



Full wwPDB EM Validation Report ⓘ

Aug 3, 2026 – 08:22 pm BST

PDB ID : 9S5E / pdb_00009s5e
EMDB ID : EMD-54595
Title : Tight class, Apo-state RyR1 in the native membrane solved by StA
Authors : Mikirtumov, V.
Deposited on : 2025-07-29
Resolution : 6.99 Å(reported)
Based on initial model : 7tzc

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

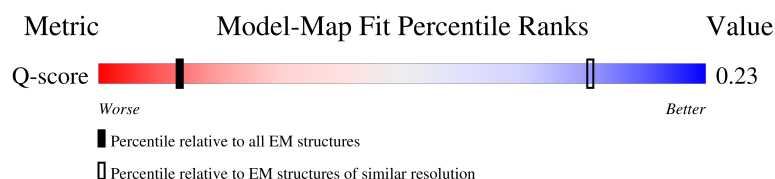
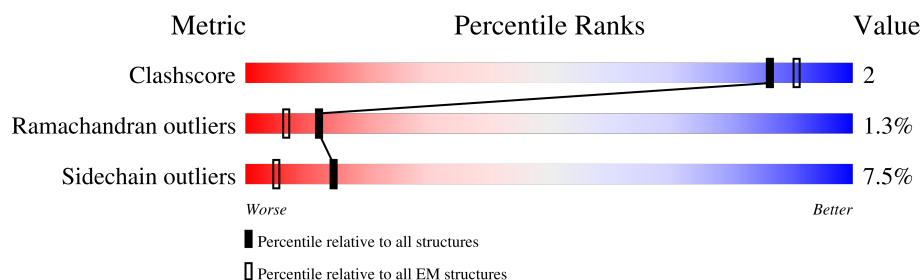
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 6.99 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	449 (6.49 - 7.46)

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

Mol	Chain	Length	Quality of chain
1	A	5037	20% 74% 12% • 13%
1	B	5037	20% 74% 11% • 13%
1	C	5037	20% 74% 11% • 13%
1	D	5037	20% 74% 12% • 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	108	41% 86% 11% ..
2	F	108	38% 87% 11% ..
2	G	108	39% 88% 10% ..
2	H	108	44% 87% 11% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 285956 atoms, of which 142276 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	4404	Total	C	H	N	O	S	0	0
			69828	22323	34740	6046	6482	237		
1	B	4404	Total	C	H	N	O	S	0	0
			69828	22323	34740	6046	6482	237		
1	C	4404	Total	C	H	N	O	S	0	0
			69828	22323	34740	6046	6482	237		
1	D	4404	Total	C	H	N	O	S	0	0
			69828	22323	34740	6046	6482	237		

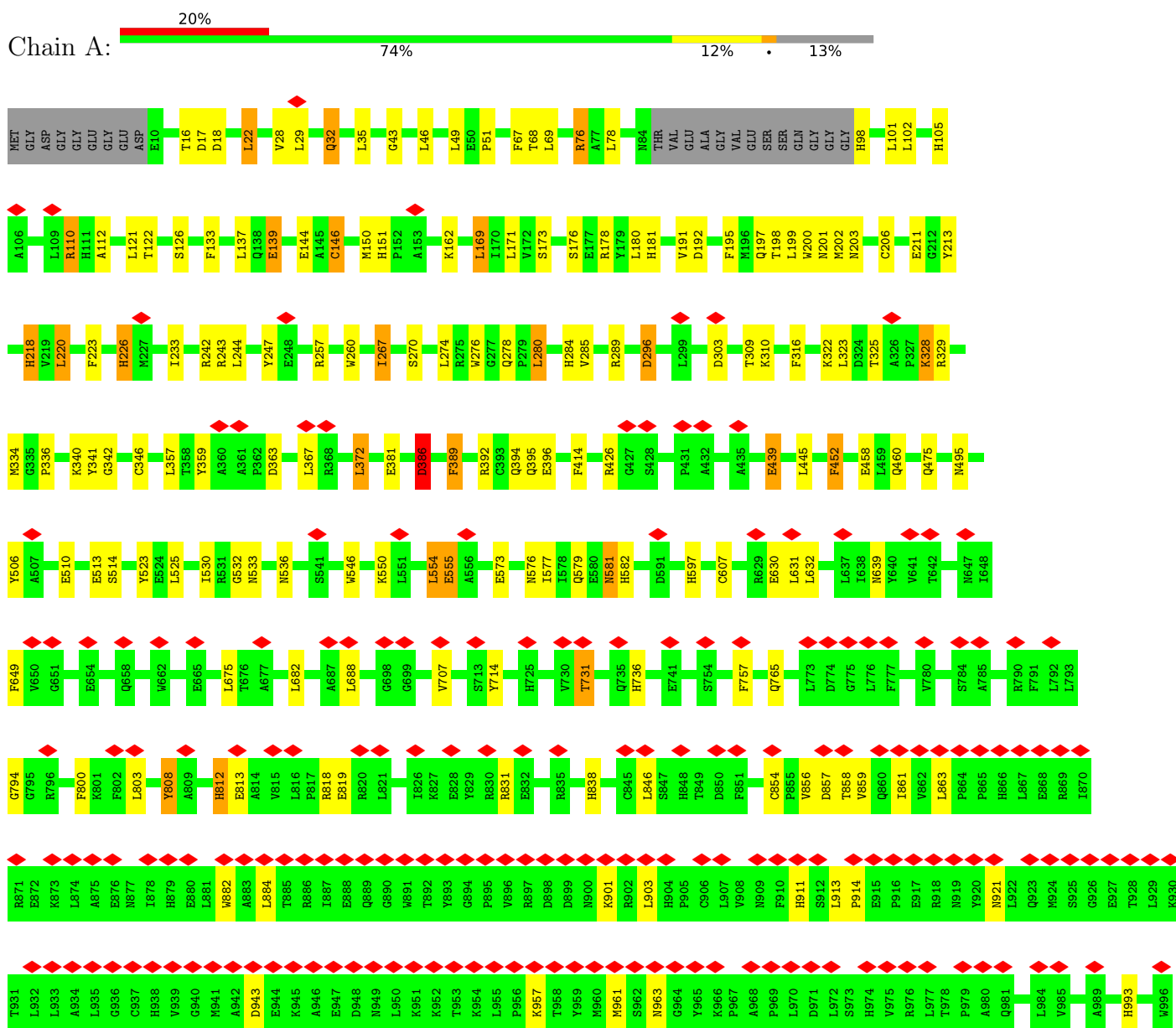
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

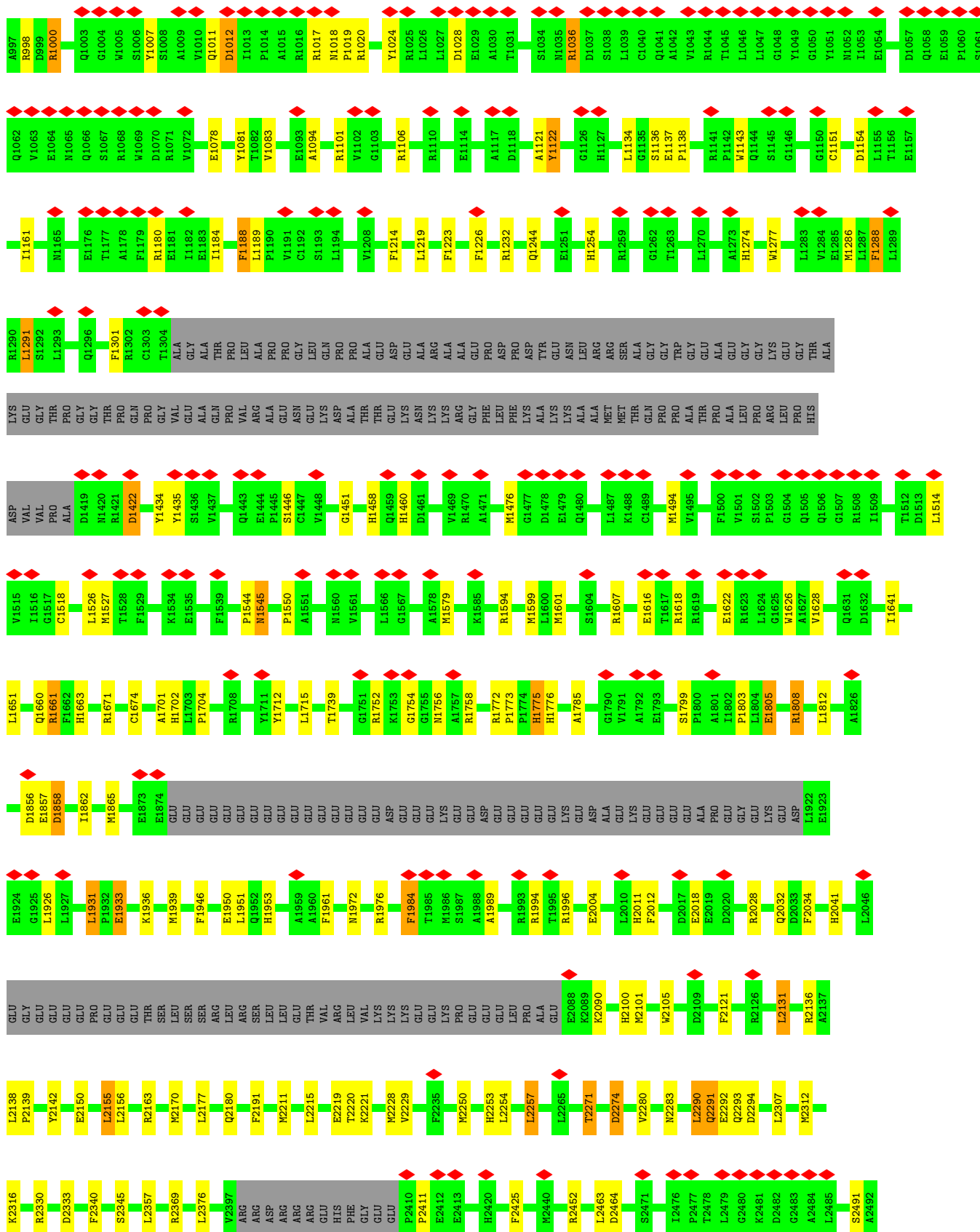
Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	F	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	G	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	H	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		

