Full wwPDB EM Validation Report

Dec 17, 2022 – 02:21 pm GMT

PDB ID	:	7A7D
EMDB ID	:	EMD-11678
Title	:	Cadherin fit into cryo-ET map
Authors	:	Sikora, M.; Ermel, U.H.; Seybold, A.; Kunz, M.; Calloni, G.; Reitz, J.; Vabulas, R.M.; Hummer, G.; Frangakis, A.S.
Deposited on	:	2020-08-28
Resolution	:	26.00 Å(reported)

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

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

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

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

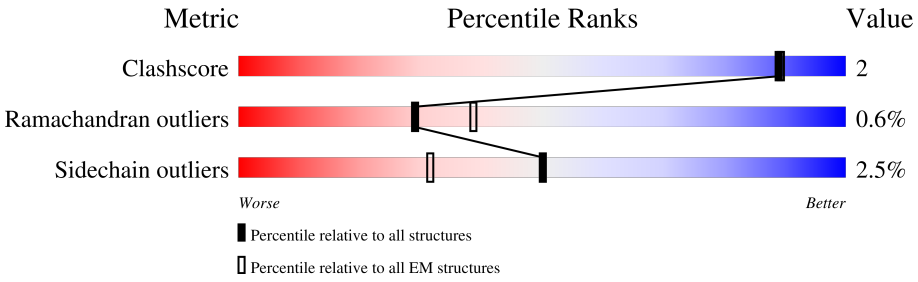
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 26.00 Å.

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



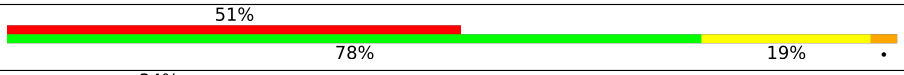
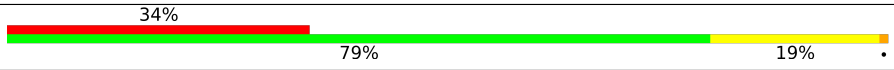
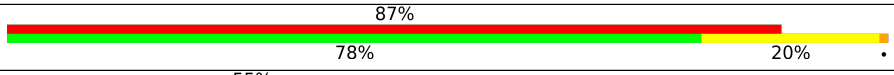
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	554	42% 77% 21% •
1	B	554	70% 81% 17% •
1	C	554	77% 79% 19% •
1	D	554	66% 78% 21% •
1	E	554	60% 77% 18% • •
1	F	554	68% 79% 18% •
1	G	554	64% 78% 20% •
2	a	544	61% 77% 21% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	b	544	
2	c	544	
2	d	544	
2	e	544	
2	f	544	
2	g	544	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 119497 atoms, of which 59136 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 Desmoglein-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	554	Total	C	H	N	O	S	0	0
			8649	2749	4294	725	870	11		
1	B	554	Total	C	H	N	O	S	0	0
			8649	2749	4294	725	870	11		
1	C	554	Total	C	H	N	O	S	0	0
			8649	2749	4294	725	870	11		
1	D	554	Total	C	H	N	O	S	0	0
			8649	2749	4294	725	870	11		
1	E	554	Total	C	H	N	O	S	0	0
			8649	2749	4294	725	870	11		
1	F	554	Total	C	H	N	O	S	0	0
			8649	2749	4294	725	870	11		
1	G	554	Total	C	H	N	O	S	0	0
			8649	2749	4294	725	870	11		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	554	HIS	GLN	conflict	UNP Q14126
B	2252	HIS	GLN	conflict	UNP Q14126
C	1120	HIS	GLN	conflict	UNP Q14126
D	1686	HIS	GLN	conflict	UNP Q14126
E	2252	HIS	GLN	conflict	UNP Q14126
F	1686	HIS	GLN	conflict	UNP Q14126
G	1120	HIS	GLN	conflict	UNP Q14126

- Molecule 2 is a protein called Desmocollin-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	a	544	Total	C	H	N	O	S	0	0
			8422	2670	4154	708	868	22		
2	b	544	Total	C	H	N	O	S	0	0
			8422	2670	4154	708	868	22		

Continued on next page...

Continued from previous page...

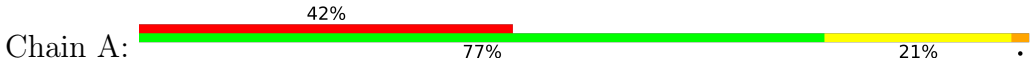
Mol	Chain	Residues	Atoms						AltConf	Trace
2	c	544	Total	C	H	N	O	S	0	0
			8422	2670	4154	708	868	22		
2	d	544	Total	C	H	N	O	S	0	0
			8422	2670	4154	708	868	22		
2	e	544	Total	C	H	N	O	S	0	0
			8422	2670	4154	708	868	22		
2	f	544	Total	C	H	N	O	S	0	0
			8422	2670	4154	708	868	22		
2	g	544	Total	C	H	N	O	S	0	0
			8422	2670	4154	708	868	22		

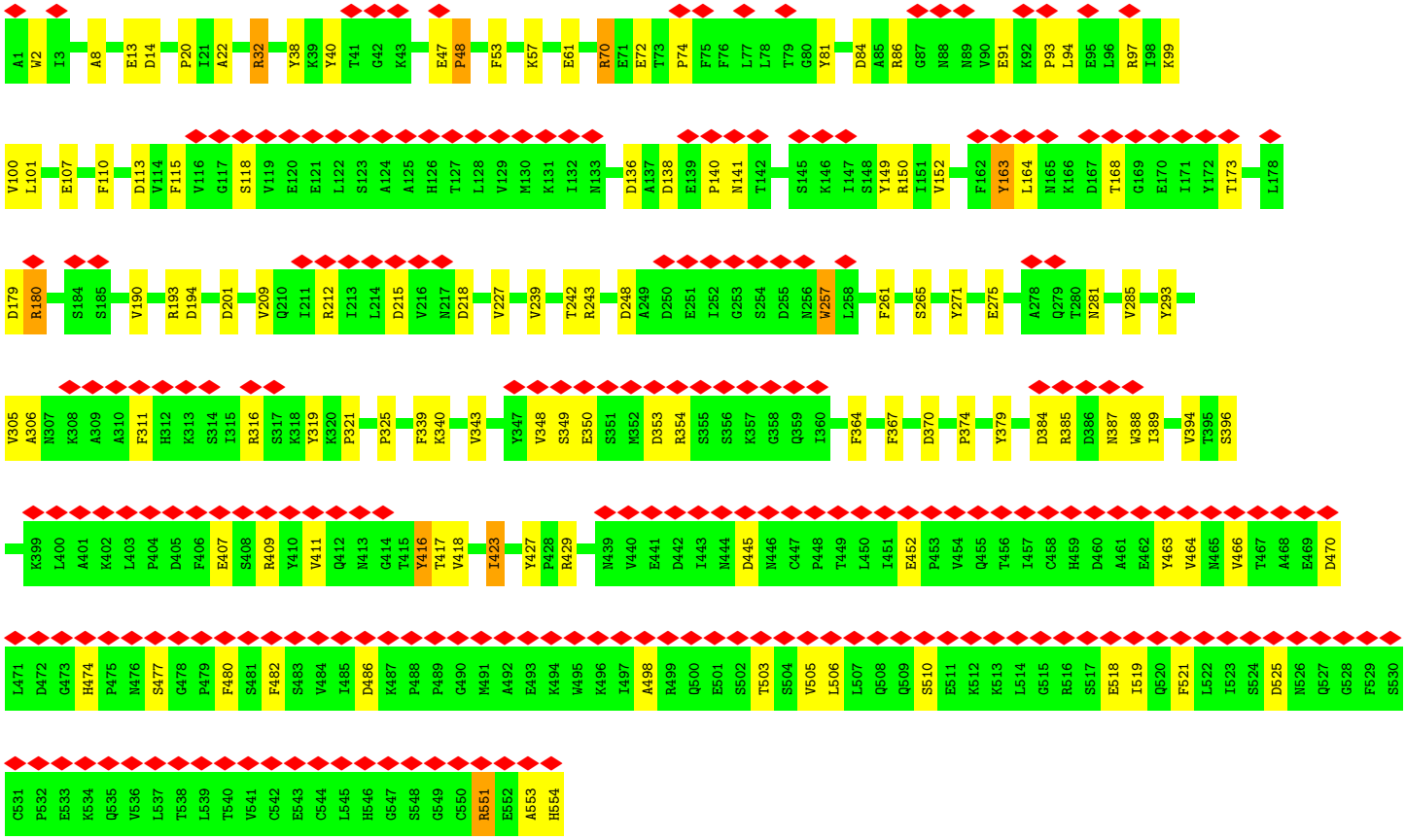
3 Residue-property plots (i)

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: Desmoglein-2

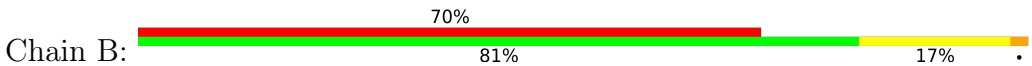
Chain A:

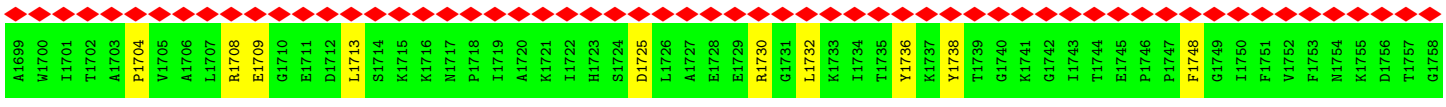


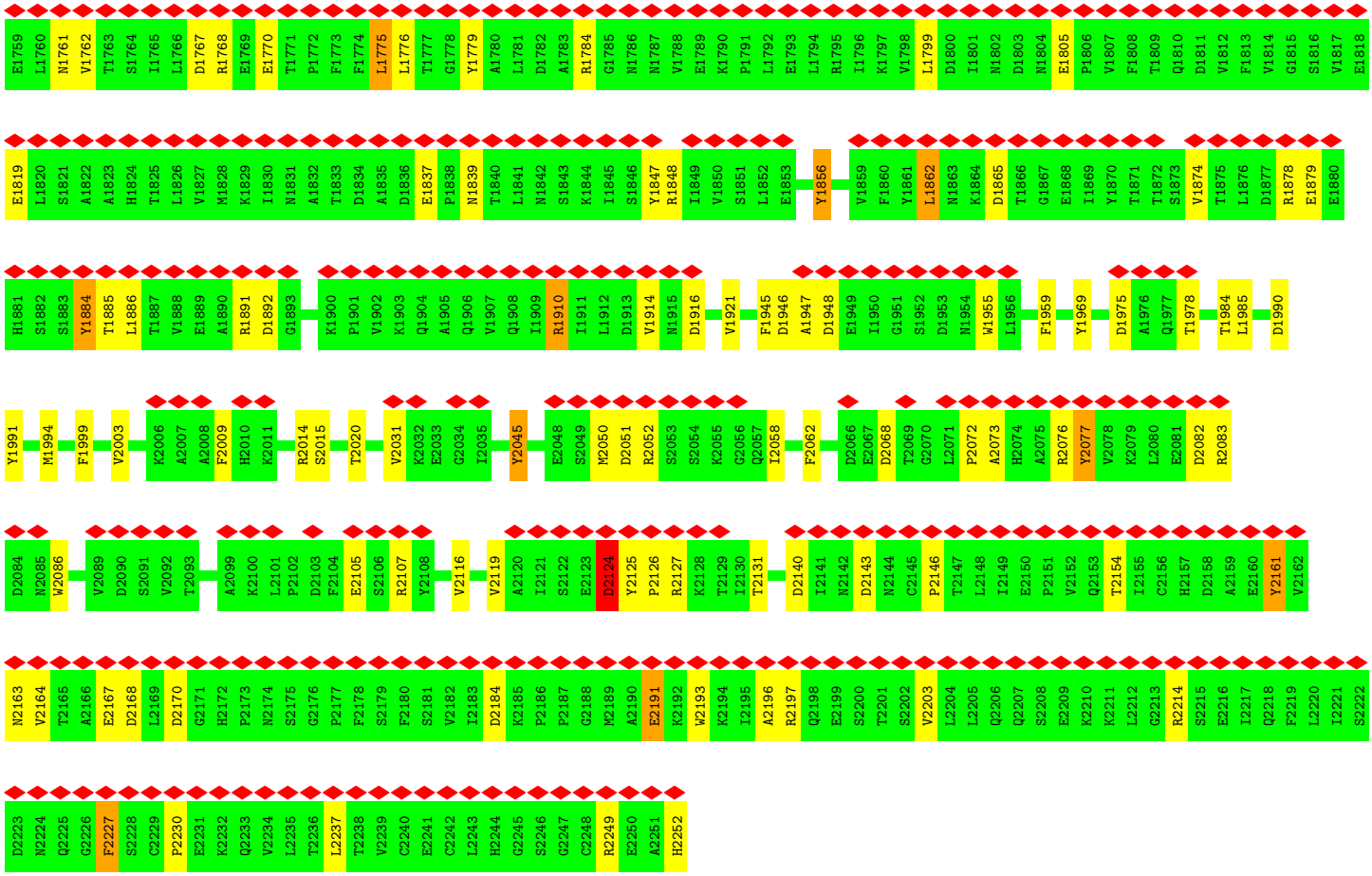


• Molecule 1: Desmoglein-2

Chain B:

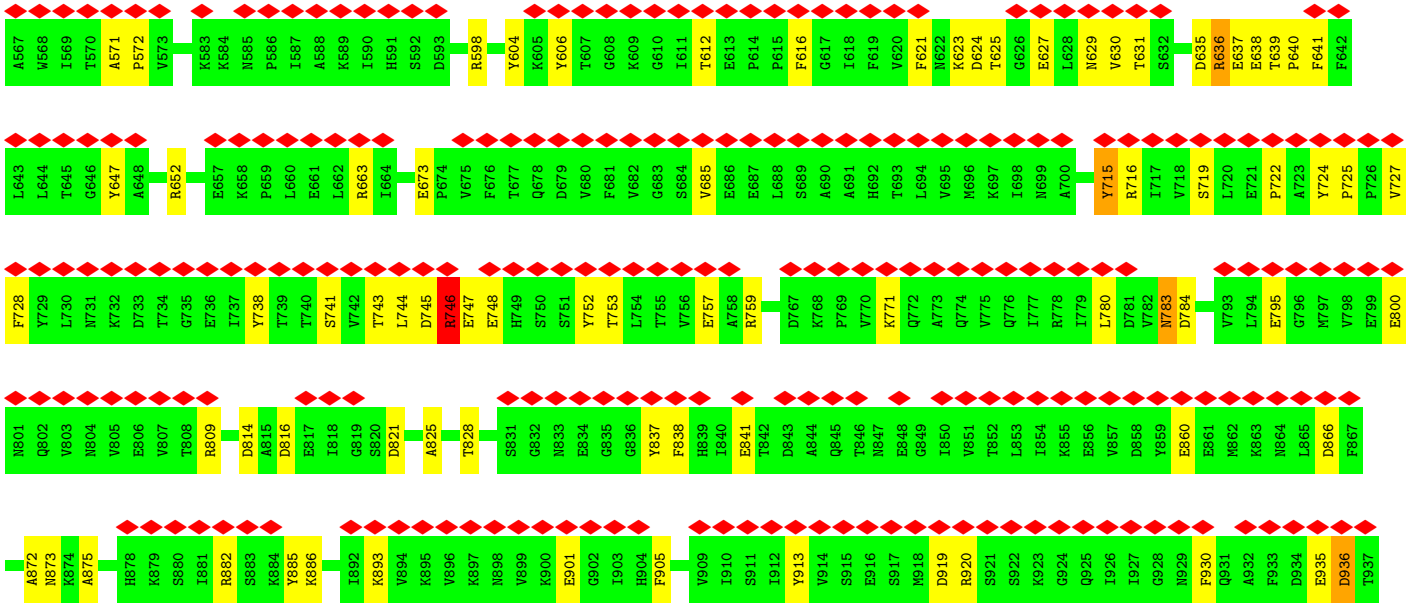


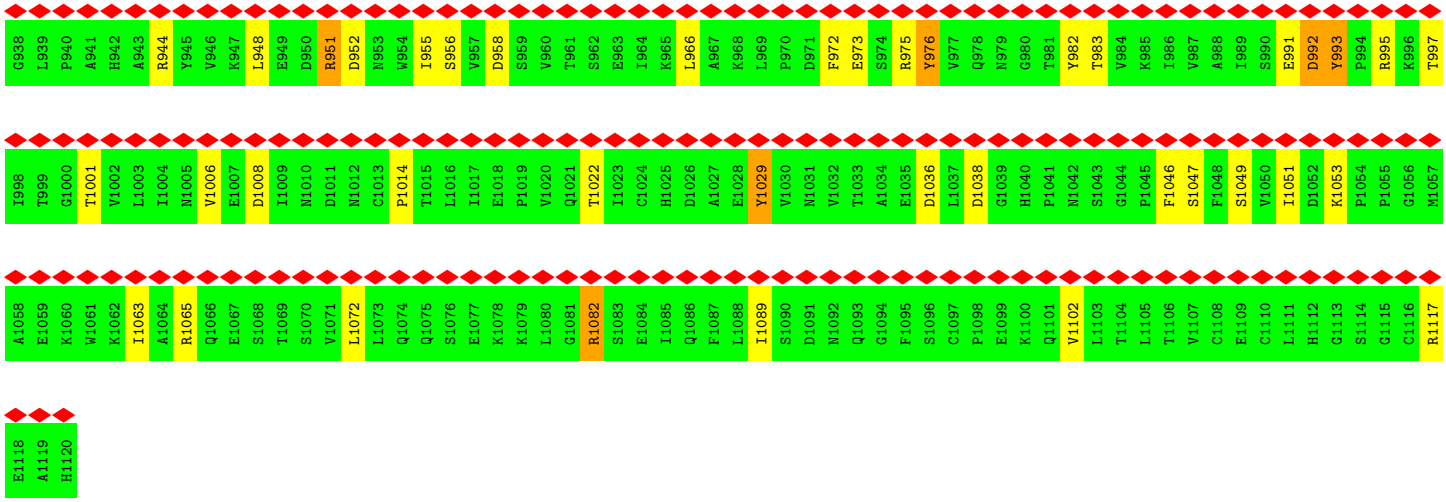




• Molecule 1: Desmoglein-2

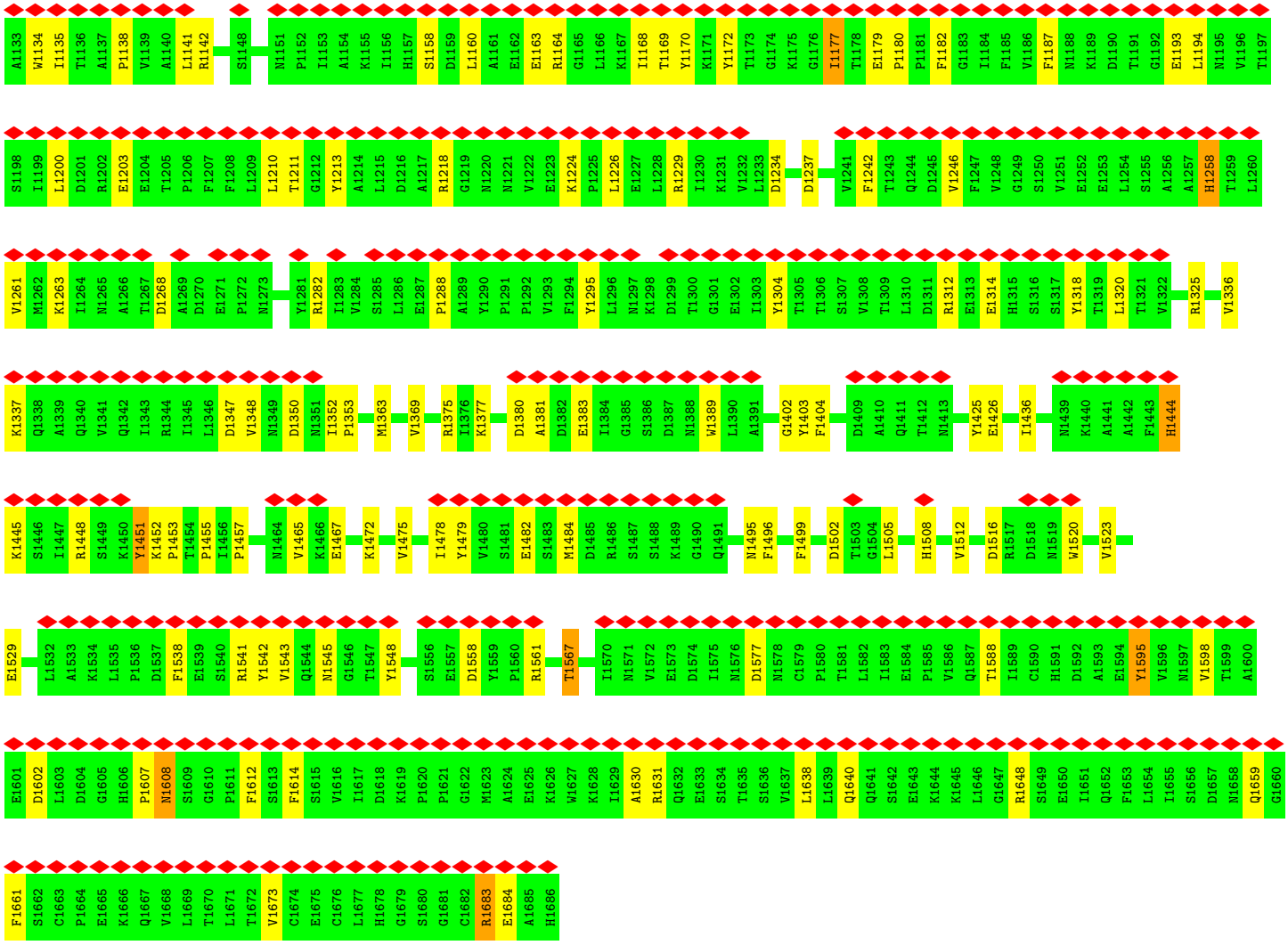
Chain C:





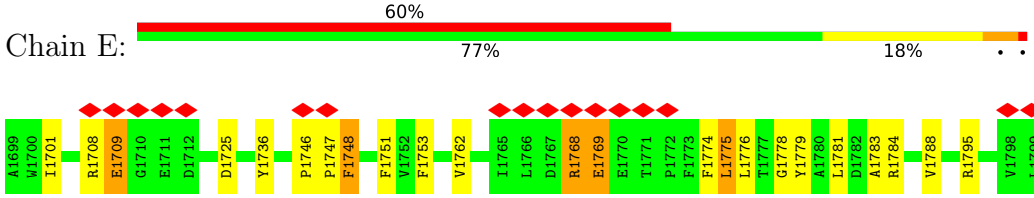
- Molecule 1: Desmoglein-2

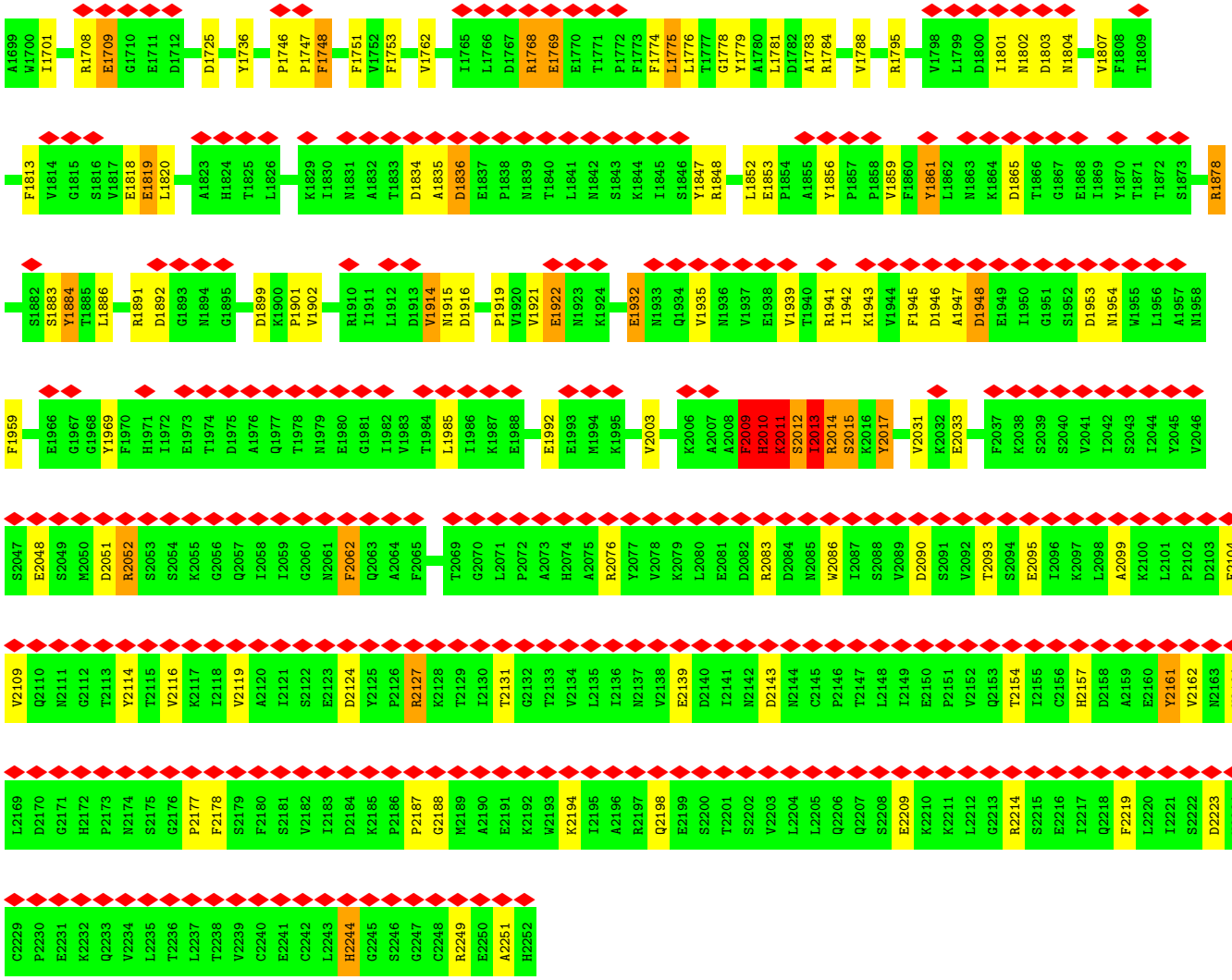
Chain D:



• Molecule 1: Desmoglein-2

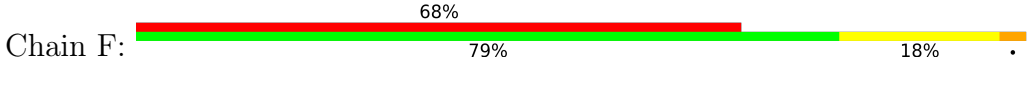
Chain E:

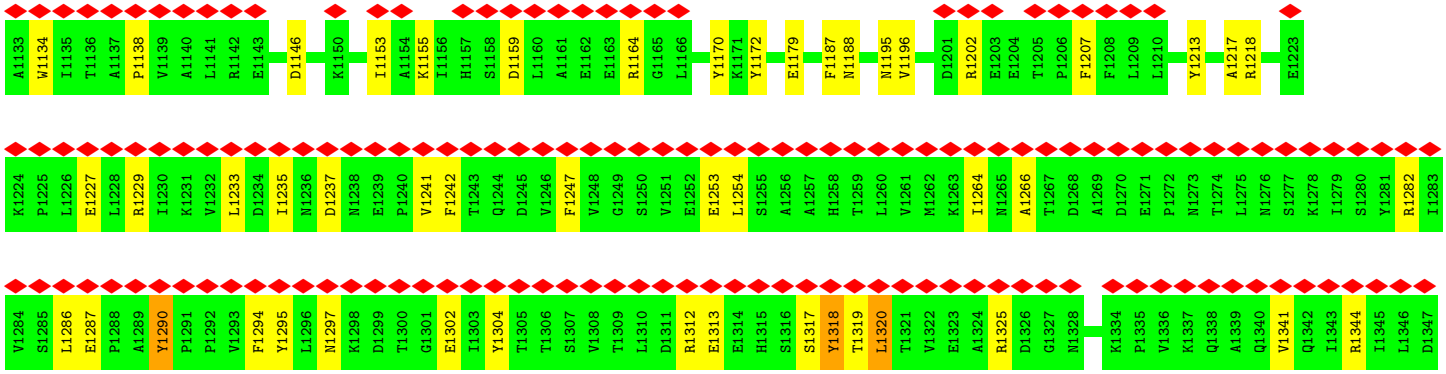


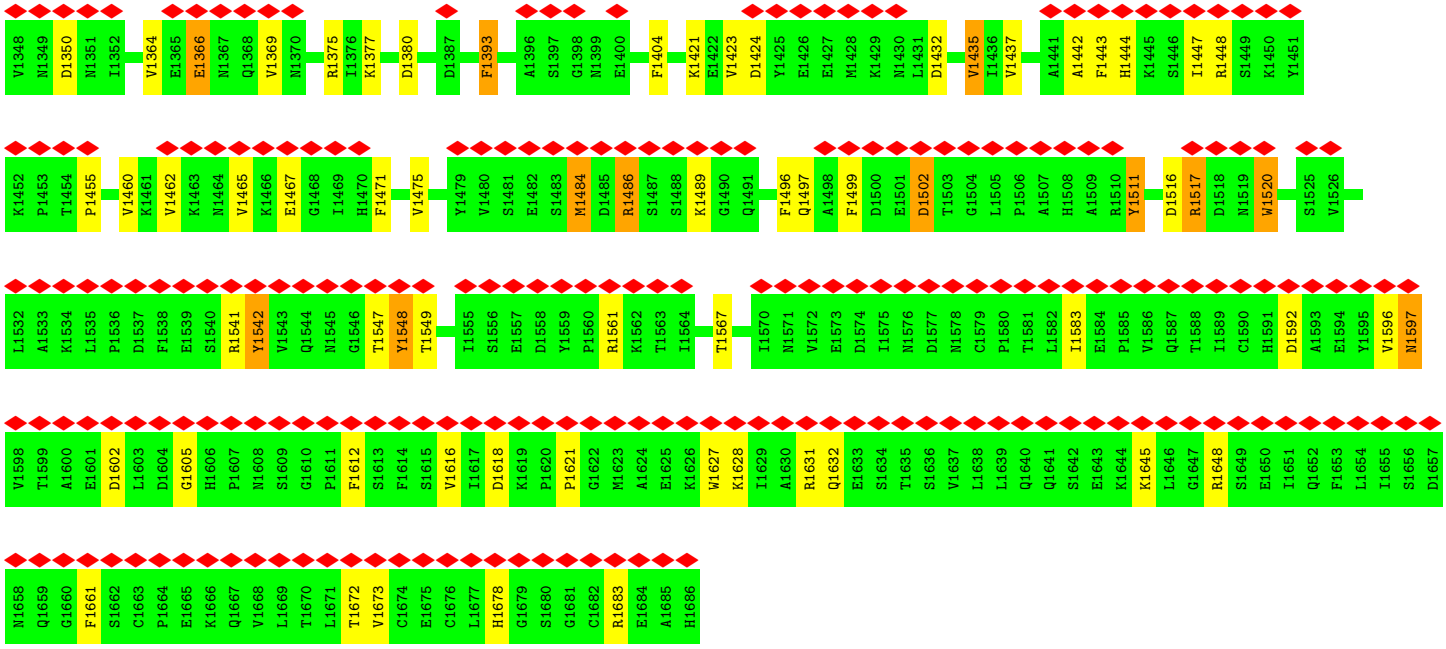


• Molecule 1: Desmoglein-2

Chain F:

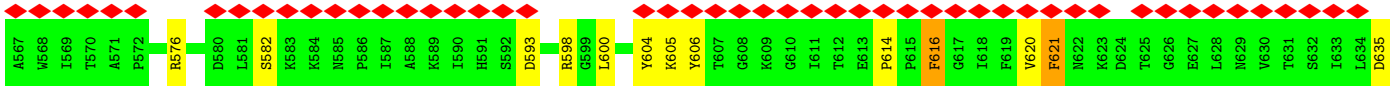


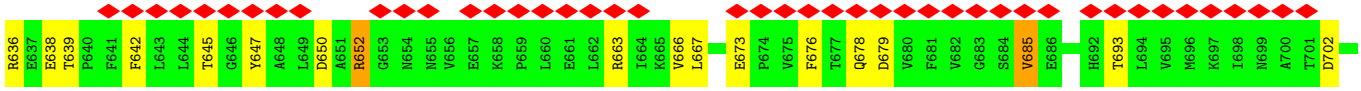


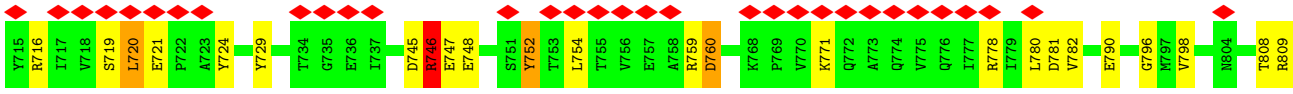


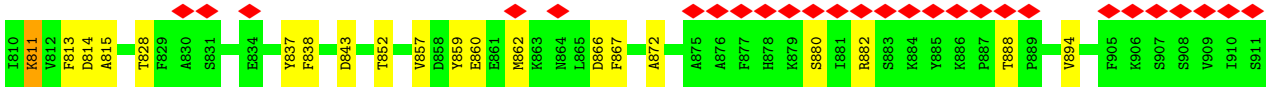
• Molecule 1: Desmoglein-2

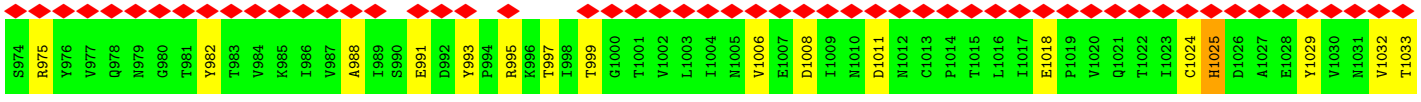
Chain G:

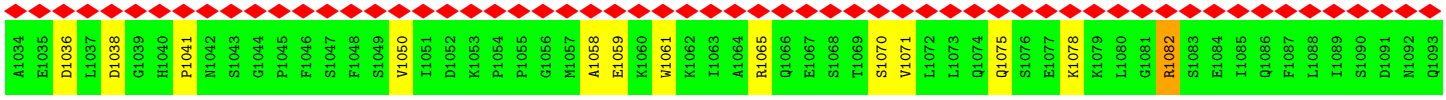


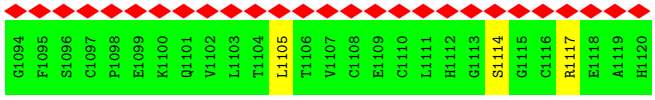






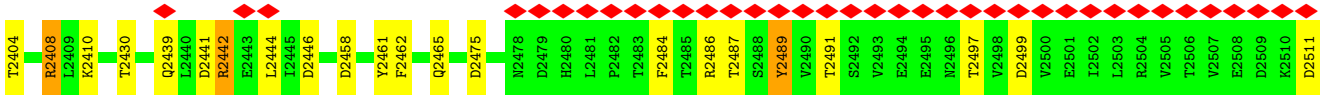


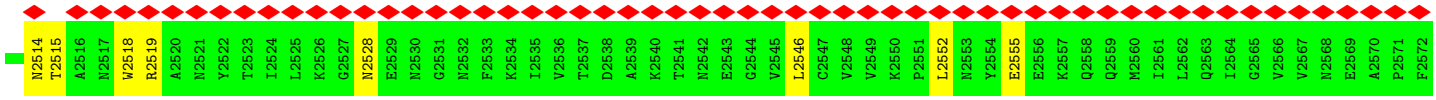


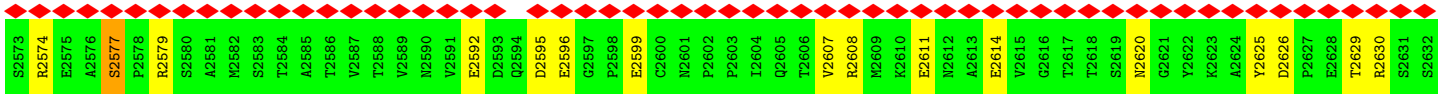


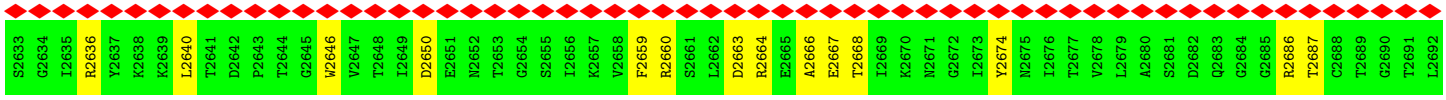
• Molecule 2: Desmocollin-2

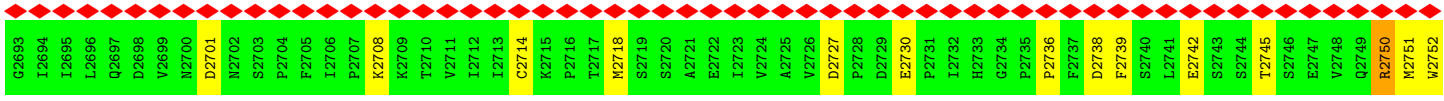
Chain a:

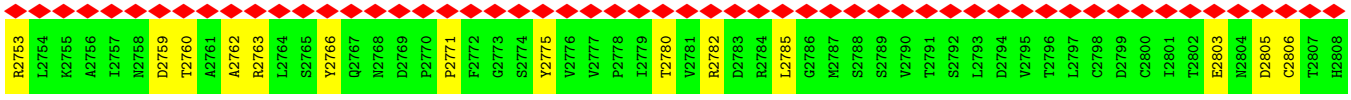






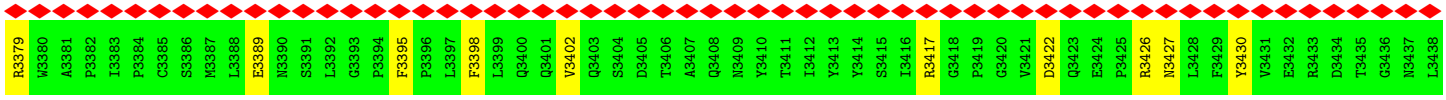


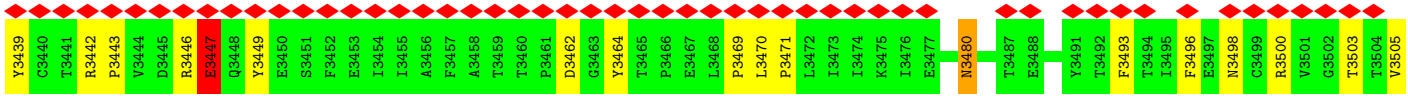


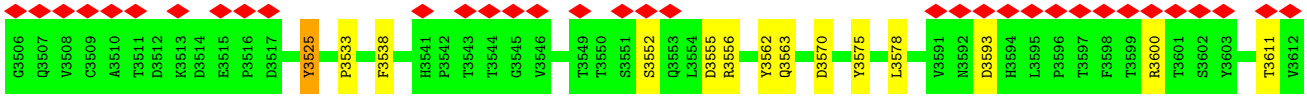


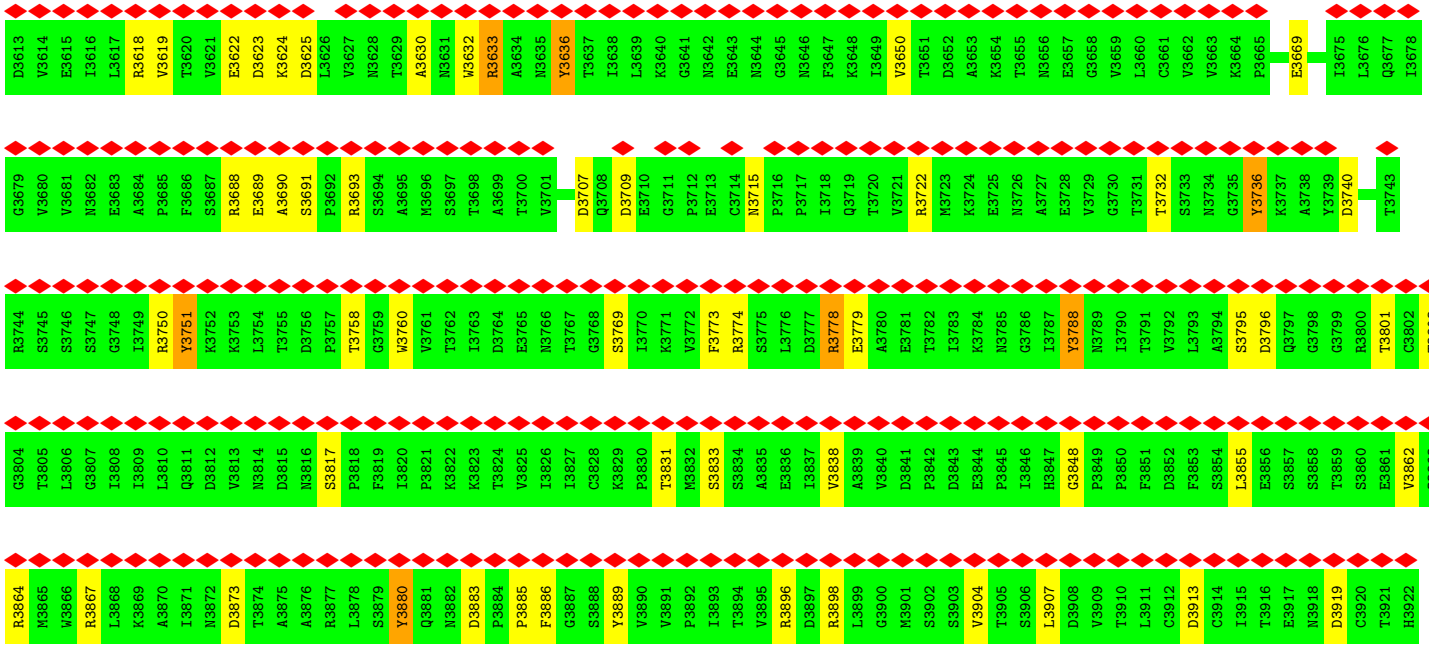
• Molecule 2: Desmocollin-2

Chain b:



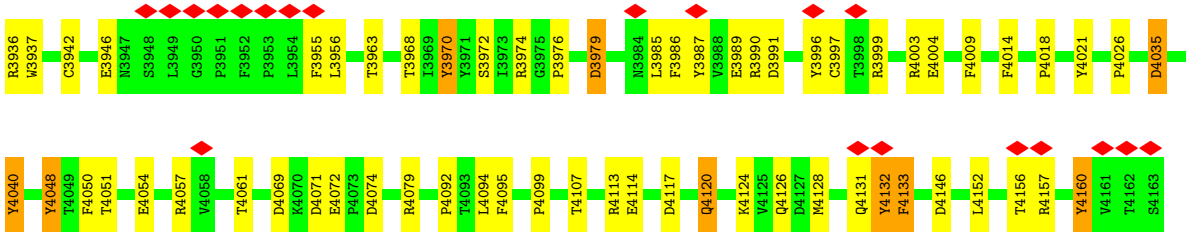






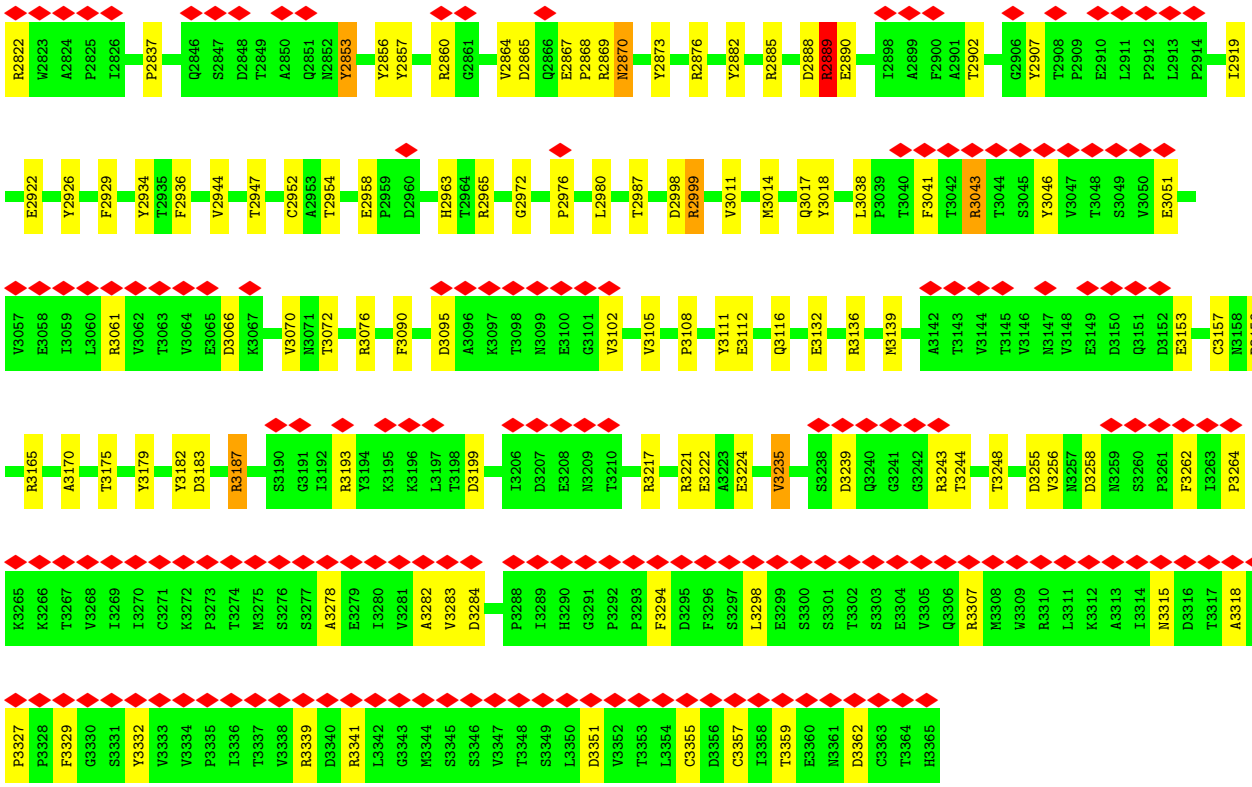
- Molecule 2: Desmocollin-2

Chain c:



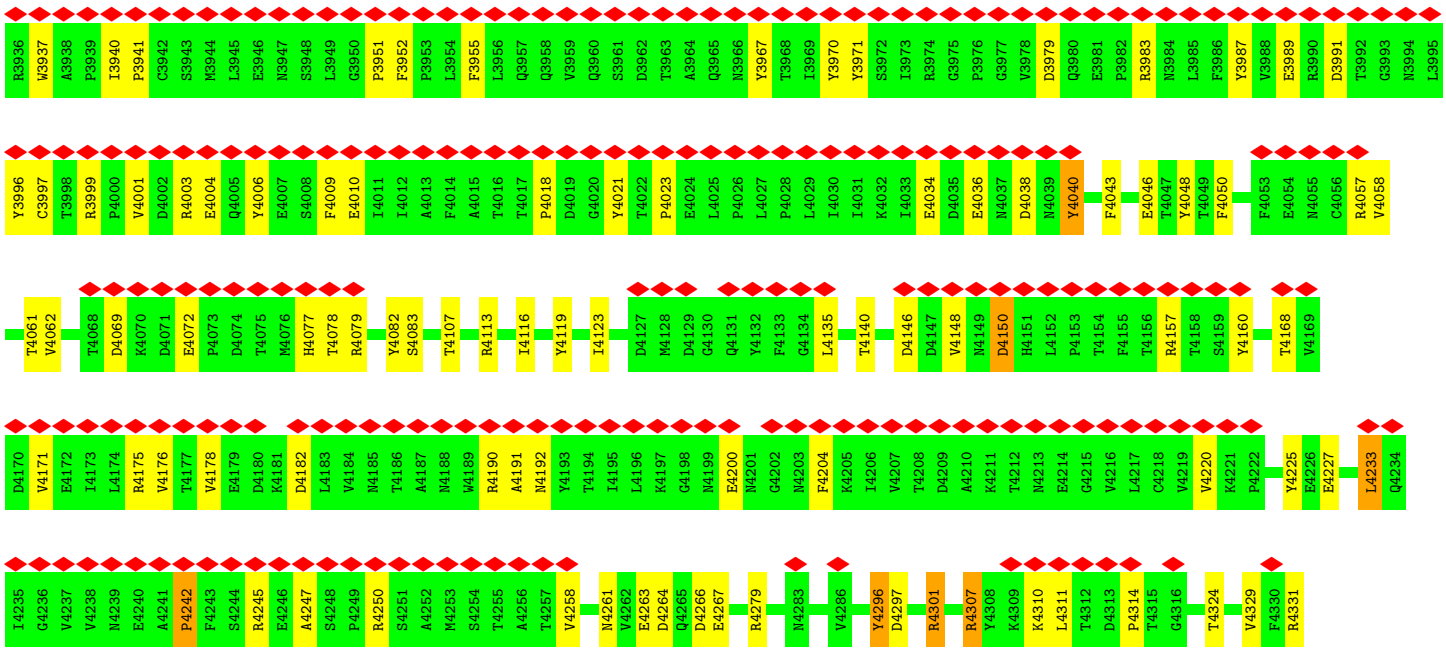
• Molecule 2: Desmocollin-2

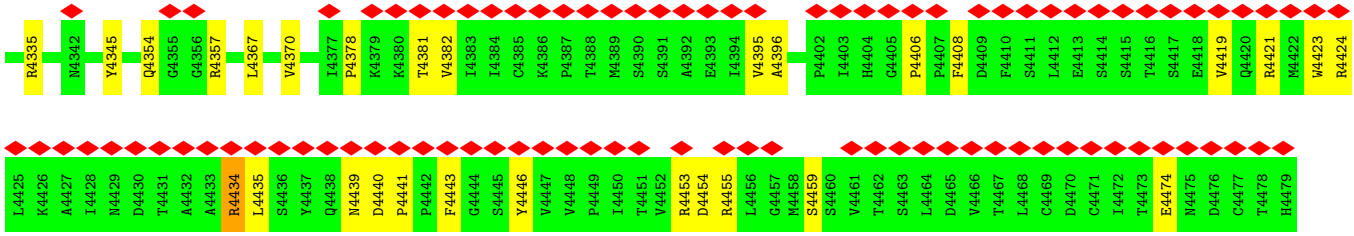
Chain d:



• Molecule 2: Desmocollin-2

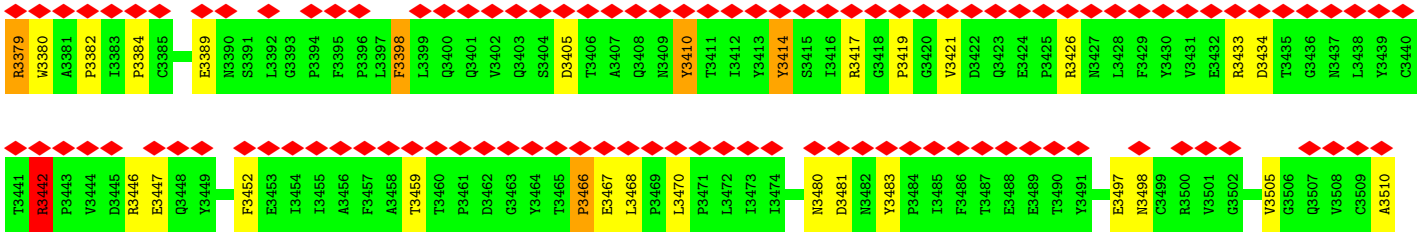
Chain e:

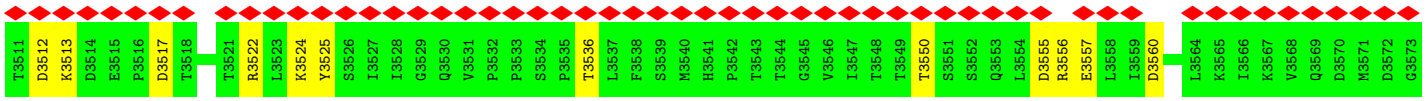


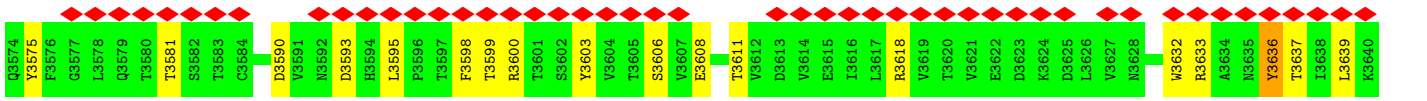


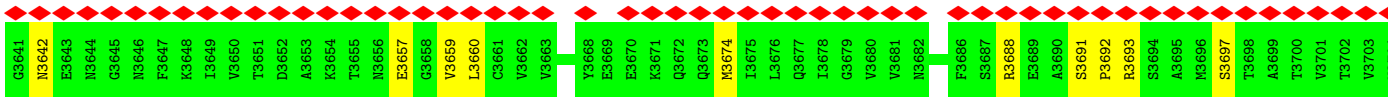
• Molecule 2: Desmocollin-2

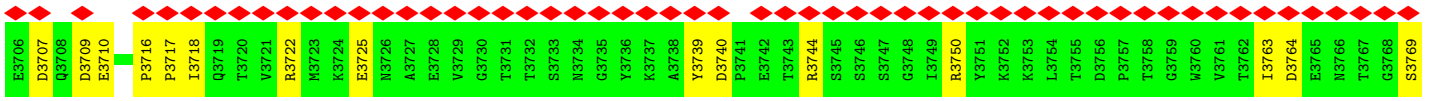
Chain f:

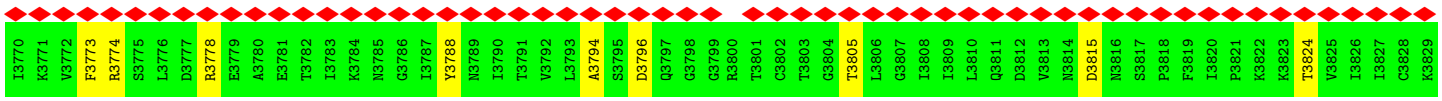


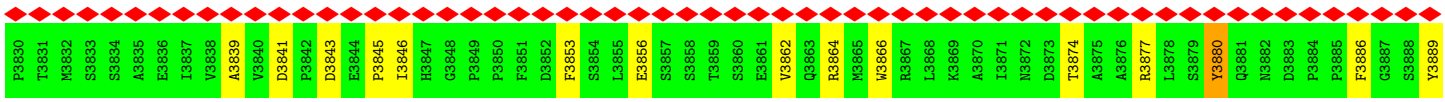


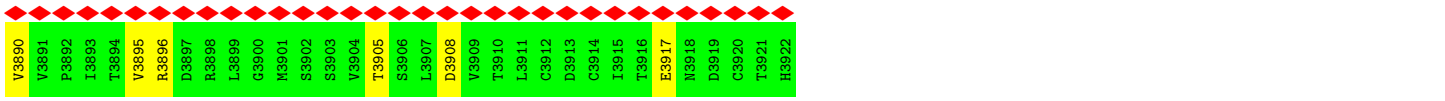






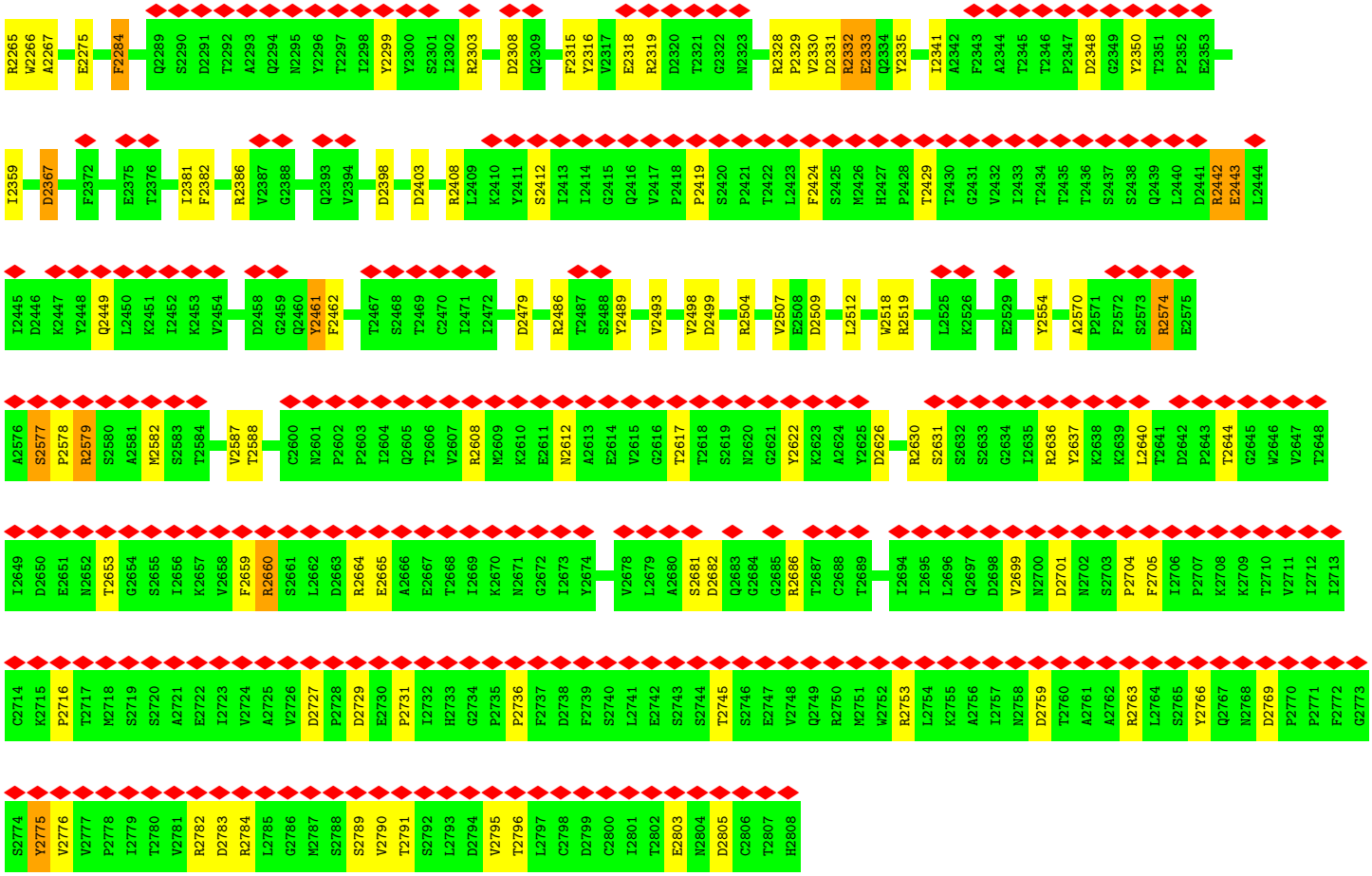






• Molecule 2: Desmocollin-2

Chain g:


R2265 W2266 A2267 E2275 F2284 Q2289 S2290 D2291 T2292 A2293 Q2294 N2295 Y2296 T2297 I2298 Y2299 Y2300 S2301 I2302 R2303 D2308 Q2309 F2315 Y2316 V2317 E2318 R2319 D2320 T2321 G2322 N2323 R2328 P2329 V2330 D2331 R2332 E2333 Q2334 Y2335 I2341 A2342 F2343 A2344 T2345 T2346 P2347 D2348 G2349 Y2350 T2351 P2352 E2353
I2359 D2367 F2372 E2375 T2376 I2381 F2382 R2386 V2387 G2388 Q2393 V2394 D2398 D2403 R2408 L2409 K2410 Y2411 S2412 I2413 I2414 G2415 Q2416 V2417 P2418 P2419 S2420 P2421 T2422 L2423 F2424 S2425 M2426 H2427 P2428 T2429 T2430 G2431 V2432 I2433 T2434 T2435 T2436 S2437 S2438 Q2439 L2440 D2441 R2442 E2443 L2444
I2445 D2446 K2447 Y2448 Q2449 L2450 K2451 I2452 K2453 V2454 D2458 G2459 Q2460 Y2461 F2462 T2467 S2468 T2469 C2470 I2471 I2472 D2479 R2486 T2487 S2488 Y2489 V2493 V2498 D2499 R2504 V2507 E2508 D2509 L2512 W2518 R2519 L2525 K2526 E2529 Y2554 A2570 P2571 F2572 S2573 R2574 E2575
A2576 S2577 P2578 R2579 S2580 A2581 M2582 S2583 T2584 V2587 T2588 C2600 N2601 P2602 P2603 I2604 Q2605 T2606 V2607 R2608 M2609 K2610 E2611 N2612 A2613 E2614 V2615 G2616 T2617 T2618 S2619 N2620 G2621 Y2622 K2623 A2624 Y2625 D2626 R2630 S2631 S2632 S2633 G2634 I2635 R2636 Y2637 K2638 K2639 L2640 T2641 D2642 P2643 T2644 G2645 W2646 V2647 T2648
I2649 D2650 E2651 N2652 T2653 G2654 S2655 I2656 K2657 V2658 F2659 R2660 S2661 L2662 D2663 R2664 E2665 A2666 E2667 T2668 I2669 K2670 N2671 G2672 I2673 Y2674 V2678 L2679 A2680 S2681 D2682 Q2683 G2684 G2685 R2686 T2687 C2688 T2689 I2694 I2695 L2696 Q2697 D2698 V2699 N2700 D2701 N2702 S2703 P2704 F2705 I2706 P2707 K2708 K2709 T2710 V2711 I2712 I2713
C2714 K2715 P2716 T2717 M2718 S2719 S2720 A2721 E2722 I2723 V2724 A2725 V2726 D2727 P2728 D2729 E2730 P2731 I2732 H2733 G2734 P2735 P2736 F2737 D2738 P2739 S2740 L2741 E2742 S2743 S2744 T2745 S2746 E2747 V2748 Q2749 R2750 M2751 W2752 R2753 L2754 K2755 A2756 I2757 N2758 D2759 T2760 A2761 A2762 R2763 L2764 S2765 Y2766 Q2767 N2768 D2769 P2770 P2771 F2772 G2773
S2774 Y2775 V2776 V2777 P2778 I2779 T2780 V2781 R2782 D2783 R2784 L2785 G2786 M2787 S2788 S2789 V2790 T2791 S2792 L2793 D2794 V2795 T2796 L2797 C2798 D2799 C2800 I2801 T2802 E2803 N2804 D2805 C2806 T2807 H2808

