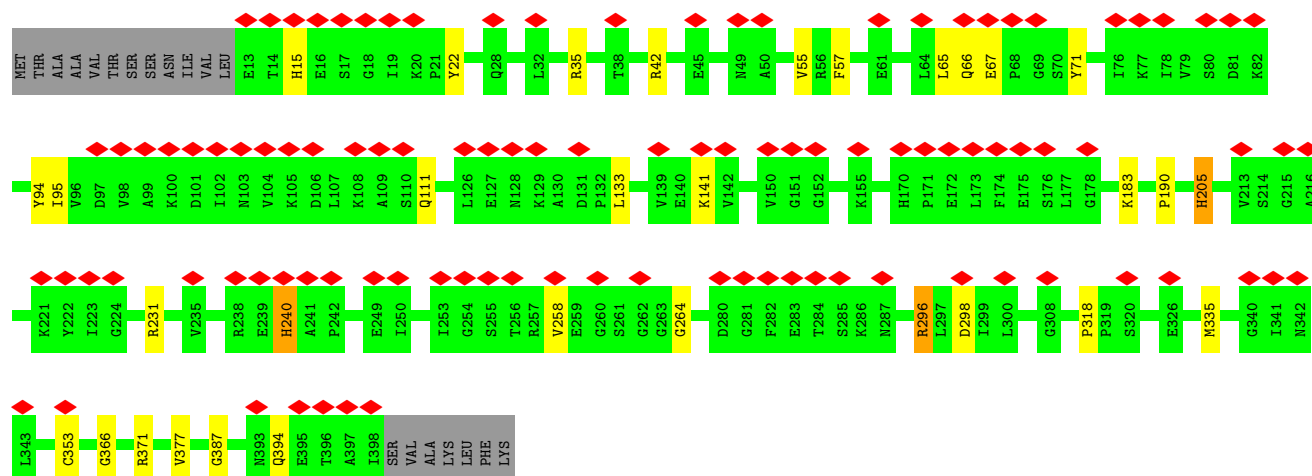
79% 7% .. 12%



Y436
L437

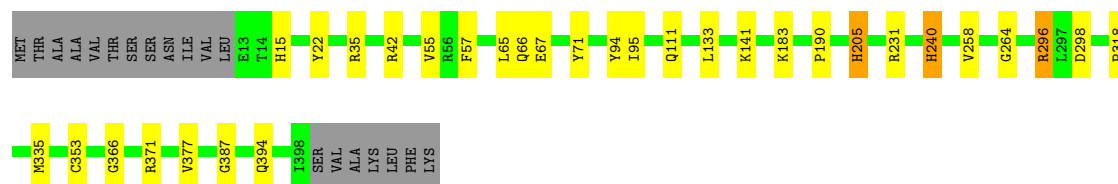
- Molecule 17: 26S protease regulatory subunit 8 homolog

Chain 1-J: 



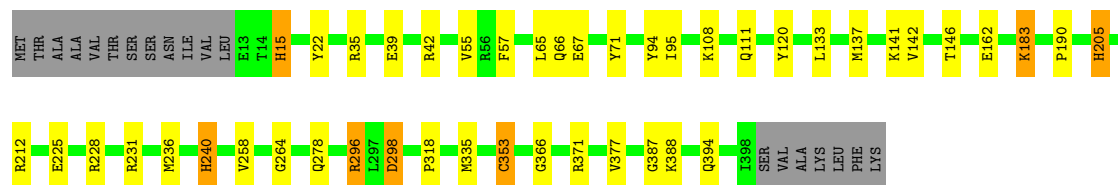
- Molecule 17: 26S protease regulatory subunit 8 homolog

Chain 2-J: 



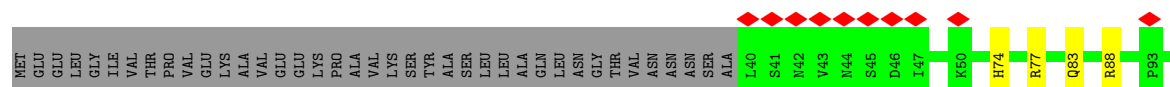
- Molecule 17: 26S protease regulatory subunit 8 homolog

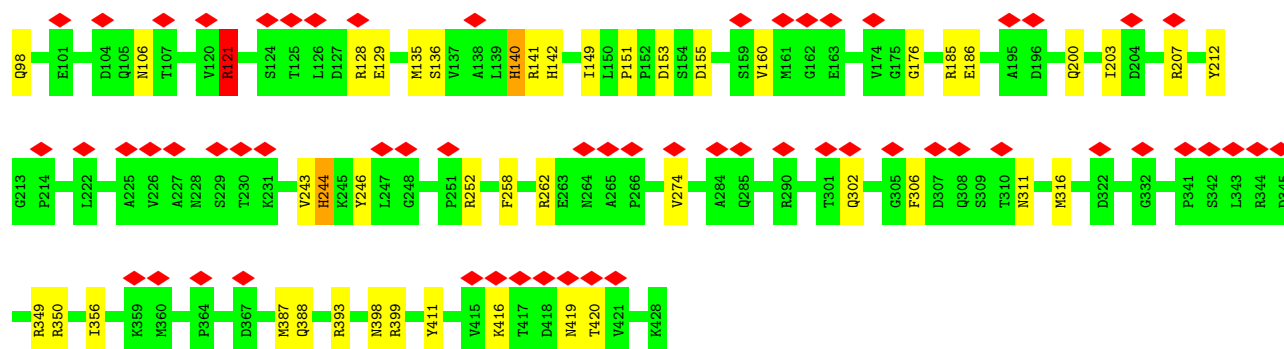
Chain 3-J: 



- Molecule 18: 26S protease regulatory subunit 6B homolog

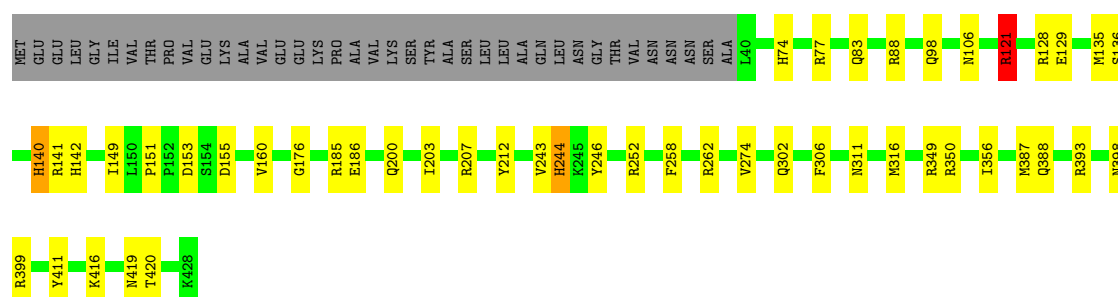
Chain 1-K: 





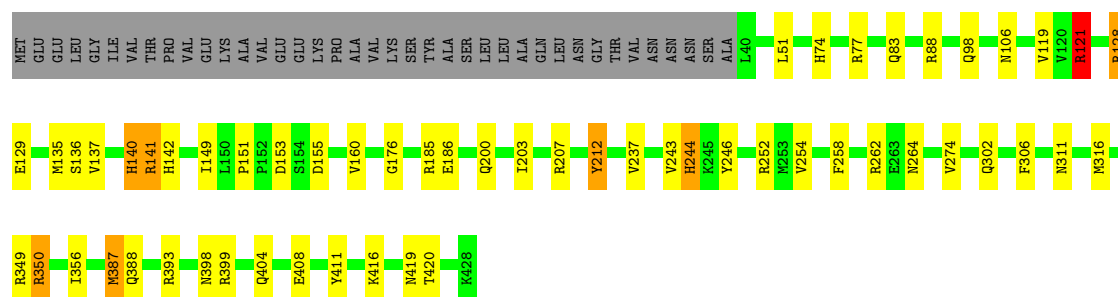
- Molecule 18: 26S protease regulatory subunit 6B homolog

Chain 2-K: 79% 11% 9%



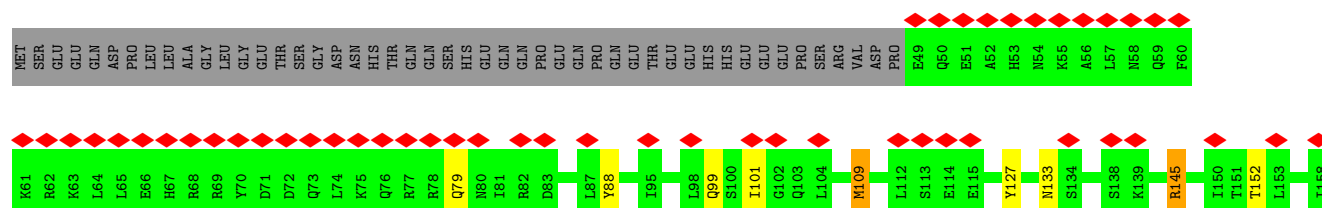
- Molecule 18: 26S protease regulatory subunit 6B homolog

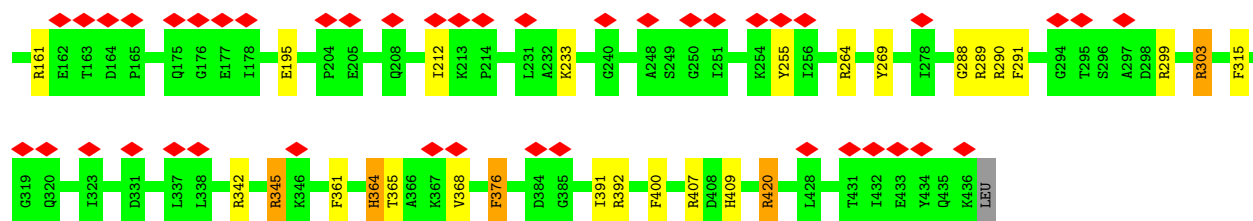
Chain 3-K: 78% 11% 9%



- Molecule 19: 26S protease subunit RPT4

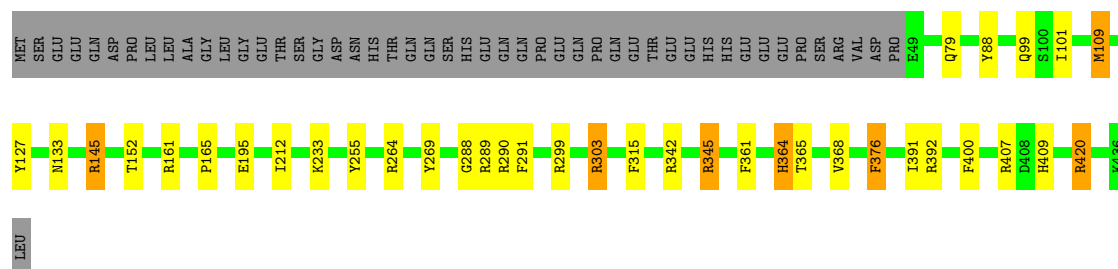
Chain 1-L: 21% 81% 7% 11%





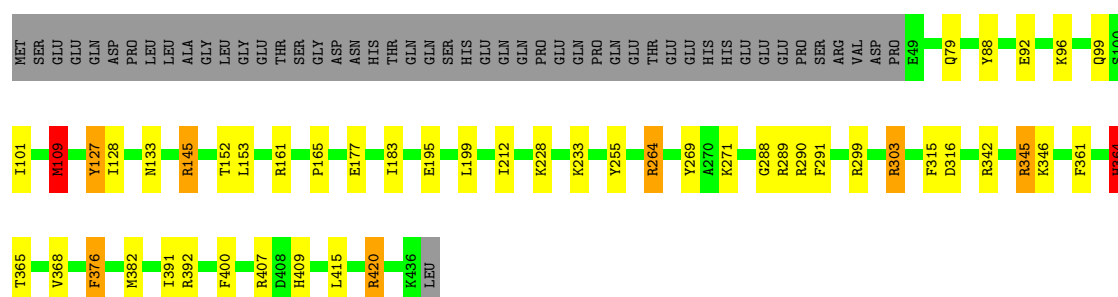
• Molecule 19: 26S protease subunit RPT4

Chain 2-L: 80% 7% 11%



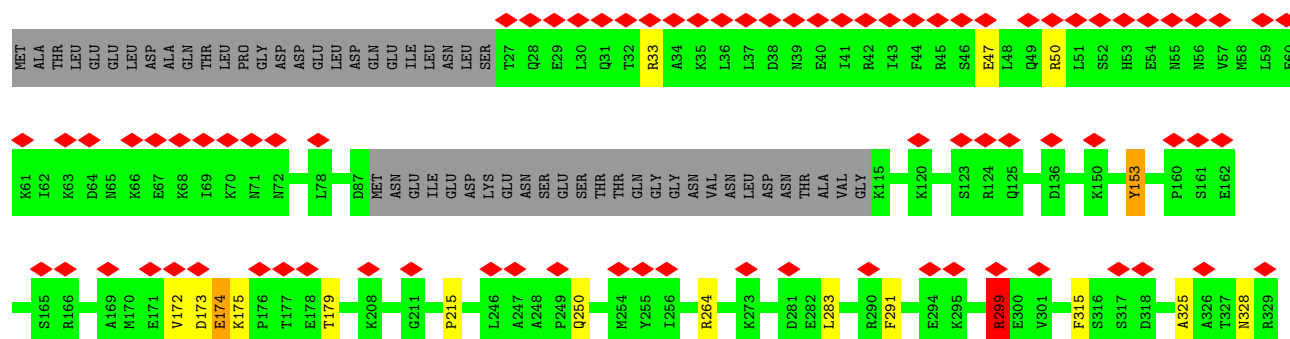
• Molecule 19: 26S protease subunit RPT4

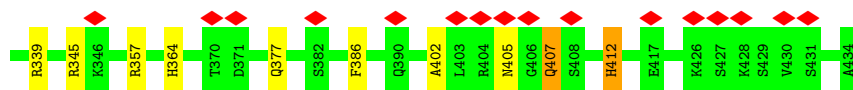
Chain 3-L: 77% 9% 11%



• Molecule 20: 26S protease regulatory subunit 6A

Chain 1-M: 22% 81% 5% 12%





- Molecule 20: 26S protease regulatory subunit 6A

Chain 2-M: 82% 5% • 12%



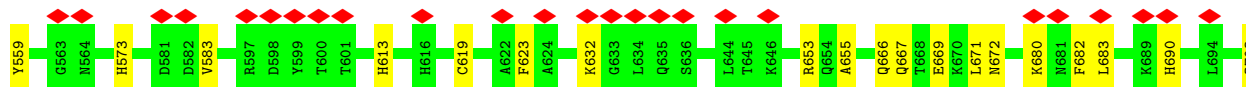
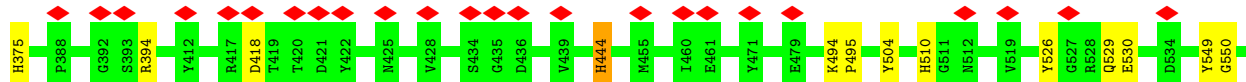
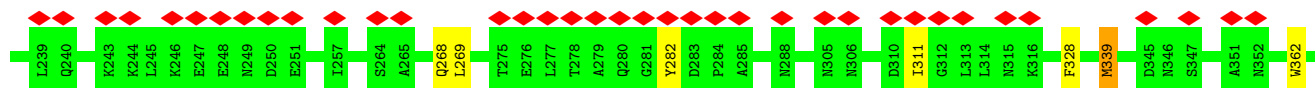
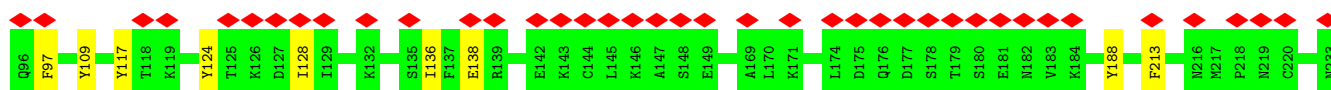
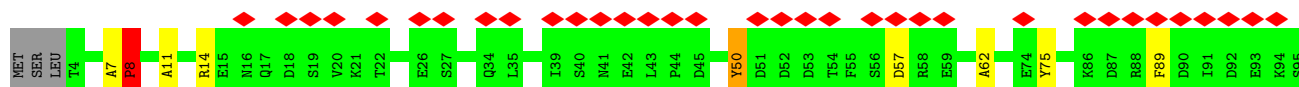
- Molecule 20: 26S protease regulatory subunit 6A

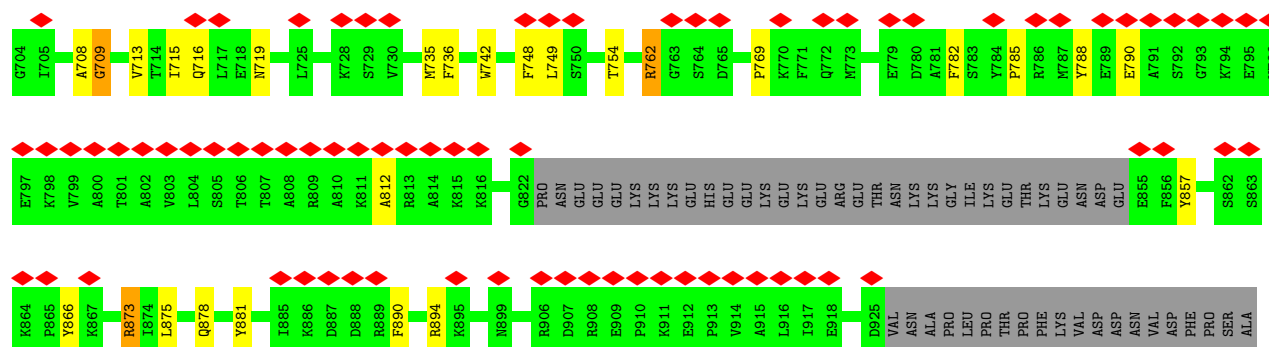
Chain 3-M: 79% 7% • 12%



- Molecule 21: 26S proteasome regulatory subunit RPN2

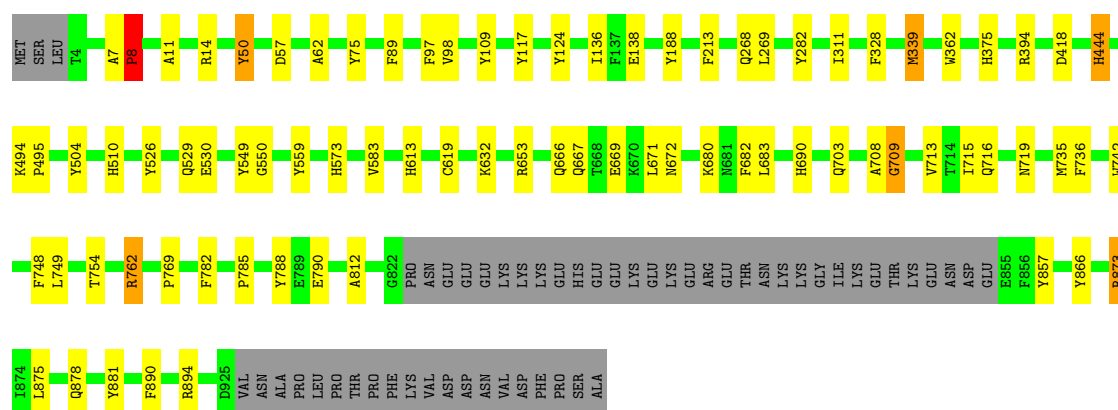
Chain 1-N: 25% 85% 8% • 6%





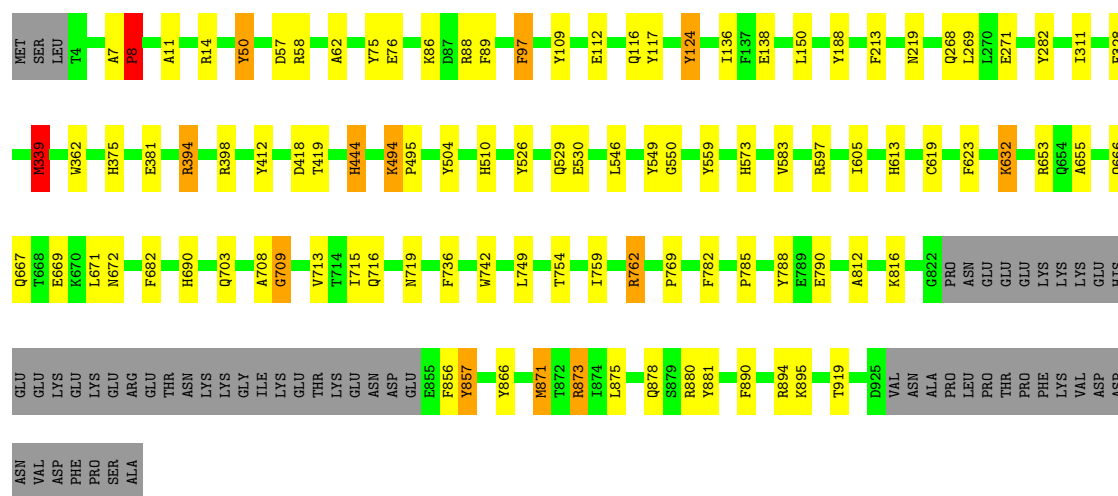
• Molecule 21: 26S proteasome regulatory subunit RPN2

Chain 2-N: 86% 8% 6%



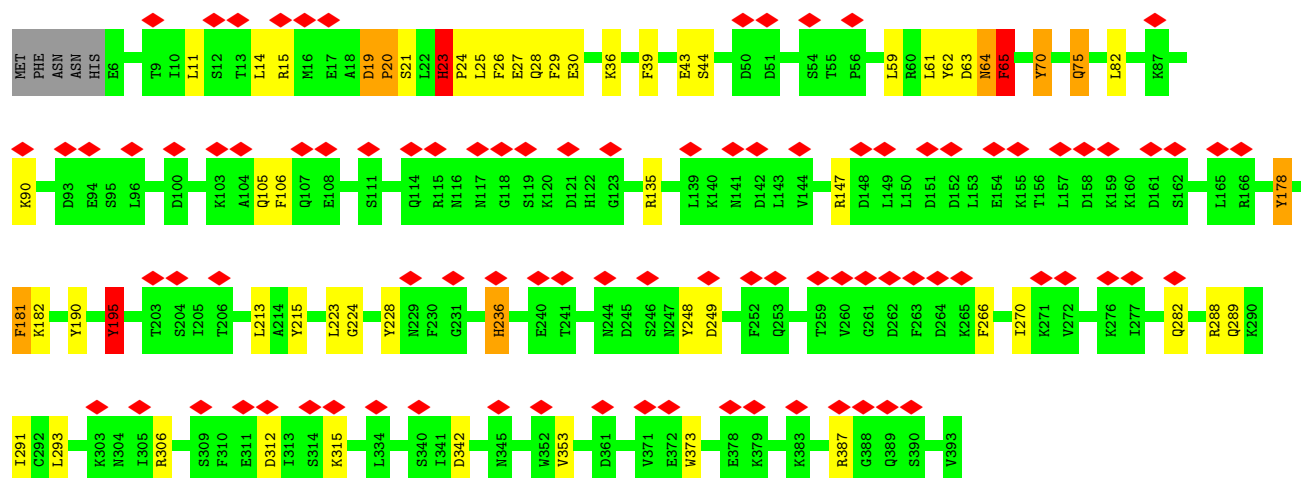
• Molecule 21: 26S proteasome regulatory subunit RPN2

Chain 3-N: 83% 9% 6%



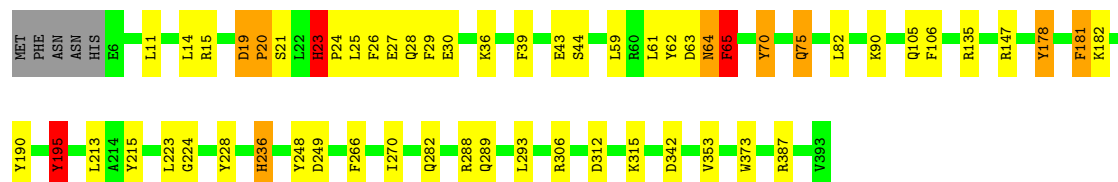
• Molecule 22: 26S proteasome regulatory subunit RPN9

Chain 1-O: 23% 84% 12% ...



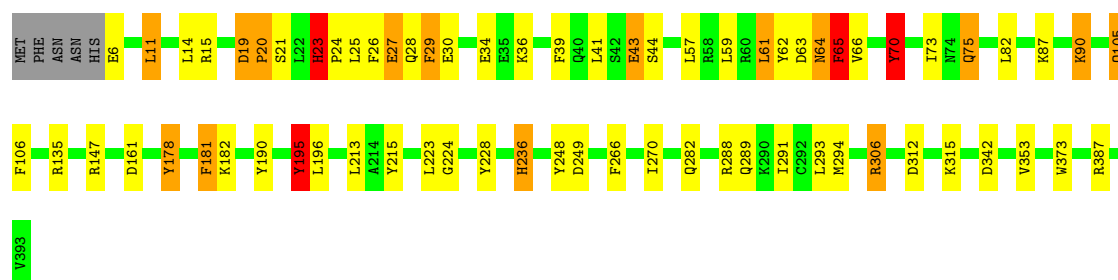
- Molecule 22: 26S proteasome regulatory subunit RPN9

Chain 2-O: 84% 12% ..



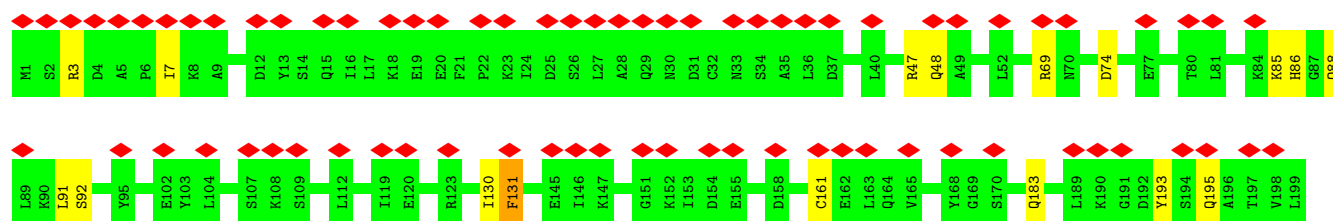
- Molecule 22: 26S proteasome regulatory subunit RPN9

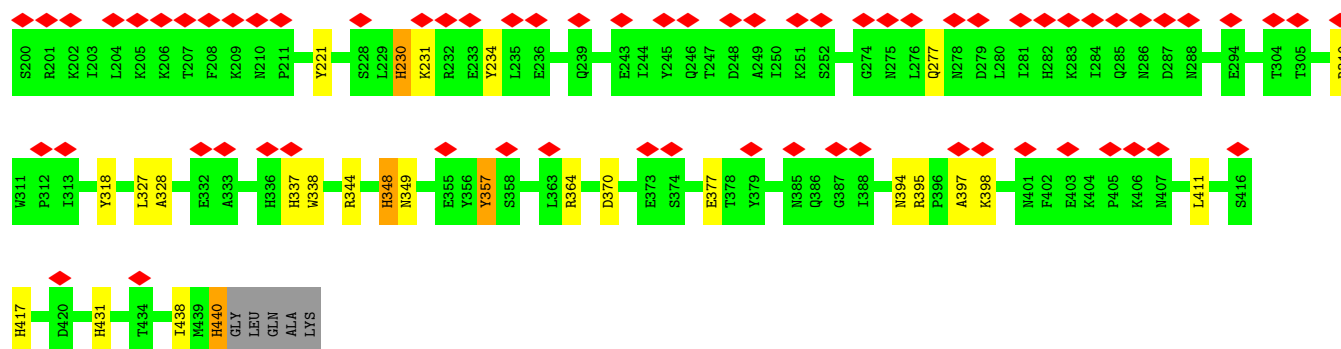
Chain 3-O: 81% 13% ..



- Molecule 23: 26S proteasome regulatory subunit RPN5

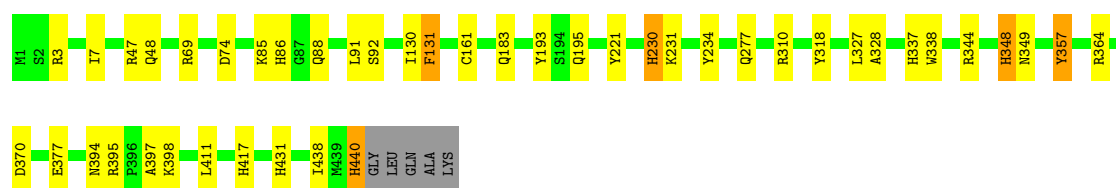
Chain 1-P: 31% 89% 9% ..





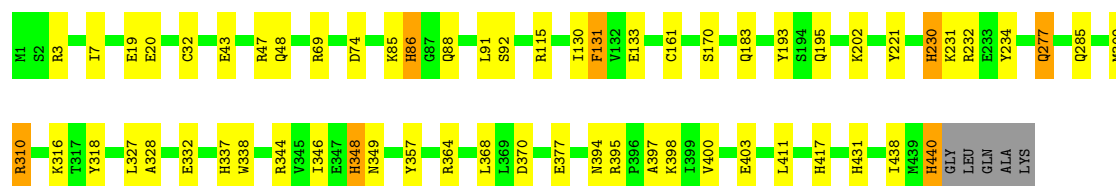
• Molecule 23: 26S proteasome regulatory subunit RPN5

Chain 2-P: 89% 9% ..



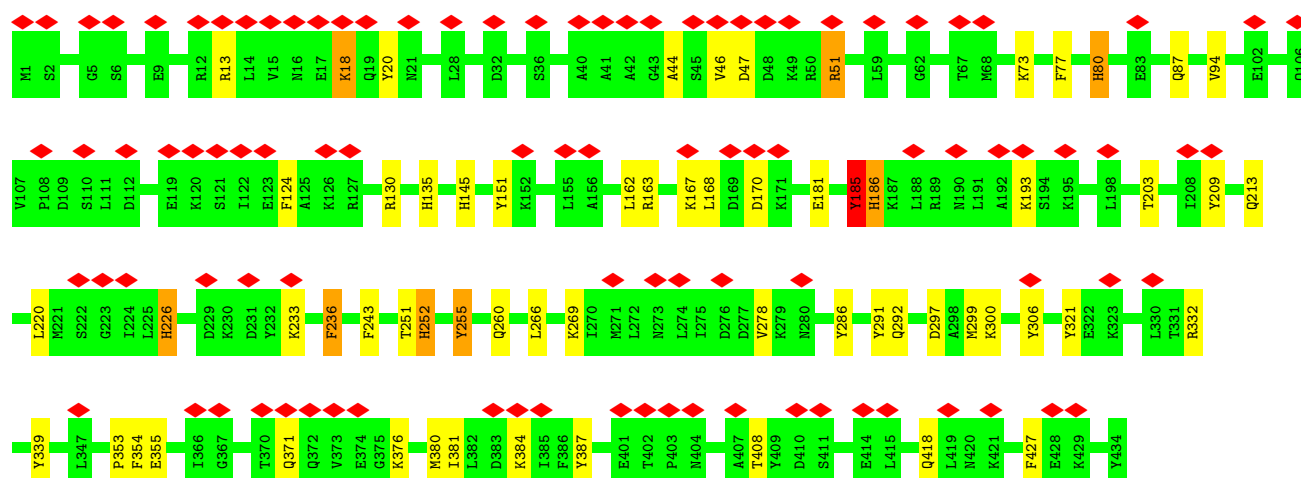
• Molecule 23: 26S proteasome regulatory subunit RPN5

Chain 3-P: 85% 12% ..

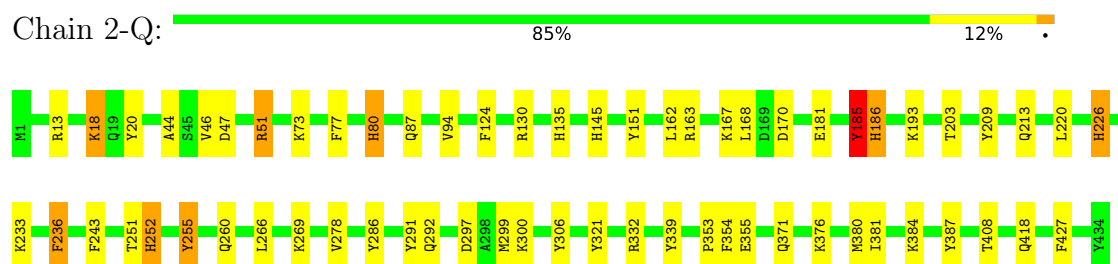


• Molecule 24: 26S proteasome regulatory subunit RPN6

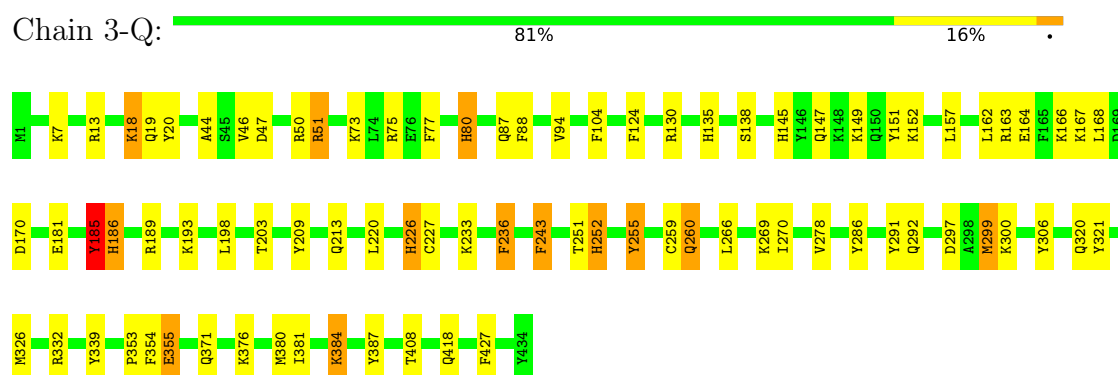
Chain 1-Q: 22% 85% 12% .



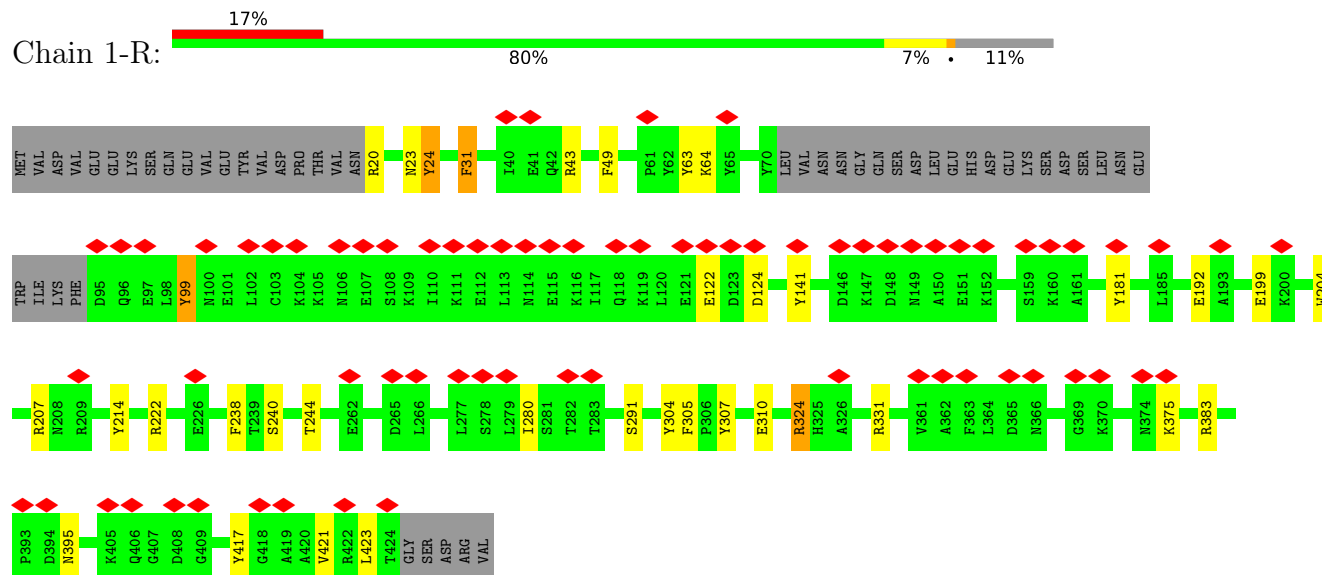
- Molecule 24: 26S proteasome regulatory subunit RPN6



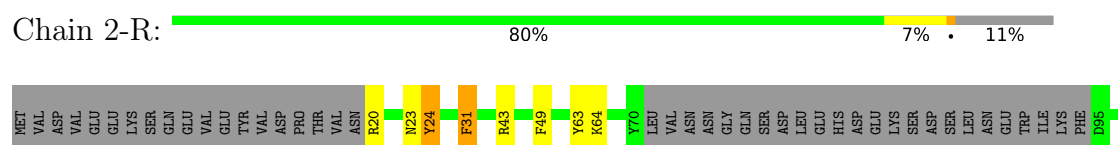
- Molecule 24: 26S proteasome regulatory subunit RPN6



- Molecule 25: 26S proteasome regulatory subunit RPN7

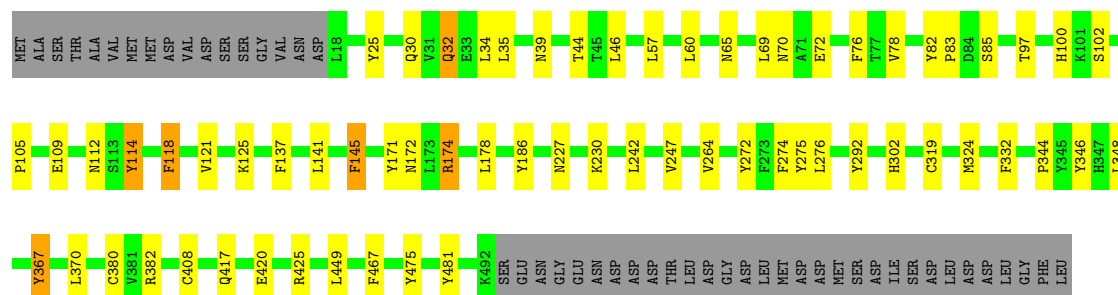


- Molecule 25: 26S proteasome regulatory subunit RPN7

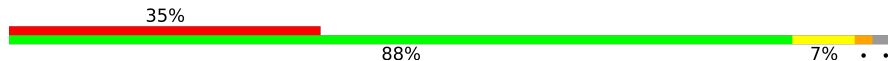


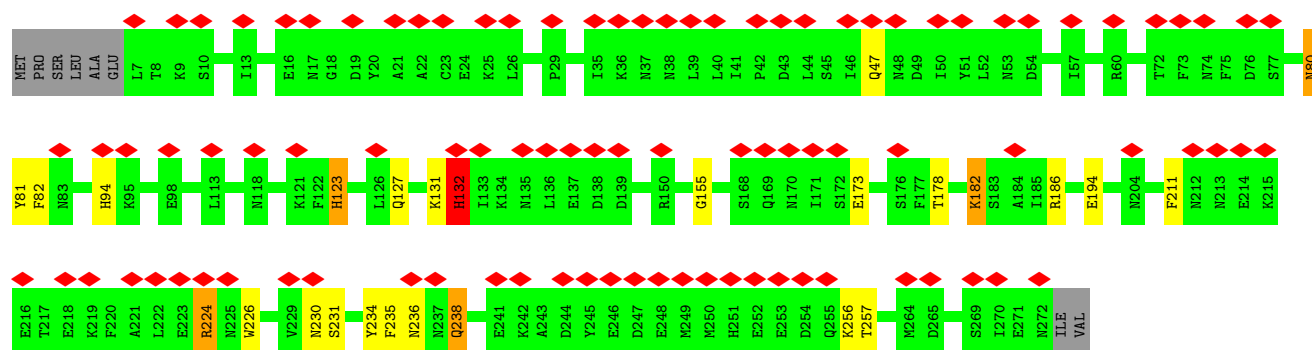
- Molecule 26: 26S proteasome regulatory subunit RPN3

Chain 3-S:  78% 11% 9%



- Molecule 27: 26S proteasome regulatory subunit RPN12

Chain 1-T:  35% 88% 7% ..



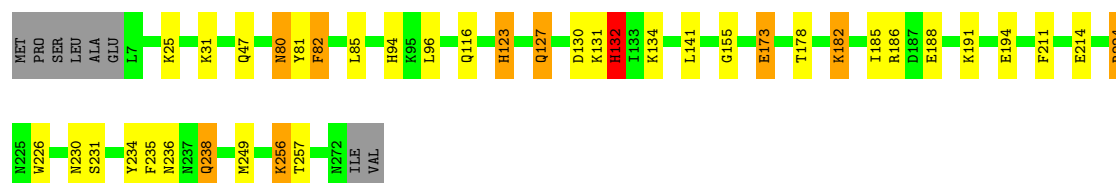
- Molecule 27: 26S proteasome regulatory subunit RPN12

Chain 2-T:  88% 7% ..



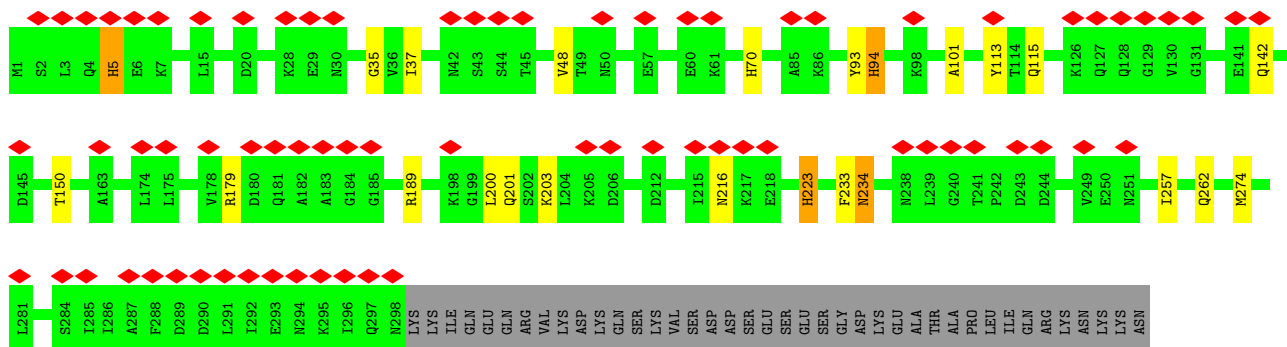
- Molecule 27: 26S proteasome regulatory subunit RPN12

Chain 3-T:  83% 11% ..



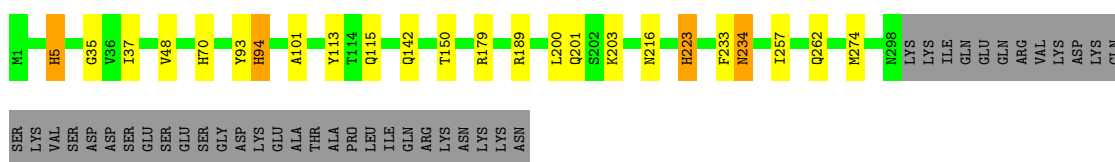
- Molecule 28: 26S proteasome regulatory subunit RPN8

Chain 1-U:  22% 81% 6% 12%



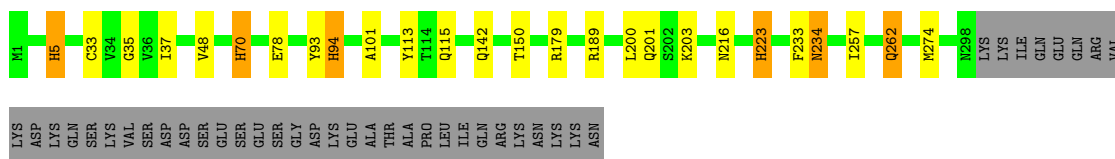
- Molecule 28: 26S proteasome regulatory subunit RPN8

Chain 2-U: 81% 6% • 12%



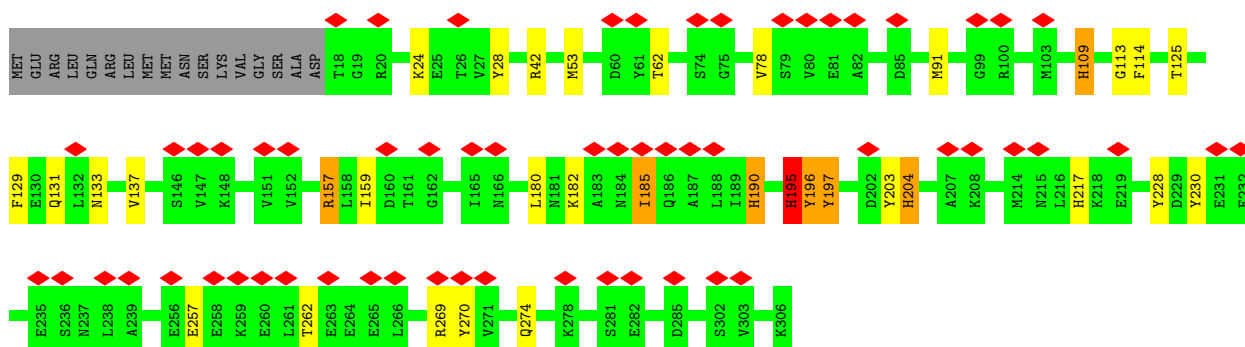
- Molecule 28: 26S proteasome regulatory subunit RPN8

Chain 3-U: 80% 6% • 12%



- Molecule 29: Ubiquitin carboxyl-terminal hydrolase RPN11

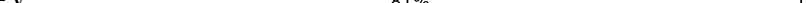
Chain 1-V: 20% 83% 8% • 6%

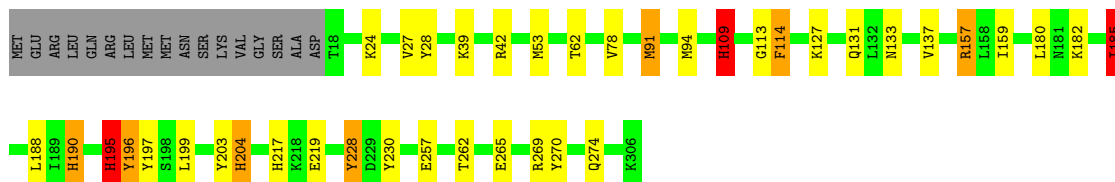


- Molecule 29: Ubiquitin carboxyl-terminal hydrolase RPN11

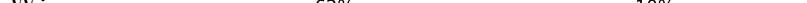
Chain 2-V: 84% 8% • 6%

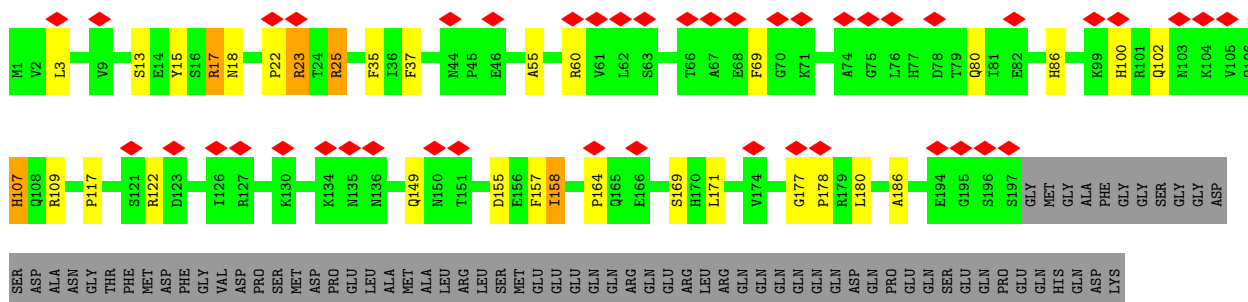
- Molecule 29: Ubiquitin carboxyl-terminal hydrolase RPN11

Chain 3-V:  81% 10% .. 6%

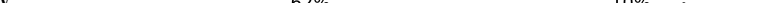


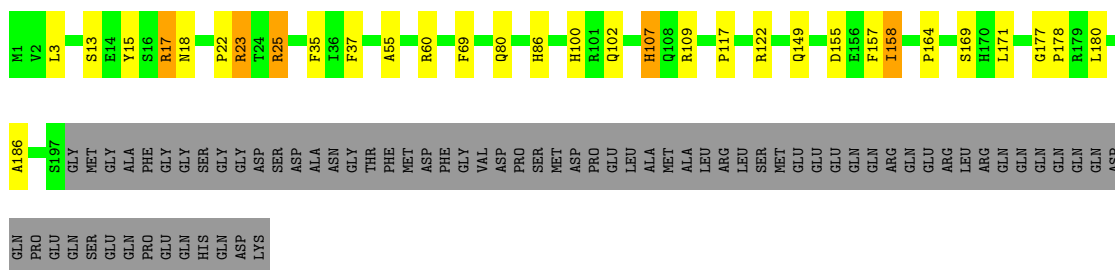
- Molecule 30: 26S proteasome regulatory subunit RPN10

Chain 1-W: 



- Molecule 30: 26S proteasome regulatory subunit RPN10

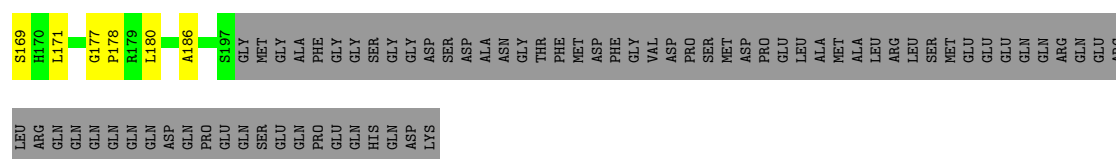
Chain 2-W:  62% 10% 26%



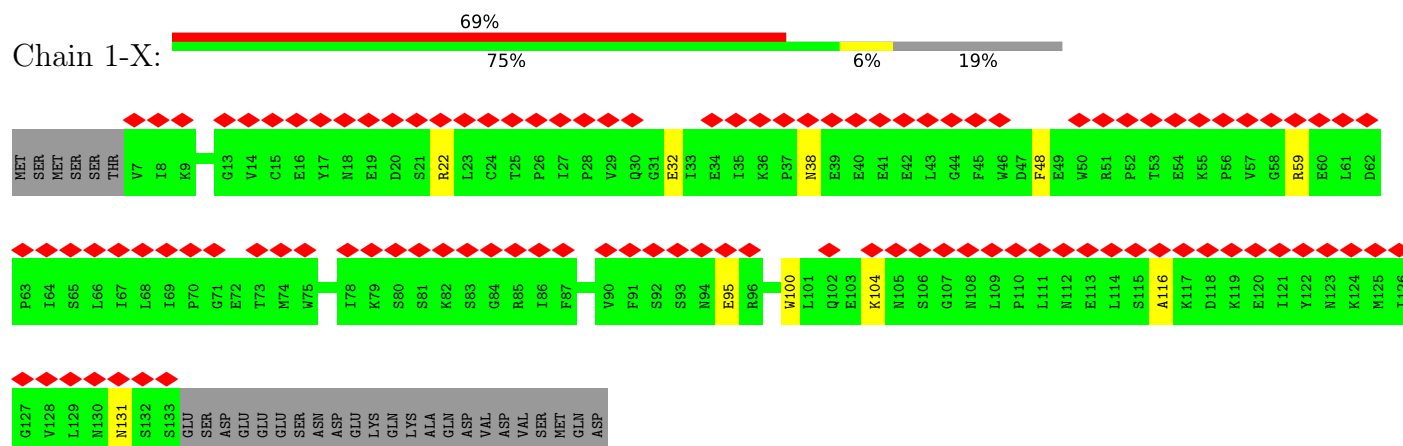
- Molecule 30: 26S proteasome regulatory subunit RPN10

Chain 3-W: 60% 11% 0 26%

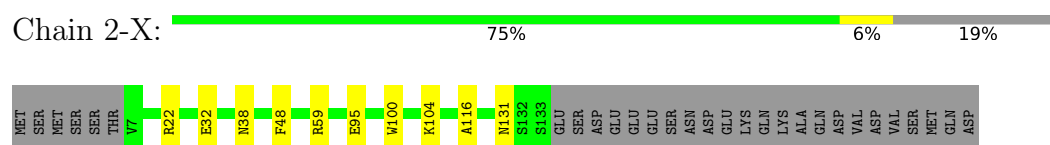




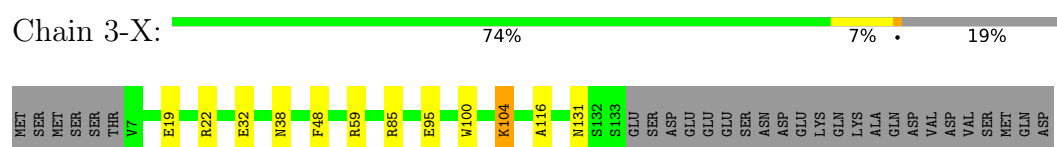
• Molecule 31: 26S proteasome regulatory subunit RPN13



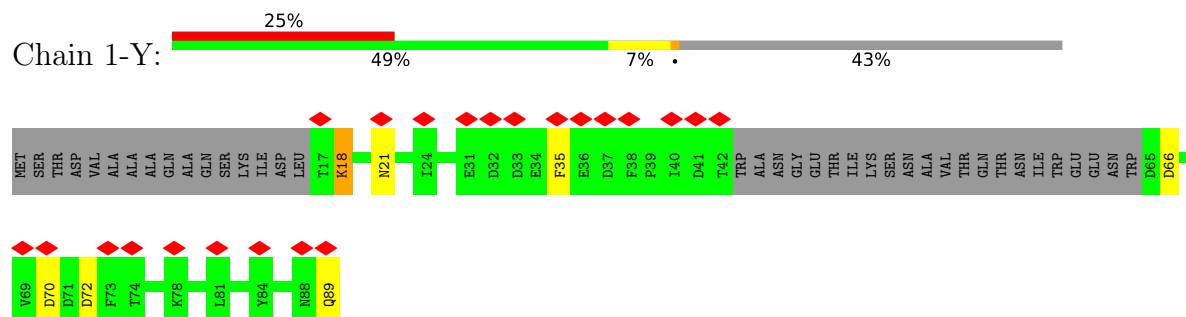
• Molecule 31: 26S proteasome regulatory subunit RPN13