3 Residue-property plots

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

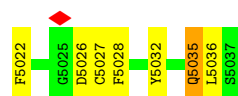
• Molecule 1: Ryanodine receptor 1



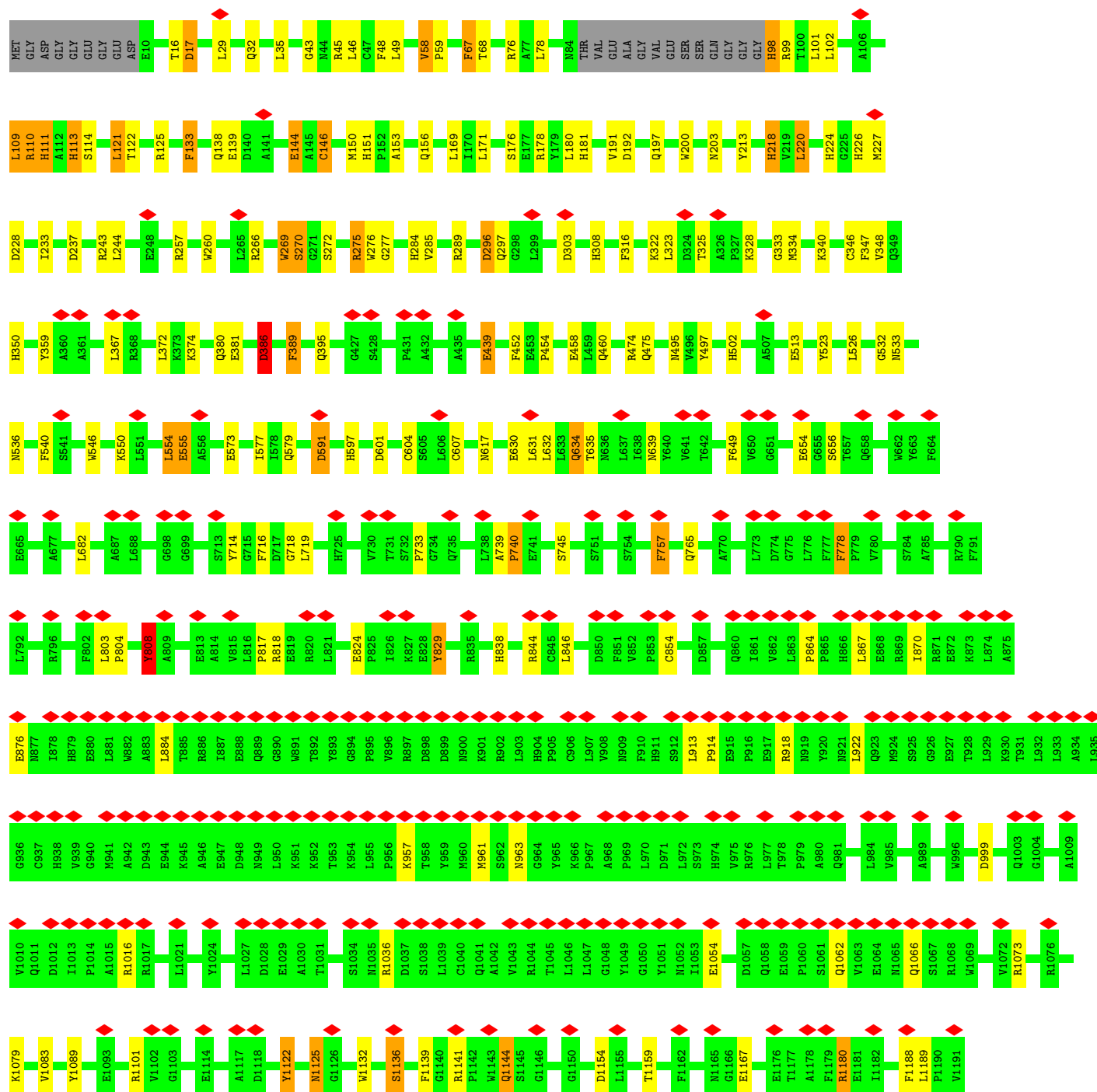
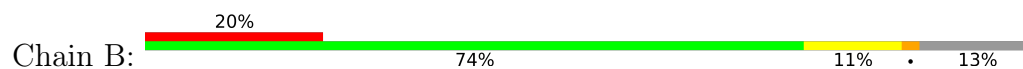