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	3656	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.95	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	64000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.210	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0133	Depositor
Map size (Å)	550.4, 550.4, 550.4	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	4.3, 4.3, 4.3	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	A	0.54	0/4438	1.98	133/6026 (2.2%)
1	B	0.54	0/4438	1.96	121/6026 (2.0%)
1	C	0.53	0/4438	1.94	118/6026 (2.0%)
1	D	0.54	0/4438	1.93	107/6026 (1.8%)
1	E	0.87	10/4438 (0.2%)	2.21	150/6026 (2.5%)
1	F	0.54	0/4438	1.98	125/6026 (2.1%)
1	G	0.54	0/4438	1.96	120/6026 (2.0%)
2	a	0.64	1/4355 (0.0%)	2.02	132/5943 (2.2%)
2	b	0.56	0/4355	1.97	116/5943 (2.0%)
2	c	0.55	0/4355	2.02	150/5943 (2.5%)
2	d	0.55	0/4355	2.01	146/5943 (2.5%)
2	e	0.56	0/4355	2.02	140/5943 (2.4%)
2	f	0.56	0/4355	1.95	119/5943 (2.0%)
2	g	0.61	2/4355 (0.0%)	2.05	137/5943 (2.3%)
All	All	0.59	13/61551 (0.0%)	2.00	1814/83783 (2.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	15
1	C	0	13
1	D	0	15
1	E	0	18
1	F	0	12
1	G	0	9
2	a	0	15
2	b	0	11
2	c	0	11
2	d	0	5

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	e	0	12
2	f	0	11
2	g	0	13
All	All	0	168

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	2010	HIS	ND1-CE1	25.77	1.99	1.34
2	a	2333	GLU	CD-OE1	-19.74	1.03	1.25
1	E	2012	SER	CB-OG	-17.47	1.19	1.42
1	E	2010	HIS	CG-ND1	17.03	1.76	1.38
1	E	2011	LYS	C-N	15.63	1.70	1.34
1	E	2010	HIS	N-CA	13.74	1.73	1.46
2	g	2333	GLU	CD-OE2	-12.77	1.11	1.25
2	g	2333	GLU	CD-OE1	-9.34	1.15	1.25
1	E	2010	HIS	CG-CD2	-8.20	1.21	1.35
1	E	1819	GLU	CD-OE2	-6.94	1.18	1.25
1	E	2010	HIS	CA-CB	-6.04	1.40	1.53
1	E	2010	HIS	C-O	5.76	1.34	1.23
1	E	2012	SER	C-N	5.47	1.46	1.34