• Molecule 31: 26S proteasome regulatory subunit RPN13

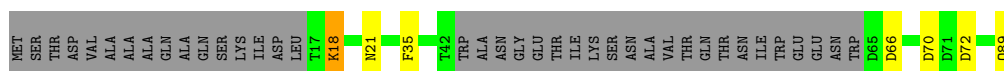


• Molecule 32: 26S proteasome complex subunit SEM1

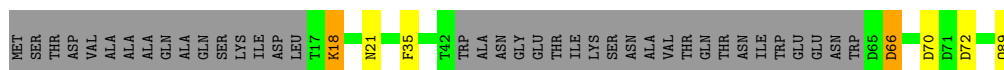


• Molecule 32: 26S proteasome complex subunit SEM1

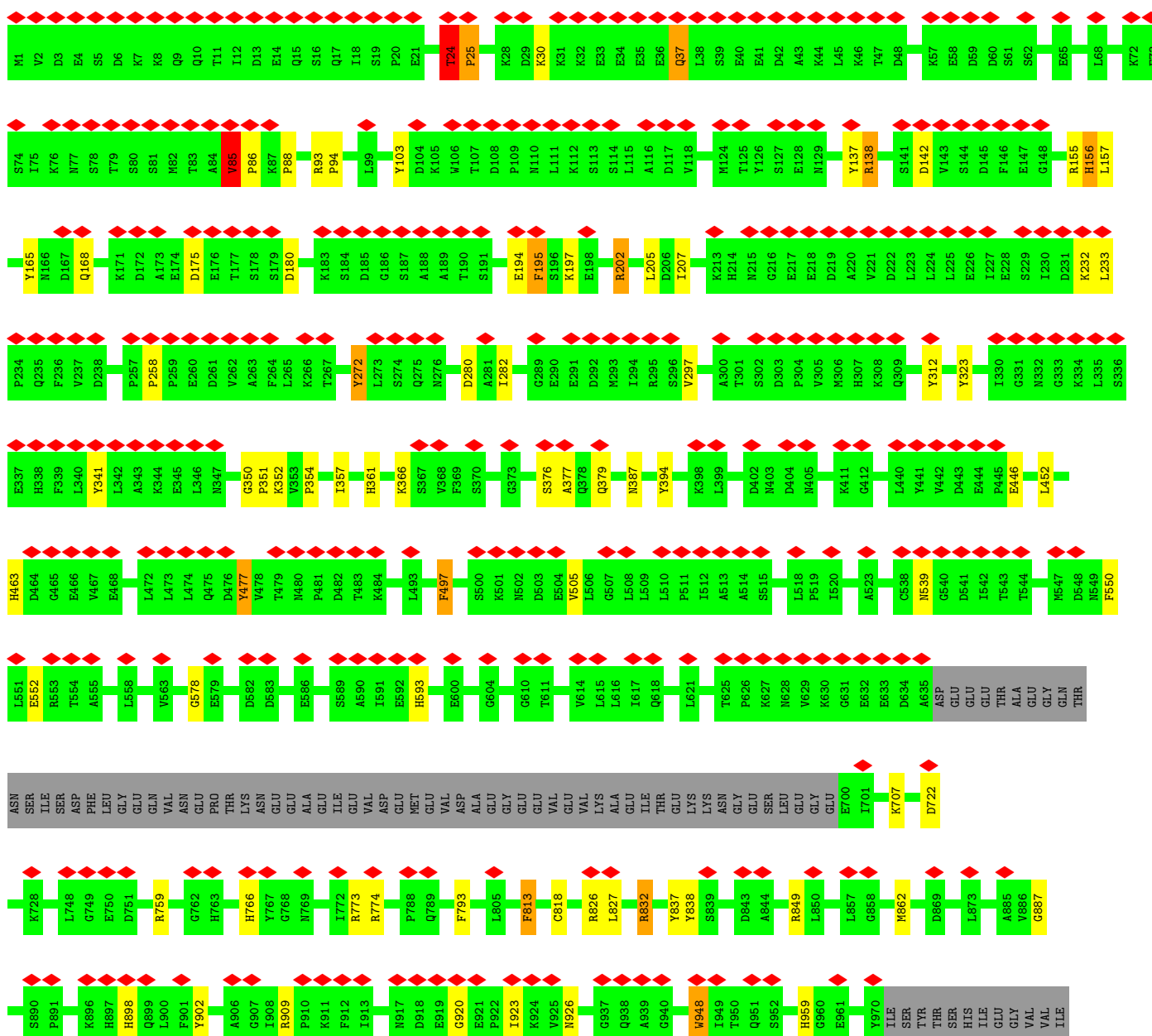
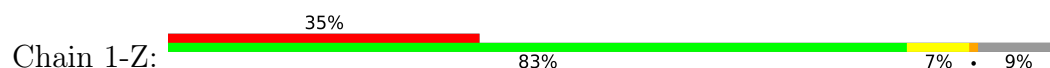




- Molecule 32: 26S proteasome complex subunit SEM1



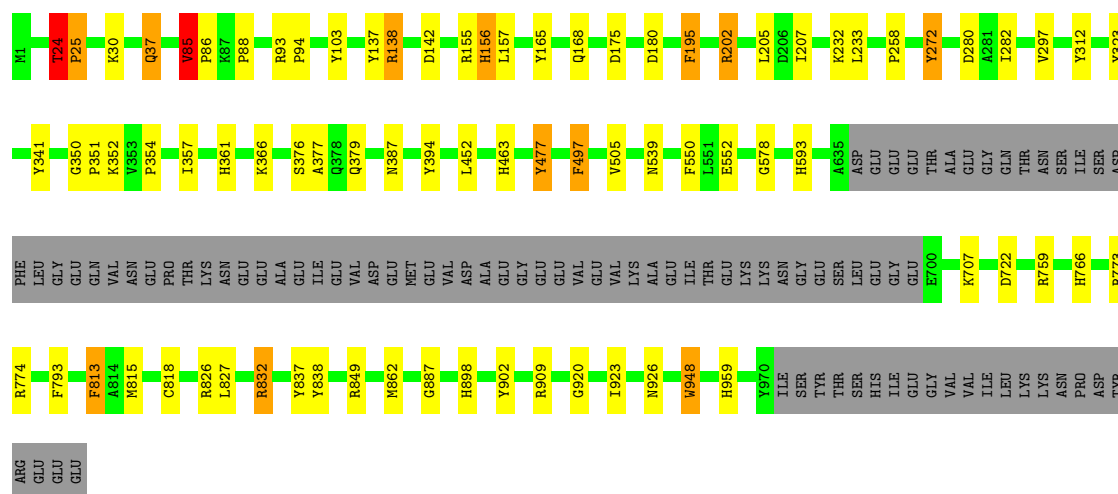
- Molecule 33: 26S proteasome regulatory subunit RPN1



LEU
LYS
LYS
ASN
PRO
ASP
TYR
ARG
GLU
GLU

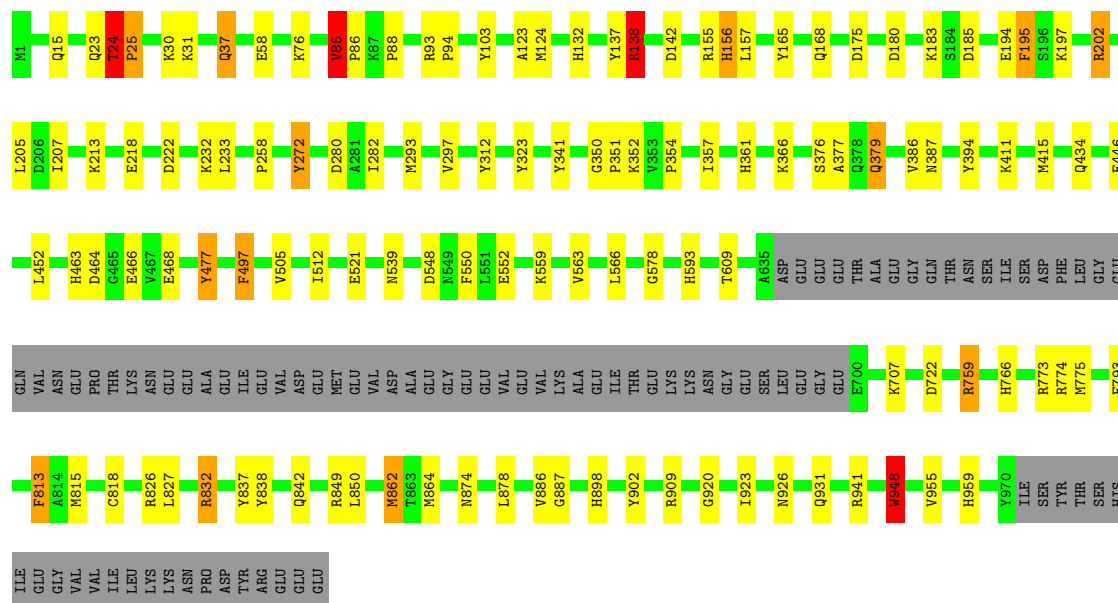
• Molecule 33: 26S proteasome regulatory subunit RPN1

Chain 2-Z:  83% 7% 9%



• Molecule 33: 26S proteasome regulatory subunit RPN1

Chain 3-Z:  79% 11% 9%



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of subtomograms used	1700	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.894	Depositor
Minimum map value	-0.848	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.091	Depositor
Recommended contour level	0.27	Depositor
Map size (Å)	890.88, 890.88, 890.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.32, 2.32, 2.32	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	1-1	0.74	0/1541	1.29	5/2087 (0.2%)
1	1-h	0.72	0/1541	1.27	6/2087 (0.3%)
1	2-1	0.74	0/1541	1.29	5/2087 (0.2%)
1	2-h	0.72	0/1541	1.27	6/2087 (0.3%)
1	3-1	0.74	0/1541	1.29	5/2087 (0.2%)
1	3-h	0.72	0/1541	1.27	6/2087 (0.3%)
2	1-2	0.74	0/1750	1.37	13/2373 (0.5%)
2	1-i	0.75	0/1750	1.34	9/2373 (0.4%)
2	2-2	0.74	0/1750	1.37	13/2373 (0.5%)
2	2-i	0.75	0/1750	1.34	9/2373 (0.4%)
2	3-2	0.74	0/1750	1.37	13/2373 (0.5%)
2	3-i	0.75	0/1750	1.34	9/2373 (0.4%)
3	1-3	0.74	0/1611	1.29	6/2174 (0.3%)
3	1-j	0.72	0/1611	1.27	5/2174 (0.2%)
3	2-3	0.74	0/1611	1.29	6/2174 (0.3%)
3	2-j	0.72	0/1611	1.27	5/2174 (0.2%)
3	3-3	0.74	0/1611	1.29	6/2174 (0.3%)
3	3-j	0.72	0/1611	1.27	5/2174 (0.2%)
4	1-4	0.74	0/1589	1.33	4/2142 (0.2%)
4	1-k	0.74	0/1589	1.34	10/2142 (0.5%)
4	2-4	0.74	0/1589	1.33	4/2142 (0.2%)
4	2-k	0.74	0/1589	1.34	10/2142 (0.5%)
4	3-4	0.74	0/1589	1.33	4/2142 (0.2%)
4	3-k	0.74	0/1589	1.34	10/2142 (0.5%)
5	1-5	0.77	0/1681	1.28	4/2274 (0.2%)
5	1-l	0.75	0/1681	1.28	3/2274 (0.1%)
5	2-5	0.77	0/1681	1.28	4/2274 (0.2%)
5	2-l	0.75	0/1681	1.28	3/2274 (0.1%)
5	3-5	0.77	0/1681	1.28	4/2274 (0.2%)
5	3-l	0.75	0/1681	1.28	3/2274 (0.1%)
6	1-6	0.74	0/1795	1.34	10/2420 (0.4%)
6	1-m	0.74	0/1795	1.33	9/2420 (0.4%)
6	2-6	0.74	0/1795	1.34	10/2420 (0.4%)
6	2-m	0.74	0/1795	1.33	9/2420 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	3-6	0.74	0/1795	1.34	10/2420 (0.4%)
6	3-m	0.74	0/1795	1.33	9/2420 (0.4%)
7	1-7	0.74	0/1821	1.31	7/2470 (0.3%)
7	1-n	0.73	0/1846	1.34	4/2503 (0.2%)
7	2-7	0.74	0/1821	1.31	7/2470 (0.3%)
7	2-n	0.73	0/1846	1.34	4/2503 (0.2%)
7	3-7	0.74	0/1821	1.31	7/2470 (0.3%)
7	3-n	0.73	0/1846	1.34	4/2503 (0.2%)
8	1-A	0.76	0/1945	1.34	6/2634 (0.2%)
8	1-a	0.75	0/1945	1.33	2/2634 (0.1%)
8	2-A	0.76	0/1945	1.34	6/2634 (0.2%)
8	2-a	0.75	0/1945	1.33	2/2634 (0.1%)
8	3-A	0.76	0/1945	1.34	6/2634 (0.2%)
8	3-a	0.75	0/1945	1.33	2/2634 (0.1%)
9	1-B	0.75	0/1952	1.30	7/2642 (0.3%)
9	1-b	0.76	0/1952	1.29	7/2642 (0.3%)
9	2-B	0.75	0/1952	1.30	7/2642 (0.3%)
9	2-b	0.76	0/1952	1.29	7/2642 (0.3%)
9	3-B	0.75	0/1952	1.30	7/2642 (0.3%)
9	3-b	0.76	0/1952	1.29	7/2642 (0.3%)
10	1-C	0.75	0/1934	1.31	7/2618 (0.3%)
10	1-c	0.76	0/1934	1.30	8/2618 (0.3%)
10	2-C	0.75	0/1934	1.31	7/2618 (0.3%)
10	2-c	0.76	0/1934	1.30	8/2618 (0.3%)
10	3-C	0.75	0/1934	1.31	7/2618 (0.3%)
10	3-c	0.76	0/1934	1.30	8/2618 (0.3%)
11	1-D	0.77	0/1910	1.34	7/2586 (0.3%)
11	1-d	0.77	0/1910	1.32	6/2586 (0.2%)
11	2-D	0.77	0/1910	1.34	7/2586 (0.3%)
11	2-d	0.77	0/1910	1.32	6/2586 (0.2%)
11	3-D	0.77	0/1910	1.34	7/2586 (0.3%)
11	3-d	0.77	0/1910	1.32	6/2586 (0.2%)
12	1-E	0.74	0/1886	1.36	6/2541 (0.2%)
12	1-e	0.73	0/1886	1.33	4/2541 (0.2%)
12	2-E	0.74	0/1886	1.36	6/2541 (0.2%)
12	2-e	0.73	0/1886	1.33	4/2541 (0.2%)
12	3-E	0.74	0/1886	1.36	6/2541 (0.2%)
12	3-e	0.73	0/1886	1.33	4/2541 (0.2%)
13	1-F	0.75	0/1823	1.34	10/2463 (0.4%)
13	1-f	0.74	0/1800	1.31	8/2433 (0.3%)
13	2-F	0.75	0/1823	1.34	10/2463 (0.4%)
13	2-f	0.74	0/1800	1.31	8/2433 (0.3%)
13	3-F	0.75	0/1823	1.34	10/2463 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
13	3-f	0.74	0/1800	1.31	8/2433 (0.3%)
14	1-G	0.74	0/1932	1.36	6/2609 (0.2%)
14	1-g	0.74	0/1932	1.34	4/2609 (0.2%)
14	2-G	0.74	0/1932	1.36	6/2609 (0.2%)
14	2-g	0.74	0/1932	1.34	4/2609 (0.2%)
14	3-G	0.74	0/1932	1.36	6/2609 (0.2%)
14	3-g	0.74	0/1932	1.34	4/2609 (0.2%)
15	1-H	0.81	0/3102	1.37	6/4175 (0.1%)
15	2-H	0.81	0/3102	1.37	6/4175 (0.1%)
15	3-H	0.81	0/3102	1.37	6/4175 (0.1%)
16	1-I	0.77	0/3061	1.37	17/4121 (0.4%)
16	2-I	0.77	0/3061	1.37	17/4121 (0.4%)
16	3-I	0.77	0/3061	1.37	17/4121 (0.4%)
17	1-J	0.81	2/3073 (0.1%)	1.37	13/4129 (0.3%)
17	2-J	0.81	2/3073 (0.1%)	1.37	13/4129 (0.3%)
17	3-J	0.81	2/3073 (0.1%)	1.37	13/4129 (0.3%)
18	1-K	0.80	0/3121	1.39	23/4213 (0.5%)
18	2-K	0.80	0/3121	1.39	23/4213 (0.5%)
18	3-K	0.80	0/3121	1.39	23/4213 (0.5%)
19	1-L	0.79	0/3128	1.37	14/4204 (0.3%)
19	2-L	0.79	0/3128	1.37	14/4204 (0.3%)
19	3-L	0.79	0/3128	1.37	14/4204 (0.3%)
20	1-M	0.75	0/3023	1.38	10/4070 (0.2%)
20	2-M	0.75	0/3023	1.38	10/4070 (0.2%)
20	3-M	0.75	0/3023	1.38	10/4070 (0.2%)
21	1-N	0.78	1/6994 (0.0%)	1.44	34/9455 (0.4%)
21	2-N	0.78	1/6994 (0.0%)	1.44	34/9455 (0.4%)
21	3-N	0.78	1/6994 (0.0%)	1.44	34/9455 (0.4%)
22	1-O	0.78	0/3247	1.53	28/4380 (0.6%)
22	2-O	0.78	0/3247	1.53	28/4380 (0.6%)
22	3-O	0.78	0/3247	1.53	28/4380 (0.6%)
23	1-P	0.78	0/3663	1.45	25/4940 (0.5%)
23	2-P	0.78	0/3663	1.45	25/4940 (0.5%)
23	3-P	0.78	0/3663	1.45	25/4940 (0.5%)
24	1-Q	0.79	0/3556	1.49	22/4787 (0.5%)
24	2-Q	0.79	0/3556	1.49	22/4787 (0.5%)
24	3-Q	0.79	0/3556	1.49	22/4787 (0.5%)
25	1-R	0.77	0/3110	1.44	11/4193 (0.3%)
25	2-R	0.77	0/3110	1.44	11/4193 (0.3%)
25	3-R	0.77	0/3110	1.44	11/4193 (0.3%)
26	1-S	0.81	0/3966	1.49	20/5355 (0.4%)
26	2-S	0.81	0/3966	1.49	20/5355 (0.4%)
26	3-S	0.81	0/3966	1.49	20/5355 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	1-T	0.77	0/2235	1.53	20/3017 (0.7%)
27	2-T	0.77	0/2235	1.53	20/3017 (0.7%)
27	3-T	0.77	0/2235	1.53	20/3017 (0.7%)
28	1-U	0.77	0/2407	1.43	13/3258 (0.4%)
28	2-U	0.77	0/2407	1.43	13/3258 (0.4%)
28	3-U	0.77	0/2407	1.43	13/3258 (0.4%)
29	1-V	0.82	1/2309 (0.0%)	1.51	15/3115 (0.5%)
29	2-V	0.82	1/2309 (0.0%)	1.51	15/3115 (0.5%)
29	3-V	0.82	1/2309 (0.0%)	1.51	15/3115 (0.5%)
30	1-W	0.80	0/1557	1.50	14/2111 (0.7%)
30	2-W	0.80	0/1557	1.50	14/2111 (0.7%)
30	3-W	0.80	0/1557	1.50	14/2111 (0.7%)
31	1-X	0.81	0/1058	1.45	6/1432 (0.4%)
31	2-X	0.81	0/1058	1.45	6/1432 (0.4%)
31	3-X	0.81	0/1058	1.45	6/1432 (0.4%)
32	1-Y	0.79	0/438	1.54	5/583 (0.9%)
32	2-Y	0.79	0/438	1.54	5/583 (0.9%)
32	3-Y	0.79	0/438	1.54	5/583 (0.9%)
33	1-Z	0.79	0/7122	1.47	42/9645 (0.4%)
33	2-Z	0.79	0/7122	1.47	42/9645 (0.4%)
33	3-Z	0.79	0/7122	1.47	42/9645 (0.4%)
All	All	0.77	12/331536 (0.0%)	1.39	1563/447756 (0.3%)

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	1-1	0	4
1	1-h	0	5
1	2-1	0	4
1	2-h	0	5
1	3-1	0	4
1	3-h	0	5
2	1-2	0	5
2	1-i	0	5
2	2-2	0	5
2	2-i	0	5
2	3-2	0	5
2	3-i	0	5
3	1-3	0	7

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
3	1-j	0	7
3	2-3	0	7
3	2-j	0	7
3	3-3	0	7
3	3-j	0	7
4	1-4	0	8
4	1-k	0	7
4	2-4	0	8
4	2-k	0	7
4	3-4	0	8
4	3-k	0	7
5	1-5	0	7
5	1-l	0	6
5	2-5	0	7
5	2-l	0	6
5	3-5	0	7
5	3-l	0	6
6	1-6	0	9
6	1-m	0	4
6	2-6	0	9
6	2-m	0	4
6	3-6	0	9
6	3-m	0	4
7	1-7	0	4
7	1-n	0	7
7	2-7	0	4
7	2-n	0	7
7	3-7	0	4
7	3-n	0	7
8	1-A	0	7
8	1-a	0	10
8	2-A	0	7
8	2-a	0	9
8	3-A	0	7
8	3-a	0	10
9	1-B	0	7
9	1-b	0	4
9	2-B	0	7
9	2-b	0	4
9	3-B	0	7
9	3-b	0	4
10	1-C	0	11

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	1-c	0	5
10	2-C	0	11
10	2-c	0	5
10	3-C	0	11
10	3-c	0	5
11	1-D	0	5
11	1-d	0	6
11	2-D	0	5
11	2-d	0	6
11	3-D	0	5
11	3-d	0	6
12	1-E	0	5
12	1-e	0	5
12	2-E	0	5
12	2-e	0	5
12	3-E	0	5
12	3-e	0	5
13	1-F	0	7
13	1-f	0	6
13	2-F	0	8
13	2-f	0	6
13	3-F	0	8
13	3-f	0	6
14	1-G	0	7
14	1-g	0	7
14	2-G	0	7
14	2-g	0	7
14	3-G	0	7
14	3-g	0	7
15	1-H	0	12
15	2-H	0	12
15	3-H	0	12
16	1-I	0	10
16	2-I	0	10
16	3-I	0	10
17	1-J	0	6
17	2-J	0	6
17	3-J	0	6
18	1-K	0	10
18	2-K	0	10
18	3-K	0	10
19	1-L	0	14

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Mol	Chain	#Chirality outliers	#Planarity outliers
19	2-L	0	14
19	3-L	0	14
20	1-M	0	7
20	2-M	0	7
20	3-M	0	7
21	1-N	0	22
21	2-N	0	22
21	3-N	0	22
22	1-O	0	12
22	2-O	0	12
22	3-O	0	12
23	1-P	0	12
23	2-P	0	12
23	3-P	0	12
24	1-Q	0	19
24	2-Q	0	19
24	3-Q	0	19
25	1-R	0	11
25	2-R	0	11
25	3-R	0	11
26	1-S	0	14
26	2-S	0	14
26	3-S	0	14
27	1-T	0	3
27	2-T	0	3
27	3-T	0	3
28	1-U	0	5
28	2-U	0	5
28	3-U	0	5
29	1-V	0	10
29	2-V	0	10
29	3-V	0	10
30	1-W	0	8
30	2-W	0	8
30	3-W	0	8
31	1-X	0	1
31	2-X	0	1
31	3-X	0	1
32	1-Y	0	1
32	2-Y	0	1
32	3-Y	0	1
33	1-Z	0	20

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Mol	Chain	#Chirality outliers	#Planarity outliers
33	2-Z	0	20
33	3-Z	0	20
All	All	0	1123

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1-J	190	PRO	CA-C	6.07	1.55	1.51
17	2-J	190	PRO	CA-C	6.07	1.55	1.51
17	3-J	190	PRO	CA-C	6.07	1.55	1.51
29	1-V	196	TYR	CA-C	5.88	1.55	1.52
29	2-V	196	TYR	CA-C	5.88	1.55	1.52
29	3-V	196	TYR	CA-C	5.88	1.55	1.52
17	1-J	318	PRO	CA-C	5.61	1.54	1.51
17	2-J	318	PRO	CA-C	5.61	1.54	1.51
17	3-J	318	PRO	CA-C	5.61	1.54	1.51
21	1-N	8	PRO	CA-CB	5.07	1.60	1.53
21	2-N	8	PRO	CA-CB	5.07	1.60	1.53
21	3-N	8	PRO	CA-CB	5.07	1.60	1.53