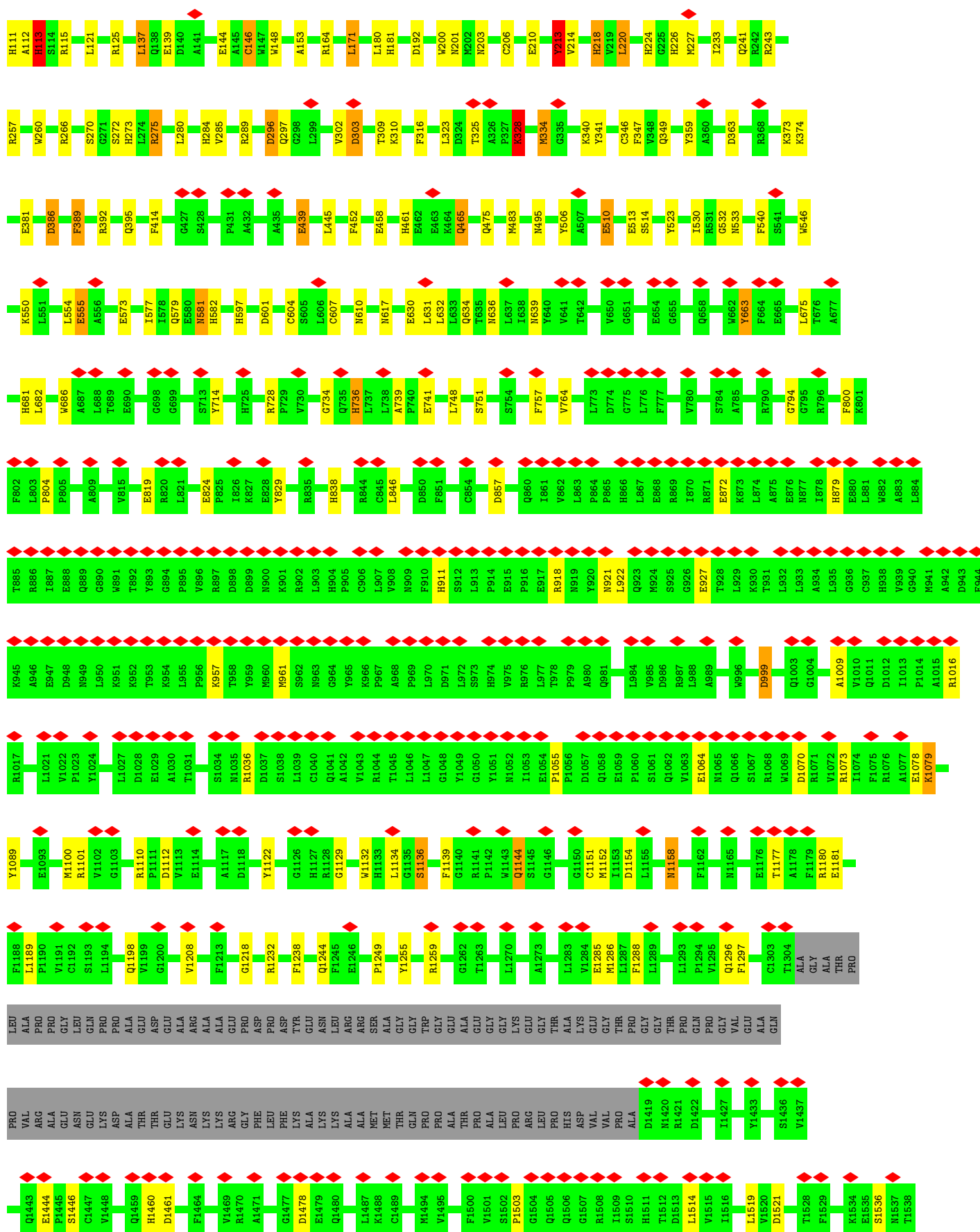


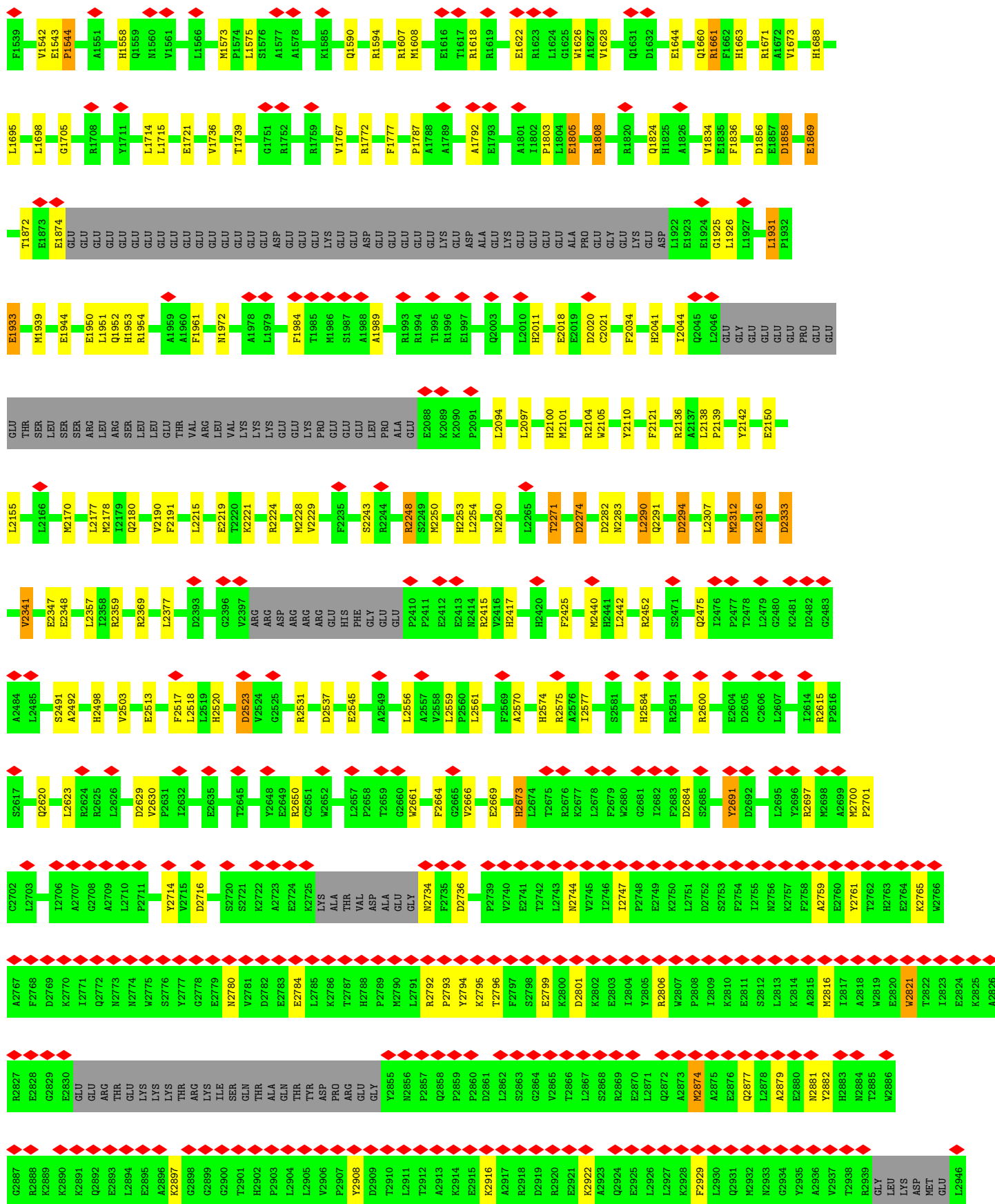
• Molecule 1: Ryanodine receptor 1

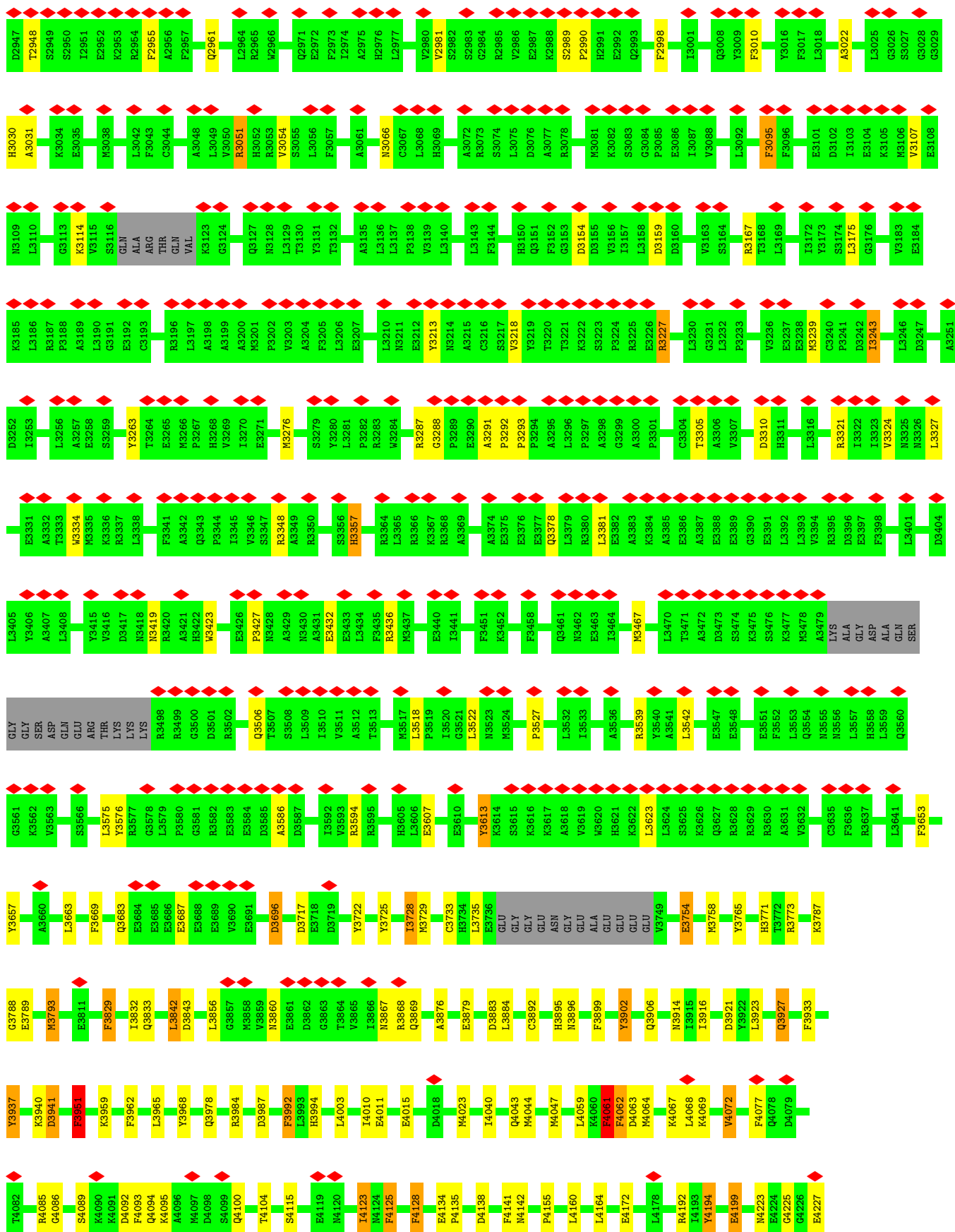




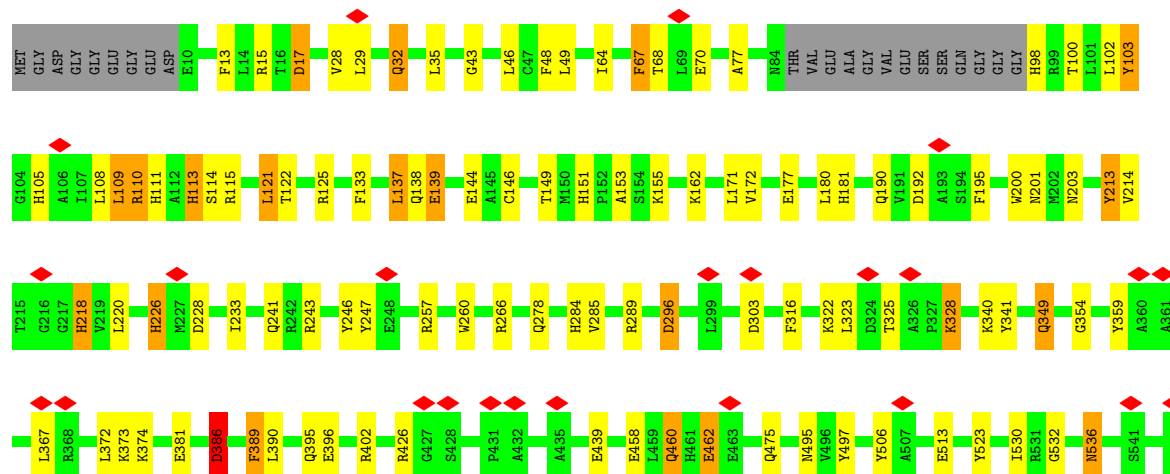
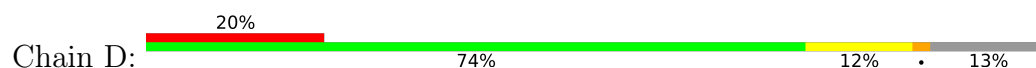
W3620	H3621	K3622	L3623	L3624	S3625	K3626	Q3627	R3628	R3629	R3630	A3631	V3632	D3633	C3635	R3636	F3637	L3641	F3653	Y3657	A3660	L3663	D3666	F3669	E3670	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	D3696	A3601	V3602	L3603	Y3604	H3605	T3609	E3610	Y3613	K3614	S3615	K3616	K3617	A3618	V3619										
A3526	P3527	L3532	I3533	A3536	R3539	Y3540	S3541	L3542	D3546	E3547	E3548	V3549	R3550	E3551	F3552	L3553	L3557	Q3560	G3561	K3562	V3563	L3575	G3578	L3579	P3580	G3581	R3582	E3583	E3584	D3585	A3586	D3587	R3595	A3601	V3602	L3603	Y3604	H3605	T3609	E3610	Y3613	K3614	S3615	K3616	K3617	A3618	V3619											
F3458	Q3461	N3462	E3463	I3464	S3468	F3469	L3470	T3471	A3472	D3473	S3474	K3475	S3476	K3477	A3478	A3479	LYS	ALA	GLY	ASP	ALA	GLN	SER	GLY	SER	ASP	GLN	GLY	ARG	THR	LYS	LYS	R3498	R3499	G3500	D3501	R3502	Q3506	T3507	S3508	L3509	T3510	V3511	A3512	T3513	M3517	T3520	N3523	K3524	C3525								
E3377	Q3378	L3379	R3380	E3382	A3383	K3384	A3385	E3386	A3387	E3388	E3389	G3390	E3391	L3392	L3393	D3396	E3397	F3398	L3401	D3404	L3405	Y3406	A3407	L3408	Y3415	V3416	D3417	N3418	N3419	A3421	H3422	G3423	E3426	P3427	N3430	A3431	E3432	E3433	L3434	F3435	R3436	M3437	E3440	I3441	H3449	N3450	K3452	R3453										
P3297	A3298	G3299	A3300	P3301	C3304	T3305	A3306	V3307	P3308	S3309	D3310	H3311	R3321	I3322	L3323	V3324	L3327	E3331	A3332	T3333	W3334	K3335	K3336	R3337	L3338	F3341	A3342	Q3343	P3344	T3345	V3346	R3347	R3348	A3349	R3350	P3351	S3356	T3359	P3360	T3361	R3364	L3365	R3366	K3367	R3368	K3371	A3374	E3375	E3376									
K3222	S3223	P3224	R3225	E3226	R3227	L3230	G3231	L3232	P3233	K3234	S3235	V3236	E3237	E3238	M3239	C3240	P3241	D3242	D3247	R3248	A3251	K3252	L3253	L3256	A3257	E3258	S3259	Y3263	T3264	E3265	M3266	F3267	H3268	V3269	I3270	E3271	M3276	P3282	R3283	W3284	W3285	E3286	R3287	G3288	P3289	E3290	A3291	P3292	P3293	A3295	L3296							