All (1814) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	2010	HIS	CG-ND1-CE1	-44.79	45.49	108.20
1	E	2010	HIS	CA-CB-CG	-28.51	65.14	113.60
1	E	2012	SER	N-CA-CB	27.63	151.94	110.50
2	a	2486	ARG	NE-CZ-NH2	20.05	130.33	120.30
1	B	2076	ARG	NE-CZ-NH1	18.93	129.77	120.30
2	b	3600	ARG	NE-CZ-NH1	18.92	129.76	120.30
1	E	2014	ARG	NE-CZ-NH1	18.67	129.64	120.30
1	E	2010	HIS	CE1-NE2-CD2	-18.32	60.80	106.60
1	F	1218	ARG	NE-CZ-NH1	18.11	129.35	120.30
2	e	4157	ARG	NE-CZ-NH1	17.42	129.01	120.30
1	C	944	ARG	NE-CZ-NH1	17.01	128.80	120.30
1	G	995	ARG	NE-CZ-NH1	16.55	128.58	120.30
2	f	3864	ARG	NE-CZ-NH1	16.31	128.46	120.30
1	D	1164	ARG	NE-CZ-NH1	16.23	128.42	120.30
1	E	2011	LYS	CA-CB-CG	16.16	148.96	113.40
1	B	1708	ARG	NE-CZ-NH1	16.12	128.36	120.30
2	a	2486	ARG	NE-CZ-NH1	-16.06	112.27	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1164	ARG	NE-CZ-NH2	-16.00	112.30	120.30
1	A	463	TYR	CB-CG-CD2	-15.91	111.45	121.00
2	b	3600	ARG	NE-CZ-NH2	-15.77	112.41	120.30
2	d	2860	ARG	NE-CZ-NH2	15.40	128.00	120.30
2	g	2763	ARG	NE-CZ-NH1	15.28	127.94	120.30
2	e	4331	ARG	NE-CZ-NH2	15.23	127.92	120.30
2	f	3877	ARG	NE-CZ-NH1	15.21	127.90	120.30
1	E	2010	HIS	CA-C-N	15.17	150.57	117.20
2	a	2574	ARG	NE-CZ-NH1	15.01	127.80	120.30
2	g	2686	ARG	NE-CZ-NH2	14.99	127.80	120.30
2	g	2486	ARG	NE-CZ-NH2	14.88	127.74	120.30
2	e	4245	ARG	NE-CZ-NH2	-14.83	112.89	120.30
1	A	316	ARG	NE-CZ-NH1	14.76	127.68	120.30
1	F	1344	ARG	NE-CZ-NH1	14.62	127.61	120.30
2	d	3187	ARG	NE-CZ-NH1	14.36	127.48	120.30
2	b	3417	ARG	NE-CZ-NH1	14.29	127.44	120.30
2	g	2332	ARG	NE-CZ-NH1	14.21	127.41	120.30
2	c	4113	ARG	NE-CZ-NH1	14.09	127.35	120.30
1	E	2012	SER	CA-C-N	-14.00	86.40	117.20
1	G	920	ARG	NE-CZ-NH1	-13.95	113.33	120.30
1	F	1517	ARG	NE-CZ-NH1	13.88	127.24	120.30
1	E	2052	ARG	NE-CZ-NH1	13.84	127.22	120.30
2	g	2686	ARG	NE-CZ-NH1	-13.82	113.39	120.30
1	G	746	ARG	NE-CZ-NH1	13.81	127.21	120.30
2	e	4079	ARG	NE-CZ-NH2	13.68	127.14	120.30
2	g	2784	ARG	NE-CZ-NH1	13.66	127.13	120.30
1	C	663	ARG	NE-CZ-NH1	13.57	127.09	120.30
2	d	2869	ARG	NE-CZ-NH2	13.56	127.08	120.30
2	g	2664	ARG	NE-CZ-NH2	-13.50	113.55	120.30
2	f	3442	ARG	NE-CZ-NH1	13.49	127.04	120.30
1	B	2107	ARG	NE-CZ-NH2	13.39	126.99	120.30
2	b	3500	ARG	NE-CZ-NH2	-13.35	113.63	120.30
2	g	2265	ARG	NE-CZ-NH1	13.33	126.96	120.30
2	c	4398	ASP	CB-CG-OD2	13.29	130.26	118.30
2	b	3778	ARG	NE-CZ-NH1	13.23	126.92	120.30
2	g	2509	ASP	CB-CG-OD2	13.22	130.19	118.30
2	a	2303	ARG	NE-CZ-NH1	13.21	126.91	120.30
2	g	2408	ARG	NE-CZ-NH2	13.16	126.88	120.30
2	a	2753	ARG	NE-CZ-NH1	13.05	126.83	120.30
2	g	2782	ARG	NE-CZ-NH1	13.01	126.80	120.30
2	g	2637	TYR	CB-CG-CD1	-13.00	113.20	121.00
2	e	4113	ARG	NE-CZ-NH1	12.90	126.75	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	d	3076	ARG	NE-CZ-NH1	12.83	126.72	120.30
2	f	3841	ASP	CB-CG-OD1	12.75	129.77	118.30
1	E	2249	ARG	NE-CZ-NH1	12.69	126.65	120.30
2	e	4455	ARG	NE-CZ-NH1	12.69	126.64	120.30
2	f	3452	PHE	CB-CG-CD2	-12.62	111.97	120.80
1	E	2013	ILE	N-CA-CB	12.59	139.75	110.80
1	B	1708	ARG	NE-CZ-NH2	-12.57	114.02	120.30
1	F	1218	ARG	NE-CZ-NH2	-12.50	114.05	120.30
1	G	576	ARG	NE-CZ-NH1	12.50	126.55	120.30
1	B	1910	ARG	NE-CZ-NH1	12.46	126.53	120.30
1	D	1179	GLU	OE1-CD-OE2	-12.45	108.36	123.30
2	a	2750	ARG	NE-CZ-NH2	12.41	126.51	120.30
2	f	3688	ARG	NE-CZ-NH1	12.37	126.49	120.30
2	a	2333	GLU	OE1-CD-OE2	-12.37	108.46	123.30
2	g	2775	TYR	CB-CG-CD2	-12.36	113.58	121.00
2	g	2331	ASP	CB-CG-OD1	-12.33	107.20	118.30
1	D	1648	ARG	NE-CZ-NH2	12.29	126.44	120.30
1	E	2010	HIS	CB-CA-C	12.28	134.95	110.40
2	a	2265	ARG	NE-CZ-NH1	12.24	126.42	120.30
1	B	2214	ARG	NE-CZ-NH1	12.22	126.41	120.30
1	C	866	ASP	CB-CG-OD1	12.21	129.28	118.30
2	g	2805	ASP	CB-CG-OD2	12.07	129.16	118.30
1	G	945	TYR	CB-CG-CD1	12.05	128.23	121.00
1	F	1592	ASP	CB-CG-OD1	12.04	129.13	118.30
2	d	2885	ARG	NE-CZ-NH1	11.96	126.28	120.30
1	B	1891	ARG	NE-CZ-NH1	11.90	126.25	120.30
2	a	2328	ARG	NE-CZ-NH1	11.90	126.25	120.30
1	F	1561	ARG	NE-CZ-NH2	-11.89	114.36	120.30
1	B	2052	ARG	NE-CZ-NH1	11.83	126.22	120.30
1	A	385	ARG	NE-CZ-NH1	11.81	126.21	120.30
2	a	2660	ARG	NE-CZ-NH1	11.80	126.20	120.30
1	A	180	ARG	NE-CZ-NH2	-11.76	114.42	120.30
2	a	2332	ARG	NE-CZ-NH2	-11.70	114.45	120.30
2	d	3136	ARG	NE-CZ-NH1	11.69	126.14	120.30
1	F	1448	ARG	NE-CZ-NH2	11.68	126.14	120.30
2	a	2519	ARG	NE-CZ-NH1	11.66	126.13	120.30
1	F	1375	ARG	NE-CZ-NH1	11.62	126.11	120.30
1	D	1380	ASP	CB-CG-OD1	11.61	128.74	118.30
1	G	814	ASP	CB-CG-OD2	11.60	128.74	118.30
1	A	218	ASP	CB-CG-OD1	11.58	128.72	118.30
1	C	882	ARG	NE-CZ-NH2	11.56	126.08	120.30
2	e	4357	ARG	NE-CZ-NH1	11.46	126.03	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	1202	ARG	CD-NE-CZ	11.42	139.58	123.60
2	d	2876	ARG	NE-CZ-NH1	11.39	126.00	120.30
1	E	2010	HIS	ND1-CE1-NE2	-11.37	84.88	109.90
1	E	2012	SER	CA-C-O	11.36	143.96	120.10
2	d	2965	ARG	NE-CZ-NH1	11.32	125.96	120.30
1	E	2010	HIS	O-C-N	-11.29	104.64	122.70
2	g	2660	ARG	NE-CZ-NH1	11.26	125.93	120.30
1	G	944	ARG	NE-CZ-NH2	11.25	125.92	120.30
1	G	621	PHE	CB-CG-CD2	-11.22	112.95	120.80
2	c	4372	ASP	CB-CG-OD1	11.20	128.38	118.30
2	d	3307	ARG	NE-CZ-NH1	11.19	125.89	120.30
2	g	2328	ARG	NE-CZ-NH2	-11.16	114.72	120.30
2	b	3623	ASP	CB-CG-OD1	11.14	128.33	118.30
1	D	1187	PHE	CB-CG-CD1	-11.12	113.02	120.80
2	g	2637	TYR	CB-CG-CD2	11.11	127.67	121.00
1	F	1282	ARG	NE-CZ-NH2	-11.11	114.74	120.30
2	b	3796	ASP	CB-CG-OD1	11.11	128.30	118.30
1	A	416	TYR	CB-CG-CD2	-11.07	114.36	121.00
2	b	3896	ARG	NE-CZ-NH1	11.04	125.82	120.30
1	A	319	TYR	CB-CG-CD1	-11.00	114.40	121.00
1	E	2127	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	G	647	TYR	CB-CG-CD1	-10.94	114.44	121.00
1	E	1779	TYR	CB-CG-CD1	-10.89	114.47	121.00
1	A	409	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	C	1065	ARG	NE-CZ-NH1	10.82	125.71	120.30
2	e	3983	ARG	NE-CZ-NH2	10.82	125.71	120.30
2	e	4357	ARG	NE-CZ-NH2	-10.81	114.89	120.30
1	G	604	TYR	CB-CG-CD1	-10.81	114.51	121.00
1	C	972	PHE	CB-CG-CD1	-10.81	113.23	120.80
1	C	663	ARG	NE-CZ-NH2	-10.81	114.90	120.30
1	E	2168	ASP	CB-CG-OD2	10.77	127.99	118.30
1	G	1117	ARG	NE-CZ-NH1	10.76	125.68	120.30
2	a	2650	ASP	CB-CG-OD2	10.75	127.97	118.30
2	c	4250	ARG	NE-CZ-NH1	10.74	125.67	120.30
2	g	2579	ARG	NE-CZ-NH2	10.71	125.66	120.30
1	G	1117	ARG	NE-CZ-NH2	-10.70	114.95	120.30
2	e	3996	TYR	CB-CG-CD2	-10.68	114.59	121.00
2	c	4331	ARG	NE-CZ-NH1	-10.68	114.96	120.30
2	e	3983	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	D	1467	GLU	OE1-CD-OE2	-10.60	110.59	123.30
1	B	1878	ARG	NE-CZ-NH2	-10.58	115.01	120.30
1	F	1618	ASP	CB-CG-OD1	10.56	127.80	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	1486	ARG	NE-CZ-NH1	10.56	125.58	120.30
2	g	2636	ARG	NE-CZ-NH1	10.49	125.55	120.30
1	D	1282	ARG	NE-CZ-NH1	10.47	125.53	120.30
2	b	3500	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	C	972	PHE	CB-CG-CD2	10.46	128.12	120.80
1	B	2184	ASP	CB-CG-OD1	10.45	127.70	118.30
2	f	3522	ARG	NE-CZ-NH2	10.44	125.52	120.30
1	E	1820	LEU	CB-CA-C	10.39	129.94	110.20
1	F	1602	ASP	CB-CG-OD2	10.38	127.64	118.30
1	E	2249	ARG	NE-CZ-NH2	-10.37	115.11	120.30
1	E	1784	ARG	NE-CZ-NH1	10.37	125.48	120.30
1	F	1179	GLU	OE1-CD-OE2	-10.37	110.86	123.30
1	B	2083	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	F	1304	TYR	CB-CG-CD1	-10.33	114.80	121.00
2	d	2860	ARG	NH1-CZ-NH2	-10.29	108.08	119.40
1	F	1325	ARG	NE-CZ-NH1	10.26	125.43	120.30
2	a	2319	ARG	NE-CZ-NH1	10.24	125.42	120.30
2	e	4307	ARG	NE-CZ-NH1	10.23	125.42	120.30
1	E	2214	ARG	NE-CZ-NH1	10.23	125.41	120.30
2	g	2701	ASP	CB-CG-OD1	10.22	127.50	118.30
2	g	2803	GLU	OE1-CD-OE2	-10.21	111.05	123.30
1	F	1146	ASP	CB-CG-OD1	-10.19	109.13	118.30
2	e	4175	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	F	1213	TYR	CB-CG-CD2	-10.15	114.91	121.00
2	b	3774	ARG	NE-CZ-NH1	10.13	125.36	120.30
2	c	4050	PHE	CB-CG-CD1	-10.13	113.71	120.80
1	B	1725	ASP	CB-CG-OD1	10.06	127.36	118.30
2	d	3339	ARG	NE-CZ-NH2	9.98	125.29	120.30
2	c	3974	ARG	NE-CZ-NH1	9.97	125.28	120.30
2	c	4003	ARG	NE-CZ-NH1	9.94	125.27	120.30
2	g	2682	ASP	CB-CG-OD2	9.92	127.22	118.30
2	g	2442	ARG	NE-CZ-NH1	9.90	125.25	120.30
2	a	2441	ASP	CB-CG-OD1	9.88	127.20	118.30
2	b	3430	TYR	CB-CG-CD2	-9.88	115.08	121.00
1	C	715	TYR	CB-CG-CD2	-9.87	115.08	121.00
2	d	3051	GLU	OE1-CD-OE2	-9.86	111.47	123.30
1	E	2076	ARG	NE-CZ-NH2	9.86	125.23	120.30
2	f	3618	ARG	NE-CZ-NH1	9.85	125.22	120.30
2	b	3633	ARG	NE-CZ-NH1	9.84	125.22	120.30
2	a	2599	GLU	OE1-CD-OE2	-9.83	111.50	123.30
1	C	1117	ARG	NE-CZ-NH1	9.83	125.22	120.30
1	E	2012	SER	CB-CA-C	-9.81	91.46	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	72	GLU	OE1-CD-OE2	-9.81	111.53	123.30
1	E	2139	GLU	OE1-CD-OE2	-9.81	111.53	123.30
2	c	4072	GLU	OE1-CD-OE2	-9.79	111.56	123.30
1	E	2104	PHE	CB-CG-CD1	-9.77	113.96	120.80
2	e	3983	ARG	NH1-CZ-NH2	-9.76	108.66	119.40
2	d	2934	TYR	CB-CG-CD2	-9.74	115.15	121.00
2	c	4335	ARG	NE-CZ-NH1	-9.73	115.43	120.30
1	G	745	ASP	CB-CG-OD1	9.73	127.06	118.30
1	D	1325	ARG	NE-CZ-NH2	9.72	125.16	120.30
1	C	814	ASP	CB-CG-OD1	9.72	127.04	118.30
2	a	2782	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	E	2013	ILE	CA-C-O	-9.69	99.74	120.10
1	F	1159	ASP	CB-CG-OD1	9.70	127.03	118.30
2	f	3722	ARG	NE-CZ-NH1	-9.67	115.46	120.30
1	A	138	ASP	CB-CG-OD1	9.64	126.97	118.30
2	c	4157	ARG	NE-CZ-NH2	9.62	125.11	120.30
2	d	3329	PHE	CB-CG-CD1	-9.60	114.08	120.80
1	E	2090	ASP	CB-CG-OD2	9.55	126.90	118.30
2	d	3332	TYR	CB-CG-CD2	-9.55	115.27	121.00
2	f	3417	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	B	1990	ASP	CB-CG-OD2	-9.54	109.72	118.30
1	F	1164	ARG	NE-CZ-NH2	-9.53	115.54	120.30
1	B	1945	PHE	CB-CG-CD2	-9.52	114.14	120.80
1	A	194	ASP	CB-CG-OD1	9.49	126.85	118.30
1	G	951	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	G	860	GLU	OE1-CD-OE2	-9.47	111.94	123.30
2	a	2579	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	D	1268	ASP	CB-CG-OD2	9.45	126.80	118.30
2	d	3090	PHE	CB-CG-CD1	-9.45	114.19	120.80
1	B	2105	GLU	OE1-CD-OE2	-9.44	111.97	123.30
1	C	624	ASP	CB-CG-OD1	9.44	126.79	118.30
2	g	2303	ARG	NE-CZ-NH1	9.42	125.01	120.30
2	c	4040	TYR	CB-CG-CD2	-9.40	115.36	121.00
2	c	4003	ARG	NE-CZ-NH2	-9.40	115.60	120.30
2	g	2775	TYR	CG-CD1-CE1	-9.39	113.79	121.30
1	C	976	TYR	CB-CG-CD2	-9.38	115.37	121.00
2	e	4245	ARG	NE-CZ-NH1	9.37	124.98	120.30
2	b	3442	ARG	NE-CZ-NH2	-9.36	115.62	120.30
2	a	2330	VAL	CA-CB-CG1	9.35	124.93	110.90
1	B	1999	PHE	CB-CG-CD1	-9.34	114.26	120.80
2	a	2519	ARG	NE-CZ-NH2	-9.33	115.63	120.30
2	f	3593	ASP	CB-CG-OD1	9.32	126.69	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	c	4357	ARG	CD-NE-CZ	9.32	136.65	123.60
1	C	995	ARG	NE-CZ-NH1	-9.28	115.66	120.30
2	d	2929	PHE	CB-CG-CD1	9.27	127.29	120.80
2	e	4225	TYR	CB-CG-CD1	-9.26	115.44	121.00
2	d	3298	LEU	CB-CG-CD1	9.23	126.69	111.00
2	e	4009	PHE	CB-CG-CD1	-9.21	114.35	120.80
1	B	2249	ARG	NE-CZ-NH2	9.17	124.89	120.30
1	F	1561	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	A	293	TYR	CB-CG-CD1	-9.14	115.52	121.00
2	c	4180	ASP	CB-CG-OD2	9.13	126.52	118.30
1	F	1375	ARG	NE-CZ-NH2	-9.11	115.75	120.30
2	b	3525	TYR	CB-CG-CD2	-9.09	115.54	121.00
2	c	4182	ASP	CB-CG-OD1	9.09	126.48	118.30
1	F	1648	ARG	NE-CZ-NH1	9.07	124.83	120.30
2	a	2398	ASP	CB-CG-OD2	9.05	126.45	118.30
2	b	3778	ARG	NH1-CZ-NH2	-9.04	109.45	119.40
1	C	652	ARG	NE-CZ-NH2	9.04	124.82	120.30
2	d	2876	ARG	NE-CZ-NH2	-9.03	115.79	120.30
2	f	3750	ARG	NE-CZ-NH2	9.03	124.81	120.30
1	F	1313	GLU	OE1-CD-OE2	-9.02	112.48	123.30
2	d	3136	ARG	NH1-CZ-NH2	-9.01	109.48	119.40
1	D	1229	ARG	NE-CZ-NH1	9.01	124.81	120.30
2	g	2398	ASP	CB-CG-OD1	9.01	126.41	118.30
2	f	3608	GLU	OE1-CD-OE2	-8.97	112.53	123.30
2	a	2555	GLU	OE1-CD-OE2	-8.93	112.58	123.30
2	d	3061	ARG	NE-CZ-NH1	-8.92	115.84	120.30
2	a	2408	ARG	NE-CZ-NH1	8.92	124.76	120.30
2	c	4050	PHE	CB-CG-CD2	8.92	127.04	120.80
2	a	2319	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	E	1781	LEU	CB-CG-CD2	8.91	126.15	111.00
1	F	1548	TYR	CB-CG-CD1	-8.91	115.66	121.00
2	e	4395	VAL	CA-CB-CG1	8.91	124.26	110.90
1	E	2012	SER	C-N-CA	8.90	143.96	121.70
2	e	4250	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	D	1577	ASP	CB-CG-OD1	8.90	126.31	118.30
2	c	4069	ASP	CB-CG-OD1	8.87	126.29	118.30
2	d	3066	ASP	CB-CG-OD2	8.87	126.28	118.30
1	D	1375	ARG	CD-NE-CZ	8.86	136.00	123.60
2	d	3170	ALA	N-CA-CB	-8.86	97.70	110.10
2	a	2727	ASP	CB-CG-OD1	8.85	126.27	118.30
2	c	4423	TRP	CD1-CG-CD2	-8.85	99.22	106.30
1	E	2013	ILE	CA-CB-CG1	8.84	127.80	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	g	2630	ARG	NE-CZ-NH2	8.83	124.71	120.30
2	e	4331	ARG	NE-CZ-NH1	-8.82	115.89	120.30
2	a	2782	ARG	NE-CZ-NH2	-8.79	115.90	120.30
2	g	2299	TYR	CB-CG-CD1	8.78	126.27	121.00
2	a	2596	GLU	OE1-CD-OE2	-8.77	112.78	123.30
2	d	2885	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	B	2068	ASP	CB-CG-OD1	8.76	126.19	118.30
1	A	261	PHE	CB-CG-CD2	8.72	126.91	120.80
1	C	616	PHE	CB-CG-CD1	-8.72	114.70	120.80
2	f	3426	ARG	NE-CZ-NH2	8.72	124.66	120.30
2	f	3788	TYR	CB-CG-CD2	-8.72	115.77	121.00
1	B	2143	ASP	CB-CG-OD2	8.71	126.14	118.30
1	E	1813	PHE	CB-CG-CD2	-8.68	114.72	120.80
2	g	2328	ARG	CD-NE-CZ	8.68	135.75	123.60
1	A	521	PHE	CB-CG-CD2	-8.67	114.73	120.80
2	g	2329	PRO	N-CA-CB	8.64	113.67	103.30
2	e	4119	TYR	CB-CG-CD2	-8.63	115.82	121.00
1	A	136	ASP	CB-CG-OD1	8.63	126.06	118.30
2	d	3284	ASP	CB-CG-OD1	8.61	126.05	118.30
2	d	2907	TYR	CB-CG-CD1	-8.60	115.84	121.00
2	c	4331	ARG	NE-CZ-NH2	8.59	124.60	120.30
1	G	1036	ASP	CB-CG-OD1	8.59	126.03	118.30
2	a	2625	TYR	CB-CG-CD2	8.58	126.15	121.00
1	A	521	PHE	CB-CG-CD1	8.57	126.80	120.80
1	B	1738	TYR	CB-CG-CD2	-8.56	115.86	121.00
1	D	1211	THR	CA-CB-CG2	-8.55	100.42	112.40
1	B	1748	PHE	CB-CG-CD2	-8.52	114.83	120.80
2	c	4317	TRP	CD1-NE1-CE2	8.52	116.66	109.00
1	E	2010	HIS	CB-CG-ND1	-8.51	101.92	123.20
2	e	4175	ARG	NH1-CZ-NH2	-8.51	110.04	119.40
1	A	407	GLU	OE1-CD-OE2	-8.51	113.09	123.30
2	g	2769	ASP	CB-CG-OD1	-8.47	110.68	118.30
1	A	248	ASP	CB-CG-OD2	8.47	125.92	118.30
1	A	150	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	D	1542	TYR	CB-CG-CD1	-8.46	115.92	121.00
2	e	4190	ARG	NE-CZ-NH2	8.45	124.53	120.30
2	d	3362	ASP	CB-CG-OD1	-8.44	110.70	118.30
1	D	1203	GLU	OE1-CD-OE2	-8.43	113.19	123.30
2	b	3398	PHE	CB-CG-CD2	-8.43	114.90	120.80
1	D	1348	VAL	O-C-N	8.43	136.18	122.70
1	E	2012	SER	CA-CB-OG	-8.43	88.45	111.20
2	g	2727	ASP	CB-CG-OD1	8.43	125.88	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	c	4071	ASP	CB-CG-OD1	8.41	125.87	118.30
1	G	716	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	F	1499	PHE	CB-CG-CD1	-8.40	114.92	120.80
2	a	2625	TYR	CZ-CE2-CD2	8.40	127.36	119.80
1	B	1959	PHE	CB-CG-CD2	-8.40	114.92	120.80
1	D	1588	THR	CA-CB-CG2	8.39	124.15	112.40
2	b	3669	GLU	OE1-CD-OE2	-8.39	113.23	123.30
1	C	598	ARG	NE-CZ-NH1	8.35	124.48	120.30
2	c	4317	TRP	NE1-CE2-CD2	-8.35	98.95	107.30
1	D	1444	HIS	N-CA-CB	8.34	125.60	110.60
1	B	2031	VAL	CA-CB-CG2	8.33	123.40	110.90
2	c	4133	PHE	CB-CG-CD2	-8.33	114.97	120.80
2	f	3446	ARG	CD-NE-CZ	8.33	135.27	123.60
2	f	3862	VAL	CG1-CB-CG2	-8.33	97.57	110.90
1	E	1884	TYR	CB-CG-CD1	-8.32	116.01	121.00
2	e	4267	GLU	OE1-CD-OE2	-8.32	113.31	123.30
2	c	4335	ARG	CD-NE-CZ	8.31	135.24	123.60
2	c	4074	ASP	CB-CG-OD2	8.30	125.77	118.30
1	E	2011	LYS	O-C-N	8.29	135.97	122.70
2	e	4335	ARG	CD-NE-CZ	8.29	135.21	123.60
2	f	3481	ASP	CB-CG-OD2	8.29	125.76	118.30
2	c	4335	ARG	NE-CZ-NH2	8.29	124.44	120.30
1	A	32	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	E	1856	TYR	CB-CG-CD1	-8.26	116.04	121.00
1	E	1848	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	D	1425	TYR	CB-CG-CD1	-8.25	116.05	121.00
2	e	3987	TYR	CB-CG-CD2	-8.23	116.06	121.00
2	a	2636	ARG	NE-CZ-NH2	8.21	124.41	120.30
1	C	901	GLU	OE1-CD-OE2	-8.21	113.45	123.30
2	a	2592	GLU	OE1-CD-OE2	-8.21	113.45	123.30
2	d	3264	PRO	N-CA-CB	8.20	113.14	103.30
2	c	3991	ASP	CB-CG-OD2	8.19	125.67	118.30
2	f	3773	PHE	CB-CG-CD2	-8.19	115.07	120.80
2	a	2350	TYR	CB-CG-CD2	-8.19	116.09	121.00
2	d	3066	ASP	OD1-CG-OD2	-8.18	107.76	123.30
2	c	4146	ASP	CB-CG-OD1	8.17	125.66	118.30
2	e	3970	TYR	CB-CG-CD1	-8.17	116.10	121.00
1	F	1369	VAL	CA-CB-CG1	8.16	123.15	110.90
2	c	4331	ARG	CD-NE-CZ	8.16	135.03	123.60
2	e	4171	VAL	CA-CB-CG2	8.16	123.14	110.90
1	B	1945	PHE	CB-CG-CD1	8.16	126.51	120.80
2	b	3593	ASP	CB-CG-OD1	8.15	125.64	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	752	TYR	CB-CG-CD1	-8.14	116.12	121.00
1	E	1884	TYR	CB-CG-CD2	8.14	125.88	121.00
1	F	1393	PHE	CB-CG-CD2	-8.13	115.11	120.80
2	e	3970	TYR	CG-CD1-CE1	-8.13	114.80	121.30
1	E	1751	PHE	CB-CG-CD2	-8.13	115.11	120.80
2	e	4079	ARG	NH1-CZ-NH2	-8.12	110.47	119.40
1	E	2143	ASP	CB-CG-OD1	8.11	125.60	118.30
2	b	3760	TRP	CG-CD2-CE3	8.09	141.18	133.90
2	d	3320	ARG	CD-NE-CZ	8.08	134.91	123.60
2	b	3913	ASP	CB-CG-OD1	-8.06	111.04	118.30
2	b	3570	ASP	CB-CG-OD1	8.06	125.56	118.30
1	A	163	TYR	CB-CG-CD1	-8.06	116.17	121.00
1	B	1984	THR	CA-CB-CG2	8.05	123.67	112.40
1	C	936	ASP	CB-CG-OD2	8.04	125.53	118.30
2	g	2316	TYR	CB-CG-CD2	-8.03	116.18	121.00
2	b	3864	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	E	1819	GLU	CB-CG-CD	8.00	135.80	114.20
1	B	2249	ARG	NE-CZ-NH1	-7.99	116.31	120.30
2	d	3066	ASP	CB-CG-OD1	7.99	125.49	118.30
1	G	1029	TYR	CB-CG-CD2	-7.98	116.21	121.00
2	a	2397	THR	CA-CB-CG2	7.97	123.56	112.40
2	f	3688	ARG	CD-NE-CZ	7.97	134.75	123.60
1	B	2072	PRO	N-CA-CB	7.96	112.86	103.30
2	c	4113	ARG	NH1-CZ-NH2	-7.94	110.66	119.40
1	F	1496	PHE	CB-CG-CD1	-7.94	115.24	120.80
1	B	1805	GLU	OE1-CD-OE2	-7.94	113.77	123.30
1	G	747	GLU	OE1-CD-OE2	-7.94	113.78	123.30
2	b	3773	PHE	CB-CG-CD1	-7.93	115.25	120.80
1	B	2125	TYR	CB-CG-CD2	-7.92	116.25	121.00
2	b	3630	ALA	N-CA-CB	-7.92	99.01	110.10
2	d	3278	ALA	N-CA-CB	-7.91	99.03	110.10
1	D	1543	VAL	CA-CB-CG2	7.91	122.76	110.90
2	g	2554	TYR	CB-CG-CD1	-7.90	116.26	121.00
1	E	1922	GLU	OE1-CD-OE2	-7.90	113.82	123.30
1	G	945	TYR	CB-CG-CD2	-7.90	116.26	121.00
2	b	3722	ARG	NE-CZ-NH2	7.89	124.25	120.30
2	g	2479	ASP	CB-CG-OD1	7.88	125.39	118.30
1	B	1948	ASP	CB-CG-OD1	7.88	125.39	118.30
2	c	4226	GLU	OE1-CD-OE2	-7.87	113.86	123.30
1	E	1891	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	D	1538	PHE	CB-CG-CD1	-7.86	115.30	120.80
2	c	4423	TRP	CG-CD2-CE3	-7.86	126.82	133.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	3838	VAL	CG1-CB-CG2	-7.85	98.35	110.90
2	e	4443	PHE	CB-CG-CD2	-7.84	115.31	120.80
1	D	1426	GLU	OE1-CD-OE2	-7.82	113.91	123.30
1	A	212	ARG	NE-CZ-NH1	-7.82	116.39	120.30
1	F	1683	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	F	1548	TYR	CB-CG-CD2	7.80	125.68	121.00
2	c	4345	TYR	CB-CG-CD1	-7.80	116.32	121.00
1	G	920	ARG	NH1-CZ-NH2	7.79	127.96	119.40
1	A	503	THR	OG1-CB-CG2	-7.77	92.13	110.00
1	C	746	ARG	NE-CZ-NH2	7.76	124.18	120.30
2	g	2769	ASP	CB-CG-OD2	7.76	125.28	118.30
1	F	1542	TYR	CB-CG-CD2	-7.76	116.34	121.00
1	B	2170	ASP	CB-CG-OD2	-7.76	111.32	118.30
2	b	3788	TYR	CB-CG-CD2	-7.75	116.35	121.00
2	c	4117	ASP	CB-CG-OD1	-7.75	111.32	118.30
1	B	2076	ARG	CD-NE-CZ	7.74	134.43	123.60
2	a	2265	ARG	NH1-CZ-NH2	-7.74	110.89	119.40
1	A	201	ASP	CB-CG-OD2	7.73	125.26	118.30
2	g	2504	ARG	CD-NE-CZ	7.73	134.42	123.60
1	F	1471	PHE	CB-CG-CD1	7.72	126.21	120.80
1	A	180	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	E	2013	ILE	O-C-N	7.72	135.05	122.70
1	E	1834	ASP	CB-CG-OD2	7.71	125.24	118.30
2	c	4132	TYR	CB-CG-CD2	-7.70	116.38	121.00
2	c	4021	TYR	CB-CG-CD2	-7.69	116.38	121.00
1	E	1819	GLU	CA-C-O	-7.69	103.95	120.10
1	B	1865	ASP	CB-CG-OD2	-7.67	111.40	118.30
2	b	3422	ASP	CB-CG-OD2	7.67	125.20	118.30
1	A	2	TRP	CG-CD2-CE3	7.66	140.79	133.90
1	F	1170	TYR	CB-CG-CD2	7.65	125.59	121.00
1	B	2146	PRO	N-CD-CG	7.65	114.67	103.20
2	a	2753	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	F	1618	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	B	1730	ARG	CD-NE-CZ	7.63	134.29	123.60
1	E	2011	LYS	C-N-CA	-7.63	102.63	121.70
1	E	2177	PRO	N-CA-CB	7.62	112.45	103.30
2	g	2736	PRO	N-CA-CB	7.62	112.45	103.30
1	F	1304	TYR	CG-CD1-CE1	-7.62	115.21	121.30
1	C	636	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	D	1529	GLU	OE1-CD-OE2	-7.61	114.16	123.30
2	f	3557	GLU	OE1-CD-OE2	-7.61	114.16	123.30
1	A	374	PRO	N-CA-CB	7.61	112.43	103.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	e	4010	GLU	CA-CB-CG	7.59	130.11	113.40
1	C	621	PHE	CB-CG-CD2	-7.59	115.49	120.80
2	g	2461	TYR	CB-CG-CD1	7.58	125.55	121.00
2	e	4150	ASP	CB-CG-OD1	7.57	125.11	118.30
2	a	2303	ARG	NH1-CZ-NH2	-7.57	111.08	119.40
1	G	729	TYR	CB-CG-CD2	7.56	125.53	121.00
1	G	729	TYR	CB-CG-CD1	-7.55	116.47	121.00
1	D	1381	ALA	CB-CA-C	7.55	121.42	110.10
2	a	2663	ASP	CB-CG-OD1	7.54	125.09	118.30
2	d	2965	ARG	NE-CZ-NH2	-7.54	116.53	120.30
2	g	2348	ASP	CB-CG-OD1	7.53	125.08	118.30
1	A	350	GLU	OE1-CD-OE2	-7.53	114.27	123.30
2	a	2369	TYR	CB-CG-CD1	-7.52	116.49	121.00
1	D	1561	ARG	CD-NE-CZ	7.52	134.12	123.60
2	g	2664	ARG	NE-CZ-NH1	7.50	124.05	120.30
2	b	3750	ARG	NE-CZ-NH2	7.49	124.05	120.30
2	f	3890	VAL	CG1-CB-CG2	-7.49	98.91	110.90
2	e	4038	ASP	CB-CG-OD2	7.49	125.04	118.30
2	a	2408	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	A	163	TYR	CG-CD1-CE1	-7.47	115.32	121.30
2	b	3774	ARG	NE-CZ-NH2	-7.47	116.56	120.30
2	b	3426	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	B	1784	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	C	745	ASP	CB-CG-OD2	7.46	125.02	118.30
1	E	1725	ASP	CB-CG-OD1	7.46	125.01	118.30
2	c	4296	TYR	CB-CG-CD2	-7.45	116.53	121.00
1	E	2167	GLU	OE1-CD-OE2	-7.45	114.36	123.30
1	E	2010	HIS	CA-C-O	-7.45	104.46	120.10
1	C	993	TYR	CB-CG-CD2	-7.44	116.53	121.00
1	G	652	ARG	NE-CZ-NH2	7.43	124.01	120.30
1	B	1990	ASP	CB-CG-OD1	7.42	124.98	118.30
1	E	1932	GLU	OE1-CD-OE2	-7.41	114.41	123.30
2	b	3422	ASP	CB-CG-OD1	-7.40	111.64	118.30
1	A	285	VAL	CA-CB-CG1	7.40	122.00	110.90
2	b	3447	GLU	OE1-CD-OE2	-7.40	114.42	123.30
2	f	3750	ARG	CD-NE-CZ	7.39	133.95	123.60
1	A	110	PHE	CB-CG-CD1	-7.39	115.63	120.80
1	G	1006	VAL	CA-CB-CG2	7.39	121.98	110.90
1	B	2076	ARG	NH1-CZ-NH2	-7.39	111.27	119.40
1	C	913	TYR	CB-CG-CD2	-7.39	116.57	121.00
1	C	860	GLU	OE1-CD-OE2	-7.38	114.44	123.30
2	c	4079	ARG	NE-CZ-NH1	7.37	123.99	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	c	4382	VAL	CA-CB-CG2	7.36	121.94	110.90
1	D	1548	TYR	CB-CG-CD1	-7.36	116.59	121.00
2	c	4434	ARG	NE-CZ-NH1	7.35	123.98	120.30
2	c	3990	ARG	NE-CZ-NH1	7.35	123.97	120.30
2	c	4168	THR	CA-CB-CG2	7.35	122.69	112.40
2	c	3989	GLU	OE1-CD-OE2	-7.34	114.49	123.30
1	E	1847	TYR	CB-CG-CD2	-7.33	116.60	121.00
1	F	1432	ASP	CB-CG-OD2	7.33	124.90	118.30
2	g	2716	PRO	N-CA-CB	7.33	112.09	103.30
2	f	3908	ASP	CB-CG-OD2	7.32	124.89	118.30
1	G	837	TYR	CB-CG-CD2	-7.32	116.61	121.00
2	c	4157	ARG	NH1-CZ-NH2	-7.31	111.36	119.40
2	g	2630	ARG	NH1-CZ-NH2	-7.31	111.36	119.40
2	g	2653	THR	CA-CB-CG2	7.30	122.62	112.40
2	d	3076	ARG	NH1-CZ-NH2	-7.30	111.37	119.40
2	c	4035	ASP	CB-CG-OD2	7.28	124.86	118.30
2	c	3936	ARG	NE-CZ-NH2	7.28	123.94	120.30
2	g	2443	GLU	OE1-CD-OE2	-7.27	114.57	123.30
1	F	1312	ARG	CD-NE-CZ	7.27	133.78	123.60
2	c	3974	ARG	NE-CZ-NH2	-7.27	116.67	120.30
2	f	3512	ASP	CB-CG-OD1	7.27	124.84	118.30
2	e	4279	ARG	NE-CZ-NH1	7.27	123.93	120.30
2	g	2579	ARG	NE-CZ-NH1	-7.26	116.67	120.30
2	e	4378	PRO	N-CA-CB	7.25	112.01	103.30
1	A	32	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	F	1432	ASP	CB-CG-OD1	-7.25	111.78	118.30
2	g	2608	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	C	637	GLU	OE1-CD-OE2	-7.25	114.60	123.30
2	e	3967	TYR	CB-CG-CD1	-7.25	116.65	121.00
2	g	2630	ARG	NE-CZ-NH1	7.25	123.92	120.30
2	e	4072	GLU	OE1-CD-OE2	-7.24	114.61	123.30
2	a	2766	TYR	CB-CG-CD2	-7.24	116.66	121.00
2	g	2636	ARG	NH1-CZ-NH2	-7.24	111.43	119.40
2	e	3951	PRO	N-CA-CB	7.24	111.99	103.30
1	B	1891	ARG	CD-NE-CZ	7.24	133.73	123.60
2	c	4434	ARG	CD-NE-CZ	7.22	133.71	123.60
2	d	3165	ARG	NE-CZ-NH2	7.22	123.91	120.30
2	e	4160	TYR	CB-CG-CD1	-7.22	116.67	121.00
1	F	1325	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	B	1946	ASP	CB-CG-OD2	7.21	124.79	118.30
2	f	3710	GLU	OE1-CD-OE2	-7.21	114.65	123.30
2	c	4048	TYR	CB-CG-CD2	-7.21	116.68	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	e	4175	ARG	NE-CZ-NH2	7.21	123.90	120.30
2	g	2665	GLU	OE1-CD-OE2	-7.20	114.66	123.30
2	c	4423	TRP	CB-CG-CD2	7.20	135.96	126.60
2	d	3179	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	C	973	GLU	OE1-CD-OE2	-7.19	114.68	123.30
2	a	2611	GLU	OE1-CD-OE2	-7.19	114.67	123.30
2	d	2929	PHE	CB-CG-CD2	-7.18	115.78	120.80
1	G	1061	TRP	CG-CD2-CE3	7.17	140.36	133.90
1	A	140	PRO	N-CA-CB	7.17	111.91	103.30
1	E	1795	ARG	CD-NE-CZ	7.17	133.64	123.60
1	F	1242	PHE	CB-CG-CD1	7.17	125.82	120.80
2	f	3446	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	G	702	ASP	CB-CG-OD2	7.16	124.75	118.30
2	b	3538	PHE	CB-CG-CD1	7.15	125.80	120.80
2	e	3970	TYR	CD1-CG-CD2	7.14	125.76	117.90
1	A	354	ARG	NE-CZ-NH1	7.13	123.87	120.30
2	c	4423	TRP	CE2-CD2-CG	7.13	113.01	107.30
1	E	1779	TYR	CB-CG-CD2	7.13	125.28	121.00
2	d	3217	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	D	1465	VAL	O-C-N	7.12	134.10	122.70
1	G	1082	ARG	NE-CZ-NH2	-7.12	116.74	120.30
2	c	4021	TYR	CB-CG-CD1	7.12	125.27	121.00
1	G	676	PHE	CB-CG-CD1	-7.12	115.82	120.80
2	a	2630	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	E	1818	GLU	CA-CB-CG	-7.11	97.77	113.40
1	B	2214	ARG	NH1-CZ-NH2	-7.10	111.59	119.40
2	b	3379	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	G	991	GLU	OE1-CD-OE2	-7.10	114.78	123.30
1	A	84	ASP	CB-CG-OD2	7.09	124.68	118.30
1	A	141	ASN	CB-CA-C	7.09	124.58	110.40
1	E	1795	ARG	NE-CZ-NH2	7.09	123.84	120.30
1	B	2083	ARG	NH1-CZ-NH2	-7.08	111.61	119.40
2	f	3889	TYR	CB-CG-CD2	7.08	125.25	121.00
1	G	621	PHE	CB-CG-CD1	7.07	125.75	120.80
2	e	4455	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	C	1117	ARG	NH1-CZ-NH2	-7.06	111.63	119.40
1	B	1991	TYR	CB-CG-CD2	-7.05	116.77	121.00
1	E	1768	ARG	NE-CZ-NH2	7.05	123.82	120.30
1	A	466	VAL	CA-CB-CG2	7.05	121.47	110.90
2	b	3919	ASP	CB-CG-OD2	7.04	124.64	118.30
1	E	1795	ARG	NE-CZ-NH1	7.04	123.82	120.30
2	f	3598	PHE	CB-CG-CD2	-7.03	115.88	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1878	ARG	NE-CZ-NH2	-7.03	116.79	120.30
2	f	3410	TYR	CB-CG-CD2	-7.02	116.79	121.00
1	A	463	TYR	CG-CD1-CE1	-7.02	115.69	121.30
2	c	4409	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	D	1383	GLU	OE1-CD-OE2	-7.01	114.89	123.30
2	c	4279	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	D	1558	ASP	CB-CG-OD1	7.00	124.60	118.30
1	F	1502	ASP	CB-CG-OD1	7.00	124.60	118.30
2	e	4146	ASP	CB-CG-OD2	7.00	124.60	118.30
2	b	3636	TYR	CD1-CE1-CZ	6.99	126.09	119.80
2	d	3136	ARG	NE-CZ-NH2	6.99	123.80	120.30
1	E	1878	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	G	582	SER	N-CA-CB	6.98	120.97	110.50
2	e	4406	PRO	N-CA-CB	6.97	111.66	103.30
1	D	1282	ARG	NE-CZ-NH2	-6.96	116.82	120.30
2	e	4009	PHE	CB-CG-CD2	6.96	125.67	120.80
2	a	2300	TYR	CB-CG-CD1	-6.96	116.83	121.00
2	d	3243	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	F	1380	ASP	CB-CG-OD1	6.95	124.55	118.30
2	d	2958	GLU	OE1-CD-OE2	-6.95	114.96	123.30
2	d	2902	THR	CA-CB-CG2	6.95	122.12	112.40
2	g	2626	ASP	CB-CG-OD2	6.94	124.55	118.30
1	F	1455	PRO	N-CA-CB	6.94	111.62	103.30
2	a	2686	ARG	CD-NE-CZ	6.94	133.31	123.60
2	d	3362	ASP	CB-CG-OD2	6.93	124.54	118.30
1	G	702	ASP	OD1-CG-OD2	-6.93	110.13	123.30
1	A	193	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	C	743	THR	CA-CB-CG2	6.93	122.10	112.40
2	a	2659	PHE	CB-CG-CD2	6.93	125.65	120.80
1	A	418	VAL	CA-CB-CG1	6.93	121.29	110.90
1	B	1878	ARG	NH1-CZ-NH2	6.92	127.02	119.40
1	B	1878	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	B	1856	TYR	CB-CG-CD2	-6.91	116.85	121.00
1	A	38	TYR	CB-CG-CD1	-6.91	116.85	121.00
1	F	1229	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	A	464	VAL	CG1-CB-CG2	-6.91	99.85	110.90
1	D	1683	ARG	NE-CZ-NH2	-6.91	116.85	120.30
2	d	3283	VAL	CA-CB-CG2	6.90	121.25	110.90
1	C	1008	ASP	CB-CG-OD1	6.90	124.51	118.30
1	E	2095	GLU	OE1-CD-OE2	-6.89	115.04	123.30
2	a	2299	TYR	CG-CD1-CE1	-6.89	115.79	121.30
1	C	976	TYR	CG-CD1-CE1	-6.88	115.79	121.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	993	TYR	CG-CD2-CE2	-6.88	115.80	121.30
2	b	3693	ARG	NE-CZ-NH1	6.88	123.74	120.30
2	c	4190	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	D	1516	ASP	CB-CG-OD1	6.87	124.48	118.30
2	d	3323	TYR	CB-CG-CD1	-6.86	116.88	121.00
1	A	463	TYR	CB-CG-CD1	6.86	125.12	121.00
2	b	3880	TYR	CB-CG-CD2	-6.86	116.89	121.00
1	E	1969	TYR	CB-CG-CD2	-6.85	116.89	121.00
1	G	780	LEU	CB-CG-CD2	6.85	122.64	111.00
2	g	2587	VAL	CA-CB-CG1	6.85	121.17	110.90
2	c	4180	ASP	OD1-CG-OD2	-6.84	110.29	123.30
2	e	4439	ASN	CB-CA-C	6.84	124.09	110.40
2	a	2646	TRP	CH2-CZ2-CE2	6.84	124.24	117.40
2	d	3239	ASP	CB-CG-OD1	-6.84	112.15	118.30
1	C	1065	ARG	NH1-CZ-NH2	-6.83	111.89	119.40
2	e	4018	PRO	N-CA-CB	6.83	111.49	103.30
2	d	2873	TYR	CB-CG-CD1	-6.82	116.91	121.00
1	E	1820	LEU	CA-CB-CG	6.82	130.98	115.30
1	D	1608	ASN	O-C-N	-6.81	111.80	122.70
2	a	2763	ARG	NE-CZ-NH2	6.81	123.71	120.30
2	d	2860	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	E	1914	VAL	CB-CA-C	-6.81	98.46	111.40
2	c	4452	VAL	CG1-CB-CG2	-6.81	100.00	110.90
1	F	1502	ASP	CB-CG-OD2	6.81	124.42	118.30
2	c	4190	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	394	VAL	CG1-CB-CG2	-6.80	100.02	110.90
2	c	4301	ARG	NE-CZ-NH1	6.79	123.69	120.30
2	g	2403	ASP	CB-CG-OD1	6.79	124.41	118.30
2	f	3618	ARG	NH1-CZ-NH2	-6.79	111.94	119.40
1	A	464	VAL	CA-CB-CG2	6.78	121.07	110.90
1	D	1182	PHE	CB-CG-CD1	-6.78	116.05	120.80
2	e	4335	ARG	NE-CZ-NH1	6.78	123.69	120.30
2	b	3525	TYR	CD1-CG-CD2	6.77	125.35	117.90
2	c	4476	ASP	CB-CG-OD1	-6.77	112.20	118.30
2	g	2775	TYR	CD1-CG-CD2	6.77	125.35	117.90
1	E	1784	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	G	811	LYS	CB-CA-C	6.77	123.93	110.40
1	G	920	ARG	CD-NE-CZ	6.77	133.07	123.60
2	b	3693	ARG	CD-NE-CZ	6.76	133.07	123.60
2	d	3046	TYR	CB-CG-CD2	-6.76	116.94	121.00
1	C	1102	VAL	CA-CB-CG2	6.76	121.04	110.90
1	E	1852	LEU	CB-CG-CD2	6.76	122.49	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	d	3224	GLU	OE1-CD-OE2	-6.76	115.19	123.30
2	d	3193	ARG	NE-CZ-NH1	-6.76	116.92	120.30
2	g	2265	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	C	638	GLU	OE1-CD-OE2	-6.75	115.20	123.30
1	F	1380	ASP	CB-CG-OD2	6.75	124.38	118.30
2	c	4307	ARG	NE-CZ-NH2	-6.75	116.93	120.30
2	d	3193	ARG	CD-NE-CZ	6.75	133.04	123.60
2	f	3497	GLU	OE1-CD-OE2	-6.74	115.21	123.30
1	C	837	TYR	CB-CG-CD2	-6.74	116.96	121.00
1	E	2108	TYR	CB-CG-CD1	-6.74	116.96	121.00
1	A	427	TYR	CB-CG-CD2	-6.73	116.96	121.00
2	c	4152	LEU	CB-CG-CD2	6.73	122.44	111.00
2	e	4082	TYR	CB-CG-CD2	-6.73	116.96	121.00
2	g	2682	ASP	CB-CG-OD1	-6.73	112.24	118.30
1	A	173	THR	CA-CB-CG2	-6.73	102.98	112.40
1	A	190	VAL	CG1-CB-CG2	-6.73	100.14	110.90
1	E	1748	PHE	CB-CG-CD1	-6.73	116.09	120.80
1	F	1631	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	D	1448	ARG	NE-CZ-NH2	-6.72	116.94	120.30
2	b	3632	TRP	NE1-CE2-CZ2	6.72	137.79	130.40
2	b	3862	VAL	CG1-CB-CG2	-6.72	100.15	110.90
2	a	2739	PHE	CB-CG-CD2	-6.71	116.10	120.80
2	e	4200	GLU	OE1-CD-OE2	-6.71	115.25	123.30
1	B	1999	PHE	CB-CG-CD2	6.71	125.49	120.80
1	E	1899	ASP	CA-CB-CG	6.70	128.15	113.40
1	A	311	PHE	CB-CG-CD1	-6.70	116.11	120.80
1	E	2178	PHE	CB-CG-CD1	6.70	125.49	120.80
2	f	3750	ARG	NH1-CZ-NH2	-6.69	112.04	119.40
2	g	2275	GLU	OE1-CD-OE2	-6.68	115.28	123.30
1	C	920	ARG	NE-CZ-NH2	6.68	123.64	120.30
2	f	3740	ASP	CB-CG-OD1	6.68	124.31	118.30
1	F	1170	TYR	CB-CG-CD1	-6.67	117.00	121.00
1	B	2193	TRP	CE2-CD2-CE3	-6.67	110.69	118.70
1	D	1268	ASP	OD1-CG-OD2	-6.67	110.63	123.30
1	D	1350	ASP	CB-CG-OD2	6.67	124.30	118.30
1	E	2014	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	F	1621	PRO	N-CA-CB	6.67	111.30	103.30
2	d	2870	ASN	CB-CA-C	6.67	123.73	110.40
1	C	872	ALA	CB-CA-C	6.66	120.10	110.10
2	d	3339	ARG	CD-NE-CZ	6.66	132.93	123.60
1	G	828	THR	CA-CB-CG2	6.66	121.73	112.40
1	G	993	TYR	CB-CG-CD1	-6.66	117.01	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1784	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	E	2168	ASP	OD1-CG-OD2	-6.65	110.66	123.30
2	c	3999	ARG	NE-CZ-NH2	6.65	123.63	120.30
1	G	814	ASP	OD1-CG-OD2	-6.65	110.66	123.30
2	a	2380	THR	CA-CB-CG2	6.65	121.70	112.40
1	A	61	GLU	OE1-CD-OE2	-6.64	115.33	123.30
2	g	2753	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	C	747	GLU	OE1-CD-OE2	-6.63	115.34	123.30
1	G	798	VAL	CA-CB-CG2	6.63	120.84	110.90
2	b	3740	ASP	CB-CG-OD2	6.62	124.26	118.30
1	G	951	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	81	TYR	CB-CG-CD1	-6.61	117.03	121.00
1	B	1985	LEU	CB-CG-CD1	6.61	122.24	111.00
2	f	3633	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	B	2161	TYR	CB-CG-CD1	-6.61	117.04	121.00
1	D	1661	PHE	CB-CG-CD1	-6.61	116.18	120.80
2	c	4307	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	B	2107	ARG	NH1-CZ-NH2	-6.60	112.14	119.40
1	E	2154	THR	CA-CB-CG2	6.60	121.64	112.40
2	f	3414	TYR	CB-CG-CD1	-6.60	117.04	121.00
2	g	2419	PRO	N-CA-CB	6.60	111.22	103.30
1	A	53	PHE	CB-CG-CD1	-6.59	116.19	120.80
2	g	2504	ARG	NE-CZ-NH2	6.59	123.60	120.30
1	A	370	ASP	CB-CG-OD2	6.59	124.23	118.30
2	f	3693	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	E	1701	ILE	CA-CB-CG2	6.58	124.06	110.90
1	F	1502	ASP	OD1-CG-OD2	-6.58	110.80	123.30
2	b	3778	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	D	1389	TRP	CH2-CZ2-CE2	6.58	123.98	117.40
2	b	3525	TYR	CG-CD1-CE1	-6.58	116.04	121.30
1	A	518	GLU	OE1-CD-OE2	-6.57	115.42	123.30
2	f	3705	VAL	CG1-CB-CG2	-6.57	100.39	110.90
2	c	4117	ASP	CB-CG-OD2	6.57	124.21	118.30
1	D	1451	TYR	CB-CG-CD1	-6.57	117.06	121.00
1	A	261	PHE	CB-CG-CD1	-6.57	116.20	120.80
2	d	3294	PHE	CB-CG-CD1	-6.57	116.20	120.80
1	C	571	ALA	CB-CA-C	6.56	119.94	110.10
2	b	3688	ARG	NE-CZ-NH1	6.56	123.58	120.30
2	c	4092	PRO	N-CA-CB	6.56	111.17	103.30
2	f	3660	LEU	CA-CB-CG	6.55	130.38	115.30
2	d	3320	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	C	1036	ASP	CB-CG-OD1	6.54	124.19	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2009	PHE	CB-CG-CD2	-6.54	116.22	120.80
1	A	152	VAL	CG1-CB-CG2	-6.54	100.44	110.90
2	d	2865	ASP	CB-CG-OD2	6.54	124.18	118.30
1	C	816	ASP	CB-CG-OD1	6.54	124.18	118.30
1	G	857	VAL	CA-CB-CG2	6.54	120.70	110.90
2	c	4351	ALA	CB-CA-C	6.54	119.91	110.10
2	e	4421	ARG	CD-NE-CZ	6.53	132.75	123.60
2	a	2499	ASP	CB-CG-OD1	6.53	124.17	118.30
2	g	2486	ARG	NE-CZ-NH1	-6.53	117.04	120.30
1	F	1648	ARG	NH1-CZ-NH2	-6.52	112.22	119.40
1	G	746	ARG	NH1-CZ-NH2	-6.52	112.22	119.40
2	f	3841	ASP	OD1-CG-OD2	-6.52	110.91	123.30
2	e	4148	VAL	CA-CB-CG2	6.52	120.67	110.90
1	B	2020	THR	CA-CB-CG2	6.50	121.51	112.40
2	e	4423	TRP	NE1-CE2-CD2	-6.50	100.80	107.30
2	f	3426	ARG	NH1-CZ-NH2	-6.50	112.25	119.40
1	F	1517	ARG	NH1-CZ-NH2	-6.50	112.25	119.40
2	b	3751	TYR	CB-CG-CD1	-6.50	117.10	121.00
2	e	4220	VAL	CA-CB-CG1	6.50	120.64	110.90
1	G	679	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	321	PRO	N-CA-CB	6.49	111.09	103.30
2	d	2856	TYR	CB-CG-CD1	-6.49	117.11	121.00
1	E	2033	GLU	OE1-CD-OE2	-6.49	115.52	123.30
2	c	4317	TRP	NE1-CE2-CZ2	6.49	137.53	130.40
1	G	752	TYR	CB-CG-CD2	-6.48	117.11	121.00
2	a	2364	ASP	CB-CG-OD2	-6.48	112.47	118.30
2	b	3578	LEU	CB-CG-CD1	-6.48	99.98	111.00
1	B	1768	ARG	CD-NE-CZ	6.48	132.67	123.60
1	F	1170	TYR	CG-CD1-CE1	6.48	126.48	121.30
1	F	1423	VAL	CG1-CB-CG2	6.48	121.27	110.90
2	e	4119	TYR	CG-CD1-CE1	-6.48	116.12	121.30
1	G	1059	GLU	OE1-CD-OE2	-6.47	115.54	123.30
2	d	3239	ASP	CB-CG-OD2	6.47	124.12	118.30
1	A	212	ARG	CD-NE-CZ	6.46	132.65	123.60
2	b	3525	TYR	CG-CD2-CE2	-6.46	116.13	121.30
2	g	2319	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	E	1861	TYR	CB-CG-CD1	-6.45	117.13	121.00
1	D	1314	GLU	OE1-CD-OE2	-6.45	115.56	123.30
1	F	1380	ASP	OD1-CG-OD2	-6.45	111.05	123.30
1	A	38	TYR	CG-CD1-CE1	-6.44	116.14	121.30
1	A	168	THR	CA-CB-CG2	6.44	121.42	112.40
2	e	3979	ASP	CB-CG-OD2	6.44	124.10	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	113	ASP	CB-CG-OD2	6.43	124.08	118.30
1	E	1795	ARG	NH1-CZ-NH2	-6.43	112.33	119.40
2	f	3433	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	E	2187	PRO	N-CA-CB	6.42	111.00	103.30
2	b	3417	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	G	867	PHE	CB-CG-CD1	-6.42	116.31	120.80
2	b	3883	ASP	CB-CG-OD1	-6.42	112.53	118.30
2	e	3991	ASP	CB-CG-OD2	6.41	124.07	118.30
2	d	2998	ASP	CB-CG-OD2	6.41	124.07	118.30
1	C	1102	VAL	CG1-CB-CG2	-6.40	100.66	110.90
1	D	1673	VAL	CG1-CB-CG2	-6.40	100.66	110.90
1	F	1302	GLU	OE1-CD-OE2	-6.40	115.62	123.30
1	G	782	VAL	CG1-CB-CG2	-6.40	100.66	110.90
2	f	3575	TYR	CG-CD2-CE2	-6.40	116.18	121.30
2	g	2318	GLU	OE1-CD-OE2	-6.39	115.63	123.30
1	C	725	PRO	N-CD-CG	6.39	112.79	103.20
2	c	4048	TYR	CG-CD2-CE2	-6.39	116.19	121.30
2	d	2882	TYR	CB-CG-CD2	-6.39	117.17	121.00
2	g	2316	TYR	CG-CD1-CE1	-6.39	116.19	121.30
1	A	93	PRO	N-CA-CB	6.39	110.97	103.30
2	e	4301	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	C	800	GLU	OE1-CD-OE2	-6.39	115.64	123.30
2	a	2296	TYR	CG-CD1-CE1	-6.38	116.19	121.30
1	G	720	LEU	CB-CG-CD1	-6.38	100.16	111.00
2	f	3659	VAL	CA-CB-CG2	6.38	120.46	110.90
2	c	3996	TYR	CB-CG-CD2	-6.37	117.18	121.00
2	c	4169	VAL	CA-CB-CG1	6.37	120.46	110.90
2	e	3952	PHE	CB-CG-CD1	-6.37	116.34	120.80
1	D	1683	ARG	NE-CZ-NH1	6.36	123.48	120.30
2	f	3447	GLU	OE1-CD-OE2	-6.35	115.67	123.30
1	D	1312	ARG	NE-CZ-NH1	6.35	123.48	120.30
2	f	3862	VAL	CA-CB-CG1	6.35	120.42	110.90
1	D	1182	PHE	CG-CD2-CE2	-6.35	113.82	120.80
1	E	1947	ALA	CB-CA-C	6.34	119.62	110.10
1	E	2014	ARG	C-N-CA	6.34	137.56	121.70
2	c	3942	CYS	CA-CB-SG	-6.34	102.58	114.00
2	a	2714	CYS	CA-CB-SG	-6.34	102.59	114.00
2	a	2730	GLU	OE1-CD-OE2	-6.34	115.70	123.30
2	e	4191	ALA	CB-CA-C	-6.34	100.59	110.10
2	b	3889	TYR	CB-CG-CD1	-6.33	117.20	121.00
1	A	149	TYR	CB-CG-CD2	-6.33	117.20	121.00
2	a	2803	GLU	OE1-CD-OE2	-6.33	115.70	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	c	4448	VAL	CG1-CB-CG2	-6.32	100.78	110.90
2	a	2763	ARG	CD-NE-CZ	6.32	132.45	123.60
1	A	86	ARG	CD-NE-CZ	6.31	132.44	123.60
2	e	4345	TYR	CD1-CE1-CZ	6.31	125.48	119.80
2	g	2622	TYR	CB-CG-CD1	-6.31	117.21	121.00
2	g	2783	ASP	CB-CG-OD1	6.31	123.98	118.30
1	F	1393	PHE	CB-CG-CD1	6.31	125.21	120.80
2	b	3464	TYR	CB-CG-CD1	-6.31	117.22	121.00
1	E	1865	ASP	CB-CG-OD1	6.30	123.97	118.30
1	F	1295	TYR	CB-CG-CD2	6.30	124.78	121.00
1	F	1350	ASP	CB-CG-OD1	6.30	123.97	118.30
2	b	3625	ASP	CB-CG-OD1	6.30	123.97	118.30
2	b	3873	ASP	CB-CG-OD1	6.30	123.97	118.30
2	e	3997	CYS	CB-CA-C	6.30	123.01	110.40
1	C	625	THR	CA-CB-CG2	6.30	121.22	112.40
1	C	882	ARG	NH1-CZ-NH2	-6.30	112.47	119.40
2	d	3327	PRO	N-CA-CB	6.30	110.86	103.30
1	A	275	GLU	OE1-CD-OE2	-6.30	115.74	123.30
1	C	636	ARG	N-CA-CB	-6.30	99.27	110.60
2	e	4046	GLU	OE1-CD-OE2	-6.30	115.75	123.30
1	G	702	ASP	CB-CG-OD1	6.29	123.97	118.30
2	d	3018	TYR	CB-CG-CD1	-6.29	117.22	121.00
2	e	4266	ASP	CB-CG-OD1	6.29	123.97	118.30
2	g	2328	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	110	PHE	CB-CG-CD2	6.29	125.20	120.80
1	C	885	TYR	CB-CG-CD2	-6.29	117.23	121.00
2	d	3255	ASP	CB-CG-OD2	6.29	123.96	118.30
2	d	2944	VAL	CA-CB-CG2	6.29	120.33	110.90
2	e	4058	VAL	CA-CB-CG1	-6.29	101.47	110.90
2	e	4242	PRO	N-CA-CB	6.29	110.84	103.30
2	c	4434	ARG	NE-CZ-NH2	-6.28	117.16	120.30
2	e	4204	PHE	CB-CG-CD2	6.28	125.20	120.80
1	G	888	THR	CA-CB-CG2	-6.28	103.61	112.40
2	g	2763	ARG	NH1-CZ-NH2	-6.28	112.50	119.40
2	g	2782	ARG	NH1-CZ-NH2	-6.28	112.50	119.40
2	f	3632	TRP	CE2-CD2-CE3	-6.27	111.17	118.70
1	C	952	ASP	CB-CG-OD2	6.27	123.94	118.30
1	B	2193	TRP	CD2-CE3-CZ3	6.26	126.94	118.80
2	b	3715	ASN	N-CA-CB	-6.26	99.32	110.60
2	f	3633	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	C	784	ASP	CB-CG-OD1	6.26	123.94	118.30
1	E	1853	GLU	OE1-CD-OE2	-6.26	115.79	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	e	4440	ASP	CB-CG-OD1	6.26	123.94	118.30
2	f	3866	TRP	CA-CB-CG	6.26	125.59	113.70
2	c	4054	GLU	OE1-CD-OE2	-6.25	115.80	123.30
2	f	3522	ARG	CD-NE-CZ	6.25	132.35	123.60
1	C	935	GLU	OE1-CD-OE2	-6.25	115.80	123.30
1	G	932	ALA	CB-CA-C	6.25	119.47	110.10
1	F	1597	ASN	CB-CA-C	6.24	122.88	110.40
2	a	2430	THR	CA-CB-CG2	6.24	121.13	112.40
2	e	4307	ARG	NH1-CZ-NH2	-6.24	112.54	119.40
2	g	2408	ARG	NH1-CZ-NH2	-6.24	112.54	119.40
1	F	1320	LEU	CB-CG-CD2	-6.24	100.40	111.00
2	a	2491	THR	CA-CB-CG2	6.23	121.13	112.40
2	f	3433	ARG	CD-NE-CZ	6.23	132.33	123.60
1	D	1425	TYR	CD1-CG-CD2	6.23	124.76	117.90
2	g	2398	ASP	OD1-CG-OD2	-6.23	111.46	123.30
2	a	2296	TYR	CB-CG-CD2	-6.23	117.26	121.00
2	e	4038	ASP	CB-CG-OD1	-6.23	112.69	118.30
1	F	1631	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	E	1709	GLU	OE1-CD-OE2	-6.21	115.84	123.30
2	g	2509	ASP	OD1-CG-OD2	-6.21	111.49	123.30
2	c	4114	GLU	OE1-CD-OE2	-6.21	115.84	123.30
1	B	1736	TYR	CB-CG-CD2	-6.21	117.27	121.00
1	C	631	THR	CA-CB-CG2	6.21	121.09	112.40
1	D	1336	VAL	CA-CB-CG2	6.21	120.22	110.90
1	F	1229	ARG	CD-NE-CZ	6.21	132.29	123.60
2	a	2674	TYR	CB-CG-CD2	6.21	124.72	121.00
2	a	2674	TYR	CB-CG-CD1	-6.21	117.28	121.00
1	C	748	GLU	N-CA-CB	-6.20	99.44	110.60
2	d	3258	ASP	CB-CA-C	6.20	122.81	110.40
1	G	647	TYR	CG-CD2-CE2	-6.20	116.34	121.30
2	g	2499	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	70	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	e	4367	LEU	CB-CG-CD2	6.18	121.51	111.00
2	e	4370	VAL	CA-CB-CG1	6.17	120.16	110.90
2	g	2303	ARG	CD-NE-CZ	6.17	132.24	123.60
1	E	2083	ARG	NE-CZ-NH2	6.17	123.39	120.30
1	B	1738	TYR	CG-CD2-CE2	-6.17	116.36	121.30
2	b	3867	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	20	PRO	N-CA-CB	6.17	110.70	103.30
1	B	2167	GLU	OE1-CD-OE2	-6.17	115.90	123.30
1	E	2127	ARG	CA-CB-CG	6.17	126.96	113.40
1	C	624	ASP	CB-CG-OD2	-6.16	112.76	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	946	VAL	CG1-CB-CG2	-6.16	101.05	110.90