All (1563) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	1-T	82	PHE	CA-CB-CG	11.04	124.84	113.80
27	2-T	82	PHE	CA-CB-CG	11.04	124.84	113.80
27	3-T	82	PHE	CA-CB-CG	11.04	124.84	113.80
33	1-Z	195	PHE	CA-CB-CG	10.31	124.11	113.80
33	2-Z	195	PHE	CA-CB-CG	10.31	124.11	113.80
33	3-Z	195	PHE	CA-CB-CG	10.31	124.11	113.80
7	1-n	216	ASN	CA-CB-CG	10.18	122.78	112.60
7	2-n	216	ASN	CA-CB-CG	10.18	122.78	112.60
7	3-n	216	ASN	CA-CB-CG	10.18	122.78	112.60
29	1-V	196	TYR	CA-C-O	10.05	125.50	119.77
29	2-V	196	TYR	CA-C-O	10.05	125.50	119.77
29	3-V	196	TYR	CA-C-O	10.05	125.50	119.77
29	1-V	114	PHE	CA-CB-CG	9.96	123.77	113.80
29	2-V	114	PHE	CA-CB-CG	9.96	123.77	113.80
29	3-V	114	PHE	CA-CB-CG	9.96	123.77	113.80
22	1-O	64	ASN	CA-CB-CG	9.90	122.50	112.60
22	2-O	64	ASN	CA-CB-CG	9.90	122.50	112.60
22	3-O	64	ASN	CA-CB-CG	9.90	122.50	112.60
19	1-L	364	HIS	CB-CG-CD2	-9.84	118.41	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2-L	364	HIS	CB-CG-CD2	-9.84	118.41	131.20
19	3-L	364	HIS	CB-CG-CD2	-9.84	118.41	131.20
10	1-c	30	HIS	CB-CG-CD2	-8.95	119.57	131.20
10	2-c	30	HIS	CB-CG-CD2	-8.95	119.57	131.20
10	3-c	30	HIS	CB-CG-CD2	-8.95	119.57	131.20
32	1-Y	21	ASN	N-CA-C	8.77	122.97	111.75
32	2-Y	21	ASN	N-CA-C	8.77	122.97	111.75
32	3-Y	21	ASN	N-CA-C	8.77	122.97	111.75
3	1-3	44	HIS	CB-CG-CD2	-8.66	119.95	131.20
3	2-3	44	HIS	CB-CG-CD2	-8.66	119.95	131.20
3	3-3	44	HIS	CB-CG-CD2	-8.66	119.95	131.20
19	1-L	376	PHE	CA-CB-CG	-8.63	105.17	113.80
19	2-L	376	PHE	CA-CB-CG	-8.63	105.17	113.80
19	3-L	376	PHE	CA-CB-CG	-8.63	105.17	113.80
15	1-H	242	PRO	N-CA-CB	8.62	108.02	103.19
15	2-H	242	PRO	N-CA-CB	8.62	108.02	103.19
15	3-H	242	PRO	N-CA-CB	8.62	108.02	103.19
6	1-6	92	ASN	CA-CB-CG	-8.61	103.99	112.60
6	2-6	92	ASN	CA-CB-CG	-8.61	103.99	112.60
6	3-6	92	ASN	CA-CB-CG	-8.61	103.99	112.60
33	1-Z	813	PHE	CA-CB-CG	-8.55	105.25	113.80
33	2-Z	813	PHE	CA-CB-CG	-8.55	105.25	113.80
33	3-Z	813	PHE	CA-CB-CG	-8.55	105.25	113.80
22	1-O	65	PHE	CA-CB-CG	-8.43	105.37	113.80
22	2-O	65	PHE	CA-CB-CG	-8.43	105.37	113.80
22	3-O	65	PHE	CA-CB-CG	-8.43	105.37	113.80
28	1-U	5	HIS	CA-CB-CG	8.21	122.01	113.80
28	2-U	5	HIS	CA-CB-CG	8.21	122.01	113.80
28	3-U	5	HIS	CA-CB-CG	8.21	122.01	113.80
27	1-T	123	HIS	CB-CG-CD2	-8.09	120.68	131.20
27	2-T	123	HIS	CB-CG-CD2	-8.09	120.68	131.20
27	3-T	123	HIS	CB-CG-CD2	-8.09	120.68	131.20
27	1-T	257	THR	CB-CA-C	7.97	125.88	116.63
27	2-T	257	THR	CB-CA-C	7.97	125.88	116.63
27	3-T	257	THR	CB-CA-C	7.97	125.88	116.63
18	1-K	302	GLN	OE1-CD-NE2	-7.94	114.66	122.60
18	2-K	302	GLN	OE1-CD-NE2	-7.94	114.66	122.60
18	3-K	302	GLN	OE1-CD-NE2	-7.94	114.66	122.60
22	1-O	223	LEU	CA-C-N	7.87	127.57	120.10
22	1-O	223	LEU	C-N-CA	7.87	127.57	120.10
22	2-O	223	LEU	CA-C-N	7.87	127.57	120.10
22	2-O	223	LEU	C-N-CA	7.87	127.57	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3-O	223	LEU	CA-C-N	7.87	127.57	120.10
22	3-O	223	LEU	C-N-CA	7.87	127.57	120.10
9	1-B	94	HIS	CB-CG-CD2	-7.77	121.10	131.20
9	2-B	94	HIS	CB-CG-CD2	-7.77	121.10	131.20
9	3-B	94	HIS	CB-CG-CD2	-7.77	121.10	131.20
24	1-Q	418	GLN	OE1-CD-NE2	-7.75	114.85	122.60
24	2-Q	418	GLN	OE1-CD-NE2	-7.75	114.85	122.60
24	3-Q	418	GLN	OE1-CD-NE2	-7.75	114.85	122.60
19	1-L	101	ILE	CB-CA-C	7.72	122.15	111.34
19	2-L	101	ILE	CB-CA-C	7.72	122.15	111.34
19	3-L	101	ILE	CB-CA-C	7.72	122.15	111.34
26	1-S	145	PHE	CA-CB-CG	-7.72	106.08	113.80
26	2-S	145	PHE	CA-CB-CG	-7.72	106.08	113.80
26	3-S	145	PHE	CA-CB-CG	-7.72	106.08	113.80
6	1-6	221	ARG	NE-CZ-NH2	7.71	126.14	119.20
6	2-6	221	ARG	NE-CZ-NH2	7.71	126.14	119.20
6	3-6	221	ARG	NE-CZ-NH2	7.71	126.14	119.20
2	1-i	114	HIS	CB-CG-CD2	-7.71	121.18	131.20
2	2-i	114	HIS	CB-CG-CD2	-7.71	121.18	131.20
2	3-i	114	HIS	CB-CG-CD2	-7.71	121.18	131.20
26	1-S	332	PHE	CA-CB-CG	7.65	121.45	113.80
26	2-S	332	PHE	CA-CB-CG	7.65	121.45	113.80
26	3-S	332	PHE	CA-CB-CG	7.65	121.45	113.80
31	1-X	100	TRP	CB-CG-CD2	7.57	137.40	126.80
31	2-X	100	TRP	CB-CG-CD2	7.57	137.40	126.80
31	3-X	100	TRP	CB-CG-CD2	7.57	137.40	126.80
33	1-Z	766	HIS	CB-CG-CD2	-7.53	121.41	131.20
33	2-Z	766	HIS	CB-CG-CD2	-7.53	121.41	131.20
33	3-Z	766	HIS	CB-CG-CD2	-7.53	121.41	131.20
16	1-I	150	HIS	CB-CG-CD2	-7.45	121.51	131.20
16	2-I	150	HIS	CB-CG-CD2	-7.45	121.51	131.20
16	3-I	150	HIS	CB-CG-CD2	-7.45	121.51	131.20
20	1-M	291	PHE	CA-CB-CG	7.40	121.20	113.80
20	2-M	291	PHE	CA-CB-CG	7.40	121.20	113.80
20	3-M	291	PHE	CA-CB-CG	7.40	121.20	113.80
4	1-k	146	HIS	CB-CG-CD2	-7.36	121.63	131.20
4	2-k	146	HIS	CB-CG-CD2	-7.36	121.63	131.20
4	3-k	146	HIS	CB-CG-CD2	-7.36	121.63	131.20
14	1-G	182	GLY	N-CA-C	-7.33	104.56	112.04
14	2-G	182	GLY	N-CA-C	-7.33	104.56	112.04
14	3-G	182	GLY	N-CA-C	-7.33	104.56	112.04
2	1-2	66	HIS	CB-CG-CD2	-7.33	121.67	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2-2	66	HIS	CB-CG-CD2	-7.33	121.67	131.20
2	3-2	66	HIS	CB-CG-CD2	-7.33	121.67	131.20
33	1-Z	387	ASN	CA-CB-CG	-7.32	105.28	112.60
33	2-Z	387	ASN	CA-CB-CG	-7.32	105.28	112.60
33	3-Z	387	ASN	CA-CB-CG	-7.32	105.28	112.60
21	1-N	703	GLN	OE1-CD-NE2	-7.27	115.33	122.60
21	2-N	703	GLN	OE1-CD-NE2	-7.27	115.33	122.60
21	3-N	703	GLN	OE1-CD-NE2	-7.27	115.33	122.60
33	1-Z	156	HIS	CB-CG-CD2	-7.22	121.81	131.20
33	2-Z	156	HIS	CB-CG-CD2	-7.22	121.81	131.20
33	3-Z	156	HIS	CB-CG-CD2	-7.22	121.81	131.20
20	1-M	412	HIS	CB-CG-CD2	-7.20	121.84	131.20
20	2-M	412	HIS	CB-CG-CD2	-7.20	121.84	131.20
20	3-M	412	HIS	CB-CG-CD2	-7.20	121.84	131.20
6	1-6	222	ASP	CA-CB-CG	7.16	119.76	112.60
6	2-6	222	ASP	CA-CB-CG	7.16	119.76	112.60
6	3-6	222	ASP	CA-CB-CG	7.16	119.76	112.60
26	1-S	172	ASN	CA-CB-CG	7.16	119.75	112.60
26	2-S	172	ASN	CA-CB-CG	7.16	119.75	112.60
26	3-S	172	ASN	CA-CB-CG	7.16	119.75	112.60
24	1-Q	186	HIS	CB-CG-CD2	-7.14	121.92	131.20
24	2-Q	186	HIS	CB-CG-CD2	-7.14	121.92	131.20
24	3-Q	186	HIS	CB-CG-CD2	-7.14	121.92	131.20
27	1-T	236	ASN	N-CA-C	7.13	119.05	111.28
27	2-T	236	ASN	N-CA-C	7.13	119.05	111.28
27	3-T	236	ASN	N-CA-C	7.13	119.05	111.28
16	1-I	365	HIS	CB-CG-CD2	-7.10	121.97	131.20
16	2-I	365	HIS	CB-CG-CD2	-7.10	121.97	131.20
16	3-I	365	HIS	CB-CG-CD2	-7.10	121.97	131.20
18	1-K	141	ARG	CD-NE-CZ	7.09	134.32	124.40
22	1-O	306	ARG	NE-CZ-NH2	7.09	125.58	119.20
18	2-K	141	ARG	CD-NE-CZ	7.09	134.32	124.40
22	2-O	306	ARG	NE-CZ-NH2	7.09	125.58	119.20
18	3-K	141	ARG	CD-NE-CZ	7.09	134.32	124.40
22	3-O	306	ARG	NE-CZ-NH2	7.09	125.58	119.20
29	1-V	196	TYR	CA-C-N	7.08	135.07	121.54
29	1-V	196	TYR	C-N-CA	7.08	135.07	121.54
29	2-V	196	TYR	CA-C-N	7.08	135.07	121.54
29	2-V	196	TYR	C-N-CA	7.08	135.07	121.54
29	3-V	196	TYR	CA-C-N	7.08	135.07	121.54
29	3-V	196	TYR	C-N-CA	7.08	135.07	121.54
19	1-L	264	ARG	NE-CZ-NH2	7.08	125.57	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2-L	264	ARG	NE-CZ-NH2	7.08	125.57	119.20
19	3-L	264	ARG	NE-CZ-NH2	7.08	125.57	119.20
27	1-T	127	GLN	CB-CG-CD	-7.08	100.57	112.60
27	2-T	127	GLN	CB-CG-CD	-7.08	100.57	112.60
27	3-T	127	GLN	CB-CG-CD	-7.08	100.57	112.60
16	1-I	319	ARG	NE-CZ-NH2	7.06	125.55	119.20
16	2-I	319	ARG	NE-CZ-NH2	7.06	125.55	119.20
16	3-I	319	ARG	NE-CZ-NH2	7.06	125.55	119.20
4	1-4	41	HIS	CB-CG-CD2	-7.04	122.04	131.20
4	2-4	41	HIS	CB-CG-CD2	-7.04	122.04	131.20
4	3-4	41	HIS	CB-CG-CD2	-7.04	122.04	131.20
33	1-Z	37	GLN	CB-CG-CD	7.04	124.57	112.60
33	2-Z	37	GLN	CB-CG-CD	7.04	124.57	112.60
33	3-Z	37	GLN	CB-CG-CD	7.04	124.57	112.60
22	1-O	59	LEU	O-C-N	-7.04	114.43	122.03
22	2-O	59	LEU	O-C-N	-7.04	114.43	122.03
22	3-O	59	LEU	O-C-N	-7.04	114.43	122.03
22	1-O	23	HIS	CB-CG-CD2	-6.99	122.11	131.20
22	2-O	23	HIS	CB-CG-CD2	-6.99	122.11	131.20
22	3-O	23	HIS	CB-CG-CD2	-6.99	122.11	131.20
22	1-O	19	ASP	CA-C-N	6.99	128.57	119.84
22	1-O	19	ASP	C-N-CA	6.99	128.57	119.84
22	2-O	19	ASP	CA-C-N	6.99	128.57	119.84
22	2-O	19	ASP	C-N-CA	6.99	128.57	119.84
22	3-O	19	ASP	CA-C-N	6.99	128.57	119.84
22	3-O	19	ASP	C-N-CA	6.99	128.57	119.84
5	1-5	207	PHE	N-CA-C	6.98	119.07	110.91
5	2-5	207	PHE	N-CA-C	6.98	119.07	110.91
5	3-5	207	PHE	N-CA-C	6.98	119.07	110.91
4	1-k	195	PHE	CA-CB-CG	6.96	120.76	113.80
4	2-k	195	PHE	CA-CB-CG	6.96	120.76	113.80
4	3-k	195	PHE	CA-CB-CG	6.96	120.76	113.80
22	1-O	236	HIS	CB-CG-CD2	-6.93	122.18	131.20
22	2-O	236	HIS	CB-CG-CD2	-6.93	122.18	131.20
22	3-O	236	HIS	CB-CG-CD2	-6.93	122.18	131.20
14	1-G	179	HIS	CB-CG-CD2	-6.92	122.20	131.20
14	2-G	179	HIS	CB-CG-CD2	-6.92	122.20	131.20
14	3-G	179	HIS	CB-CG-CD2	-6.92	122.20	131.20
25	1-R	31	PHE	CA-CB-CG	-6.91	106.89	113.80
25	2-R	31	PHE	CA-CB-CG	-6.91	106.89	113.80
25	3-R	31	PHE	CA-CB-CG	-6.91	106.89	113.80
30	1-W	107	HIS	CB-CG-CD2	-6.89	122.24	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	2-W	107	HIS	CB-CG-CD2	-6.89	122.24	131.20
30	3-W	107	HIS	CB-CG-CD2	-6.89	122.24	131.20
24	1-Q	226	HIS	CB-CG-CD2	-6.89	122.25	131.20
24	2-Q	226	HIS	CB-CG-CD2	-6.89	122.25	131.20
24	3-Q	226	HIS	CB-CG-CD2	-6.89	122.25	131.20
25	1-R	20	ARG	NE-CZ-NH2	6.88	125.39	119.20
25	2-R	20	ARG	NE-CZ-NH2	6.88	125.39	119.20
25	3-R	20	ARG	NE-CZ-NH2	6.88	125.39	119.20
14	1-g	179	HIS	CB-CG-CD2	-6.88	122.25	131.20
14	2-g	179	HIS	CB-CG-CD2	-6.88	122.25	131.20
14	3-g	179	HIS	CB-CG-CD2	-6.88	122.25	131.20
28	1-U	5	HIS	CB-CG-CD2	-6.88	122.26	131.20
28	2-U	5	HIS	CB-CG-CD2	-6.88	122.26	131.20
28	3-U	5	HIS	CB-CG-CD2	-6.88	122.26	131.20
9	1-B	190	HIS	CA-CB-CG	-6.87	106.93	113.80
9	2-B	190	HIS	CA-CB-CG	-6.87	106.93	113.80
9	3-B	190	HIS	CA-CB-CG	-6.87	106.93	113.80
19	1-L	290	ARG	NE-CZ-NH2	6.86	125.38	119.20
19	2-L	290	ARG	NE-CZ-NH2	6.86	125.38	119.20
19	3-L	290	ARG	NE-CZ-NH2	6.86	125.38	119.20
15	1-H	80	HIS	CB-CG-CD2	-6.86	122.29	131.20
15	2-H	80	HIS	CB-CG-CD2	-6.86	122.29	131.20
15	3-H	80	HIS	CB-CG-CD2	-6.86	122.29	131.20
7	1-7	156	ARG	CB-CG-CD	6.85	127.06	111.30
7	2-7	156	ARG	CB-CG-CD	6.85	127.06	111.30
7	3-7	156	ARG	CB-CG-CD	6.85	127.06	111.30
1	1-1	38	HIS	CB-CG-CD2	-6.81	122.35	131.20
1	2-1	38	HIS	CB-CG-CD2	-6.81	122.35	131.20
1	3-1	38	HIS	CB-CG-CD2	-6.81	122.35	131.20
21	1-N	754	THR	CB-CA-C	6.77	117.46	109.47
21	2-N	754	THR	CB-CA-C	6.77	117.46	109.47
21	3-N	754	THR	CB-CA-C	6.77	117.46	109.47
30	1-W	13	SER	O-C-N	-6.74	114.73	122.68
30	2-W	13	SER	O-C-N	-6.74	114.73	122.68
30	3-W	13	SER	O-C-N	-6.74	114.73	122.68
4	1-k	41	HIS	CB-CG-CD2	-6.72	122.46	131.20
4	2-k	41	HIS	CB-CG-CD2	-6.72	122.46	131.20
4	3-k	41	HIS	CB-CG-CD2	-6.72	122.46	131.20
13	1-f	8	ASP	CA-CB-CG	6.71	119.31	112.60
13	2-f	8	ASP	CA-CB-CG	6.71	119.31	112.60
13	3-f	8	ASP	CA-CB-CG	6.71	119.31	112.60
29	1-V	217	HIS	CB-CG-CD2	-6.70	122.48	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	2-V	217	HIS	CB-CG-CD2	-6.70	122.48	131.20
29	3-V	217	HIS	CB-CG-CD2	-6.70	122.48	131.20
7	1-7	187	ARG	NE-CZ-NH2	6.69	125.22	119.20
7	2-7	187	ARG	NE-CZ-NH2	6.69	125.22	119.20
7	3-7	187	ARG	NE-CZ-NH2	6.69	125.22	119.20
33	1-Z	258	PRO	N-CA-C	6.68	118.85	110.70
33	2-Z	258	PRO	N-CA-C	6.68	118.85	110.70
33	3-Z	258	PRO	N-CA-C	6.68	118.85	110.70
25	1-R	375	LYS	CB-CG-CD	6.64	126.58	111.30
25	2-R	375	LYS	CB-CG-CD	6.64	126.58	111.30
25	3-R	375	LYS	CB-CG-CD	6.64	126.58	111.30
12	1-e	172	GLN	OE1-CD-NE2	-6.62	115.97	122.60
12	2-e	172	GLN	OE1-CD-NE2	-6.62	115.97	122.60
12	3-e	172	GLN	OE1-CD-NE2	-6.62	115.97	122.60
21	1-N	97	PHE	CA-CB-CG	-6.62	107.18	113.80
21	2-N	97	PHE	CA-CB-CG	-6.62	107.18	113.80
21	3-N	97	PHE	CA-CB-CG	-6.62	107.18	113.80
3	1-j	47	HIS	CB-CG-CD2	-6.61	122.60	131.20
3	2-j	47	HIS	CB-CG-CD2	-6.61	122.60	131.20
3	3-j	47	HIS	CB-CG-CD2	-6.61	122.60	131.20
33	1-Z	948	TRP	CB-CG-CD2	6.61	136.06	126.80
33	2-Z	948	TRP	CB-CG-CD2	6.61	136.06	126.80
33	3-Z	948	TRP	CB-CG-CD2	6.61	136.06	126.80
24	1-Q	163	ARG	NE-CZ-NH2	6.61	125.15	119.20
24	2-Q	163	ARG	NE-CZ-NH2	6.61	125.15	119.20
24	3-Q	163	ARG	NE-CZ-NH2	6.61	125.15	119.20
25	1-R	383	ARG	NE-CZ-NH2	6.60	125.14	119.20
25	2-R	383	ARG	NE-CZ-NH2	6.60	125.14	119.20
25	3-R	383	ARG	NE-CZ-NH2	6.60	125.14	119.20
33	1-Z	25	PRO	N-CD-CG	6.58	113.07	103.20
33	2-Z	25	PRO	N-CD-CG	6.58	113.07	103.20
33	3-Z	25	PRO	N-CD-CG	6.58	113.07	103.20
23	1-P	230	HIS	CB-CG-CD2	-6.58	122.65	131.20
23	2-P	230	HIS	CB-CG-CD2	-6.58	122.65	131.20
23	3-P	230	HIS	CB-CG-CD2	-6.58	122.65	131.20
3	1-3	156	ASN	N-CA-C	6.57	120.61	111.74
3	2-3	156	ASN	N-CA-C	6.57	120.61	111.74
3	3-3	156	ASN	N-CA-C	6.57	120.61	111.74
21	1-N	682	PHE	CA-CB-CG	6.56	120.36	113.80
21	2-N	682	PHE	CA-CB-CG	6.56	120.36	113.80
21	3-N	682	PHE	CA-CB-CG	6.56	120.36	113.80
18	1-K	207	ARG	NE-CZ-NH2	6.55	125.09	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2-K	207	ARG	NE-CZ-NH2	6.55	125.09	119.20
18	3-K	207	ARG	NE-CZ-NH2	6.55	125.09	119.20
12	1-e	65	HIS	CB-CG-CD2	-6.54	122.70	131.20
12	2-e	65	HIS	CB-CG-CD2	-6.54	122.70	131.20
12	3-e	65	HIS	CB-CG-CD2	-6.54	122.70	131.20
21	1-N	762	ARG	NE-CZ-NH2	6.51	125.06	119.20
21	2-N	762	ARG	NE-CZ-NH2	6.51	125.06	119.20
21	3-N	762	ARG	NE-CZ-NH2	6.51	125.06	119.20
1	1-h	38	HIS	CB-CG-CD2	-6.50	122.75	131.20
1	2-h	38	HIS	CB-CG-CD2	-6.50	122.75	131.20
1	3-h	38	HIS	CB-CG-CD2	-6.50	122.75	131.20
2	1-2	19	ARG	NE-CZ-NH2	6.48	125.03	119.20
2	2-2	19	ARG	NE-CZ-NH2	6.48	125.03	119.20
2	3-2	19	ARG	NE-CZ-NH2	6.48	125.03	119.20
24	1-Q	124	PHE	CA-CB-CG	6.47	120.27	113.80
24	2-Q	124	PHE	CA-CB-CG	6.47	120.27	113.80
24	3-Q	124	PHE	CA-CB-CG	6.47	120.27	113.80
12	1-E	83	HIS	CB-CG-CD2	-6.45	122.81	131.20
12	2-E	83	HIS	CB-CG-CD2	-6.45	122.81	131.20
12	3-E	83	HIS	CB-CG-CD2	-6.45	122.81	131.20
18	1-K	140	HIS	CB-CG-CD2	-6.45	122.82	131.20
18	2-K	140	HIS	CB-CG-CD2	-6.45	122.82	131.20
18	3-K	140	HIS	CB-CG-CD2	-6.45	122.82	131.20
21	1-N	8	PRO	N-CA-CB	-6.45	96.48	103.25
21	2-N	8	PRO	N-CA-CB	-6.45	96.48	103.25
21	3-N	8	PRO	N-CA-CB	-6.45	96.48	103.25
3	1-j	168	GLN	CB-CG-CD	6.44	123.56	112.60
3	2-j	168	GLN	CB-CG-CD	6.44	123.56	112.60
3	3-j	168	GLN	CB-CG-CD	6.44	123.56	112.60
29	1-V	190	HIS	CB-CG-CD2	-6.44	122.83	131.20
29	2-V	190	HIS	CB-CG-CD2	-6.44	122.83	131.20
29	3-V	190	HIS	CB-CG-CD2	-6.44	122.83	131.20
2	1-2	116	HIS	CA-CB-CG	-6.43	107.37	113.80
2	2-2	116	HIS	CA-CB-CG	-6.43	107.37	113.80
2	3-2	116	HIS	CA-CB-CG	-6.43	107.37	113.80
20	1-M	407	GLN	OE1-CD-NE2	-6.42	116.18	122.60
20	2-M	407	GLN	OE1-CD-NE2	-6.42	116.18	122.60
20	3-M	407	GLN	OE1-CD-NE2	-6.42	116.18	122.60
33	1-Z	361	HIS	CA-CB-CG	-6.42	107.38	113.80
33	2-Z	361	HIS	CA-CB-CG	-6.42	107.38	113.80
33	3-Z	361	HIS	CA-CB-CG	-6.42	107.38	113.80
33	1-Z	463	HIS	CB-CG-CD2	-6.41	122.86	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2-Z	463	HIS	CB-CG-CD2	-6.41	122.86	131.20
33	3-Z	463	HIS	CB-CG-CD2	-6.41	122.86	131.20
30	1-W	18	ASN	CA-CB-CG	6.41	119.01	112.60
30	2-W	18	ASN	CA-CB-CG	6.41	119.01	112.60
30	3-W	18	ASN	CA-CB-CG	6.41	119.01	112.60
6	1-m	28	ARG	NE-CZ-NH2	6.41	124.97	119.20
6	2-m	28	ARG	NE-CZ-NH2	6.41	124.97	119.20
6	3-m	28	ARG	NE-CZ-NH2	6.41	124.97	119.20
32	1-Y	72	ASP	CA-CB-CG	-6.40	106.20	112.60
32	2-Y	72	ASP	CA-CB-CG	-6.40	106.20	112.60
32	3-Y	72	ASP	CA-CB-CG	-6.40	106.20	112.60
5	1-5	69	ARG	NE-CZ-NH2	6.40	124.96	119.20
12	1-E	139	HIS	CB-CG-CD2	-6.40	122.88	131.20
30	1-W	22	PRO	CA-C-N	6.40	133.22	121.70
30	1-W	22	PRO	C-N-CA	6.40	133.22	121.70
5	2-5	69	ARG	NE-CZ-NH2	6.40	124.96	119.20
12	2-E	139	HIS	CB-CG-CD2	-6.40	122.88	131.20
30	2-W	22	PRO	CA-C-N	6.40	133.22	121.70
30	2-W	22	PRO	C-N-CA	6.40	133.22	121.70
5	3-5	69	ARG	NE-CZ-NH2	6.40	124.96	119.20
12	3-E	139	HIS	CB-CG-CD2	-6.40	122.88	131.20
30	3-W	22	PRO	CA-C-N	6.40	133.22	121.70
30	3-W	22	PRO	C-N-CA	6.40	133.22	121.70
23	1-P	92	SER	N-CA-C	6.39	117.93	110.97
23	2-P	92	SER	N-CA-C	6.39	117.93	110.97
23	3-P	92	SER	N-CA-C	6.39	117.93	110.97
27	1-T	80	ASN	CA-CB-CG	6.39	118.99	112.60
27	2-T	80	ASN	CA-CB-CG	6.39	118.99	112.60
27	3-T	80	ASN	CA-CB-CG	6.39	118.99	112.60
15	1-H	420	ARG	NE-CZ-NH2	6.37	124.93	119.20
15	2-H	420	ARG	NE-CZ-NH2	6.37	124.93	119.20
15	3-H	420	ARG	NE-CZ-NH2	6.37	124.93	119.20
16	1-I	265	ARG	NH1-CZ-NH2	-6.36	111.03	119.30
16	2-I	265	ARG	NH1-CZ-NH2	-6.36	111.03	119.30
16	3-I	265	ARG	NH1-CZ-NH2	-6.36	111.03	119.30
27	1-T	132	HIS	CA-CB-CG	6.35	120.15	113.80
27	2-T	132	HIS	CA-CB-CG	6.35	120.15	113.80
27	3-T	132	HIS	CA-CB-CG	6.35	120.15	113.80
20	1-M	364	HIS	CB-CG-CD2	-6.34	122.96	131.20
20	2-M	364	HIS	CB-CG-CD2	-6.34	122.96	131.20
20	3-M	364	HIS	CB-CG-CD2	-6.34	122.96	131.20
13	1-f	109	HIS	CB-CG-CD2	-6.32	122.99	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	2-f	109	HIS	CB-CG-CD2	-6.32	122.99	131.20
13	3-f	109	HIS	CB-CG-CD2	-6.32	122.99	131.20
1	1-1	29	ARG	NE-CZ-NH2	6.30	124.87	119.20
1	2-1	29	ARG	NE-CZ-NH2	6.30	124.87	119.20
1	3-1	29	ARG	NE-CZ-NH2	6.30	124.87	119.20
18	1-K	77	ARG	NE-CZ-NH2	6.30	124.87	119.20
18	2-K	77	ARG	NE-CZ-NH2	6.30	124.87	119.20
18	3-K	77	ARG	NE-CZ-NH2	6.30	124.87	119.20
3	1-j	197	ARG	CD-NE-CZ	6.29	133.21	124.40
3	2-j	197	ARG	CD-NE-CZ	6.29	133.21	124.40
3	3-j	197	ARG	CD-NE-CZ	6.29	133.21	124.40
7	1-n	62	HIS	CB-CG-CD2	-6.27	123.05	131.20
7	2-n	62	HIS	CB-CG-CD2	-6.27	123.05	131.20
7	3-n	62	HIS	CB-CG-CD2	-6.27	123.05	131.20
1	1-h	103	ASP	CA-CB-CG	6.27	118.87	112.60
1	2-h	103	ASP	CA-CB-CG	6.27	118.87	112.60
1	3-h	103	ASP	CA-CB-CG	6.27	118.87	112.60
12	1-E	189	GLU	CB-CG-CD	6.26	123.25	112.60
22	1-O	387	ARG	CB-CG-CD	6.26	125.71	111.30
12	2-E	189	GLU	CB-CG-CD	6.26	123.25	112.60
22	2-O	387	ARG	CB-CG-CD	6.26	125.71	111.30
12	3-E	189	GLU	CB-CG-CD	6.26	123.25	112.60
22	3-O	387	ARG	CB-CG-CD	6.26	125.71	111.30
15	1-H	353	PHE	CA-CB-CG	6.26	120.06	113.80
15	2-H	353	PHE	CA-CB-CG	6.26	120.06	113.80
15	3-H	353	PHE	CA-CB-CG	6.26	120.06	113.80
31	1-X	48	PHE	CA-CB-CG	6.26	120.06	113.80
31	2-X	48	PHE	CA-CB-CG	6.26	120.06	113.80
31	3-X	48	PHE	CA-CB-CG	6.26	120.06	113.80
30	1-W	109	ARG	NE-CZ-NH2	6.25	124.82	119.20
30	2-W	109	ARG	NE-CZ-NH2	6.25	124.82	119.20
30	3-W	109	ARG	NE-CZ-NH2	6.25	124.82	119.20
24	1-Q	251	THR	N-CA-C	6.24	120.60	112.92
24	2-Q	251	THR	N-CA-C	6.24	120.60	112.92
24	3-Q	251	THR	N-CA-C	6.24	120.60	112.92
23	1-P	86	HIS	CB-CG-CD2	-6.23	123.11	131.20
23	2-P	86	HIS	CB-CG-CD2	-6.23	123.11	131.20
23	3-P	86	HIS	CB-CG-CD2	-6.23	123.11	131.20
17	1-J	231	ARG	NE-CZ-NH2	6.21	124.79	119.20
17	2-J	231	ARG	NE-CZ-NH2	6.21	124.79	119.20
17	3-J	231	ARG	NE-CZ-NH2	6.21	124.79	119.20
29	1-V	204	HIS	CB-CG-CD2	-6.20	123.14	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	2-V	204	HIS	CB-CG-CD2	-6.20	123.14	131.20
29	3-V	204	HIS	CB-CG-CD2	-6.20	123.14	131.20
5	1-5	104	TYR	CB-CG-CD2	-6.20	111.50	120.80
28	1-U	223	HIS	CB-CG-CD2	-6.20	123.14	131.20
5	2-5	104	TYR	CB-CG-CD2	-6.20	111.50	120.80
28	2-U	223	HIS	CB-CG-CD2	-6.20	123.14	131.20
5	3-5	104	TYR	CB-CG-CD2	-6.20	111.50	120.80
28	3-U	223	HIS	CB-CG-CD2	-6.20	123.14	131.20
21	1-N	14	ARG	NE-CZ-NH2	6.17	124.76	119.20
31	1-X	32	GLU	CB-CG-CD	-6.17	102.10	112.60
6	1-m	79	HIS	CB-CG-CD2	-6.17	123.17	131.20
21	2-N	14	ARG	NE-CZ-NH2	6.17	124.76	119.20
31	2-X	32	GLU	CB-CG-CD	-6.17	102.10	112.60
6	2-m	79	HIS	CB-CG-CD2	-6.17	123.17	131.20
21	3-N	14	ARG	NE-CZ-NH2	6.17	124.76	119.20
31	3-X	32	GLU	CB-CG-CD	-6.17	102.10	112.60
6	3-m	79	HIS	CB-CG-CD2	-6.17	123.17	131.20
24	1-Q	243	PHE	CA-CB-CG	-6.16	107.64	113.80
24	2-Q	243	PHE	CA-CB-CG	-6.16	107.64	113.80
24	3-Q	243	PHE	CA-CB-CG	-6.16	107.64	113.80
10	1-C	181	ASP	CA-CB-CG	-6.14	106.46	112.60
23	1-P	348	HIS	CB-CG-CD2	-6.14	123.22	131.20
10	2-C	181	ASP	CA-CB-CG	-6.14	106.46	112.60
23	2-P	348	HIS	CB-CG-CD2	-6.14	123.22	131.20
10	3-C	181	ASP	CA-CB-CG	-6.14	106.46	112.60
23	3-P	348	HIS	CB-CG-CD2	-6.14	123.22	131.20
15	1-H	186	PRO	N-CA-CB	6.14	108.78	103.31
15	2-H	186	PRO	N-CA-CB	6.14	108.78	103.31
15	3-H	186	PRO	N-CA-CB	6.14	108.78	103.31
10	1-C	3	ARG	NE-CZ-NH2	6.14	124.72	119.20
10	2-C	3	ARG	NE-CZ-NH2	6.14	124.72	119.20
10	3-C	3	ARG	NE-CZ-NH2	6.14	124.72	119.20
20	1-M	299	ARG	NE-CZ-NH2	6.11	124.70	119.20
20	2-M	299	ARG	NE-CZ-NH2	6.11	124.70	119.20
20	3-M	299	ARG	NE-CZ-NH2	6.11	124.70	119.20
2	1-2	207	ARG	NE-CZ-NH2	6.10	124.69	119.20
2	2-2	207	ARG	NE-CZ-NH2	6.10	124.69	119.20
2	3-2	207	ARG	NE-CZ-NH2	6.10	124.69	119.20
23	1-P	88	GLN	OE1-CD-NE2	-6.07	116.53	122.60
23	2-P	88	GLN	OE1-CD-NE2	-6.07	116.53	122.60
23	3-P	88	GLN	OE1-CD-NE2	-6.07	116.53	122.60
27	1-T	235	PHE	CA-CB-CG	6.07	119.87	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	2-T	235	PHE	CA-CB-CG	6.07	119.87	113.80
27	3-T	235	PHE	CA-CB-CG	6.07	119.87	113.80
18	1-K	141	ARG	NE-CZ-NH2	6.07	124.66	119.20
18	2-K	141	ARG	NE-CZ-NH2	6.07	124.66	119.20
18	3-K	141	ARG	NE-CZ-NH2	6.07	124.66	119.20
10	1-C	49	ARG	NE-CZ-NH2	6.07	124.66	119.20
10	2-C	49	ARG	NE-CZ-NH2	6.07	124.66	119.20
10	3-C	49	ARG	NE-CZ-NH2	6.07	124.66	119.20
28	1-U	234	ASN	CA-CB-CG	-6.06	106.54	112.60
28	2-U	234	ASN	CA-CB-CG	-6.06	106.54	112.60
28	3-U	234	ASN	CA-CB-CG	-6.06	106.54	112.60
33	1-Z	759	ARG	CD-NE-CZ	6.06	132.88	124.40
33	2-Z	759	ARG	CD-NE-CZ	6.06	132.88	124.40
33	3-Z	759	ARG	CD-NE-CZ	6.06	132.88	124.40
23	1-P	48	GLN	OE1-CD-NE2	-6.01	116.59	122.60
23	2-P	48	GLN	OE1-CD-NE2	-6.01	116.59	122.60
23	3-P	48	GLN	OE1-CD-NE2	-6.01	116.59	122.60
24	1-Q	292	GLN	OE1-CD-NE2	-6.01	116.59	122.60
24	2-Q	292	GLN	OE1-CD-NE2	-6.01	116.59	122.60
24	3-Q	292	GLN	OE1-CD-NE2	-6.01	116.59	122.60
1	1-h	120	HIS	CB-CG-CD2	-6.01	123.39	131.20
1	2-h	120	HIS	CB-CG-CD2	-6.01	123.39	131.20
1	3-h	120	HIS	CB-CG-CD2	-6.01	123.39	131.20
19	1-L	420	ARG	NE-CZ-NH2	6.00	124.60	119.20
19	2-L	420	ARG	NE-CZ-NH2	6.00	124.60	119.20
19	3-L	420	ARG	NE-CZ-NH2	6.00	124.60	119.20
8	1-a	200	HIS	CB-CG-CD2	-6.00	123.41	131.20
8	2-a	200	HIS	CB-CG-CD2	-6.00	123.41	131.20
8	3-a	200	HIS	CB-CG-CD2	-6.00	123.41	131.20
4	1-4	93	ARG	NE-CZ-NH2	5.99	124.59	119.20
4	2-4	93	ARG	NE-CZ-NH2	5.99	124.59	119.20
4	3-4	93	ARG	NE-CZ-NH2	5.99	124.59	119.20
22	1-O	63	ASP	O-C-N	5.99	128.32	122.09
22	2-O	63	ASP	O-C-N	5.99	128.32	122.09
22	3-O	63	ASP	O-C-N	5.99	128.32	122.09
12	1-e	83	HIS	CB-CG-CD2	-5.97	123.44	131.20
12	2-e	83	HIS	CB-CG-CD2	-5.97	123.44	131.20
12	3-e	83	HIS	CB-CG-CD2	-5.97	123.44	131.20
28	1-U	94	HIS	CB-CG-CD2	-5.97	123.44	131.20
9	1-b	13	SER	CA-C-N	5.97	125.67	119.82
9	1-b	13	SER	C-N-CA	5.97	125.67	119.82
28	2-U	94	HIS	CB-CG-CD2	-5.97	123.44	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2-b	13	SER	CA-C-N	5.97	125.67	119.82
9	2-b	13	SER	C-N-CA	5.97	125.67	119.82
28	3-U	94	HIS	CB-CG-CD2	-5.97	123.44	131.20
9	3-b	13	SER	CA-C-N	5.97	125.67	119.82
9	3-b	13	SER	C-N-CA	5.97	125.67	119.82
6	1-m	102	PHE	CA-CB-CG	-5.96	107.84	113.80
6	2-m	102	PHE	CA-CB-CG	-5.96	107.84	113.80
6	3-m	102	PHE	CA-CB-CG	-5.96	107.84	113.80
2	1-i	109	HIS	CB-CG-CD2	-5.96	123.45	131.20
2	2-i	109	HIS	CB-CG-CD2	-5.96	123.45	131.20
2	3-i	109	HIS	CB-CG-CD2	-5.96	123.45	131.20
21	1-N	328	PHE	CA-CB-CG	5.96	119.76	113.80
21	2-N	328	PHE	CA-CB-CG	5.96	119.76	113.80
21	3-N	328	PHE	CA-CB-CG	5.96	119.76	113.80
22	1-O	342	ASP	CA-CB-CG	5.95	118.55	112.60
22	2-O	342	ASP	CA-CB-CG	5.95	118.55	112.60
22	3-O	342	ASP	CA-CB-CG	5.95	118.55	112.60
17	1-J	298	ASP	CA-CB-CG	5.94	118.54	112.60
33	1-Z	497	PHE	CA-CB-CG	-5.94	107.86	113.80
17	2-J	298	ASP	CA-CB-CG	5.94	118.54	112.60
33	2-Z	497	PHE	CA-CB-CG	-5.94	107.86	113.80
17	3-J	298	ASP	CA-CB-CG	5.94	118.54	112.60
33	3-Z	497	PHE	CA-CB-CG	-5.94	107.86	113.80
27	1-T	230	ASN	CA-CB-CG	5.93	118.53	112.60
27	2-T	230	ASN	CA-CB-CG	5.93	118.53	112.60
27	3-T	230	ASN	CA-CB-CG	5.93	118.53	112.60
23	1-P	440	HIS	CB-CG-CD2	-5.93	123.49	131.20
23	2-P	440	HIS	CB-CG-CD2	-5.93	123.49	131.20
23	3-P	440	HIS	CB-CG-CD2	-5.93	123.49	131.20
22	1-O	224	GLY	N-CA-C	5.92	118.74	111.93
22	2-O	224	GLY	N-CA-C	5.92	118.74	111.93
22	3-O	224	GLY	N-CA-C	5.92	118.74	111.93
11	1-d	120	GLN	CB-CG-CD	-5.91	102.56	112.60
11	2-d	120	GLN	CB-CG-CD	-5.91	102.56	112.60
11	3-d	120	GLN	CB-CG-CD	-5.91	102.56	112.60
32	1-Y	89	GLN	OE1-CD-NE2	-5.90	116.70	122.60
32	2-Y	89	GLN	OE1-CD-NE2	-5.90	116.70	122.60
32	3-Y	89	GLN	OE1-CD-NE2	-5.90	116.70	122.60
26	1-S	380	CYS	CA-CB-SG	-5.89	100.85	114.40
26	2-S	380	CYS	CA-CB-SG	-5.89	100.85	114.40
26	3-S	380	CYS	CA-CB-SG	-5.89	100.85	114.40
18	1-K	186	GLU	CB-CG-CD	-5.89	102.59	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2-K	186	GLU	CB-CG-CD	-5.89	102.59	112.60
18	3-K	186	GLU	CB-CG-CD	-5.89	102.59	112.60
7	1-n	3	GLN	OE1-CD-NE2	-5.89	116.71	122.60
7	2-n	3	GLN	OE1-CD-NE2	-5.89	116.71	122.60
7	3-n	3	GLN	OE1-CD-NE2	-5.89	116.71	122.60
5	1-l	192	ASP	CA-CB-CG	-5.88	106.72	112.60
5	2-l	192	ASP	CA-CB-CG	-5.88	106.72	112.60
5	3-l	192	ASP	CA-CB-CG	-5.88	106.72	112.60
2	1-2	93	HIS	CB-CG-CD2	-5.88	123.56	131.20
24	1-Q	135	HIS	CB-CG-CD2	-5.88	123.56	131.20
2	2-2	93	HIS	CB-CG-CD2	-5.88	123.56	131.20
24	2-Q	135	HIS	CB-CG-CD2	-5.88	123.56	131.20
2	3-2	93	HIS	CB-CG-CD2	-5.88	123.56	131.20
24	3-Q	135	HIS	CB-CG-CD2	-5.88	123.56	131.20
11	1-d	4	ARG	NE-CZ-NH2	5.87	124.48	119.20
2	1-i	23	GLY	CA-C-N	5.87	125.97	119.87
2	1-i	23	GLY	C-N-CA	5.87	125.97	119.87
11	2-d	4	ARG	NE-CZ-NH2	5.87	124.48	119.20
2	2-i	23	GLY	CA-C-N	5.87	125.97	119.87
2	2-i	23	GLY	C-N-CA	5.87	125.97	119.87
11	3-d	4	ARG	NE-CZ-NH2	5.87	124.48	119.20
2	3-i	23	GLY	CA-C-N	5.87	125.97	119.87
2	3-i	23	GLY	C-N-CA	5.87	125.97	119.87
21	1-N	653	ARG	NE-CZ-NH2	5.87	124.48	119.20
22	1-O	70	TYR	CA-CB-CG	5.87	124.46	113.90
21	2-N	653	ARG	NE-CZ-NH2	5.87	124.48	119.20
22	2-O	70	TYR	CA-CB-CG	5.87	124.46	113.90
21	3-N	653	ARG	NE-CZ-NH2	5.87	124.48	119.20
22	3-O	70	TYR	CA-CB-CG	5.87	124.46	113.90
21	1-N	667	GLN	OE1-CD-NE2	-5.86	116.74	122.60
21	2-N	667	GLN	OE1-CD-NE2	-5.86	116.74	122.60
21	3-N	667	GLN	OE1-CD-NE2	-5.86	116.74	122.60
22	1-O	23	HIS	CA-CB-CG	5.86	119.66	113.80
22	2-O	23	HIS	CA-CB-CG	5.86	119.66	113.80
22	3-O	23	HIS	CA-CB-CG	5.86	119.66	113.80
6	1-6	101	ARG	NE-CZ-NH2	5.85	124.47	119.20
6	2-6	101	ARG	NE-CZ-NH2	5.85	124.47	119.20
6	3-6	101	ARG	NE-CZ-NH2	5.85	124.47	119.20
21	1-N	268	GLN	OE1-CD-NE2	-5.85	116.75	122.60
21	2-N	268	GLN	OE1-CD-NE2	-5.85	116.75	122.60
21	3-N	268	GLN	OE1-CD-NE2	-5.85	116.75	122.60
23	1-P	377	GLU	CB-CG-CD	-5.84	102.67	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2-P	377	GLU	CB-CG-CD	-5.84	102.67	112.60
23	3-P	377	GLU	CB-CG-CD	-5.84	102.67	112.60
11	1-d	136	PHE	CA-CB-CG	-5.84	107.96	113.80
11	2-d	136	PHE	CA-CB-CG	-5.84	107.96	113.80
11	3-d	136	PHE	CA-CB-CG	-5.84	107.96	113.80
28	1-U	179	ARG	NE-CZ-NH2	5.83	124.45	119.20
28	2-U	179	ARG	NE-CZ-NH2	5.83	124.45	119.20
28	3-U	179	ARG	NE-CZ-NH2	5.83	124.45	119.20
14	1-G	178	HIS	CB-CG-CD2	-5.83	123.62	131.20
14	2-G	178	HIS	CB-CG-CD2	-5.83	123.62	131.20
14	3-G	178	HIS	CB-CG-CD2	-5.83	123.62	131.20
33	1-Z	898	HIS	CB-CG-CD2	-5.83	123.63	131.20
33	2-Z	898	HIS	CB-CG-CD2	-5.83	123.63	131.20
33	3-Z	898	HIS	CB-CG-CD2	-5.83	123.63	131.20
31	1-X	100	TRP	CB-CG-CD1	-5.82	118.18	126.90
3	1-j	187	TYR	CB-CG-CD1	-5.82	112.08	120.80
31	2-X	100	TRP	CB-CG-CD1	-5.82	118.18	126.90
3	2-j	187	TYR	CB-CG-CD1	-5.82	112.08	120.80
31	3-X	100	TRP	CB-CG-CD1	-5.82	118.18	126.90
3	3-j	187	TYR	CB-CG-CD1	-5.82	112.08	120.80
21	1-N	510	HIS	CB-CG-CD2	-5.81	123.64	131.20
21	2-N	510	HIS	CB-CG-CD2	-5.81	123.64	131.20
21	3-N	510	HIS	CB-CG-CD2	-5.81	123.64	131.20
13	1-f	19	PHE	CA-CB-CG	5.81	119.61	113.80
13	2-f	19	PHE	CA-CB-CG	5.81	119.61	113.80
13	3-f	19	PHE	CA-CB-CG	5.81	119.61	113.80
2	1-2	160	GLN	OE1-CD-NE2	-5.81	116.79	122.60
2	2-2	160	GLN	OE1-CD-NE2	-5.81	116.79	122.60
2	3-2	160	GLN	OE1-CD-NE2	-5.81	116.79	122.60
23	1-P	364	ARG	CB-CG-CD	5.80	124.65	111.30
23	2-P	364	ARG	CB-CG-CD	5.80	124.65	111.30
23	3-P	364	ARG	CB-CG-CD	5.80	124.65	111.30
26	1-S	76	PHE	CA-CB-CG	5.80	119.60	113.80
26	2-S	76	PHE	CA-CB-CG	5.80	119.60	113.80
26	3-S	76	PHE	CA-CB-CG	5.80	119.60	113.80
16	1-I	151	HIS	CB-CG-CD2	-5.80	123.67	131.20
16	2-I	151	HIS	CB-CG-CD2	-5.80	123.67	131.20
16	3-I	151	HIS	CB-CG-CD2	-5.80	123.67	131.20
17	1-J	57	PHE	CA-CB-CG	5.79	119.59	113.80
17	2-J	57	PHE	CA-CB-CG	5.79	119.59	113.80
17	3-J	57	PHE	CA-CB-CG	5.79	119.59	113.80
33	1-Z	232	LYS	N-CA-C	5.79	118.36	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2-Z	232	LYS	N-CA-C	5.79	118.36	111.71
33	3-Z	232	LYS	N-CA-C	5.79	118.36	111.71
12	1-E	114	ARG	N-CA-CB	-5.78	102.19	110.57
12	2-E	114	ARG	N-CA-CB	-5.78	102.19	110.57
12	3-E	114	ARG	N-CA-CB	-5.78	102.19	110.57
5	1-5	73	ARG	NE-CZ-NH2	5.78	124.40	119.20
5	2-5	73	ARG	NE-CZ-NH2	5.78	124.40	119.20
5	3-5	73	ARG	NE-CZ-NH2	5.78	124.40	119.20
27	1-T	256	LYS	CA-CB-CG	5.77	125.64	114.10
27	2-T	256	LYS	CA-CB-CG	5.77	125.64	114.10
27	3-T	256	LYS	CA-CB-CG	5.77	125.64	114.10
33	1-Z	550	PHE	CA-CB-CG	5.76	119.56	113.80
33	2-Z	550	PHE	CA-CB-CG	5.76	119.56	113.80
33	3-Z	550	PHE	CA-CB-CG	5.76	119.56	113.80
16	1-I	174	ASP	CA-CB-CG	5.75	118.35	112.60
16	2-I	174	ASP	CA-CB-CG	5.75	118.35	112.60
16	3-I	174	ASP	CA-CB-CG	5.75	118.35	112.60
11	1-D	139	ARG	NE-CZ-NH2	5.74	124.37	119.20
11	2-D	139	ARG	NE-CZ-NH2	5.74	124.37	119.20
11	3-D	139	ARG	NE-CZ-NH2	5.74	124.37	119.20
9	1-b	216	ASP	CA-CB-CG	5.73	118.33	112.60
9	2-b	216	ASP	CA-CB-CG	5.73	118.33	112.60
9	3-b	216	ASP	CA-CB-CG	5.73	118.33	112.60
33	1-Z	165	TYR	CA-CB-CG	5.72	124.19	113.90
33	2-Z	165	TYR	CA-CB-CG	5.72	124.19	113.90
33	3-Z	165	TYR	CA-CB-CG	5.72	124.19	113.90
21	1-N	57	ASP	CA-CB-CG	-5.71	106.89	112.60
21	2-N	57	ASP	CA-CB-CG	-5.71	106.89	112.60
21	3-N	57	ASP	CA-CB-CG	-5.71	106.89	112.60
29	1-V	109	HIS	CA-CB-CG	5.71	119.51	113.80
29	2-V	109	HIS	CA-CB-CG	5.71	119.51	113.80
29	3-V	109	HIS	CA-CB-CG	5.71	119.51	113.80
9	1-b	20	GLN	OE1-CD-NE2	-5.70	116.90	122.60
9	2-b	20	GLN	OE1-CD-NE2	-5.70	116.90	122.60
9	3-b	20	GLN	OE1-CD-NE2	-5.70	116.90	122.60
25	1-R	23	ASN	OD1-CG-ND2	-5.69	116.91	122.60
25	2-R	23	ASN	OD1-CG-ND2	-5.69	116.91	122.60
25	3-R	23	ASN	OD1-CG-ND2	-5.69	116.91	122.60
28	1-U	216	ASN	OD1-CG-ND2	-5.69	116.91	122.60
28	2-U	216	ASN	OD1-CG-ND2	-5.69	116.91	122.60
28	3-U	216	ASN	OD1-CG-ND2	-5.69	116.91	122.60
17	1-J	111	GLN	OE1-CD-NE2	-5.68	116.92	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1-f	59	GLN	OE1-CD-NE2	-5.68	116.92	122.60
2	1-i	160	GLN	OE1-CD-NE2	-5.68	116.92	122.60
17	2-J	111	GLN	OE1-CD-NE2	-5.68	116.92	122.60
13	2-f	59	GLN	OE1-CD-NE2	-5.68	116.92	122.60
2	2-i	160	GLN	OE1-CD-NE2	-5.68	116.92	122.60
17	3-J	111	GLN	OE1-CD-NE2	-5.68	116.92	122.60
13	3-f	59	GLN	OE1-CD-NE2	-5.68	116.92	122.60
2	3-i	160	GLN	OE1-CD-NE2	-5.68	116.92	122.60
20	1-M	33	ARG	NE-CZ-NH2	5.68	124.31	119.20
20	2-M	33	ARG	NE-CZ-NH2	5.68	124.31	119.20
20	3-M	33	ARG	NE-CZ-NH2	5.68	124.31	119.20
21	1-N	311	ILE	CA-C-N	5.66	126.37	120.03
21	1-N	311	ILE	C-N-CA	5.66	126.37	120.03
21	2-N	311	ILE	CA-C-N	5.66	126.37	120.03
21	2-N	311	ILE	C-N-CA	5.66	126.37	120.03
21	3-N	311	ILE	CA-C-N	5.66	126.37	120.03
21	3-N	311	ILE	C-N-CA	5.66	126.37	120.03
18	1-K	121	ARG	NE-CZ-NH2	5.66	124.29	119.20
23	1-P	337	HIS	CB-CG-CD2	-5.66	123.84	131.20
18	2-K	121	ARG	NE-CZ-NH2	5.66	124.29	119.20
23	2-P	337	HIS	CB-CG-CD2	-5.66	123.84	131.20
18	3-K	121	ARG	NE-CZ-NH2	5.66	124.29	119.20
23	3-P	337	HIS	CB-CG-CD2	-5.66	123.84	131.20
23	1-P	86	HIS	CA-CB-CG	5.65	119.45	113.80
23	2-P	86	HIS	CA-CB-CG	5.65	119.45	113.80
23	3-P	86	HIS	CA-CB-CG	5.65	119.45	113.80
8	1-A	15	ARG	NE-CZ-NH2	5.64	124.28	119.20
8	2-A	15	ARG	NE-CZ-NH2	5.64	124.28	119.20
8	3-A	15	ARG	NE-CZ-NH2	5.64	124.28	119.20
33	1-Z	707	LYS	CA-C-N	5.63	126.19	119.94
33	1-Z	707	LYS	C-N-CA	5.63	126.19	119.94
33	2-Z	707	LYS	CA-C-N	5.63	126.19	119.94
33	2-Z	707	LYS	C-N-CA	5.63	126.19	119.94
33	3-Z	707	LYS	CA-C-N	5.63	126.19	119.94
33	3-Z	707	LYS	C-N-CA	5.63	126.19	119.94
8	1-A	47	GLN	OE1-CD-NE2	-5.62	116.98	122.60
8	2-A	47	GLN	OE1-CD-NE2	-5.62	116.98	122.60
8	3-A	47	GLN	OE1-CD-NE2	-5.62	116.98	122.60
29	1-V	157	ARG	NE-CZ-NH2	5.62	124.26	119.20
29	2-V	157	ARG	NE-CZ-NH2	5.62	124.26	119.20
29	3-V	157	ARG	NE-CZ-NH2	5.62	124.26	119.20
25	1-R	43	ARG	NE-CZ-NH2	5.62	124.26	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-h	53	GLN	OE1-CD-NE2	-5.62	116.98	122.60
25	2-R	43	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	2-h	53	GLN	OE1-CD-NE2	-5.62	116.98	122.60
25	3-R	43	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	3-h	53	GLN	OE1-CD-NE2	-5.62	116.98	122.60
13	1-F	163	ARG	NE-CZ-NH2	5.62	124.25	119.20
13	2-F	163	ARG	NE-CZ-NH2	5.62	124.25	119.20
13	3-F	163	ARG	NE-CZ-NH2	5.62	124.25	119.20
22	1-O	75	GLN	OE1-CD-NE2	-5.61	116.99	122.60
22	2-O	75	GLN	OE1-CD-NE2	-5.61	116.99	122.60
22	3-O	75	GLN	OE1-CD-NE2	-5.61	116.99	122.60
16	1-I	347	LYS	CB-CA-C	5.61	118.86	109.89
16	2-I	347	LYS	CB-CA-C	5.61	118.86	109.89
16	3-I	347	LYS	CB-CA-C	5.61	118.86	109.89
14	1-G	240	GLN	OE1-CD-NE2	-5.61	116.99	122.60
14	2-G	240	GLN	OE1-CD-NE2	-5.61	116.99	122.60
14	3-G	240	GLN	OE1-CD-NE2	-5.61	116.99	122.60
10	1-C	123	GLN	OE1-CD-NE2	-5.60	117.00	122.60
10	2-C	123	GLN	OE1-CD-NE2	-5.60	117.00	122.60
10	3-C	123	GLN	OE1-CD-NE2	-5.60	117.00	122.60
2	1-2	86	HIS	CB-CG-CD2	-5.60	123.92	131.20
10	1-c	13	SER	CA-C-N	5.60	125.27	119.56
10	1-c	13	SER	C-N-CA	5.60	125.27	119.56
2	2-2	86	HIS	CB-CG-CD2	-5.60	123.92	131.20
10	2-c	13	SER	CA-C-N	5.60	125.27	119.56
10	2-c	13	SER	C-N-CA	5.60	125.27	119.56
2	3-2	86	HIS	CB-CG-CD2	-5.60	123.92	131.20
10	3-c	13	SER	CA-C-N	5.60	125.27	119.56
10	3-c	13	SER	C-N-CA	5.60	125.27	119.56
8	1-A	166	GLN	OE1-CD-NE2	-5.59	117.01	122.60
8	2-A	166	GLN	OE1-CD-NE2	-5.59	117.01	122.60
8	3-A	166	GLN	OE1-CD-NE2	-5.59	117.01	122.60
18	1-K	399	ARG	NE-CZ-NH2	5.59	124.23	119.20
18	2-K	399	ARG	NE-CZ-NH2	5.59	124.23	119.20
18	3-K	399	ARG	NE-CZ-NH2	5.59	124.23	119.20
33	1-Z	156	HIS	CA-CB-CG	5.58	119.38	113.80
33	2-Z	156	HIS	CA-CB-CG	5.58	119.38	113.80
33	3-Z	156	HIS	CA-CB-CG	5.58	119.38	113.80
8	1-A	18	GLN	OE1-CD-NE2	-5.57	117.03	122.60
8	2-A	18	GLN	OE1-CD-NE2	-5.57	117.03	122.60
8	3-A	18	GLN	OE1-CD-NE2	-5.57	117.03	122.60
29	1-V	195	HIS	CB-CG-CD2	-5.57	123.96	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	2-V	195	HIS	CB-CG-CD2	-5.57	123.96	131.20
29	3-V	195	HIS	CB-CG-CD2	-5.57	123.96	131.20
24	1-Q	80	HIS	CB-CG-CD2	-5.57	123.96	131.20
24	2-Q	80	HIS	CB-CG-CD2	-5.57	123.96	131.20
24	3-Q	80	HIS	CB-CG-CD2	-5.57	123.96	131.20
19	1-L	290	ARG	N-CA-C	5.56	117.34	111.28
19	2-L	290	ARG	N-CA-C	5.56	117.34	111.28
19	3-L	290	ARG	N-CA-C	5.56	117.34	111.28
10	1-C	134	PHE	CA-CB-CG	5.56	119.36	113.80
26	1-S	32	GLN	OE1-CD-NE2	-5.56	117.04	122.60
10	2-C	134	PHE	CA-CB-CG	5.56	119.36	113.80
26	2-S	32	GLN	OE1-CD-NE2	-5.56	117.04	122.60
10	3-C	134	PHE	CA-CB-CG	5.56	119.36	113.80
26	3-S	32	GLN	OE1-CD-NE2	-5.56	117.04	122.60
26	1-S	85	SER	CA-C-N	5.55	128.51	120.79
26	1-S	85	SER	C-N-CA	5.55	128.51	120.79
28	1-U	201	GLN	OE1-CD-NE2	-5.55	117.05	122.60
26	2-S	85	SER	CA-C-N	5.55	128.51	120.79
26	2-S	85	SER	C-N-CA	5.55	128.51	120.79
28	2-U	201	GLN	OE1-CD-NE2	-5.55	117.05	122.60
26	3-S	85	SER	CA-C-N	5.55	128.51	120.79
26	3-S	85	SER	C-N-CA	5.55	128.51	120.79
28	3-U	201	GLN	OE1-CD-NE2	-5.55	117.05	122.60
13	1-F	4	ASN	CA-CB-CG	5.55	118.15	112.60
13	2-F	4	ASN	CA-CB-CG	5.55	118.15	112.60
13	3-F	4	ASN	CA-CB-CG	5.55	118.15	112.60
29	1-V	185	ILE	CA-C-N	5.54	128.02	120.54
29	1-V	185	ILE	C-N-CA	5.54	128.02	120.54
29	2-V	185	ILE	CA-C-N	5.54	128.02	120.54
29	2-V	185	ILE	C-N-CA	5.54	128.02	120.54
29	3-V	185	ILE	CA-C-N	5.54	128.02	120.54
29	3-V	185	ILE	C-N-CA	5.54	128.02	120.54
2	1-2	85	GLN	OE1-CD-NE2	-5.54	117.06	122.60
2	2-2	85	GLN	OE1-CD-NE2	-5.54	117.06	122.60
2	3-2	85	GLN	OE1-CD-NE2	-5.54	117.06	122.60
9	1-B	20	GLN	OE1-CD-NE2	-5.54	117.06	122.60
9	2-B	20	GLN	OE1-CD-NE2	-5.54	117.06	122.60
9	3-B	20	GLN	OE1-CD-NE2	-5.54	117.06	122.60
18	1-K	349	ARG	NE-CZ-NH2	5.53	124.18	119.20
18	2-K	349	ARG	NE-CZ-NH2	5.53	124.18	119.20
18	3-K	349	ARG	NE-CZ-NH2	5.53	124.18	119.20
14	1-g	16	ARG	NE-CZ-NH2	5.53	124.17	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2-g	16	ARG	NE-CZ-NH2	5.53	124.17	119.20
14	3-g	16	ARG	NE-CZ-NH2	5.53	124.17	119.20
33	1-Z	180	ASP	CB-CA-C	-5.52	101.93	109.28
33	2-Z	180	ASP	CB-CA-C	-5.52	101.93	109.28
33	3-Z	180	ASP	CB-CA-C	-5.52	101.93	109.28
14	1-g	224	HIS	CB-CG-CD2	-5.52	124.03	131.20
14	2-g	224	HIS	CB-CG-CD2	-5.52	124.03	131.20
14	3-g	224	HIS	CB-CG-CD2	-5.52	124.03	131.20
7	1-7	41	ARG	NE-CZ-NH2	5.50	124.15	119.20
30	1-W	17	ARG	NE-CZ-NH2	5.50	124.15	119.20
30	1-W	80	GLN	OE1-CD-NE2	-5.50	117.10	122.60
7	2-7	41	ARG	NE-CZ-NH2	5.50	124.15	119.20
30	2-W	17	ARG	NE-CZ-NH2	5.50	124.15	119.20
30	2-W	80	GLN	OE1-CD-NE2	-5.50	117.10	122.60
7	3-7	41	ARG	NE-CZ-NH2	5.50	124.15	119.20
30	3-W	17	ARG	NE-CZ-NH2	5.50	124.15	119.20
30	3-W	80	GLN	OE1-CD-NE2	-5.50	117.10	122.60
17	1-J	35	ARG	NE-CZ-NH2	5.50	124.15	119.20
17	2-J	35	ARG	NE-CZ-NH2	5.50	124.15	119.20
17	3-J	35	ARG	NE-CZ-NH2	5.50	124.15	119.20
17	1-J	240	HIS	CB-CG-CD2	-5.49	124.06	131.20
17	2-J	240	HIS	CB-CG-CD2	-5.49	124.06	131.20
17	3-J	240	HIS	CB-CG-CD2	-5.49	124.06	131.20
24	1-Q	44	ALA	N-CA-CB	-5.48	102.52	110.47
24	2-Q	44	ALA	N-CA-CB	-5.48	102.52	110.47
24	3-Q	44	ALA	N-CA-CB	-5.48	102.52	110.47
16	1-I	128	TYR	CB-CG-CD1	-5.48	112.58	120.80
16	2-I	128	TYR	CB-CG-CD1	-5.48	112.58	120.80
16	3-I	128	TYR	CB-CG-CD1	-5.48	112.58	120.80
27	1-T	132	HIS	CB-CG-CD2	-5.47	124.08	131.20
27	2-T	132	HIS	CB-CG-CD2	-5.47	124.08	131.20
27	3-T	132	HIS	CB-CG-CD2	-5.47	124.08	131.20
6	1-m	197	GLN	OE1-CD-NE2	-5.47	117.13	122.60
6	2-m	197	GLN	OE1-CD-NE2	-5.47	117.13	122.60
6	3-m	197	GLN	OE1-CD-NE2	-5.47	117.13	122.60
23	1-P	195	GLN	OE1-CD-NE2	-5.47	117.13	122.60
23	2-P	195	GLN	OE1-CD-NE2	-5.47	117.13	122.60
23	3-P	195	GLN	OE1-CD-NE2	-5.47	117.13	122.60
33	1-Z	379	GLN	OE1-CD-NE2	-5.46	117.14	122.60
33	2-Z	379	GLN	OE1-CD-NE2	-5.46	117.14	122.60
33	3-Z	379	GLN	OE1-CD-NE2	-5.46	117.14	122.60
23	1-P	349	ASN	CA-CB-CG	5.46	118.06	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2-P	349	ASN	CA-CB-CG	5.46	118.06	112.60
23	3-P	349	ASN	CA-CB-CG	5.46	118.06	112.60
11	1-D	164	ARG	NE-CZ-NH2	5.46	124.11	119.20
11	2-D	164	ARG	NE-CZ-NH2	5.46	124.11	119.20
11	3-D	164	ARG	NE-CZ-NH2	5.46	124.11	119.20
4	1-4	35	THR	CA-CB-CG2	5.45	119.77	110.50
23	1-P	364	ARG	NE-CZ-NH2	5.45	124.11	119.20
4	2-4	35	THR	CA-CB-CG2	5.45	119.77	110.50
23	2-P	364	ARG	NE-CZ-NH2	5.45	124.11	119.20
4	3-4	35	THR	CA-CB-CG2	5.45	119.77	110.50
23	3-P	364	ARG	NE-CZ-NH2	5.45	124.11	119.20
17	1-J	183	LYS	CA-C-N	5.45	126.85	121.62
17	1-J	183	LYS	C-N-CA	5.45	126.85	121.62
17	2-J	183	LYS	CA-C-N	5.45	126.85	121.62
17	2-J	183	LYS	C-N-CA	5.45	126.85	121.62
17	3-J	183	LYS	CA-C-N	5.45	126.85	121.62
17	3-J	183	LYS	C-N-CA	5.45	126.85	121.62
16	1-I	215	PRO	N-CA-CB	5.44	106.24	103.19
16	2-I	215	PRO	N-CA-CB	5.44	106.24	103.19
16	3-I	215	PRO	N-CA-CB	5.44	106.24	103.19
6	1-6	95	HIS	CA-CB-CG	-5.44	108.36	113.80
6	2-6	95	HIS	CA-CB-CG	-5.44	108.36	113.80
6	3-6	95	HIS	CA-CB-CG	-5.44	108.36	113.80
21	1-N	550	GLY	CA-C-N	5.43	125.97	119.94
21	1-N	550	GLY	C-N-CA	5.43	125.97	119.94
29	1-V	133	ASN	OD1-CG-ND2	-5.43	117.17	122.60
30	1-W	100	HIS	CB-CG-CD2	-5.43	124.13	131.20
21	2-N	550	GLY	CA-C-N	5.43	125.97	119.94
21	2-N	550	GLY	C-N-CA	5.43	125.97	119.94
29	2-V	133	ASN	OD1-CG-ND2	-5.43	117.17	122.60
30	2-W	100	HIS	CB-CG-CD2	-5.43	124.13	131.20
21	3-N	550	GLY	CA-C-N	5.43	125.97	119.94
21	3-N	550	GLY	C-N-CA	5.43	125.97	119.94
29	3-V	133	ASN	OD1-CG-ND2	-5.43	117.17	122.60
30	3-W	100	HIS	CB-CG-CD2	-5.43	124.13	131.20
24	1-Q	371	GLN	OE1-CD-NE2	-5.43	117.17	122.60
24	2-Q	371	GLN	OE1-CD-NE2	-5.43	117.17	122.60
24	3-Q	371	GLN	OE1-CD-NE2	-5.43	117.17	122.60
7	1-7	26	ASN	OD1-CG-ND2	-5.42	117.18	122.60
24	1-Q	213	GLN	OE1-CD-NE2	-5.42	117.18	122.60
7	2-7	26	ASN	OD1-CG-ND2	-5.42	117.18	122.60
24	2-Q	213	GLN	OE1-CD-NE2	-5.42	117.18	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	3-7	26	ASN	OD1-CG-ND2	-5.42	117.18	122.60
24	3-Q	213	GLN	OE1-CD-NE2	-5.42	117.18	122.60
22	1-O	28	GLN	OE1-CD-NE2	-5.42	117.18	122.60
22	2-O	28	GLN	OE1-CD-NE2	-5.42	117.18	122.60
22	3-O	28	GLN	OE1-CD-NE2	-5.42	117.18	122.60
32	1-Y	18	LYS	CA-C-N	5.42	127.48	120.44
32	1-Y	18	LYS	C-N-CA	5.42	127.48	120.44
32	2-Y	18	LYS	CA-C-N	5.42	127.48	120.44
32	2-Y	18	LYS	C-N-CA	5.42	127.48	120.44
32	3-Y	18	LYS	CA-C-N	5.42	127.48	120.44
32	3-Y	18	LYS	C-N-CA	5.42	127.48	120.44
16	1-I	161	GLN	OE1-CD-NE2	-5.41	117.19	122.60
16	2-I	161	GLN	OE1-CD-NE2	-5.41	117.19	122.60
16	3-I	161	GLN	OE1-CD-NE2	-5.41	117.19	122.60
24	1-Q	353	PRO	N-CA-CB	5.41	108.49	103.46
30	1-W	25	ARG	NE-CZ-NH2	5.41	124.07	119.20
24	2-Q	353	PRO	N-CA-CB	5.41	108.49	103.46
30	2-W	25	ARG	NE-CZ-NH2	5.41	124.07	119.20
24	3-Q	353	PRO	N-CA-CB	5.41	108.49	103.46
30	3-W	25	ARG	NE-CZ-NH2	5.41	124.07	119.20
13	1-F	42	HIS	CB-CG-CD2	-5.41	124.17	131.20
13	2-F	42	HIS	CB-CG-CD2	-5.41	124.17	131.20
13	3-F	42	HIS	CB-CG-CD2	-5.41	124.17	131.20
13	1-F	7	GLY	CA-C-N	5.41	131.87	121.54
13	1-F	7	GLY	C-N-CA	5.41	131.87	121.54
13	2-F	7	GLY	CA-C-N	5.41	131.87	121.54
13	2-F	7	GLY	C-N-CA	5.41	131.87	121.54
13	3-F	7	GLY	CA-C-N	5.41	131.87	121.54
13	3-F	7	GLY	C-N-CA	5.41	131.87	121.54
11	1-D	125	ARG	NE-CZ-NH2	5.41	124.06	119.20
11	2-D	125	ARG	NE-CZ-NH2	5.41	124.06	119.20
11	3-D	125	ARG	NE-CZ-NH2	5.41	124.06	119.20
24	1-Q	233	LYS	CB-CG-CD	5.40	123.73	111.30
24	2-Q	233	LYS	CB-CG-CD	5.40	123.73	111.30
24	3-Q	233	LYS	CB-CG-CD	5.40	123.73	111.30
8	1-A	75	ASN	OD1-CG-ND2	-5.40	117.20	122.60
8	2-A	75	ASN	OD1-CG-ND2	-5.40	117.20	122.60
8	3-A	75	ASN	OD1-CG-ND2	-5.40	117.20	122.60
4	1-k	51	GLY	CA-C-N	5.40	127.78	120.38
4	1-k	51	GLY	C-N-CA	5.40	127.78	120.38
4	2-k	51	GLY	CA-C-N	5.40	127.78	120.38
4	2-k	51	GLY	C-N-CA	5.40	127.78	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3-k	51	GLY	CA-C-N	5.40	127.78	120.38
4	3-k	51	GLY	C-N-CA	5.40	127.78	120.38
3	1-3	79	ARG	CB-CG-CD	5.40	123.72	111.30
3	2-3	79	ARG	CB-CG-CD	5.40	123.72	111.30
3	3-3	79	ARG	CB-CG-CD	5.40	123.72	111.30
33	1-Z	552	GLU	CB-CG-CD	-5.39	103.44	112.60
33	2-Z	552	GLU	CB-CG-CD	-5.39	103.44	112.60
33	3-Z	552	GLU	CB-CG-CD	-5.39	103.44	112.60
3	1-3	168	GLN	OE1-CD-NE2	-5.39	117.21	122.60
3	2-3	168	GLN	OE1-CD-NE2	-5.39	117.21	122.60
3	3-3	168	GLN	OE1-CD-NE2	-5.39	117.21	122.60
19	1-L	79	GLN	OE1-CD-NE2	-5.38	117.22	122.60
19	2-L	79	GLN	OE1-CD-NE2	-5.38	117.22	122.60
19	3-L	79	GLN	OE1-CD-NE2	-5.38	117.22	122.60
4	1-k	96	ARG	NE-CZ-NH2	5.38	124.04	119.20
4	2-k	96	ARG	NE-CZ-NH2	5.38	124.04	119.20
4	3-k	96	ARG	NE-CZ-NH2	5.38	124.04	119.20
13	1-F	17	ARG	NE-CZ-NH2	5.37	124.04	119.20
13	2-F	17	ARG	NE-CZ-NH2	5.37	124.04	119.20
13	3-F	17	ARG	NE-CZ-NH2	5.37	124.04	119.20
3	1-3	27	ARG	NE-CZ-NH2	5.37	124.03	119.20
21	1-N	878	GLN	OE1-CD-NE2	-5.37	117.23	122.60
3	2-3	27	ARG	NE-CZ-NH2	5.37	124.03	119.20
21	2-N	878	GLN	OE1-CD-NE2	-5.37	117.23	122.60
3	3-3	27	ARG	NE-CZ-NH2	5.37	124.03	119.20
21	3-N	878	GLN	OE1-CD-NE2	-5.37	117.23	122.60
17	1-J	394	GLN	OE1-CD-NE2	-5.37	117.23	122.60
27	1-T	224	ARG	NE-CZ-NH2	5.37	124.03	119.20
17	2-J	394	GLN	OE1-CD-NE2	-5.37	117.23	122.60
27	2-T	224	ARG	NE-CZ-NH2	5.37	124.03	119.20
17	3-J	394	GLN	OE1-CD-NE2	-5.37	117.23	122.60
27	3-T	224	ARG	NE-CZ-NH2	5.37	124.03	119.20
13	1-F	40	ASN	OD1-CG-ND2	-5.37	117.23	122.60
19	1-L	407	ARG	NE-CZ-NH2	5.37	124.03	119.20
13	2-F	40	ASN	OD1-CG-ND2	-5.37	117.23	122.60
19	2-L	407	ARG	NE-CZ-NH2	5.37	124.03	119.20
13	3-F	40	ASN	OD1-CG-ND2	-5.37	117.23	122.60
19	3-L	407	ARG	NE-CZ-NH2	5.37	124.03	119.20
27	1-T	94	HIS	CB-CG-CD2	-5.36	124.23	131.20
27	2-T	94	HIS	CB-CG-CD2	-5.36	124.23	131.20
27	3-T	94	HIS	CB-CG-CD2	-5.36	124.23	131.20
10	1-c	226	GLN	OE1-CD-NE2	-5.36	117.24	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	2-c	226	GLN	OE1-CD-NE2	-5.36	117.24	122.60
10	3-c	226	GLN	OE1-CD-NE2	-5.36	117.24	122.60
16	1-I	291	ARG	NE-CZ-NH2	5.36	124.03	119.20
16	2-I	291	ARG	NE-CZ-NH2	5.36	124.03	119.20
16	3-I	291	ARG	NE-CZ-NH2	5.36	124.03	119.20
18	1-K	350	ARG	NE-CZ-NH2	5.36	124.02	119.20
30	1-W	25	ARG	NH1-CZ-NH2	-5.36	112.33	119.30
18	2-K	350	ARG	NE-CZ-NH2	5.36	124.02	119.20
30	2-W	25	ARG	NH1-CZ-NH2	-5.36	112.33	119.30
18	3-K	350	ARG	NE-CZ-NH2	5.36	124.02	119.20
30	3-W	25	ARG	NH1-CZ-NH2	-5.36	112.33	119.30
16	1-I	205	PRO	CA-C-N	5.36	127.77	120.54
16	1-I	205	PRO	C-N-CA	5.36	127.77	120.54
33	1-Z	826	ARG	NE-CZ-NH2	5.36	124.02	119.20
16	2-I	205	PRO	CA-C-N	5.36	127.77	120.54
16	2-I	205	PRO	C-N-CA	5.36	127.77	120.54
33	2-Z	826	ARG	NE-CZ-NH2	5.36	124.02	119.20
16	3-I	205	PRO	CA-C-N	5.36	127.77	120.54
16	3-I	205	PRO	C-N-CA	5.36	127.77	120.54
33	3-Z	826	ARG	NE-CZ-NH2	5.36	124.02	119.20
4	1-4	195	PHE	CA-CB-CG	5.35	119.15	113.80
4	2-4	195	PHE	CA-CB-CG	5.35	119.15	113.80
4	3-4	195	PHE	CA-CB-CG	5.35	119.15	113.80
21	1-N	719	ASN	CB-CA-C	-5.35	102.32	110.88
21	2-N	719	ASN	CB-CA-C	-5.35	102.32	110.88
21	3-N	719	ASN	CB-CA-C	-5.35	102.32	110.88
2	1-i	86	HIS	CB-CG-CD2	-5.34	124.25	131.20
2	2-i	86	HIS	CB-CG-CD2	-5.34	124.25	131.20
2	3-i	86	HIS	CB-CG-CD2	-5.34	124.25	131.20
11	1-D	56	ARG	NE-CZ-NH2	5.34	124.01	119.20
11	2-D	56	ARG	NE-CZ-NH2	5.34	124.01	119.20
11	3-D	56	ARG	NE-CZ-NH2	5.34	124.01	119.20
10	1-C	93	HIS	CB-CG-CD2	-5.34	124.26	131.20
10	2-C	93	HIS	CB-CG-CD2	-5.34	124.26	131.20
10	3-C	93	HIS	CB-CG-CD2	-5.34	124.26	131.20
2	1-2	186	TYR	CB-CG-CD2	-5.34	112.79	120.80
25	1-R	192	GLU	CB-CG-CD	5.34	121.67	112.60
28	1-U	262	GLN	CB-CG-CD	5.34	121.67	112.60
31	1-X	59	ARG	NE-CZ-NH2	5.34	124.00	119.20
2	2-2	186	TYR	CB-CG-CD2	-5.34	112.79	120.80
25	2-R	192	GLU	CB-CG-CD	5.34	121.67	112.60
28	2-U	262	GLN	CB-CG-CD	5.34	121.67	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	2-X	59	ARG	NE-CZ-NH2	5.34	124.00	119.20
2	3-2	186	TYR	CB-CG-CD2	-5.34	112.79	120.80
25	3-R	192	GLU	CB-CG-CD	5.34	121.67	112.60
28	3-U	262	GLN	CB-CG-CD	5.34	121.67	112.60
31	3-X	59	ARG	NE-CZ-NH2	5.34	124.00	119.20
33	1-Z	773	ARG	NE-CZ-NH2	5.33	124.00	119.20
33	2-Z	773	ARG	NE-CZ-NH2	5.33	124.00	119.20
33	3-Z	773	ARG	NE-CZ-NH2	5.33	124.00	119.20
22	1-O	306	ARG	CD-NE-CZ	5.33	131.87	124.40
10	1-c	20	GLN	OE1-CD-NE2	-5.33	117.27	122.60
22	2-O	306	ARG	CD-NE-CZ	5.33	131.87	124.40
10	2-c	20	GLN	OE1-CD-NE2	-5.33	117.27	122.60
22	3-O	306	ARG	CD-NE-CZ	5.33	131.87	124.40
10	3-c	20	GLN	OE1-CD-NE2	-5.33	117.27	122.60
8	1-a	18	GLN	OE1-CD-NE2	-5.33	117.27	122.60
8	2-a	18	GLN	OE1-CD-NE2	-5.33	117.27	122.60
8	3-a	18	GLN	OE1-CD-NE2	-5.33	117.27	122.60
2	1-2	91	GLN	OE1-CD-NE2	-5.33	117.27	122.60
2	2-2	91	GLN	OE1-CD-NE2	-5.33	117.27	122.60
2	3-2	91	GLN	OE1-CD-NE2	-5.33	117.27	122.60
5	1-l	104	TYR	CB-CG-CD2	-5.33	112.81	120.80
5	2-l	104	TYR	CB-CG-CD2	-5.33	112.81	120.80
5	3-l	104	TYR	CB-CG-CD2	-5.33	112.81	120.80
22	1-O	181	PHE	CB-CA-C	-5.32	101.96	110.79
22	2-O	181	PHE	CB-CA-C	-5.32	101.96	110.79
22	3-O	181	PHE	CB-CA-C	-5.32	101.96	110.79
22	1-O	65	PHE	CB-CA-C	5.32	120.35	109.55
24	1-Q	185	TYR	CB-CG-CD2	-5.32	112.82	120.80
22	2-O	65	PHE	CB-CA-C	5.32	120.35	109.55
24	2-Q	185	TYR	CB-CG-CD2	-5.32	112.82	120.80
22	3-O	65	PHE	CB-CA-C	5.32	120.35	109.55
24	3-Q	185	TYR	CB-CG-CD2	-5.32	112.82	120.80
29	1-V	131	GLN	CB-CA-C	-5.32	101.81	110.85
29	2-V	131	GLN	CB-CA-C	-5.32	101.81	110.85
29	3-V	131	GLN	CB-CA-C	-5.32	101.81	110.85
19	1-L	109	MET	CG-SD-CE	-5.32	89.20	100.90
19	2-L	109	MET	CG-SD-CE	-5.32	89.20	100.90
19	3-L	109	MET	CG-SD-CE	-5.32	89.20	100.90
22	1-O	20	PRO	N-CA-C	5.31	123.41	112.47
30	1-W	158	ILE	CA-CB-CG2	5.31	119.53	110.50
22	2-O	20	PRO	N-CA-C	5.31	123.41	112.47
30	2-W	158	ILE	CA-CB-CG2	5.31	119.53	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3-O	20	PRO	N-CA-C	5.31	123.41	112.47
30	3-W	158	ILE	CA-CB-CG2	5.31	119.53	110.50
9	1-B	151	ASP	CB-CA-C	5.31	117.81	109.37
20	1-M	250	GLN	OE1-CD-NE2	-5.31	117.29	122.60
31	1-X	131	ASN	CA-CB-CG	5.31	117.91	112.60
9	2-B	151	ASP	CB-CA-C	5.31	117.81	109.37
20	2-M	250	GLN	OE1-CD-NE2	-5.31	117.29	122.60
31	2-X	131	ASN	CA-CB-CG	5.31	117.91	112.60
9	3-B	151	ASP	CB-CA-C	5.31	117.81	109.37
20	3-M	250	GLN	OE1-CD-NE2	-5.31	117.29	122.60
31	3-X	131	ASN	CA-CB-CG	5.31	117.91	112.60
18	1-K	153	ASP	CA-CB-CG	5.31	117.91	112.60
27	1-T	123	HIS	CA-CB-CG	-5.31	108.49	113.80
18	2-K	153	ASP	CA-CB-CG	5.31	117.91	112.60
27	2-T	123	HIS	CA-CB-CG	-5.31	108.49	113.80
18	3-K	153	ASP	CA-CB-CG	5.31	117.91	112.60
27	3-T	123	HIS	CA-CB-CG	-5.31	108.49	113.80
24	1-Q	51	ARG	CA-C-N	5.30	127.82	120.29
24	1-Q	51	ARG	C-N-CA	5.30	127.82	120.29
29	1-V	109	HIS	CB-CG-CD2	-5.30	124.31	131.20
24	2-Q	51	ARG	CA-C-N	5.30	127.82	120.29
24	2-Q	51	ARG	C-N-CA	5.30	127.82	120.29
29	2-V	109	HIS	CB-CG-CD2	-5.30	124.31	131.20
24	3-Q	51	ARG	CA-C-N	5.30	127.82	120.29
24	3-Q	51	ARG	C-N-CA	5.30	127.82	120.29
29	3-V	109	HIS	CB-CG-CD2	-5.30	124.31	131.20
15	1-H	357	ARG	NE-CZ-NH2	5.30	123.97	119.20
15	2-H	357	ARG	NE-CZ-NH2	5.30	123.97	119.20
15	3-H	357	ARG	NE-CZ-NH2	5.30	123.97	119.20
23	1-P	370	ASP	CB-CA-C	5.30	120.97	110.42
23	2-P	370	ASP	CB-CA-C	5.30	120.97	110.42
23	3-P	370	ASP	CB-CA-C	5.30	120.97	110.42
10	1-c	218	GLY	CA-C-N	5.29	131.65	121.54
10	1-c	218	GLY	C-N-CA	5.29	131.65	121.54
10	2-c	218	GLY	CA-C-N	5.29	131.65	121.54
10	2-c	218	GLY	C-N-CA	5.29	131.65	121.54
10	3-c	218	GLY	CA-C-N	5.29	131.65	121.54
10	3-c	218	GLY	C-N-CA	5.29	131.65	121.54
7	1-7	131	ASN	OD1-CG-ND2	-5.29	117.31	122.60
7	2-7	131	ASN	OD1-CG-ND2	-5.29	117.31	122.60
7	3-7	131	ASN	OD1-CG-ND2	-5.29	117.31	122.60
23	1-P	344	ARG	NE-CZ-NH2	5.29	123.96	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2-P	344	ARG	NE-CZ-NH2	5.29	123.96	119.20
23	3-P	344	ARG	NE-CZ-NH2	5.29	123.96	119.20
18	1-K	200	GLN	OE1-CD-NE2	-5.29	117.31	122.60
18	2-K	200	GLN	OE1-CD-NE2	-5.29	117.31	122.60
18	3-K	200	GLN	OE1-CD-NE2	-5.29	117.31	122.60
21	1-N	529	GLN	OE1-CD-NE2	-5.29	117.31	122.60
11	1-d	53	GLN	OE1-CD-NE2	-5.29	117.31	122.60
21	2-N	529	GLN	OE1-CD-NE2	-5.29	117.31	122.60
11	2-d	53	GLN	OE1-CD-NE2	-5.29	117.31	122.60
21	3-N	529	GLN	OE1-CD-NE2	-5.29	117.31	122.60
11	3-d	53	GLN	OE1-CD-NE2	-5.29	117.31	122.60
33	1-Z	24	THR	CA-C-N	5.29	126.45	119.84
33	1-Z	24	THR	C-N-CA	5.29	126.45	119.84
33	2-Z	24	THR	CA-C-N	5.29	126.45	119.84
33	2-Z	24	THR	C-N-CA	5.29	126.45	119.84
33	3-Z	24	THR	CA-C-N	5.29	126.45	119.84
33	3-Z	24	THR	C-N-CA	5.29	126.45	119.84
11	1-d	68	HIS	CB-CG-CD2	-5.29	124.33	131.20
11	2-d	68	HIS	CB-CG-CD2	-5.29	124.33	131.20
11	3-d	68	HIS	CB-CG-CD2	-5.29	124.33	131.20
21	1-N	715	ILE	CB-CA-C	5.28	118.44	111.21
27	1-T	81	TYR	CA-C-N	5.28	127.61	120.38
27	1-T	81	TYR	C-N-CA	5.28	127.61	120.38
21	2-N	715	ILE	CB-CA-C	5.28	118.44	111.21
27	2-T	81	TYR	CA-C-N	5.28	127.61	120.38
27	2-T	81	TYR	C-N-CA	5.28	127.61	120.38
21	3-N	715	ILE	CB-CA-C	5.28	118.44	111.21
27	3-T	81	TYR	CA-C-N	5.28	127.61	120.38
27	3-T	81	TYR	C-N-CA	5.28	127.61	120.38
33	1-Z	959	HIS	CB-CG-CD2	-5.28	124.34	131.20
33	2-Z	959	HIS	CB-CG-CD2	-5.28	124.34	131.20
33	3-Z	959	HIS	CB-CG-CD2	-5.28	124.34	131.20
20	1-M	345	ARG	NE-CZ-NH2	5.27	123.95	119.20
23	1-P	231	LYS	CA-C-N	5.27	131.54	123.47
23	1-P	231	LYS	C-N-CA	5.27	131.54	123.47
20	2-M	345	ARG	NE-CZ-NH2	5.27	123.95	119.20
23	2-P	231	LYS	CA-C-N	5.27	131.54	123.47
23	2-P	231	LYS	C-N-CA	5.27	131.54	123.47
20	3-M	345	ARG	NE-CZ-NH2	5.27	123.95	119.20
23	3-P	231	LYS	CA-C-N	5.27	131.54	123.47
23	3-P	231	LYS	C-N-CA	5.27	131.54	123.47
12	1-e	91	HIS	CA-CB-CG	-5.27	108.53	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	2-e	91	HIS	CA-CB-CG	-5.27	108.53	113.80
12	3-e	91	HIS	CA-CB-CG	-5.27	108.53	113.80
17	1-J	296	ARG	NE-CZ-NH2	5.26	123.94	119.20
7	1-n	187	ARG	NE-CZ-NH2	5.26	123.94	119.20
17	2-J	296	ARG	NE-CZ-NH2	5.26	123.94	119.20
7	2-n	187	ARG	NE-CZ-NH2	5.26	123.94	119.20
17	3-J	296	ARG	NE-CZ-NH2	5.26	123.94	119.20
7	3-n	187	ARG	NE-CZ-NH2	5.26	123.94	119.20
25	1-R	222	ARG	NE-CZ-NH2	5.26	123.93	119.20
25	2-R	222	ARG	NE-CZ-NH2	5.26	123.93	119.20
25	3-R	222	ARG	NE-CZ-NH2	5.26	123.93	119.20
18	1-K	244	HIS	CA-CB-CG	-5.26	108.54	113.80
18	2-K	244	HIS	CA-CB-CG	-5.26	108.54	113.80
18	3-K	244	HIS	CA-CB-CG	-5.26	108.54	113.80
28	1-U	70	HIS	CB-CG-CD2	-5.25	124.37	131.20
13	1-f	42	HIS	CB-CG-CD2	-5.25	124.37	131.20
28	2-U	70	HIS	CB-CG-CD2	-5.25	124.37	131.20
13	2-f	42	HIS	CB-CG-CD2	-5.25	124.37	131.20
28	3-U	70	HIS	CB-CG-CD2	-5.25	124.37	131.20
13	3-f	42	HIS	CB-CG-CD2	-5.25	124.37	131.20
14	1-G	83	HIS	CB-CG-CD2	-5.25	124.38	131.20
14	2-G	83	HIS	CB-CG-CD2	-5.25	124.38	131.20
14	3-G	83	HIS	CB-CG-CD2	-5.25	124.38	131.20
19	1-L	289	ARG	NE-CZ-NH2	5.25	123.92	119.20
14	1-g	111	ARG	NE-CZ-NH2	5.25	123.92	119.20
5	1-l	191	HIS	CB-CG-CD2	-5.25	124.38	131.20
19	2-L	289	ARG	NE-CZ-NH2	5.25	123.92	119.20
14	2-g	111	ARG	NE-CZ-NH2	5.25	123.92	119.20
5	2-l	191	HIS	CB-CG-CD2	-5.25	124.38	131.20
19	3-L	289	ARG	NE-CZ-NH2	5.25	123.92	119.20
14	3-g	111	ARG	NE-CZ-NH2	5.25	123.92	119.20
5	3-l	191	HIS	CB-CG-CD2	-5.25	124.38	131.20
26	1-S	467	PHE	CA-CB-CG	5.24	119.04	113.80
26	2-S	467	PHE	CA-CB-CG	5.24	119.04	113.80
26	3-S	467	PHE	CA-CB-CG	5.24	119.04	113.80
17	1-J	371	ARG	NE-CZ-NH2	5.24	123.91	119.20
17	2-J	371	ARG	NE-CZ-NH2	5.24	123.91	119.20
17	3-J	371	ARG	NE-CZ-NH2	5.24	123.91	119.20
3	1-3	63	ASN	CA-CB-CG	-5.24	107.36	112.60
22	1-O	147	ARG	NE-CZ-NH2	5.24	123.91	119.20
27	1-T	82	PHE	N-CA-CB	-5.24	102.21	110.06
3	2-3	63	ASN	CA-CB-CG	-5.24	107.36	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2-O	147	ARG	NE-CZ-NH2	5.24	123.91	119.20
27	2-T	82	PHE	N-CA-CB	-5.24	102.21	110.06
3	3-3	63	ASN	CA-CB-CG	-5.24	107.36	112.60
22	3-O	147	ARG	NE-CZ-NH2	5.24	123.91	119.20
27	3-T	82	PHE	N-CA-CB	-5.24	102.21	110.06
13	1-F	116	GLN	OE1-CD-NE2	-5.23	117.37	122.60
26	1-S	65	ASN	CA-CB-CG	5.23	117.83	112.60
13	2-F	116	GLN	OE1-CD-NE2	-5.23	117.37	122.60
26	2-S	65	ASN	CA-CB-CG	5.23	117.83	112.60
13	3-F	116	GLN	OE1-CD-NE2	-5.23	117.37	122.60
26	3-S	65	ASN	CA-CB-CG	5.23	117.83	112.60
33	1-Z	88	PRO	N-CA-CB	5.22	109.03	103.39
33	2-Z	88	PRO	N-CA-CB	5.22	109.03	103.39
33	3-Z	88	PRO	N-CA-CB	5.22	109.03	103.39
10	1-c	159	TRP	CB-CG-CD2	5.22	134.11	126.80
10	2-c	159	TRP	CB-CG-CD2	5.22	134.11	126.80
10	3-c	159	TRP	CB-CG-CD2	5.22	134.11	126.80
26	1-S	227	ASN	CA-C-N	5.22	127.28	120.28
26	1-S	227	ASN	C-N-CA	5.22	127.28	120.28
3	1-j	44	HIS	CB-CG-CD2	-5.22	124.42	131.20
26	2-S	227	ASN	CA-C-N	5.22	127.28	120.28
26	2-S	227	ASN	C-N-CA	5.22	127.28	120.28
3	2-j	44	HIS	CB-CG-CD2	-5.22	124.42	131.20
26	3-S	227	ASN	CA-C-N	5.22	127.28	120.28
26	3-S	227	ASN	C-N-CA	5.22	127.28	120.28
3	3-j	44	HIS	CB-CG-CD2	-5.22	124.42	131.20
13	1-f	20	GLN	OE1-CD-NE2	-5.22	117.38	122.60
4	1-k	8	ARG	NE-CZ-NH2	5.22	123.90	119.20
13	2-f	20	GLN	OE1-CD-NE2	-5.22	117.38	122.60
4	2-k	8	ARG	NE-CZ-NH2	5.22	123.90	119.20
13	3-f	20	GLN	OE1-CD-NE2	-5.22	117.38	122.60
4	3-k	8	ARG	NE-CZ-NH2	5.22	123.90	119.20
19	1-L	133	ASN	OD1-CG-ND2	-5.21	117.39	122.60
19	2-L	133	ASN	OD1-CG-ND2	-5.21	117.39	122.60
19	3-L	133	ASN	OD1-CG-ND2	-5.21	117.39	122.60
21	1-N	418	ASP	CA-CB-CG	5.21	117.81	112.60
21	2-N	418	ASP	CA-CB-CG	5.21	117.81	112.60
21	3-N	418	ASP	CA-CB-CG	5.21	117.81	112.60
13	1-F	85	ASN	OD1-CG-ND2	-5.21	117.39	122.60
13	2-F	85	ASN	OD1-CG-ND2	-5.21	117.39	122.60
13	3-F	85	ASN	OD1-CG-ND2	-5.21	117.39	122.60
23	1-P	277	GLN	OE1-CD-NE2	-5.21	117.39	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2-P	277	GLN	OE1-CD-NE2	-5.21	117.39	122.60
23	3-P	277	GLN	OE1-CD-NE2	-5.21	117.39	122.60
21	1-N	719	ASN	CA-CB-CG	5.21	117.81	112.60
21	2-N	719	ASN	CA-CB-CG	5.21	117.81	112.60
21	3-N	719	ASN	CA-CB-CG	5.21	117.81	112.60
21	1-N	138	GLU	CB-CG-CD	5.20	121.44	112.60
21	2-N	138	GLU	CB-CG-CD	5.20	121.44	112.60
21	3-N	138	GLU	CB-CG-CD	5.20	121.44	112.60
11	1-d	109	ARG	NE-CZ-NH2	5.20	123.88	119.20
11	2-d	109	ARG	NE-CZ-NH2	5.20	123.88	119.20
11	3-d	109	ARG	NE-CZ-NH2	5.20	123.88	119.20
17	1-J	15	HIS	CB-CG-CD2	-5.20	124.45	131.20
17	2-J	15	HIS	CB-CG-CD2	-5.20	124.45	131.20
17	3-J	15	HIS	CB-CG-CD2	-5.20	124.45	131.20
18	1-K	83	GLN	OE1-CD-NE2	-5.19	117.41	122.60
18	2-K	83	GLN	OE1-CD-NE2	-5.19	117.41	122.60
18	3-K	83	GLN	OE1-CD-NE2	-5.19	117.41	122.60
11	1-D	53	GLN	OE1-CD-NE2	-5.19	117.41	122.60
11	2-D	53	GLN	OE1-CD-NE2	-5.19	117.41	122.60
11	3-D	53	GLN	OE1-CD-NE2	-5.19	117.41	122.60
26	1-S	46	LEU	CA-C-N	5.19	131.45	121.54
26	1-S	46	LEU	C-N-CA	5.19	131.45	121.54
26	2-S	46	LEU	CA-C-N	5.19	131.45	121.54
26	2-S	46	LEU	C-N-CA	5.19	131.45	121.54
26	3-S	46	LEU	CA-C-N	5.19	131.45	121.54
26	3-S	46	LEU	C-N-CA	5.19	131.45	121.54
17	1-J	205	HIS	CB-CG-CD2	-5.18	124.46	131.20
33	1-Z	205	LEU	CA-C-N	5.18	127.49	120.65
33	1-Z	205	LEU	C-N-CA	5.18	127.49	120.65
17	2-J	205	HIS	CB-CG-CD2	-5.18	124.46	131.20
33	2-Z	205	LEU	CA-C-N	5.18	127.49	120.65
33	2-Z	205	LEU	C-N-CA	5.18	127.49	120.65
17	3-J	205	HIS	CB-CG-CD2	-5.18	124.46	131.20
33	3-Z	205	LEU	CA-C-N	5.18	127.49	120.65
33	3-Z	205	LEU	C-N-CA	5.18	127.49	120.65
26	1-S	420	GLU	CB-CA-C	-5.18	102.19	110.79
26	2-S	420	GLU	CB-CA-C	-5.18	102.19	110.79
26	3-S	420	GLU	CB-CA-C	-5.18	102.19	110.79
6	1-m	106	TYR	CB-CG-CD1	-5.17	113.04	120.80
6	2-m	106	TYR	CB-CG-CD1	-5.17	113.04	120.80
6	3-m	106	TYR	CB-CG-CD1	-5.17	113.04	120.80
21	1-N	375	HIS	CA-CB-CG	5.17	118.97	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	1-b	246	ARG	NE-CZ-NH2	5.17	123.86	119.20
1	1-h	91	ASP	CA-CB-CG	5.17	117.77	112.60
21	2-N	375	HIS	CA-CB-CG	5.17	118.97	113.80
9	2-b	246	ARG	NE-CZ-NH2	5.17	123.86	119.20
1	2-h	91	ASP	CA-CB-CG	5.17	117.77	112.60
21	3-N	375	HIS	CA-CB-CG	5.17	118.97	113.80
9	3-b	246	ARG	NE-CZ-NH2	5.17	123.86	119.20
1	3-h	91	ASP	CA-CB-CG	5.17	117.77	112.60
25	1-R	310	GLU	CB-CA-C	-5.17	102.21	110.79
25	2-R	310	GLU	CB-CA-C	-5.17	102.21	110.79
25	3-R	310	GLU	CB-CA-C	-5.17	102.21	110.79
28	1-U	142	GLN	OE1-CD-NE2	-5.17	117.43	122.60
28	2-U	142	GLN	OE1-CD-NE2	-5.17	117.43	122.60
28	3-U	142	GLN	OE1-CD-NE2	-5.17	117.43	122.60
8	1-A	111	ARG	CD-NE-CZ	5.16	131.62	124.40
12	1-E	208	ASN	OD1-CG-ND2	-5.16	117.44	122.60
8	2-A	111	ARG	CD-NE-CZ	5.16	131.62	124.40
12	2-E	208	ASN	OD1-CG-ND2	-5.16	117.44	122.60
8	3-A	111	ARG	CD-NE-CZ	5.16	131.62	124.40
12	3-E	208	ASN	OD1-CG-ND2	-5.16	117.44	122.60
23	1-P	74	ASP	CA-CB-CG	-5.16	107.44	112.60
33	1-Z	759	ARG	NE-CZ-NH2	5.16	123.84	119.20
23	2-P	74	ASP	CA-CB-CG	-5.16	107.44	112.60
33	2-Z	759	ARG	NE-CZ-NH2	5.16	123.84	119.20
23	3-P	74	ASP	CA-CB-CG	-5.16	107.44	112.60
33	3-Z	759	ARG	NE-CZ-NH2	5.16	123.84	119.20
6	1-6	102	PHE	CA-CB-CG	-5.15	108.65	113.80
6	2-6	102	PHE	CA-CB-CG	-5.15	108.65	113.80
6	3-6	102	PHE	CA-CB-CG	-5.15	108.65	113.80
2	1-2	116	HIS	CB-CG-CD2	-5.15	124.50	131.20
2	2-2	116	HIS	CB-CG-CD2	-5.15	124.50	131.20
2	3-2	116	HIS	CB-CG-CD2	-5.15	124.50	131.20
7	1-7	149	HIS	CB-CG-CD2	-5.15	124.50	131.20
7	2-7	149	HIS	CB-CG-CD2	-5.15	124.50	131.20
7	3-7	149	HIS	CB-CG-CD2	-5.15	124.50	131.20
6	1-6	106	TYR	CB-CG-CD1	-5.15	113.08	120.80
28	1-U	115	GLN	CB-CG-CD	5.15	121.35	112.60
33	1-Z	168	GLN	OE1-CD-NE2	-5.15	117.45	122.60
6	2-6	106	TYR	CB-CG-CD1	-5.15	113.08	120.80
28	2-U	115	GLN	CB-CG-CD	5.15	121.35	112.60
33	2-Z	168	GLN	OE1-CD-NE2	-5.15	117.45	122.60
6	3-6	106	TYR	CB-CG-CD1	-5.15	113.08	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	3-U	115	GLN	CB-CG-CD	5.15	121.35	112.60
33	3-Z	168	GLN	OE1-CD-NE2	-5.15	117.45	122.60
18	1-K	74	HIS	CB-CG-CD2	-5.15	124.51	131.20
9	1-b	234	ARG	NE-CZ-NH2	5.15	123.83	119.20
18	2-K	74	HIS	CB-CG-CD2	-5.15	124.51	131.20
9	2-b	234	ARG	NE-CZ-NH2	5.15	123.83	119.20
18	3-K	74	HIS	CB-CG-CD2	-5.15	124.51	131.20
9	3-b	234	ARG	NE-CZ-NH2	5.15	123.83	119.20
27	1-T	238	GLN	OE1-CD-NE2	-5.15	117.45	122.60
27	2-T	238	GLN	OE1-CD-NE2	-5.15	117.45	122.60
27	3-T	238	GLN	OE1-CD-NE2	-5.15	117.45	122.60
18	1-K	142	HIS	CB-CG-CD2	-5.14	124.51	131.20
27	1-T	182	LYS	CB-CA-C	-5.14	101.94	110.68
18	2-K	142	HIS	CB-CG-CD2	-5.14	124.51	131.20
27	2-T	182	LYS	CB-CA-C	-5.14	101.94	110.68
18	3-K	142	HIS	CB-CG-CD2	-5.14	124.51	131.20
27	3-T	182	LYS	CB-CA-C	-5.14	101.94	110.68
13	1-f	145	GLU	CB-CG-CD	-5.14	103.86	112.60
13	2-f	145	GLU	CB-CG-CD	-5.14	103.86	112.60
13	3-f	145	GLU	CB-CG-CD	-5.14	103.86	112.60
12	1-E	65	HIS	CB-CG-CD2	-5.14	124.52	131.20
12	2-E	65	HIS	CB-CG-CD2	-5.14	124.52	131.20
12	3-E	65	HIS	CB-CG-CD2	-5.14	124.52	131.20
18	1-K	98	GLN	OE1-CD-NE2	-5.14	117.46	122.60
19	1-L	303	ARG	NE-CZ-NH2	5.14	123.83	119.20
18	2-K	98	GLN	OE1-CD-NE2	-5.14	117.46	122.60
19	2-L	303	ARG	NE-CZ-NH2	5.14	123.83	119.20
18	3-K	98	GLN	OE1-CD-NE2	-5.14	117.46	122.60
19	3-L	303	ARG	NE-CZ-NH2	5.14	123.83	119.20
2	1-i	206	PRO	N-CA-CB	5.13	108.10	103.33
2	2-i	206	PRO	N-CA-CB	5.13	108.10	103.33
2	3-i	206	PRO	N-CA-CB	5.13	108.10	103.33
16	1-I	150	HIS	CA-CB-CG	5.13	118.93	113.80
16	2-I	150	HIS	CA-CB-CG	5.13	118.93	113.80
16	3-I	150	HIS	CA-CB-CG	5.13	118.93	113.80
18	1-K	151	PRO	CA-C-N	5.13	124.82	119.64
18	1-K	151	PRO	C-N-CA	5.13	124.82	119.64
18	2-K	151	PRO	CA-C-N	5.13	124.82	119.64
18	2-K	151	PRO	C-N-CA	5.13	124.82	119.64
18	3-K	151	PRO	CA-C-N	5.13	124.82	119.64
18	3-K	151	PRO	C-N-CA	5.13	124.82	119.64
20	1-M	377	GLN	OE1-CD-NE2	-5.12	117.47	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1-S	39	ASN	CA-CB-CG	5.12	117.72	112.60
2	1-i	116	HIS	CA-CB-CG	-5.12	108.67	113.80
20	2-M	377	GLN	OE1-CD-NE2	-5.12	117.47	122.60
26	2-S	39	ASN	CA-CB-CG	5.12	117.72	112.60
2	2-i	116	HIS	CA-CB-CG	-5.12	108.67	113.80
20	3-M	377	GLN	OE1-CD-NE2	-5.12	117.47	122.60
26	3-S	39	ASN	CA-CB-CG	5.12	117.72	112.60
2	3-i	116	HIS	CA-CB-CG	-5.12	108.67	113.80
1	1-1	185	ARG	NE-CZ-NH2	5.12	123.81	119.20
24	1-Q	18	LYS	CB-CG-CD	5.12	123.09	111.30
1	2-1	185	ARG	NE-CZ-NH2	5.12	123.81	119.20
24	2-Q	18	LYS	CB-CG-CD	5.12	123.09	111.30
1	3-1	185	ARG	NE-CZ-NH2	5.12	123.81	119.20
24	3-Q	18	LYS	CB-CG-CD	5.12	123.09	111.30
21	1-N	672	ASN	CA-C-N	5.12	124.91	119.28
21	1-N	672	ASN	C-N-CA	5.12	124.91	119.28
21	2-N	672	ASN	CA-C-N	5.12	124.91	119.28
21	2-N	672	ASN	C-N-CA	5.12	124.91	119.28
21	3-N	672	ASN	CA-C-N	5.12	124.91	119.28
21	3-N	672	ASN	C-N-CA	5.12	124.91	119.28
6	1-6	178	GLU	CB-CG-CD	-5.12	103.90	112.60
23	1-P	47	ARG	NE-CZ-NH2	5.12	123.81	119.20
6	2-6	178	GLU	CB-CG-CD	-5.12	103.90	112.60
23	2-P	47	ARG	NE-CZ-NH2	5.12	123.81	119.20
6	3-6	178	GLU	CB-CG-CD	-5.12	103.90	112.60
23	3-P	47	ARG	NE-CZ-NH2	5.12	123.81	119.20
33	1-Z	85	VAL	N-CA-C	5.12	119.93	108.88
33	2-Z	85	VAL	N-CA-C	5.12	119.93	108.88
33	3-Z	85	VAL	N-CA-C	5.12	119.93	108.88
21	1-N	583	VAL	CB-CA-C	-5.11	105.16	112.22
22	1-O	288	ARG	NE-CZ-NH2	5.11	123.80	119.20
30	1-W	177	GLY	CA-C-N	5.11	126.23	119.84
30	1-W	177	GLY	C-N-CA	5.11	126.23	119.84
21	2-N	583	VAL	CB-CA-C	-5.11	105.16	112.22
22	2-O	288	ARG	NE-CZ-NH2	5.11	123.80	119.20
30	2-W	177	GLY	CA-C-N	5.11	126.23	119.84
30	2-W	177	GLY	C-N-CA	5.11	126.23	119.84
21	3-N	583	VAL	CB-CA-C	-5.11	105.16	112.22
22	3-O	288	ARG	NE-CZ-NH2	5.11	123.80	119.20
30	3-W	177	GLY	CA-C-N	5.11	126.23	119.84
30	3-W	177	GLY	C-N-CA	5.11	126.23	119.84
7	1-7	104	ARG	NE-CZ-NH2	5.11	123.80	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	2-7	104	ARG	NE-CZ-NH2	5.11	123.80	119.20
7	3-7	104	ARG	NE-CZ-NH2	5.11	123.80	119.20
2	1-i	144	GLN	OE1-CD-NE2	-5.11	117.49	122.60
2	2-i	144	GLN	OE1-CD-NE2	-5.11	117.49	122.60
2	3-i	144	GLN	OE1-CD-NE2	-5.11	117.49	122.60
26	1-S	100	HIS	CB-CG-CD2	-5.11	124.56	131.20
26	1-S	382	ARG	NE-CZ-NH2	5.11	123.80	119.20
27	1-T	47	GLN	OE1-CD-NE2	-5.11	117.49	122.60
28	1-U	115	GLN	OE1-CD-NE2	-5.11	117.49	122.60
26	2-S	100	HIS	CB-CG-CD2	-5.11	124.56	131.20
26	2-S	382	ARG	NE-CZ-NH2	5.11	123.80	119.20
27	2-T	47	GLN	OE1-CD-NE2	-5.11	117.49	122.60
28	2-U	115	GLN	OE1-CD-NE2	-5.11	117.49	122.60
26	3-S	100	HIS	CB-CG-CD2	-5.11	124.56	131.20
26	3-S	382	ARG	NE-CZ-NH2	5.11	123.80	119.20
27	3-T	47	GLN	OE1-CD-NE2	-5.11	117.49	122.60
28	3-U	115	GLN	OE1-CD-NE2	-5.11	117.49	122.60
11	1-D	176	ASN	CA-CB-CG	-5.11	107.49	112.60
16	1-I	303	GLN	OE1-CD-NE2	-5.11	117.49	122.60
26	1-S	417	GLN	OE1-CD-NE2	-5.11	117.50	122.60
11	2-D	176	ASN	CA-CB-CG	-5.11	107.49	112.60
16	2-I	303	GLN	OE1-CD-NE2	-5.11	117.49	122.60
26	2-S	417	GLN	OE1-CD-NE2	-5.11	117.50	122.60
11	3-D	176	ASN	CA-CB-CG	-5.11	107.49	112.60
16	3-I	303	GLN	OE1-CD-NE2	-5.11	117.49	122.60
26	3-S	417	GLN	OE1-CD-NE2	-5.11	117.50	122.60
24	1-Q	162	LEU	N-CA-CB	-5.10	102.58	110.13
24	2-Q	162	LEU	N-CA-CB	-5.10	102.58	110.13
24	3-Q	162	LEU	N-CA-CB	-5.10	102.58	110.13
20	1-M	328	ASN	CA-CB-CG	5.10	117.70	112.60
20	2-M	328	ASN	CA-CB-CG	5.10	117.70	112.60
20	3-M	328	ASN	CA-CB-CG	5.10	117.70	112.60
21	1-N	716	GLN	OE1-CD-NE2	-5.10	117.50	122.60
21	2-N	716	GLN	OE1-CD-NE2	-5.10	117.50	122.60
21	3-N	716	GLN	OE1-CD-NE2	-5.10	117.50	122.60
22	1-O	20	PRO	CA-N-CD	-5.10	104.86	112.00
23	1-P	431	HIS	CB-CG-CD2	-5.10	124.57	131.20
33	1-Z	948	TRP	CB-CG-CD1	-5.10	119.25	126.90
22	2-O	20	PRO	CA-N-CD	-5.10	104.86	112.00
23	2-P	431	HIS	CB-CG-CD2	-5.10	124.57	131.20
33	2-Z	948	TRP	CB-CG-CD1	-5.10	119.25	126.90
22	3-O	20	PRO	CA-N-CD	-5.10	104.86	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	3-P	431	HIS	CB-CG-CD2	-5.10	124.57	131.20
33	3-Z	948	TRP	CB-CG-CD1	-5.10	119.25	126.90
22	1-O	282	GLN	OE1-CD-NE2	-5.10	117.50	122.60
22	2-O	282	GLN	OE1-CD-NE2	-5.10	117.50	122.60
22	3-O	282	GLN	OE1-CD-NE2	-5.10	117.50	122.60
6	1-6	2	PHE	CA-CB-CG	5.09	118.89	113.80
21	1-N	619	CYS	CA-C-N	5.09	125.59	119.94
21	1-N	619	CYS	C-N-CA	5.09	125.59	119.94
23	1-P	91	LEU	CA-C-N	5.09	127.37	120.65
23	1-P	91	LEU	C-N-CA	5.09	127.37	120.65
6	2-6	2	PHE	CA-CB-CG	5.09	118.89	113.80
21	2-N	619	CYS	CA-C-N	5.09	125.59	119.94
21	2-N	619	CYS	C-N-CA	5.09	125.59	119.94
23	2-P	91	LEU	CA-C-N	5.09	127.37	120.65
23	2-P	91	LEU	C-N-CA	5.09	127.37	120.65
6	3-6	2	PHE	CA-CB-CG	5.09	118.89	113.80
21	3-N	619	CYS	CA-C-N	5.09	125.59	119.94
21	3-N	619	CYS	C-N-CA	5.09	125.59	119.94
23	3-P	91	LEU	CA-C-N	5.09	127.37	120.65
23	3-P	91	LEU	C-N-CA	5.09	127.37	120.65
2	1-2	22	GLN	OE1-CD-NE2	-5.08	117.52	122.60
2	2-2	22	GLN	OE1-CD-NE2	-5.08	117.52	122.60
2	3-2	22	GLN	OE1-CD-NE2	-5.08	117.52	122.60
33	1-Z	175	ASP	CA-CB-CG	5.08	117.68	112.60
33	2-Z	175	ASP	CA-CB-CG	5.08	117.68	112.60
33	3-Z	175	ASP	CA-CB-CG	5.08	117.68	112.60
1	1-1	53	GLN	OE1-CD-NE2	-5.07	117.53	122.60
19	1-L	99	GLN	OE1-CD-NE2	-5.07	117.53	122.60
33	1-Z	202	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	2-1	53	GLN	OE1-CD-NE2	-5.07	117.53	122.60
19	2-L	99	GLN	OE1-CD-NE2	-5.07	117.53	122.60
33	2-Z	202	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	3-1	53	GLN	OE1-CD-NE2	-5.07	117.53	122.60
19	3-L	99	GLN	OE1-CD-NE2	-5.07	117.53	122.60
33	3-Z	202	ARG	NE-CZ-NH2	5.07	123.76	119.20
33	1-Z	539	ASN	OD1-CG-ND2	-5.07	117.53	122.60
33	2-Z	539	ASN	OD1-CG-ND2	-5.07	117.53	122.60
33	3-Z	539	ASN	OD1-CG-ND2	-5.07	117.53	122.60
10	1-C	20	GLN	OE1-CD-NE2	-5.07	117.53	122.60
21	1-N	812	ALA	CA-C-N	5.07	127.38	120.54
21	1-N	812	ALA	C-N-CA	5.07	127.38	120.54
13	1-f	116	GLN	OE1-CD-NE2	-5.07	117.53	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	2-C	20	GLN	OE1-CD-NE2	-5.07	117.53	122.60
21	2-N	812	ALA	CA-C-N	5.07	127.38	120.54
21	2-N	812	ALA	C-N-CA	5.07	127.38	120.54
13	2-f	116	GLN	OE1-CD-NE2	-5.07	117.53	122.60
10	3-C	20	GLN	OE1-CD-NE2	-5.07	117.53	122.60
21	3-N	812	ALA	CA-C-N	5.07	127.38	120.54
21	3-N	812	ALA	C-N-CA	5.07	127.38	120.54
13	3-f	116	GLN	OE1-CD-NE2	-5.07	117.53	122.60
18	1-K	185	ARG	NE-CZ-NH2	5.06	123.76	119.20
22	1-O	195	TYR	CB-CG-CD2	-5.06	113.21	120.80
18	2-K	185	ARG	NE-CZ-NH2	5.06	123.76	119.20
22	2-O	195	TYR	CB-CG-CD2	-5.06	113.21	120.80
18	3-K	185	ARG	NE-CZ-NH2	5.06	123.76	119.20
22	3-O	195	TYR	CB-CG-CD2	-5.06	113.21	120.80
26	1-S	174	ARG	NE-CZ-NH2	5.06	123.75	119.20
9	1-b	30	GLN	OE1-CD-NE2	-5.06	117.54	122.60
26	2-S	174	ARG	NE-CZ-NH2	5.06	123.75	119.20
9	2-b	30	GLN	OE1-CD-NE2	-5.06	117.54	122.60
26	3-S	174	ARG	NE-CZ-NH2	5.06	123.75	119.20
9	3-b	30	GLN	OE1-CD-NE2	-5.06	117.54	122.60
13	1-F	90	GLN	OE1-CD-NE2	-5.06	117.54	122.60
13	2-F	90	GLN	OE1-CD-NE2	-5.06	117.54	122.60
13	3-F	90	GLN	OE1-CD-NE2	-5.06	117.54	122.60
6	1-m	76	HIS	CB-CG-CD2	-5.05	124.63	131.20
6	2-m	76	HIS	CB-CG-CD2	-5.05	124.63	131.20
6	3-m	76	HIS	CB-CG-CD2	-5.05	124.63	131.20
9	1-B	178	ARG	NE-CZ-NH2	5.05	123.75	119.20
9	2-B	178	ARG	NE-CZ-NH2	5.05	123.75	119.20
9	3-B	178	ARG	NE-CZ-NH2	5.05	123.75	119.20
16	1-I	343	ARG	NE-CZ-NH2	5.05	123.74	119.20
4	1-k	52	ASP	CA-C-N	5.05	127.00	120.44
4	1-k	52	ASP	C-N-CA	5.05	127.00	120.44
16	2-I	343	ARG	NE-CZ-NH2	5.05	123.74	119.20
4	2-k	52	ASP	CA-C-N	5.05	127.00	120.44
4	2-k	52	ASP	C-N-CA	5.05	127.00	120.44
16	3-I	343	ARG	NE-CZ-NH2	5.05	123.74	119.20
4	3-k	52	ASP	CA-C-N	5.05	127.00	120.44
4	3-k	52	ASP	C-N-CA	5.05	127.00	120.44
14	1-G	59	LYS	N-CA-CB	-5.04	102.75	110.26
14	2-G	59	LYS	N-CA-CB	-5.04	102.75	110.26
14	3-G	59	LYS	N-CA-CB	-5.04	102.75	110.26
22	1-O	105	GLN	CB-CG-CD	5.04	121.17	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2-O	105	GLN	CB-CG-CD	5.04	121.17	112.60
22	3-O	105	GLN	CB-CG-CD	5.04	121.17	112.60
4	1-k	74	GLU	CB-CG-CD	5.04	121.17	112.60
6	1-m	101	ARG	NE-CZ-NH2	5.04	123.73	119.20
4	2-k	74	GLU	CB-CG-CD	5.04	121.17	112.60
6	2-m	101	ARG	NE-CZ-NH2	5.04	123.73	119.20
4	3-k	74	GLU	CB-CG-CD	5.04	121.17	112.60
6	3-m	101	ARG	NE-CZ-NH2	5.04	123.73	119.20
2	1-2	186	TYR	CB-CG-CD1	5.03	128.35	120.80
2	2-2	186	TYR	CB-CG-CD1	5.03	128.35	120.80
2	3-2	186	TYR	CB-CG-CD1	5.03	128.35	120.80
16	1-I	332	GLU	CB-CG-CD	5.03	121.15	112.60
23	1-P	69	ARG	NE-CZ-NH2	5.03	123.73	119.20
33	1-Z	351	PRO	CA-C-N	5.03	127.02	120.28
33	1-Z	351	PRO	C-N-CA	5.03	127.02	120.28
16	2-I	332	GLU	CB-CG-CD	5.03	121.15	112.60
23	2-P	69	ARG	NE-CZ-NH2	5.03	123.73	119.20
33	2-Z	351	PRO	CA-C-N	5.03	127.02	120.28
33	2-Z	351	PRO	C-N-CA	5.03	127.02	120.28
16	3-I	332	GLU	CB-CG-CD	5.03	121.15	112.60
23	3-P	69	ARG	NE-CZ-NH2	5.03	123.73	119.20
33	3-Z	351	PRO	CA-C-N	5.03	127.02	120.28
33	3-Z	351	PRO	C-N-CA	5.03	127.02	120.28
6	1-6	137	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	1-h	62	HIS	CB-CG-CD2	-5.03	124.66	131.20
6	1-m	79	HIS	CA-CB-CG	-5.03	108.77	113.80
6	2-6	137	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	2-h	62	HIS	CB-CG-CD2	-5.03	124.66	131.20
6	2-m	79	HIS	CA-CB-CG	-5.03	108.77	113.80
6	3-6	137	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	3-h	62	HIS	CB-CG-CD2	-5.03	124.66	131.20
6	3-m	79	HIS	CA-CB-CG	-5.03	108.77	113.80
1	1-1	195	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	2-1	195	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	3-1	195	GLN	OE1-CD-NE2	-5.03	117.57	122.60
11	1-D	4	ARG	NE-CZ-NH2	5.02	123.72	119.20
11	2-D	4	ARG	NE-CZ-NH2	5.02	123.72	119.20
11	3-D	4	ARG	NE-CZ-NH2	5.02	123.72	119.20
24	1-Q	87	GLN	OE1-CD-NE2	-5.02	117.58	122.60
24	2-Q	87	GLN	OE1-CD-NE2	-5.02	117.58	122.60
24	3-Q	87	GLN	OE1-CD-NE2	-5.02	117.58	122.60
21	1-N	444	HIS	CB-CG-CD2	-5.02	124.68	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2-N	444	HIS	CB-CG-CD2	-5.02	124.68	131.20
21	3-N	444	HIS	CB-CG-CD2	-5.02	124.68	131.20
24	1-Q	145	HIS	CA-CB-CG	5.01	118.81	113.80
24	2-Q	145	HIS	CA-CB-CG	5.01	118.81	113.80
24	3-Q	145	HIS	CA-CB-CG	5.01	118.81	113.80
18	1-K	244	HIS	CB-CG-CD2	-5.01	124.69	131.20
33	1-Z	138	ARG	CB-CG-CD	5.01	122.83	111.30
6	1-m	195	HIS	CB-CG-CD2	-5.01	124.69	131.20
18	2-K	244	HIS	CB-CG-CD2	-5.01	124.69	131.20
33	2-Z	138	ARG	CB-CG-CD	5.01	122.83	111.30
6	2-m	195	HIS	CB-CG-CD2	-5.01	124.69	131.20
18	3-K	244	HIS	CB-CG-CD2	-5.01	124.69	131.20
33	3-Z	138	ARG	CB-CG-CD	5.01	122.83	111.30
6	3-m	195	HIS	CB-CG-CD2	-5.01	124.69	131.20
9	1-B	13	SER	CA-C-N	5.01	124.67	119.56
9	1-B	13	SER	C-N-CA	5.01	124.67	119.56
9	2-B	13	SER	CA-C-N	5.01	124.67	119.56
9	2-B	13	SER	C-N-CA	5.01	124.67	119.56
9	3-B	13	SER	CA-C-N	5.01	124.67	119.56
9	3-B	13	SER	C-N-CA	5.01	124.67	119.56
18	1-K	252	ARG	NE-CZ-NH2	5.00	123.70	119.20
25	1-R	199	GLU	CA-C-N	5.00	126.94	120.44
25	1-R	199	GLU	C-N-CA	5.00	126.94	120.44
33	1-Z	722	ASP	CA-CB-CG	5.00	117.60	112.60
18	2-K	252	ARG	NE-CZ-NH2	5.00	123.70	119.20
25	2-R	199	GLU	CA-C-N	5.00	126.94	120.44
25	2-R	199	GLU	C-N-CA	5.00	126.94	120.44
33	2-Z	722	ASP	CA-CB-CG	5.00	117.60	112.60
18	3-K	252	ARG	NE-CZ-NH2	5.00	123.70	119.20
25	3-R	199	GLU	CA-C-N	5.00	126.94	120.44
25	3-R	199	GLU	C-N-CA	5.00	126.94	120.44
33	3-Z	722	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (1123) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-1	102	TYR	Sidechain
1	1-1	189	TYR	Sidechain
1	1-1	29	ARG	Sidechain
1	1-1	61	TYR	Sidechain
2	1-2	114	HIS	Sidechain