G3153	D3154	V3155	I3156	I3157	L3158	D3159	D3160	V3163	S3164	L3169	I3172	Y3173	S3174	T3177	T3178	K3179	N3180	V3183	E3184	K3185	L3186	R3187	P3188	A3189	L3190	G3191	E3192	R3196	L3197	A3198	A3199	P3202	V3203	A3204	F3205	L3206	E3207	P3208	Q3209	L3210	N3211	E3212	Y3213	N3214	A3215	C3216	S3217	Y3218	T3220	T3221								
S3074	L3075	D3076	A3077	R3078	N3081	K3082	S3083	G3084	P3085	E3086	L3087	V3088	L3092	F3095	F3096	E3101	D3102	T3103	E3104	S3105	K3106	V3107	E3108	N3109	L3110	R3111	G3112	G3113	V3115	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	Q3127	N3128	L3129	T3132	A3135	L3136	L3137	P3138	V3139	L3140	L3143	F3144									
H2976	L2977	V2980	V2981	R2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992	F2998	N3007	Q3008	Y3009	F3010	F3017	L3018	S3019	T3020	V3024	L3025	G3026	A3031	K3034	E3035	M3038	L3042	F3043	C3044	A3048	L3049	V3050	R3051	H3052	L3056	F3057	A3061	C3067	L3068	H3069	I3070	L3071	A3072	R3073													
Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	V2935	A2936	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	GLU	L2946	D2947	T2948	S2949	S2950	L2951	E2952	K2953	R2954	F2955	A2956	F2957	L2964	R2965	W2966	Q2971	F2973	A2975			
H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	S2863	K2802	E2803	I2804	S2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	S2813	K2814	A2815	M2816	L2817	A2818	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	Q2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	C2899	G2900	T2901	H2902	P2903	L2904	V2906	P2907
THR	VAL	ASP	ALA	GLY	N2734	F2735	D2736	T2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	I2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	I2755	I2756	K2757	F2758	A2759	E2760	V2761	T2762	K2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	I2771	Q2772	K2773	N2774	W2775	S2776	Y2777	G2778	E2779	W2780	V2781	D2782	E2783	E2784	I2785	K2786	T2787