2	b	3650	VAL	CA-CB-CG1	6.16	120.14	110.90
2	d	2869	ARG	NH1-CZ-NH2	-6.16	112.63	119.40
2	b	3469	PRO	N-CA-CB	6.15	110.69	103.30
1	C	809	ARG	NE-CZ-NH1	6.14	123.37	120.30
2	d	2873	TYR	CG-CD2-CE2	-6.13	116.39	121.30
1	D	1163	GLU	OE1-CD-OE2	-6.13	115.95	123.30
1	A	13	GLU	OE1-CD-OE2	-6.13	115.95	123.30
2	e	4003	ARG	NE-CZ-NH2	6.13	123.36	120.30
2	d	3179	TYR	CB-CG-CD1	6.12	124.67	121.00
2	g	2489	TYR	CB-CG-CD1	-6.12	117.33	121.00
1	G	778	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	1767	ASP	CB-CG-OD2	6.12	123.81	118.30
2	f	3864	ARG	NH1-CZ-NH2	-6.12	112.67	119.40
1	B	1959	PHE	CB-CG-CD1	6.11	125.08	120.80
2	a	2608	ARG	NE-CZ-NH1	6.11	123.35	120.30
2	f	3600	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	E	2223	ASP	CB-CG-OD2	-6.10	112.81	118.30
2	e	4408	PHE	CB-CG-CD2	-6.10	116.53	120.80
1	F	1159	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	E	1708	ARG	CD-NE-CZ	6.10	132.13	123.60
2	c	4057	ARG	NE-CZ-NH1	6.10	123.35	120.30
2	c	3997	CYS	CA-CB-SG	-6.09	103.05	114.00
2	c	4179	GLU	CB-CG-CD	-6.09	97.76	114.20
2	c	4014	PHE	CB-CG-CD1	-6.08	116.54	120.80
2	c	4160	TYR	CG-CD2-CE2	-6.08	116.43	121.30
2	f	3886	PHE	CB-CG-CD2	-6.08	116.54	120.80
2	b	3402	VAL	CA-CB-CG2	6.08	120.02	110.90
2	b	3622	GLU	OE1-CD-OE2	-6.08	116.01	123.30
1	F	1448	ARG	CD-NE-CZ	6.07	132.10	123.60
2	e	4263	GLU	OE1-CD-OE2	-6.07	116.01	123.30
1	D	1141	LEU	CB-CG-CD2	6.07	121.31	111.00
1	F	1424	ASP	CB-CG-OD2	-6.07	112.84	118.30
2	d	3341	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	E	1856	TYR	CG-CD2-CE2	-6.07	116.45	121.30
2	f	3815	ASP	CB-CG-OD1	6.07	123.76	118.30
1	B	1969	TYR	CG-CD1-CE1	-6.06	116.45	121.30
1	E	2107	ARG	NE-CZ-NH1	6.06	123.33	120.30
2	d	3105	VAL	CG1-CB-CG2	-6.06	101.20	110.90
2	f	3763	ILE	CA-CB-CG2	6.06	123.02	110.90
2	b	3919	ASP	OD1-CG-OD2	-6.06	111.79	123.30
1	A	339	PHE	CB-CG-CD1	6.05	125.04	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	d	3111	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	A	305	VAL	CG1-CB-CG2	-6.05	101.22	110.90
1	C	606	TYR	CD1-CE1-CZ	-6.05	114.36	119.80
2	f	3877	ARG	NH1-CZ-NH2	-6.05	112.75	119.40
2	a	2614	GLU	OE1-CD-OE2	-6.05	116.04	123.30
1	E	2083	ARG	NE-CZ-NH1	-6.05	117.28	120.30
2	e	4140	THR	CA-CB-CG2	6.05	120.86	112.40
2	b	3496	PHE	CB-CG-CD1	-6.04	116.57	120.80
2	g	2729	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	C	745	ASP	OD1-CG-OD2	-6.04	111.82	123.30
2	a	2291	ASP	CB-CG-OD2	6.04	123.74	118.30
2	c	4446	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	D	1602	ASP	CB-CG-OD2	6.04	123.73	118.30
1	B	2227	PHE	CB-CG-CD1	6.04	125.03	120.80
2	f	3805	THR	CA-CB-CG2	6.03	120.84	112.40
1	B	1762	VAL	CA-CB-CG1	6.03	119.94	110.90
1	F	1467	GLU	OE1-CD-OE2	-6.03	116.06	123.30
2	b	3493	PHE	CB-CG-CD1	6.03	125.02	120.80
2	b	3690	ALA	N-CA-CB	-6.03	101.67	110.10
2	c	4279	ARG	NE-CZ-NH2	6.03	123.31	120.30
1	C	944	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	E	1945	PHE	CB-CG-CD2	-6.02	116.59	120.80
2	f	3642	ASN	CB-CA-C	6.02	122.44	110.40
2	e	4023	PRO	N-CA-CB	6.02	110.52	103.30
2	c	3987	TYR	N-CA-CB	-6.02	99.77	110.60
2	e	4001	VAL	CA-CB-CG2	6.01	119.92	110.90
1	G	1018	GLU	OE1-CD-OE2	-6.01	116.09	123.30
1	E	2076	ARG	NH1-CZ-NH2	-6.01	112.79	119.40
1	G	1065	ARG	CD-NE-CZ	6.01	132.01	123.60
2	d	3318	ALA	N-CA-CB	-6.01	101.69	110.10
1	D	1425	TYR	CG-CD2-CE2	-6.00	116.50	121.30
1	F	1462	VAL	CA-CB-CG2	6.00	119.90	110.90
2	c	4132	TYR	CG-CD2-CE2	-6.00	116.50	121.30
2	f	3522	ARG	NH1-CZ-NH2	-6.00	112.80	119.40
2	d	2856	TYR	CD1-CG-CD2	6.00	124.49	117.90
1	G	576	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	B	1874	VAL	CA-CB-CG1	5.99	119.89	110.90
1	B	1767	ASP	CB-CG-OD1	5.99	123.69	118.30
2	b	3795	SER	C-N-CA	5.99	136.68	121.70
2	a	2398	ASP	OD1-CG-OD2	-5.99	111.93	123.30
2	d	2822	ARG	CD-NE-CZ	5.98	131.98	123.60
1	A	271	TYR	CB-CG-CD2	5.98	124.59	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	988	ALA	CB-CA-C	5.98	119.07	110.10
1	E	1916	ASP	CB-CG-OD1	5.98	123.68	118.30
1	D	1242	PHE	CB-CG-CD2	-5.98	116.61	120.80
1	E	2086	TRP	CD1-CG-CD2	-5.97	101.52	106.30
2	f	3380	TRP	CD2-CE3-CZ3	5.97	126.57	118.80
1	D	1520	TRP	CA-CB-CG	5.97	125.05	113.70
2	c	4190	ARG	CD-NE-CZ	5.97	131.96	123.60
2	e	4455	ARG	CD-NE-CZ	-5.97	115.25	123.60
2	b	3430	TYR	CG-CD2-CE2	-5.96	116.53	121.30
1	G	600	LEU	CB-CG-CD2	5.96	121.13	111.00
2	c	4412	LEU	CB-CG-CD1	5.96	121.12	111.00
2	g	2574	ARG	NE-CZ-NH2	5.95	123.28	120.30
1	B	2161	TYR	CG-CD2-CE2	-5.95	116.54	121.30
2	g	2745	THR	O-C-N	-5.95	113.18	122.70
1	D	1218	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	F	1592	ASP	OD1-CG-OD2	-5.94	112.01	123.30
1	F	1318	TYR	CG-CD1-CE1	-5.94	116.55	121.30
2	f	3636	TYR	CB-CG-CD2	-5.94	117.44	121.00
2	f	3845	PRO	N-CA-CB	5.94	110.42	103.30
2	f	3889	TYR	CB-CG-CD1	-5.94	117.44	121.00
1	D	1261	VAL	CA-CB-CG2	5.93	119.79	110.90
1	E	2031	VAL	CA-CB-CG1	5.93	119.79	110.90
1	D	1479	TYR	CG-CD1-CE1	-5.92	116.56	121.30
1	E	1919	PRO	N-CD-CG	5.92	112.08	103.20
1	A	445	ASP	CB-CG-OD2	5.92	123.63	118.30
2	a	2771	PRO	N-CD-CG	5.92	112.08	103.20
1	E	2013	ILE	N-CA-C	-5.92	95.03	111.00
1	G	866	ASP	CA-CB-CG	5.91	126.39	113.40
1	F	1187	PHE	CD1-CE1-CZ	-5.91	113.01	120.10
2	c	3979	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	C	752	TYR	CG-CD1-CE1	-5.90	116.58	121.30
2	a	2762	ALA	N-CA-CB	-5.90	101.84	110.10
2	d	3182	TYR	CB-CG-CD1	-5.90	117.46	121.00
1	D	1320	LEU	CB-CG-CD1	5.90	121.03	111.00
1	A	505	VAL	CA-CB-CG2	5.90	119.75	110.90
2	g	2462	PHE	CB-CG-CD2	5.90	124.93	120.80
2	b	3736	TYR	CB-CG-CD1	-5.89	117.46	121.00
2	f	3908	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	G	1058	ALA	CB-CA-C	5.89	118.94	110.10
2	f	3718	ILE	CA-CB-CG1	5.89	122.19	111.00
2	e	4040	TYR	CZ-CE2-CD2	-5.89	114.50	119.80
2	c	4468	LEU	CB-CG-CD1	5.88	121.00	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	3552	SER	O-C-N	-5.88	113.29	122.70
1	B	1891	ARG	NH1-CZ-NH2	-5.88	112.93	119.40
2	g	2803	GLU	CG-CD-OE2	5.88	130.06	118.30
2	d	3095	ASP	CB-CG-OD2	5.88	123.59	118.30
1	B	2168	ASP	CB-CG-OD2	5.87	123.58	118.30
2	a	2806	CYS	CA-CB-SG	5.87	124.56	114.00
1	E	2048	GLU	OE1-CD-OE2	-5.87	116.26	123.30
1	G	882	ARG	NE-CZ-NH1	-5.86	117.37	120.30
2	c	3976	PRO	N-CA-CB	5.86	110.33	103.30
2	e	4423	TRP	CD1-NE1-CE2	5.86	114.27	109.00
1	A	248	ASP	OD1-CG-OD2	-5.86	112.17	123.30
1	G	754	LEU	CA-CB-CG	5.86	128.77	115.30
1	D	1170	TYR	CB-CG-CD2	-5.85	117.49	121.00
2	c	4308	TYR	CB-CG-CD1	-5.85	117.49	121.00
1	C	913	TYR	CG-CD1-CE1	-5.85	116.62	121.30
2	e	4378	PRO	N-CD-CG	5.84	111.97	103.20
2	e	4424	ARG	NE-CZ-NH1	5.84	123.22	120.30
2	f	3722	ARG	CD-NE-CZ	5.84	131.78	123.60
1	B	1969	TYR	CB-CG-CD1	-5.84	117.50	121.00
1	D	1347	ASP	CB-CG-OD1	5.84	123.56	118.30
2	e	4378	PRO	CA-N-CD	-5.84	103.32	111.50
2	b	3623	ASP	OD1-CG-OD2	-5.84	112.21	123.30
2	c	4187	ALA	N-CA-CB	-5.84	101.92	110.10
1	C	958	ASP	CB-CG-OD1	5.84	123.55	118.30
2	f	3843	ASP	CB-CG-OD1	-5.84	113.05	118.30
1	E	2223	ASP	CB-CG-OD1	5.83	123.55	118.30
2	d	2980	LEU	CB-CG-CD2	5.83	120.92	111.00
2	d	2919	ILE	CA-CB-CG1	5.83	122.08	111.00
1	A	136	ASP	OD1-CG-OD2	-5.83	112.22	123.30
2	g	2367	ASP	CB-CG-OD1	-5.83	113.05	118.30
1	A	498	ALA	CB-CA-C	5.83	118.84	110.10
2	c	4348	THR	CA-CB-CG2	5.83	120.56	112.40
1	G	642	PHE	CB-CG-CD2	-5.82	116.72	120.80
1	D	1337	LYS	CB-CA-C	5.82	122.04	110.40
1	G	620	VAL	CA-CB-CG2	5.82	119.63	110.90
2	e	4182	ASP	CB-CA-C	5.82	122.04	110.40
2	f	3560	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	1713	LEU	CB-CG-CD2	5.81	120.88	111.00
1	A	385	ARG	CD-NE-CZ	5.81	131.74	123.60
2	c	4454	ASP	CB-CG-OD1	5.81	123.53	118.30
1	C	1038	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	F	1547	THR	CA-CB-CG2	5.80	120.52	112.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	a	2595	ASP	CB-CG-OD1	5.80	123.52	118.30
2	f	3560	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	B	1767	ASP	OD1-CG-OD2	-5.80	112.28	123.30
1	A	385	ARG	NH1-CZ-NH2	-5.79	113.03	119.40
1	G	663	ARG	CD-NE-CZ	5.79	131.70	123.60
2	g	2381	ILE	CA-C-O	-5.79	107.94	120.10
2	a	2701	ASP	CB-CG-OD1	5.79	123.51	118.30
1	C	841	GLU	OE1-CD-OE2	-5.79	116.36	123.30
1	C	975	ARG	NE-CZ-NH1	5.78	123.19	120.30
2	e	4419	VAL	CB-CA-C	5.78	122.39	111.40
2	d	3235	VAL	CA-CB-CG2	5.78	119.57	110.90
2	e	4021	TYR	CB-CG-CD1	-5.78	117.53	121.00
2	e	4459	SER	N-CA-CB	-5.78	101.83	110.50
1	C	1049	SER	N-CA-CB	-5.78	101.84	110.50
1	G	729	TYR	CZ-CE2-CD2	-5.77	114.60	119.80
2	d	3112	GLU	OE1-CD-OE2	-5.77	116.38	123.30
2	f	3905	THR	CA-CB-CG2	5.77	120.48	112.40
1	C	1029	TYR	CG-CD2-CE2	-5.77	116.69	121.30
2	e	3970	TYR	CG-CD2-CE2	-5.77	116.69	121.30
1	E	2090	ASP	OD1-CG-OD2	-5.76	112.35	123.30
1	F	1404	PHE	CB-CG-CD1	5.76	124.83	120.80
2	c	4402	PRO	N-CD-CG	5.76	111.85	103.20
2	a	2458	ASP	CB-CG-OD1	-5.76	113.11	118.30
2	b	3503	THR	CA-CB-CG2	5.76	120.46	112.40
2	b	3562	TYR	CG-CD1-CE1	-5.76	116.69	121.30
2	f	3467	GLU	OE1-CD-OE2	-5.76	116.39	123.30
2	a	2650	ASP	OD1-CG-OD2	-5.76	112.36	123.30
2	e	4382	VAL	CG1-CB-CG2	-5.76	101.69	110.90
2	d	3038	LEU	CB-CG-CD1	5.75	120.78	111.00
2	d	3244	THR	OG1-CB-CG2	-5.75	96.76	110.00
1	E	2119	VAL	CA-CB-CG2	-5.75	102.27	110.90
2	a	2718	MET	CG-SD-CE	-5.75	91.00	100.20
2	c	4301	ARG	NH1-CZ-NH2	-5.75	113.07	119.40
2	c	4312	THR	CA-CB-OG1	5.75	121.08	109.00
2	d	2870	ASN	N-CA-CB	-5.75	100.25	110.60
2	f	3839	ALA	CB-CA-C	5.75	118.73	110.10
2	e	3999	ARG	NE-CZ-NH1	5.75	123.17	120.30
2	f	3517	ASP	CB-CG-OD2	5.74	123.47	118.30
1	G	771	LYS	O-C-N	-5.74	113.51	122.70
2	e	4036	GLU	OE1-CD-OE2	5.74	130.19	123.30
2	a	2444	LEU	CB-CA-C	5.74	121.11	110.20
1	A	57	LYS	N-CA-CB	-5.74	100.27	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	e	4119	TYR	CD1-CG-CD2	5.74	124.21	117.90
2	f	3556	ARG	CD-NE-CZ	5.74	131.63	123.60
2	g	2461	TYR	CB-CG-CD2	-5.74	117.56	121.00
2	c	4071	ASP	CB-CG-OD2	-5.73	113.14	118.30
2	e	4157	ARG	NH1-CZ-NH2	-5.73	113.10	119.40
1	E	2015	SER	O-C-N	-5.73	113.53	122.70
2	d	3359	THR	C-N-CA	5.73	136.02	121.70
2	e	4001	VAL	CA-CB-CG1	5.72	119.48	110.90
1	D	1193	GLU	OE1-CD-OE2	5.72	130.16	123.30
2	c	4398	ASP	OD1-CG-OD2	-5.72	112.44	123.30
1	G	635	ASP	N-CA-CB	-5.72	100.31	110.60
2	c	4061	THR	CA-CB-CG2	5.72	120.40	112.40
1	D	1455	PRO	N-CA-CB	5.71	110.16	103.30
2	a	2752	TRP	NE1-CE2-CZ2	5.71	136.69	130.40
1	D	1661	PHE	CB-CG-CD2	5.71	124.80	120.80
2	c	4132	TYR	CG-CD1-CE1	-5.71	116.73	121.30
2	d	2889	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	B	1847	TYR	CB-CG-CD1	-5.71	117.58	121.00
2	g	2705	PHE	CG-CD2-CE2	-5.71	114.53	120.80
1	A	409	ARG	NH1-CZ-NH2	-5.70	113.13	119.40
1	G	759	ARG	CD-NE-CZ	5.70	131.59	123.60
1	G	843	ASP	CB-CG-OD2	5.70	123.43	118.30
1	D	1598	VAL	CA-CB-CG2	5.70	119.45	110.90
2	e	4077	HIS	C-N-CA	5.70	135.95	121.70
1	C	1117	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	G	919	ASP	CB-CG-OD1	-5.70	113.17	118.30
2	a	2727	ASP	OD1-CG-OD2	-5.70	112.48	123.30
2	d	2987	THR	CA-CB-CG2	5.70	120.37	112.40
1	C	825	ALA	CB-CA-C	5.69	118.64	110.10
1	D	1648	ARG	NH1-CZ-NH2	-5.69	113.14	119.40
1	G	1029	TYR	CB-CG-CD1	5.69	124.42	121.00
2	a	2365	GLU	OE1-CD-OE2	-5.69	116.47	123.30
1	G	852	THR	CA-CB-OG1	-5.69	97.05	109.00
1	F	1344	ARG	NE-CZ-NH2	-5.69	117.46	120.30
2	g	2493	VAL	CA-CB-CG2	5.69	119.43	110.90
1	F	1475	VAL	CG1-CB-CG2	-5.68	101.81	110.90
2	a	2410	LYS	C-N-CA	5.68	135.91	121.70
2	c	4133	PHE	CB-CG-CD1	5.68	124.78	120.80
2	f	3379	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	G	638	GLU	OE1-CD-OE2	-5.68	116.48	123.30
1	B	1955	TRP	CB-CG-CD1	-5.68	119.62	127.00
1	G	894	VAL	CA-CB-CG2	5.68	119.42	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	551	ARG	NE-CZ-NH2	-5.68	117.46	120.30
2	e	3970	TYR	CB-CG-CD2	-5.68	117.59	121.00
2	b	3389	GLU	OE1-CD-OE2	-5.68	116.49	123.30
1	G	666	VAL	CG1-CB-CG2	-5.67	101.82	110.90
2	a	2775	TYR	CG-CD1-CE1	-5.67	116.76	121.30
2	g	2315	PHE	CB-CG-CD2	-5.67	116.83	120.80
2	b	3562	TYR	CB-CG-CD1	-5.67	117.60	121.00
2	b	3889	TYR	CG-CD2-CE2	-5.67	116.77	121.30
1	B	2214	ARG	CD-NE-CZ	5.67	131.53	123.60
1	E	1762	VAL	CA-CB-CG1	5.67	119.40	110.90
2	a	2363	GLU	OE1-CD-OE2	-5.67	116.50	123.30
1	A	209	VAL	CG1-CB-CG2	-5.66	101.84	110.90
2	g	2329	PRO	CA-N-CD	-5.66	103.58	111.50
1	E	2086	TRP	CE2-CD2-CG	5.66	111.83	107.30
2	b	3919	ASP	CB-CG-OD1	5.66	123.39	118.30
1	F	1295	TYR	CG-CD1-CE1	5.66	125.83	121.30
2	b	3470	LEU	CB-CG-CD2	-5.66	101.39	111.00
2	d	3248	THR	N-CA-CB	5.66	121.05	110.30
1	D	1213	TYR	CB-CG-CD2	-5.65	117.61	121.00
2	c	4345	TYR	CG-CD2-CE2	-5.65	116.78	121.30
2	d	2856	TYR	CG-CD1-CE1	-5.65	116.78	121.30
1	F	1364	VAL	CA-CB-CG2	5.65	119.37	110.90
2	f	3555	ASP	CB-CG-OD2	5.65	123.38	118.30
2	c	4440	ASP	CB-CG-OD1	-5.64	113.22	118.30
2	a	2751	MET	CA-CB-CG	5.64	122.88	113.30
2	e	4113	ARG	NH1-CZ-NH2	-5.64	113.20	119.40
1	F	1153	ILE	CA-CB-CG2	-5.63	99.63	110.90
1	C	627	GLU	OE1-CD-OE2	-5.63	116.55	123.30
2	f	3707	ASP	CB-CG-OD2	5.63	123.36	118.30
2	g	2704	PRO	N-CA-CB	5.63	110.05	103.30
1	C	838	PHE	CG-CD2-CE2	-5.62	114.61	120.80
1	E	2108	TYR	CG-CD2-CE2	-5.62	116.80	121.30
2	g	2686	ARG	CD-NE-CZ	5.62	131.47	123.60
1	E	1836	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	E	2244	HIS	CB-CA-C	5.62	121.64	110.40
1	F	1567	THR	OG1-CB-CG2	-5.62	97.08	110.00
2	b	3624	LYS	N-CA-CB	-5.62	100.48	110.60
2	b	3760	TRP	CD2-CE3-CZ3	5.62	126.10	118.80
2	c	4225	TYR	CB-CG-CD1	-5.62	117.63	121.00
1	A	306	ALA	N-CA-CB	-5.61	102.25	110.10
2	e	3989	GLU	OE1-CD-OE2	-5.61	116.57	123.30
2	e	4446	TYR	CD1-CE1-CZ	5.61	124.85	119.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	1304	TYR	CD1-CE1-CZ	5.61	124.85	119.80
2	g	2791	THR	O-C-N	-5.61	113.73	122.70
2	b	3907	LEU	CB-CG-CD2	5.60	120.53	111.00
2	a	2461	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	E	2162	VAL	CA-CB-CG1	5.60	119.30	110.90
1	B	2003	VAL	CA-CB-CG2	5.60	119.30	110.90
2	c	4423	TRP	CG-CD1-NE1	5.60	115.70	110.10
1	E	2062	PHE	CB-CG-CD1	-5.60	116.88	120.80
2	e	4048	TYR	CD1-CE1-CZ	-5.59	114.77	119.80
2	f	3389	GLU	OE1-CD-OE2	-5.59	116.59	123.30
2	f	3739	TYR	CB-CG-CD2	-5.59	117.64	121.00
1	A	388	TRP	NE1-CE2-CZ2	5.59	136.55	130.40
1	F	1496	PHE	CG-CD1-CE1	-5.59	114.65	120.80
1	B	2124	ASP	CB-CG-OD1	5.59	123.33	118.30
2	d	2999	ARG	NE-CZ-NH2	5.59	123.09	120.30
1	F	1632	GLN	OE1-CD-NE2	-5.59	109.05	121.90
1	A	506	LEU	CB-CG-CD1	5.59	120.50	111.00
1	B	1991	TYR	CG-CD1-CE1	-5.59	116.83	121.30
1	E	2011	LYS	CA-C-O	-5.59	108.37	120.10
2	f	3405	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	115	PHE	CB-CG-CD1	-5.58	116.89	120.80
1	C	572	PRO	N-CD-CG	5.58	111.58	103.20
2	e	4178	VAL	CG1-CB-CG2	-5.58	101.97	110.90
2	g	2608	ARG	CD-NE-CZ	5.58	131.42	123.60
1	G	650	ASP	CB-CG-OD1	5.58	123.32	118.30
2	g	2783	ASP	CA-CB-CG	5.58	125.68	113.40
2	f	3434	ASP	CB-CG-OD2	5.58	123.32	118.30
1	G	838	PHE	CG-CD1-CE1	-5.58	114.66	120.80
2	b	3611	THR	CA-CB-OG1	5.58	120.72	109.00
2	c	4317	TRP	CE2-CD2-CG	5.58	111.76	107.30
2	g	2507	VAL	CA-CB-CG2	5.58	119.27	110.90
1	C	685	VAL	CA-CB-CG2	5.57	119.26	110.90
1	D	1213	TYR	CG-CD1-CE1	-5.57	116.84	121.30
1	E	1847	TYR	CG-CD1-CE1	-5.57	116.84	121.30
2	g	2267	ALA	CB-CA-C	5.57	118.46	110.10
1	G	997	THR	OG1-CB-CG2	-5.57	97.19	110.00
1	E	2086	TRP	CE2-CD2-CE3	-5.57	112.01	118.70
1	G	1011	ASP	CB-CG-OD2	5.57	123.31	118.30
2	a	2332	ARG	CD-NE-CZ	5.57	131.40	123.60
2	f	3717	PRO	N-CA-CB	5.57	109.98	103.30
1	D	1495	ASN	CB-CA-C	5.56	121.53	110.40
1	G	645	THR	CA-CB-CG2	-5.56	104.61	112.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	d	3221	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	c	4072	GLU	CG-CD-OE2	5.56	129.41	118.30
2	d	3183	ASP	CB-CG-OD2	5.56	123.30	118.30
1	F	1672	THR	CA-CB-CG2	5.56	120.18	112.40
2	d	2998	ASP	CB-CG-OD1	-5.56	113.30	118.30
2	a	2780	THR	CA-CB-CG2	5.55	120.18	112.40
2	d	3018	TYR	CG-CD2-CE2	-5.55	116.86	121.30
2	d	2837	PRO	N-CD-CG	5.55	111.52	103.20
2	d	3139	MET	CB-CA-C	5.55	121.50	110.40
2	e	4069	ASP	CB-CG-OD1	5.55	123.29	118.30
2	a	2663	ASP	CB-CG-OD2	-5.55	113.31	118.30
2	a	2759	ASP	CB-CG-OD2	5.55	123.29	118.30
1	F	1297	ASN	CB-CA-C	5.54	121.49	110.40
1	F	1511	TYR	CA-CB-CG	5.54	123.93	113.40
2	a	2552	LEU	O-C-N	-5.54	113.83	122.70
1	D	1134	TRP	NE1-CE2-CZ2	5.54	136.50	130.40
1	F	1155	LYS	N-CA-CB	-5.54	100.62	110.60
2	f	3880	TYR	CZ-CE2-CD2	-5.54	114.81	119.80
2	g	2791	THR	OG1-CB-CG2	-5.54	97.25	110.00
1	D	1179	GLU	CG-CD-OE2	5.54	129.38	118.30
1	E	1775	LEU	CB-CG-CD2	-5.54	101.59	111.00
2	c	4329	VAL	CA-CB-CG1	5.53	119.20	110.90
2	d	3357	CYS	CA-CB-SG	5.53	123.96	114.00
1	F	1227	GLU	OE1-CD-OE2	-5.53	116.67	123.30
2	g	2265	ARG	CD-NE-CZ	5.53	131.34	123.60
2	g	2776	VAL	CA-CB-CG2	5.53	119.19	110.90
1	F	1442	ALA	N-CA-CB	-5.53	102.37	110.10
1	A	22	ALA	CB-CA-C	5.52	118.39	110.10
1	D	1516	ASP	CB-CA-C	5.52	121.45	110.40
2	g	2489	TYR	CB-CG-CD2	5.52	124.31	121.00
2	g	2608	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	F	1369	VAL	CG1-CB-CG2	-5.52	102.07	110.90
2	d	3102	VAL	CG1-CB-CG2	-5.52	102.07	110.90
1	F	1344	ARG	CD-NE-CZ	5.52	131.32	123.60
1	F	1541	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	343	VAL	CA-CB-CG1	5.51	119.17	110.90
2	c	4204	PHE	CB-CG-CD2	-5.51	116.94	120.80
1	A	149	TYR	CD1-CE1-CZ	5.51	124.76	119.80
2	d	2926	TYR	CA-CB-CG	5.51	123.87	113.40
2	e	4018	PRO	CA-N-CD	-5.51	103.78	111.50
1	B	1848	ARG	NE-CZ-NH1	5.51	123.06	120.30
2	a	2630	ARG	CD-NE-CZ	5.51	131.31	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	c	4026	PRO	N-CD-CG	5.51	111.46	103.20
2	d	3339	ARG	NE-CZ-NH1	-5.51	117.55	120.30
2	f	3421	VAL	CA-CB-CG1	5.51	119.16	110.90
2	b	3443	PRO	N-CA-CB	5.50	109.91	103.30
1	D	1567	THR	N-CA-CB	-5.50	99.84	110.30
2	a	2625	TYR	CB-CG-CD1	-5.50	117.70	121.00
2	c	3974	ARG	CD-NE-CZ	5.50	131.30	123.60
2	c	4189	TRP	CB-CG-CD2	5.50	133.75	126.60
1	E	1781	LEU	CB-CG-CD1	-5.50	101.65	111.00
1	G	720	LEU	CB-CA-C	5.50	120.65	110.20
2	e	4247	ALA	N-CA-CB	-5.50	102.40	110.10
2	d	3262	PHE	CG-CD2-CE2	-5.50	114.75	120.80
1	D	1631	ARG	CD-NE-CZ	5.50	131.29	123.60
2	f	3774	ARG	NE-CZ-NH2	5.49	123.05	120.30
2	d	2876	ARG	CD-NE-CZ	5.49	131.29	123.60
2	f	3590	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	2197	ARG	NE-CZ-NH2	5.49	123.04	120.30
1	F	1548	TYR	CZ-CE2-CD2	-5.49	114.86	119.80
2	d	3175	THR	OG1-CB-CG2	-5.49	97.38	110.00
1	F	1312	ARG	NE-CZ-NH1	5.49	123.04	120.30
2	f	3426	ARG	NE-CZ-NH1	5.49	123.04	120.30
2	g	2332	ARG	NH1-CZ-NH2	-5.49	113.37	119.40
2	e	4250	ARG	NH1-CZ-NH2	-5.48	113.37	119.40
1	G	1032	VAL	CA-CB-CG2	5.48	119.12	110.90
2	a	2386	ARG	CD-NE-CZ	5.48	131.28	123.60
2	b	3618	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	G	1041	PRO	N-CD-CG	5.48	111.42	103.20
2	g	2805	ASP	CB-CG-OD1	-5.48	113.37	118.30
2	d	2922	GLU	OE1-CD-OE2	-5.48	116.73	123.30
1	E	2116	VAL	CG1-CB-CG2	-5.47	102.14	110.90
2	d	3323	TYR	CD1-CG-CD2	5.47	123.92	117.90
2	g	2790	VAL	CA-CB-CG2	5.47	119.11	110.90
1	A	482	PHE	CZ-CE2-CD2	5.47	126.67	120.10
2	a	2736	PRO	N-CA-CB	5.47	109.87	103.30
2	f	3524	LYS	O-C-N	-5.47	113.94	122.70
1	D	1200	LEU	CB-CG-CD2	5.47	120.30	111.00
1	D	1541	ARG	CB-CA-C	5.47	121.34	110.40
1	G	598	ARG	NE-CZ-NH2	-5.47	117.57	120.30
2	b	3439	TYR	CB-CG-CD1	-5.47	117.72	121.00
2	b	3722	ARG	NH1-CZ-NH2	-5.47	113.38	119.40
1	B	2143	ASP	OD1-CG-OD2	-5.46	112.92	123.30
1	D	1404	PHE	CB-CG-CD2	5.46	124.62	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	3493	PHE	CB-CG-CD2	-5.46	116.97	120.80
2	b	3538	PHE	CB-CG-CD2	-5.46	116.98	120.80
1	E	2014	ARG	NH1-CZ-NH2	-5.46	113.40	119.40
2	b	3480	ASN	C-N-CA	5.46	135.35	121.70
2	f	3398	PHE	CB-CG-CD1	5.46	124.62	120.80
1	B	1947	ALA	CB-CA-C	5.46	118.28	110.10
1	C	1029	TYR	CD1-CG-CD2	5.45	123.90	117.90
1	G	754	LEU	CB-CG-CD1	5.45	120.27	111.00
2	a	2275	GLU	OE1-CD-OE2	-5.45	116.76	123.30
2	a	2384	ASN	CB-CA-C	5.45	121.31	110.40
2	d	3041	PHE	CB-CG-CD1	-5.45	116.98	120.80
1	A	100	VAL	CG1-CB-CG2	-5.45	102.18	110.90
1	D	1312	ARG	CD-NE-CZ	5.45	131.23	123.60
2	g	2699	VAL	CA-CB-CG1	-5.45	102.72	110.90
1	F	1447	ILE	O-C-N	5.45	131.42	122.70
2	f	3744	ARG	CD-NE-CZ	5.45	131.23	123.60
2	d	3255	ASP	OD1-CG-OD2	-5.44	112.96	123.30
1	C	725	PRO	CA-N-CD	-5.44	103.88	111.50
1	G	913	TYR	CB-CG-CD1	-5.44	117.74	121.00
2	b	3471	PRO	N-CA-CB	5.44	109.83	103.30
2	d	3307	ARG	NH1-CZ-NH2	-5.44	113.42	119.40
2	b	3636	TYR	CB-CG-CD1	5.44	124.26	121.00
1	G	729	TYR	CG-CD2-CE2	5.43	125.65	121.30
2	a	2626	ASP	CB-CG-OD1	5.43	123.19	118.30
2	e	4078	THR	CA-CB-CG2	5.43	120.00	112.40
2	c	4372	ASP	CB-CA-C	5.43	121.26	110.40
2	d	2963	HIS	C-N-CA	5.43	135.28	121.70
2	d	3017	GLN	OE1-CD-NE2	-5.43	109.41	121.90
1	B	1709	GLU	OE1-CD-OE2	-5.43	116.79	123.30
1	F	1673	VAL	CA-CB-CG1	5.43	119.04	110.90
2	f	3581	THR	CA-CB-CG2	5.43	120.00	112.40
1	D	1226	LEU	CB-CA-C	5.42	120.51	110.20
2	b	3758	THR	N-CA-CB	5.42	120.61	110.30
2	d	3199	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	E	1914	VAL	N-CA-C	5.42	125.64	111.00
2	b	3632	TRP	CD1-NE1-CE2	5.42	113.88	109.00
2	e	4329	VAL	CG1-CB-CG2	-5.42	102.23	110.90
2	f	3603	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	C	930	PHE	CB-CG-CD2	-5.42	117.01	120.80
1	D	1213	TYR	CD1-CE1-CZ	5.42	124.68	119.80
2	e	4043	PHE	CB-CG-CD2	-5.42	117.01	120.80
1	E	1985	LEU	N-CA-CB	-5.42	99.57	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	1548	TYR	O-C-N	-5.42	114.03	122.70
2	g	2644	THR	CA-CB-OG1	5.42	120.38	109.00
2	c	4263	GLU	OE1-CD-OE2	-5.42	116.80	123.30
1	A	486	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	2126	PRO	N-CA-CB	5.41	109.80	103.30
1	B	2163	ASN	N-CA-CB	-5.41	100.86	110.60
1	D	1348	VAL	CA-C-N	-5.41	105.30	117.20
1	E	2161	TYR	CB-CG-CD1	-5.41	117.75	121.00
2	c	4180	ASP	CB-CG-OD1	5.41	123.17	118.30
1	C	640	PRO	O-C-N	5.41	131.35	122.70
1	C	744	LEU	CB-CG-CD1	5.40	120.18	111.00
1	C	1001	THR	CA-CB-CG2	5.40	119.96	112.40
2	e	4258	VAL	CA-CB-CG1	5.40	119.00	110.90
1	A	118	SER	C-N-CA	5.40	135.20	121.70
1	E	1892	ASP	CB-CG-OD2	-5.40	113.44	118.30
2	a	2752	TRP	NE1-CE2-CD2	-5.40	101.90	107.30
2	c	4369	ASP	CB-CG-OD2	5.40	123.16	118.30
1	D	1288	PRO	N-CA-CB	5.40	109.78	103.30
2	c	4128	MET	CA-CB-CG	5.40	122.47	113.30
1	B	2146	PRO	CA-N-CD	-5.40	103.95	111.50
2	b	3449	TYR	CG-CD2-CE2	-5.40	116.98	121.30
2	e	4175	ARG	CD-NE-CZ	5.40	131.16	123.60
1	F	1549	THR	OG1-CB-CG2	-5.39	97.59	110.00
1	G	1036	ASP	OD1-CG-OD2	-5.39	113.05	123.30
1	A	316	ARG	NH1-CZ-NH2	-5.39	113.47	119.40
1	D	1353	PRO	N-CA-CB	5.39	109.77	103.30
2	c	3937	TRP	NE1-CE2-CZ2	5.39	136.33	130.40
2	d	2873	TYR	CD1-CE1-CZ	-5.39	114.95	119.80
2	e	4190	ARG	CD-NE-CZ	5.39	131.14	123.60
2	g	2631	SER	N-CA-CB	-5.39	102.42	110.50
1	G	995	ARG	NH1-CZ-NH2	-5.38	113.48	119.40
2	d	3043	ARG	CD-NE-CZ	5.38	131.13	123.60
1	A	2	TRP	CD2-CE3-CZ3	5.38	125.79	118.80
1	G	676	PHE	CG-CD2-CE2	-5.38	114.89	120.80
1	A	243	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	G	760	ASP	CA-CB-CG	5.37	125.22	113.40
2	a	2579	ARG	NH1-CZ-NH2	-5.37	113.49	119.40
2	d	2888	ASP	CB-CG-OD2	5.37	123.13	118.30
1	F	1683	ARG	CD-NE-CZ	5.37	131.12	123.60
2	c	4293	TYR	CA-CB-CG	5.37	123.60	113.40
2	d	3255	ASP	C-N-CA	5.37	135.12	121.70
2	g	2284	PHE	CB-CG-CD1	-5.37	117.04	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	3886	PHE	CB-CG-CD2	-5.37	117.04	120.80
1	D	1169	THR	CA-CB-CG2	5.37	119.91	112.40
1	E	2165	THR	CA-CB-CG2	5.37	119.91	112.40
2	e	4176	VAL	CA-CB-CG1	5.37	118.95	110.90
2	e	4263	GLU	CA-CB-CG	5.37	125.20	113.40
1	B	1916	ASP	CB-CG-OD1	5.36	123.13	118.30
1	B	2077	TYR	CE1-CZ-CE2	-5.36	111.22	119.80
2	f	3716	PRO	N-CA-CB	5.36	109.73	103.30
1	F	1661	PHE	CB-CG-CD1	5.36	124.55	120.80
2	c	4297	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	2077	TYR	CA-CB-CG	5.36	123.58	113.40
1	F	1253	GLU	OE1-CD-OE2	-5.36	116.87	123.30
1	F	1511	TYR	CB-CG-CD1	-5.36	117.79	121.00
2	a	2646	TRP	CZ3-CH2-CZ2	-5.36	115.17	121.60
2	d	3165	ARG	CD-NE-CZ	5.36	131.10	123.60
2	d	3221	ARG	CD-NE-CZ	5.36	131.10	123.60
1	A	470	ASP	CB-CG-OD2	5.35	123.12	118.30
2	g	2753	ARG	N-CA-CB	-5.35	100.96	110.60
2	c	4094	LEU	O-C-N	-5.35	114.14	122.70
2	e	4062	VAL	CB-CA-C	5.35	121.57	111.40
1	E	2164	VAL	CA-CB-CG1	5.35	118.92	110.90
2	f	3382	PRO	CA-N-CD	-5.35	104.01	111.50
2	f	3856	GLU	O-C-N	-5.35	114.14	122.70
1	C	866	ASP	OD1-CG-OD2	-5.34	113.15	123.30
1	F	1377	LYS	CB-CA-C	5.34	121.09	110.40
1	D	1595	TYR	CB-CG-CD1	-5.34	117.79	121.00
2	a	2515	THR	N-CA-CB	5.34	120.45	110.30
2	b	3803	THR	C-N-CA	5.34	133.51	122.30
2	f	3466	PRO	CA-N-CD	-5.34	104.02	111.50
2	e	4057	ARG	CD-NE-CZ	5.34	131.07	123.60
1	A	215	ASP	CB-CG-OD2	-5.34	113.50	118.30
2	e	4116	ILE	CA-CB-CG1	5.34	121.14	111.00
2	f	3382	PRO	N-CA-CB	5.34	109.70	103.30
1	F	1616	VAL	CG1-CB-CG2	-5.33	102.37	110.90
1	G	809	ARG	NE-CZ-NH1	5.33	122.96	120.30
2	a	2266	TRP	CD1-NE1-CE2	5.33	113.80	109.00
2	c	4095	PHE	CB-CG-CD1	-5.33	117.07	120.80
2	d	2954	THR	CA-CB-CG2	5.33	119.86	112.40
1	A	149	TYR	CG-CD1-CE1	-5.32	117.04	121.30
2	c	3955	PHE	CB-CG-CD1	-5.32	117.07	120.80
1	C	992	ASP	CB-CG-OD1	5.32	123.09	118.30
2	a	2742	GLU	O-C-N	5.32	131.22	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1862	LEU	CB-CG-CD1	5.32	120.04	111.00
1	B	1969	TYR	CD1-CG-CD2	5.32	123.75	117.90
1	B	2116	VAL	CG1-CB-CG2	-5.32	102.39	110.90
1	C	951	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	E	1948	ASP	CB-CG-OD2	5.32	123.09	118.30
1	F	1612	PHE	CB-CG-CD2	5.32	124.52	120.80
2	a	2484	PHE	N-CA-CB	-5.31	101.04	110.60
1	C	780	LEU	CB-CG-CD2	5.31	120.03	111.00
2	c	4132	TYR	CD1-CG-CD2	5.31	123.74	117.90
2	a	2528	ASN	N-CA-CB	-5.31	101.05	110.60
1	A	257	TRP	CA-CB-CG	5.31	123.78	113.70
2	c	4198	GLY	C-N-CA	5.31	134.97	121.70
2	c	4208	THR	OG1-CB-CG2	-5.31	97.80	110.00
1	F	1233	LEU	CB-CG-CD1	5.30	120.02	111.00
2	b	3709	ASP	CB-CG-OD2	5.30	123.07	118.30
2	f	3896	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	C	1006	VAL	CA-CB-CG2	5.30	118.85	110.90
1	E	1859	VAL	CA-CB-CG2	5.30	118.85	110.90
1	G	598	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	g	2783	ASP	CB-CG-OD2	-5.30	113.53	118.30
2	a	2555	GLU	CG-CD-OE1	5.30	128.90	118.30
1	B	2140	ASP	CB-CG-OD1	5.29	123.06	118.30
2	a	2408	ARG	CD-NE-CZ	5.29	131.01	123.60
2	g	2588	THR	O-C-N	-5.29	114.23	122.70
1	E	1708	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	G	975	ARG	CD-NE-CZ	5.29	131.01	123.60
2	c	4189	TRP	NE1-CE2-CZ2	5.29	136.22	130.40
2	d	2865	ASP	CB-CG-OD1	-5.29	113.54	118.30
2	e	4396	ALA	CB-CA-C	5.29	118.03	110.10
1	B	2073	ALA	N-CA-CB	-5.29	102.70	110.10
2	a	2708	LYS	CB-CA-C	5.29	120.97	110.40
1	F	1648	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	F	1421	LYS	O-C-N	-5.28	114.26	122.70
2	a	2574	ARG	NH1-CZ-NH2	-5.28	113.59	119.40
2	a	2664	ARG	NE-CZ-NH2	5.28	122.94	120.30
2	b	3505	VAL	CA-CB-CG1	5.28	118.81	110.90
1	F	1196	VAL	CA-CB-CG1	5.27	118.81	110.90
2	c	4124	LYS	N-CA-CB	-5.27	101.11	110.60
1	G	1114	SER	N-CA-CB	-5.27	102.59	110.50
2	f	3774	ARG	CD-NE-CZ	5.27	130.98	123.60
1	G	894	VAL	CG1-CB-CG2	-5.27	102.47	110.90
2	b	3439	TYR	CB-CG-CD2	5.27	124.16	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	d	2972	GLY	C-N-CA	5.27	134.88	121.70
2	d	3014	MET	CG-SD-CE	5.27	108.63	100.20
1	A	194	ASP	O-C-N	5.27	132.16	123.20
2	e	4454	ASP	CB-CG-OD1	5.27	123.04	118.30
1	B	2003	VAL	CG1-CB-CG2	-5.26	102.48	110.90
1	F	1237	ASP	CB-CG-OD1	5.26	123.04	118.30
2	e	4157	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	g	2498	VAL	CA-CB-CG1	5.26	118.80	110.90
1	G	999	THR	CA-CB-OG1	5.26	120.05	109.00
2	d	3116	GLN	N-CA-CB	-5.26	101.13	110.60
1	F	1435	VAL	CA-CB-CG2	5.26	118.79	110.90
2	b	3533	PRO	N-CD-CG	5.26	111.09	103.20
1	C	886	LYS	N-CA-CB	-5.26	101.13	110.60
1	D	1142	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	d	3165	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	F	1341	VAL	CA-CB-CG1	5.26	118.79	110.90
1	B	1975	ASP	CB-CG-OD2	5.26	123.03	118.30
1	C	771	LYS	C-N-CA	5.26	134.84	121.70
1	G	693	THR	N-CA-CB	5.26	120.29	110.30
2	a	2318	GLU	OE1-CD-OE2	-5.26	116.99	123.30
2	c	3956	LEU	O-C-N	-5.25	114.29	122.70
2	d	3153	GLU	OE1-CD-OE2	-5.25	117.00	123.30
2	a	2752	TRP	CD1-NE1-CE2	5.25	113.73	109.00
2	f	3917	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	E	1939	VAL	CA-CB-CG2	5.25	118.77	110.90
2	g	2727	ASP	OD1-CG-OD2	-5.25	113.33	123.30
1	G	782	VAL	O-C-N	5.24	131.08	122.70
1	A	480	PHE	CZ-CE2-CD2	-5.24	113.81	120.10
2	d	2999	ARG	NE-CZ-NH1	-5.24	117.68	120.30
2	g	2570	ALA	CB-CA-C	5.24	117.96	110.10
2	g	2498	VAL	CA-CB-CG2	5.24	118.76	110.90
1	A	384	ASP	CB-CG-OD1	5.24	123.01	118.30
2	c	4267	GLU	OE1-CD-OE2	-5.24	117.02	123.30
2	f	3470	LEU	CB-CG-CD1	5.24	119.90	111.00
2	g	2753	ARG	CD-NE-CZ	5.24	130.93	123.60
1	D	1607	PRO	N-CD-CG	5.23	111.05	103.20
1	G	975	ARG	NE-CZ-NH2	5.23	122.92	120.30
2	a	2446	ASP	CB-CG-OD1	5.23	123.01	118.30
2	d	2907	TYR	CB-CG-CD2	5.23	124.14	121.00
2	g	2617	THR	CA-CB-CG2	-5.23	105.08	112.40
1	B	1879	GLU	N-CA-CB	5.23	120.01	110.60
1	B	2051	ASP	CB-CG-OD1	5.23	123.00	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	c	4099	PRO	N-CA-CB	5.23	109.57	103.30
1	C	1072	LEU	CB-CG-CD1	5.23	119.88	111.00
1	A	525	ASP	CA-CB-CG	5.22	124.89	113.40
1	C	630	VAL	CG1-CB-CG2	-5.22	102.54	110.90
1	C	1082	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	E	1992	GLU	OE1-CD-OE2	-5.22	117.03	123.30
1	E	2099	ALA	CB-CA-C	5.22	117.94	110.10
2	c	4476	ASP	CB-CG-OD2	5.22	123.00	118.30
2	f	3510	ALA	N-CA-CB	-5.22	102.78	110.10
1	C	893	LYS	N-CA-CB	-5.22	101.20	110.60
1	A	452	GLU	OE1-CD-OE2	-5.22	117.03	123.30
1	B	2140	ASP	C-N-CA	5.22	134.75	121.70
1	F	1266	ALA	N-CA-CB	-5.22	102.79	110.10
2	e	3987	TYR	CB-CG-CD1	5.22	124.13	121.00
1	B	1761	ASN	O-C-N	-5.22	114.35	122.70
2	e	4331	ARG	CD-NE-CZ	5.22	130.90	123.60
1	E	1820	LEU	N-CA-CB	-5.21	99.97	110.40
1	A	94	LEU	CB-CA-C	5.21	120.10	110.20
1	C	948	LEU	C-N-CA	5.21	134.73	121.70
2	a	2745	THR	CA-CB-CG2	5.21	119.69	112.40
2	g	2519	ARG	CD-NE-CZ	5.21	130.90	123.60
1	E	1941	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	E	2198	GLN	CA-CB-CG	-5.21	101.94	113.40
2	a	2775	TYR	CB-CG-CD1	-5.21	117.88	121.00
2	g	2636	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	E	2051	ASP	CB-CG-OD2	5.21	122.99	118.30
2	b	3898	ARG	CA-CB-CG	5.21	124.85	113.40
2	e	4233	LEU	CB-CG-CD1	5.21	119.85	111.00
1	A	22	ALA	N-CA-CB	-5.20	102.81	110.10
1	A	325	PRO	C-N-CA	5.20	134.71	121.70
1	E	2017	TYR	N-CA-CB	-5.20	101.23	110.60
2	d	3090	PHE	CB-CG-CD2	5.20	124.44	120.80
1	A	74	PRO	N-CD-CG	5.20	111.00	103.20
1	A	91	GLU	OE1-CD-OE2	-5.20	117.06	123.30
1	A	348	VAL	CA-CB-CG2	5.20	118.70	110.90
2	a	2738	ASP	CB-CG-OD2	5.20	122.98	118.30
2	b	3555	ASP	CB-CG-OD2	5.20	122.98	118.30
2	d	3282	ALA	CB-CA-C	5.20	117.90	110.10
1	B	2193	TRP	CE2-CD2-CG	5.20	111.46	107.30
1	C	716	ARG	NE-CZ-NH2	5.20	122.90	120.30
2	b	3880	TYR	CG-CD2-CE2	-5.20	117.14	121.30
2	f	3657	GLU	OE1-CD-OE2	-5.20	117.06	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1377	LYS	N-CA-CB	-5.20	101.25	110.60
2	g	2659	PHE	CB-CG-CD1	-5.20	117.16	120.80
1	D	1224	LYS	CA-CB-CG	5.19	124.83	113.40
2	f	3725	GLU	OE1-CD-OE2	-5.19	117.07	123.30
1	C	719	SER	N-CA-CB	5.19	118.29	110.50
2	f	3709	ASP	C-N-CA	5.19	134.68	121.70
2	d	3243	ARG	CD-NE-CZ	5.19	130.87	123.60
2	f	3794	ALA	O-C-N	-5.19	114.39	122.70
2	d	3222	GLU	OE1-CD-OE2	-5.19	117.07	123.30
1	D	1234	ASP	CB-CG-OD1	-5.18	113.63	118.30
1	D	1684	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	G	813	PHE	CB-CG-CD1	-5.18	117.17	120.80
2	a	2607	VAL	CB-CA-C	-5.18	101.56	111.40
2	c	3970	TYR	CZ-CE2-CD2	-5.18	115.14	119.80
1	A	14	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	411	VAL	CG1-CB-CG2	-5.18	102.61	110.90
1	D	1512	VAL	CG1-CB-CG2	-5.18	102.61	110.90
2	e	4021	TYR	CB-CG-CD2	5.18	124.11	121.00
1	E	1946	ASP	CB-CG-OD1	5.18	122.96	118.30
1	E	2009	PHE	O-C-N	-5.18	114.42	122.70
1	G	872	ALA	N-CA-CB	-5.18	102.85	110.10
2	b	3760	TRP	CE2-CD2-CE3	-5.18	112.49	118.70
2	g	2582	MET	N-CA-CB	-5.18	101.28	110.60
1	D	1246	VAL	CA-CB-CG1	5.17	118.66	110.90
2	d	2868	PRO	N-CA-CB	5.17	109.51	103.30
2	f	3611	THR	C-N-CA	5.17	134.63	121.70
1	A	97	ARG	CD-NE-CZ	5.17	130.84	123.60
1	C	606	TYR	CG-CD2-CE2	-5.17	117.16	121.30
1	D	1648	ARG	CD-NE-CZ	5.17	130.84	123.60
1	E	2209	GLU	CB-CA-C	-5.17	100.06	110.40
2	e	4435	LEU	CB-CG-CD1	5.17	119.79	111.00
2	a	2666	ALA	N-CA-CB	-5.17	102.86	110.10
2	c	4018	PRO	N-CA-CB	5.17	109.50	103.30
1	B	1837	GLU	OE1-CD-OE2	-5.17	117.10	123.30
1	B	2193	TRP	NE1-CE2-CD2	-5.17	102.13	107.30
2	c	3986	PHE	CD1-CE1-CZ	5.17	126.30	120.10
1	D	1595	TYR	CG-CD1-CE1	-5.17	117.17	121.30
2	d	3157	CYS	CA-CB-SG	5.17	123.30	114.00
2	e	3967	TYR	CB-CG-CD2	5.17	124.10	121.00
2	a	2441	ASP	O-C-N	-5.17	114.44	122.70
1	B	1892	ASP	CB-CG-OD1	5.16	122.95	118.30
1	C	621	PHE	CB-CG-CD1	5.16	124.41	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	716	ARG	CD-NE-CZ	5.16	130.83	123.60
1	C	724	TYR	CD1-CG-CD2	5.16	123.58	117.90
1	G	1050	VAL	CA-CB-CG2	5.16	118.64	110.90
2	d	2936	PHE	CB-CG-CD2	-5.16	117.19	120.80
1	B	1921	VAL	CA-CB-CG1	5.16	118.64	110.90
1	D	1210	LEU	CB-CG-CD2	5.16	119.76	111.00
2	a	2687	THR	CA-CB-CG2	5.15	119.62	112.40
2	e	4310	LYS	CA-CB-CG	5.15	124.74	113.40
1	F	1673	VAL	CG1-CB-CG2	-5.15	102.66	110.90
2	a	2489	TYR	CB-CG-CD2	-5.15	117.91	121.00
2	e	3996	TYR	CB-CG-CD1	5.15	124.09	121.00
1	A	271	TYR	CB-CG-CD1	-5.15	117.91	121.00
1	B	2083	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	G	721	GLU	N-CA-CB	-5.15	101.33	110.60
2	a	2611	GLU	N-CA-CB	-5.15	101.33	110.60
2	d	3072	THR	CA-CB-CG2	5.15	119.61	112.40
2	e	4354	GLN	CG-CD-OE1	5.15	131.90	121.60
1	F	1549	THR	CA-CB-CG2	5.15	119.61	112.40
1	B	2058	ILE	CA-CB-CG2	5.15	121.19	110.90
1	B	2082	ASP	CB-CG-OD1	5.15	122.93	118.30
1	C	875	ALA	CB-CA-C	5.15	117.82	110.10
2	c	4051	THR	C-N-CA	5.15	134.57	121.70
1	A	163	TYR	CD1-CE1-CZ	5.15	124.43	119.80
1	F	1602	ASP	OD1-CG-OD2	-5.15	113.52	123.30
1	B	2203	VAL	CA-CB-CG2	5.14	118.62	110.90
1	F	1616	VAL	CA-CB-CG1	5.14	118.62	110.90
2	c	4344	ILE	CA-CB-CG2	5.14	121.19	110.90
2	d	2952	CYS	CA-CB-SG	-5.14	104.74	114.00
2	g	2784	ARG	NH1-CZ-NH2	-5.14	113.74	119.40
2	g	2796	THR	CA-CB-CG2	5.14	119.60	112.40
2	d	2853	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	E	2086	TRP	NE1-CE2-CD2	-5.14	102.16	107.30
2	a	2514	ASN	CB-CA-C	5.14	120.68	110.40
2	c	4186	THR	CA-CB-OG1	5.14	119.79	109.00
2	g	2350	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	A	510	SER	O-C-N	-5.14	114.48	122.70
1	B	2164	VAL	CA-CB-CG2	5.14	118.61	110.90
1	D	1187	PHE	CG-CD1-CE1	-5.14	115.15	120.80
2	d	3187	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
1	F	1134	TRP	CD1-NE1-CE2	5.13	113.62	109.00
2	a	2497	THR	CA-CB-CG2	5.13	119.59	112.40
2	c	4069	ASP	OD1-CG-OD2	-5.13	113.55	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	a	2331	ASP	CB-CG-OD2	5.13	122.92	118.30
2	d	3108	PRO	N-CD-CG	5.13	110.89	103.20
2	e	4434	ARG	NE-CZ-NH2	-5.13	117.73	120.30
2	e	4453	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	C	722	PRO	CA-N-CD	-5.13	104.32	111.50
1	E	2251	ALA	N-CA-CB	-5.13	102.92	110.10
1	G	748	GLU	CA-C-N	-5.13	105.92	117.20
2	f	3639	LEU	CB-CG-CD1	-5.13	102.28	111.00
1	A	242	THR	CA-CB-CG2	5.12	119.58	112.40
1	A	179	ASP	CB-CG-OD1	5.12	122.91	118.30
2	d	2867	GLU	CB-CG-CD	-5.12	100.37	114.20
1	C	635	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	C	1046	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	D	1548	TYR	CB-CG-CD2	5.12	124.07	121.00
2	g	2330	VAL	CA-CB-CG1	5.12	118.58	110.90
2	g	2716	PRO	CA-N-CD	-5.12	104.33	111.50
1	F	1188	ASN	CB-CA-C	5.12	120.64	110.40
2	a	2518	TRP	CG-CD1-NE1	-5.12	104.98	110.10
2	c	3946	GLU	OE1-CD-OE2	-5.12	117.16	123.30
2	f	3637	THR	O-C-N	5.12	130.89	122.70
1	G	678	GLN	O-C-N	-5.12	114.51	122.70
1	G	1008	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	1063	ILE	CA-CB-CG2	-5.12	100.67	110.90
1	E	1969	TYR	CB-CG-CD1	5.12	124.07	121.00
2	d	3061	ARG	CD-NE-CZ	5.12	130.76	123.60
2	e	4297	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	B	1994	MET	CB-CA-C	5.11	120.62	110.40
1	B	1770	GLU	OE1-CD-OE2	-5.11	117.17	123.30
2	b	3779	GLU	OE1-CD-OE2	-5.11	117.17	123.30
1	A	239	VAL	CA-CB-CG2	5.10	118.56	110.90
1	G	685	VAL	CA-CB-CG2	5.10	118.55	110.90
2	b	3732	THR	CA-CB-OG1	5.10	119.72	109.00
2	g	2335	TYR	CB-CG-CD1	5.10	124.06	121.00
1	F	1605	GLY	O-C-N	-5.10	114.54	122.70
1	G	593	ASP	CB-CG-OD1	5.10	122.89	118.30
1	D	1369	VAL	CA-CB-CG1	5.10	118.55	110.90
1	B	1856	TYR	CG-CD2-CE2	-5.10	117.22	121.30
1	G	972	PHE	CB-CG-CD2	-5.10	117.23	120.80
2	b	3848	GLY	CA-C-O	-5.10	111.43	120.60
1	A	417	THR	OG1-CB-CG2	5.09	121.72	110.00
1	G	667	LEU	CB-CG-CD1	-5.09	102.34	111.00
2	b	3709	ASP	CB-CG-OD1	-5.09	113.71	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	c	3999	ARG	NE-CZ-NH1	-5.09	117.75	120.30
2	d	3011	VAL	CA-CB-CG1	5.09	118.54	110.90
2	f	3692	PRO	N-CA-CB	5.09	109.41	103.30
2	g	2424	PHE	CB-CG-CD1	-5.09	117.23	120.80
2	d	2860	ARG	CD-NE-CZ	5.09	130.73	123.60
2	g	2512	LEU	CB-CG-CD1	5.09	119.66	111.00
2	b	3446	ARG	NE-CZ-NH1	-5.09	117.76	120.30
2	g	2578	PRO	N-CD-CG	5.09	110.83	103.20
2	g	2640	LEU	CB-CG-CD1	-5.09	102.35	111.00
1	D	1478	ILE	O-C-N	-5.09	114.56	122.70
2	g	2382	PHE	CB-CG-CD1	-5.09	117.24	120.80
2	g	2763	ARG	CD-NE-CZ	5.09	130.72	123.60
1	E	1948	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	F	1290	TYR	CG-CD1-CE1	-5.09	117.23	121.30
1	C	641	PHE	CB-CG-CD1	5.08	124.36	120.80
1	A	179	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	C	913	TYR	CD1-CG-CD2	5.08	123.49	117.90
1	F	1366	GLU	OE1-CD-OE2	-5.08	117.20	123.30
2	d	3321	LEU	CB-CA-C	5.08	119.86	110.20
1	E	1921	VAL	CA-CB-CG2	5.08	118.52	110.90
1	C	757	GLU	OE1-CD-OE2	-5.08	117.21	123.30
1	G	815	ALA	CB-CA-C	5.08	117.72	110.10
2	c	3972	SER	O-C-N	5.08	130.82	122.70
2	e	3971	TYR	CD1-CE1-CZ	5.08	124.37	119.80
2	f	3632	TRP	CD2-CE2-CZ2	5.08	128.39	122.30
1	F	1207	PHE	CB-CG-CD1	-5.07	117.25	120.80
1	C	1029	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	E	1884	TYR	CD1-CE1-CZ	5.07	124.36	119.80
2	d	3315	ASN	CB-CA-C	5.07	120.54	110.40
2	a	2667	GLU	OE1-CD-OE2	-5.07	117.22	123.30
2	f	3618	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	E	2109	VAL	CA-CB-CG1	5.07	118.50	110.90
1	G	859	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	A	416	TYR	CD1-CE1-CZ	5.07	124.36	119.80
2	d	3159	PRO	N-CA-CB	5.07	109.38	103.30
2	b	3578	LEU	CB-CG-CD2	5.06	119.61	111.00
1	C	746	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	D	1263	LYS	C-N-CA	5.06	134.35	121.70
1	E	1935	VAL	CA-CB-CG1	5.06	118.49	110.90
1	F	1312	ARG	CB-CG-CD	5.06	124.75	111.60
2	b	3563	GLN	CA-CB-CG	5.06	124.53	113.40
2	f	3774	ARG	NH1-CZ-NH2	-5.06	113.83	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	e	4227	GLU	C-N-CA	5.06	134.34	121.70
1	E	2116	VAL	CA-CB-CG1	5.05	118.48	110.90
2	c	4357	ARG	NE-CZ-NH2	-5.05	117.77	120.30
2	f	3525	TYR	CB-CG-CD1	-5.05	117.97	121.00
2	c	4222	PRO	N-CD-CG	5.05	110.78	103.20
1	D	1505	LEU	CB-CG-CD2	5.05	119.59	111.00
1	F	1520	TRP	NE1-CE2-CD2	-5.05	102.25	107.30
2	a	2646	TRP	NE1-CE2-CZ2	5.05	135.96	130.40
2	g	2705	PHE	CB-CG-CD2	-5.05	117.27	120.80
1	C	612	THR	CA-CB-OG1	5.05	119.60	109.00
2	e	4378	PRO	O-C-N	-5.05	114.62	122.70
1	C	612	THR	OG1-CB-CG2	-5.05	98.39	110.00
2	a	2760	THR	O-C-N	-5.04	114.63	122.70
1	B	1946	ASP	OD1-CG-OD2	-5.04	113.72	123.30
1	B	2077	TYR	CZ-CE2-CD2	5.04	124.34	119.80
1	B	2086	TRP	CD1-NE1-CE2	5.04	113.54	109.00
1	C	944	ARG	NH1-CZ-NH2	-5.04	113.85	119.40
1	A	141	ASN	N-CA-CB	-5.04	101.53	110.60
2	f	3575	TYR	CB-CG-CD2	-5.04	117.97	121.00
2	f	3599	THR	N-CA-CB	5.04	119.88	110.30
2	g	2266	TRP	CD1-CG-CD2	-5.04	102.27	106.30
2	c	4455	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	519	ILE	CG1-CB-CG2	-5.04	100.31	111.40
1	B	2196	ALA	N-CA-CB	-5.04	103.05	110.10
2	a	2660	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	b	3889	TYR	CZ-CE2-CD2	5.04	124.33	119.80
2	f	3796	ASP	O-C-N	-5.04	114.64	122.70
1	A	293	TYR	CZ-CE2-CD2	-5.04	115.27	119.80
1	C	944	ARG	CD-NE-CZ	5.04	130.65	123.60
1	C	991	GLU	C-N-CA	5.04	134.29	121.70
1	G	966	LEU	CB-CG-CD2	-5.04	102.44	111.00
1	G	1024	CYS	CA-CB-SG	5.04	123.06	114.00
1	G	1038	ASP	CB-CG-OD1	5.04	122.83	118.30
1	A	48	PRO	N-CD-CG	5.03	110.75	103.20
2	a	2404	THR	CA-CB-OG1	5.03	119.57	109.00
1	A	227	VAL	CA-CB-CG1	5.03	118.44	110.90
2	c	3968	THR	OG1-CB-CG2	-5.03	98.43	110.00
2	c	4120	GLN	O-C-N	-5.03	114.65	122.70
1	E	1953	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	997	THR	CA-CB-CG2	5.03	119.44	112.40
1	D	1258	HIS	CB-CA-C	5.03	120.46	110.40
2	g	2341	ILE	CA-CB-CG1	5.03	120.55	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	8	ALA	N-CA-CB	5.03	117.14	110.10
2	e	4279	ARG	NE-CZ-NH2	-5.03	117.79	120.30
2	g	2303	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	D	1389	TRP	CZ3-CH2-CZ2	-5.02	115.57	121.60
1	A	388	TRP	CE2-CD2-CG	5.02	111.32	107.30
1	A	482	PHE	CG-CD1-CE1	5.02	126.33	120.80
1	D	1543	VAL	C-N-CA	5.02	134.26	121.70
1	B	1775	LEU	CB-CG-CD2	5.02	119.53	111.00
1	C	821	ASP	CB-CG-OD1	5.02	122.82	118.30
2	b	3636	TYR	CG-CD1-CE1	-5.02	117.28	121.30
2	b	3732	THR	OG1-CB-CG2	-5.02	98.45	110.00
2	e	4296	TYR	CG-CD1-CE1	-5.02	117.28	121.30
2	f	3505	VAL	C-N-CA	5.02	132.84	122.30
2	a	2640	LEU	CB-CG-CD1	-5.02	102.47	111.00
1	B	1847	TYR	CB-CG-CD2	5.01	124.01	121.00
2	e	4441	PRO	CA-N-CD	-5.01	104.48	111.50
2	g	2630	ARG	CD-NE-CZ	5.01	130.62	123.60
1	C	715	TYR	CD1-CE1-CZ	-5.01	115.29	119.80
1	C	738	TYR	CD1-CE1-CZ	-5.01	115.29	119.80
1	A	388	TRP	NE1-CE2-CD2	-5.01	102.29	107.30
1	E	2062	PHE	CG-CD1-CE1	-5.01	115.29	120.80
1	E	2095	GLU	CA-CB-CG	5.01	124.42	113.40
2	a	2439	GLN	CG-CD-OE1	5.01	131.61	121.60
1	B	2252	HIS	CA-CB-CG	5.00	122.11	113.60
1	D	1457	PRO	N-CD-CG	5.00	110.71	103.20
2	a	2377	TYR	CB-CG-CD1	-5.00	118.00	121.00
2	c	4470	ASP	O-C-N	-5.00	114.69	122.70
2	b	3636	TYR	CB-CG-CD2	-5.00	118.00	121.00
2	e	4048	TYR	CB-CG-CD2	-5.00	118.00	121.00
1	B	2191	GLU	CA-CB-CG	5.00	124.40	113.40
1	D	1180	PRO	N-CA-CB	5.00	109.30	103.30
2	b	3707	ASP	CB-CG-OD2	5.00	122.80	118.30
2	d	2934	TYR	CG-CD2-CE2	-5.00	117.30	121.30