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Mol	Chain	Res	Type	Group
2	1-2	116	HIS	Sidechain
2	1-2	188	ARG	Sidechain
2	1-2	36	ARG	Sidechain
2	1-2	97	TYR	Sidechain
3	1-3	187	TYR	Sidechain
3	1-3	197	ARG	Sidechain
3	1-3	198	TYR	Sidechain
3	1-3	202	ARG	Sidechain
3	1-3	44	HIS	Sidechain
3	1-3	45	TYR	Sidechain
3	1-3	47	HIS	Sidechain
4	1-4	107	TYR	Sidechain
4	1-4	135	TYR	Sidechain
4	1-4	139	TYR	Sidechain
4	1-4	146	HIS	Sidechain
4	1-4	195	PHE	Sidechain
4	1-4	59	TYR	Sidechain
4	1-4	73	TYR	Sidechain
4	1-4	8	ARG	Sidechain
5	1-5	104	TYR	Sidechain
5	1-5	113	TYR	Sidechain
5	1-5	114	TYR	Sidechain
5	1-5	121	ARG	Sidechain
5	1-5	170	TYR	Sidechain
5	1-5	207	PHE	Sidechain
5	1-5	69	ARG	Sidechain
6	1-6	105	TYR	Sidechain
6	1-6	106	TYR	Sidechain
6	1-6	123	TYR	Sidechain
6	1-6	125	PHE	Sidechain
6	1-6	213	ARG	Sidechain
6	1-6	44	PHE	Sidechain
6	1-6	5	TYR	Sidechain
6	1-6	79	HIS	Sidechain
6	1-6	98	TYR	Sidechain
7	1-7	129	TYR	Sidechain
7	1-7	30	TYR	Sidechain
7	1-7	76	TYR	Sidechain
7	1-7	95	TYR	Sidechain
8	1-A	119	TYR	Sidechain
8	1-A	122	ARG	Sidechain
8	1-A	224	PHE	Sidechain

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Mol	Chain	Res	Type	Group
8	1-A	235	ARG	Sidechain
8	1-A	62	TYR	Sidechain
8	1-A	64	PHE	Sidechain
8	1-A	99	TYR	Sidechain
9	1-B	104	TYR	Sidechain
9	1-B	128	ARG	Sidechain
9	1-B	148	TYR	Sidechain
9	1-B	156	TYR	Sidechain
9	1-B	190	HIS	Sidechain
9	1-B	82	TYR	Sidechain
9	1-B	94	HIS	Sidechain
10	1-C	136	TYR	Sidechain
10	1-C	139	TYR	Sidechain
10	1-C	145	TYR	Sidechain
10	1-C	17	ARG	Sidechain
10	1-C	179	TYR	Sidechain
10	1-C	19	TYR	Sidechain
10	1-C	207	TYR	Sidechain
10	1-C	225	TYR	Sidechain
10	1-C	30	HIS	Sidechain
10	1-C	49	ARG	Sidechain
10	1-C	97	TYR	Sidechain
11	1-D	110	TYR	Sidechain
11	1-D	118	TYR	Sidechain
11	1-D	20	TYR	Sidechain
11	1-D	230	TYR	Sidechain
11	1-D	88	ARG	Sidechain
12	1-E	145	TYR	Sidechain
12	1-E	157	TYR	Sidechain
12	1-E	2	ARG	Sidechain
12	1-E	83	HIS	Sidechain
12	1-E	95	TYR	Sidechain
13	1-F	2	ARG	Sidechain
13	1-F	224	TYR	Sidechain
13	1-F	38	ARG	Sidechain
13	1-F	5	TYR	Sidechain
13	1-F	58	TYR	Sidechain
13	1-F	81	ARG	Sidechain
13	1-F	93	TYR	Sidechain
14	1-G	11	PHE	Sidechain
14	1-G	122	TYR	Sidechain
14	1-G	145	TYR	Sidechain

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Mol	Chain	Res	Type	Group
14	1-G	179	HIS	Sidechain
14	1-G	4	TYR	Sidechain
14	1-G	87	ARG	Sidechain
14	1-G	89	ARG	Sidechain
15	1-H	145	TYR	Sidechain
15	1-H	155	PHE	Sidechain
15	1-H	181	TYR	Sidechain
15	1-H	271	PHE	Sidechain
15	1-H	389	PHE	Sidechain
15	1-H	392	HIS	Sidechain
15	1-H	434	ARG	Sidechain
15	1-H	45	TYR	Sidechain
15	1-H	454	TYR	Sidechain
15	1-H	466	TYR	Sidechain
15	1-H	62	ARG	Sidechain
15	1-H	80	HIS	Sidechain
16	1-I	128	TYR	Sidechain
16	1-I	129	TYR	Sidechain
16	1-I	150	HIS	Sidechain
16	1-I	181	TYR	Sidechain
16	1-I	265	ARG	Sidechain
16	1-I	304	ARG	Sidechain
16	1-I	319	ARG	Sidechain
16	1-I	365	HIS	Sidechain
16	1-I	422	ARG	Sidechain
16	1-I	436	TYR	Sidechain
17	1-J	205	HIS	Sidechain
17	1-J	22	TYR	Sidechain
17	1-J	296	ARG	Sidechain
17	1-J	42	ARG	Sidechain
17	1-J	71	TYR	Sidechain
17	1-J	94	TYR	Sidechain
18	1-K	121	ARG	Sidechain
18	1-K	128	ARG	Sidechain
18	1-K	140	HIS	Sidechain
18	1-K	212	TYR	Sidechain
18	1-K	244	HIS	Sidechain
18	1-K	246	TYR	Sidechain
18	1-K	258	PHE	Sidechain
18	1-K	393	ARG	Sidechain
18	1-K	411	TYR	Sidechain
18	1-K	88	ARG	Sidechain

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Mol	Chain	Res	Type	Group
19	1-L	127	TYR	Sidechain
19	1-L	145	ARG	Sidechain
19	1-L	255	TYR	Sidechain
19	1-L	269	TYR	Sidechain
19	1-L	299	ARG	Sidechain
19	1-L	315	PHE	Sidechain
19	1-L	342	ARG	Sidechain
19	1-L	345	ARG	Sidechain
19	1-L	364	HIS	Sidechain
19	1-L	376	PHE	Sidechain
19	1-L	392	ARG	Sidechain
19	1-L	409	HIS	Sidechain
19	1-L	420	ARG	Sidechain
19	1-L	88	TYR	Sidechain
20	1-M	153	TYR	Sidechain
20	1-M	264	ARG	Sidechain
20	1-M	299	ARG	Sidechain
20	1-M	339	ARG	Sidechain
20	1-M	357	ARG	Sidechain
20	1-M	386	PHE	Sidechain
20	1-M	412	HIS	Sidechain
21	1-N	109	TYR	Sidechain
21	1-N	117	TYR	Sidechain
21	1-N	188	TYR	Sidechain
21	1-N	213	PHE	Sidechain
21	1-N	282	TYR	Sidechain
21	1-N	394	ARG	Sidechain
21	1-N	444	HIS	Sidechain
21	1-N	50	TYR	Sidechain
21	1-N	504	TYR	Sidechain
21	1-N	526	TYR	Sidechain
21	1-N	549	TYR	Sidechain
21	1-N	559	TYR	Sidechain
21	1-N	573	HIS	Sidechain
21	1-N	690	HIS	Sidechain
21	1-N	75	TYR	Sidechain
21	1-N	782	PHE	Sidechain
21	1-N	788	TYR	Sidechain
21	1-N	866	TYR	Sidechain
21	1-N	873	ARG	Sidechain
21	1-N	881	TYR	Sidechain
21	1-N	890	PHE	Sidechain

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Mol	Chain	Res	Type	Group
21	1-N	894	ARG	Sidechain
22	1-O	135	ARG	Sidechain
22	1-O	178	TYR	Sidechain
22	1-O	181	PHE	Sidechain
22	1-O	190	TYR	Sidechain
22	1-O	195	TYR	Sidechain
22	1-O	215	TYR	Sidechain
22	1-O	228	TYR	Sidechain
22	1-O	23	HIS	Sidechain
22	1-O	236	HIS	Sidechain
22	1-O	248	TYR	Sidechain
22	1-O	65	PHE	Sidechain
22	1-O	70	TYR	Sidechain
23	1-P	131	PHE	Sidechain
23	1-P	193	TYR	Sidechain
23	1-P	221	TYR	Sidechain
23	1-P	230	HIS	Sidechain
23	1-P	234	TYR	Sidechain
23	1-P	3	ARG	Sidechain
23	1-P	310	ARG	Sidechain
23	1-P	318	TYR	Sidechain
23	1-P	348	HIS	Sidechain
23	1-P	357	TYR	Sidechain
23	1-P	417	HIS	Sidechain
23	1-P	440	HIS	Sidechain
24	1-Q	13	ARG	Sidechain
24	1-Q	151	TYR	Sidechain
24	1-Q	185	TYR	Sidechain
24	1-Q	186	HIS	Sidechain
24	1-Q	20	TYR	Sidechain
24	1-Q	209	TYR	Sidechain
24	1-Q	226	HIS	Sidechain
24	1-Q	236	PHE	Sidechain
24	1-Q	252	HIS	Sidechain
24	1-Q	255	TYR	Sidechain
24	1-Q	286	TYR	Sidechain
24	1-Q	291	TYR	Sidechain
24	1-Q	306	TYR	Sidechain
24	1-Q	321	TYR	Sidechain
24	1-Q	332	ARG	Sidechain
24	1-Q	339	TYR	Sidechain
24	1-Q	354	PHE	Sidechain

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Mol	Chain	Res	Type	Group
24	1-Q	387	TYR	Sidechain
24	1-Q	80	HIS	Sidechain
25	1-R	141	TYR	Sidechain
25	1-R	181	TYR	Sidechain
25	1-R	214	TYR	Sidechain
25	1-R	24	TYR	Sidechain
25	1-R	304	TYR	Sidechain
25	1-R	305	PHE	Sidechain
25	1-R	324	ARG	Sidechain
25	1-R	331	ARG	Sidechain
25	1-R	49	PHE	Sidechain
25	1-R	63	TYR	Sidechain
25	1-R	99	TYR	Sidechain
26	1-S	114	TYR	Sidechain
26	1-S	118	PHE	Sidechain
26	1-S	145	PHE	Sidechain
26	1-S	174	ARG	Sidechain
26	1-S	186	TYR	Sidechain
26	1-S	25	TYR	Sidechain
26	1-S	274	PHE	Sidechain
26	1-S	275	TYR	Sidechain
26	1-S	292	TYR	Sidechain
26	1-S	302	HIS	Sidechain
26	1-S	346	TYR	Sidechain
26	1-S	367	TYR	Sidechain
26	1-S	481	TYR	Sidechain
26	1-S	82	TYR	Sidechain
27	1-T	123	HIS	Sidechain
27	1-T	132	HIS	Sidechain
27	1-T	234	TYR	Sidechain
28	1-U	113	TYR	Sidechain
28	1-U	189	ARG	Sidechain
28	1-U	223	HIS	Sidechain
28	1-U	5	HIS	Sidechain
28	1-U	94	HIS	Sidechain
29	1-V	109	HIS	Sidechain
29	1-V	190	HIS	Sidechain
29	1-V	195	HIS	Sidechain
29	1-V	197	TYR	Sidechain
29	1-V	203	TYR	Sidechain
29	1-V	204	HIS	Sidechain
29	1-V	230	TYR	Sidechain

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Mol	Chain	Res	Type	Group
29	1-V	269	ARG	Sidechain
29	1-V	270	TYR	Sidechain
29	1-V	42	ARG	Sidechain
30	1-W	107	HIS	Sidechain
30	1-W	122	ARG	Sidechain
30	1-W	157	PHE	Sidechain
30	1-W	17	ARG	Sidechain
30	1-W	23	ARG	Sidechain
30	1-W	25	ARG	Sidechain
30	1-W	60	ARG	Sidechain
30	1-W	86	HIS	Sidechain
31	1-X	22	ARG	Sidechain
32	1-Y	35	PHE	Sidechain
33	1-Z	103	TYR	Sidechain
33	1-Z	137	TYR	Sidechain
33	1-Z	138	ARG	Sidechain
33	1-Z	155	ARG	Sidechain
33	1-Z	156	HIS	Sidechain
33	1-Z	195	PHE	Sidechain
33	1-Z	202	ARG	Sidechain
33	1-Z	272	TYR	Sidechain
33	1-Z	312	TYR	Sidechain
33	1-Z	341	TYR	Sidechain
33	1-Z	394	TYR	Sidechain
33	1-Z	477	TYR	Sidechain
33	1-Z	593	HIS	Sidechain
33	1-Z	774	ARG	Sidechain
33	1-Z	813	PHE	Sidechain
33	1-Z	832	ARG	Sidechain
33	1-Z	837	TYR	Sidechain
33	1-Z	838	TYR	Sidechain
33	1-Z	849	ARG	Sidechain
33	1-Z	902	TYR	Sidechain
8	1-a	126	ARG	Sidechain
8	1-a	15	ARG	Sidechain
8	1-a	153	TYR	Sidechain
8	1-a	157	TYR	Sidechain
8	1-a	17	TYR	Sidechain
8	1-a	184	HIS	Sidechain
8	1-a	21	TYR	Sidechain
8	1-a	224	PHE	Sidechain
8	1-a	62	TYR	Sidechain

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Mol	Chain	Res	Type	Group
8	1-a	64	PHE	Sidechain
9	1-b	104	TYR	Sidechain
9	1-b	156	TYR	Sidechain
9	1-b	4	ARG	Sidechain
9	1-b	94	HIS	Sidechain
10	1-c	143	TYR	Sidechain
10	1-c	19	TYR	Sidechain
10	1-c	30	HIS	Sidechain
10	1-c	4	ARG	Sidechain
10	1-c	97	TYR	Sidechain
11	1-d	118	TYR	Sidechain
11	1-d	136	PHE	Sidechain
11	1-d	139	ARG	Sidechain
11	1-d	146	TYR	Sidechain
11	1-d	164	ARG	Sidechain
11	1-d	195	ARG	Sidechain
12	1-e	145	TYR	Sidechain
12	1-e	157	TYR	Sidechain
12	1-e	65	HIS	Sidechain
12	1-e	94	TYR	Sidechain
12	1-e	95	TYR	Sidechain
13	1-f	106	ARG	Sidechain
13	1-f	109	HIS	Sidechain
13	1-f	19	PHE	Sidechain
13	1-f	5	TYR	Sidechain
13	1-f	58	TYR	Sidechain
13	1-f	93	TYR	Sidechain
14	1-g	11	PHE	Sidechain
14	1-g	111	ARG	Sidechain
14	1-g	115	TYR	Sidechain
14	1-g	122	TYR	Sidechain
14	1-g	179	HIS	Sidechain
14	1-g	74	TYR	Sidechain
14	1-g	83	HIS	Sidechain
1	1-h	102	TYR	Sidechain
1	1-h	185	ARG	Sidechain
1	1-h	188	PHE	Sidechain
1	1-h	61	TYR	Sidechain
1	1-h	87	TYR	Sidechain
2	1-i	114	HIS	Sidechain
2	1-i	116	HIS	Sidechain
2	1-i	124	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	1-i	90	TYR	Sidechain
2	1-i	97	TYR	Sidechain
3	1-j	102	TYR	Sidechain
3	1-j	187	TYR	Sidechain
3	1-j	198	TYR	Sidechain
3	1-j	43	PHE	Sidechain
3	1-j	44	HIS	Sidechain
3	1-j	45	TYR	Sidechain
3	1-j	47	HIS	Sidechain
4	1-k	107	TYR	Sidechain
4	1-k	135	TYR	Sidechain
4	1-k	146	HIS	Sidechain
4	1-k	59	TYR	Sidechain
4	1-k	73	TYR	Sidechain
4	1-k	8	ARG	Sidechain
4	1-k	98	TYR	Sidechain
5	1-l	104	TYR	Sidechain
5	1-l	114	TYR	Sidechain
5	1-l	144	TYR	Sidechain
5	1-l	191	HIS	Sidechain
5	1-l	207	PHE	Sidechain
5	1-l	90	TYR	Sidechain
6	1-m	105	TYR	Sidechain
6	1-m	106	TYR	Sidechain
6	1-m	137	ARG	Sidechain
6	1-m	79	HIS	Sidechain
7	1-n	156	ARG	Sidechain
7	1-n	185	TYR	Sidechain
7	1-n	30	TYR	Sidechain
7	1-n	62	HIS	Sidechain
7	1-n	65	ARG	Sidechain
7	1-n	76	TYR	Sidechain
7	1-n	95	TYR	Sidechain
1	2-1	102	TYR	Sidechain
1	2-1	189	TYR	Sidechain
1	2-1	29	ARG	Sidechain
1	2-1	61	TYR	Sidechain
2	2-2	114	HIS	Sidechain
2	2-2	116	HIS	Sidechain
2	2-2	188	ARG	Sidechain
2	2-2	36	ARG	Sidechain
2	2-2	97	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	2-3	187	TYR	Sidechain
3	2-3	197	ARG	Sidechain
3	2-3	198	TYR	Sidechain
3	2-3	202	ARG	Sidechain
3	2-3	44	HIS	Sidechain
3	2-3	45	TYR	Sidechain
3	2-3	47	HIS	Sidechain
4	2-4	107	TYR	Sidechain
4	2-4	135	TYR	Sidechain
4	2-4	139	TYR	Sidechain
4	2-4	146	HIS	Sidechain
4	2-4	195	PHE	Sidechain
4	2-4	59	TYR	Sidechain
4	2-4	73	TYR	Sidechain
4	2-4	8	ARG	Sidechain
5	2-5	104	TYR	Sidechain
5	2-5	113	TYR	Sidechain
5	2-5	114	TYR	Sidechain
5	2-5	121	ARG	Sidechain
5	2-5	170	TYR	Sidechain
5	2-5	207	PHE	Sidechain
5	2-5	69	ARG	Sidechain
6	2-6	105	TYR	Sidechain
6	2-6	106	TYR	Sidechain
6	2-6	123	TYR	Sidechain
6	2-6	125	PHE	Sidechain
6	2-6	213	ARG	Sidechain
6	2-6	44	PHE	Sidechain
6	2-6	5	TYR	Sidechain
6	2-6	79	HIS	Sidechain
6	2-6	98	TYR	Sidechain
7	2-7	129	TYR	Sidechain
7	2-7	30	TYR	Sidechain
7	2-7	76	TYR	Sidechain
7	2-7	95	TYR	Sidechain
8	2-A	119	TYR	Sidechain
8	2-A	122	ARG	Sidechain
8	2-A	224	PHE	Sidechain
8	2-A	235	ARG	Sidechain
8	2-A	62	TYR	Sidechain
8	2-A	64	PHE	Sidechain
8	2-A	99	TYR	Sidechain