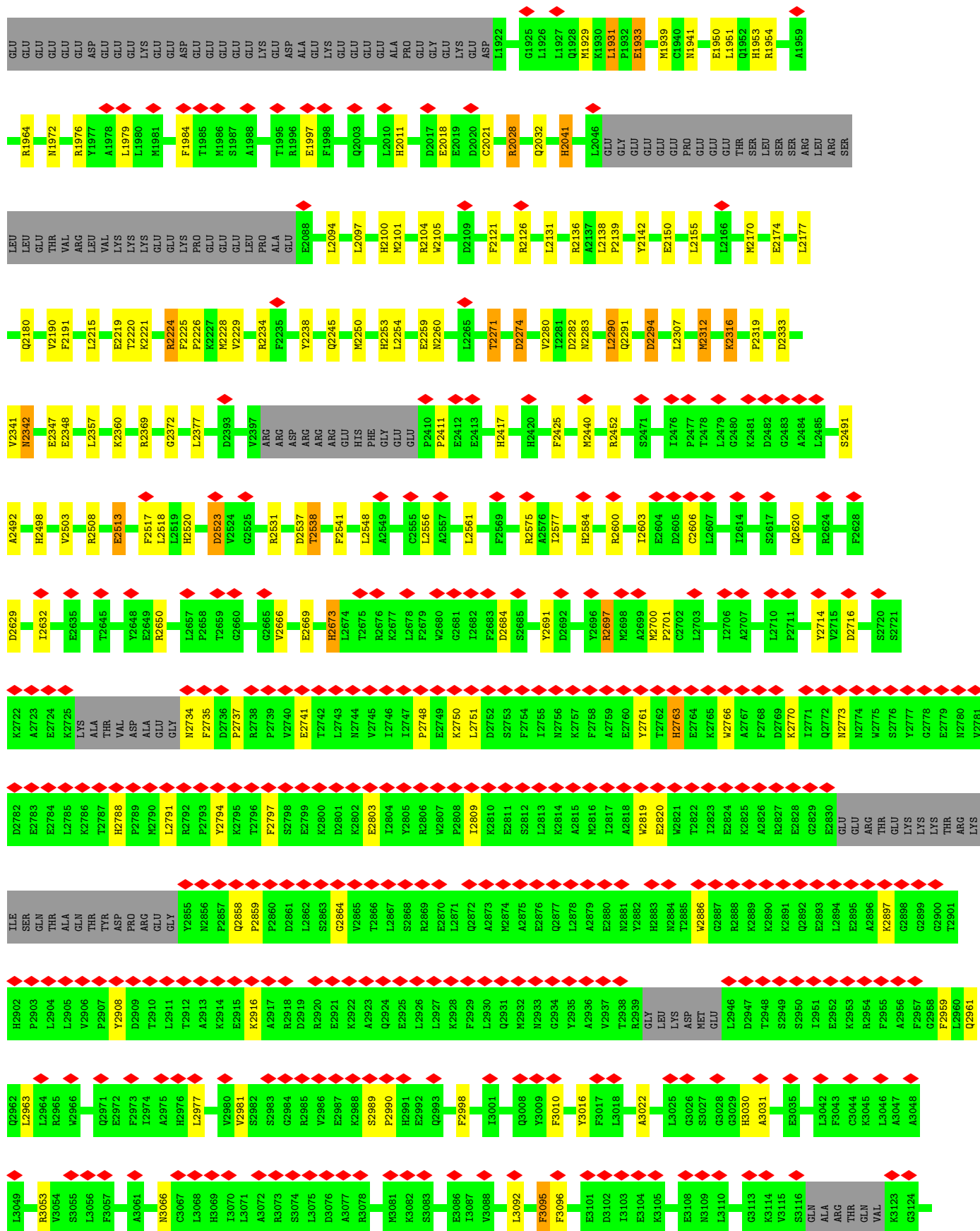




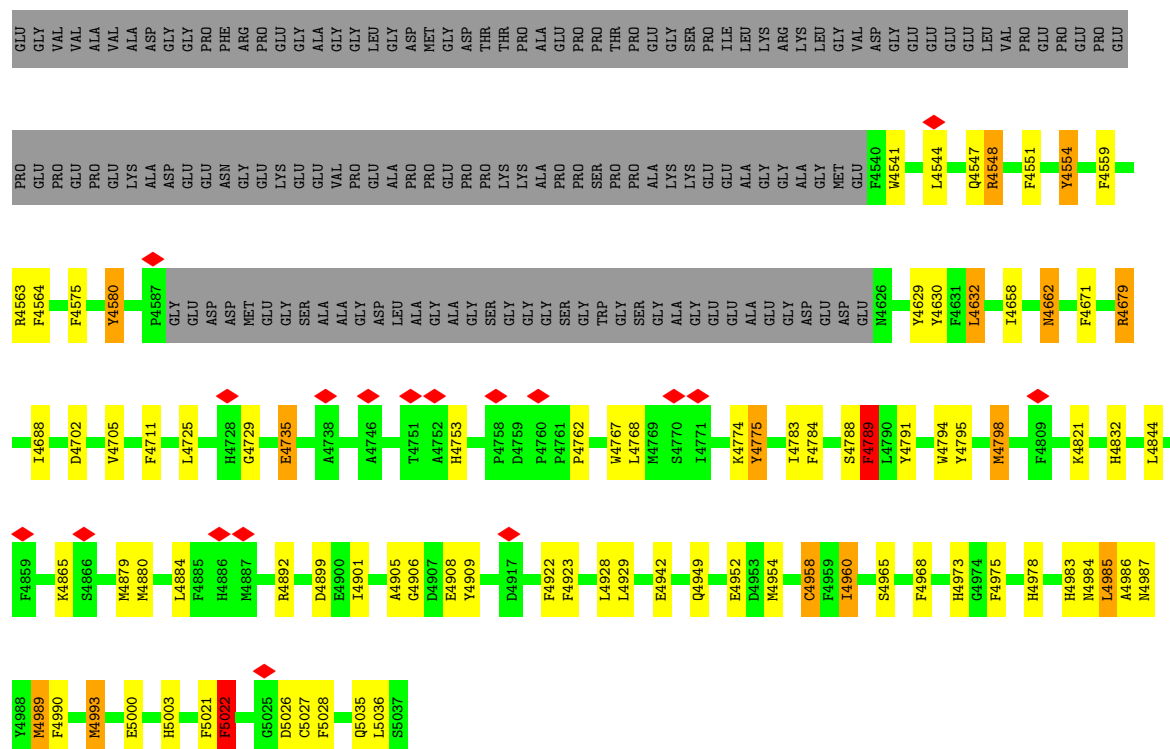
- Molecule 1: Ryanodine receptor 1



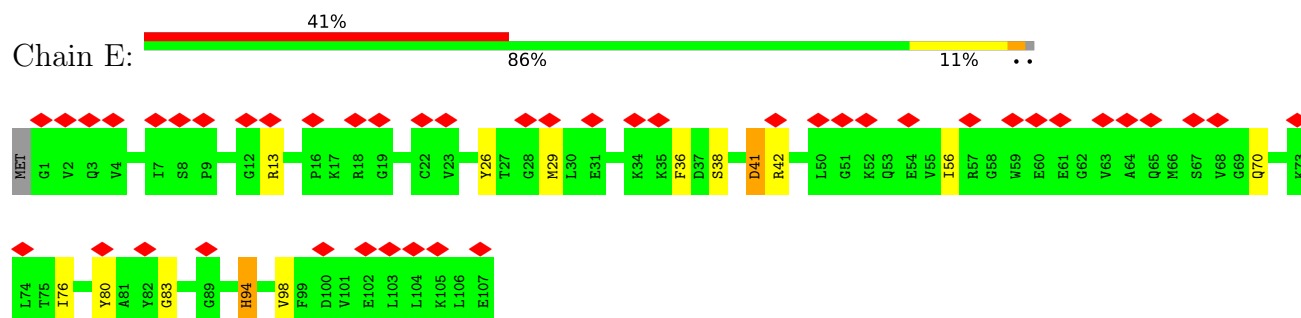




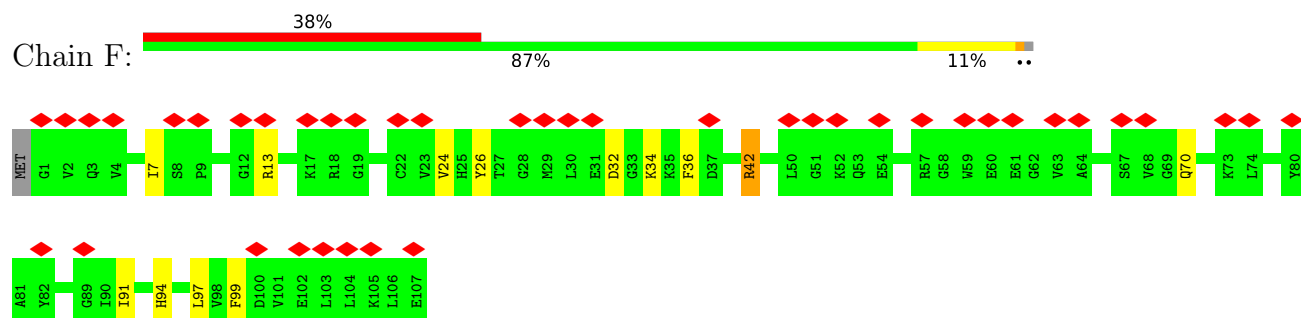




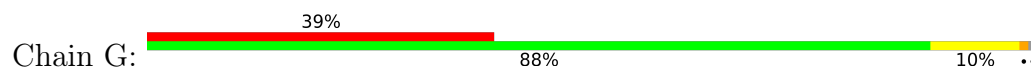
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

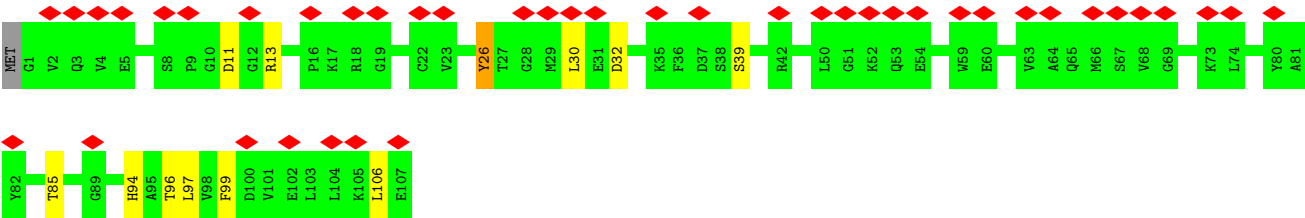


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

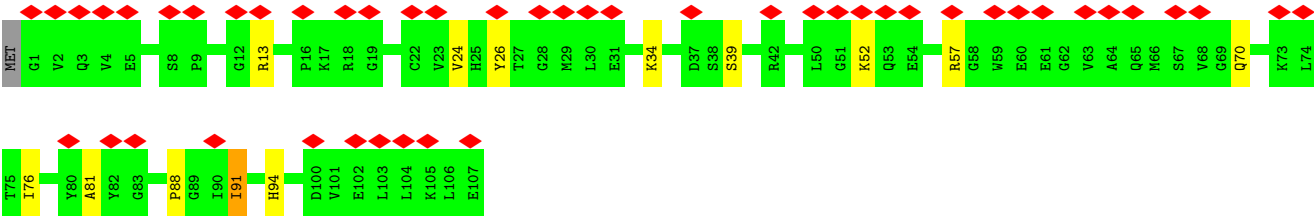
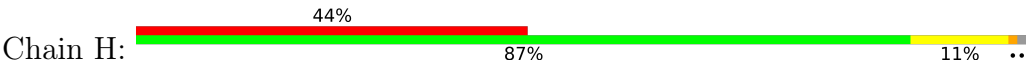


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A





• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of subtomograms used	1088	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	132	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	64000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.706	Depositor
Minimum map value	-0.417	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.105	Depositor
Map size (Å)	496.74, 496.74, 496.74	wwPDB
Map dimensions	170, 170, 170	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.922, 2.922, 2.922	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	0.82	0/35885	1.47	227/48603 (0.5%)
1	B	0.81	0/35885	1.46	228/48603 (0.5%)
1	C	0.82	0/35885	1.47	218/48603 (0.4%)
1	D	0.82	1/35885 (0.0%)	1.47	215/48603 (0.4%)
2	E	0.78	0/851	1.50	4/1146 (0.3%)
2	F	0.77	0/851	1.44	5/1146 (0.4%)
2	G	0.78	0/851	1.44	1/1146 (0.1%)
2	H	0.79	0/851	1.47	5/1146 (0.4%)
All	All	0.82	1/146944 (0.0%)	1.47	903/198996 (0.5%)

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	44
1	B	0	40
1	C	0	45
1	D	0	52
2	E	0	1
2	F	0	1
All	All	0	183

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	2859	PRO	CA-C	5.61	1.54	1.51