There are no chirality outliers.

All (168) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	ARG	Sidechain
1	A	32	ARG	Sidechain
1	A	40	TYR	Sidechain
1	A	416	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	429	ARG	Sidechain
1	A	474	HIS	Sidechain
1	A	477	SER	Peptide
1	A	551	ARG	Sidechain
1	B	1704	PRO	Peptide,Mainchain
1	B	1779	TYR	Sidechain
1	B	1799	LEU	Peptide
1	B	1856	TYR	Sidechain
1	B	1862	LEU	Peptide
1	B	1884	TYR	Sidechain
1	B	1910	ARG	Sidechain
1	B	2014	ARG	Sidechain
1	B	2045	TYR	Sidechain
1	B	2077	TYR	Sidechain
1	B	2127	ARG	Sidechain
1	B	2154	THR	Peptide
1	B	2161	TYR	Sidechain
1	B	2191	GLU	Mainchain
1	C	1029	TYR	Sidechain
1	C	1082	ARG	Sidechain
1	C	604	TYR	Sidechain
1	C	636	ARG	Sidechain
1	C	647	TYR	Sidechain
1	C	715	TYR	Sidechain
1	C	746	ARG	Sidechain
1	C	759	ARG	Sidechain
1	C	905	PHE	Sidechain
1	C	951	ARG	Sidechain
1	C	976	TYR	Sidechain
1	C	982	TYR	Sidechain
1	C	993	TYR	Sidechain
1	D	1138	PRO	Peptide
1	D	1172	TYR	Sidechain
1	D	1295	TYR	Sidechain
1	D	1304	TYR	Sidechain
1	D	1318	TYR	Sidechain
1	D	1352	ILE	Mainchain
1	D	1403	TYR	Sidechain
1	D	1436	ILE	Mainchain
1	D	1451	TYR	Sidechain
1	D	1508	HIS	Sidechain
1	D	1608	ASN	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	1612	PHE	Mainchain
1	D	1614	PHE	Sidechain
1	D	1659	GLN	Peptide
1	D	1683	ARG	Mainchain
1	E	1736	TYR	Sidechain
1	E	1748	PHE	Sidechain
1	E	1753	PHE	Sidechain
1	E	1774	PHE	Sidechain
1	E	1778	GLY	Mainchain
1	E	1861	TYR	Sidechain
1	E	1932	GLU	Sidechain
1	E	2009	PHE	Mainchain
1	E	2010	HIS	Peptide,Sidechain
1	E	2013	ILE	Peptide
1	E	2014	ARG	Mainchain
1	E	2052	ARG	Sidechain
1	E	2108	TYR	Sidechain
1	E	2114	TYR	Sidechain
1	E	2127	ARG	Sidechain
1	E	2161	TYR	Peptide
1	E	2219	PHE	Peptide
1	F	1138	PRO	Peptide
1	F	1172	TYR	Sidechain
1	F	1195	ASN	Mainchain
1	F	1290	TYR	Sidechain
1	F	1294	PHE	Sidechain
1	F	1318	TYR	Sidechain
1	F	1443	PHE	Sidechain
1	F	1486	ARG	Sidechain
1	F	1511	TYR	Sidechain
1	F	1628	LYS	Mainchain
1	F	1645	LYS	Mainchain
1	F	1678	HIS	Sidechain
1	G	606	TYR	Sidechain
1	G	616	PHE	Sidechain
1	G	652	ARG	Sidechain
1	G	724	TYR	Sidechain
1	G	746	ARG	Sidechain
1	G	752	TYR	Sidechain
1	G	930	PHE	Peptide
1	G	943	ALA	Mainchain
1	G	982	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	a	2284	PHE	Sidechain
2	a	2296	TYR	Sidechain
2	a	2308	ASP	Peptide
2	a	2315	PHE	Sidechain
2	a	2316	TYR	Sidechain
2	a	2333	GLU	Sidechain
2	a	2350	TYR	Sidechain
2	a	2386	ARG	Sidechain
2	a	2402	PRO	Mainchain
2	a	2408	ARG	Sidechain
2	a	2442	ARG	Sidechain
2	a	2462	PHE	Sidechain
2	a	2475	ASP	Peptide
2	a	2620	ASN	Peptide
2	a	2750	ARG	Sidechain
2	b	3395	PHE	Sidechain
2	b	3525	TYR	Sidechain
2	b	3575	TYR	Sidechain
2	b	3633	ARG	Sidechain
2	b	3636	TYR	Sidechain
2	b	3736	TYR	Sidechain
2	b	3751	TYR	Sidechain
2	b	3769	SER	Mainchain
2	b	3788	TYR	Sidechain
2	b	3833	SER	Peptide
2	b	3880	TYR	Sidechain
2	c	3979	ASP	Peptide
2	c	4035	ASP	Peptide
2	c	4040	TYR	Sidechain
2	c	4048	TYR	Sidechain
2	c	4131	GLN	Sidechain
2	c	4132	TYR	Sidechain
2	c	4160	TYR	Sidechain
2	c	4220	VAL	Mainchain
2	c	4279	ARG	Mainchain
2	c	4293	TYR	Sidechain
2	c	4455	ARG	Sidechain
2	d	2853	TYR	Sidechain
2	d	2857	TYR	Sidechain
2	d	2889	ARG	Sidechain
2	d	3043	ARG	Sidechain
2	d	3187	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	e	3941	PRO	Peptide
2	e	3955	PHE	Sidechain
2	e	4006	TYR	Sidechain
2	e	4034	GLU	Peptide
2	e	4040	TYR	Sidechain
2	e	4192	ASN	Peptide
2	e	4261	ASN	Mainchain
2	e	4264	ASP	Peptide
2	e	4296	TYR	Peptide
2	e	4301	ARG	Sidechain
2	e	4307	ARG	Sidechain
2	e	4434	ARG	Sidechain
2	f	3379	ARG	Sidechain
2	f	3398	PHE	Sidechain
2	f	3410	TYR	Sidechain
2	f	3414	TYR	Sidechain
2	f	3442	ARG	Sidechain
2	f	3483	TYR	Sidechain
2	f	3513	LYS	Peptide
2	f	3636	TYR	Sidechain
2	f	3764	ASP	Peptide
2	f	3853	PHE	Sidechain
2	f	3880	TYR	Sidechain
2	g	2284	PHE	Mainchain
2	g	2386	ARG	Sidechain
2	g	2412	SER	Peptide
2	g	2442	ARG	Sidechain
2	g	2443	GLU	Sidechain
2	g	2461	TYR	Sidechain
2	g	2574	ARG	Sidechain
2	g	2579	ARG	Sidechain
2	g	2660	ARG	Sidechain
2	g	2766	TYR	Sidechain
2	g	2775	TYR	Sidechain
2	g	2789	SER	Peptide
2	g	2795	VAL	Mainchain