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Mol	Chain	Res	Type	Group
9	2-B	104	TYR	Sidechain
9	2-B	128	ARG	Sidechain
9	2-B	148	TYR	Sidechain
9	2-B	156	TYR	Sidechain
9	2-B	190	HIS	Sidechain
9	2-B	82	TYR	Sidechain
9	2-B	94	HIS	Sidechain
10	2-C	136	TYR	Sidechain
10	2-C	139	TYR	Sidechain
10	2-C	145	TYR	Sidechain
10	2-C	17	ARG	Sidechain
10	2-C	179	TYR	Sidechain
10	2-C	19	TYR	Sidechain
10	2-C	207	TYR	Sidechain
10	2-C	225	TYR	Sidechain
10	2-C	30	HIS	Sidechain
10	2-C	49	ARG	Sidechain
10	2-C	97	TYR	Sidechain
11	2-D	110	TYR	Sidechain
11	2-D	118	TYR	Sidechain
11	2-D	20	TYR	Sidechain
11	2-D	230	TYR	Sidechain
11	2-D	88	ARG	Sidechain
12	2-E	145	TYR	Sidechain
12	2-E	157	TYR	Sidechain
12	2-E	2	ARG	Sidechain
12	2-E	83	HIS	Sidechain
12	2-E	95	TYR	Sidechain
13	2-F	2	ARG	Sidechain
13	2-F	224	TYR	Sidechain
13	2-F	232	TYR	Sidechain
13	2-F	38	ARG	Sidechain
13	2-F	5	TYR	Sidechain
13	2-F	58	TYR	Sidechain
13	2-F	81	ARG	Sidechain
13	2-F	93	TYR	Sidechain
14	2-G	11	PHE	Sidechain
14	2-G	122	TYR	Sidechain
14	2-G	145	TYR	Sidechain
14	2-G	179	HIS	Sidechain
14	2-G	4	TYR	Sidechain
14	2-G	87	ARG	Sidechain

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Mol	Chain	Res	Type	Group
14	2-G	89	ARG	Sidechain
15	2-H	145	TYR	Sidechain
15	2-H	155	PHE	Sidechain
15	2-H	181	TYR	Sidechain
15	2-H	271	PHE	Sidechain
15	2-H	389	PHE	Sidechain
15	2-H	392	HIS	Sidechain
15	2-H	434	ARG	Sidechain
15	2-H	45	TYR	Sidechain
15	2-H	454	TYR	Sidechain
15	2-H	466	TYR	Sidechain
15	2-H	62	ARG	Sidechain
15	2-H	80	HIS	Sidechain
16	2-I	128	TYR	Sidechain
16	2-I	129	TYR	Sidechain
16	2-I	150	HIS	Sidechain
16	2-I	181	TYR	Sidechain
16	2-I	265	ARG	Sidechain
16	2-I	304	ARG	Sidechain
16	2-I	319	ARG	Sidechain
16	2-I	365	HIS	Sidechain
16	2-I	422	ARG	Sidechain
16	2-I	436	TYR	Sidechain
17	2-J	205	HIS	Sidechain
17	2-J	22	TYR	Sidechain
17	2-J	296	ARG	Sidechain
17	2-J	42	ARG	Sidechain
17	2-J	71	TYR	Sidechain
17	2-J	94	TYR	Sidechain
18	2-K	121	ARG	Sidechain
18	2-K	128	ARG	Sidechain
18	2-K	140	HIS	Sidechain
18	2-K	212	TYR	Sidechain
18	2-K	244	HIS	Sidechain
18	2-K	246	TYR	Sidechain
18	2-K	258	PHE	Sidechain
18	2-K	393	ARG	Sidechain
18	2-K	411	TYR	Sidechain
18	2-K	88	ARG	Sidechain
19	2-L	127	TYR	Sidechain
19	2-L	145	ARG	Sidechain
19	2-L	255	TYR	Sidechain

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Mol	Chain	Res	Type	Group
19	2-L	269	TYR	Sidechain
19	2-L	299	ARG	Sidechain
19	2-L	315	PHE	Sidechain
19	2-L	342	ARG	Sidechain
19	2-L	345	ARG	Sidechain
19	2-L	364	HIS	Sidechain
19	2-L	376	PHE	Sidechain
19	2-L	392	ARG	Sidechain
19	2-L	409	HIS	Sidechain
19	2-L	420	ARG	Sidechain
19	2-L	88	TYR	Sidechain
20	2-M	153	TYR	Sidechain
20	2-M	264	ARG	Sidechain
20	2-M	299	ARG	Sidechain
20	2-M	339	ARG	Sidechain
20	2-M	357	ARG	Sidechain
20	2-M	386	PHE	Sidechain
20	2-M	412	HIS	Sidechain
21	2-N	109	TYR	Sidechain
21	2-N	117	TYR	Sidechain
21	2-N	188	TYR	Sidechain
21	2-N	213	PHE	Sidechain
21	2-N	282	TYR	Sidechain
21	2-N	394	ARG	Sidechain
21	2-N	444	HIS	Sidechain
21	2-N	50	TYR	Sidechain
21	2-N	504	TYR	Sidechain
21	2-N	526	TYR	Sidechain
21	2-N	549	TYR	Sidechain
21	2-N	559	TYR	Sidechain
21	2-N	573	HIS	Sidechain
21	2-N	690	HIS	Sidechain
21	2-N	75	TYR	Sidechain
21	2-N	782	PHE	Sidechain
21	2-N	788	TYR	Sidechain
21	2-N	866	TYR	Sidechain
21	2-N	873	ARG	Sidechain
21	2-N	881	TYR	Sidechain
21	2-N	890	PHE	Sidechain
21	2-N	894	ARG	Sidechain
22	2-O	135	ARG	Sidechain
22	2-O	178	TYR	Sidechain

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Mol	Chain	Res	Type	Group
22	2-O	181	PHE	Sidechain
22	2-O	190	TYR	Sidechain
22	2-O	195	TYR	Sidechain
22	2-O	215	TYR	Sidechain
22	2-O	228	TYR	Sidechain
22	2-O	23	HIS	Sidechain
22	2-O	236	HIS	Sidechain
22	2-O	248	TYR	Sidechain
22	2-O	65	PHE	Sidechain
22	2-O	70	TYR	Sidechain
23	2-P	131	PHE	Sidechain
23	2-P	193	TYR	Sidechain
23	2-P	221	TYR	Sidechain
23	2-P	230	HIS	Sidechain
23	2-P	234	TYR	Sidechain
23	2-P	3	ARG	Sidechain
23	2-P	310	ARG	Sidechain
23	2-P	318	TYR	Sidechain
23	2-P	348	HIS	Sidechain
23	2-P	357	TYR	Sidechain
23	2-P	417	HIS	Sidechain
23	2-P	440	HIS	Sidechain
24	2-Q	13	ARG	Sidechain
24	2-Q	151	TYR	Sidechain
24	2-Q	185	TYR	Sidechain
24	2-Q	186	HIS	Sidechain
24	2-Q	20	TYR	Sidechain
24	2-Q	209	TYR	Sidechain
24	2-Q	226	HIS	Sidechain
24	2-Q	236	PHE	Sidechain
24	2-Q	252	HIS	Sidechain
24	2-Q	255	TYR	Sidechain
24	2-Q	286	TYR	Sidechain
24	2-Q	291	TYR	Sidechain
24	2-Q	306	TYR	Sidechain
24	2-Q	321	TYR	Sidechain
24	2-Q	332	ARG	Sidechain
24	2-Q	339	TYR	Sidechain
24	2-Q	354	PHE	Sidechain
24	2-Q	387	TYR	Sidechain
24	2-Q	80	HIS	Sidechain
25	2-R	141	TYR	Sidechain

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Mol	Chain	Res	Type	Group
25	2-R	181	TYR	Sidechain
25	2-R	214	TYR	Sidechain
25	2-R	24	TYR	Sidechain
25	2-R	304	TYR	Sidechain
25	2-R	305	PHE	Sidechain
25	2-R	324	ARG	Sidechain
25	2-R	331	ARG	Sidechain
25	2-R	49	PHE	Sidechain
25	2-R	63	TYR	Sidechain
25	2-R	99	TYR	Sidechain
26	2-S	114	TYR	Sidechain
26	2-S	118	PHE	Sidechain
26	2-S	145	PHE	Sidechain
26	2-S	174	ARG	Sidechain
26	2-S	186	TYR	Sidechain
26	2-S	25	TYR	Sidechain
26	2-S	274	PHE	Sidechain
26	2-S	275	TYR	Sidechain
26	2-S	292	TYR	Sidechain
26	2-S	302	HIS	Sidechain
26	2-S	346	TYR	Sidechain
26	2-S	367	TYR	Sidechain
26	2-S	481	TYR	Sidechain
26	2-S	82	TYR	Sidechain
27	2-T	123	HIS	Sidechain
27	2-T	132	HIS	Sidechain
27	2-T	234	TYR	Sidechain
28	2-U	113	TYR	Sidechain
28	2-U	189	ARG	Sidechain
28	2-U	223	HIS	Sidechain
28	2-U	5	HIS	Sidechain
28	2-U	94	HIS	Sidechain
29	2-V	109	HIS	Sidechain
29	2-V	190	HIS	Sidechain
29	2-V	195	HIS	Sidechain
29	2-V	197	TYR	Sidechain
29	2-V	203	TYR	Sidechain
29	2-V	204	HIS	Sidechain
29	2-V	230	TYR	Sidechain
29	2-V	269	ARG	Sidechain
29	2-V	270	TYR	Sidechain
29	2-V	42	ARG	Sidechain

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Mol	Chain	Res	Type	Group
30	2-W	107	HIS	Sidechain
30	2-W	122	ARG	Sidechain
30	2-W	157	PHE	Sidechain
30	2-W	17	ARG	Sidechain
30	2-W	23	ARG	Sidechain
30	2-W	25	ARG	Sidechain
30	2-W	60	ARG	Sidechain
30	2-W	86	HIS	Sidechain
31	2-X	22	ARG	Sidechain
32	2-Y	35	PHE	Sidechain
33	2-Z	103	TYR	Sidechain
33	2-Z	137	TYR	Sidechain
33	2-Z	138	ARG	Sidechain
33	2-Z	155	ARG	Sidechain
33	2-Z	156	HIS	Sidechain
33	2-Z	195	PHE	Sidechain
33	2-Z	202	ARG	Sidechain
33	2-Z	272	TYR	Sidechain
33	2-Z	312	TYR	Sidechain
33	2-Z	341	TYR	Sidechain
33	2-Z	394	TYR	Sidechain
33	2-Z	477	TYR	Sidechain
33	2-Z	593	HIS	Sidechain
33	2-Z	774	ARG	Sidechain
33	2-Z	813	PHE	Sidechain
33	2-Z	832	ARG	Sidechain
33	2-Z	837	TYR	Sidechain
33	2-Z	838	TYR	Sidechain
33	2-Z	849	ARG	Sidechain
33	2-Z	902	TYR	Sidechain
8	2-a	126	ARG	Sidechain
8	2-a	15	ARG	Sidechain
8	2-a	153	TYR	Sidechain
8	2-a	157	TYR	Sidechain
8	2-a	17	TYR	Sidechain
8	2-a	21	TYR	Sidechain
8	2-a	224	PHE	Sidechain
8	2-a	62	TYR	Sidechain
8	2-a	64	PHE	Sidechain
9	2-b	104	TYR	Sidechain
9	2-b	156	TYR	Sidechain
9	2-b	4	ARG	Sidechain

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Mol	Chain	Res	Type	Group
9	2-b	94	HIS	Sidechain
10	2-c	143	TYR	Sidechain
10	2-c	19	TYR	Sidechain
10	2-c	30	HIS	Sidechain
10	2-c	4	ARG	Sidechain
10	2-c	97	TYR	Sidechain
11	2-d	118	TYR	Sidechain
11	2-d	136	PHE	Sidechain
11	2-d	139	ARG	Sidechain
11	2-d	146	TYR	Sidechain
11	2-d	164	ARG	Sidechain
11	2-d	195	ARG	Sidechain
12	2-e	145	TYR	Sidechain
12	2-e	157	TYR	Sidechain
12	2-e	65	HIS	Sidechain
12	2-e	94	TYR	Sidechain
12	2-e	95	TYR	Sidechain
13	2-f	106	ARG	Sidechain
13	2-f	109	HIS	Sidechain
13	2-f	19	PHE	Sidechain
13	2-f	5	TYR	Sidechain
13	2-f	58	TYR	Sidechain
13	2-f	93	TYR	Sidechain
14	2-g	11	PHE	Sidechain
14	2-g	111	ARG	Sidechain
14	2-g	115	TYR	Sidechain
14	2-g	122	TYR	Sidechain
14	2-g	179	HIS	Sidechain
14	2-g	74	TYR	Sidechain
14	2-g	83	HIS	Sidechain
1	2-h	102	TYR	Sidechain
1	2-h	185	ARG	Sidechain
1	2-h	188	PHE	Sidechain
1	2-h	61	TYR	Sidechain
1	2-h	87	TYR	Sidechain
2	2-i	114	HIS	Sidechain
2	2-i	116	HIS	Sidechain
2	2-i	124	TYR	Sidechain
2	2-i	90	TYR	Sidechain
2	2-i	97	TYR	Sidechain
3	2-j	102	TYR	Sidechain
3	2-j	187	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	2-j	198	TYR	Sidechain
3	2-j	43	PHE	Sidechain
3	2-j	44	HIS	Sidechain
3	2-j	45	TYR	Sidechain
3	2-j	47	HIS	Sidechain
4	2-k	107	TYR	Sidechain
4	2-k	135	TYR	Sidechain
4	2-k	146	HIS	Sidechain
4	2-k	59	TYR	Sidechain
4	2-k	73	TYR	Sidechain
4	2-k	8	ARG	Sidechain
4	2-k	98	TYR	Sidechain
5	2-l	104	TYR	Sidechain
5	2-l	114	TYR	Sidechain
5	2-l	144	TYR	Sidechain
5	2-l	191	HIS	Sidechain
5	2-l	207	PHE	Sidechain
5	2-l	90	TYR	Sidechain
6	2-m	105	TYR	Sidechain
6	2-m	106	TYR	Sidechain
6	2-m	137	ARG	Sidechain
6	2-m	79	HIS	Sidechain
7	2-n	156	ARG	Sidechain
7	2-n	185	TYR	Sidechain
7	2-n	30	TYR	Sidechain
7	2-n	62	HIS	Sidechain
7	2-n	65	ARG	Sidechain
7	2-n	76	TYR	Sidechain
7	2-n	95	TYR	Sidechain
1	3-1	102	TYR	Sidechain
1	3-1	189	TYR	Sidechain
1	3-1	29	ARG	Sidechain
1	3-1	61	TYR	Sidechain
2	3-2	114	HIS	Sidechain
2	3-2	116	HIS	Sidechain
2	3-2	188	ARG	Sidechain
2	3-2	36	ARG	Sidechain
2	3-2	97	TYR	Sidechain
3	3-3	187	TYR	Sidechain
3	3-3	197	ARG	Sidechain
3	3-3	198	TYR	Sidechain
3	3-3	202	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	3-3	44	HIS	Sidechain
3	3-3	45	TYR	Sidechain
3	3-3	47	HIS	Sidechain
4	3-4	107	TYR	Sidechain
4	3-4	135	TYR	Sidechain
4	3-4	139	TYR	Sidechain
4	3-4	146	HIS	Sidechain
4	3-4	195	PHE	Sidechain
4	3-4	59	TYR	Sidechain
4	3-4	73	TYR	Sidechain
4	3-4	8	ARG	Sidechain
5	3-5	104	TYR	Sidechain
5	3-5	113	TYR	Sidechain
5	3-5	114	TYR	Sidechain
5	3-5	121	ARG	Sidechain
5	3-5	170	TYR	Sidechain
5	3-5	207	PHE	Sidechain
5	3-5	69	ARG	Sidechain
6	3-6	105	TYR	Sidechain
6	3-6	106	TYR	Sidechain
6	3-6	123	TYR	Sidechain
6	3-6	125	PHE	Sidechain
6	3-6	213	ARG	Sidechain
6	3-6	44	PHE	Sidechain
6	3-6	5	TYR	Sidechain
6	3-6	79	HIS	Sidechain
6	3-6	98	TYR	Sidechain
7	3-7	129	TYR	Sidechain
7	3-7	30	TYR	Sidechain
7	3-7	76	TYR	Sidechain
7	3-7	95	TYR	Sidechain
8	3-A	119	TYR	Sidechain
8	3-A	122	ARG	Sidechain
8	3-A	224	PHE	Sidechain
8	3-A	235	ARG	Sidechain
8	3-A	62	TYR	Sidechain
8	3-A	64	PHE	Sidechain
8	3-A	99	TYR	Sidechain
9	3-B	104	TYR	Sidechain
9	3-B	128	ARG	Sidechain
9	3-B	148	TYR	Sidechain
9	3-B	156	TYR	Sidechain

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Mol	Chain	Res	Type	Group
9	3-B	190	HIS	Sidechain
9	3-B	82	TYR	Sidechain
9	3-B	94	HIS	Sidechain
10	3-C	136	TYR	Sidechain
10	3-C	139	TYR	Sidechain
10	3-C	145	TYR	Sidechain
10	3-C	17	ARG	Sidechain
10	3-C	179	TYR	Sidechain
10	3-C	19	TYR	Sidechain
10	3-C	207	TYR	Sidechain
10	3-C	225	TYR	Sidechain
10	3-C	30	HIS	Sidechain
10	3-C	49	ARG	Sidechain
10	3-C	97	TYR	Sidechain
11	3-D	110	TYR	Sidechain
11	3-D	118	TYR	Sidechain
11	3-D	20	TYR	Sidechain
11	3-D	230	TYR	Sidechain
11	3-D	88	ARG	Sidechain
12	3-E	145	TYR	Sidechain
12	3-E	157	TYR	Sidechain
12	3-E	2	ARG	Sidechain
12	3-E	83	HIS	Sidechain
12	3-E	95	TYR	Sidechain
13	3-F	2	ARG	Sidechain
13	3-F	224	TYR	Sidechain
13	3-F	232	TYR	Sidechain
13	3-F	38	ARG	Sidechain
13	3-F	5	TYR	Sidechain
13	3-F	58	TYR	Sidechain
13	3-F	81	ARG	Sidechain
13	3-F	93	TYR	Sidechain
14	3-G	11	PHE	Sidechain
14	3-G	122	TYR	Sidechain
14	3-G	145	TYR	Sidechain
14	3-G	179	HIS	Sidechain
14	3-G	4	TYR	Sidechain
14	3-G	87	ARG	Sidechain
14	3-G	89	ARG	Sidechain
15	3-H	145	TYR	Sidechain
15	3-H	155	PHE	Sidechain
15	3-H	181	TYR	Sidechain

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Mol	Chain	Res	Type	Group
15	3-H	271	PHE	Sidechain
15	3-H	389	PHE	Sidechain
15	3-H	392	HIS	Sidechain
15	3-H	434	ARG	Sidechain
15	3-H	45	TYR	Sidechain
15	3-H	454	TYR	Sidechain
15	3-H	466	TYR	Sidechain
15	3-H	62	ARG	Sidechain
15	3-H	80	HIS	Sidechain
16	3-I	128	TYR	Sidechain
16	3-I	129	TYR	Sidechain
16	3-I	150	HIS	Sidechain
16	3-I	181	TYR	Sidechain
16	3-I	265	ARG	Sidechain
16	3-I	304	ARG	Sidechain
16	3-I	319	ARG	Sidechain
16	3-I	365	HIS	Sidechain
16	3-I	422	ARG	Sidechain
16	3-I	436	TYR	Sidechain
17	3-J	205	HIS	Sidechain
17	3-J	22	TYR	Sidechain
17	3-J	296	ARG	Sidechain
17	3-J	42	ARG	Sidechain
17	3-J	71	TYR	Sidechain
17	3-J	94	TYR	Sidechain
18	3-K	121	ARG	Sidechain
18	3-K	128	ARG	Sidechain
18	3-K	140	HIS	Sidechain
18	3-K	212	TYR	Sidechain
18	3-K	244	HIS	Sidechain
18	3-K	246	TYR	Sidechain
18	3-K	258	PHE	Sidechain
18	3-K	393	ARG	Sidechain
18	3-K	411	TYR	Sidechain
18	3-K	88	ARG	Sidechain
19	3-L	127	TYR	Sidechain
19	3-L	145	ARG	Sidechain
19	3-L	255	TYR	Sidechain
19	3-L	269	TYR	Sidechain
19	3-L	299	ARG	Sidechain
19	3-L	315	PHE	Sidechain
19	3-L	342	ARG	Sidechain

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Mol	Chain	Res	Type	Group
19	3-L	345	ARG	Sidechain
19	3-L	364	HIS	Sidechain
19	3-L	376	PHE	Sidechain
19	3-L	392	ARG	Sidechain
19	3-L	409	HIS	Sidechain
19	3-L	420	ARG	Sidechain
19	3-L	88	TYR	Sidechain
20	3-M	153	TYR	Sidechain
20	3-M	264	ARG	Sidechain
20	3-M	299	ARG	Sidechain
20	3-M	339	ARG	Sidechain
20	3-M	357	ARG	Sidechain
20	3-M	386	PHE	Sidechain
20	3-M	412	HIS	Sidechain
21	3-N	109	TYR	Sidechain
21	3-N	117	TYR	Sidechain
21	3-N	188	TYR	Sidechain
21	3-N	213	PHE	Sidechain
21	3-N	282	TYR	Sidechain
21	3-N	394	ARG	Sidechain
21	3-N	444	HIS	Sidechain
21	3-N	50	TYR	Sidechain
21	3-N	504	TYR	Sidechain
21	3-N	526	TYR	Sidechain
21	3-N	549	TYR	Sidechain
21	3-N	559	TYR	Sidechain
21	3-N	573	HIS	Sidechain
21	3-N	690	HIS	Sidechain
21	3-N	75	TYR	Sidechain
21	3-N	782	PHE	Sidechain
21	3-N	788	TYR	Sidechain
21	3-N	866	TYR	Sidechain
21	3-N	873	ARG	Sidechain
21	3-N	881	TYR	Sidechain
21	3-N	890	PHE	Sidechain
21	3-N	894	ARG	Sidechain
22	3-O	135	ARG	Sidechain
22	3-O	178	TYR	Sidechain
22	3-O	181	PHE	Sidechain
22	3-O	190	TYR	Sidechain
22	3-O	195	TYR	Sidechain
22	3-O	215	TYR	Sidechain

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Mol	Chain	Res	Type	Group
22	3-O	228	TYR	Sidechain
22	3-O	23	HIS	Sidechain
22	3-O	236	HIS	Sidechain
22	3-O	248	TYR	Sidechain
22	3-O	65	PHE	Sidechain
22	3-O	70	TYR	Sidechain
23	3-P	131	PHE	Sidechain
23	3-P	193	TYR	Sidechain
23	3-P	221	TYR	Sidechain
23	3-P	230	HIS	Sidechain
23	3-P	234	TYR	Sidechain
23	3-P	3	ARG	Sidechain
23	3-P	310	ARG	Sidechain
23	3-P	318	TYR	Sidechain
23	3-P	348	HIS	Sidechain
23	3-P	357	TYR	Sidechain
23	3-P	417	HIS	Sidechain
23	3-P	440	HIS	Sidechain
24	3-Q	13	ARG	Sidechain
24	3-Q	151	TYR	Sidechain
24	3-Q	185	TYR	Sidechain
24	3-Q	186	HIS	Sidechain
24	3-Q	20	TYR	Sidechain
24	3-Q	209	TYR	Sidechain
24	3-Q	226	HIS	Sidechain
24	3-Q	236	PHE	Sidechain
24	3-Q	252	HIS	Sidechain
24	3-Q	255	TYR	Sidechain
24	3-Q	286	TYR	Sidechain
24	3-Q	291	TYR	Sidechain
24	3-Q	306	TYR	Sidechain
24	3-Q	321	TYR	Sidechain
24	3-Q	332	ARG	Sidechain
24	3-Q	339	TYR	Sidechain
24	3-Q	354	PHE	Sidechain
24	3-Q	387	TYR	Sidechain
24	3-Q	80	HIS	Sidechain
25	3-R	141	TYR	Sidechain
25	3-R	181	TYR	Sidechain
25	3-R	214	TYR	Sidechain
25	3-R	24	TYR	Sidechain
25	3-R	304	TYR	Sidechain

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Mol	Chain	Res	Type	Group
25	3-R	305	PHE	Sidechain
25	3-R	324	ARG	Sidechain
25	3-R	331	ARG	Sidechain
25	3-R	49	PHE	Sidechain
25	3-R	63	TYR	Sidechain
25	3-R	99	TYR	Sidechain
26	3-S	114	TYR	Sidechain
26	3-S	118	PHE	Sidechain
26	3-S	145	PHE	Sidechain
26	3-S	174	ARG	Sidechain
26	3-S	186	TYR	Sidechain
26	3-S	25	TYR	Sidechain
26	3-S	274	PHE	Sidechain
26	3-S	275	TYR	Sidechain
26	3-S	292	TYR	Sidechain
26	3-S	302	HIS	Sidechain
26	3-S	346	TYR	Sidechain
26	3-S	367	TYR	Sidechain
26	3-S	481	TYR	Sidechain
26	3-S	82	TYR	Sidechain
27	3-T	123	HIS	Sidechain
27	3-T	132	HIS	Sidechain
27	3-T	234	TYR	Sidechain
28	3-U	113	TYR	Sidechain
28	3-U	189	ARG	Sidechain
28	3-U	223	HIS	Sidechain
28	3-U	5	HIS	Sidechain
28	3-U	94	HIS	Sidechain
29	3-V	109	HIS	Sidechain
29	3-V	190	HIS	Sidechain
29	3-V	195	HIS	Sidechain
29	3-V	197	TYR	Sidechain
29	3-V	203	TYR	Sidechain
29	3-V	204	HIS	Sidechain
29	3-V	230	TYR	Sidechain
29	3-V	269	ARG	Sidechain
29	3-V	270	TYR	Sidechain
29	3-V	42	ARG	Sidechain
30	3-W	107	HIS	Sidechain
30	3-W	122	ARG	Sidechain
30	3-W	157	PHE	Sidechain
30	3-W	17	ARG	Sidechain

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Mol	Chain	Res	Type	Group
30	3-W	23	ARG	Sidechain
30	3-W	25	ARG	Sidechain
30	3-W	60	ARG	Sidechain
30	3-W	86	HIS	Sidechain
31	3-X	22	ARG	Sidechain
32	3-Y	35	PHE	Sidechain
33	3-Z	103	TYR	Sidechain
33	3-Z	137	TYR	Sidechain
33	3-Z	138	ARG	Sidechain
33	3-Z	155	ARG	Sidechain
33	3-Z	156	HIS	Sidechain
33	3-Z	195	PHE	Sidechain
33	3-Z	202	ARG	Sidechain
33	3-Z	272	TYR	Sidechain
33	3-Z	312	TYR	Sidechain
33	3-Z	341	TYR	Sidechain
33	3-Z	394	TYR	Sidechain
33	3-Z	477	TYR	Sidechain
33	3-Z	593	HIS	Sidechain
33	3-Z	774	ARG	Sidechain
33	3-Z	813	PHE	Sidechain
33	3-Z	832	ARG	Sidechain
33	3-Z	837	TYR	Sidechain
33	3-Z	838	TYR	Sidechain
33	3-Z	849	ARG	Sidechain
33	3-Z	902	TYR	Sidechain
8	3-a	126	ARG	Sidechain
8	3-a	15	ARG	Sidechain
8	3-a	153	TYR	Sidechain
8	3-a	157	TYR	Sidechain
8	3-a	17	TYR	Sidechain
8	3-a	184	HIS	Sidechain
8	3-a	21	TYR	Sidechain
8	3-a	224	PHE	Sidechain
8	3-a	62	TYR	Sidechain
8	3-a	64	PHE	Sidechain
9	3-b	104	TYR	Sidechain
9	3-b	156	TYR	Sidechain
9	3-b	4	ARG	Sidechain
9	3-b	94	HIS	Sidechain
10	3-c	143	TYR	Sidechain
10	3-c	19	TYR	Sidechain

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Mol	Chain	Res	Type	Group
10	3-c	30	HIS	Sidechain
10	3-c	4	ARG	Sidechain
10	3-c	97	TYR	Sidechain
11	3-d	118	TYR	Sidechain
11	3-d	136	PHE	Sidechain
11	3-d	139	ARG	Sidechain
11	3-d	146	TYR	Sidechain
11	3-d	164	ARG	Sidechain
11	3-d	195	ARG	Sidechain
12	3-e	145	TYR	Sidechain
12	3-e	157	TYR	Sidechain
12	3-e	65	HIS	Sidechain
12	3-e	94	TYR	Sidechain
12	3-e	95	TYR	Sidechain
13	3-f	106	ARG	Sidechain
13	3-f	109	HIS	Sidechain
13	3-f	19	PHE	Sidechain
13	3-f	5	TYR	Sidechain
13	3-f	58	TYR	Sidechain
13	3-f	93	TYR	Sidechain
14	3-g	11	PHE	Sidechain
14	3-g	111	ARG	Sidechain
14	3-g	115	TYR	Sidechain
14	3-g	122	TYR	Sidechain
14	3-g	179	HIS	Sidechain
14	3-g	74	TYR	Sidechain
14	3-g	83	HIS	Sidechain
1	3-h	102	TYR	Sidechain
1	3-h	185	ARG	Sidechain
1	3-h	188	PHE	Sidechain
1	3-h	61	TYR	Sidechain
1	3-h	87	TYR	Sidechain
2	3-i	114	HIS	Sidechain
2	3-i	116	HIS	Sidechain
2	3-i	124	TYR	Sidechain
2	3-i	90	TYR	Sidechain
2	3-i	97	TYR	Sidechain
3	3-j	102	TYR	Sidechain
3	3-j	187	TYR	Sidechain
3	3-j	198	TYR	Sidechain
3	3-j	43	PHE	Sidechain
3	3-j	44	HIS	Sidechain

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Mol	Chain	Res	Type	Group
3	3-j	45	TYR	Sidechain
3	3-j	47	HIS	Sidechain
4	3-k	107	TYR	Sidechain
4	3-k	135	TYR	Sidechain
4	3-k	146	HIS	Sidechain
4	3-k	59	TYR	Sidechain
4	3-k	73	TYR	Sidechain
4	3-k	8	ARG	Sidechain
4	3-k	98	TYR	Sidechain
5	3-l	104	TYR	Sidechain
5	3-l	114	TYR	Sidechain
5	3-l	144	TYR	Sidechain
5	3-l	191	HIS	Sidechain
5	3-l	207	PHE	Sidechain
5	3-l	90	TYR	Sidechain
6	3-m	105	TYR	Sidechain
6	3-m	106	TYR	Sidechain
6	3-m	137	ARG	Sidechain
6	3-m	79	HIS	Sidechain
7	3-n	156	ARG	Sidechain
7	3-n	185	TYR	Sidechain
7	3-n	30	TYR	Sidechain
7	3-n	62	HIS	Sidechain
7	3-n	65	ARG	Sidechain
7	3-n	76	TYR	Sidechain
7	3-n	95	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-1	1512	1479	1481	3	0
1	1-h	1512	1479	1481	5	0
1	2-1	1512	1479	1481	3	0
1	2-h	1512	1479	1481	3	0
1	3-1	1512	1479	1481	3	0
1	3-h	1512	1479	1481	4	0
2	1-2	1719	1717	1719	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1-i	1719	1717	1719	1	0
2	2-2	1719	1717	1719	7	0
2	2-i	1719	1717	1719	0	0
2	3-2	1719	1717	1719	7	0
2	3-i	1719	1717	1719	1	0
3	1-3	1581	1572	1574	5	0
3	1-j	1581	1572	1574	5	0
3	2-3	1581	1572	1574	5	0
3	2-j	1581	1572	1574	4	0
3	3-3	1581	1572	1574	5	0
3	3-j	1581	1572	1574	6	0
4	1-4	1561	1569	1569	3	0
4	1-k	1561	1569	1569	3	0
4	2-4	1561	1569	1569	3	0
4	2-k	1561	1569	1569	3	0
4	3-4	1561	1569	1569	2	0
4	3-k	1561	1569	1569	3	0
5	1-5	1644	1593	1595	3	0
5	1-l	1644	1593	1595	2	0
5	2-5	1644	1593	1595	2	0
5	2-l	1644	1593	1595	1	0
5	3-5	1644	1593	1595	2	0
5	3-l	1644	1593	1595	2	0
6	1-6	1757	1709	1711	1	0
6	1-m	1757	1709	1711	7	0
6	2-6	1757	1709	1711	1	0
6	2-m	1757	1709	1711	7	0
6	3-6	1757	1709	1711	1	0
6	3-m	1757	1709	1711	7	0
7	1-7	1790	1791	1793	5	0
7	1-n	1815	1819	1821	8	0
7	2-7	1790	1791	1793	5	0
7	2-n	1815	1819	1821	8	0
7	3-7	1790	1791	1793	5	0
7	3-n	1815	1819	1821	9	0
8	1-A	1907	1902	1901	7	0
8	1-a	1907	1902	1901	4	0
8	2-A	1907	1902	1901	6	0
8	2-a	1907	1902	1901	4	0
8	3-A	1907	1902	1901	6	0
8	3-a	1907	1902	1901	4	0
9	1-B	1915	1929	1929	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	1-b	1915	1929	1929	4	0
9	2-B	1915	1929	1929	8	0
9	2-b	1915	1929	1929	4	0
9	3-B	1915	1929	1929	9	0
9	3-b	1915	1929	1929	4	0
10	1-C	1904	1902	1904	5	0
10	1-c	1904	1902	1904	4	0
10	2-C	1904	1902	1904	5	0
10	2-c	1904	1902	1904	5	0
10	3-C	1904	1902	1904	4	0
10	3-c	1904	1902	1904	5	0
11	1-D	1881	1893	1895	7	0
11	1-d	1881	1893	1895	4	0
11	2-D	1881	1893	1895	7	0
11	2-d	1881	1893	1895	4	0
11	3-D	1881	1893	1895	7	0
11	3-d	1881	1893	1895	4	0
12	1-E	1861	1837	1839	3	0
12	1-e	1861	1837	1839	7	0
12	2-E	1861	1837	1839	3	0
12	2-e	1861	1837	1839	8	0
12	3-E	1861	1837	1839	3	0
12	3-e	1861	1837	1839	8	0
13	1-F	1795	1800	1800	4	0
13	1-f	1773	1778	1775	2	0
13	2-F	1795	1800	1800	5	0
13	2-f	1773	1778	1775	2	0
13	3-F	1795	1800	1800	4	0
13	3-f	1773	1778	1775	1	0
14	1-G	1892	1885	1883	6	0
14	1-g	1892	1884	1883	5	0
14	2-G	1892	1885	1883	6	0
14	2-g	1892	1884	1883	5	0
14	3-G	1892	1885	1883	6	0
14	3-g	1892	1884	1883	6	0
15	1-H	3053	3130	3127	17	0
15	2-H	3053	3130	3127	17	0
15	3-H	3053	3130	3127	16	0
16	1-I	3022	3093	3092	9	0
16	2-I	3022	3093	3092	9	0
16	3-I	3022	3093	3092	10	0
17	1-J	3033	3157	3156	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	2-J	3033	3157	3156	9	0
17	3-J	3033	3157	3156	9	0
18	1-K	3078	3142	3141	13	0
18	2-K	3078	3142	3141	13	0
18	3-K	3078	3142	3141	13	0
19	1-L	3082	3158	3157	12	0
19	2-L	3082	3158	3157	13	0
19	3-L	3082	3158	3157	14	0
20	1-M	2986	3057	3055	8	0
20	2-M	2986	3057	3055	7	0
20	3-M	2986	3057	3055	7	0
21	1-N	6882	6961	6959	34	0
21	2-N	6882	6961	6959	35	0
21	3-N	6882	6961	6959	34	0
22	1-O	3186	3214	3213	39	0
22	2-O	3186	3214	3213	37	0
22	3-O	3186	3214	3213	39	0
23	1-P	3608	3694	3694	8	0
23	2-P	3608	3694	3694	8	0
23	3-P	3608	3694	3694	7	0
24	1-Q	3499	3524	3524	22	0
24	2-Q	3499	3524	3524	22	0
24	3-Q	3499	3524	3524	24	0
25	1-R	3060	3085	3083	10	0
25	2-R	3060	3085	3083	10	0
25	3-R	3060	3085	3083	10	0
26	1-S	3894	3939	3938	14	0
26	2-S	3894	3939	3938	14	0
26	3-S	3894	3939	3938	14	0
27	1-T	2192	2162	2161	10	0
27	2-T	2192	2162	2161	10	0
27	3-T	2192	2162	2161	10	0
28	1-U	2373	2403	2403	12	0
28	2-U	2373	2403	2403	12	0
28	3-U	2373	2403	2403	12	0
29	1-V	2274	2275	2273	24	0
29	2-V	2274	2275	2273	23	0
29	3-V	2274	2275	2273	22	0
30	1-W	1534	1542	1542	7	0
30	2-W	1534	1542	1542	7	0
30	3-W	1534	1542	1542	7	0
31	1-X	1032	1018	1017	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	2-X	1032	1018	1017	1	0
31	3-X	1032	1018	1017	1	0
32	1-Y	435	396	394	1	0
32	2-Y	435	396	394	1	0
32	3-Y	435	396	394	1	0
33	1-Z	7005	6934	6932	37	0
33	2-Z	7005	6934	6932	36	0
33	3-Z	7005	6934	6932	37	0
All	All	326007	327135	327150	1091	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 2.