All (903) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	41	ASP	CA-CB-CG	12.77	125.37	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4077	PHE	CA-CB-CG	9.76	123.56	113.80
1	C	2794	TYR	N-CA-C	9.14	121.25	111.28
1	C	3293	PRO	N-CA-C	8.84	121.49	110.70
1	B	1539	PHE	CA-CB-CG	8.61	122.41	113.80
1	C	1858	ASP	CA-CB-CG	8.45	121.05	112.60
1	A	3293	PRO	N-CA-C	8.34	120.88	110.70
1	A	3154	ASP	CA-CB-CG	8.17	120.77	112.60
1	A	3527	PRO	N-CA-C	8.15	124.65	113.65
1	A	4065	PHE	CA-CB-CG	8.03	121.83	113.80
1	B	3527	PRO	N-CA-C	7.96	124.39	113.65
1	A	3586	ALA	N-CA-C	7.90	122.49	113.01
1	C	105	HIS	N-CA-C	7.88	122.48	109.95
1	C	4870	ASP	CA-CB-CG	7.84	120.44	112.60
1	B	4077	PHE	CA-CB-CG	7.80	121.60	113.80
1	B	591	ASP	CA-CB-CG	7.76	120.36	112.60
1	A	2869	ARG	N-CA-C	7.70	119.67	111.28
1	A	203	ASN	CB-CA-C	7.69	121.87	109.41
1	B	3951	PHE	CA-CB-CG	-7.69	106.11	113.80
1	C	1158	ASN	CA-CB-CG	7.63	120.23	112.60
1	C	2440	MET	N-CA-C	7.61	119.21	111.07
1	D	386	ASP	CA-CB-CG	7.59	120.19	112.60
1	C	3095	PHE	CA-CB-CG	-7.58	106.22	113.80
1	D	591	ASP	CA-CB-CG	7.58	120.18	112.60
1	B	2283	ASN	CA-CB-CG	-7.56	105.04	112.60
1	B	4719	PHE	CA-CB-CG	7.56	121.36	113.80
1	B	45	ARG	NE-CZ-NH2	7.52	125.97	119.20
1	C	1249	PRO	N-CA-CB	7.48	107.11	103.22
1	A	4922	PHE	CA-CB-CG	-7.47	106.33	113.80
1	C	200	TRP	N-CA-C	7.45	120.39	109.07
1	C	2011	HIS	CA-CB-CG	-7.43	106.37	113.80
1	C	751	SER	CA-C-N	7.42	124.92	120.24
1	C	751	SER	C-N-CA	7.42	124.92	120.24
2	G	32	ASP	CA-CB-CG	7.42	120.03	112.60
1	B	2044	ILE	N-CA-C	7.40	118.13	110.36
1	B	3095	PHE	CA-CB-CG	-7.39	106.41	113.80
1	D	1521	ASP	CA-CB-CG	-7.39	105.21	112.60
1	D	2523	ASP	CA-CB-CG	7.37	119.97	112.60
1	D	3899	PHE	CA-CB-CG	-7.33	106.47	113.80
1	B	1521	ASP	CA-CB-CG	-7.31	105.29	112.60
1	A	386	ASP	CA-CB-CG	7.30	119.90	112.60
1	A	2283	ASN	CA-CB-CG	-7.29	105.31	112.60
1	B	59	PRO	N-CA-CB	7.28	107.00	103.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4092	ASP	CA-CB-CG	7.26	119.86	112.60
1	D	3951	PHE	CA-CB-CG	-7.26	106.54	113.80
1	D	15	ARG	NE-CZ-NH2	7.25	125.73	119.20
1	A	4775	TYR	CA-CB-CG	7.23	126.91	113.90
1	A	3636	PHE	CA-CB-CG	7.23	121.03	113.80
1	A	1101	ARG	NE-CZ-NH2	7.22	125.70	119.20
1	B	3899	PHE	CA-CB-CG	-7.20	106.60	113.80
1	B	289	ARG	NE-CZ-NH2	7.19	125.67	119.20
1	B	2523	ASP	CA-CB-CG	7.17	119.77	112.60
1	A	3095	PHE	CA-CB-CG	-7.14	106.66	113.80
1	D	1189	LEU	N-CA-C	7.14	116.53	108.25
1	C	4225	GLY	CA-C-N	7.12	130.66	121.27
1	C	4225	GLY	C-N-CA	7.12	130.66	121.27
1	C	3987	ASP	CA-CB-CG	7.09	119.69	112.60
1	D	4077	PHE	N-CA-C	7.08	119.08	111.36
1	C	4223	ASN	CA-CB-CG	-7.06	105.54	112.60
1	D	4922	PHE	CA-CB-CG	-7.05	106.75	113.80
1	B	3539	ARG	NE-CZ-NH2	7.03	125.53	119.20
1	D	3095	PHE	CA-CB-CG	-7.01	106.79	113.80
1	D	1055	PRO	N-CA-CB	7.00	106.86	103.22
1	A	296	ASP	CA-CB-CG	7.00	119.60	112.60
1	A	2684	ASP	CA-CB-CG	6.99	119.59	112.60
1	D	3527	PRO	N-CA-C	6.97	123.06	113.65
1	B	386	ASP	CA-CB-CG	6.96	119.56	112.60
1	D	732	SER	N-CA-C	6.95	114.47	108.22
1	D	1136	SER	N-CA-C	6.94	119.99	109.23
1	B	3154	ASP	CA-CB-CG	6.94	119.54	112.60
1	C	2629	ASP	CA-C-N	6.90	124.59	120.24
1	C	2629	ASP	C-N-CA	6.90	124.59	120.24
1	D	289	ARG	NE-CZ-NH2	6.90	125.41	119.20
1	B	4223	ASN	CA-CB-CG	-6.89	105.71	112.60
1	C	4077	PHE	N-CA-C	6.89	118.87	111.36
1	D	203	ASN	CB-CA-C	6.89	120.57	109.41
1	B	296	ASP	CA-CB-CG	6.85	119.45	112.60
1	C	2796	THR	N-CA-C	6.83	123.86	113.61
1	C	4922	PHE	CA-CB-CG	-6.83	106.97	113.80
1	B	4922	PHE	CA-CB-CG	-6.82	106.98	113.80
1	D	3154	ASP	CA-CB-CG	6.81	119.41	112.60
1	D	3144	PHE	CA-CB-CG	-6.80	107.00	113.80
1	C	1055	PRO	N-CA-CB	6.80	106.75	103.22
1	D	2283	ASN	CA-CB-CG	-6.78	105.82	112.60
1	A	3304	CYS	N-CA-C	6.78	119.68	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2215	LEU	CA-C-N	6.76	127.43	120.00
1	D	2215	LEU	C-N-CA	6.76	127.43	120.00
1	C	2584	HIS	CA-CB-CG	6.75	120.55	113.80
1	C	2795	LYS	N-CA-C	6.75	119.47	111.71
1	A	1858	ASP	CA-CB-CG	6.75	119.35	112.60
1	A	200	TRP	N-CA-C	6.75	119.58	108.99
1	C	201	ASN	CA-CB-CG	6.74	119.34	112.60
1	D	1158	ASN	CA-CB-CG	6.74	119.34	112.60
1	D	4223	ASN	CA-CB-CG	-6.73	105.87	112.60
1	D	4168	GLU	CA-C-N	6.71	129.27	120.28
1	D	4168	GLU	C-N-CA	6.71	129.27	120.28
1	B	3829	PHE	CA-CB-CG	-6.71	107.09	113.80
1	D	3896	ASN	CA-CB-CG	-6.70	105.90	112.60
1	A	854	CYS	N-CA-C	6.69	114.25	108.22
1	A	3987	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	2584	HIS	CA-CB-CG	6.67	120.47	113.80
1	D	3868	ARG	NE-CZ-NH2	6.67	125.20	119.20
1	C	2793	PRO	CA-C-N	6.66	129.20	120.28
1	C	2793	PRO	C-N-CA	6.66	129.20	120.28
1	A	2629	ASP	CA-C-N	6.63	124.42	120.24
1	A	2629	ASP	C-N-CA	6.63	124.42	120.24
1	C	389	PHE	CA-CB-CG	6.63	120.43	113.80
1	D	751	SER	CA-C-N	6.62	125.63	120.33
1	D	751	SER	C-N-CA	6.62	125.63	120.33
1	D	2121	PHE	CA-CB-CG	-6.62	107.18	113.80
1	A	4168	GLU	CA-C-N	6.62	129.45	120.38
1	A	4168	GLU	C-N-CA	6.62	129.45	120.38
1	C	218	HIS	CB-CG-CD2	-6.62	122.60	131.20
1	B	200	TRP	N-CA-C	6.62	119.38	108.99
1	D	3987	ASP	CA-CB-CG	6.62	119.22	112.60
1	B	864	PRO	N-CA-CB	6.61	106.89	103.19
1	D	1101	ARG	NE-CZ-NH2	6.60	125.14	119.20
1	D	4662	ASN	CA-CB-CG	6.59	119.19	112.60
1	C	296	ASP	CA-CB-CG	6.58	119.18	112.60
1	A	328	LYS	CA-C-N	6.58	134.11	121.54
1	A	328	LYS	C-N-CA	6.58	134.11	121.54
1	C	4679	ARG	CD-NE-CZ	6.58	133.61	124.40
1	C	2523	ASP	CA-CB-CG	6.57	119.17	112.60
1	D	3432	GLU	CB-CA-C	-6.56	99.90	110.79
1	B	3883	ASP	CA-CB-CG	6.55	119.15	112.60
1	A	3432	GLU	CB-CA-C	-6.55	99.91	110.79
1	C	2714	TYR	N-CA-C	6.55	119.39	110.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2713	ASP	CA-CB-CG	6.54	119.14	112.60
1	A	2523	ASP	CA-CB-CG	6.53	119.13	112.60
2	H	91	ILE	CB-CA-C	6.53	115.72	109.33
1	A	260	TRP	N-CA-C	6.52	119.34	109.23
1	B	3987	ASP	CA-CB-CG	6.52	119.12	112.60
1	D	4702	ASP	CA-CB-CG	6.52	119.12	112.60
1	A	3350	ARG	NE-CZ-NH2	6.51	125.06	119.20
1	D	3586	ALA	N-CA-C	6.51	120.83	113.01
1	B	3523	ASN	CA-CB-CG	6.51	119.11	112.60
1	B	2673	HIS	CB-CG-CD2	-6.51	122.74	131.20
1	C	2121	PHE	CA-CB-CG	-6.50	107.30	113.80
1	C	2684	ASP	CA-CB-CG	6.50	119.10	112.60
1	D	1858	ASP	CA-CB-CG	6.49	119.09	112.60
1	C	3432	GLU	CB-CA-C	-6.49	100.02	110.79
1	C	452	PHE	CA-CB-CG	-6.49	107.31	113.80
1	D	218	HIS	CB-CG-CD2	-6.47	122.79	131.20
1	B	2274	ASP	CA-CB-CG	6.47	119.07	112.60
1	D	296	ASP	CA-CB-CG	6.47	119.07	112.60
1	D	4240	ASP	CA-CB-CG	6.47	119.07	112.60
1	B	1223	PHE	CA-CB-CG	6.46	120.27	113.80
1	A	4223	ASN	CA-CB-CG	-6.46	106.14	112.60
1	B	2121	PHE	CA-CB-CG	-6.46	107.34	113.80
1	C	260	TRP	N-CA-C	6.45	119.22	109.23
1	B	4662	ASN	CA-CB-CG	6.44	119.04	112.60
1	D	2673	HIS	CB-CG-CD2	-6.44	122.82	131.20