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	A	4355	4294	4294	10	0
1	B	4355	4294	4291	8	0
1	C	4355	4294	4291	6	0
1	D	4355	4294	4291	15	0
1	E	4355	4294	4291	55	0
1	F	4355	4294	4291	11	0
1	G	4355	4294	4291	7	0
2	a	4268	4154	4151	0	0
2	b	4268	4154	4150	0	0
2	c	4268	4154	4151	0	0
2	d	4268	4154	4151	0	0
2	e	4268	4154	4151	0	0
2	f	4268	4154	4151	0	0
2	g	4268	4154	4151	0	0
All	All	60361	59136	59096	110	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 (110) 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)
1:E:2010:HIS:CG	1:E:2010:HIS:ND1	1.76	1.54
1:E:2010:HIS:N	1:E:2010:HIS:CA	1.73	1.51
1:E:2011:LYS:C	1:E:2012:SER:N	1.70	1.42
1:E:1769:GLU:CG	1:E:1835:ALA:HB1	1.51	1.38
1:E:1769:GLU:HG2	1:E:1835:ALA:CB	1.60	1.31
1:E:2010:HIS:ND1	1:E:2010:HIS:CE1	1.99	1.31
1:D:1444:HIS:CE1	1:D:1445:LYS:HG2	1.71	1.26
1:E:2010:HIS:ND1	1:E:2010:HIS:CA	2.16	1.08
1:E:2010:HIS:ND1	1:E:2010:HIS:HA	1.61	1.05
1:E:1804:ASN:ND2	1:E:1835:ALA:HB3	1.74	1.02
1:E:1802:ASN:HA	1:E:1836:ASP:OD1	1.65	0.96
1:E:1804:ASN:CG	1:E:1835:ALA:HB3	1.91	0.91
1:E:2012:SER:H	1:E:2013:ILE:HB	1.33	0.89
1:E:1769:GLU:HG2	1:E:1835:ALA:HB1	0.87	0.87
1:E:2011:LYS:C	1:E:2012:SER:CA	2.47	0.82
1:D:1444:HIS:ND1	1:D:1445:LYS:HG2	1.95	0.81
1:E:1709:GLU:OE1	1:E:1803:ASP:OD2	1.99	0.81
1:D:1444:HIS:HE1	1:D:1445:LYS:HG2	1.39	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1804:ASN:ND2	1:E:1835:ALA:CB	2.46	0.79
1:E:2012:SER:N	1:E:2013:ILE:CA	2.42	0.75
1:E:2010:HIS:ND1	1:E:2010:HIS:NE2	2.34	0.74
1:E:2010:HIS:N	1:E:2010:HIS:CB	2.48	0.73
1:E:2010:HIS:ND1	1:E:2010:HIS:CD2	2.49	0.71
1:E:1802:ASN:OD1	1:E:1836:ASP:OD2	2.08	0.71
1:B:1819:GLU:HG3	1:B:1914:VAL:HG22	1.73	0.71
1:E:2012:SER:H	1:E:2013:ILE:CA	2.07	0.68
1:E:2010:HIS:ND1	1:E:2010:HIS:CB	2.57	0.66
1:E:2009:PHE:C	1:E:2010:HIS:CA	2.61	0.65
1:D:1444:HIS:CG	1:D:1445:LYS:H	2.14	0.65
1:E:1769:GLU:CD	1:E:1804:ASN:ND2	2.49	0.65
1:E:2012:SER:H	1:E:2013:ILE:CB	2.09	0.65
1:A:99:LYS:HE2	1:A:101:LEU:HD21	1.79	0.64
1:F:1596:VAL:HG12	1:F:1627:TRP:CZ3	2.33	0.64
1:E:1769:GLU:HG2	1:E:1835:ALA:HB2	1.75	0.63
1:C:1014:PRO:HG2	1:C:1089:ILE:HG22	1.83	0.61
1:F:1254:LEU:HD13	1:F:1444:HIS:CE1	2.36	0.60
1:E:2012:SER:N	1:E:2013:ILE:HB	2.13	0.60
1:E:1769:GLU:CD	1:E:1835:ALA:HB1	2.20	0.59
1:E:1802:ASN:CA	1:E:1836:ASP:OD1	2.47	0.58
1:F:1393:PHE:CE2	1:F:1437:VAL:HG12	2.40	0.57
1:E:2010:HIS:CD2	1:E:2011:LYS:N	2.73	0.57
1:C:727:VAL:HG23	1:C:728:PHE:CD2	2.40	0.55
1:D:1444:HIS:ND1	1:D:1445:LYS:CG	2.68	0.55
1:D:1444:HIS:ND1	1:D:1445:LYS:N	2.52	0.55
1:D:1595:TYR:HB3	1:D:1638:LEU:HD11	1.89	0.55
1:E:1769:GLU:HG3	1:E:1835:ALA:HB1	1.75	0.55
1:E:1709:GLU:OE1	1:E:1803:ASP:CG	2.44	0.54
1:G:1033:THR:HG22	1:G:1070:SER:HB3	1.91	0.52
1:A:340:LYS:HE3	1:A:367:PHE:CE1	2.45	0.52
1:D:1444:HIS:CG	1:D:1445:LYS:N	2.77	0.52
1:A:99:LYS:HE2	1:A:101:LEU:CD2	2.39	0.52
1:E:1801:ILE:O	1:E:1836:ASP:OD1	2.28	0.51
1:D:1630:ALA:HB2	1:D:1640:GLN:HB2	1.92	0.51
1:E:1915:ASN:CG	1:E:1954:ASN:HB3	2.31	0.51
1:A:554:HIS:CB	1:B:2050:MET:HG2	2.41	0.50
1:E:1804:ASN:OD1	1:E:1835:ALA:HB3	2.09	0.50
1:B:2119:VAL:HG12	1:B:2131:THR:HG22	1.93	0.50
1:D:1475:VAL:HG23	1:D:1567:THR:HB	1.95	0.49
1:B:1819:GLU:CG	1:B:1914:VAL:HG22	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1802:ASN:HA	1:E:1836:ASP:CG	2.32	0.49
1:B:1885:THR:HG22	1:B:1886:LEU:N	2.28	0.49
1:E:1915:ASN:OD1	1:E:1948:ASP:OD2	2.30	0.49
1:E:2011:LYS:C	1:E:2012:SER:C	2.73	0.48
1:A:423:ILE:N	1:A:423:ILE:HD12	2.28	0.47
1:A:553:ALA:HB1	1:B:2227:PHE:CD1	2.49	0.47
1:C:1051:ILE:HG22	1:C:1053:LYS:H	1.79	0.47
1:E:1775:LEU:C	1:E:1776:LEU:HD12	2.35	0.47
1:D:1177:ILE:HD11	1:D:1194:LEU:HD11	1.97	0.46
1:E:1819:GLU:HG3	1:E:1914:VAL:HG22	1.97	0.46
1:G:605:LYS:HA	1:G:621:PHE:CE1	2.51	0.46
1:C:955:ILE:HG22	1:C:966:LEU:HA	1.97	0.46
1:D:1472:LYS:HE3	1:D:1499:PHE:CG	2.50	0.46
1:E:1804:ASN:HD21	1:E:1835:ALA:CB	2.26	0.46
1:E:1769:GLU:CD	1:E:1804:ASN:HD21	2.18	0.45
1:E:1915:ASN:HD21	1:E:1954:ASN:HA	1.81	0.45
1:C:783:ASN:HD21	1:C:873:ASN:HB2	1.82	0.45
1:E:1915:ASN:ND2	1:E:1954:ASN:HA	2.32	0.44
1:B:1775:LEU:HD23	1:B:1776:LEU:N	2.32	0.44
1:F:1366:GLU:HB2	1:F:1465:VAL:HG22	1.99	0.44
1:F:1517:ARG:HB3	1:F:1542:TYR:CD2	2.52	0.44
1:E:1804:ASN:HD21	1:E:1835:ALA:HB3	1.71	0.44
1:F:1319:THR:C	1:F:1320:LEU:HD12	2.38	0.43
1:A:47:GLU:HB3	1:A:48:PRO:HD2	2.01	0.43
1:E:1914:VAL:HB	1:E:2010:HIS:HB2	2.00	0.43
1:A:379:TYR:CE1	1:A:396:SER:HB3	2.54	0.43
1:F:1286:LEU:HD12	1:F:1287:GLU:H	1.84	0.43
1:E:1819:GLU:CG	1:E:1914:VAL:HG22	2.49	0.43
1:B:1732:LEU:HD23	1:B:1732:LEU:HA	1.88	0.43
1:D:1452:LYS:HA	1:D:1453:PRO:HD3	1.93	0.43
1:G:796:GLY:HA2	1:G:808:THR:HB	2.00	0.42
1:G:790:GLU:HB2	1:G:811:LYS:HE2	2.00	0.42
1:E:1802:ASN:CG	1:E:1836:ASP:OD2	2.58	0.42
1:A:340:LYS:HE3	1:A:367:PHE:CZ	2.55	0.42
1:F:1247:PHE:CD2	1:F:1264:ILE:HG22	2.55	0.42
1:E:1922:GLU:OE1	1:E:1943:LYS:HE2	2.20	0.42
1:C:1047:SER:O	1:C:1089:ILE:HG23	2.20	0.41
1:E:2013:ILE:HG23	1:E:2017:TYR:HB3	2.02	0.41
1:D:1444:HIS:CE1	1:D:1445:LYS:CG	2.67	0.41
1:G:1075:GLN:HB3	1:G:1078:LYS:H	1.85	0.41
1:E:2012:SER:N	1:E:2013:ILE:CB	2.77	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1160:LEU:HB2	1:D:1168:ILE:HD11	2.03	0.41
1:F:1484:MET:H	1:F:1484:MET:HG3	1.71	0.41
1:A:257:TRP:CZ2	1:A:281:ASN:HB2	2.56	0.41
1:E:1709:GLU:OE1	1:E:1803:ASP:OD1	2.39	0.41
1:G:1082:ARG:HA	1:G:1105:LEU:O	2.20	0.41
1:E:1959:PHE:CE2	1:E:2003:VAL:HG23	2.56	0.41
1:G:614:PRO:HB3	1:G:616:PHE:CE1	2.57	0.40
1:F:1583:ILE:HD13	1:F:1583:ILE:HG21	1.83	0.40
1:E:1746:PRO:HA	1:E:1747:PRO:C	2.41	0.40
1:F:1520:TRP:CD1	1:F:1548:TYR:CZ	3.10	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	A	552/554 (100%)	513 (93%)	39 (7%)	0	100	100
1	B	552/554 (100%)	512 (93%)	38 (7%)	2 (0%)	34	72
1	C	552/554 (100%)	516 (94%)	32 (6%)	4 (1%)	22	63
1	D	552/554 (100%)	516 (94%)	34 (6%)	2 (0%)	34	72
1	E	552/554 (100%)	510 (92%)	32 (6%)	10 (2%)	8	40
1	F	552/554 (100%)	516 (94%)	33 (6%)	3 (0%)	29	69
1	G	552/554 (100%)	517 (94%)	33 (6%)	2 (0%)	34	72
2	a	542/544 (100%)	505 (93%)	33 (6%)	4 (1%)	22	63
2	b	542/544 (100%)	505 (93%)	31 (6%)	6 (1%)	14	52
2	c	542/544 (100%)	499 (92%)	42 (8%)	1 (0%)	47	81
2	d	542/544 (100%)	493 (91%)	47 (9%)	2 (0%)	34	72
2	e	542/544 (100%)	501 (92%)	38 (7%)	3 (1%)	25	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	f	542/544 (100%)	498 (92%)	39 (7%)	5 (1%)	17 57
2	g	542/544 (100%)	499 (92%)	40 (7%)	3 (1%)	25 66
All	All	7658/7686 (100%)	7100 (93%)	511 (7%)	47 (1%)	29 66

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	992	ASP
1	E	1783	ALA
1	E	2010	HIS
1	E	2011	LYS
1	E	2013	ILE
2	a	2577	SER
2	b	3427	ASN
2	b	3691	SER
2	d	2864	VAL
2	e	4242	PRO
2	f	3498	ASN
2	f	3691	SER
2	g	2577	SER
1	B	2124	ASP
1	C	741	SER
1	D	1402	GLY
1	F	1489	LYS
1	G	1025	HIS
2	a	2367	ASP
2	d	3070	VAL
2	g	2759	ASP
1	B	2015	SER
1	E	2015	SER
1	E	2244	HIS
1	F	1217	ALA
2	b	3689	GLU
2	b	3855	LEU
2	g	2367	ASP
1	C	795	GLU
1	E	1902	VAL
1	F	1516	ASP
2	c	4166	GLU
2	e	4474	GLU
2	f	3480	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	2124	ASP
1	G	880	SER
2	a	2511	ASP
2	f	3419	PRO
1	C	783	ASN
2	b	3447	GLU
1	E	2188	GLY
2	e	4314	PRO
2	b	3885	PRO
1	D	1177	ILE
1	E	1788	VAL
2	f	3384	PRO
2	a	2282	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	492/492 (100%)	481 (98%)	11 (2%)	52	71
1	B	492/492 (100%)	484 (98%)	8 (2%)	62	79
1	C	492/492 (100%)	480 (98%)	12 (2%)	49	69
1	D	492/492 (100%)	481 (98%)	11 (2%)	52	71
1	E	492/492 (100%)	478 (97%)	14 (3%)	43	65
1	F	492/492 (100%)	483 (98%)	9 (2%)	59	77
1	G	492/492 (100%)	477 (97%)	15 (3%)	41	63
2	a	494/494 (100%)	479 (97%)	15 (3%)	41	63
2	b	494/494 (100%)	483 (98%)	11 (2%)	52	71
2	c	494/494 (100%)	479 (97%)	15 (3%)	41	63
2	d	494/494 (100%)	483 (98%)	11 (2%)	52	71
2	e	494/494 (100%)	479 (97%)	15 (3%)	41	63
2	f	494/494 (100%)	478 (97%)	16 (3%)	39	61
2	g	494/494 (100%)	483 (98%)	11 (2%)	52	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6902/6902 (100%)	6728 (98%)	174 (2%)	50 68