All (1091) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:339:MET:HA	21:N:709:GLY:N	1.73	1.04
21:N:339:MET:HA	21:N:709:GLY:N	1.73	1.04
33:Z:30:LYS:CG	33:Z:37:GLN:HB3	1.89	1.02
21:N:339:MET:HA	21:N:709:GLY:N	1.73	1.02
33:Z:30:LYS:CG	33:Z:37:GLN:HB3	1.89	1.01
33:Z:30:LYS:CG	33:Z:37:GLN:HB3	1.89	1.00
33:Z:24:THR:HB	33:Z:25:PRO:CD	1.94	0.97
33:Z:24:THR:HB	33:Z:25:PRO:CD	1.94	0.97
33:Z:24:THR:HB	33:Z:25:PRO:CD	1.94	0.96
33:Z:24:THR:HB	33:Z:25:PRO:HD3	1.49	0.95
33:Z:30:LYS:HG3	33:Z:37:GLN:HB3	1.51	0.93
33:Z:24:THR:HB	33:Z:25:PRO:HD3	1.49	0.92
33:Z:24:THR:HB	33:Z:25:PRO:HD3	1.49	0.91
33:Z:30:LYS:HG3	33:Z:37:GLN:HB3	1.51	0.91
33:Z:30:LYS:HG3	33:Z:37:GLN:HB3	1.51	0.91
21:N:339:MET:HA	21:N:709:GLY:CA	2.06	0.85
21:N:339:MET:HA	21:N:709:GLY:CA	2.06	0.84
21:N:339:MET:HA	21:N:709:GLY:CA	2.06	0.84
33:Z:30:LYS:HG3	33:Z:37:GLN:CB	2.08	0.84
21:N:339:MET:C	21:N:709:GLY:HA3	2.04	0.82
33:Z:30:LYS:HG3	33:Z:37:GLN:CB	2.08	0.82
33:Z:30:LYS:HG3	33:Z:37:GLN:CB	2.08	0.82
21:N:339:MET:C	21:N:709:GLY:HA3	2.04	0.81
21:N:339:MET:C	21:N:709:GLY:HA3	2.04	0.81
29:V:53:MET:HE1	29:V:137:VAL:CG2	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:V:53:MET:HE1	29:V:137:VAL:CG2	2.11	0.80
29:V:53:MET:HE1	29:V:137:VAL:CG2	2.12	0.80
21:N:339:MET:CA	21:N:709:GLY:HA3	2.12	0.80
22:O:25:LEU:HD11	22:O:61:LEU:HG	1.64	0.80
21:N:339:MET:CA	21:N:709:GLY:HA3	2.12	0.79
22:O:25:LEU:HD11	22:O:61:LEU:HG	1.64	0.79
21:N:339:MET:CA	21:N:709:GLY:HA3	2.12	0.79
22:O:25:LEU:HD11	22:O:61:LEU:HG	1.64	0.78
21:N:339:MET:HA	21:N:709:GLY:H	1.47	0.77
21:N:11:ALA:HB1	27:T:80:ASN:CG	2.10	0.77
21:N:339:MET:HA	21:N:709:GLY:H	1.47	0.77
21:N:339:MET:HA	21:N:709:GLY:H	1.47	0.77
21:N:11:ALA:HB1	27:T:80:ASN:CG	2.10	0.76
21:N:11:ALA:HB1	27:T:80:ASN:CG	2.10	0.76
33:Z:30:LYS:CG	33:Z:37:GLN:CB	2.64	0.75
21:N:708:ALA:HB1	21:N:713:VAL:HG22	1.71	0.73
33:Z:30:LYS:CG	33:Z:37:GLN:CB	2.64	0.73
22:O:25:LEU:HD12	22:O:65:PHE:CD2	2.24	0.73
22:O:25:LEU:HD12	22:O:65:PHE:CD2	2.24	0.73
22:O:25:LEU:HD12	22:O:65:PHE:CD2	2.24	0.72
21:N:708:ALA:HB1	21:N:713:VAL:HG22	1.71	0.72
21:N:708:ALA:HB1	21:N:713:VAL:HG22	1.71	0.71
33:Z:30:LYS:CG	33:Z:37:GLN:CB	2.64	0.70
3:3:185:VAL:HG22	3:3:198:TYR:CE2	2.29	0.68
21:N:339:MET:HA	21:N:709:GLY:HA3	1.74	0.68
3:3:185:VAL:HG22	3:3:198:TYR:CE2	2.29	0.68
19:L:152:THR:HG22	29:V:113:GLY:HA3	1.77	0.67
19:L:152:THR:HG22	29:V:113:GLY:HA3	1.77	0.67
19:L:152:THR:HG22	29:V:113:GLY:HA3	1.77	0.67
3:3:185:VAL:HG22	3:3:198:TYR:CE2	2.29	0.67
21:N:339:MET:HA	21:N:709:GLY:HA3	1.74	0.66
10:C:149:THR:HG22	10:C:159:TRP:HE1	1.63	0.64
10:C:149:THR:HG22	10:C:159:TRP:HE1	1.62	0.64
29:V:157:ARG:H	29:V:196:TYR:HB2	1.64	0.63
7:n:178:VAL:HG12	7:n:182:ARG:HH22	1.63	0.63
33:Z:282:ILE:HG12	33:Z:297:VAL:HG11	1.81	0.62
21:N:11:ALA:CB	27:T:80:ASN:CG	2.72	0.62
22:O:25:LEU:HB3	22:O:65:PHE:CE2	2.35	0.62
7:n:178:VAL:HG12	7:n:182:ARG:HH22	1.64	0.62
29:V:157:ARG:H	29:V:196:TYR:HB2	1.64	0.62
33:Z:282:ILE:HG12	33:Z:297:VAL:HG11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:11:ALA:CB	27:T:80:ASN:CG	2.72	0.62
33:Z:948:TRP:H	33:Z:948:TRP:CD1	2.17	0.62
7:n:178:VAL:HG12	7:n:182:ARG:HH22	1.64	0.62
10:C:149:THR:HG22	10:C:159:TRP:HE1	1.62	0.62
22:O:25:LEU:HB3	22:O:65:PHE:CE2	2.35	0.62
33:Z:282:ILE:HG12	33:Z:297:VAL:HG11	1.81	0.61
21:N:11:ALA:CB	27:T:80:ASN:CG	2.72	0.61
22:O:29:PHE:CD2	22:O:65:PHE:CE1	2.89	0.61
22:O:29:PHE:CD2	22:O:65:PHE:CE1	2.89	0.61
22:O:25:LEU:HB3	22:O:65:PHE:CE2	2.35	0.61
25:R:421:VAL:HG21	28:U:274:MET:SD	2.41	0.61
33:Z:24:THR:CB	33:Z:25:PRO:CD	2.75	0.61
25:R:421:VAL:HG21	28:U:274:MET:SD	2.41	0.61
29:V:24:LYS:HG3	29:V:196:TYR:CD1	2.36	0.61
33:Z:948:TRP:H	33:Z:948:TRP:CD1	2.17	0.61
29:V:157:ARG:H	29:V:196:TYR:HB2	1.64	0.61
22:O:29:PHE:CD2	22:O:65:PHE:CE1	2.89	0.60
19:L:152:THR:HG22	29:V:113:GLY:CA	2.31	0.60
19:L:152:THR:HG22	29:V:113:GLY:CA	2.31	0.60
33:Z:24:THR:CB	33:Z:25:PRO:HD3	2.28	0.60
29:V:24:LYS:HG3	29:V:196:TYR:CD1	2.36	0.60
33:Z:85:VAL:HB	33:Z:86:PRO:HD3	1.84	0.60
25:R:421:VAL:HG21	28:U:274:MET:SD	2.41	0.60
33:Z:24:THR:CB	33:Z:25:PRO:HD3	2.28	0.60
33:Z:948:TRP:CD1	33:Z:948:TRP:H	2.17	0.59
14:g:87:ARG:HE	14:g:91:GLU:CD	2.10	0.59
33:Z:85:VAL:HB	33:Z:86:PRO:HD3	1.84	0.59
14:g:87:ARG:HE	14:g:91:GLU:CD	2.10	0.59
29:V:24:LYS:HG3	29:V:196:TYR:CD1	2.36	0.59
21:N:708:ALA:CB	21:N:713:VAL:HG22	2.33	0.59
24:Q:297:ASP:HA	24:Q:300:LYS:HE2	1.85	0.59
26:S:121:VAL:HG13	26:S:125:LYS:CE	2.33	0.59
19:L:152:THR:HG22	29:V:113:GLY:CA	2.31	0.59
26:S:121:VAL:HG13	26:S:125:LYS:CE	2.33	0.59
21:N:708:ALA:CB	21:N:713:VAL:HG22	2.33	0.59
26:S:121:VAL:HG13	26:S:125:LYS:CE	2.33	0.59
14:g:175:LEU:HD11	14:g:195:ILE:HD11	1.85	0.59
21:N:11:ALA:HB1	27:T:80:ASN:CB	2.33	0.58
33:Z:24:THR:HB	33:Z:25:PRO:HD2	1.81	0.58
21:N:708:ALA:CB	21:N:713:VAL:HG22	2.33	0.58
14:g:87:ARG:HE	14:g:91:GLU:CD	2.10	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:g:175:LEU:HD11	14:g:195:ILE:HD11	1.85	0.58
33:Z:24:THR:HB	33:Z:25:PRO:HD2	1.81	0.58
26:S:121:VAL:HG13	26:S:125:LYS:HE2	1.86	0.58
33:Z:24:THR:CB	33:Z:25:PRO:HD3	2.28	0.58
24:Q:297:ASP:HA	24:Q:300:LYS:HE2	1.85	0.58
33:Z:85:VAL:HB	33:Z:86:PRO:HD3	1.84	0.58
14:g:175:LEU:HD11	14:g:195:ILE:HD11	1.85	0.57
26:S:121:VAL:HG13	26:S:125:LYS:HE2	1.86	0.57
24:Q:260:GLN:HE21	24:Q:260:GLN:C	2.12	0.57
8:a:234:GLU:CD	8:a:235:ARG:HH22	2.12	0.57
25:R:64:LYS:HE2	25:R:99:TYR:CZ	2.40	0.57
8:a:234:GLU:CD	8:a:235:ARG:HH22	2.12	0.57
22:O:14:LEU:HD22	22:O:23:HIS:CD2	2.40	0.57
26:S:121:VAL:HG13	26:S:125:LYS:HE2	1.86	0.57
24:Q:260:GLN:HE21	24:Q:260:GLN:C	2.12	0.57
25:R:64:LYS:HE2	25:R:99:TYR:CZ	2.40	0.57
22:O:26:PHE:HA	22:O:29:PHE:CD2	2.39	0.57
8:a:234:GLU:CD	8:a:235:ARG:HH22	2.12	0.57
18:K:243:VAL:HG21	19:L:303:ARG:HD3	1.86	0.57
21:N:11:ALA:HB1	27:T:80:ASN:CB	2.33	0.57
24:Q:297:ASP:HA	24:Q:300:LYS:HE2	1.85	0.57
22:O:26:PHE:HA	22:O:29:PHE:CD2	2.39	0.57
15:H:66:LYS:HA	15:H:66:LYS:HE2	1.87	0.57
21:N:11:ALA:HB1	27:T:80:ASN:CB	2.33	0.57
22:O:14:LEU:HD22	22:O:23:HIS:CD2	2.40	0.57
22:O:26:PHE:HA	22:O:29:PHE:CD2	2.39	0.57
24:Q:260:GLN:HE21	24:Q:260:GLN:C	2.12	0.56
33:Z:24:THR:CB	33:Z:25:PRO:CD	2.75	0.56
18:K:243:VAL:HG21	19:L:303:ARG:HD3	1.86	0.56
33:Z:30:LYS:HG2	33:Z:37:GLN:HB3	1.84	0.56
22:O:14:LEU:HD22	22:O:23:HIS:CD2	2.40	0.56
18:K:243:VAL:HG21	19:L:303:ARG:HD3	1.86	0.56
12:e:37:GLY:HA2	12:e:145:TYR:CE1	2.40	0.56
12:e:37:GLY:HA2	12:e:145:TYR:CE1	2.41	0.56
15:H:66:LYS:HA	15:H:66:LYS:HE2	1.87	0.56
33:Z:24:THR:HB	33:Z:25:PRO:HD2	1.81	0.56
29:V:28:TYR:CD1	29:V:62:THR:HG23	2.41	0.56
15:H:223:GLU:HB2	15:H:373:ARG:HH22	1.71	0.56
25:R:64:LYS:HE2	25:R:99:TYR:CZ	2.40	0.55
29:V:28:TYR:CD1	29:V:62:THR:HG23	2.41	0.55
12:e:37:GLY:HA2	12:e:145:TYR:CE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:V:28:TYR:CD1	29:V:62:THR:HG23	2.41	0.55
29:V:157:ARG:HB3	29:V:196:TYR:CD2	2.42	0.55
15:H:223:GLU:HB2	15:H:373:ARG:HH22	1.71	0.55
29:V:53:MET:HE1	29:V:137:VAL:HG22	1.89	0.55
15:H:66:LYS:HA	15:H:66:LYS:HE2	1.87	0.55
29:V:157:ARG:HB3	29:V:196:TYR:CD2	2.42	0.55
17:J:335:MET:SD	17:J:377:VAL:HG21	2.47	0.55
21:N:339:MET:O	21:N:709:GLY:HA3	2.06	0.55
25:R:204:TRP:CD1	25:R:207:ARG:HH11	2.25	0.55
15:H:310:GLU:CD	15:H:356:ASN:HD21	2.15	0.55
29:V:157:ARG:HB3	29:V:196:TYR:CD2	2.42	0.55
15:H:310:GLU:CD	15:H:356:ASN:HD21	2.15	0.55
18:K:135:MET:HE3	18:K:136:SER:O	2.07	0.54
18:K:135:MET:HE3	18:K:136:SER:O	2.07	0.54
15:H:223:GLU:HB2	15:H:373:ARG:HH22	1.71	0.54
21:N:339:MET:O	21:N:709:GLY:HA3	2.06	0.54
18:K:135:MET:HE3	18:K:136:SER:O	2.07	0.54
15:H:310:GLU:CD	15:H:356:ASN:HD21	2.15	0.54
17:J:335:MET:SD	17:J:377:VAL:HG21	2.47	0.54
24:Q:220:LEU:HD11	24:Q:260:GLN:HE22	1.73	0.54
25:R:204:TRP:CD1	25:R:207:ARG:HH11	2.25	0.54
11:D:37:LYS:HE3	11:D:37:LYS:HA	1.89	0.54
25:R:204:TRP:CD1	25:R:207:ARG:HH11	2.25	0.54
15:H:246:ILE:HD11	15:H:352:MET:HE3	1.90	0.54
11:D:37:LYS:HE3	11:D:37:LYS:HA	1.89	0.53
21:N:339:MET:O	21:N:709:GLY:HA3	2.06	0.53
28:U:37:ILE:CG2	28:U:48:VAL:HG13	2.38	0.53
17:J:335:MET:SD	17:J:377:VAL:HG21	2.47	0.53
15:H:246:ILE:HD11	15:H:352:MET:HE3	1.90	0.53
24:Q:220:LEU:HD11	24:Q:260:GLN:HE22	1.73	0.53
15:H:246:ILE:HD11	15:H:352:MET:HE3	1.90	0.53
22:O:373:TRP:CH2	28:U:233:PHE:CD1	2.97	0.53
27:T:194:GLU:CD	27:T:224:ARG:HH12	2.17	0.53
33:Z:30:LYS:HG2	33:Z:37:GLN:HB3	1.84	0.53
12:E:37:GLY:HA2	12:E:145:TYR:CE1	2.44	0.53
31:X:104:LYS:HA	31:X:104:LYS:HE2	1.91	0.53
28:U:37:ILE:CG2	28:U:48:VAL:HG13	2.38	0.53
8:A:72:MET:HE3	8:A:74:VAL:CG2	2.39	0.53
29:V:53:MET:HE1	29:V:137:VAL:HG22	1.89	0.53
11:d:37:LYS:HE2	11:d:37:LYS:HA	1.91	0.53
22:O:266:PHE:CZ	22:O:270:ILE:HG13	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:X:104:LYS:HA	31:X:104:LYS:HE2	1.91	0.53
22:O:266:PHE:CZ	22:O:270:ILE:HG13	2.44	0.53
24:Q:220:LEU:HD11	24:Q:260:GLN:HE22	1.73	0.53
29:V:91:MET:HE3	29:V:91:MET:HA	1.91	0.53
22:O:289:GLN:OE1	22:O:293:LEU:HD11	2.09	0.53
28:U:37:ILE:CG2	28:U:48:VAL:HG13	2.38	0.53
29:V:28:TYR:CE1	29:V:62:THR:HG23	2.44	0.53
22:O:373:TRP:CH2	28:U:233:PHE:CD1	2.97	0.52
12:E:37:GLY:HA2	12:E:145:TYR:CE1	2.44	0.52
22:O:373:TRP:CH2	28:U:233:PHE:CD1	2.97	0.52
22:O:289:GLN:OE1	22:O:293:LEU:HD11	2.09	0.52
6:m:4:PRO:HG3	7:n:107:MET:SD	2.50	0.52
21:N:50:TYR:CD2	21:N:62:ALA:HB2	2.45	0.52
22:O:289:GLN:OE1	22:O:293:LEU:HD11	2.09	0.52
29:V:28:TYR:CE1	29:V:62:THR:HG23	2.44	0.52
29:V:91:MET:HE3	29:V:91:MET:HA	1.91	0.52
33:Z:272:TYR:CE1	33:Z:280:ASP:HB3	2.45	0.52
27:T:194:GLU:CD	27:T:224:ARG:HH12	2.17	0.52
22:O:266:PHE:CZ	22:O:270:ILE:HG13	2.44	0.52
24:Q:94:VAL:HG11	24:Q:130:ARG:HH12	1.75	0.52
11:D:37:LYS:HE3	11:D:37:LYS:HA	1.89	0.52
29:V:28:TYR:CE1	29:V:62:THR:HG23	2.44	0.52
22:O:11:LEU:HA	22:O:27:GLU:HB2	1.92	0.52
8:A:72:MET:HE3	8:A:74:VAL:CG2	2.39	0.52
27:T:194:GLU:CD	27:T:224:ARG:HH12	2.17	0.52
8:A:72:MET:HE3	8:A:74:VAL:CG2	2.39	0.52
10:C:149:THR:HG22	10:C:159:TRP:NE1	2.25	0.52
11:d:37:LYS:HE2	11:d:37:LYS:HA	1.91	0.52
12:E:37:GLY:HA2	12:E:145:TYR:CE1	2.44	0.52
29:V:53:MET:HE1	29:V:137:VAL:HG23	1.92	0.52
6:m:4:PRO:HG3	7:n:107:MET:SD	2.50	0.52
6:m:4:PRO:HG3	7:n:107:MET:SD	2.50	0.52
26:S:425:ARG:HD2	27:T:155:GLY:HA2	1.92	0.52
11:d:37:LYS:HE2	11:d:37:LYS:HA	1.91	0.52
21:N:50:TYR:CD2	21:N:62:ALA:HB2	2.45	0.52
22:O:25:LEU:HD11	22:O:61:LEU:CG	2.38	0.52
22:O:25:LEU:HD11	22:O:61:LEU:CG	2.38	0.51
22:O:11:LEU:HA	22:O:27:GLU:HB2	1.92	0.51
24:Q:94:VAL:HG11	24:Q:130:ARG:HH12	1.74	0.51
29:V:91:MET:HE3	29:V:91:MET:HA	1.91	0.51
1:h:155:ILE:HG21	1:h:175:MET:SD	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:24:THR:CB	33:Z:25:PRO:CD	2.75	0.51
33:Z:272:TYR:CE1	33:Z:280:ASP:HB3	2.45	0.51
21:N:50:TYR:CD2	21:N:62:ALA:HB2	2.45	0.51
26:S:425:ARG:HD2	27:T:155:GLY:HA2	1.91	0.51
33:Z:272:TYR:CE1	33:Z:280:ASP:HB3	2.45	0.51
22:O:373:TRP:CH2	28:U:233:PHE:CE1	2.99	0.51
21:N:339:MET:CA	21:N:709:GLY:CA	2.75	0.51
22:O:11:LEU:HA	22:O:27:GLU:HB2	1.92	0.51
23:P:411:LEU:H	23:P:411:LEU:HD12	1.76	0.51
9:B:66:LEU:HD13	9:B:235:PHE:CD2	2.46	0.51
22:O:373:TRP:CH2	28:U:233:PHE:CE1	2.99	0.51
24:Q:376:LYS:HE3	24:Q:380:MET:SD	2.51	0.51
22:O:266:PHE:CE1	22:O:270:ILE:HG13	2.46	0.51
8:a:93:ALA:HB1	1:h:61:TYR:CE1	2.46	0.51
2:2:42:TRP:CZ3	2:2:176:CYS:HB2	2.46	0.51
22:O:25:LEU:HD21	22:O:61:LEU:HG	1.93	0.51
24:Q:297:ASP:HA	24:Q:300:LYS:CE	2.41	0.51
9:B:66:LEU:HD13	9:B:235:PHE:CD2	2.46	0.51
22:O:373:TRP:CH2	28:U:233:PHE:CE1	2.99	0.51
31:X:104:LYS:HA	31:X:104:LYS:HE2	1.91	0.51
10:C:149:THR:HG22	10:C:159:TRP:NE1	2.25	0.51
22:O:25:LEU:HD21	22:O:61:LEU:HG	1.93	0.51
22:O:25:LEU:HD21	22:O:61:LEU:HG	1.93	0.51
24:Q:376:LYS:HE3	24:Q:380:MET:SD	2.51	0.51
26:S:425:ARG:HD2	27:T:155:GLY:HA2	1.92	0.51
2:2:42:TRP:CZ3	2:2:176:CYS:HB2	2.46	0.51
33:Z:793:PHE:CB	33:Z:832:ARG:HE	2.24	0.51
1:h:155:ILE:HG21	1:h:175:MET:SD	2.51	0.51
19:L:233:LYS:HE2	20:M:315:PHE:CE2	2.46	0.51
33:Z:793:PHE:CB	33:Z:832:ARG:HE	2.24	0.51
24:Q:94:VAL:HG11	24:Q:130:ARG:HH12	1.74	0.50
24:Q:297:ASP:HA	24:Q:300:LYS:CE	2.41	0.50
25:R:423:LEU:HD22	32:Y:18:LYS:HG2	1.93	0.50
23:P:394:ASN:HD21	24:Q:355:GLU:CD	2.19	0.50
23:P:411:LEU:H	23:P:411:LEU:HD12	1.76	0.50
8:a:93:ALA:HB1	1:h:61:TYR:CE1	2.46	0.50
19:L:233:LYS:HE2	20:M:315:PHE:CE2	2.46	0.50
29:V:53:MET:HE1	29:V:137:VAL:HG22	1.89	0.50
1:h:155:ILE:HG21	1:h:175:MET:SD	2.51	0.50
33:Z:793:PHE:CB	33:Z:832:ARG:HE	2.24	0.50
23:P:411:LEU:H	23:P:411:LEU:HD12	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:129:TYR:CE1	7:7:137:TYR:CE2	3.00	0.50
21:N:494:LYS:HE3	21:N:495:PRO:HD2	1.94	0.50
23:P:394:ASN:HD21	24:Q:355:GLU:CD	2.20	0.50
21:N:494:LYS:HE3	21:N:495:PRO:HD2	1.94	0.50
22:O:266:PHE:CE1	22:O:270:ILE:HG13	2.46	0.50
9:B:66:LEU:HD13	9:B:235:PHE:CD2	2.46	0.50
18:K:356:ILE:HG21	18:K:387:MET:HG2	1.94	0.50
22:O:266:PHE:CE1	22:O:270:ILE:HG13	2.46	0.50
29:V:53:MET:HE1	29:V:137:VAL:HG23	1.92	0.50
8:a:93:ALA:HB1	1:h:61:TYR:CE1	2.46	0.50
19:L:233:LYS:HE2	20:M:315:PHE:CE2	2.47	0.50
24:Q:297:ASP:HA	24:Q:300:LYS:CE	2.41	0.50
23:P:394:ASN:HD21	24:Q:355:GLU:CD	2.19	0.50
18:K:356:ILE:HG21	18:K:387:MET:HG2	1.94	0.50
24:Q:73:LYS:HE3	24:Q:77:PHE:CE2	2.47	0.50
24:Q:266:LEU:HD22	24:Q:278:VAL:HG13	1.93	0.50
25:R:423:LEU:HD22	32:Y:18:LYS:HG2	1.93	0.50
29:V:53:MET:HE1	29:V:137:VAL:HG23	1.92	0.50
21:N:494:LYS:HE3	21:N:495:PRO:HD2	1.93	0.50
24:Q:376:LYS:HE3	24:Q:380:MET:SD	2.50	0.50
2:2:42:TRP:CZ3	2:2:176:CYS:HB2	2.46	0.50
7:7:129:TYR:CE1	7:7:137:TYR:CE2	3.00	0.50
7:n:208:PHE:CD2	7:n:210:LYS:HE3	2.47	0.50
19:L:361:PHE:CD1	19:L:391:ILE:HG23	2.47	0.50
30:W:158:ILE:HG23	30:W:169:SER:HB2	1.94	0.50
24:Q:266:LEU:HD22	24:Q:278:VAL:HG13	1.93	0.50
17:J:366:GLY:HA3	18:K:203:ILE:HG21	1.94	0.49
18:K:129:GLU:HG2	29:V:274:GLN:H	1.77	0.49
24:Q:73:LYS:HE3	24:Q:77:PHE:CE2	2.47	0.49
25:R:423:LEU:HD22	32:Y:18:LYS:HG2	1.93	0.49
10:C:149:THR:HG22	10:C:159:TRP:NE1	2.25	0.49
27:T:226:TRP:CD1	27:T:238:GLN:HE21	2.30	0.49
12:e:58:LYS:HA	12:e:70:MET:SD	2.52	0.49
7:n:208:PHE:CD2	7:n:210:LYS:HE3	2.47	0.49
19:L:361:PHE:CD1	19:L:391:ILE:HG23	2.47	0.49
12:e:58:LYS:HA	12:e:70:MET:SD	2.52	0.49
17:J:366:GLY:HA3	18:K:203:ILE:HG21	1.94	0.49
33:Z:832:ARG:HA	33:Z:832:ARG:NE	2.28	0.49
18:K:129:GLU:HG2	29:V:274:GLN:H	1.77	0.49
30:W:158:ILE:HG23	30:W:169:SER:HB2	1.94	0.49
17:J:366:GLY:HA3	18:K:203:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:39:PHE:CZ	30:W:15:TYR:CZ	3.00	0.49
33:Z:832:ARG:HA	33:Z:832:ARG:NE	2.27	0.49
18:K:129:GLU:HG2	29:V:274:GLN:H	1.77	0.49
24:Q:266:LEU:HD22	24:Q:278:VAL:HG13	1.93	0.49
22:O:39:PHE:CZ	30:W:15:TYR:CZ	3.01	0.49
7:7:129:TYR:CE1	7:7:137:TYR:CE2	3.00	0.49
9:b:66:LEU:HD13	9:b:235:PHE:CD2	2.48	0.49
10:C:42:GLY:HA2	10:C:145:TYR:CZ	2.48	0.49
10:C:42:GLY:HA2	10:C:145:TYR:CZ	2.48	0.49
18:K:356:ILE:HG21	18:K:387:MET:HG2	1.94	0.49
12:e:58:LYS:HA	12:e:70:MET:SD	2.52	0.49
19:L:361:PHE:CD1	19:L:391:ILE:HG23	2.47	0.49
9:b:66:LEU:HD13	9:b:235:PHE:CD2	2.48	0.49
11:d:195:ARG:HH12	11:d:237:GLU:CD	2.21	0.49
15:H:66:LYS:HE3	16:I:75:PHE:CE2	2.48	0.49
16:I:148:LEU:CD2	17:J:95:ILE:HD13	2.43	0.49
23:P:395:ARG:C	23:P:397:ALA:H	2.21	0.49
27:T:226:TRP:CD1	27:T:238:GLN:HE21	2.30	0.49
7:n:150:MET:HE1	7:n:187:ARG:HG2	1.95	0.49
15:H:66:LYS:HE3	16:I:75:PHE:CE2	2.48	0.49
27:T:226:TRP:CD1	27:T:238:GLN:HE21	2.30	0.49
23:P:395:ARG:C	23:P:397:ALA:H	2.21	0.49
24:Q:73:LYS:HE3	24:Q:77:PHE:CE2	2.47	0.49
17:J:55:VAL:HG23	21:N:613:HIS:CD2	2.48	0.48
7:n:208:PHE:CD2	7:n:210:LYS:HE3	2.47	0.48
22:O:39:PHE:CZ	30:W:15:TYR:CZ	3.00	0.48
23:P:395:ARG:C	23:P:397:ALA:H	2.21	0.48
15:H:66:LYS:HE3	16:I:75:PHE:CE2	2.48	0.48
33:Z:30:LYS:HG2	33:Z:37:GLN:HB3	1.84	0.48
11:d:195:ARG:HH12	11:d:237:GLU:CD	2.21	0.48
17:J:55:VAL:HG23	21:N:613:HIS:CD2	2.48	0.48
21:N:632:LYS:HE3	21:N:632:LYS:HA	1.95	0.48
13:F:175:LEU:HA	13:F:178:PHE:CE2	2.49	0.48
33:Z:354:PRO:HA	33:Z:357:ILE:HG12	1.96	0.48
33:Z:832:ARG:HA	33:Z:832:ARG:NE	2.27	0.48
21:N:632:LYS:HE3	21:N:632:LYS:HA	1.96	0.48
10:C:42:GLY:HA2	10:C:145:TYR:CZ	2.48	0.48
16:I:319:ARG:HH21	16:I:319:ARG:HG2	1.79	0.48
22:O:25:LEU:HD11	22:O:61:LEU:CG	2.38	0.48
33:Z:93:ARG:HB3	33:Z:94:PRO:HD3	1.95	0.48
16:I:319:ARG:HH21	16:I:319:ARG:HG2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:K:106:ASN:HD21	18:K:121:ARG:NH1	2.12	0.48
26:S:70:ASN:HA	26:S:72:GLU:CD	2.38	0.48
8:a:72:MET:HE3	8:a:74:VAL:CG2	2.44	0.48
8:a:72:MET:HE3	8:a:74:VAL:CG2	2.44	0.48
13:F:175:LEU:HA	13:F:178:PHE:CE2	2.48	0.48
26:S:70:ASN:HA	26:S:72:GLU:CD	2.38	0.48
9:b:66:LEU:HD13	9:b:235:PHE:CD2	2.48	0.48
24:Q:236:PHE:CE1	24:Q:269:LYS:HE2	2.48	0.48
6:m:93:ILE:HA	6:m:96:LEU:HD12	1.95	0.48
24:Q:236:PHE:CE1	24:Q:269:LYS:HE2	2.48	0.48
33:Z:93:ARG:HB3	33:Z:94:PRO:HD3	1.95	0.48
18:K:106:ASN:HD21	18:K:121:ARG:NH1	2.12	0.48
33:Z:354:PRO:HA	33:Z:357:ILE:HG12	1.96	0.48
26:S:70:ASN:HA	26:S:72:GLU:CD	2.38	0.48
6:m:93:ILE:HA	6:m:96:LEU:HD12	1.95	0.48
9:b:36:GLY:C	9:b:37:ILE:HD12	2.39	0.48
13:F:175:LEU:HA	13:F:178:PHE:CE2	2.48	0.48
8:a:72:MET:HE3	8:a:74:VAL:CG2	2.44	0.48
6:m:93:ILE:HA	6:m:96:LEU:HD12	1.95	0.48
15:H:224:VAL:HG23	15:H:373:ARG:HH21	1.79	0.48
21:N:632:LYS:HE3	21:N:632:LYS:HA	1.96	0.48
16:I:319:ARG:HH21	16:I:319:ARG:HG2	1.79	0.48
17:J:55:VAL:HG23	21:N:613:HIS:CD2	2.48	0.48
9:b:36:GLY:C	9:b:37:ILE:HD12	2.39	0.48
7:n:150:MET:HE1	7:n:187:ARG:HG2	1.95	0.47
2:2:25:ILE:HG21	3:3:146:PHE:CD2	2.50	0.47
18:K:262:ARG:HA	18:K:311:ASN:HD21	1.79	0.47
22:O:195:TYR:CZ	22:O:213:LEU:HD13	2.49	0.47
30:W:158:ILE:HG23	30:W:169:SER:HB2	1.94	0.47
33:Z:354:PRO:HA	33:Z:357:ILE:HG12	1.96	0.47
22:O:75:GLN:C	22:O:75:GLN:CD	2.82	0.47
18:K:262:ARG:HA	18:K:311:ASN:HD21	1.80	0.47
22:O:75:GLN:C	22:O:75:GLN:CD	2.82	0.47
33:Z:93:ARG:HB3	33:Z:94:PRO:HD3	1.95	0.47
24:Q:299:MET:HE3	24:Q:299:MET:HA	1.97	0.47
11:d:195:ARG:HH12	11:d:237:GLU:CD	2.21	0.47
7:n:150:MET:HE1	7:n:187:ARG:HG2	1.95	0.47
24:Q:236:PHE:CE1	24:Q:269:LYS:HE2	2.49	0.47
33:Z:323:TYR:CD2	33:Z:862:MET:SD	3.07	0.47
12:e:37:GLY:HA2	12:e:145:TYR:CZ	2.50	0.47
9:B:187:ASP:HA	24:Q:130:ARG:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:387:GLY:HA3	24:Q:203:THR:HG23	1.97	0.47
33:Z:323:TYR:CD2	33:Z:862:MET:SD	3.07	0.47
9:b:36:GLY:C	9:b:37:ILE:HD12	2.39	0.47
10:c:42:GLY:HA2	10:c:145:TYR:CZ	2.50	0.47
9:B:187:ASP:HA	24:Q:130:ARG:HD2	1.97	0.47
15:H:224:VAL:HG23	15:H:373:ARG:HH21	1.79	0.47
16:I:148:LEU:CD2	17:J:95:ILE:HD13	2.43	0.47
12:e:37:GLY:HA2	12:e:145:TYR:CZ	2.50	0.47
3:3:19:CYS:HA	3:3:111:ILE:HD11	1.97	0.47
22:O:75:GLN:C	22:O:75:GLN:CD	2.82	0.47
23:P:161:CYS:HA	23:P:183:GLN:NE2	2.30	0.47
2:2:25:ILE:HG21	3:3:146:PHE:CD2	2.50	0.47
9:B:187:ASP:HA	24:Q:130:ARG:HD2	1.97	0.47
12:e:37:GLY:HA2	12:e:145:TYR:CZ	2.50	0.47
16:I:148:LEU:CD2	17:J:95:ILE:HD13	2.43	0.47
27:T:186:ARG:CD	27:T:211:PHE:CE1	2.98	0.47
10:c:42:GLY:HA2	10:c:145:TYR:CZ	2.50	0.47
28:U:37:ILE:HG23	28:U:48:VAL:CG1	2.45	0.47
11:d:187:GLU:CD	11:d:187:GLU:H	2.23	0.47
22:O:195:TYR:CZ	22:O:213:LEU:HD13	2.49	0.47
11:d:187:GLU:CD	11:d:187:GLU:H	2.23	0.47
33:Z:30:LYS:CD	33:Z:37:GLN:HB3	2.44	0.47
23:P:161:CYS:HA	23:P:183:GLN:NE2	2.30	0.47
2:2:25:ILE:HG21	3:3:146:PHE:CD2	2.50	0.46
22:O:195:TYR:CZ	22:O:213:LEU:HD13	2.49	0.46
10:c:95:GLN:HB3	3:j:68:TYR:CD1	2.51	0.46
3:3:19:CYS:HA	3:3:111:ILE:HD11	1.97	0.46
28:U:37:ILE:HG23	28:U:48:VAL:CG1	2.45	0.46
33:Z:323:TYR:CD2	33:Z:862:MET:SD	3.07	0.46
33:Z:827:LEU:HD23	33:Z:827:LEU:C	2.40	0.46
6:6:209:LYS:CD	6:6:209:LYS:H	2.28	0.46
29:V:24:LYS:CG	29:V:196:TYR:CD1	2.98	0.46
33:Z:827:LEU:HD23	33:Z:827:LEU:C	2.40	0.46
33:Z:832:ARG:CZ	33:Z:832:ARG:HB3	2.45	0.46
3:3:19:CYS:HA	3:3:111:ILE:HD11	1.97	0.46
15:H:224:VAL:HG23	15:H:373:ARG:HH21	1.79	0.46
23:P:161:CYS:HA	23:P:183:GLN:NE2	2.30	0.46
12:e:221:LYS:HE3	12:e:221:LYS:HA	1.98	0.46
20:M:47:GLU:HG3	20:M:50:ARG:HH22	1.80	0.46
33:Z:909:ARG:HE	33:Z:923:ILE:HD11	1.80	0.46
18:K:106:ASN:HD21	18:K:121:ARG:NH1	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:K:262:ARG:HA	18:K:311:ASN:HD21	1.79	0.46
6:6:209:LYS:CD	6:6:209:LYS:H	2.28	0.46
20:M:47:GLU:HG3	20:M:50:ARG:HH22	1.80	0.46
33:Z:827:LEU:HD23	33:Z:827:LEU:C	2.40	0.46
21:N:339:MET:CA	21:N:709:GLY:CA	2.75	0.46
10:c:95:GLN:HB3	3:j:68:TYR:CD1	2.51	0.46
4:4:173:PRO:HG2	4:4:174:MET:SD	2.56	0.46
18:K:306:PHE:CE2	18:K:311:ASN:HB3	2.50	0.46
21:N:339:MET:O	21:N:709:GLY:CA	2.63	0.46
25:R:238:PHE:CE2	25:R:240:SER:HA	2.50	0.46
21:N:339:MET:O	21:N:709:GLY:CA	2.63	0.46
12:e:221:LYS:HE3	12:e:221:LYS:HA	1.98	0.46
18:K:135:MET:HE1	18:K:149:ILE:HB	1.97	0.46
24:Q:299:MET:HE3	24:Q:299:MET:HA	1.96	0.46
25:R:24:TYR:CE1	25:R:244:THR:HA	2.51	0.46
30:W:35:PHE:CZ	30:W:186:ALA:HB2	2.51	0.46
4:k:172:MET:CE	4:k:176:PHE:CD1	2.99	0.46
6:6:209:LYS:CD	6:6:209:LYS:H	2.28	0.46
24:Q:299:MET:HE3	24:Q:299:MET:HA	1.96	0.46
29:V:24:LYS:CG	29:V:196:TYR:CE1	2.99	0.46
20:M:402:ALA:HA	20:M:407:GLN:NE2	2.31	0.46
24:Q:181:GLU:HG2	24:Q:185:TYR:CE2	2.50	0.46
30:W:35:PHE:CZ	30:W:186:ALA:HB2	2.51	0.46
4:4:173:PRO:HG2	4:4:174:MET:SD	2.56	0.46
24:Q:181:GLU:HG2	24:Q:185:TYR:CE2	2.51	0.46
29:V:24:LYS:CG	29:V:196:TYR:CD1	2.98	0.46
10:c:42:GLY:HA2	10:c:145:TYR:CZ	2.50	0.46
11:d:187:GLU:CD	11:d:187:GLU:H	2.23	0.46
8:A:72:MET:HE1	8:A:85:ALA:HB2	1.97	0.46
15:H:280:VAL:HG11	16:I:304:ARG:CZ	2.46	0.46
17:J:387:GLY:HA3	24:Q:203:THR:HG23	1.97	0.46
33:Z:30:LYS:HG2	33:Z:37:GLN:CB	2.44	0.46
33:Z:909:ARG:HE	33:Z:923:ILE:HD11	1.80	0.46
29:V:24:LYS:CG	29:V:196:TYR:CD1	2.98	0.46
22:O:75:GLN:NE2	22:O:106:PHE:CE2	2.83	0.46
33:Z:909:ARG:HE	33:Z:923:ILE:HD11	1.80	0.46
27:T:186:ARG:CD	27:T:211:PHE:CE1	2.98	0.46
17:J:387:GLY:HA3	24:Q:203:THR:HG23	1.97	0.46
25:R:238:PHE:CE2	25:R:240:SER:HA	2.50	0.46
28:U:37:ILE:HG23	28:U:48:VAL:CG1	2.45	0.46
20:M:402:ALA:HA	20:M:407:GLN:NE2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:238:PHE:CE2	25:R:240:SER:HA	2.50	0.46
29:V:24:LYS:CG	29:V:196:TYR:CE1	2.99	0.46
33:Z:832:ARG:CZ	33:Z:832:ARG:HB3	2.45	0.46
30:W:35:PHE:CZ	30:W:186:ALA:HB2	2.51	0.46
33:Z:832:ARG:CZ	33:Z:832:ARG:HB3	2.45	0.46
24:Q:408:THR:CG2	28:U:257:ILE:HD11	2.46	0.46
18:K:135:MET:HE1	18:K:149:ILE:HB	1.97	0.46
24:Q:427:PHE:CE1	25:R:417:TYR:CD1	3.04	0.46
10:c:95:GLN:HB3	3:j:68:TYR:CD1	2.51	0.46
17:J:95:ILE:N	17:J:95:ILE:HD12	2.31	0.45
9:B:118:MET:SD	9:B:152:PRO:HA	2.57	0.45
20:M:402:ALA:HA	20:M:407:GLN:NE2	2.31	0.45
12:e:221:LYS:HE3	12:e:221:LYS:HA	1.98	0.45
4:k:172:MET:CE	4:k:176:PHE:CD1	2.99	0.45
4:4:173:PRO:HG2	4:4:174:MET:SD	2.56	0.45
29:V:24:LYS:CG	29:V:196:TYR:CE1	2.99	0.45
18:K:306:PHE:CE2	18:K:311:ASN:HB3	2.50	0.45
21:N:339:MET:O	21:N:709:GLY:CA	2.64	0.45
25:R:291:SER:HB3	25:R:307:TYR:CE1	2.52	0.45
26:S:272:TYR:CE2	26:S:276:LEU:HD11	2.52	0.45
10:c:180:LYS:HE3	10:c:183:MET:HA	1.98	0.45
29:V:159:ILE:HG13	29:V:196:TYR:CD2	2.52	0.45
4:k:168:LEU:HB3	4:k:172:MET:HE2	1.99	0.45
18:K:306:PHE:CE2	18:K:311:ASN:HB3	2.50	0.45
20:M:47:GLU:HG3	20:M:50:ARG:HH22	1.80	0.45
26:S:60:LEU:C	26:S:60:LEU:HD13	2.41	0.45
6:m:66:LYS:N	6:m:66:LYS:HE2	2.32	0.45
26:S:60:LEU:C	26:S:60:LEU:HD13	2.41	0.45
33:Z:452:LEU:HD22	33:Z:477:TYR:CD2	2.52	0.45
11:D:146:TYR:CZ	11:D:156:SER:HB2	2.52	0.45
15:H:280:VAL:HG11	16:I:304:ARG:CZ	2.46	0.45
17:J:95:ILE:N	17:J:95:ILE:HD12	2.31	0.45
6:m:66:LYS:N	6:m:66:LYS:HE2	2.32	0.45
24:Q:408:THR:CG2	28:U:257:ILE:HD11	2.46	0.45
27:T:186:ARG:CD	27:T:211:PHE:CE1	2.98	0.45
33:Z:452:LEU:HD22	33:Z:477:TYR:CD2	2.52	0.45
19:L:365:THR:HA	19:L:368:VAL:HG22	1.99	0.45
24:Q:408:THR:CG2	28:U:257:ILE:HD11	2.46	0.45
26:S:60:LEU:C	26:S:60:LEU:HD13	2.41	0.45
11:D:118:TYR:CD2	11:D:124:VAL:HG11	2.52	0.45
24:Q:181:GLU:HG2	24:Q:185:TYR:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:291:SER:HB3	25:R:307:TYR:CE1	2.52	0.45
33:Z:452:LEU:HD22	33:Z:477:TYR:CD2	2.52	0.45
15:H:311:ILE:HD11	15:H:353:PHE:CD2	2.52	0.45
22:O:64:ASN:HB2	22:O:65:PHE:CD2	2.52	0.45
4:k:172:MET:CE	4:k:176:PHE:CD1	2.99	0.45
4:k:168:LEU:HB3	4:k:172:MET:HE2	1.99	0.45
15:H:77:ALA:HB3	15:H:78:PRO:HD3	1.98	0.45
20:M:172:VAL:HG22	20:M:174:GLU:H	1.81	0.45
9:B:118:MET:SD	9:B:152:PRO:HA	2.57	0.45
18:K:135:MET:HE1	18:K:149:ILE:HB	1.97	0.45
24:Q:427:PHE:CE1	25:R:417:TYR:CD1	3.04	0.45
25:R:291:SER:HB3	25:R:307:TYR:CE1	2.52	0.45
8:A:72:MET:HE1	8:A:85:ALA:HB2	1.97	0.45
22:O:29:PHE:CD1	22:O:29:PHE:C	2.95	0.45
19:L:365:THR:HA	19:L:368:VAL:HG22	1.99	0.45
25:R:31:PHE:CE1	25:R:324:ARG:NH1	2.85	0.45
26:S:137:PHE:CE1	26:S:141:LEU:HD11	2.52	0.45
33:Z:30:LYS:HG2	33:Z:37:GLN:CB	2.44	0.45
12:E:37:GLY:HA2	12:E:145:TYR:CZ	2.52	0.45
26:S:137:PHE:CE1	26:S:141:LEU:HD11	2.51	0.45
2:2:132:LEU:HD23	7:n:149:HIS:CB	2.47	0.45
12:e:99:ILE:HD13	12:e:99:ILE:H	1.82	0.45
2:2:132:LEU:HD23	7:n:149:HIS:CB	2.47	0.45
9:B:118:MET:SD	9:B:152:PRO:HA	2.57	0.45
11:D:118:TYR:CD2	11:D:124:VAL:HG11	2.52	0.45
25:R:31:PHE:CE1	25:R:324:ARG:NH1	2.85	0.45
26:S:137:PHE:CE1	26:S:141:LEU:HD11	2.52	0.45
2:2:132:LEU:HD11	7:n:150:MET:SD	2.57	0.45
8:A:72:MET:HE1	8:A:85:ALA:HB2	1.97	0.45
25:R:24:TYR:CE1	25:R:244:THR:HA	2.51	0.45
26:S:272:TYR:CE2	26:S:276:LEU:HD11	2.52	0.45
22:O:29:PHE:CD1	22:O:29:PHE:C	2.95	0.45
22:O:39:PHE:CZ	30:W:15:TYR:CE1	3.05	0.45
26:S:272:TYR:CE2	26:S:276:LEU:HD11	2.51	0.45
15:H:280:VAL:HG11	16:I:304:ARG:CZ	2.46	0.45
15:H:311:ILE:HD11	15:H:353:PHE:CD2	2.52	0.45
22:O:39:PHE:CZ	30:W:15:TYR:CE1	3.05	0.45
22:O:75:GLN:NE2	22:O:106:PHE:CE2	2.83	0.45
24:Q:427:PHE:CE1	25:R:417:TYR:CD1	3.04	0.45
17:J:95:ILE:N	17:J:95:ILE:HD12	2.31	0.45
18:K:398:ASN:CB	23:P:130:ILE:HG23	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:T:178:THR:HG22	27:T:182:LYS:HE3	1.99	0.45
33:Z:93:ARG:HB3	33:Z:94:PRO:CD	2.47	0.45
33:Z:793:PHE:CG	33:Z:832:ARG:NE	2.85	0.45
20:M:405:ASN:HD22	20:M:407:GLN:NE2	2.15	0.44
29:V:159:ILE:HG13	29:V:196:TYR:CD2	2.52	0.44
33:Z:30:LYS:CD	33:Z:37:GLN:HB3	2.44	0.44
12:E:37:GLY:HA2	12:E:145:TYR:CZ	2.52	0.44
33:Z:30:LYS:HG2	33:Z:37:GLN:CB	2.44	0.44
11:D:118:TYR:CD2	11:D:124:VAL:HG11	2.52	0.44
15:H:77:ALA:HB3	15:H:78:PRO:CD	2.48	0.44
20:M:172:VAL:HG22	20:M:174:GLU:H	1.81	0.44
25:R:24:TYR:CE1	25:R:244:THR:HA	2.51	0.44
4:k:168:LEU:HB3	4:k:172:MET:HE2	1.99	0.44
21:N:669:GLU:CD	21:N:785:PRO:HB3	2.43	0.44
22:O:62:TYR:CZ	22:O:82:LEU:HD13	2.53	0.44
3:3:97:ARG:HA	3:3:97:ARG:NE	2.33	0.44
9:B:187:ASP:HA	24:Q:130:ARG:CD	2.47	0.44
33:Z:93:ARG:HB3	33:Z:94:PRO:CD	2.47	0.44
19:L:365:THR:HA	19:L:368:VAL:HG22	1.99	0.44
25:R:31:PHE:CE1	25:R:324:ARG:NH1	2.85	0.44
29:V:159:ILE:HG13	29:V:196:TYR:CD2	2.52	0.44
15:H:77:ALA:HB3	15:H:78:PRO:CD	2.47	0.44
15:H:77:ALA:HB3	15:H:78:PRO:HD3	1.98	0.44
9:b:97:TYR:CE2	9:b:105:PRO:HA	2.53	0.44
11:D:146:TYR:CZ	11:D:156:SER:HB2	2.52	0.44
15:H:77:ALA:HB3	15:H:78:PRO:CD	2.47	0.44
18:K:155:ASP:C	19:L:109:MET:HE1	2.43	0.44
22:O:64:ASN:HB2	22:O:65:PHE:CD2	2.52	0.44
26:S:137:PHE:CZ	26:S:141:LEU:HD11	2.53	0.44
14:g:175:LEU:CD1	14:g:195:ILE:HD11	2.48	0.44
6:m:66:LYS:N	6:m:66:LYS:HE2	2.32	0.44
18:K:398:ASN:CB	23:P:130:ILE:HG23	2.47	0.44
22:O:62:TYR:CZ	22:O:82:LEU:HD13	2.53	0.44
29:V:159:ILE:HD11	29:V:196:TYR:CD1	2.53	0.44
10:c:180:LYS:HE3	10:c:183:MET:HA	1.98	0.44
14:g:205:GLU:CD	14:g:205:GLU:H	2.25	0.44
29:V:159:ILE:HD11	29:V:196:TYR:CD1	2.53	0.44
2:2:132:LEU:HD11	7:n:150:MET:SD	2.57	0.44
8:A:11:SER:HB3	8:A:17:TYR:CE2	2.53	0.44
15:H:77:ALA:HB3	15:H:78:PRO:HD3	1.98	0.44
20:M:172:VAL:HG22	20:M:174:GLU:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:97:TYR:CE2	9:b:105:PRO:HA	2.52	0.44
22:O:39:PHE:CZ	30:W:15:TYR:CE1	3.05	0.44
22:O:64:ASN:HB2	22:O:65:PHE:CD2	2.52	0.44
30:W:15:TYR:CE2	30:W:117:PRO:HD2	2.53	0.44
4:4:36:ARG:HE	4:4:57:ALA:HB3	1.83	0.44
12:E:37:GLY:HA2	12:E:145:TYR:CZ	2.52	0.44
13:F:86:TYR:CG	13:F:114:LYS:HE2	2.52	0.44
21:N:873:ARG:CZ	21:N:875:LEU:HD21	2.48	0.44
8:A:45:ILE:HG22	8:A:216:VAL:HG22	2.00	0.44
15:H:274:VAL:HG11	15:H:279:LEU:HD21	2.00	0.44
21:N:669:GLU:CD	21:N:785:PRO:HB3	2.43	0.44
27:T:178:THR:HG22	27:T:182:LYS:HE3	1.99	0.44
9:b:97:TYR:CE2	9:b:105:PRO:HA	2.53	0.44
21:N:669:GLU:CD	21:N:785:PRO:HB3	2.43	0.44
33:Z:93:ARG:HB3	33:Z:94:PRO:CD	2.47	0.44
2:2:132:LEU:HD23	7:n:149:HIS:CB	2.47	0.44
15:H:311:ILE:HD11	15:H:353:PHE:CD2	2.52	0.44
22:O:64:ASN:HB3	22:O:65:PHE:CE2	2.53	0.44
33:Z:793:PHE:CG	33:Z:832:ARG:NE	2.86	0.44
22:O:62:TYR:CZ	22:O:82:LEU:HD13	2.53	0.44
22:O:64:ASN:HB3	22:O:65:PHE:CE2	2.53	0.44
13:F:86:TYR:CG	13:F:114:LYS:HE2	2.53	0.44
14:G:74:TYR:CE2	14:G:81:GLY:HA3	2.53	0.44
21:N:873:ARG:CZ	21:N:875:LEU:HD21	2.48	0.44
29:V:159:ILE:HD11	29:V:196:TYR:CD1	2.53	0.44
12:e:65:HIS:CD2	12:e:65:HIS:H	2.36	0.44
14:G:74:TYR:CE2	14:G:81:GLY:HA3	2.53	0.44
15:H:233:GLU:H	15:H:233:GLU:CD	2.26	0.44
21:N:873:ARG:CZ	21:N:875:LEU:HD21	2.48	0.44
2:2:132:LEU:HD11	7:n:150:MET:SD	2.57	0.44
11:D:146:TYR:CZ	11:D:156:SER:HB2	2.52	0.44
16:I:409:MET:SD	16:I:409:MET:C	3.01	0.44
33:Z:194:GLU:CD	33:Z:197:LYS:HZ1	2.26	0.44
5:l:144:TYR:C	5:l:145:LYS:HE2	2.43	0.44
33:Z:793:PHE:CG	33:Z:832:ARG:NE	2.86	0.44
5:l:144:TYR:C	5:l:145:LYS:HE2	2.43	0.44
26:S:137:PHE:CZ	26:S:141:LEU:HD11	2.53	0.44
29:V:180:LEU:HB3	29:V:182:LYS:HE3	1.99	0.44
22:O:353:VAL:HG22	28:U:234:ASN:CG	2.43	0.44
4:4:36:ARG:HE	4:4:57:ALA:HB3	1.83	0.43
16:I:409:MET:SD	16:I:409:MET:C	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:11:ALA:HB1	27:T:80:ASN:HB2	2.00	0.43
22:O:25:LEU:HD11	22:O:61:LEU:CD2	2.48	0.43
12:e:99:ILE:HD13	12:e:99:ILE:H	1.82	0.43
15:H:233:GLU:H	15:H:233:GLU:CD	2.26	0.43
18:K:155:ASP:C	19:L:109:MET:HE1	2.43	0.43
20:M:405:ASN:HD22	20:M:407:GLN:NE2	2.15	0.43
28:U:37:ILE:HG23	28:U:48:VAL:HG13	2.00	0.43
8:a:45:ILE:HG22	8:a:216:VAL:HG22	2.00	0.43
1:1:190:PRO:HA	1:1:193:TYR:CZ	2.53	0.43
17:J:65:LEU:C	17:J:67:GLU:H	2.26	0.43
18:K:398:ASN:CB	23:P:130:ILE:HG23	2.47	0.43
24:Q:255:TYR:CD2	24:Q:255:TYR:C	2.96	0.43
27:T:178:THR:HG22	27:T:182:LYS:HE3	1.99	0.43
33:Z:194:GLU:CD	33:Z:197:LYS:HZ1	2.27	0.43
8:A:11:SER:HB3	8:A:17:TYR:CE2	2.53	0.43
7:7:76:TYR:CE2	14:G:89:ARG:HD3	2.54	0.43
30:W:155:ASP:HB2	30:W:171:LEU:HD22	1.99	0.43
10:c:180:LYS:HE3	10:c:183:MET:HA	1.98	0.43
14:g:175:LEU:CD1	14:g:195:ILE:HD11	2.48	0.43
22:O:64:ASN:HB3	22:O:65:PHE:CE2	2.53	0.43
26:S:121:VAL:HG13	26:S:125:LYS:HE3	2.00	0.43
12:e:99:ILE:HD13	12:e:99:ILE:H	1.82	0.43
24:Q:167:LYS:HE3	24:Q:168:LEU:CD2	2.48	0.43
28:U:37:ILE:HG23	28:U:48:VAL:HG13	2.00	0.43
30:W:155:ASP:HB2	30:W:171:LEU:HD22	1.99	0.43
9:B:187:ASP:HA	24:Q:130:ARG:CD	2.47	0.43
10:c:99:LYS:CE	3:j:68:TYR:CD1	3.01	0.43
3:3:97:ARG:NE	3:3:97:ARG:HA	2.33	0.43
11:D:191:LYS:HE2	11:D:234:ILE:CG1	2.49	0.43
16:I:102:ASN:HA	16:I:103:PRO:C	2.43	0.43
21:N:671:LEU:HA	21:N:857:TYR:CD2	2.53	0.43
22:O:25:LEU:HD11	22:O:61:LEU:CD2	2.48	0.43
22:O:25:LEU:N	22:O:25:LEU:HD22	2.33	0.43
29:V:180:LEU:HB3	29:V:182:LYS:HE3	1.99	0.43
14:g:205:GLU:CD	14:g:205:GLU:H	2.25	0.43
16:I:102:ASN:HA	16:I:103:PRO:C	2.43	0.43
18:K:155:ASP:C	19:L:109:MET:HE1	2.43	0.43
20:M:405:ASN:HD22	20:M:407:GLN:NE2	2.15	0.43
22:O:25:LEU:N	22:O:25:LEU:HD22	2.33	0.43
22:O:75:GLN:NE2	22:O:106:PHE:CE2	2.83	0.43
23:P:338:TRP:CD1	23:P:338:TRP:C	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:163:ARG:HD2	13:f:201:ARG:HD3	2.00	0.43
8:A:45:ILE:HG22	8:A:216:VAL:HG22	2.00	0.43
16:I:102:ASN:HA	16:I:103:PRO:C	2.43	0.43
22:O:25:LEU:HD11	22:O:61:LEU:CD2	2.48	0.43
22:O:25:LEU:HD13	22:O:25:LEU:HA	1.74	0.43
29:V:159:ILE:HG13	29:V:196:TYR:HA	2.00	0.43
30:W:15:TYR:CE2	30:W:117:PRO:HD2	2.53	0.43
8:A:45:ILE:HG22	8:A:216:VAL:HG22	2.00	0.43
13:F:86:TYR:CG	13:F:114:LYS:HE2	2.53	0.43
16:I:409:MET:SD	16:I:409:MET:C	3.01	0.43
22:O:29:PHE:C	22:O:29:PHE:CD1	2.95	0.43
27:T:131:LYS:HE2	27:T:132:HIS:CE1	2.54	0.43
10:c:99:LYS:CE	3:j:68:TYR:CD1	3.01	0.43
8:A:11:SER:HB3	8:A:17:TYR:CE2	2.53	0.43
26:S:137:PHE:CZ	26:S:141:LEU:HD11	2.53	0.43
33:Z:30:LYS:CD	33:Z:37:GLN:HB3	2.44	0.43
12:e:65:HIS:CD2	12:e:65:HIS:H	2.36	0.43
7:7:76:TYR:CE2	14:G:89:ARG:HD3	2.54	0.43
9:B:187:ASP:HA	24:Q:130:ARG:CD	2.47	0.43
11:D:68:HIS:CD2	11:D:69:VAL:HG23	2.54	0.43
22:O:353:VAL:HG22	28:U:234:ASN:CG	2.43	0.43
30:W:155:ASP:HB2	30:W:171:LEU:HD22	1.99	0.43
13:f:163:ARG:HD2	13:f:201:ARG:HD3	2.00	0.43
6:m:160:TYR:CG	6:m:166:GLY:HA2	2.54	0.43
11:D:68:HIS:CD2	11:D:69:VAL:HG23	2.54	0.43
22:O:353:VAL:HG22	28:U:234:ASN:CG	2.43	0.43
11:D:68:HIS:CD2	11:D:69:VAL:HG23	2.54	0.43
21:N:11:ALA:HB1	27:T:80:ASN:HB2	2.00	0.43
14:g:205:GLU:CD	14:g:205:GLU:H	2.25	0.43
21:N:339:MET:CA	21:N:709:GLY:CA	2.75	0.43
24:Q:167:LYS:HE3	24:Q:168:LEU:CD2	2.48	0.43
12:e:64:ARG:HD3	12:e:219:GLY:HA3	2.01	0.43
8:A:126:ARG:HH11	14:G:121:LEU:HD13	1.84	0.43
9:B:68:THR:HB	9:B:69:PRO:CD	2.49	0.43
11:D:191:LYS:HE2	11:D:234:ILE:CG1	2.49	0.43
6:m:160:TYR:CG	6:m:166:GLY:HA2	2.54	0.43
11:D:191:LYS:HE2	11:D:234:ILE:CG1	2.49	0.43
18:K:274:VAL:HG11	18:K:316:MET:SD	2.59	0.43
27:T:131:LYS:HE2	27:T:132:HIS:CE1	2.54	0.43
6:m:160:TYR:CG	6:m:166:GLY:HA2	2.54	0.43
18:K:274:VAL:HG11	18:K:316:MET:SD	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:190:PRO:HA	1:1:193:TYR:CZ	2.53	0.43
33:Z:818:CYS:SG	33:Z:832:ARG:NH2	2.92	0.43
1:1:190:PRO:HA	1:1:193:TYR:CZ	2.53	0.43
3:3:97:ARG:HA	3:3:97:ARG:NE	2.33	0.43
29:V:159:ILE:HG13	29:V:196:TYR:HA	2.00	0.43
30:W:15:TYR:CE2	30:W:117:PRO:HD2	2.53	0.43
24:Q:255:TYR:CD2	24:Q:255:TYR:C	2.96	0.43
5:l:144:TYR:C	5:l:145:LYS:HE2	2.43	0.43
15:H:192:ASP:HB3	15:H:289:ARG:CZ	2.49	0.43
29:V:180:LEU:HB3	29:V:182:LYS:HE3	2.00	0.43
33:Z:30:LYS:HG3	33:Z:37:GLN:CD	2.44	0.43
15:H:192:ASP:HB3	15:H:289:ARG:CZ	2.49	0.43
19:L:145:ARG:HE	19:L:161:ARG:HA	1.84	0.43
33:Z:30:LYS:HG3	33:Z:37:GLN:CD	2.44	0.43
19:L:145:ARG:HE	19:L:161:ARG:HA	1.84	0.43
6:m:4:PRO:CG	7:n:107:MET:SD	3.07	0.43
1:1:28:ASN:HB3	1:1:31:THR:HG23	2.01	0.43
17:J:65:LEU:C	17:J:67:GLU:H	2.26	0.43
22:O:312:ASP:O	22:O:315:LYS:HE3	2.19	0.43
15:H:233:GLU:H	15:H:233:GLU:CD	2.26	0.42
15:H:274:VAL:HG11	15:H:279:LEU:HD21	2.00	0.42
22:O:29:PHE:CG	22:O:30:GLU:N	2.87	0.42
23:P:438:ILE:HG21	28:U:101:ALA:H	1.84	0.42
27:T:131:LYS:HE2	27:T:132:HIS:CE1	2.54	0.42
22:O:29:PHE:CG	22:O:30:GLU:N	2.87	0.42
7:7:126:PHE:CD1	7:7:126:PHE:C	2.97	0.42
9:B:66:LEU:HD13	9:B:235:PHE:CG	2.54	0.42
17:J:133:LEU:HD23	17:J:240:HIS:CG	2.54	0.42
24:Q:255:TYR:C	24:Q:255:TYR:CD2	2.96	0.42
8:A:126:ARG:HH11	14:G:121:LEU:HD13	1.84	0.42
20:M:173:ASP:CG	20:M:175:LYS:HZ1	2.27	0.42
15:H:192:ASP:HB3	15:H:289:ARG:CZ	2.49	0.42
17:J:258:VAL:HA	17:J:264:GLY:H	1.84	0.42
18:K:274:VAL:HG11	18:K:316:MET:SD	2.59	0.42
8:a:45:ILE:HG22	8:a:216:VAL:HG22	2.00	0.42
12:e:64:ARG:HD3	12:e:219:GLY:HA3	2.01	0.42
14:G:74:TYR:CE2	14:G:81:GLY:HA3	2.53	0.42
15:H:274:VAL:HG11	15:H:279:LEU:HD21	2.00	0.42
17:J:133:LEU:HD23	17:J:240:HIS:CG	2.54	0.42
21:N:11:ALA:HB1	27:T:80:ASN:HB2	2.00	0.42
8:a:45:ILE:HG22	8:a:216:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:65:LEU:C	17:J:67:GLU:H	2.26	0.42
8:A:126:ARG:HH11	14:G:121:LEU:HD13	1.84	0.42
12:E:80:MET:SD	12:E:132:VAL:CG1	3.08	0.42
21:N:671:LEU:HA	21:N:857:TYR:CD2	2.53	0.42
7:7:126:PHE:CD1	7:7:126:PHE:C	2.97	0.42
9:B:68:THR:HB	9:B:69:PRO:CD	2.49	0.42
17:J:258:VAL:HA	17:J:264:GLY:H	1.84	0.42
21:N:269:LEU:HD13	21:N:269:LEU:C	2.44	0.42
22:O:25:LEU:HD13	22:O:25:LEU:HA	1.74	0.42
22:O:312:ASP:O	22:O:315:LYS:HE3	2.19	0.42
10:c:99:LYS:CE	3:j:68:TYR:CD1	3.01	0.42
7:7:126:PHE:CD1	7:7:126:PHE:C	2.97	0.42
7:7:208:PHE:CD2	7:7:210:LYS:HE3	2.55	0.42
21:N:666:GLN:HE21	21:N:713:VAL:C	2.27	0.42
21:N:671:LEU:HA	21:N:857:TYR:CD2	2.53	0.42
22:O:312:ASP:O	22:O:315:LYS:HE3	2.19	0.42
33:Z:30:LYS:HG3	33:Z:37:GLN:CD	2.44	0.42
33:Z:85:VAL:HG12	33:Z:86:PRO:N	2.34	0.42
22:O:29:PHE:CG	22:O:30:GLU:N	2.87	0.42
33:Z:818:CYS:SG	33:Z:832:ARG:NH2	2.92	0.42
13:f:163:ARG:HD2	13:f:201:ARG:HD3	2.00	0.42
12:E:80:MET:SD	12:E:132:VAL:CG1	3.08	0.42
19:L:145:ARG:HD3	19:L:161:ARG:HE	1.84	0.42
21:N:666:GLN:HE21	21:N:713:VAL:C	2.27	0.42
1:1:28:ASN:HB3	1:1:31:THR:HG23	2.01	0.42
21:N:362:TRP:CD2	21:N:742:TRP:CH2	3.08	0.42
28:U:35:GLY:HA3	28:U:93:TYR:CE2	2.55	0.42
8:A:124:TYR:CE1	8:A:125:MET:HG2	2.55	0.42
15:H:227:LEU:HD13	15:H:234:ARG:HH22	1.85	0.42
17:J:258:VAL:HA	17:J:264:GLY:H	1.84	0.42
23:P:338:TRP:CD1	23:P:338:TRP:C	2.97	0.42
7:7:208:PHE:CD2	7:7:210:LYS:HE3	2.55	0.42
21:N:362:TRP:CD2	21:N:742:TRP:CH2	3.08	0.42
23:P:338:TRP:CD1	23:P:338:TRP:C	2.97	0.42
28:U:37:ILE:HG23	28:U:48:VAL:HG13	2.00	0.42
14:G:137:VAL:HG23	14:G:215:CYS:SG	2.60	0.42
23:P:438:ILE:HG21	28:U:101:ALA:H	1.84	0.42
12:e:65:HIS:H	12:e:65:HIS:CD2	2.36	0.42
24:Q:167:LYS:HE3	24:Q:168:LEU:CD2	2.49	0.42
26:S:121:VAL:HG13	26:S:125:LYS:HE3	2.00	0.42
6:m:4:PRO:CG	7:n:107:MET:SD	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:227:LEU:HD13	15:H:234:ARG:HH22	1.84	0.42
16:I:378:GLU:CD	16:I:378:GLU:H	2.28	0.42
19:L:195:GLU:CD	19:L:345:ARG:HH22	2.28	0.42
26:S:344:PRO:HA	26:S:367:TYR:CE2	2.55	0.42
9:b:61:LEU:O	9:b:63:LYS:HE2	2.20	0.42
1:1:11:GLY:HA2	1:1:102:TYR:CE1	2.55	0.42
29:V:196:TYR:HB3	29:V:197:TYR:H	1.47	0.42
22:O:25:LEU:N	22:O:25:LEU:HD22	2.33	0.42
12:e:64:ARG:HD3	12:e:219:GLY:HA3	2.01	0.42
7:7:91:TYR:CE2	13:F:100:ARG:HD3	2.55	0.42
28:U:200:LEU:HA	28:U:203:LYS:HE3	2.02	0.42
4:4:36:ARG:HE	4:4:57:ALA:HB3	1.83	0.42
12:E:80:MET:SD	12:E:132:VAL:CG1	3.08	0.42
21:N:269:LEU:HD13	21:N:269:LEU:C	2.44	0.42
21:N:762:ARG:H	21:N:769:PRO:HD3	1.85	0.42
26:S:78:VAL:HA	26:S:105:PRO:HA	2.01	0.42
9:B:68:THR:HB	9:B:69:PRO:CD	2.49	0.42
22:O:178:TYR:CD1	22:O:182:LYS:HE2	2.55	0.42
1:1:28:ASN:HB3	1:1:31:THR:HG23	2.01	0.42
10:C:205:LEU:HD23	10:C:243:ILE:HG21	2.02	0.42
14:G:137:VAL:HG23	14:G:215:CYS:SG	2.60	0.42
23:P:357:TYR:CD1	23:P:357:TYR:N	2.88	0.42
26:S:78:VAL:HA	26:S:105:PRO:HA	2.01	0.42
33:Z:818:CYS:SG	33:Z:832:ARG:NH2	2.92	0.42
5:5:159:ARG:CZ	5:5:163:ALA:HB2	2.50	0.42
7:7:76:TYR:CE2	14:G:89:ARG:HD3	2.54	0.42
7:7:91:TYR:CE2	13:F:100:ARG:HD3	2.55	0.42
22:O:11:LEU:HG	22:O:27:GLU:CG	2.50	0.42
26:S:121:VAL:HG13	26:S:125:LYS:HE3	2.00	0.42
26:S:344:PRO:HA	26:S:367:TYR:CE2	2.54	0.42
33:Z:497:PHE:CD2	33:Z:505:VAL:HG21	2.55	0.42
14:g:175:LEU:CD1	14:g:195:ILE:HD11	2.48	0.42
7:7:91:TYR:CE2	13:F:100:ARG:HD3	2.55	0.42
19:L:145:ARG:HE	19:L:161:ARG:HA	1.84	0.42
23:P:438:ILE:HG21	28:U:101:ALA:H	1.84	0.42
1:1:11:GLY:HA2	1:1:102:TYR:CE1	2.55	0.42
21:N:530:GLU:CD	21:N:530:GLU:H	2.28	0.42
33:Z:497:PHE:CD2	33:Z:505:VAL:HG21	2.55	0.42
6:m:4:PRO:CG	7:n:107:MET:SD	3.07	0.42
8:A:124:TYR:CE1	8:A:125:MET:HG2	2.55	0.42
9:B:66:LEU:HD13	9:B:235:PHE:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:15:ARG:HH11	22:O:24:PRO:CB	2.33	0.42
9:B:122:THR:HG22	9:B:129:PRO:HG3	2.02	0.42
14:G:137:VAL:HG23	14:G:215:CYS:SG	2.60	0.42
19:L:400:PHE:CZ	20:M:215:PRO:HG2	2.55	0.42
21:N:666:GLN:HE21	21:N:713:VAL:C	2.28	0.42
33:Z:85:VAL:HG12	33:Z:86:PRO:N	2.34	0.42
33:Z:272:TYR:CZ	33:Z:280:ASP:HB3	2.55	0.42
1:h:61:TYR:CD2	1:h:61:TYR:C	2.98	0.41
5:5:18:SER:HB3	5:5:174:SER:H	1.85	0.41
16:I:378:GLU:H	16:I:378:GLU:CD	2.28	0.41
21:N:98:VAL:HG12	21:N:98:VAL:O	2.20	0.41
29:V:159:ILE:HG13	29:V:196:TYR:HA	2.00	0.41
4:k:8:ARG:HH21	4:k:8:ARG:HG2	1.86	0.41
2:2:142:TRP:CH2	2:2:144:GLN:HA	2.55	0.41
26:S:344:PRO:HA	26:S:367:TYR:CE2	2.54	0.41
28:U:35:GLY:HA3	28:U:93:TYR:CE2	2.55	0.41
33:Z:497:PHE:CD2	33:Z:505:VAL:HG21	2.55	0.41
24:Q:381:ILE:O	24:Q:384:LYS:HE3	2.20	0.41
29:V:196:TYR:HB3	29:V:197:TYR:H	1.47	0.41
3:3:187:TYR:CZ	3:3:196:LYS:HE3	2.56	0.41
11:D:94:HIS:CD2	11:D:98:LEU:HD13	2.55	0.41
19:L:145:ARG:HD3	19:L:161:ARG:HE	1.84	0.41
22:O:26:PHE:HA	22:O:29:PHE:CE2	2.56	0.41
33:Z:157:LEU:HB3	33:Z:207:ILE:HD12	2.02	0.41
5:5:18:SER:HB3	5:5:174:SER:H	1.85	0.41
19:L:195:GLU:CD	19:L:345:ARG:HH22	2.28	0.41
22:O:15:ARG:HH11	22:O:24:PRO:CB	2.33	0.41
9:b:61:LEU:O	9:b:63:LYS:HE2	2.20	0.41
9:B:66:LEU:HD13	9:B:235:PHE:CG	2.54	0.41
15:H:227:LEU:HD22	15:H:234:ARG:HH22	1.86	0.41
22:O:11:LEU:HG	22:O:27:GLU:CG	2.50	0.41
33:Z:85:VAL:HG12	33:Z:86:PRO:N	2.34	0.41
33:Z:350:GLY:HA3	33:Z:352:LYS:HE2	2.02	0.41
9:B:122:THR:HG22	9:B:129:PRO:HG3	2.02	0.41
14:G:134:PHE:CZ	14:G:145:TYR:HB2	2.56	0.41
30:W:37:PHE:CE1	30:W:69:PHE:CE1	3.09	0.41
33:Z:272:TYR:CZ	33:Z:280:ASP:HB3	2.55	0.41
11:d:146:TYR:CZ	11:d:156:SER:HB2	2.56	0.41
1:h:61:TYR:CD2	1:h:61:TYR:C	2.98	0.41
22:O:14:LEU:HD13	22:O:23:HIS:CG	2.55	0.41
26:S:78:VAL:HA	26:S:105:PRO:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:V:157:ARG:N	29:V:196:TYR:HB2	2.33	0.41
14:g:4:TYR:CE2	14:g:13:PRO:HD3	2.55	0.41
2:2:142:TRP:CH2	2:2:144:GLN:HA	2.56	0.41
8:A:124:TYR:CE1	8:A:125:MET:HG2	2.55	0.41
14:G:134:PHE:CZ	14:G:145:TYR:HB2	2.56	0.41
22:O:15:ARG:HH11	22:O:24:PRO:CB	2.33	0.41
26:S:112:ASN:HB2	26:S:114:TYR:CE1	2.56	0.41
29:V:228:TYR:CD1	29:V:228:TYR:N	2.88	0.41
11:d:146:TYR:CZ	11:d:156:SER:HB2	2.55	0.41
4:k:8:ARG:HG2	4:k:8:ARG:HH21	1.86	0.41
2:2:104:ASP:HB2	2:2:105:PRO:CD	2.51	0.41
9:B:149:GLN:HB3	9:B:159:TRP:HE1	1.86	0.41
14:G:111:ARG:HA	14:G:111:ARG:HH21	1.86	0.41
17:J:133:LEU:HD23	17:J:240:HIS:CG	2.54	0.41
21:N:124:TYR:CD1	21:N:124:TYR:N	2.89	0.41
33:Z:832:ARG:CZ	33:Z:832:ARG:CB	2.99	0.41
9:B:149:GLN:HB3	9:B:159:TRP:HE1	1.86	0.41
13:F:80:ALA:HB2	13:F:129:VAL:HG21	2.02	0.41
21:N:362:TRP:CD2	21:N:742:TRP:CH2	3.08	0.41
21:N:762:ARG:H	21:N:769:PRO:HD3	1.85	0.41
22:O:11:LEU:HG	22:O:27:GLU:CG	2.50	0.41
29:V:228:TYR:CD1	29:V:228:TYR:N	2.88	0.41
6:m:121:ALA:HB2	6:m:133:ARG:CZ	2.51	0.41
4:4:36:ARG:CZ	4:4:58:GLU:HG2	2.51	0.41
21:N:762:ARG:H	21:N:769:PRO:HD3	1.85	0.41
33:Z:272:TYR:CZ	33:Z:280:ASP:HB3	2.55	0.41
14:g:4:TYR:CE2	14:g:13:PRO:HD3	2.55	0.41
15:H:227:LEU:HD22	15:H:234:ARG:HH22	1.86	0.41
22:O:178:TYR:CD1	22:O:182:LYS:HE2	2.55	0.41
14:g:4:TYR:CE2	14:g:13:PRO:HD3	2.55	0.41
6:m:121:ALA:HB2	6:m:133:ARG:CZ	2.51	0.41
22:O:178:TYR:CD1	22:O:182:LYS:HE2	2.55	0.41
2:2:142:TRP:CH2	2:2:144:GLN:HA	2.56	0.41
11:D:29:THR:HG23	16:I:437:LEU:CD2	2.50	0.41
21:N:7:ALA:HB3	21:N:8:PRO:HD2	2.03	0.41
22:O:14:LEU:HD13	22:O:23:HIS:CG	2.55	0.41
23:P:357:TYR:N	23:P:357:TYR:CD1	2.88	0.41
1:1:11:GLY:HA2	1:1:102:TYR:CE1	2.55	0.41
2:2:132:LEU:HD11	7:n:150:MET:CG	2.51	0.41
22:O:26:PHE:HA	22:O:29:PHE:CE2	2.55	0.41
18:K:388:GLN:HA	19:L:212:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:V:157:ARG:N	29:V:196:TYR:HB2	2.33	0.41
3:j:17:LYS:HE3	3:j:18:ASP:HB2	2.02	0.41
6:m:205:LEU:HD21	6:m:214:LYS:HE2	2.03	0.41
16:I:81:ILE:HG22	16:I:84:PRO:HD2	2.02	0.41
19:L:400:PHE:CZ	20:M:215:PRO:HG2	2.56	0.41
21:N:735:MET:HE3	21:N:748:PHE:CZ	2.56	0.41
21:N:736:PHE:CD1	21:N:749:LEU:HB2	2.56	0.41
26:S:112:ASN:HB2	26:S:114:TYR:CE1	2.56	0.41
3:3:187:TYR:CZ	3:3:196:LYS:HE3	2.55	0.41
7:7:208:PHE:CD2	7:7:210:LYS:HE3	2.55	0.41
21:N:530:GLU:CD	21:N:530:GLU:H	2.28	0.41
28:U:200:LEU:HA	28:U:203:LYS:HE3	2.02	0.41
29:V:24:LYS:HB2	29:V:196:TYR:CE1	2.56	0.41
11:d:146:TYR:CZ	11:d:156:SER:HB2	2.56	0.41
3:j:17:LYS:HE3	3:j:18:ASP:HB2	2.02	0.41
9:B:122:THR:HG22	9:B:129:PRO:HG3	2.02	0.41
22:O:61:LEU:CD2	22:O:61:LEU:C	2.94	0.41
29:V:180:LEU:CB	29:V:182:LYS:HE3	2.51	0.41
10:C:205:LEU:HD23	10:C:243:ILE:HG21	2.02	0.41
9:b:61:LEU:O	9:b:63:LYS:HE2	2.20	0.41
21:N:269:LEU:HD13	21:N:269:LEU:C	2.44	0.41
22:O:61:LEU:CD2	22:O:61:LEU:C	2.94	0.41
22:O:90:LYS:HE2	22:O:90:LYS:O	2.21	0.41
29:V:180:LEU:CB	29:V:182:LYS:HE3	2.51	0.41
3:3:187:TYR:CZ	3:3:196:LYS:HE3	2.56	0.41
9:B:149:GLN:HB3	9:B:159:TRP:HE1	1.86	0.41
15:H:289:ARG:CZ	15:H:290:MET:HA	2.51	0.41
16:I:100:ARG:HA	16:I:150:HIS:CE1	2.56	0.41
20:M:283:LEU:HD11	20:M:325:ALA:HB1	2.03	0.41
21:N:124:TYR:CD1	21:N:124:TYR:N	2.89	0.41
24:Q:408:THR:HG23	28:U:257:ILE:HD11	2.03	0.41
29:V:24:LYS:HB2	29:V:196:TYR:CE1	2.56	0.41
13:f:175:LEU:HA	13:f:178:PHE:CE2	2.56	0.41
4:4:36:ARG:CZ	4:4:58:GLU:HG2	2.51	0.41
13:F:80:ALA:HB2	13:F:129:VAL:HG21	2.02	0.41
18:K:388:GLN:HA	19:L:212:ILE:HD11	2.03	0.41
21:N:530:GLU:CD	21:N:530:GLU:H	2.28	0.41
22:O:195:TYR:CD1	22:O:195:TYR:C	2.99	0.41
29:V:180:LEU:CB	29:V:182:LYS:HE3	2.51	0.41
33:Z:350:GLY:HA3	33:Z:352:LYS:HE2	2.02	0.41
10:C:205:LEU:HD23	10:C:243:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:29:THR:HG23	16:I:437:LEU:CD2	2.50	0.41
15:H:227:LEU:HD22	15:H:234:ARG:HH22	1.86	0.41
16:I:100:ARG:HA	16:I:150:HIS:CE1	2.56	0.41
16:I:378:GLU:CD	16:I:378:GLU:H	2.28	0.41
21:N:124:TYR:CD1	21:N:124:TYR:N	2.89	0.41
21:N:736:PHE:CD1	21:N:749:LEU:HB2	2.56	0.41
24:Q:381:ILE:O	24:Q:384:LYS:HE3	2.20	0.41
25:R:122:GLU:C	25:R:124:ASP:H	2.29	0.41
26:S:112:ASN:HB2	26:S:114:TYR:CE1	2.56	0.41
33:Z:157:LEU:HB3	33:Z:207:ILE:HD12	2.02	0.41
33:Z:350:GLY:HA3	33:Z:352:LYS:HE2	2.02	0.41
1:h:61:TYR:CD2	1:h:61:TYR:C	2.98	0.41
2:i:215:GLU:CD	3:j:197:ARG:HE	2.29	0.41
22:O:26:PHE:HA	22:O:29:PHE:CE2	2.55	0.41
26:S:401:LYS:HE2	26:S:442:PHE:CE1	2.56	0.41
33:Z:832:ARG:CZ	33:Z:832:ARG:CB	2.99	0.41
22:O:29:PHE:CD2	22:O:65:PHE:CZ	3.09	0.41
24:Q:408:THR:HG23	28:U:257:ILE:HD11	2.03	0.41
5:5:159:ARG:CZ	5:5:163:ALA:HB2	2.50	0.41
19:L:145:ARG:HD3	19:L:161:ARG:HE	1.84	0.41
21:N:89:PHE:CZ	21:N:136:ILE:HD11	2.56	0.41
33:Z:832:ARG:CZ	33:Z:832:ARG:CB	2.99	0.41
14:g:172:LEU:HD22	14:g:195:ILE:HD13	2.03	0.41
4:k:8:ARG:HG2	4:k:8:ARG:HH21	1.85	0.41
2:2:132:LEU:HD11	7:n:150:MET:CG	2.51	0.40
21:N:7:ALA:HB3	21:N:8:PRO:HD2	2.03	0.40
21:N:128:ILE:H	21:N:128:ILE:HD12	1.86	0.40
21:N:735:MET:HE3	21:N:748:PHE:CZ	2.56	0.40
28:U:35:GLY:HA3	28:U:93:TYR:CE2	2.55	0.40
6:m:121:ALA:HB2	6:m:133:ARG:CZ	2.51	0.40
2:2:132:LEU:HD11	7:n:150:MET:CG	2.51	0.40
15:H:192:ASP:N	15:H:193:PRO:CD	2.84	0.40
15:H:227:LEU:HD13	15:H:234:ARG:HH22	1.84	0.40
15:H:289:ARG:CZ	15:H:290:MET:HA	2.51	0.40
25:R:122:GLU:C	25:R:124:ASP:H	2.29	0.40
10:c:99:LYS:HE3	3:j:68:TYR:CD1	2.56	0.40
2:2:104:ASP:HB2	2:2:105:PRO:CD	2.51	0.40
11:D:94:HIS:CD2	11:D:98:LEU:HD13	2.55	0.40
14:G:111:ARG:HH21	14:G:111:ARG:HA	1.86	0.40
19:L:127:TYR:CE2	19:L:153:LEU:HD13	2.56	0.40
21:N:97:PHE:CZ	26:S:171:TYR:CZ	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:759:ILE:HG23	21:N:871:MET:SD	2.62	0.40
22:O:195:TYR:CD1	22:O:195:TYR:C	2.99	0.40
5:5:159:ARG:CZ	5:5:163:ALA:HB2	2.50	0.40
9:B:204:PHE:CE2	9:B:247:LEU:HD22	2.56	0.40
11:D:94:HIS:CD2	11:D:98:LEU:HD13	2.55	0.40
13:F:178:PHE:CD1	13:F:178:PHE:C	2.99	0.40
22:O:29:PHE:CD2	22:O:65:PHE:CZ	3.09	0.40
29:V:125:THR:HG22	29:V:129:PHE:CE2	2.56	0.40
30:W:37:PHE:CE1	30:W:69:PHE:CE1	3.09	0.40
33:Z:157:LEU:HB3	33:Z:207:ILE:HD12	2.02	0.40
33:Z:446:GLU:N	33:Z:446:GLU:CD	2.80	0.40
3:j:148:MET:HG2	3:j:169:ALA:HA	2.04	0.40
21:N:89:PHE:CZ	21:N:136:ILE:HD11	2.56	0.40
29:V:125:THR:HG22	29:V:129:PHE:CE2	2.56	0.40
9:B:204:PHE:CE2	9:B:247:LEU:HD22	2.56	0.40
15:H:289:ARG:CZ	15:H:290:MET:HA	2.51	0.40
19:L:165:PRO:HD3	20:M:83:VAL:HG13	2.04	0.40
21:N:7:ALA:HB3	21:N:8:PRO:HD2	2.03	0.40
21:N:623:PHE:CZ	21:N:655:ALA:CB	3.04	0.40
24:Q:185:TYR:CE2	24:Q:193:LYS:HG3	2.56	0.40
30:W:37:PHE:CE1	30:W:69:PHE:CE1	3.09	0.40
3:j:148:MET:HG2	3:j:169:ALA:HA	2.04	0.40
2:2:104:ASP:HB2	2:2:105:PRO:CD	2.51	0.40
5:5:54:PHE:CD1	5:5:54:PHE:C	3.00	0.40
8:A:91:GLU:CD	8:A:111:ARG:HE	2.30	0.40
11:D:29:THR:HG23	16:I:437:LEU:CD2	2.50	0.40
14:G:111:ARG:HA	14:G:111:ARG:HH21	1.86	0.40
21:N:623:PHE:CZ	21:N:655:ALA:CB	3.04	0.40
21:N:680:LYS:HA	21:N:683:LEU:HD12	2.04	0.40
21:N:736:PHE:CD1	21:N:749:LEU:HB2	2.56	0.40
22:O:14:LEU:HD13	22:O:23:HIS:CG	2.55	0.40
22:O:90:LYS:O	22:O:90:LYS:HE2	2.21	0.40
22:O:195:TYR:CD1	22:O:195:TYR:C	2.99	0.40
22:O:266:PHE:CD1	22:O:291:ILE:HG13	2.57	0.40
26:S:83:PRO:HG2	26:S:84:ASP:H	1.87	0.40
1:h:3:ILE:HD12	1:h:44:CYS:HB2	2.04	0.40
1:h:156:LYS:HE2	1:h:156:LYS:HB3	1.94	0.40
19:L:165:PRO:HD3	20:M:83:VAL:HG13	2.04	0.40
19:L:195:GLU:CD	19:L:345:ARG:HH22	2.28	0.40
21:N:50:TYR:CD1	21:N:50:TYR:C	3.00	0.40
22:O:90:LYS:O	22:O:90:LYS:HE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:V:157:ARG:N	29:V:196:TYR:HB2	2.33	0.40
3:j:17:LYS:HE3	3:j:18:ASP:HB2	2.02	0.40
16:I:81:ILE:HG22	16:I:84:PRO:HD2	2.02	0.40
18:K:388:GLN:HA	19:L:212:ILE:HD11	2.03	0.40
22:O:29:PHE:CD2	22:O:65:PHE:CZ	3.09	0.40
24:Q:236:PHE:CE1	24:Q:269:LYS:CE	3.05	0.40
24:Q:408:THR:HG23	28:U:257:ILE:HD11	2.03	0.40
10:c:99:LYS:HE3	3:j:68:TYR:CD1	2.57	0.40
10:C:63:GLU:N	10:C:63:GLU:CD	2.80	0.40
15:H:192:ASP:N	15:H:193:PRO:CD	2.84	0.40
19:L:400:PHE:CZ	20:M:215:PRO:HG2	2.55	0.40
21:N:89:PHE:CZ	21:N:136:ILE:HD11	2.56	0.40
25:R:122:GLU:C	25:R:124:ASP:H	2.29	0.40
21:N:680:LYS:HA	21:N:683:LEU:HD12	2.04	0.40
33:Z:815:MET:HB3	33:Z:832:ARG:NH1	2.37	0.40
13:f:175:LEU:HA	13:f:178:PHE:CE2	2.56	0.40
6:m:125:PHE:CD1	6:m:131:TYR:HB3	2.57	0.40
14:G:134:PHE:CZ	14:G:145:TYR:HB2	2.56	0.40
24:Q:243:PHE:CD2	24:Q:243:PHE:C	3.00	0.40
33:Z:123:ALA:HA	33:Z:132:HIS:CD2	2.57	0.40
12:e:91:HIS:CG	12:e:99:ILE:CG2	3.05	0.40
1:h:3:ILE:HD12	1:h:44:CYS:HB2	2.04	0.40
6:m:205:LEU:HD21	6:m:214:LYS:HE2	2.03	0.40
5:5:18:SER:HB3	5:5:174:SER:H	1.85	0.40
24:Q:185:TYR:CE2	24:Q:193:LYS:HG3	2.56	0.40
2:i:215:GLU:CD	3:j:197:ARG:HE	2.29	0.40
5:l:144:TYR:O	5:l:145:LYS:HE2	2.22	0.40
10:C:63:GLU:N	10:C:63:GLU:CD	2.80	0.40
13:F:178:PHE:CD1	13:F:178:PHE:C	2.99	0.40
22:O:25:LEU:HA	22:O:25:LEU:HD13	1.74	0.40
24:Q:185:TYR:CE2	24:Q:193:LYS:HG3	2.56	0.40
24:Q:381:ILE:O	24:Q:384:LYS:HE3	2.20	0.40
26:S:83:PRO:HG2	26:S:84:ASP:H	1.87	0.40
26:S:401:LYS:HE2	26:S:442:PHE:CE1	2.56	0.40
28:U:200:LEU:HA	28:U:203:LYS:HE3	2.02	0.40
29:V:24:LYS:HB2	29:V:196:TYR:CE1	2.56	0.40
12:e:91:HIS:CG	12:e:99:ILE:CG2	3.05	0.40
22:O:266:PHE:CD1	22:O:291:ILE:HG13	2.57	0.40
26:S:57:LEU:HD23	26:S:57:LEU:C	2.47	0.40
5:l:144:TYR:O	5:l:145:LYS:HE2	2.22	0.40
7:n:150:MET:HE2	7:n:183:VAL:CG1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-1	194/215 (90%)	190 (98%)	4 (2%)	0	100	100
1	1-h	194/215 (90%)	186 (96%)	8 (4%)	0	100	100
1	2-1	194/215 (90%)	190 (98%)	4 (2%)	0	100	100
1	2-h	194/215 (90%)	186 (96%)	8 (4%)	0	100	100
1	3-1	194/215 (90%)	190 (98%)	4 (2%)	0	100	100
1	3-h	194/215 (90%)	186 (96%)	8 (4%)	0	100	100
2	1-2	224/261 (86%)	210 (94%)	13 (6%)	1 (0%)	30	67
2	1-i	224/261 (86%)	215 (96%)	9 (4%)	0	100	100
2	2-2	224/261 (86%)	210 (94%)	13 (6%)	1 (0%)	30	67
2	2-i	224/261 (86%)	215 (96%)	9 (4%)	0	100	100
2	3-2	224/261 (86%)	210 (94%)	13 (6%)	1 (0%)	30	67
2	3-i	224/261 (86%)	215 (96%)	9 (4%)	0	100	100
3	1-3	202/205 (98%)	189 (94%)	10 (5%)	3 (2%)	8	40
3	1-j	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
3	2-3	202/205 (98%)	189 (94%)	10 (5%)	3 (2%)	8	40
3	2-j	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
3	3-3	202/205 (98%)	189 (94%)	10 (5%)	3 (2%)	8	40
3	3-j	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
4	1-4	193/198 (98%)	191 (99%)	1 (0%)	1 (0%)	24	63
4	1-k	193/198 (98%)	185 (96%)	8 (4%)	0	100	100
4	2-4	193/198 (98%)	191 (99%)	1 (0%)	1 (0%)	24	63
4	2-k	193/198 (98%)	185 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	3-4	193/198 (98%)	191 (99%)	1 (0%)	1 (0%)	24	63
4	3-k	193/198 (98%)	185 (96%)	8 (4%)	0	100	100
5	1-5	210/287 (73%)	196 (93%)	13 (6%)	1 (0%)	24	63
5	1-l	210/287 (73%)	199 (95%)	11 (5%)	0	100	100
5	2-5	210/287 (73%)	196 (93%)	13 (6%)	1 (0%)	24	63
5	2-l	210/287 (73%)	199 (95%)	11 (5%)	0	100	100
5	3-5	210/287 (73%)	196 (93%)	13 (6%)	1 (0%)	24	63
5	3-l	210/287 (73%)	199 (95%)	11 (5%)	0	100	100
6	1-6	220/241 (91%)	212 (96%)	7 (3%)	1 (0%)	24	63
6	1-m	220/241 (91%)	212 (96%)	7 (3%)	1 (0%)	24	63
6	2-6	220/241 (91%)	212 (96%)	7 (3%)	1 (0%)	24	63
6	2-m	220/241 (91%)	212 (96%)	7 (3%)	1 (0%)	24	63
6	3-6	220/241 (91%)	212 (96%)	7 (3%)	1 (0%)	24	63
6	3-m	220/241 (91%)	212 (96%)	7 (3%)	1 (0%)	24	63
7	1-7	227/266 (85%)	211 (93%)	13 (6%)	3 (1%)	9	42
7	1-n	230/266 (86%)	223 (97%)	6 (3%)	1 (0%)	30	67
7	2-7	227/266 (85%)	211 (93%)	13 (6%)	3 (1%)	9	42
7	2-n	230/266 (86%)	223 (97%)	6 (3%)	1 (0%)	30	67
7	3-7	227/266 (85%)	211 (93%)	13 (6%)	3 (1%)	9	42
7	3-n	230/266 (86%)	223 (97%)	6 (3%)	1 (0%)	30	67
8	1-A	239/252 (95%)	232 (97%)	6 (2%)	1 (0%)	30	67
8	1-a	239/252 (95%)	232 (97%)	6 (2%)	1 (0%)	30	67
8	2-A	239/252 (95%)	232 (97%)	6 (2%)	1 (0%)	30	67
8	2-a	239/252 (95%)	232 (97%)	6 (2%)	1 (0%)	30	67
8	3-A	239/252 (95%)	232 (97%)	6 (2%)	1 (0%)	30	67
8	3-a	239/252 (95%)	232 (97%)	6 (2%)	1 (0%)	30	67
9	1-B	248/250 (99%)	244 (98%)	3 (1%)	1 (0%)	30	67
9	1-b	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
9	2-B	248/250 (99%)	244 (98%)	3 (1%)	1 (0%)	30	67
9	2-b	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
9	3-B	248/250 (99%)	244 (98%)	3 (1%)	1 (0%)	30	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	3-b	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
10	1-C	242/258 (94%)	236 (98%)	6 (2%)	0	100	100
10	1-c	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	30	67
10	2-C	242/258 (94%)	236 (98%)	6 (2%)	0	100	100
10	2-c	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	30	67
10	3-C	242/258 (94%)	236 (98%)	6 (2%)	0	100	100
10	3-c	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	30	67
11	1-D	238/254 (94%)	227 (95%)	7 (3%)	4 (2%)	7	36
11	1-d	238/254 (94%)	228 (96%)	7 (3%)	3 (1%)	9	42
11	2-D	238/254 (94%)	227 (95%)	7 (3%)	4 (2%)	7	36
11	2-d	238/254 (94%)	228 (96%)	7 (3%)	3 (1%)	9	42
11	3-D	238/254 (94%)	227 (95%)	7 (3%)	4 (2%)	7	36
11	3-d	238/254 (94%)	228 (96%)	7 (3%)	3 (1%)	9	42
12	1-E	240/260 (92%)	234 (98%)	6 (2%)	0	100	100
12	1-e	240/260 (92%)	233 (97%)	4 (2%)	3 (1%)	9	42
12	2-E	240/260 (92%)	234 (98%)	6 (2%)	0	100	100
12	2-e	240/260 (92%)	233 (97%)	4 (2%)	3 (1%)	9	42
12	3-E	240/260 (92%)	234 (98%)	6 (2%)	0	100	100
12	3-e	240/260 (92%)	233 (97%)	4 (2%)	3 (1%)	9	42
13	1-F	231/234 (99%)	218 (94%)	9 (4%)	4 (2%)	7	36
13	1-f	229/234 (98%)	218 (95%)	10 (4%)	1 (0%)	30	67
13	2-F	231/234 (99%)	218 (94%)	9 (4%)	4 (2%)	7	36
13	2-f	229/234 (98%)	218 (95%)	10 (4%)	1 (0%)	30	67
13	3-F	231/234 (99%)	218 (94%)	9 (4%)	4 (2%)	7	36
13	3-f	229/234 (98%)	218 (95%)	10 (4%)	1 (0%)	30	67
14	1-G	241/288 (84%)	232 (96%)	8 (3%)	1 (0%)	30	67
14	1-g	241/288 (84%)	228 (95%)	12 (5%)	1 (0%)	30	67
14	2-G	241/288 (84%)	232 (96%)	8 (3%)	1 (0%)	30	67
14	2-g	241/288 (84%)	228 (95%)	12 (5%)	1 (0%)	30	67
14	3-G	241/288 (84%)	232 (96%)	8 (3%)	1 (0%)	30	67
14	3-g	241/288 (84%)	228 (95%)	12 (5%)	1 (0%)	30	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	1-H	386/467 (83%)	351 (91%)	28 (7%)	7 (2%)	6	34
15	2-H	386/467 (83%)	351 (91%)	28 (7%)	7 (2%)	6	34
15	3-H	386/467 (83%)	351 (91%)	28 (7%)	7 (2%)	6	34
16	1-I	383/437 (88%)	355 (93%)	25 (6%)	3 (1%)	16	54
16	2-I	383/437 (88%)	355 (93%)	25 (6%)	3 (1%)	16	54
16	3-I	383/437 (88%)	355 (93%)	25 (6%)	3 (1%)	16	54
17	1-J	384/405 (95%)	364 (95%)	17 (4%)	3 (1%)	16	54
17	2-J	384/405 (95%)	364 (95%)	17 (4%)	3 (1%)	16	54
17	3-J	384/405 (95%)	364 (95%)	17 (4%)	3 (1%)	16	54
18	1-K	387/428 (90%)	366 (95%)	16 (4%)	5 (1%)	9	42
18	2-K	387/428 (90%)	366 (95%)	16 (4%)	5 (1%)	9	42
18	3-K	387/428 (90%)	366 (95%)	16 (4%)	5 (1%)	9	42
19	1-L	386/437 (88%)	362 (94%)	22 (6%)	2 (0%)	24	63
19	2-L	386/437 (88%)	362 (94%)	22 (6%)	2 (0%)	24	63
19	3-L	386/437 (88%)	362 (94%)	22 (6%)	2 (0%)	24	63
20	1-M	377/434 (87%)	346 (92%)	27 (7%)	4 (1%)	11	46
20	2-M	377/434 (87%)	346 (92%)	27 (7%)	4 (1%)	11	46
20	3-M	377/434 (87%)	346 (92%)	27 (7%)	4 (1%)	11	46
21	1-N	886/945 (94%)	833 (94%)	49 (6%)	4 (0%)	24	63
21	2-N	886/945 (94%)	833 (94%)	49 (6%)	4 (0%)	24	63
21	3-N	886/945 (94%)	833 (94%)	48 (5%)	5 (1%)	21	59
22	1-O	386/393 (98%)	360 (93%)	19 (5%)	7 (2%)	6	34
22	2-O	386/393 (98%)	360 (93%)	19 (5%)	7 (2%)	6	34
22	3-O	386/393 (98%)	359 (93%)	20 (5%)	7 (2%)	6	34
23	1-P	438/445 (98%)	412 (94%)	20 (5%)	6 (1%)	9	40
23	2-P	438/445 (98%)	412 (94%)	20 (5%)	6 (1%)	9	40
23	3-P	438/445 (98%)	412 (94%)	20 (5%)	6 (1%)	9	40
24	1-Q	432/434 (100%)	400 (93%)	26 (6%)	6 (1%)	9	40
24	2-Q	432/434 (100%)	400 (93%)	26 (6%)	6 (1%)	9	40
24	3-Q	432/434 (100%)	400 (93%)	26 (6%)	6 (1%)	9	40
25	1-R	377/429 (88%)	361 (96%)	14 (4%)	2 (0%)	24	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	2-R	377/429 (88%)	361 (96%)	14 (4%)	2 (0%)	24	63
25	3-R	377/429 (88%)	361 (96%)	14 (4%)	2 (0%)	24	63
26	1-S	473/523 (90%)	447 (94%)	19 (4%)	7 (2%)	8	40
26	2-S	473/523 (90%)	447 (94%)	19 (4%)	7 (2%)	8	40
26	3-S	473/523 (90%)	447 (94%)	19 (4%)	7 (2%)	8	40
27	1-T	264/274 (96%)	245 (93%)	17 (6%)	2 (1%)	16	54
27	2-T	264/274 (96%)	245 (93%)	17 (6%)	2 (1%)	16	54
27	3-T	264/274 (96%)	245 (93%)	17 (6%)	2 (1%)	16	54
28	1-U	296/338 (88%)	283 (96%)	12 (4%)	1 (0%)	36	72
28	2-U	296/338 (88%)	283 (96%)	12 (4%)	1 (0%)	36	72
28	3-U	296/338 (88%)	283 (96%)	12 (4%)	1 (0%)	36	72
29	1-V	287/306 (94%)	263 (92%)	19 (7%)	5 (2%)	7	36
29	2-V	287/306 (94%)	263 (92%)	19 (7%)	5 (2%)	7	36
29	3-V	287/306 (94%)	263 (92%)	19 (7%)	5 (2%)	7	36
30	1-W	195/268 (73%)	176 (90%)	11 (6%)	8 (4%)	2	18
30	2-W	195/268 (73%)	176 (90%)	11 (6%)	8 (4%)	2	18
30	3-W	195/268 (73%)	176 (90%)	11 (6%)	8 (4%)	2	18
31	1-X	125/156 (80%)	111 (89%)	11 (9%)	3 (2%)	4	27
31	2-X	125/156 (80%)	111 (89%)	11 (9%)	3 (2%)	4	27
31	3-X	125/156 (80%)	111 (89%)	11 (9%)	3 (2%)	4	27
32	1-Y	47/89 (53%)	41 (87%)	4 (8%)	2 (4%)	2	17
32	2-Y	47/89 (53%)	41 (87%)	4 (8%)	2 (4%)	2	17
32	3-Y	47/89 (53%)	41 (87%)	4 (8%)	2 (4%)	2	17
33	1-Z	902/993 (91%)	827 (92%)	64 (7%)	11 (1%)	10	44
33	2-Z	902/993 (91%)	827 (92%)	64 (7%)	11 (1%)	10	44
33	3-Z	902/993 (91%)	827 (92%)	64 (7%)	11 (1%)	10	44
All	All	41130/45417 (91%)	38849 (94%)	1917 (5%)	364 (1%)	16	51