1	D	2011	HIS	CA-CB-CG	-6.43	107.37	113.80
1	D	3066	ASN	CA-CB-CG	-6.41	106.19	112.60
1	A	3829	PHE	CA-CB-CG	-6.41	107.39	113.80
1	B	3896	ASN	CA-CB-CG	-6.38	106.22	112.60
1	A	1137	GLU	CA-C-N	6.38	126.29	119.85
1	A	1137	GLU	C-N-CA	6.38	126.29	119.85
1	B	1663	HIS	CA-CB-CG	-6.38	107.42	113.80
1	A	4662	ASN	CA-CB-CG	6.37	118.97	112.60
1	C	540	PHE	CA-CB-CG	-6.36	107.44	113.80
1	D	2271	THR	N-CA-C	6.36	115.63	108.25
1	D	4821	LYS	N-CA-C	6.36	119.02	111.71
1	A	4198	SER	CA-C-N	6.35	129.07	120.38
1	A	4198	SER	C-N-CA	6.35	129.07	120.38
1	C	386	ASP	CA-CB-CG	6.34	118.94	112.60
1	B	1858	ASP	CA-CB-CG	6.34	118.94	112.60
1	D	2797	PHE	CA-CB-CG	6.33	120.13	113.80
1	A	1671	ARG	NE-CZ-NH2	6.32	124.89	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2121	PHE	CA-CB-CG	-6.32	107.48	113.80
1	A	4638	TYR	CA-C-N	6.31	129.91	120.31
1	A	4638	TYR	C-N-CA	6.31	129.91	120.31
1	B	2011	HIS	CA-CB-CG	-6.31	107.49	113.80
1	A	289	ARG	NE-CZ-NH2	6.31	124.88	119.20
1	D	389	PHE	CA-CB-CG	6.31	120.11	113.80
1	C	2274	ASP	CA-CB-CG	6.30	118.91	112.60
1	D	2260	ASN	CA-CB-CG	-6.30	106.30	112.60
1	B	4832	HIS	CA-CB-CG	-6.30	107.50	113.80
1	D	2274	ASP	CA-CB-CG	6.30	118.90	112.60
1	A	3051	ARG	NE-CZ-NH2	6.29	124.87	119.20
1	B	1189	LEU	N-CA-C	6.29	115.55	108.25
1	D	2714	TYR	N-CA-C	6.29	118.84	110.53
1	A	3066	ASN	CA-CB-CG	-6.29	106.31	112.60
1	A	3984	ARG	NE-CZ-NH2	6.29	124.86	119.20
1	D	243	ARG	NE-CZ-NH2	6.29	124.86	119.20
1	A	1036	ARG	NE-CZ-NH2	6.29	124.86	119.20
1	D	2221	LYS	CA-C-N	6.27	130.04	120.82
1	D	2221	LYS	C-N-CA	6.27	130.04	120.82
1	A	2736	ASP	CA-CB-CG	6.27	118.87	112.60
1	C	203	ASN	CB-CA-C	6.25	119.53	109.41
1	C	4240	ASP	CA-CB-CG	6.24	118.84	112.60
1	B	3051	ARG	NE-CZ-NH2	6.24	124.82	119.20
1	B	260	TRP	N-CA-C	6.24	118.90	109.23
1	C	392	ARG	NE-CZ-NH2	6.24	124.81	119.20
1	C	3527	PRO	N-CA-C	6.24	122.07	113.65
1	B	2714	TYR	N-CA-C	6.21	118.94	110.55
1	D	4541	TRP	N-CA-C	6.21	117.72	111.07
1	D	3010	PHE	CA-CB-CG	-6.20	107.60	113.80
1	B	452	PHE	CA-CB-CG	-6.20	107.60	113.80
1	B	778	PHE	CA-CB-CG	6.20	120.00	113.80
1	A	2011	HIS	CA-CB-CG	-6.19	107.61	113.80
1	C	1736	VAL	N-CA-C	6.18	114.97	107.61
1	C	4662	ASN	CA-CB-CG	6.18	118.78	112.60
1	D	201	ASN	CA-CB-CG	6.17	118.77	112.60
1	B	2126	ARG	NE-CZ-NH2	6.17	124.75	119.20
1	D	838	HIS	CB-CG-CD2	-6.17	123.19	131.20
1	C	3883	ASP	CA-CB-CG	6.16	118.76	112.60
2	H	24	VAL	N-CA-C	6.16	117.23	108.42
1	D	3914	ASN	CA-CB-CG	-6.15	106.45	112.60
1	B	4702	ASP	CA-CB-CG	6.15	118.75	112.60
1	C	4923	PHE	CA-CB-CG	-6.15	107.65	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3636	PHE	CA-CB-CG	6.15	119.95	113.80
1	D	639	ASN	CA-CB-CG	6.14	118.74	112.60
1	D	218	HIS	CA-CB-CG	-6.14	107.66	113.80
1	C	284	HIS	CB-CG-CD2	-6.13	123.23	131.20
1	A	4709	PRO	CA-C-N	6.12	133.24	121.54
1	A	4709	PRO	C-N-CA	6.12	133.24	121.54
1	C	3717	ASP	CA-CB-CG	6.12	118.72	112.60
1	D	3883	ASP	CA-CB-CG	6.12	118.72	112.60
2	F	32	ASP	CA-CB-CG	6.12	118.72	112.60
1	C	2673	HIS	CB-CG-CD2	-6.12	123.24	131.20
1	D	4923	PHE	CA-CB-CG	-6.12	107.68	113.80
1	A	3180	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	C	316	PHE	CA-CB-CG	6.11	119.91	113.80
1	D	4832	HIS	CA-CB-CG	-6.11	107.69	113.80
1	C	3892	CYS	N-CA-CB	-6.10	101.47	110.49
1	D	3829	PHE	CA-CB-CG	-6.08	107.72	113.80
1	B	2260	ASN	CA-CB-CG	-6.08	106.52	112.60
1	C	1461	ASP	CA-CB-CG	6.08	118.68	112.60
1	D	1663	HIS	CA-CB-CG	-6.08	107.72	113.80
1	B	218	HIS	CB-CG-CD2	-6.07	123.30	131.20
1	B	2271	THR	N-CA-C	6.07	115.29	108.25
1	B	4240	ASP	CA-CB-CG	6.07	118.67	112.60
1	D	4061	PHE	CA-CB-CG	6.07	119.87	113.80
1	A	2673	HIS	CB-CG-CD2	-6.06	123.32	131.20
1	C	1478	ASP	CA-CB-CG	6.06	118.66	112.60
1	C	4061	PHE	CA-CB-CG	6.06	119.86	113.80
1	B	3934	TYR	N-CA-C	6.05	117.54	111.07
1	D	3066	ASN	CB-CA-C	6.04	120.81	110.79
1	A	2683	PHE	CA-CB-CG	6.03	119.83	113.80
1	C	2498	HIS	CB-CG-CD2	-6.03	123.36	131.20
1	C	1136	SER	N-CA-C	6.03	118.58	109.23
1	D	2684	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	3218	VAL	N-CA-C	6.03	116.77	110.62
1	B	2684	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	4993	MET	CB-CA-C	-6.03	100.79	110.79
1	A	1136	SER	N-CA-C	6.02	118.57	109.23
1	C	3436	ARG	NE-CZ-NH2	6.02	124.62	119.20
1	A	3010	PHE	CA-CB-CG	-6.02	107.78	113.80
1	A	5019	TRP	CA-C-N	6.02	130.32	120.63
1	A	5019	TRP	C-N-CA	6.02	130.32	120.63
1	D	2221	LYS	N-CA-C	6.02	118.09	110.33
1	C	533	ASN	CA-C-N	6.02	128.62	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	533	ASN	C-N-CA	6.02	128.62	120.38
1	C	1663	HIS	CA-CB-CG	-6.01	107.78	113.80
1	A	3969	ILE	N-CA-C	6.00	119.98	113.43
1	C	1189	LEU	N-CA-C	6.00	115.21	108.25
1	C	303	ASP	CA-CB-CG	5.99	118.59	112.60
1	C	3066	ASN	CA-CB-CG	-5.99	106.61	112.60
1	C	3218	VAL	N-CA-C	5.99	116.77	110.72
1	D	2440	MET	N-CA-C	5.99	117.81	111.28
1	D	1558	HIS	CB-CG-CD2	-5.99	123.42	131.20
1	A	4240	ASP	CA-CB-CG	5.99	118.58	112.60
1	C	4832	HIS	CA-CB-CG	-5.99	107.81	113.80
1	C	999	ASP	CA-CB-CG	5.97	118.57	112.60
1	A	328	LYS	N-CA-C	5.97	118.49	109.23
1	B	3207	GLU	CA-C-N	5.97	125.67	119.82
1	B	3207	GLU	C-N-CA	5.97	125.67	119.82
1	B	3717	ASP	CA-CB-CG	5.97	118.57	112.60
1	D	2584	HIS	CA-CB-CG	5.97	119.77	113.80
1	A	2136	ARG	NE-CZ-NH2	5.96	124.57	119.20
1	A	203	ASN	CA-CB-CG	-5.96	106.64	112.60
1	D	260	TRP	N-CA-C	5.96	118.24	109.24
1	C	4563	ARG	NE-CZ-NH2	5.96	124.56	119.20
1	C	5018	CYS	N-CA-CB	-5.96	101.73	110.49
1	A	4821	LYS	N-CA-C	5.96	118.56	111.71
1	C	3051	ARG	NE-CZ-NH2	5.96	124.56	119.20
1	A	2274	ASP	CA-CB-CG	5.94	118.54	112.60
1	B	3321	ARG	NE-CZ-NH2	5.94	124.55	119.20
1	B	454	PRO	N-CA-CB	5.94	106.31	103.22
1	B	4784	PHE	CA-CB-CG	5.94	119.74	113.80
1	D	4767	TRP	CB-CA-C	5.94	122.28	110.17
1	D	4784	PHE	CA-CB-CG	5.93	119.73	113.80
1	C	1575	LEU	N-CA-C	5.93	117.82	111.36
1	C	1671	ARG	NE-CZ-NH2	5.93	124.53	119.20
1	C	2747	ILE	N-CA-CB	-5.92	107.74	111.83
1	D	4702	ASP	CB-CA-C	-5.92	99.30	110.67
1	A	2498	HIS	CB-CG-CD2	-5.92	123.51	131.20
1	B	4993	MET	CB-CA-C	-5.91	100.98	110.79
1	C	2556	LEU	N-CA-CB	-5.91	102.73	110.59
1	C	4072	VAL	N-CA-C	5.91	121.62	109.34
1	C	3896	ASN	CA-CB-CG	-5.90	106.70	112.60
1	D	3705	PHE	CA-CB-CG	5.89	119.69	113.80
1	A	1223	PHE	CA-CB-CG	5.89	119.69	113.80
1	B	203	ASN	CA-C-N	5.89	125.86	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	ASN	C-N-CA	5.89	125.86	120.03
1	C	4679	ARG	NE-CZ-NH2	5.89	124.50	119.20
1	A	284	HIS	CB-CG-CD2	-5.88	123.55	131.20
1	A	5018	CYS	N-CA-CB	-5.88	101.79	110.49
1	B	1808	ARG	NE-CZ-NH2	5.88	124.49	119.20
1	D	1671	ARG	NE-CZ-NH2	5.87	124.48	119.20
1	B	1461	ASP	CA-CB-CG	5.86	118.46	112.60
1	B	3526	ALA	CA-C-N	5.86	125.72	119.28
1	B	3526	ALA	C-N-CA	5.86	125.72	119.28