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ARG
1	A	107	GLU
1	A	163	TYR
1	A	164	LEU
1	A	265	SER
1	A	349	SER
1	A	353	ASP
1	A	364	PHE
1	A	387	ASN
1	A	389	ILE
1	A	423	ILE
1	B	1839	ASN
1	B	1884	TYR
1	B	1978	THR
1	B	2045	TYR
1	B	2062	PHE
1	B	2124	ASP
1	B	2230	PRO
1	B	2237	LEU
1	C	623	LYS
1	C	629	ASN
1	C	639	THR
1	C	673	GLU
1	C	746	ARG
1	C	753	THR
1	C	828	THR
1	C	919	ASP
1	C	936	ASP
1	C	956	SER
1	C	983	THR
1	C	1022	THR
1	D	1135	ILE
1	D	1158	SER
1	D	1237	ASP
1	D	1258	HIS
1	D	1363	MET
1	D	1482	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1484	MET
1	D	1496	PHE
1	D	1502	ASP
1	D	1523	VAL
1	D	1545	ASN
1	E	1768	ARG
1	E	1769	GLU
1	E	1807	VAL
1	E	1878	ARG
1	E	1883	SER
1	E	1884	TYR
1	E	1886	LEU
1	E	1901	PRO
1	E	1942	ILE
1	E	2062	PHE
1	E	2093	THR
1	E	2131	THR
1	E	2157	HIS
1	E	2194	LYS
1	F	1235	ILE
1	F	1241	VAL
1	F	1317	SER
1	F	1435	VAL
1	F	1460	VAL
1	F	1484	MET
1	F	1497	GLN
1	F	1502	ASP
1	F	1597	ASN
1	G	636	ARG
1	G	639	THR
1	G	673	GLU
1	G	685	VAL
1	G	719	SER
1	G	720	LEU
1	G	746	ARG
1	G	760	ASP
1	G	781	ASP
1	G	862	MET
1	G	942	HIS
1	G	955	ILE
1	G	964	ILE
1	G	1025	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	1071	VAL
2	a	2292	THR
2	a	2332	ARG
2	a	2333	GLU
2	a	2354	LEU
2	a	2381	ILE
2	a	2442	ARG
2	a	2465	GLN
2	a	2487	THR
2	a	2489	TYR
2	a	2546	LEU
2	a	2577	SER
2	a	2629	THR
2	a	2668	THR
2	a	2785	LEU
2	a	2805	ASP
2	b	3447	GLU
2	b	3462	ASP
2	b	3480	ASN
2	b	3498	ASN
2	b	3556	ARG
2	b	3619	VAL
2	b	3778	ARG
2	b	3801	THR
2	b	3817	SER
2	b	3831	THR
2	b	3904	VAL
2	c	3963	THR
2	c	3970	TYR
2	c	3985	LEU
2	c	4004	GLU
2	c	4009	PHE
2	c	4107	THR
2	c	4120	GLN
2	c	4126	GLN
2	c	4133	PHE
2	c	4156	THR
2	c	4183	LEU
2	c	4233	LEU
2	c	4290	SER
2	c	4308	TYR
2	c	4312	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	d	2870	ASN
2	d	2889	ARG
2	d	2890	GLU
2	d	2947	THR
2	d	2976	PRO
2	d	2999	ARG
2	d	3132	GLU
2	d	3235	VAL
2	d	3256	VAL
2	d	3351	ASP
2	d	3355	CYS
2	e	3937	TRP
2	e	3940	ILE
2	e	4004	GLU
2	e	4050	PHE
2	e	4061	THR
2	e	4083	SER
2	e	4107	THR
2	e	4123	ILE
2	e	4135	LEU
2	e	4150	ASP
2	e	4168	THR
2	e	4233	LEU
2	e	4311	LEU
2	e	4324	THR
2	e	4381	THR
2	f	3442	ARG
2	f	3459	THR
2	f	3466	PRO
2	f	3468	LEU
2	f	3536	THR
2	f	3550	THR
2	f	3595	LEU
2	f	3606	SER
2	f	3674	MET
2	f	3697	SER
2	f	3769	SER
2	f	3778	ARG
2	f	3824	THR
2	f	3846	ILE
2	f	3874	THR
2	f	3895	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	g	2308	ASP
2	g	2332	ARG
2	g	2333	GLU
2	g	2359	ILE
2	g	2429	THR
2	g	2449	GLN
2	g	2518	TRP
2	g	2577	SER
2	g	2612	ASN
2	g	2681	SER
2	g	2731	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	217	ASN
1	A	444	ASN
1	D	1236	ASN
1	D	1349	ASN
1	D	1351	ASN
1	E	1804	ASN
1	E	1915	ASN
1	E	2010	HIS
1	F	1349	ASN
1	F	1367	ASN
1	G	783	ASN
1	G	904	HIS
1	G	1010	ASN
2	a	2568	ASN
2	b	3814	ASN
2	c	3994	ASN
2	c	4039	ASN
2	c	4371	ASN
2	d	3035	ASN
2	d	3158	ASN
2	d	3257	ASN
2	e	4144	ASN
2	e	4149	ASN
2	f	3592	ASN
2	f	3814	ASN
2	g	2480	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	g	2568	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	2011:LYS	C	2012:SER	N	1.70

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11678. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

6.1.1 Primary map

X

Y

Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 64

Y Index: 64

Z Index: 64

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: 62

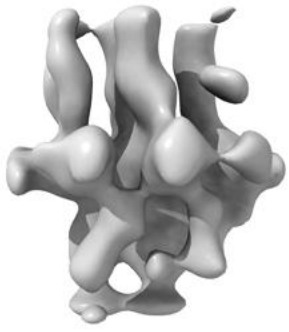
Y Index: 66

Z Index: 66

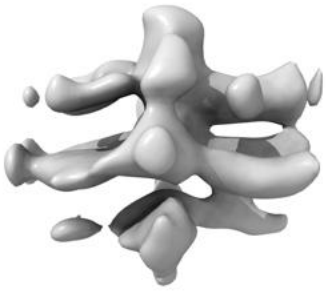
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

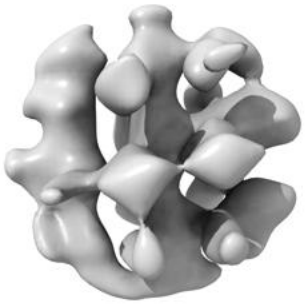
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0133. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

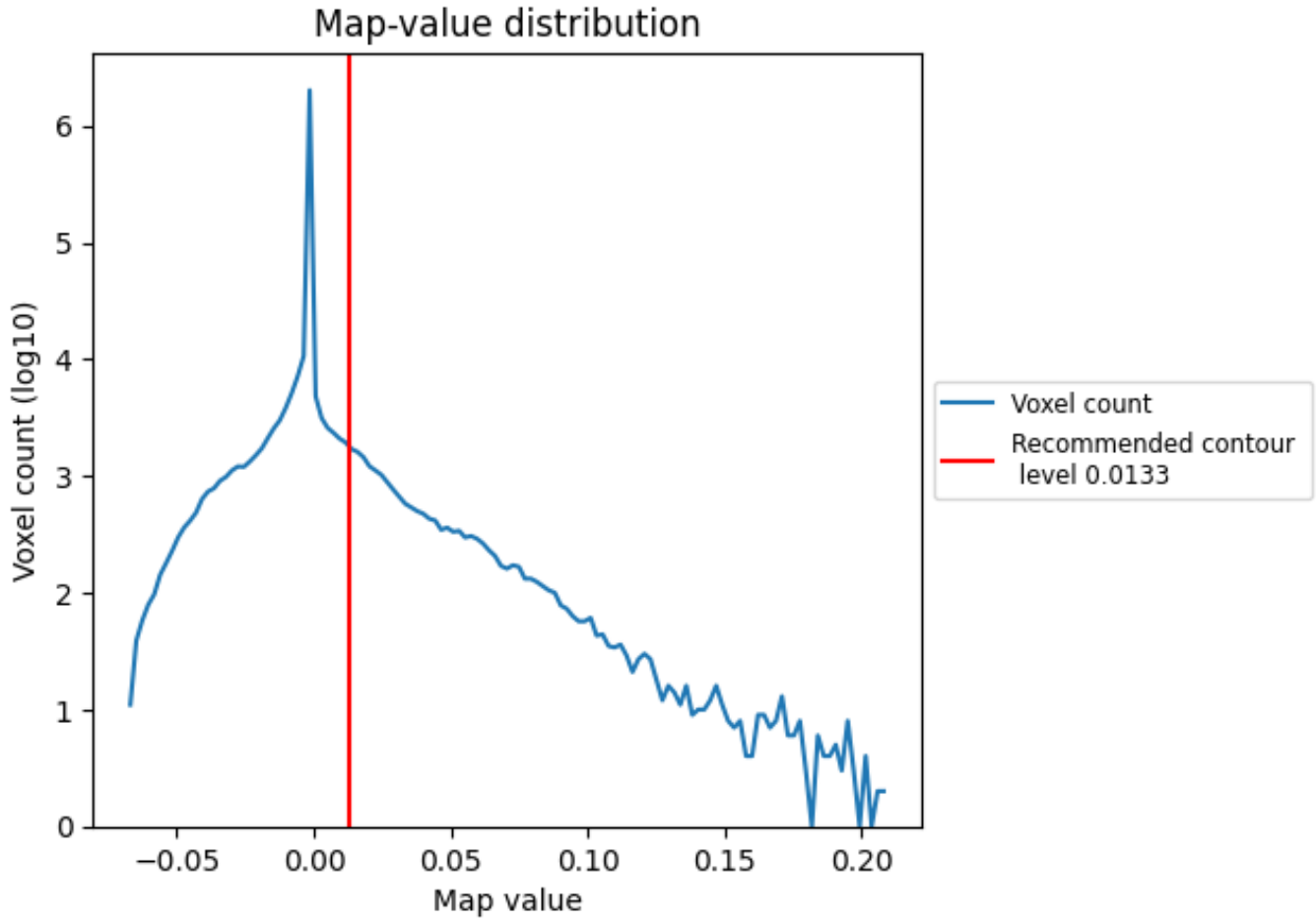
6.5 Mask visualisation (i)

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

7 Map analysis

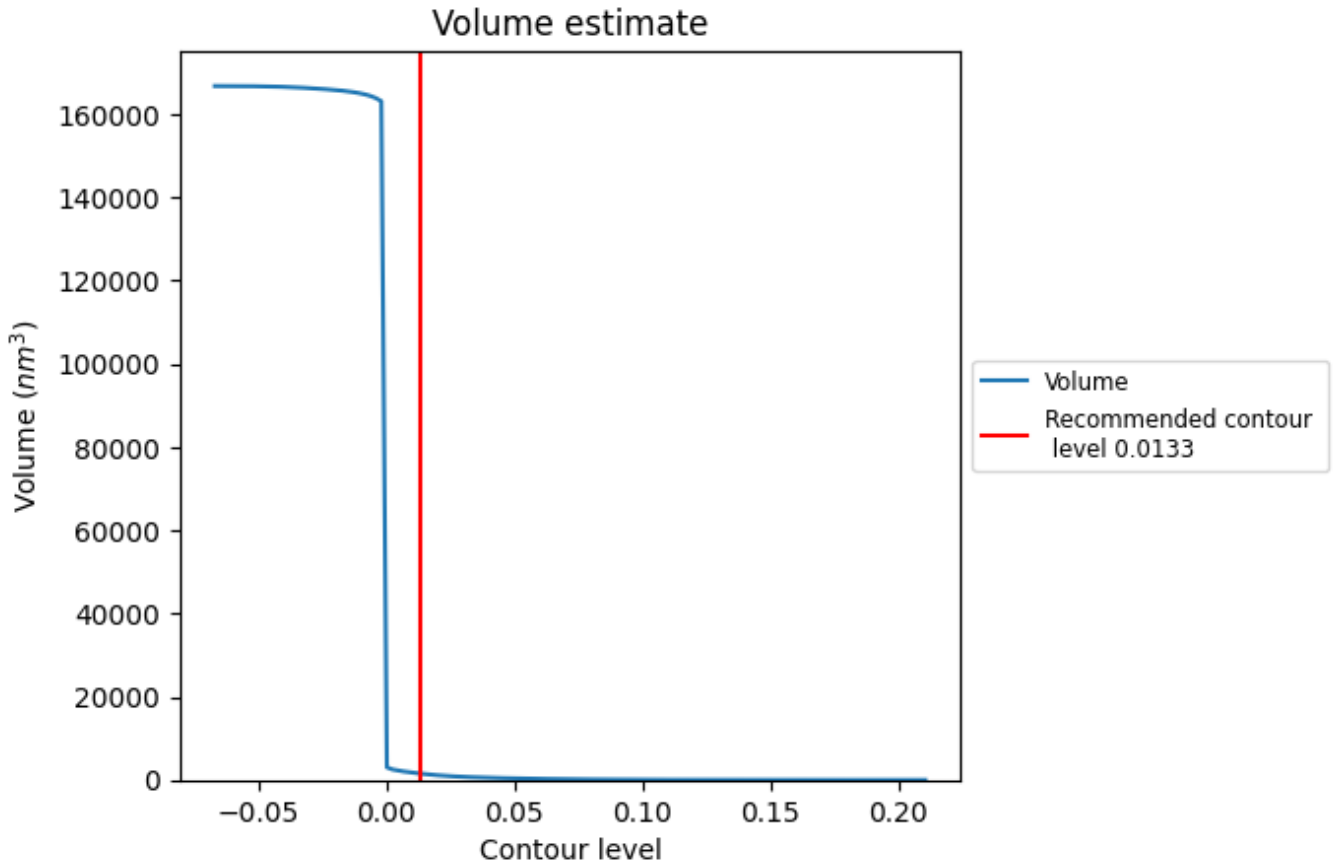
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

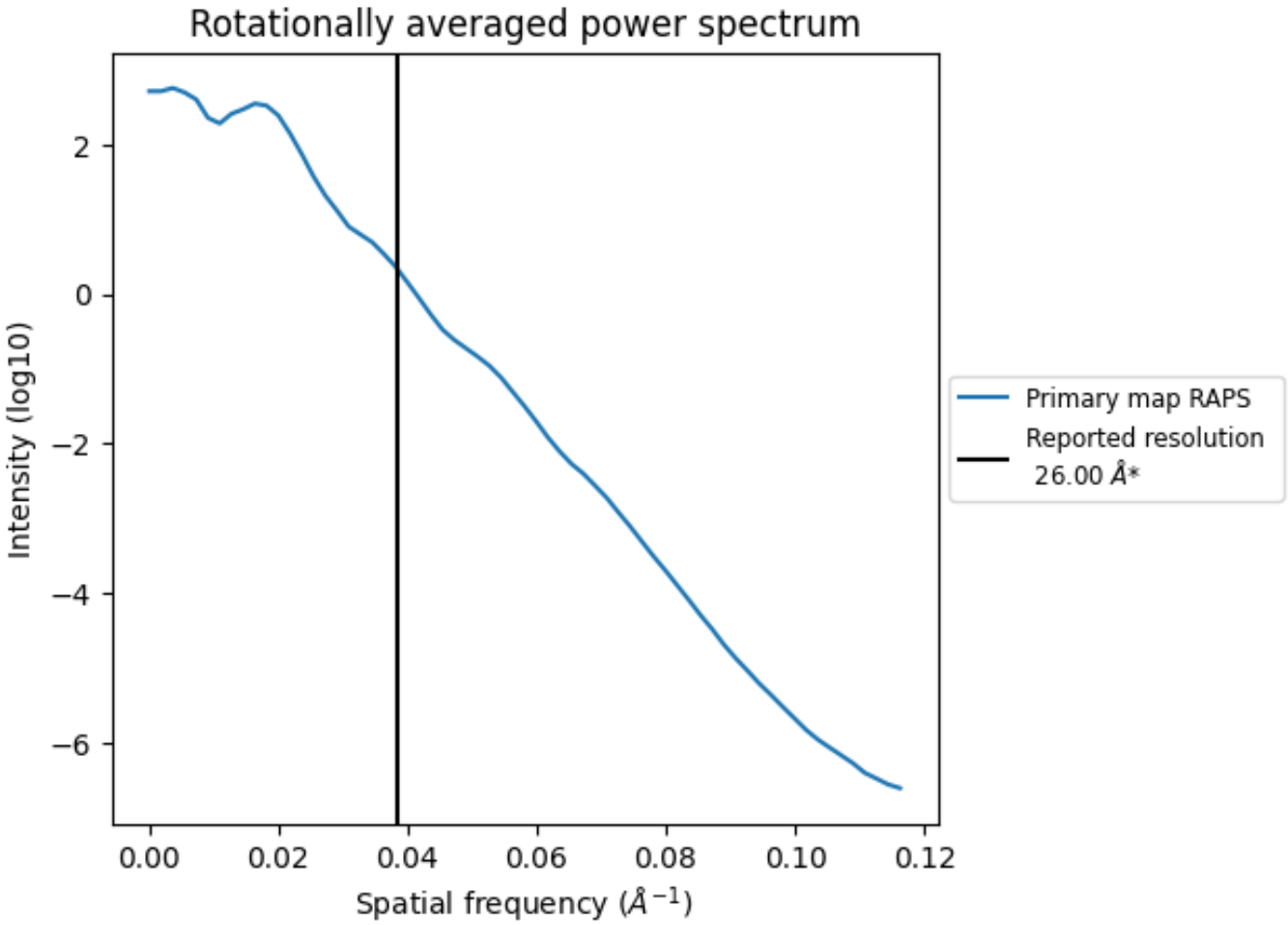
7.2 Volume estimate



The volume at the recommended contour level is 1526 nm^3; this corresponds to an approximate mass of 1378 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

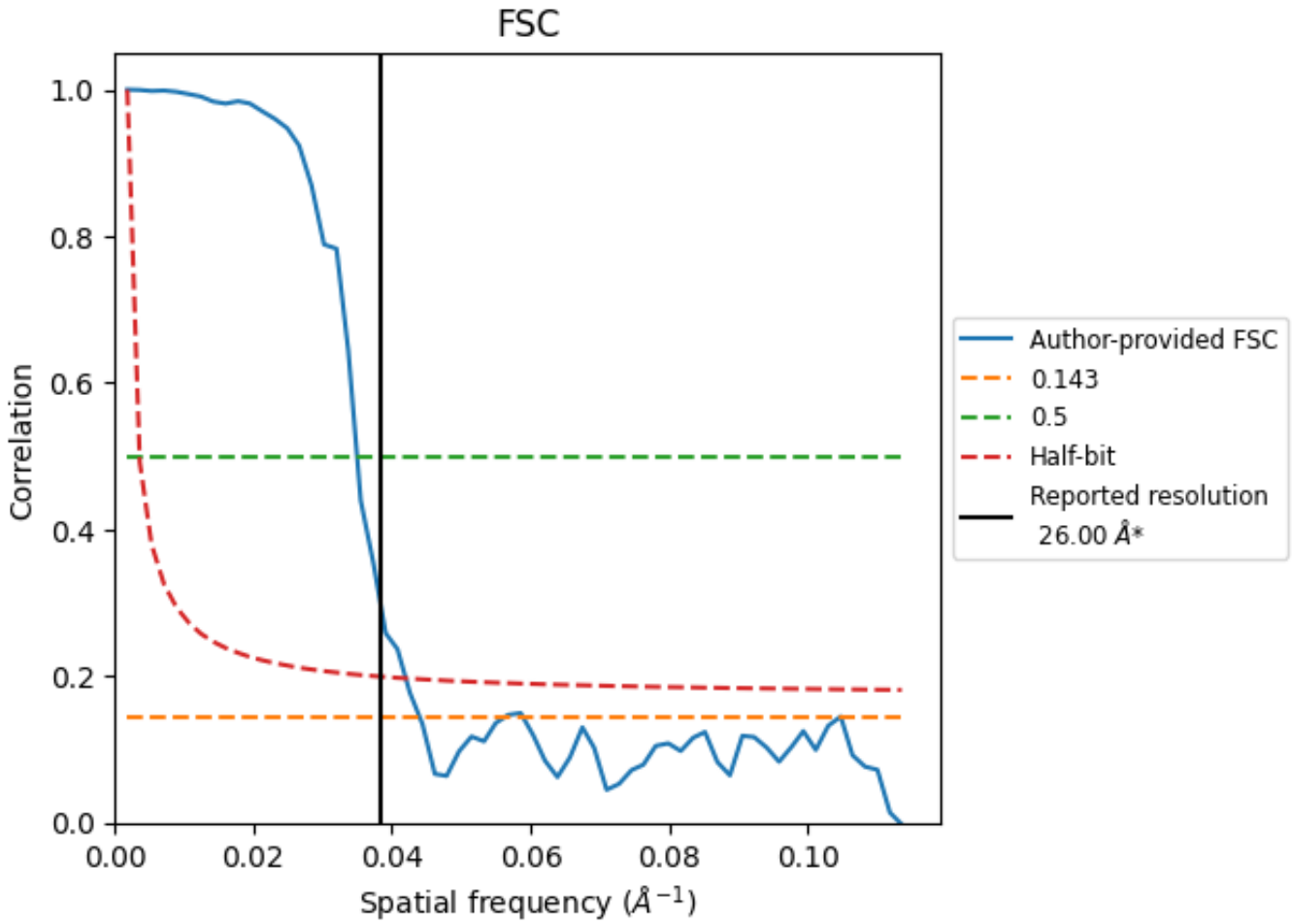


*Reported resolution corresponds to spatial frequency of 0.038 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.038 Å^{-1}

8.2 Resolution estimates (i)

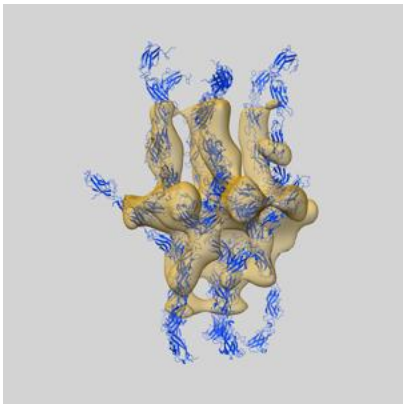
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	26.00	-
Author-provided FSC curve	22.73	28.57	23.81
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

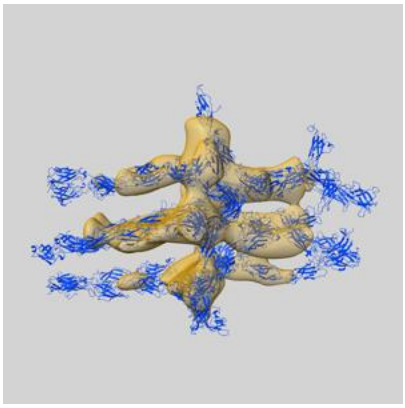
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11678 and PDB model 7A7D. Per-residue inclusion information can be found in section 3 on page 6.

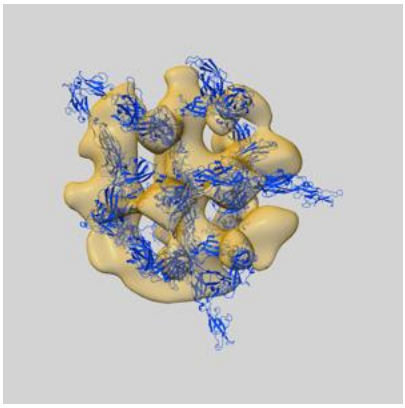
9.1 Map-model overlay



X



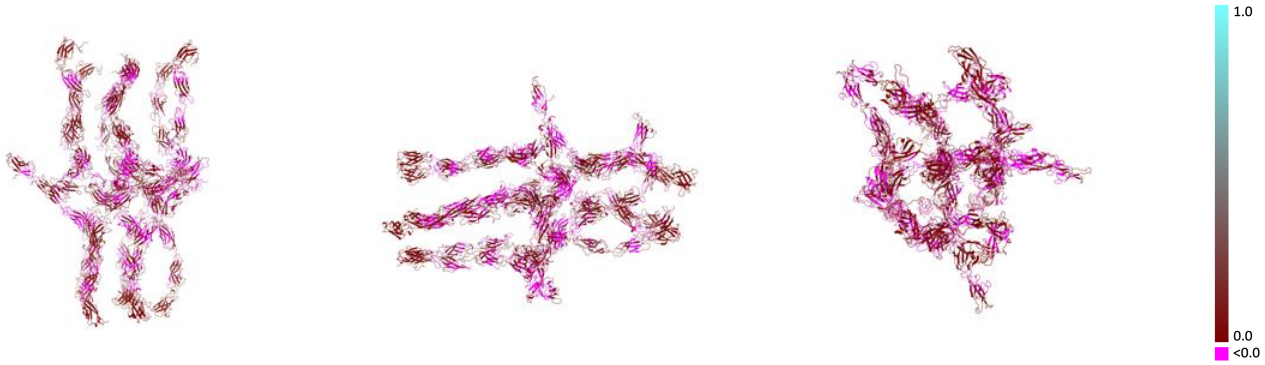
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0133 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

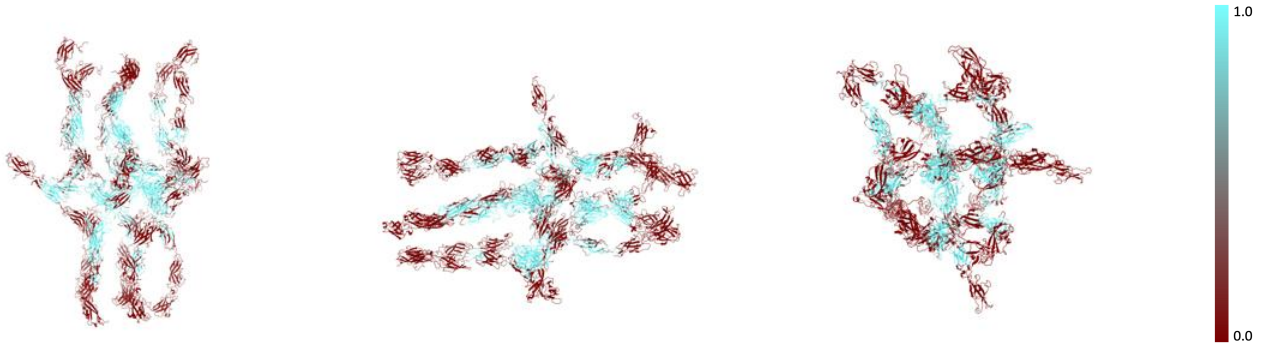
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

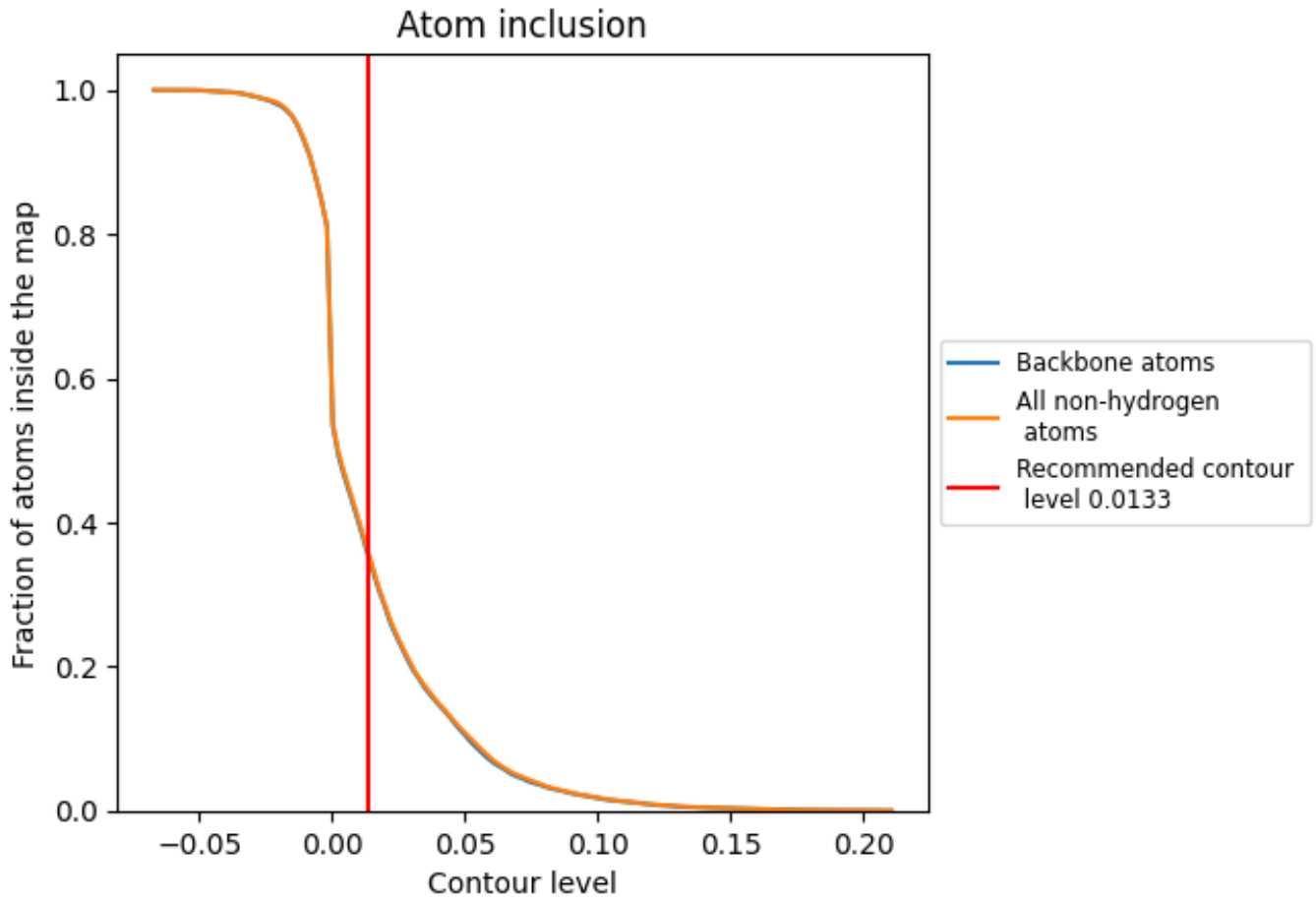
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0133).

9.4 Atom inclusion (i)



At the recommended contour level, 36% of all backbone atoms, 36% 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 (0.0133) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3615	0.0190
A	0.5617	0.0360
B	0.2968	0.0080
C	0.2207	0.0050
D	0.3273	0.0090
E	0.3843	0.0380
F	0.2945	0.0190
G	0.3454	0.0280
a	0.4007	0.0340
b	0.1989	0.0090
c	0.4870	0.0250
d	0.6420	0.0160
e	0.3782	0.0050
f	0.1095	0.0080
g	0.4446	0.0270