All (364) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	1-F	8	ASP
16	1-I	84	PRO

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Mol	Chain	Res	Type
16	1-I	125	MET
22	1-O	19	ASP
22	1-O	20	PRO
22	1-O	21	SER
22	1-O	36	LYS
22	1-O	43	GLU
23	1-P	398	LYS
24	1-Q	51	ARG
33	1-Z	24	THR
33	1-Z	85	VAL
13	2-F	8	ASP
16	2-I	84	PRO
16	2-I	125	MET
22	2-O	19	ASP
22	2-O	20	PRO
22	2-O	21	SER
22	2-O	36	LYS
22	2-O	43	GLU
23	2-P	398	LYS
24	2-Q	51	ARG
33	2-Z	24	THR
33	2-Z	85	VAL
13	3-F	8	ASP
16	3-I	84	PRO
16	3-I	125	MET
22	3-O	19	ASP
22	3-O	20	PRO
22	3-O	21	SER
22	3-O	36	LYS
22	3-O	43	GLU
23	3-P	398	LYS
24	3-Q	51	ARG
33	3-Z	24	THR
33	3-Z	85	VAL
3	1-3	182	TRP
9	1-B	17	LYS
11	1-D	2	TYR
13	1-F	124	GLY
13	1-F	204	SER
14	1-G	77	LEU
15	1-H	303	ALA
16	1-I	86	GLU

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Mol	Chain	Res	Type
17	1-J	141	LYS
17	1-J	353	CYS
20	1-M	299	ARG
21	1-N	339	MET
21	1-N	709	GLY
26	1-S	83	PRO
30	1-W	180	LEU
31	1-X	116	ALA
33	1-Z	142	ASP
33	1-Z	920	GLY
11	1-d	202	GLN
12	1-e	122	GLU
13	1-f	52	ALA
3	2-3	182	TRP
9	2-B	17	LYS
11	2-D	2	TYR
13	2-F	124	GLY
13	2-F	204	SER
14	2-G	77	LEU
15	2-H	303	ALA
16	2-I	86	GLU
17	2-J	141	LYS
17	2-J	353	CYS
20	2-M	299	ARG
21	2-N	339	MET
21	2-N	709	GLY
26	2-S	83	PRO
30	2-W	180	LEU
31	2-X	116	ALA
33	2-Z	142	ASP
33	2-Z	920	GLY
11	2-d	202	GLN
12	2-e	122	GLU
13	2-f	52	ALA
3	3-3	182	TRP
9	3-B	17	LYS
11	3-D	2	TYR
13	3-F	124	GLY
13	3-F	204	SER
14	3-G	77	LEU
15	3-H	303	ALA
16	3-I	86	GLU

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Mol	Chain	Res	Type
17	3-J	141	LYS
17	3-J	353	CYS
20	3-M	299	ARG
21	3-N	339	MET
21	3-N	709	GLY
26	3-S	83	PRO
30	3-W	180	LEU
31	3-X	116	ALA
33	3-Z	142	ASP
33	3-Z	920	GLY
11	3-d	202	GLN
12	3-e	122	GLU
13	3-f	52	ALA
8	1-A	51	PRO
11	1-D	203	THR
15	1-H	77	ALA
15	1-H	179	SER
15	1-H	324	GLY
18	1-K	416	LYS
18	1-K	419	ASN
18	1-K	420	THR
20	1-M	153	TYR
22	1-O	249	ASP
23	1-P	327	LEU
24	1-Q	18	LYS
24	1-Q	252	HIS
25	1-R	280	ILE
26	1-S	69	LEU
27	1-T	173	GLU
28	1-U	150	THR
29	1-V	78	VAL
29	1-V	195	HIS
30	1-W	23	ARG
30	1-W	149	GLN
31	1-X	38	ASN
33	1-Z	233	LEU
33	1-Z	366	LYS
33	1-Z	376	SER
33	1-Z	887	GLY
10	1-c	51	VAL
11	1-d	203	THR
11	1-d	204	GLY

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Mol	Chain	Res	Type
8	2-A	51	PRO
11	2-D	203	THR
15	2-H	77	ALA
15	2-H	179	SER
15	2-H	324	GLY
18	2-K	416	LYS
18	2-K	419	ASN
18	2-K	420	THR
20	2-M	153	TYR
22	2-O	249	ASP
23	2-P	327	LEU
24	2-Q	18	LYS
24	2-Q	252	HIS
25	2-R	280	ILE
26	2-S	44	THR
26	2-S	69	LEU
27	2-T	173	GLU
28	2-U	150	THR
29	2-V	78	VAL
29	2-V	195	HIS
30	2-W	23	ARG
30	2-W	149	GLN
31	2-X	38	ASN
33	2-Z	233	LEU
33	2-Z	366	LYS
33	2-Z	376	SER
33	2-Z	887	GLY
10	2-c	51	VAL
11	2-d	203	THR
11	2-d	204	GLY
8	3-A	51	PRO
11	3-D	203	THR
15	3-H	77	ALA
15	3-H	179	SER
15	3-H	324	GLY
18	3-K	416	LYS
18	3-K	419	ASN
18	3-K	420	THR
20	3-M	153	TYR
22	3-O	249	ASP
23	3-P	327	LEU
24	3-Q	18	LYS

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Mol	Chain	Res	Type
24	3-Q	252	HIS
25	3-R	280	ILE
26	3-S	69	LEU
27	3-T	173	GLU
28	3-U	150	THR
29	3-V	78	VAL
29	3-V	195	HIS
30	3-W	23	ARG
30	3-W	149	GLN
31	3-X	38	ASN
33	3-Z	233	LEU
33	3-Z	366	LYS
33	3-Z	376	SER
33	3-Z	887	GLY
10	3-c	51	VAL
11	3-d	203	THR
11	3-d	204	GLY
2	1-2	145	ASP
6	1-6	200	ASP
7	1-7	10	SER
7	1-7	216	ASN
17	1-J	66	GLN
19	1-L	291	PHE
20	1-M	174	GLU
20	1-M	179	THR
21	1-N	790	GLU
22	1-O	44	SER
23	1-P	85	LYS
23	1-P	131	PHE
24	1-Q	170	ASP
26	1-S	44	THR
26	1-S	97	THR
29	1-V	185	ILE
29	1-V	257	GLU
29	1-V	262	THR
30	1-W	55	ALA
31	1-X	95	GLU
32	1-Y	66	ASP
33	1-Z	926	ASN
8	1-a	123	ALA
12	1-e	45	ARG
12	1-e	123	GLU

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Mol	Chain	Res	Type
14	1-g	219	GLU
6	1-m	200	ASP
7	1-n	9	THR
2	2-2	145	ASP
6	2-6	200	ASP
7	2-7	10	SER
7	2-7	216	ASN
17	2-J	66	GLN
19	2-L	291	PHE
20	2-M	174	GLU
20	2-M	179	THR
21	2-N	790	GLU
22	2-O	44	SER
23	2-P	85	LYS
23	2-P	131	PHE
24	2-Q	170	ASP
26	2-S	97	THR
29	2-V	185	ILE
29	2-V	257	GLU
29	2-V	262	THR
30	2-W	55	ALA
31	2-X	95	GLU
32	2-Y	66	ASP
33	2-Z	926	ASN
8	2-a	123	ALA
12	2-e	45	ARG
12	2-e	123	GLU
6	2-m	200	ASP
7	2-n	9	THR
2	3-2	145	ASP
6	3-6	200	ASP
7	3-7	10	SER
7	3-7	216	ASN
17	3-J	66	GLN
19	3-L	291	PHE
20	3-M	174	GLU
20	3-M	179	THR
21	3-N	790	GLU
22	3-O	44	SER
23	3-P	85	LYS
23	3-P	131	PHE
24	3-Q	170	ASP

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Mol	Chain	Res	Type
26	3-S	44	THR
26	3-S	97	THR
29	3-V	185	ILE
29	3-V	257	GLU
29	3-V	262	THR
30	3-W	55	ALA
31	3-X	95	GLU
32	3-Y	66	ASP
33	3-Z	926	ASN
8	3-a	123	ALA
12	3-e	45	ARG
12	3-e	123	GLU
14	3-g	219	GLU
6	3-m	200	ASP
7	3-n	9	THR
3	1-3	125	LEU
7	1-7	78	ASN
11	1-D	99	GLU
11	1-D	100	ASP
18	1-K	160	VAL
23	1-P	328	ALA
24	1-Q	46	VAL
24	1-Q	47	ASP
25	1-R	395	ASN
26	1-S	102	SER
30	1-W	3	LEU
30	1-W	178	PRO
32	1-Y	70	ASP
3	2-3	125	LEU
7	2-7	78	ASN
11	2-D	99	GLU
11	2-D	100	ASP
18	2-K	160	VAL
23	2-P	328	ALA
24	2-Q	46	VAL
24	2-Q	47	ASP
25	2-R	395	ASN
26	2-S	102	SER
30	2-W	3	LEU
30	2-W	178	PRO
32	2-Y	70	ASP
14	2-g	219	GLU

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Mol	Chain	Res	Type
3	3-3	125	LEU
7	3-7	78	ASN
11	3-D	99	GLU
11	3-D	100	ASP
18	3-K	160	VAL
23	3-P	328	ALA
24	3-Q	46	VAL
24	3-Q	47	ASP
25	3-R	395	ASN
26	3-S	102	SER
30	3-W	3	LEU
30	3-W	178	PRO
32	3-Y	70	ASP
33	3-Z	377	ALA
18	1-K	176	GLY
19	1-L	288	GLY
21	1-N	8	PRO
23	1-P	7	ILE
26	1-S	118	PHE
26	1-S	449	LEU
27	1-T	231	SER
30	1-W	102	GLN
33	1-Z	377	ALA
18	2-K	176	GLY
19	2-L	288	GLY
21	2-N	8	PRO
23	2-P	7	ILE
26	2-S	118	PHE
26	2-S	449	LEU
27	2-T	231	SER
30	2-W	102	GLN
33	2-Z	377	ALA
18	3-K	176	GLY
19	3-L	288	GLY
21	3-N	8	PRO
21	3-N	856	PHE
23	3-P	7	ILE
26	3-S	118	PHE
26	3-S	449	LEU
27	3-T	231	SER
30	3-W	102	GLN
15	1-H	193	PRO

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Mol	Chain	Res	Type
15	1-H	311	ILE
15	2-H	193	PRO
15	2-H	311	ILE
15	3-H	193	PRO
15	3-H	311	ILE
15	1-H	315	GLY
33	1-Z	578	GLY
15	2-H	315	GLY
33	2-Z	578	GLY
15	3-H	315	GLY
33	3-Z	578	GLY
30	1-W	164	PRO
3	2-3	183	GLY
30	2-W	164	PRO
13	3-F	220	PRO
30	3-W	164	PRO
3	1-3	183	GLY
4	1-4	9	VAL
13	1-F	220	PRO
4	2-4	9	VAL
13	2-F	220	PRO
3	3-3	183	GLY
4	3-4	9	VAL
5	1-5	94	GLY
5	2-5	94	GLY
5	3-5	94	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3-1	162/178 (91%)	156 (96%)	6 (4%)	30	51
1	3-h	162/178 (91%)	152 (94%)	10 (6%)	16	38
2	3-2	185/214 (86%)	182 (98%)	3 (2%)	55	70
2	3-i	185/214 (86%)	175 (95%)	10 (5%)	20	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3-3	172/173 (99%)	168 (98%)	4 (2%)	44	64
3	3-j	172/173 (99%)	167 (97%)	5 (3%)	37	58
4	3-4	173/175 (99%)	167 (96%)	6 (4%)	32	53
4	3-k	173/175 (99%)	165 (95%)	8 (5%)	24	45
5	3-5	169/235 (72%)	166 (98%)	3 (2%)	51	68
5	3-l	169/235 (72%)	158 (94%)	11 (6%)	15	37
6	3-6	185/201 (92%)	179 (97%)	6 (3%)	34	56
6	3-m	185/201 (92%)	174 (94%)	11 (6%)	18	39
7	3-7	195/224 (87%)	189 (97%)	6 (3%)	35	56
7	3-n	198/224 (88%)	186 (94%)	12 (6%)	17	38
8	3-A	206/210 (98%)	198 (96%)	8 (4%)	28	49
8	3-a	206/210 (98%)	194 (94%)	12 (6%)	18	40
9	3-B	209/209 (100%)	205 (98%)	4 (2%)	50	67
9	3-b	209/209 (100%)	193 (92%)	16 (8%)	12	32
10	3-C	203/216 (94%)	195 (96%)	8 (4%)	28	49
10	3-c	203/216 (94%)	196 (97%)	7 (3%)	32	54
11	3-D	212/226 (94%)	200 (94%)	12 (6%)	18	40
11	3-d	212/226 (94%)	202 (95%)	10 (5%)	23	45
12	3-E	198/215 (92%)	186 (94%)	12 (6%)	17	38
12	3-e	198/215 (92%)	187 (94%)	11 (6%)	19	40
13	3-F	192/193 (100%)	182 (95%)	10 (5%)	21	42
13	3-f	190/193 (98%)	182 (96%)	8 (4%)	26	48
14	3-G	201/239 (84%)	195 (97%)	6 (3%)	36	57
14	3-g	201/239 (84%)	194 (96%)	7 (4%)	32	53
15	3-H	330/399 (83%)	315 (96%)	15 (4%)	24	46
16	3-I	342/385 (89%)	331 (97%)	11 (3%)	34	56
17	3-J	336/352 (96%)	319 (95%)	17 (5%)	21	42
18	3-K	342/374 (91%)	329 (96%)	13 (4%)	29	50
19	3-L	332/377 (88%)	317 (96%)	15 (4%)	24	46
20	3-M	329/375 (88%)	317 (96%)	12 (4%)	31	52
21	3-N	745/797 (94%)	718 (96%)	27 (4%)	31	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	3-O	363/368 (99%)	342 (94%)	21 (6%)	18	40
23	3-P	412/415 (99%)	392 (95%)	20 (5%)	22	43
24	3-Q	391/391 (100%)	367 (94%)	24 (6%)	17	38
25	3-R	333/379 (88%)	319 (96%)	14 (4%)	26	48
26	3-S	447/489 (91%)	431 (96%)	16 (4%)	31	52
27	3-T	249/256 (97%)	232 (93%)	17 (7%)	14	36
28	3-U	271/308 (88%)	267 (98%)	4 (2%)	57	72
29	3-V	253/268 (94%)	240 (95%)	13 (5%)	21	42
30	3-W	171/230 (74%)	162 (95%)	9 (5%)	20	41
31	3-X	116/144 (81%)	113 (97%)	3 (3%)	40	62
32	3-Y	50/81 (62%)	49 (98%)	1 (2%)	48	66
33	3-Z	773/850 (91%)	730 (94%)	43 (6%)	19	40
All	All	11910/13054 (91%)	11383 (96%)	527 (4%)	27	47

All (527) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3-1	31	THR
1	3-1	43	CYS
1	3-1	104	ASP
1	3-1	126	ILE
1	3-1	148	LYS
1	3-1	195	GLN
2	3-2	85	GLN
2	3-2	145	ASP
2	3-2	176	CYS
3	3-3	17	LYS
3	3-3	65	MET
3	3-3	96	GLU
3	3-3	154	GLU
4	3-4	3	ILE
4	3-4	37	GLN
4	3-4	78	GLN
4	3-4	110	LYS
4	3-4	126	VAL
4	3-4	183	ILE
5	3-5	104	TYR
5	3-5	106	ARG

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Mol	Chain	Res	Type
5	3-5	149	SER
6	3-6	34	SER
6	3-6	42	LYS
6	3-6	80	ASN
6	3-6	122	VAL
6	3-6	134	GLU
6	3-6	206	ILE
7	3-7	104	ARG
7	3-7	106	LYS
7	3-7	129	TYR
7	3-7	187	ARG
7	3-7	213	GLN
7	3-7	216	ASN
8	3-A	41	CYS
8	3-A	111	ARG
8	3-A	112	MET
8	3-A	122	ARG
8	3-A	124	TYR
8	3-A	211	LYS
8	3-A	220	THR
8	3-A	241	GLU
9	3-B	13	SER
9	3-B	20	GLN
9	3-B	108	LYS
9	3-B	182	GLU
10	3-C	26	GLU
10	3-C	38	MET
10	3-C	57	GLU
10	3-C	63	GLU
10	3-C	79	LEU
10	3-C	180	LYS
10	3-C	181	ASP
10	3-C	237	ILE
11	3-D	7	SER
11	3-D	16	PHE
11	3-D	37	LYS
11	3-D	85	GLU
11	3-D	116	GLN
11	3-D	149	GLU
11	3-D	164	ARG
11	3-D	180	LYS
11	3-D	224	SER

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Mol	Chain	Res	Type
11	3-D	226	GLU
11	3-D	237	GLU
11	3-D	240	GLU
12	3-E	17	GLU
12	3-E	54	ASP
12	3-E	58	LYS
12	3-E	70	MET
12	3-E	82	GLU
12	3-E	97	GLU
12	3-E	102	GLU
12	3-E	108	VAL
12	3-E	114	ARG
12	3-E	176	LEU
12	3-E	208	ASN
12	3-E	221	LYS
13	3-F	2	ARG
13	3-F	3	ASN
13	3-F	4	ASN
13	3-F	29	LYS
13	3-F	50	ARG
13	3-F	73	LEU
13	3-F	85	ASN
13	3-F	125	ARG
13	3-F	172	GLU
13	3-F	188	LEU
14	3-G	5	ASP
14	3-G	111	ARG
14	3-G	139	LYS
14	3-G	148	GLU
14	3-G	166	GLN
14	3-G	215	CYS
15	3-H	69	VAL
15	3-H	107	LYS
15	3-H	151	GLN
15	3-H	173	ARG
15	3-H	190	ARG
15	3-H	208	TYR
15	3-H	249	TYR
15	3-H	289	ARG
15	3-H	297	MET
15	3-H	311	ILE
15	3-H	326	ASP

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Mol	Chain	Res	Type
15	3-H	333	MET
15	3-H	359	ASN
15	3-H	367	ARG
15	3-H	425	GLU
16	3-I	58	LYS
16	3-I	150	HIS
16	3-I	174	ASP
16	3-I	254	GLN
16	3-I	265	ARG
16	3-I	309	LEU
16	3-I	319	ARG
16	3-I	333	THR
16	3-I	359	LYS
16	3-I	366	THR
16	3-I	409	MET
17	3-J	15	HIS
17	3-J	39	GLU
17	3-J	108	LYS
17	3-J	120	TYR
17	3-J	137	MET
17	3-J	142	VAL
17	3-J	146	THR
17	3-J	162	GLU
17	3-J	183	LYS
17	3-J	212	ARG
17	3-J	225	GLU
17	3-J	228	ARG
17	3-J	236	MET
17	3-J	278	GLN
17	3-J	298	ASP
17	3-J	353	CYS
17	3-J	388	LYS
18	3-K	51	LEU
18	3-K	119	VAL
18	3-K	128	ARG
18	3-K	137	VAL
18	3-K	141	ARG
18	3-K	212	TYR
18	3-K	237	VAL
18	3-K	254	VAL
18	3-K	264	ASN
18	3-K	350	ARG

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Mol	Chain	Res	Type
18	3-K	387	MET
18	3-K	404	GLN
18	3-K	408	GLU
19	3-L	92	GLU
19	3-L	96	LYS
19	3-L	109	MET
19	3-L	128	ILE
19	3-L	177	GLU
19	3-L	183	ILE
19	3-L	199	LEU
19	3-L	228	LYS
19	3-L	264	ARG
19	3-L	271	LYS
19	3-L	316	ASP
19	3-L	346	LYS
19	3-L	364	HIS
19	3-L	382	MET
19	3-L	415	LEU
20	3-M	85	VAL
20	3-M	129	LEU
20	3-M	145	LEU
20	3-M	151	ASP
20	3-M	162	GLU
20	3-M	238	GLN
20	3-M	263	VAL
20	3-M	302	GLN
20	3-M	339	ARG
20	3-M	373	ASP
20	3-M	426	LYS
20	3-M	427	SER
21	3-N	58	ARG
21	3-N	76	GLU
21	3-N	86	LYS
21	3-N	88	ARG
21	3-N	112	GLU
21	3-N	116	GLN
21	3-N	124	TYR
21	3-N	150	LEU
21	3-N	219	ASN
21	3-N	271	GLU
21	3-N	339	MET
21	3-N	381	GLU

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Mol	Chain	Res	Type
21	3-N	394	ARG
21	3-N	398	ARG
21	3-N	412	TYR
21	3-N	419	THR
21	3-N	494	LYS
21	3-N	546	LEU
21	3-N	597	ARG
21	3-N	605	ILE
21	3-N	632	LYS
21	3-N	816	LYS
21	3-N	857	TYR
21	3-N	871	MET
21	3-N	880	ARG
21	3-N	895	LYS
21	3-N	919	THR
22	3-O	6	GLU
22	3-O	11	LEU
22	3-O	23	HIS
22	3-O	27	GLU
22	3-O	29	PHE
22	3-O	34	GLU
22	3-O	41	LEU
22	3-O	43	GLU
22	3-O	57	LEU
22	3-O	61	LEU
22	3-O	66	VAL
22	3-O	70	TYR
22	3-O	73	ILE
22	3-O	87	LYS
22	3-O	90	LYS
22	3-O	105	GLN
22	3-O	161	ASP
22	3-O	195	TYR
22	3-O	196	LEU
22	3-O	294	MET
22	3-O	306	ARG
23	3-P	19	GLU
23	3-P	20	GLU
23	3-P	32	CYS
23	3-P	43	GLU
23	3-P	86	HIS
23	3-P	115	ARG

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Mol	Chain	Res	Type
23	3-P	133	GLU
23	3-P	170	SER
23	3-P	202	LYS
23	3-P	232	ARG
23	3-P	277	GLN
23	3-P	285	GLN
23	3-P	309	MET
23	3-P	310	ARG
23	3-P	316	LYS
23	3-P	332	GLU
23	3-P	346	ILE
23	3-P	368	LEU
23	3-P	400	VAL
23	3-P	403	GLU
24	3-Q	7	LYS
24	3-Q	19	GLN
24	3-Q	50	ARG
24	3-Q	75	ARG
24	3-Q	88	PHE
24	3-Q	104	PHE
24	3-Q	138	SER
24	3-Q	147	GLN
24	3-Q	149	LYS
24	3-Q	152	LYS
24	3-Q	157	LEU
24	3-Q	164	GLU
24	3-Q	166	LYS
24	3-Q	189	ARG
24	3-Q	198	LEU
24	3-Q	227	CYS
24	3-Q	259	CYS
24	3-Q	260	GLN
24	3-Q	270	ILE
24	3-Q	299	MET
24	3-Q	320	GLN
24	3-Q	326	MET
24	3-Q	355	GLU
24	3-Q	384	LYS
25	3-R	25	GLU
25	3-R	49	PHE
25	3-R	57	GLU
25	3-R	58	GLU

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Mol	Chain	Res	Type
25	3-R	96	GLN
25	3-R	110	ILE
25	3-R	119	LYS
25	3-R	132	GLN
25	3-R	160	LYS
25	3-R	192	GLU
25	3-R	229	LYS
25	3-R	331	ARG
25	3-R	343	GLU
25	3-R	416	LYS
26	3-S	30	GLN
26	3-S	32	GLN
26	3-S	34	LEU
26	3-S	35	LEU
26	3-S	109	GLU
26	3-S	178	LEU
26	3-S	230	LYS
26	3-S	242	LEU
26	3-S	247	VAL
26	3-S	264	VAL
26	3-S	319	CYS
26	3-S	324	MET
26	3-S	348	LEU
26	3-S	370	LEU
26	3-S	408	CYS
26	3-S	475	TYR
27	3-T	25	LYS
27	3-T	31	LYS
27	3-T	82	PHE
27	3-T	85	LEU
27	3-T	96	LEU
27	3-T	116	GLN
27	3-T	127	GLN
27	3-T	130	ASP
27	3-T	134	LYS
27	3-T	141	LEU
27	3-T	173	GLU
27	3-T	185	ILE
27	3-T	188	GLU
27	3-T	191	LYS
27	3-T	214	GLU
27	3-T	249	MET

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Mol	Chain	Res	Type
27	3-T	256	LYS
28	3-U	33	CYS
28	3-U	70	HIS
28	3-U	78	GLU
28	3-U	262	GLN
29	3-V	27	VAL
29	3-V	39	LYS
29	3-V	91	MET
29	3-V	94	MET
29	3-V	109	HIS
29	3-V	114	PHE
29	3-V	127	LYS
29	3-V	185	ILE
29	3-V	188	LEU
29	3-V	199	LEU
29	3-V	219	GLU
29	3-V	228	TYR
29	3-V	265	GLU
30	3-W	3	LEU
30	3-W	17	ARG
30	3-W	20	ASP
30	3-W	104	LYS
30	3-W	127	ARG
30	3-W	139	VAL
30	3-W	149	GLN
30	3-W	154	LEU
30	3-W	157	PHE
31	3-X	19	GLU
31	3-X	85	ARG
31	3-X	104	LYS
32	3-Y	66	ASP
33	3-Z	15	GLN
33	3-Z	23	GLN
33	3-Z	31	LYS
33	3-Z	58	GLU
33	3-Z	76	LYS
33	3-Z	124	MET
33	3-Z	138	ARG
33	3-Z	183	LYS
33	3-Z	185	ASP
33	3-Z	213	LYS
33	3-Z	218	GLU

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Mol	Chain	Res	Type
33	3-Z	222	ASP
33	3-Z	293	MET
33	3-Z	379	GLN
33	3-Z	386	VAL
33	3-Z	411	LYS
33	3-Z	415	MET
33	3-Z	434	GLN
33	3-Z	446	GLU
33	3-Z	464	ASP
33	3-Z	466	GLU
33	3-Z	468	GLU
33	3-Z	512	ILE
33	3-Z	521	GLU
33	3-Z	548	ASP
33	3-Z	559	LYS
33	3-Z	563	VAL
33	3-Z	566	LEU
33	3-Z	609	THR
33	3-Z	759	ARG
33	3-Z	775	MET
33	3-Z	815	MET
33	3-Z	842	GLN
33	3-Z	850	LEU
33	3-Z	862	MET
33	3-Z	864	MET
33	3-Z	874	ASN
33	3-Z	878	LEU
33	3-Z	886	VAL
33	3-Z	931	GLN
33	3-Z	941	ARG
33	3-Z	948	TRP
33	3-Z	955	VAL
8	3-a	41	CYS
8	3-a	69	THR
8	3-a	82	ARG
8	3-a	94	GLU
8	3-a	101	TYR
8	3-a	122	ARG
8	3-a	124	TYR
8	3-a	166	GLN
8	3-a	200	HIS
8	3-a	211	LYS

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Mol	Chain	Res	Type
8	3-a	223	LYS
8	3-a	225	PHE
9	3-b	1	MET
9	3-b	20	GLN
9	3-b	32	VAL
9	3-b	37	ILE
9	3-b	61	LEU
9	3-b	63	LYS
9	3-b	92	VAL
9	3-b	108	LYS
9	3-b	119	GLN
9	3-b	127	VAL
9	3-b	133	SER
9	3-b	172	LYS
9	3-b	197	LYS
9	3-b	216	ASP
9	3-b	231	LYS
9	3-b	250	LEU
10	3-c	4	ARG
10	3-c	18	LEU
10	3-c	95	GLN
10	3-c	121	TYR
10	3-c	209	ARG
10	3-c	223	GLU
10	3-c	235	LYS
11	3-d	37	LYS
11	3-d	77	ASN
11	3-d	169	VAL
11	3-d	175	LYS
11	3-d	180	LYS
11	3-d	181	GLU
11	3-d	187	GLU
11	3-d	192	LEU
11	3-d	223	SER
11	3-d	235	GLU
12	3-e	17	GLU
12	3-e	20	LEU
12	3-e	35	LYS
12	3-e	43	GLU
12	3-e	45	ARG
12	3-e	52	GLU
12	3-e	82	GLU

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Mol	Chain	Res	Type
12	3-e	99	ILE
12	3-e	102	GLU
12	3-e	126	MET
12	3-e	182	SER
13	3-f	9	THR
13	3-f	11	THR
13	3-f	38	ARG
13	3-f	71	LEU
13	3-f	99	ASN
13	3-f	118	ASN
13	3-f	188	LEU
13	3-f	206	THR
14	3-g	48	LYS
14	3-g	51	THR
14	3-g	140	ASN
14	3-g	146	MET
14	3-g	150	SER
14	3-g	172	LEU
14	3-g	215	CYS
1	3-h	9	LYS
1	3-h	14	LEU
1	3-h	43	CYS
1	3-h	44	CYS
1	3-h	62	HIS
1	3-h	76	GLU
1	3-h	84	GLU
1	3-h	90	LYS
1	3-h	103	ASP
1	3-h	161	GLN
2	3-i	17	ASP
2	3-i	22	GLN
2	3-i	41	ILE
2	3-i	85	GLN
2	3-i	127	LEU
2	3-i	143	LYS
2	3-i	144	GLN
2	3-i	176	CYS
2	3-i	215	GLU
2	3-i	221	CYS
3	3-j	17	LYS
3	3-j	27	ARG
3	3-j	43	PHE

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Mol	Chain	Res	Type
3	3-j	133	LYS
3	3-j	168	GLN
4	3-k	3	ILE
4	3-k	52	ASP
4	3-k	61	GLN
4	3-k	82	SER
4	3-k	92	ILE
4	3-k	126	VAL
4	3-k	174	MET
4	3-k	175	ASP
5	3-l	4	LEU
5	3-l	69	ARG
5	3-l	70	GLU
5	3-l	84	SER
5	3-l	86	LEU
5	3-l	108	GLU
5	3-l	145	LYS
5	3-l	149	SER
5	3-l	159	ARG
5	3-l	170	TYR
5	3-l	211	ILE
6	3-m	22	VAL
6	3-m	42	LYS
6	3-m	66	LYS
6	3-m	80	ASN
6	3-m	115	ASP
6	3-m	150	LEU
6	3-m	167	LYS
6	3-m	179	GLU
6	3-m	209	LYS
6	3-m	210	ASP
6	3-m	221	ARG
7	3-n	3	GLN
7	3-n	26	ASN
7	3-n	70	LEU
7	3-n	104	ARG
7	3-n	105	SER
7	3-n	120	GLN
7	3-n	124	ASP
7	3-n	161	ARG
7	3-n	167	LYS
7	3-n	175	GLU

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Mol	Chain	Res	Type
7	3-n	187	ARG
7	3-n	216	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (199) such sidechains are listed below:

Mol	Chain	Res	Type
1	3-1	92	ASN
1	3-1	145	ASN
2	3-2	66	HIS
2	3-2	86	HIS
2	3-2	93	HIS
2	3-2	160	GLN
2	3-2	172	ASN
3	3-3	203	GLN
4	3-4	112	ASN
5	3-5	176	ASN
5	3-5	190	ASN
6	3-6	79	HIS
7	3-7	18	ASN
7	3-7	108	ASN
7	3-7	120	GLN
8	3-A	30	ASN
9	3-B	205	ASN
10	3-C	102	ASN
10	3-C	146	GLN
10	3-C	167	ASN
11	3-D	94	HIS
11	3-D	116	GLN
11	3-D	228	ASN
12	3-E	83	HIS
13	3-F	51	ASN
13	3-F	99	ASN
13	3-F	109	HIS
13	3-F	116	GLN
13	3-F	118	ASN
13	3-F	147	GLN
13	3-F	151	ASN
13	3-F	198	GLN
13	3-F	209	ASN
14	3-G	29	ASN
14	3-G	83	HIS
14	3-G	119	HIS

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Mol	Chain	Res	Type
14	3-G	143	HIS
14	3-G	166	GLN
14	3-G	191	GLN
15	3-H	89	GLN
15	3-H	182	ASN
15	3-H	330	GLN
15	3-H	339	GLN
16	3-I	78	ASN
16	3-I	102	ASN
16	3-I	150	HIS
16	3-I	312	GLN
16	3-I	393	GLN
17	3-J	15	HIS
17	3-J	25	GLN
17	3-J	49	ASN
17	3-J	52	ASN
17	3-J	170	HIS
17	3-J	240	HIS
17	3-J	394	GLN
18	3-K	200	GLN
18	3-K	319	ASN
19	3-L	53	HIS
19	3-L	76	GLN
19	3-L	80	ASN
19	3-L	93	ASN
19	3-L	99	GLN
19	3-L	103	GLN
19	3-L	175	GLN
19	3-L	409	HIS
19	3-L	435	GLN
20	3-M	55	ASN
20	3-M	149	ASN
20	3-M	311	GLN
20	3-M	405	ASN
21	3-N	34	GLN
21	3-N	249	ASN
21	3-N	280	GLN
21	3-N	300	ASN
21	3-N	308	ASN
21	3-N	315	ASN
21	3-N	336	ASN
21	3-N	472	ASN

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Mol	Chain	Res	Type
21	3-N	565	ASN
21	3-N	580	ASN
21	3-N	613	HIS
21	3-N	614	ASN
21	3-N	688	ASN
21	3-N	690	HIS
21	3-N	747	HIS
22	3-O	105	GLN
22	3-O	177	GLN
22	3-O	244	ASN
22	3-O	253	GLN
22	3-O	354	GLN
22	3-O	362	GLN
23	3-P	178	GLN
23	3-P	183	GLN
23	3-P	246	GLN
23	3-P	296	GLN
23	3-P	386	GLN
23	3-P	394	ASN
23	3-P	410	GLN
24	3-Q	54	GLN
24	3-Q	147	GLN
24	3-Q	190	ASN
24	3-Q	260	GLN
24	3-Q	273	ASN
24	3-Q	315	ASN
24	3-Q	320	GLN
24	3-Q	405	GLN
25	3-R	35	GLN
25	3-R	130	GLN
25	3-R	136	ASN
25	3-R	143	GLN
25	3-R	195	ASN
25	3-R	340	GLN
26	3-S	32	GLN
26	3-S	65	ASN
26	3-S	112	ASN
26	3-S	135	ASN
26	3-S	139	HIS
26	3-S	154	GLN
26	3-S	166	ASN
26	3-S	177	ASN

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Mol	Chain	Res	Type
26	3-S	235	ASN
26	3-S	243	ASN
26	3-S	290	ASN
26	3-S	312	GLN
26	3-S	347	HIS
26	3-S	437	ASN
26	3-S	450	ASN
26	3-S	488	GLN
27	3-T	93	ASN
27	3-T	132	HIS
28	3-U	50	ASN
28	3-U	75	ASN
28	3-U	127	GLN
28	3-U	216	ASN
28	3-U	251	ASN
28	3-U	260	ASN
28	3-U	297	GLN
29	3-V	73	GLN
29	3-V	97	GLN
29	3-V	111	HIS
29	3-V	193	ASN
29	3-V	220	GLN
30	3-W	12	ASN
30	3-W	44	ASN
30	3-W	58	ASN
30	3-W	100	HIS
30	3-W	106	GLN
30	3-W	108	GLN
31	3-X	123	ASN
31	3-X	130	ASN
33	3-Z	129	ASN
33	3-Z	215	ASN
33	3-Z	275	GLN
33	3-Z	364	ASN
33	3-Z	380	ASN
33	3-Z	763	HIS
33	3-Z	789	GLN
33	3-Z	810	ASN
33	3-Z	868	ASN
33	3-Z	898	HIS
33	3-Z	926	ASN
33	3-Z	959	HIS

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Mol	Chain	Res	Type
8	3-a	30	ASN
8	3-a	175	ASN
9	3-b	123	GLN
10	3-c	58	GLN
11	3-d	202	GLN
12	3-e	106	GLN
12	3-e	207	ASN
13	3-f	4	ASN
13	3-f	116	GLN
13	3-f	120	GLN
13	3-f	209	ASN
14	3-g	58	GLN
14	3-g	123	ASN
14	3-g	203	ASN
1	3-h	62	HIS
1	3-h	92	ASN
1	3-h	106	ASN
1	3-h	120	HIS
1	3-h	145	ASN
2	3-i	10	ASN
2	3-i	22	GLN
2	3-i	91	GLN
2	3-i	116	HIS
2	3-i	144	GLN
2	3-i	165	ASN
2	3-i	172	ASN
3	3-j	63	ASN
3	3-j	112	ASN
4	3-k	37	GLN
4	3-k	78	GLN
5	3-l	176	ASN
6	3-m	95	HIS
7	3-n	37	ASN
7	3-n	61	GLN
7	3-n	120	GLN
7	3-n	122	ASN
7	3-n	213	GLN

5.3.3 RNA ⓘ

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.

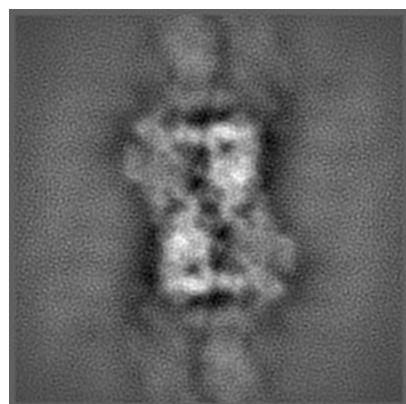
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60960. These allow visual inspection of the internal detail of the map and identification of artifacts.

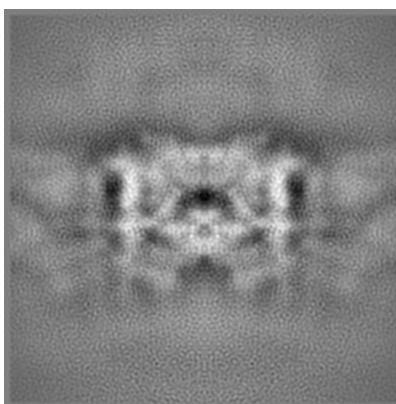
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

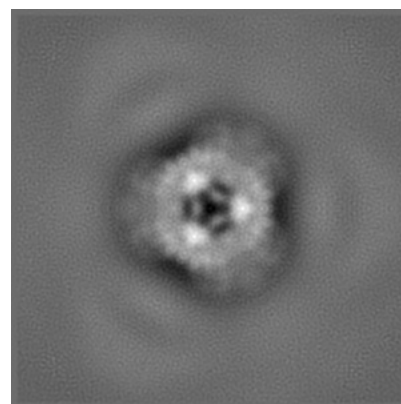
6.1.1 Primary map



X

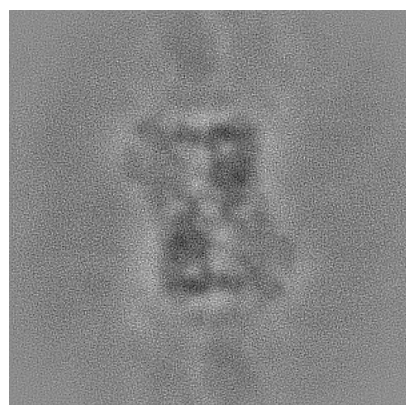


Y

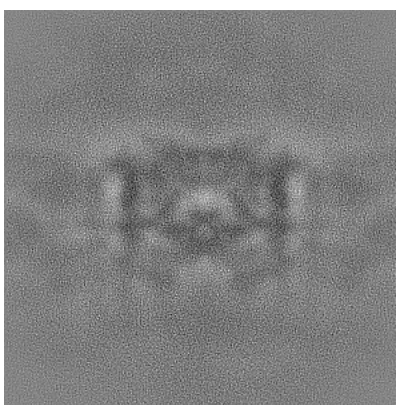


Z

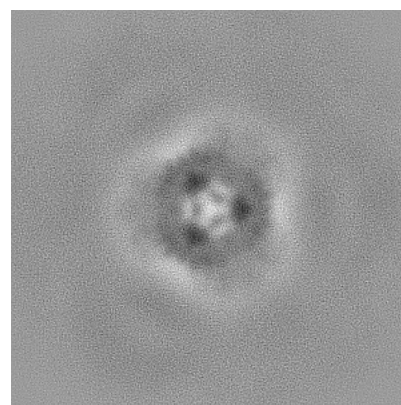
6.1.2 Raw map



X



Y

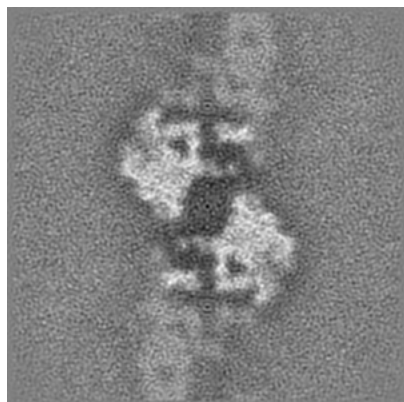


Z

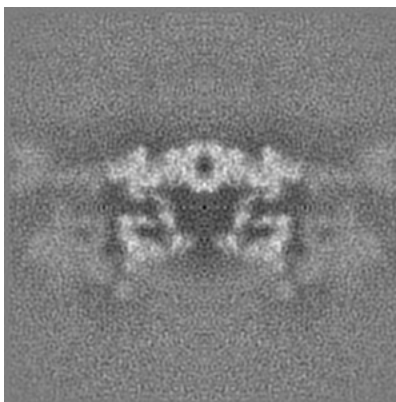
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

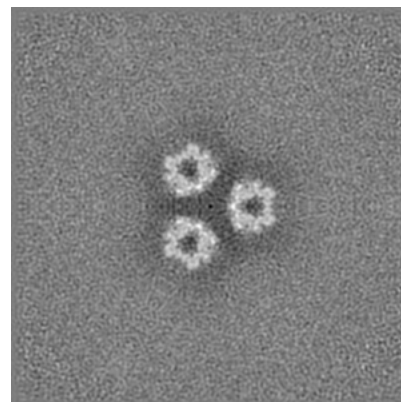
6.2.1 Primary map



X Index: 192

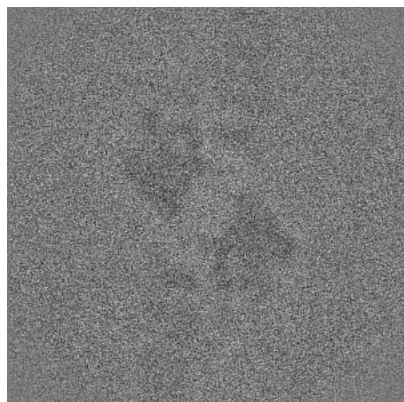


Y Index: 192

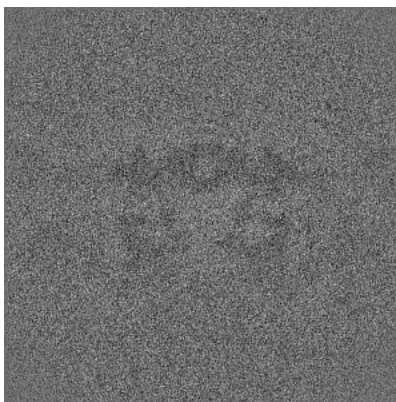


Z Index: 192

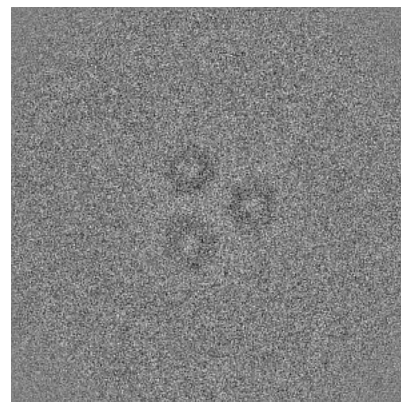
6.2.2 Raw map



X Index: 192



Y Index: 192

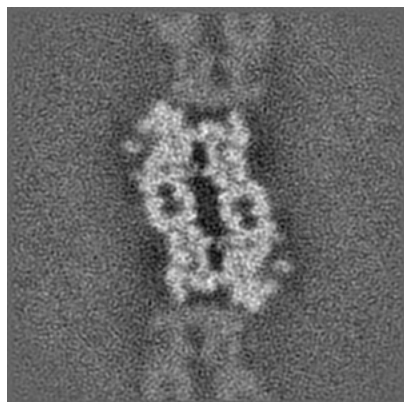


Z Index: 192

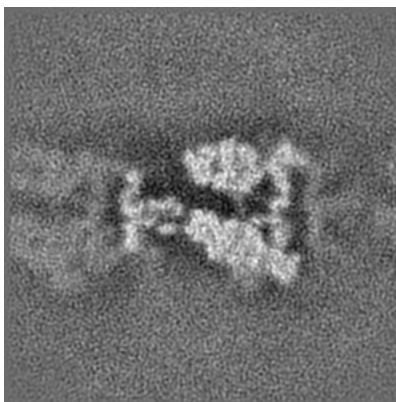
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

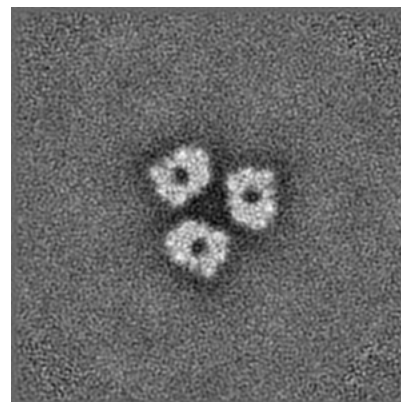
6.3.1 Primary map



X Index: 176

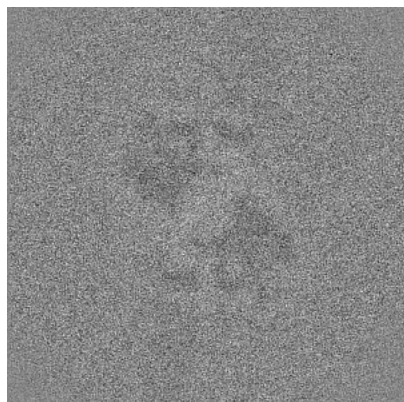


Y Index: 209

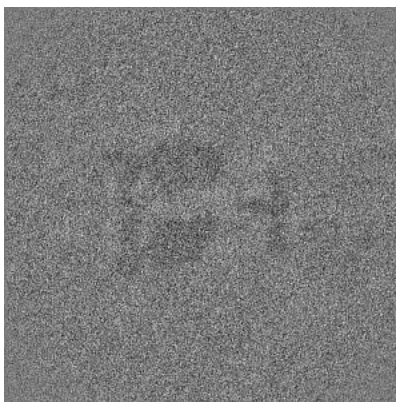


Z Index: 205

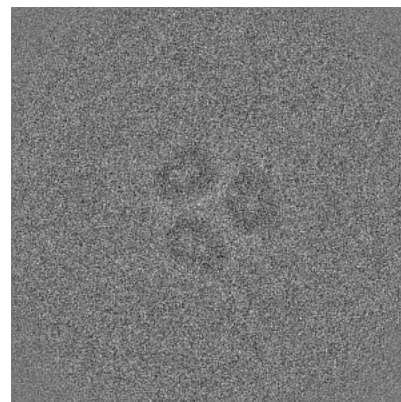
6.3.2 Raw map



X Index: 194



Y Index: 178

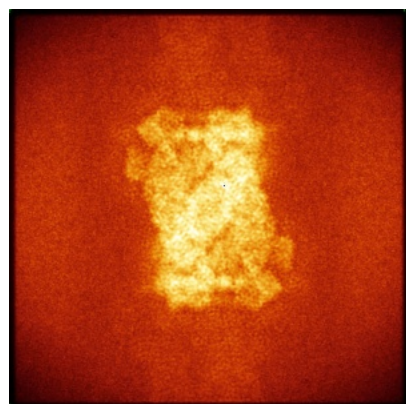


Z Index: 199

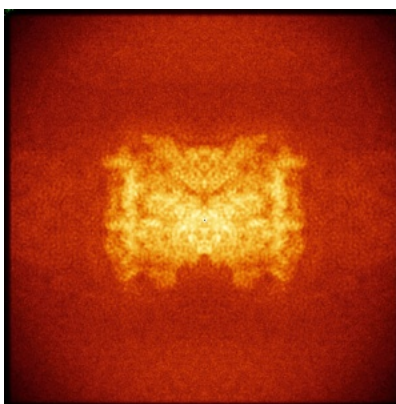
The images above show the largest variance slices of the map in three orthogonal directions.

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

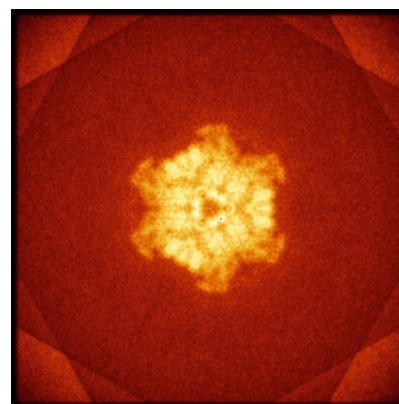
6.4.1 Primary map



X

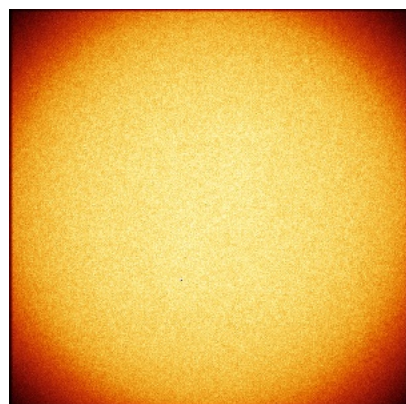


Y

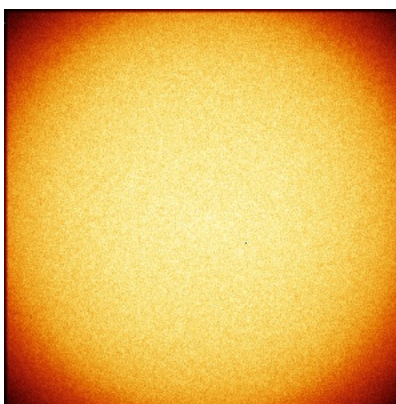


Z

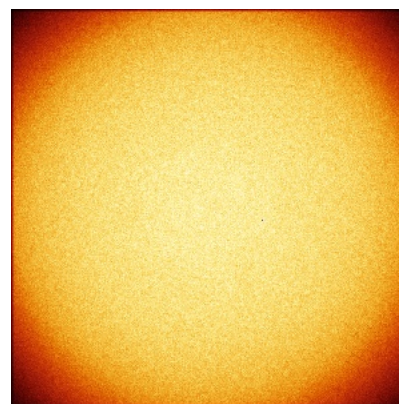
6.4.2 Raw map



X



Y

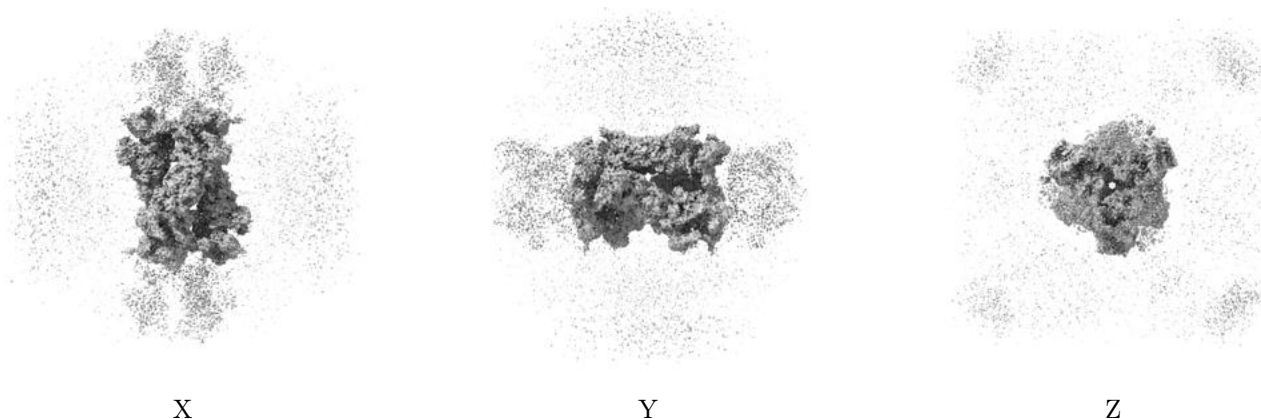


Z

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

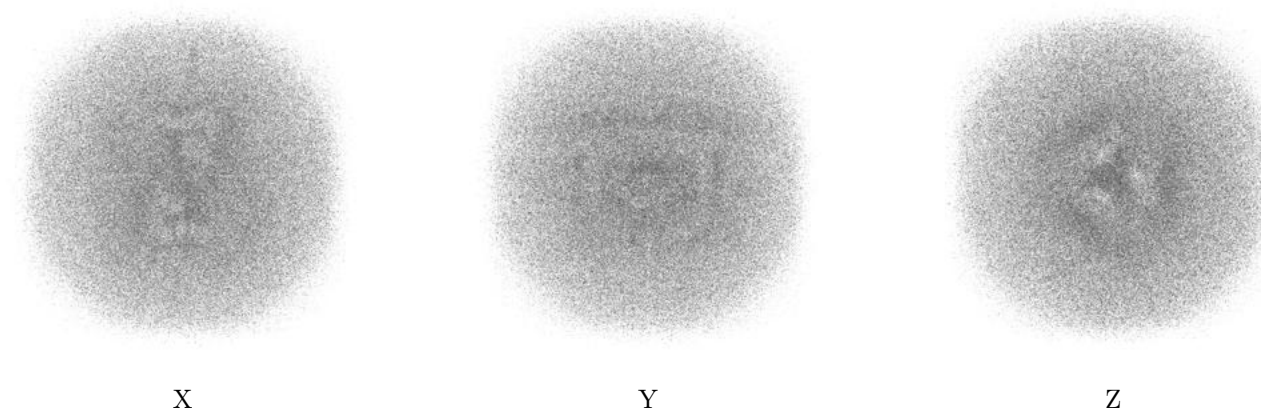
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.27. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

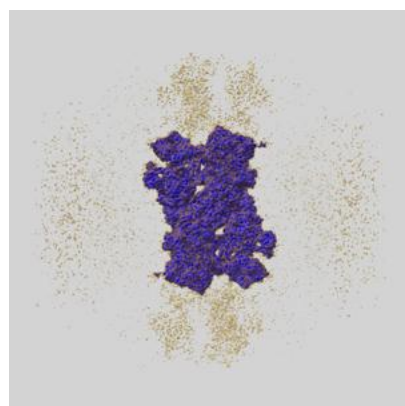
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

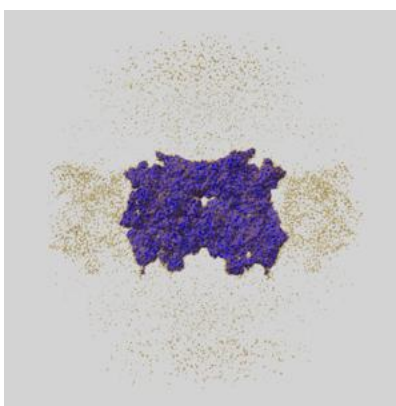
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

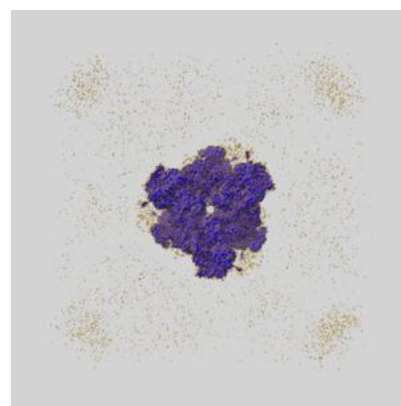
6.6.1 emd_60960_msk_1.map [i](#)



X



Y

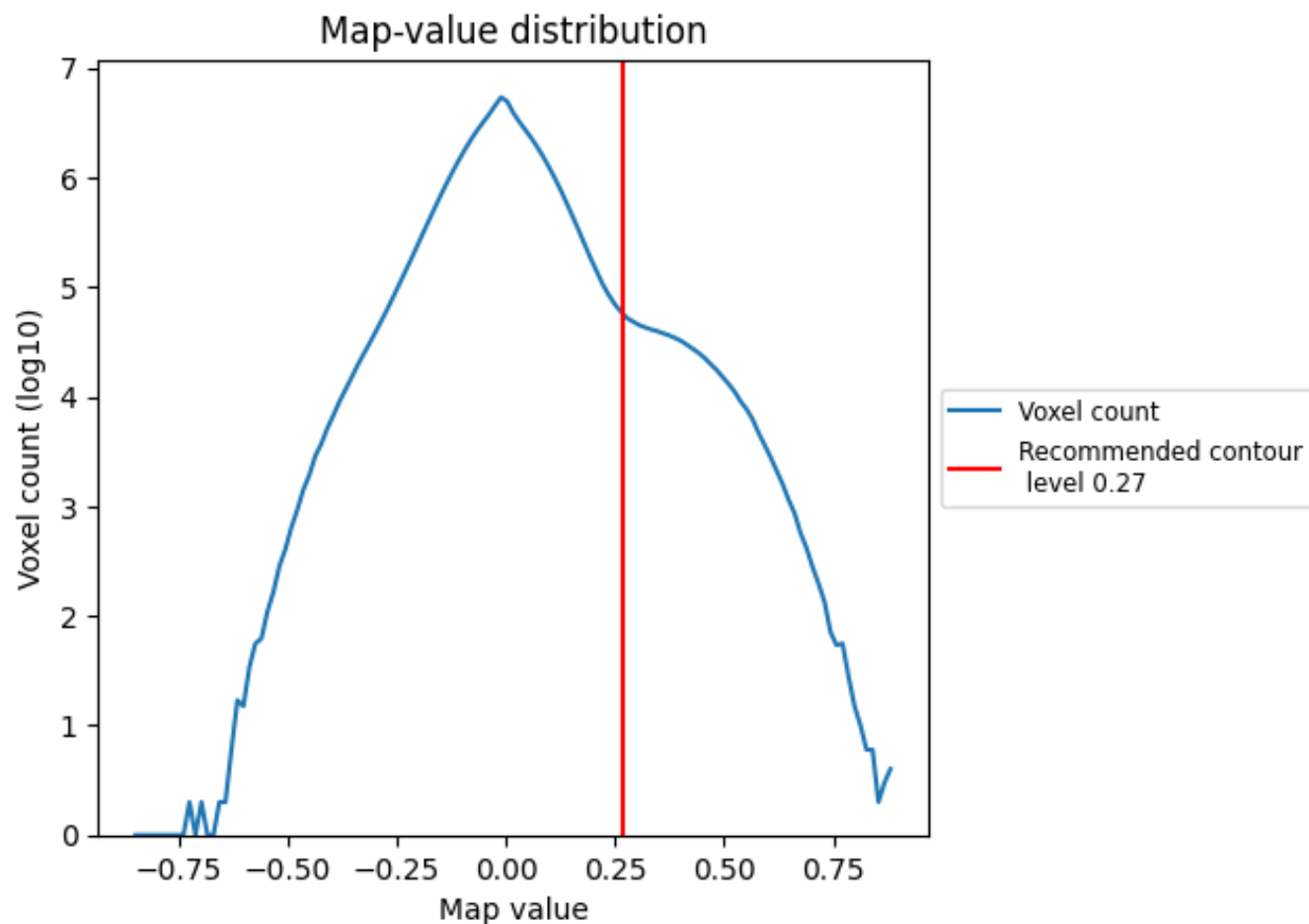


Z

7 Map analysis [i](#)

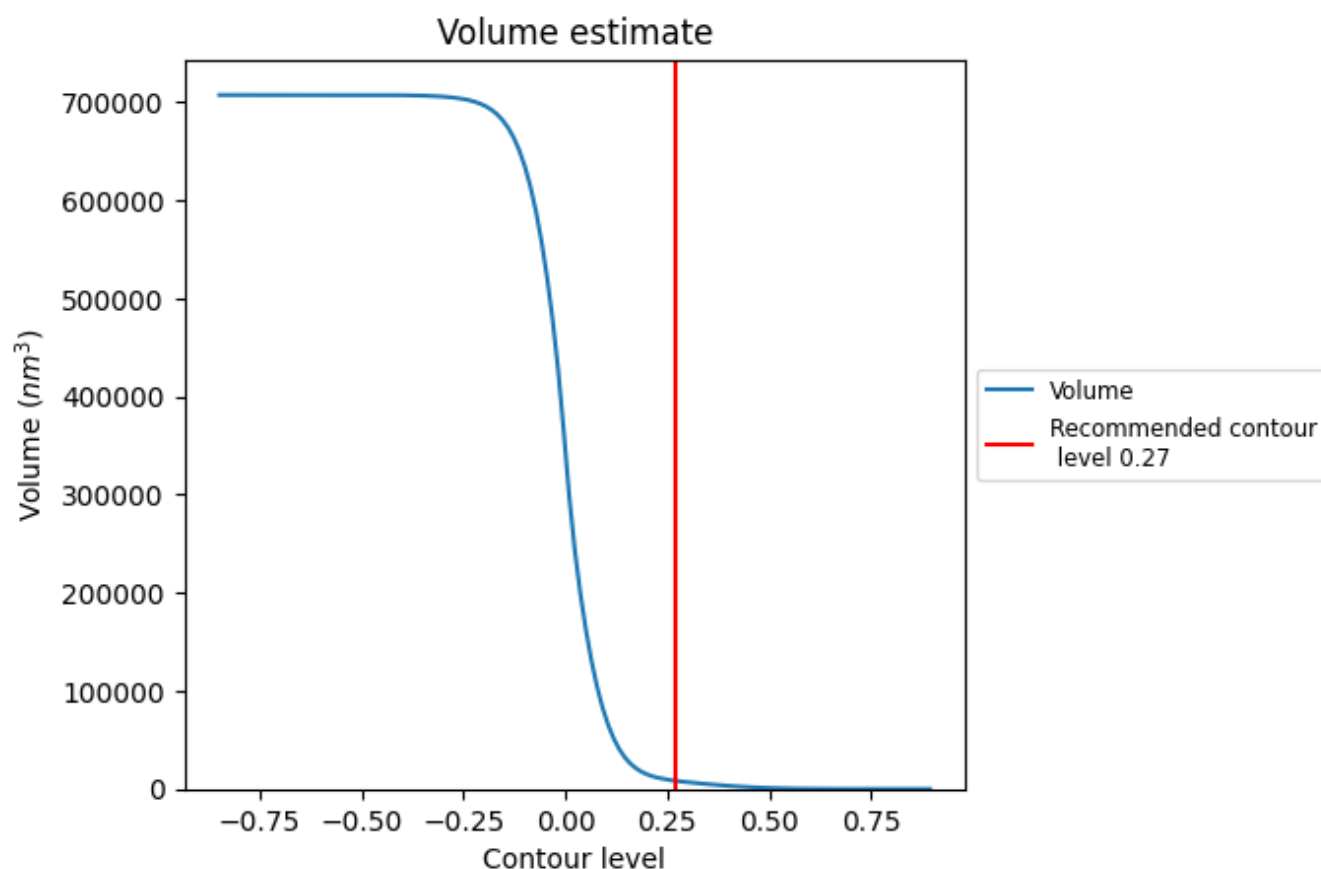
This section contains the results of statistical analysis of the map.

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.

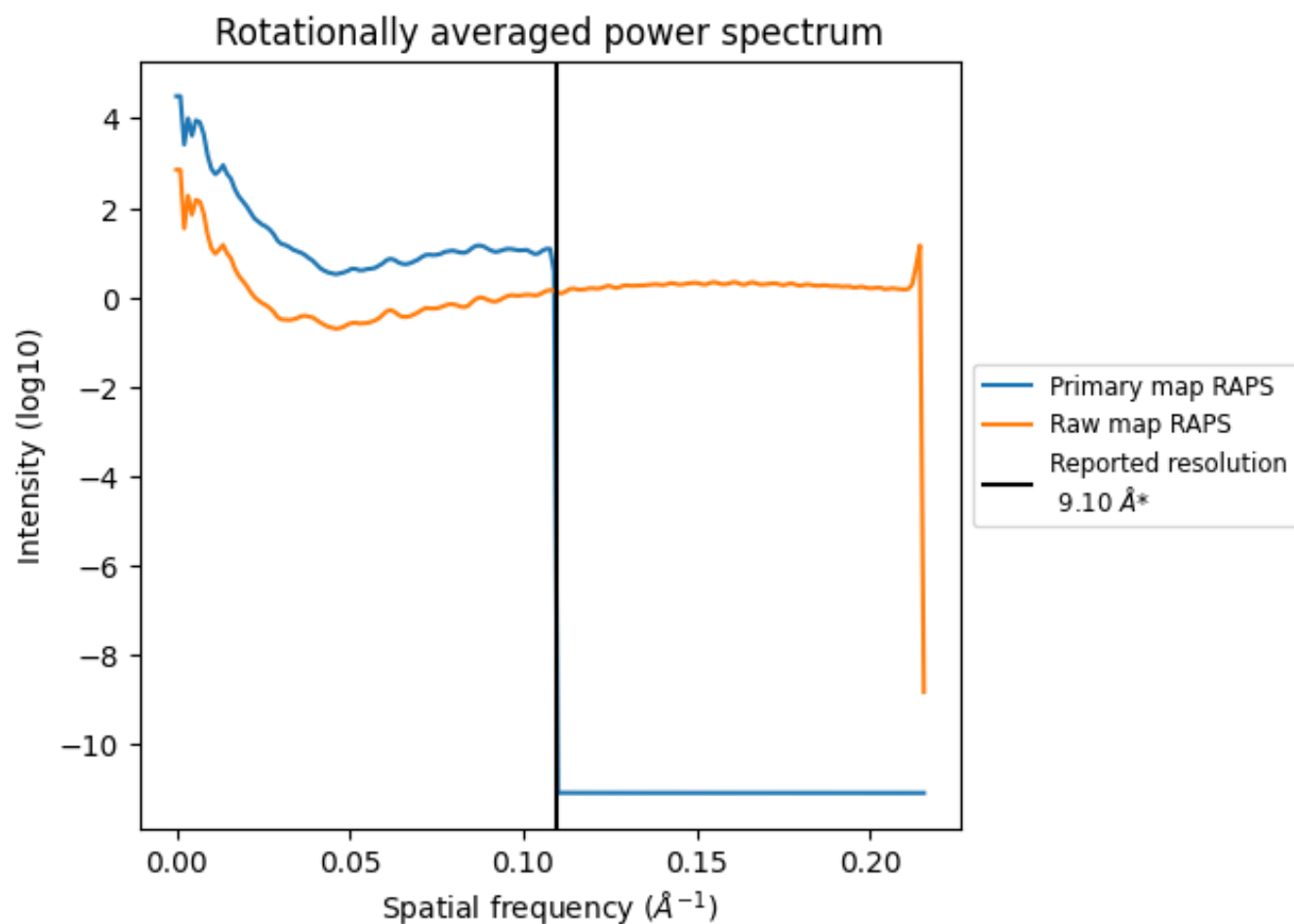
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 8289 nm^3 ; this corresponds to an approximate mass of 7488 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 ⓘ

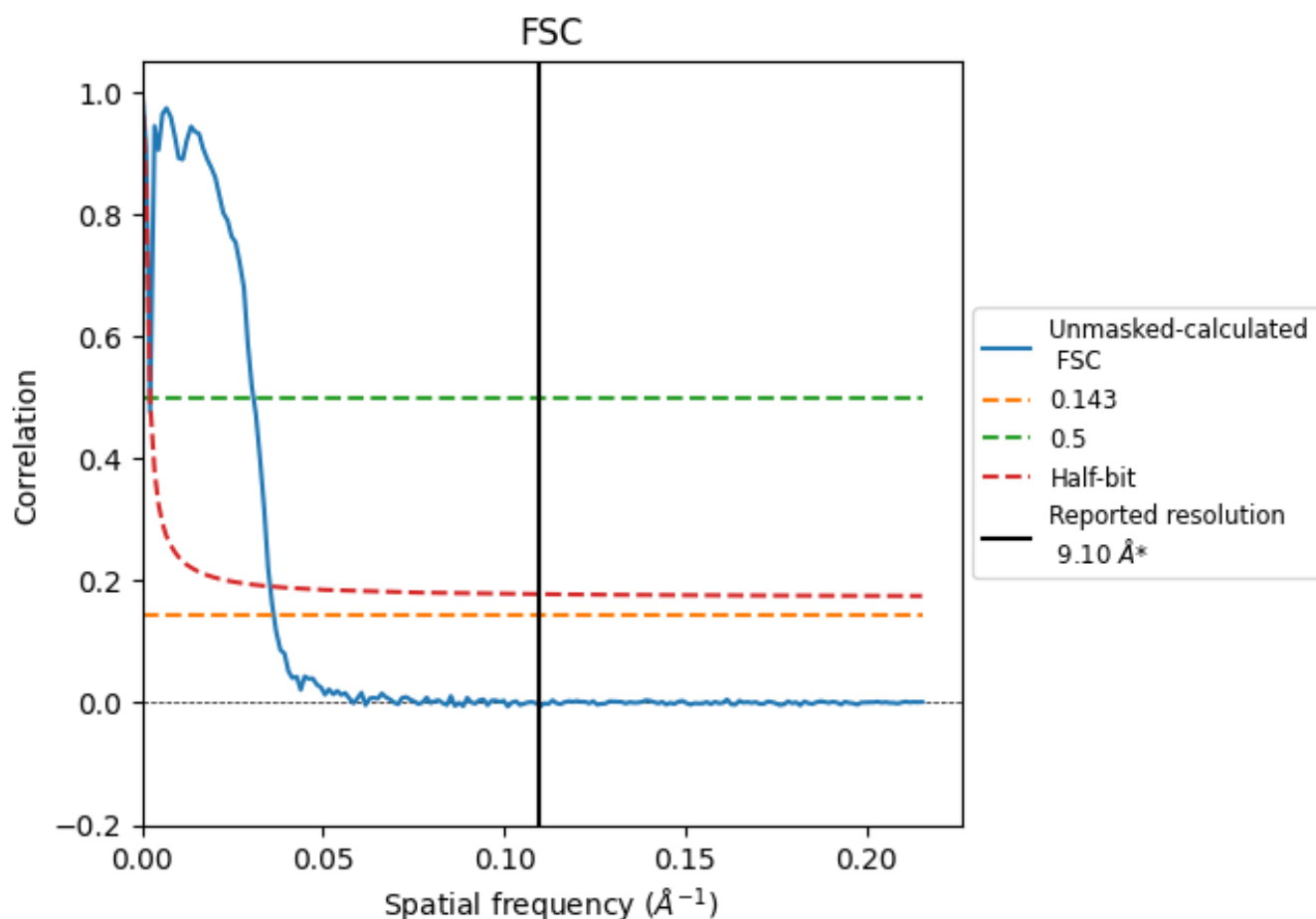


*Reported resolution corresponds to spatial frequency of 0.110 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.110 $\text{\AA}^{-1}$

8.2 Resolution estimates

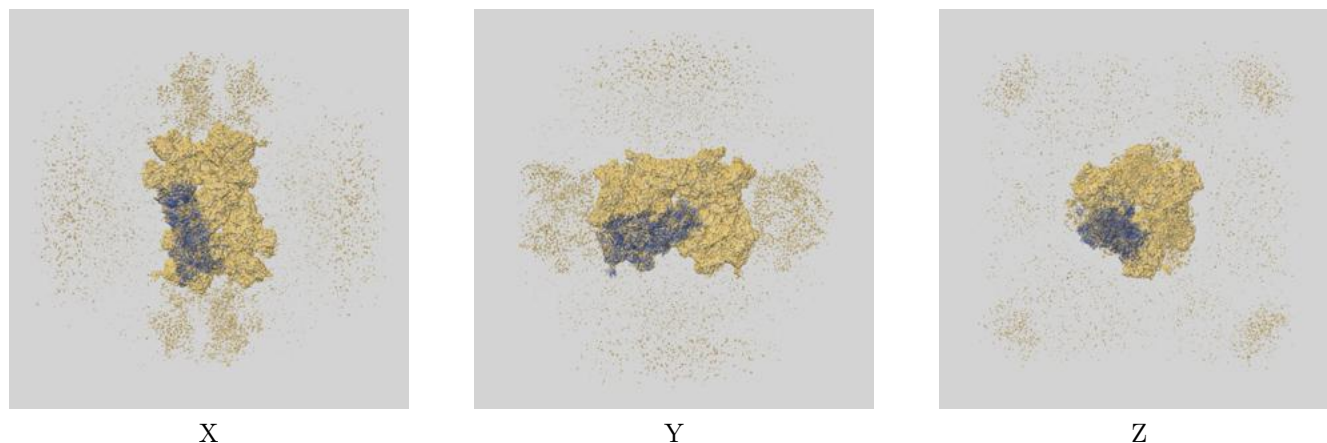
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	27.47	454.55	500.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 27.47 differs from the reported value 9.1 by more than 10 %

9 Map-model fit [i](#)

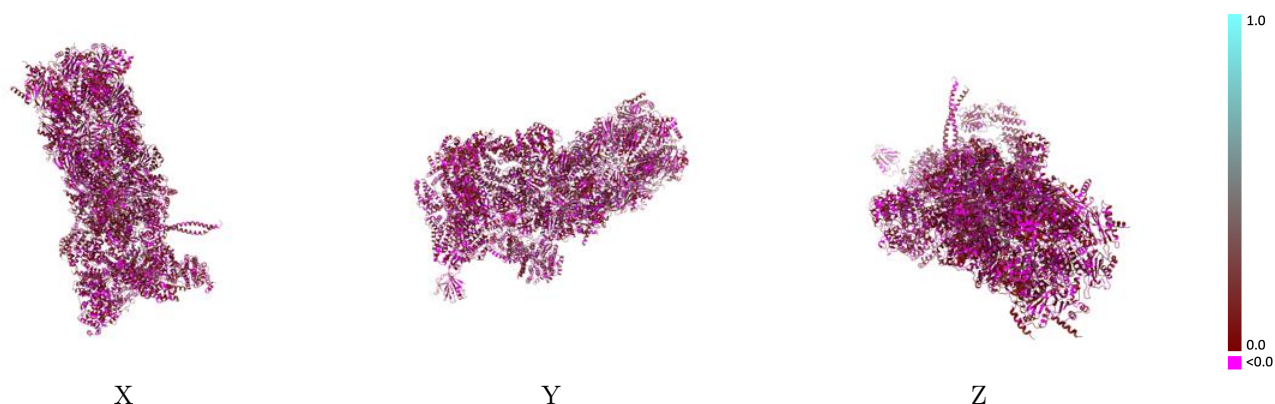
This section contains information regarding the fit between EMDB map EMD-60960 and PDB model 9IWR. Per-residue inclusion information can be found in section 3 on page 19.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.27 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](#)

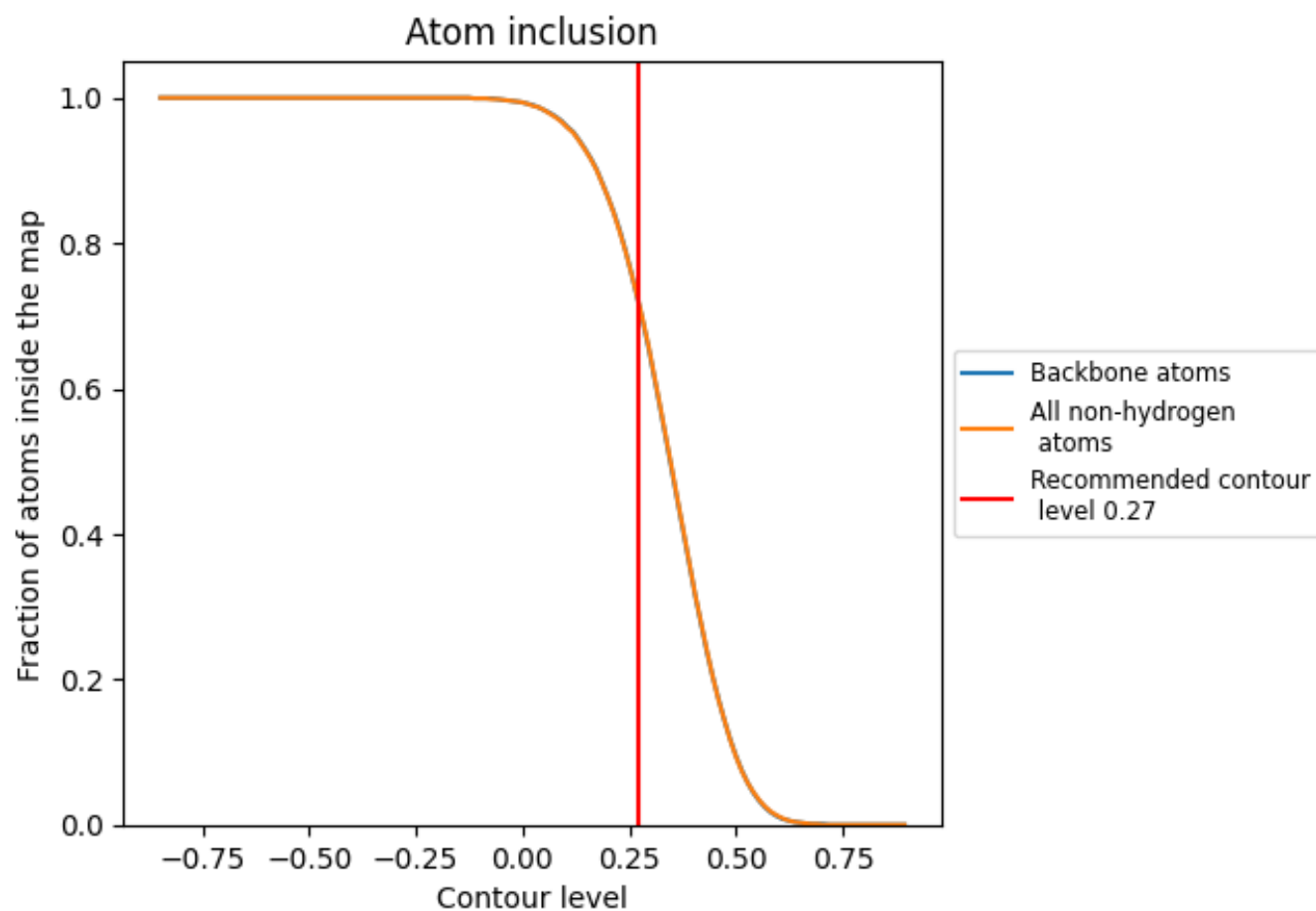


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 72% 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 (0.27) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7230	 0.0580
1	 0.8610	 0.0680
2	 0.8010	 0.0650
3	 0.8250	 0.0630
4	 0.7490	 0.0650
5	 0.8380	 0.0770
6	 0.7980	 0.0650
7	 0.8440	 0.0620
A	 0.7610	 0.0410
B	 0.7770	 0.0590
C	 0.7800	 0.0600
D	 0.7560	 0.0630
E	 0.7430	 0.0430
F	 0.7910	 0.0610
G	 0.8410	 0.0770
H	 0.7070	 0.0540
I	 0.6900	 0.0640
J	 0.6660	 0.0690
K	 0.7390	 0.0690
L	 0.6910	 0.0520
M	 0.6990	 0.0630
N	 0.6680	 0.0490
O	 0.6970	 0.0740
P	 0.6330	 0.0660
Q	 0.7220	 0.0770
R	 0.7430	 0.0680
S	 0.6860	 0.0390
T	 0.6100	 0.0430
U	 0.6920	 0.0570
V	 0.7200	 0.0430
W	 0.7280	 0.0570
X	 0.1580	 0.0210
Y	 0.4880	 0.0490
Z	 0.5700	 0.0430
a	 0.7650	 0.0460



Continued on next page...

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Chain	Atom inclusion	Q-score
b	 0.8070	 0.0570
c	 0.7890	 0.0560
d	 0.7420	 0.0660
e	 0.7150	 0.0470
f	 0.7750	 0.0540
g	 0.7960	 0.0580
h	 0.8740	 0.0720
i	 0.8330	 0.0630
j	 0.8630	 0.0600
k	 0.7740	 0.0500
l	 0.8280	 0.0600
m	 0.8290	 0.0600
n	 0.8450	 0.0520