2	F	70	GLN	OE1-CD-NE2	-5.86	116.74	122.60
1	D	1478	ASP	CA-CB-CG	5.85	118.45	112.60
1	D	1984	PHE	CA-CB-CG	5.85	119.65	113.80
1	A	3867	ASN	CA-C-N	5.84	130.70	122.46
1	A	3867	ASN	C-N-CA	5.84	130.70	122.46
1	A	3587	ASP	N-CA-C	5.84	117.72	108.79
1	A	4784	PHE	CA-CB-CG	5.84	119.64	113.80
1	A	218	HIS	CB-CG-CD2	-5.84	123.61	131.20
1	A	1808	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	B	3292	PRO	N-CA-C	5.83	117.82	110.70
1	A	1663	HIS	CA-CB-CG	-5.83	107.97	113.80
1	D	1594	ARG	NE-CZ-NH2	5.82	124.44	119.20
1	B	284	HIS	CB-CG-CD2	-5.82	123.64	131.20
1	C	3010	PHE	CA-CB-CG	-5.81	107.99	113.80
1	C	1101	ARG	NE-CZ-NH2	5.81	124.43	119.20
1	C	181	HIS	N-CA-C	5.81	119.02	109.72
1	C	2248	ARG	NE-CZ-NH2	5.81	124.43	119.20
1	D	2191	PHE	CA-CB-CG	-5.81	107.99	113.80
1	D	4070	ASP	CA-CB-CG	5.81	118.41	112.60
1	B	1503	PRO	CA-C-N	5.81	125.62	120.10
1	B	1503	PRO	C-N-CA	5.81	125.62	120.10
2	F	24	VAL	N-CA-C	5.81	116.72	108.42
1	D	4198	SER	CA-C-N	5.81	128.33	120.38
1	D	4198	SER	C-N-CA	5.81	128.33	120.38
1	B	2253	HIS	CA-CB-CG	-5.80	108.00	113.80
1	A	2794	TYR	N-CA-C	5.79	118.37	111.71
1	B	4225	GLY	N-CA-C	5.79	118.59	111.93
1	C	243	ARG	NE-CZ-NH2	5.79	124.41	119.20
1	C	4821	LYS	N-CA-C	5.78	118.36	111.71
1	C	302	VAL	N-CA-C	5.78	118.00	108.99
1	A	3883	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	4679	ARG	CD-NE-CZ	5.78	132.49	124.40
1	C	1521	ASP	CA-CB-CG	-5.78	106.82	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1671	ARG	NE-CZ-NH2	5.77	124.40	119.20
1	B	4061	PHE	CA-CB-CG	5.77	119.57	113.80
1	B	1984	PHE	CA-CB-CG	5.77	119.57	113.80
1	C	328	LYS	CA-C-N	5.77	129.46	120.75
1	C	328	LYS	C-N-CA	5.77	129.46	120.75
1	A	357	LEU	N-CA-CB	-5.77	100.48	110.17
1	B	4821	LYS	N-CA-C	5.77	118.34	111.71
1	C	4993	MET	CB-CA-C	-5.77	101.22	110.79
1	C	4142	ASN	CA-CB-CG	-5.76	106.84	112.60
1	A	2271	THR	N-CA-C	5.75	114.92	108.25
1	D	2629	ASP	CA-C-N	5.75	123.86	120.24
1	D	2629	ASP	C-N-CA	5.75	123.86	120.24
1	D	2136	ARG	NE-CZ-NH2	5.75	124.37	119.20
1	D	1036	ARG	NE-CZ-NH2	5.75	124.37	119.20
1	D	1808	ARG	NE-CZ-NH2	5.75	124.37	119.20
1	A	243	ARG	NE-CZ-NH2	5.74	124.37	119.20
1	A	1775	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	B	3506	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	C	3992	PHE	CA-CB-CG	5.74	119.54	113.80
1	A	2090	LYS	CA-C-N	5.73	125.20	119.24
1	A	2090	LYS	C-N-CA	5.73	125.20	119.24
1	D	1736	VAL	N-CA-C	5.73	114.43	107.61
1	D	2556	LEU	N-CA-CB	-5.73	102.97	110.59
1	D	4077	PHE	CA-CB-CG	5.73	119.53	113.80
1	A	1989	ALA	N-CA-C	5.73	118.47	111.82
1	C	1144	GLN	OE1-CD-NE2	-5.73	116.87	122.60
1	B	3348	ARG	NE-CZ-NH2	5.73	124.36	119.20
1	B	1136	SER	N-CA-C	5.72	118.10	109.23
1	B	2652	TRP	N-CA-C	5.72	118.26	111.33
1	A	2714	TYR	N-CA-C	5.72	118.57	110.50
1	A	2345	SER	N-CA-C	5.72	118.36	110.35
1	A	220	LEU	N-CA-C	5.72	116.95	108.60
1	C	1503	PRO	CA-C-N	5.71	125.77	120.34
1	C	1503	PRO	C-N-CA	5.71	125.77	120.34
1	D	3387	ALA	N-CA-C	5.71	118.24	111.33
1	B	4923	PHE	CA-CB-CG	-5.71	108.09	113.80
1	D	226	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	C	203	ASN	CA-C-N	5.71	125.68	120.03
1	C	203	ASN	C-N-CA	5.71	125.68	120.03
1	A	169	LEU	N-CA-C	5.71	118.54	109.81
1	B	1856	ASP	CA-CB-CG	5.70	118.30	112.60
1	B	181	HIS	N-CA-C	5.70	119.01	109.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	284	HIS	CB-CG-CD2	-5.70	123.79	131.20
1	A	203	ASN	CA-C-N	5.70	125.67	120.03
1	A	203	ASN	C-N-CA	5.70	125.67	120.03
1	B	2191	PHE	CA-CB-CG	-5.70	108.11	113.80
1	C	328	LYS	N-CA-C	5.70	117.42	110.41
1	A	1856	ASP	CA-CB-CG	5.69	118.29	112.60
1	D	838	HIS	CA-CB-CG	5.69	119.49	113.80
1	B	2673	HIS	CA-CB-CG	5.68	119.48	113.80
1	D	4679	ARG	CD-NE-CZ	5.67	132.34	124.40
1	D	1772	ARG	NE-CZ-NH2	5.67	124.31	119.20
1	A	803	LEU	CA-C-N	5.67	126.22	120.38
1	A	803	LEU	C-N-CA	5.67	126.22	120.38
1	D	4775	TYR	CA-CB-CG	5.67	124.11	113.90
1	C	1808	ARG	NE-CZ-NH2	5.67	124.30	119.20
1	D	2600	ARG	NE-CZ-NH2	5.67	124.30	119.20
1	A	3717	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	4563	ARG	NE-CZ-NH2	5.67	124.30	119.20
1	B	5018	CYS	N-CA-CB	-5.66	102.42	110.58
1	A	4923	PHE	CA-CB-CG	-5.66	108.14	113.80
1	C	1208	VAL	N-CA-C	5.65	116.38	110.62
1	C	3167	ARG	NE-CZ-NH2	5.64	124.28	119.20
1	A	2294	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	4958	CYS	CA-CB-SG	-5.63	101.44	114.40
1	D	4942	GLU	N-CA-CB	-5.63	101.85	110.01
1	B	5019	TRP	CA-C-N	5.63	132.29	121.54
1	B	5019	TRP	C-N-CA	5.63	132.29	121.54
1	C	2294	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	2821	TRP	CA-CB-CG	5.63	124.29	113.60
1	B	1702	HIS	CB-CG-CD2	-5.62	123.89	131.20
1	B	4198	SER	CA-C-N	5.62	128.08	120.38
1	B	4198	SER	C-N-CA	5.62	128.08	120.38
1	D	4679	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	B	3180	ASN	CA-CB-CG	5.62	118.22	112.60
1	C	2191	PHE	CA-CB-CG	-5.62	108.18	113.80
1	B	4559	PHE	N-CA-C	5.61	117.08	111.07
1	C	289	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	D	629	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	A	4832	HIS	CA-CB-CG	-5.61	108.19	113.80
1	A	151	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	C	2697	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	D	2763	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	D	200	TRP	N-CA-C	5.60	117.78	108.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3350	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	C	1777	PHE	CA-CB-CG	5.60	119.40	113.80
1	A	3052	HIS	CA-C-N	5.59	129.63	120.63
1	A	3052	HIS	C-N-CA	5.59	129.63	120.63
1	B	3227	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	A	2215	LEU	CA-C-N	5.59	126.15	120.00
1	A	2215	LEU	C-N-CA	5.59	126.15	120.00
1	B	4065	PHE	CA-CB-CG	5.59	119.39	113.80
1	C	4043	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	A	201	ASN	CA-CB-CG	5.59	118.19	112.60
1	C	3114	LYS	N-CA-C	5.58	118.09	111.33
1	A	316	PHE	CA-CB-CG	5.58	119.38	113.80
1	D	2100	HIS	CA-CB-CG	5.58	119.38	113.80
1	D	2716	ASP	N-CA-C	5.57	117.44	109.14
1	A	533	ASN	CA-C-N	5.57	128.01	120.38
1	A	533	ASN	C-N-CA	5.57	128.01	120.38
1	A	831	ARG	NE-CZ-NH2	5.56	124.21	119.20
1	A	226	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	B	2798	SER	N-CA-C	5.56	115.36	108.19
1	C	3829	PHE	CA-CB-CG	-5.56	108.24	113.80
1	C	5019	TRP	CA-C-N	5.56	132.16	121.54
1	C	5019	TRP	C-N-CA	5.56	132.16	121.54
1	A	3387	ALA	N-CA-C	5.56	118.05	111.33
1	B	533	ASN	CA-C-N	5.55	127.99	120.38
1	B	533	ASN	C-N-CA	5.55	127.99	120.38
1	D	647	ASN	CA-CB-CG	5.55	118.15	112.60
1	D	1688	HIS	CB-CG-CD2	-5.55	123.98	131.20
1	C	3771	HIS	CB-CG-CD2	-5.55	123.98	131.20
1	C	3867	ASN	CA-C-N	5.55	130.71	122.82
1	C	3867	ASN	C-N-CA	5.55	130.71	122.82
1	A	2673	HIS	CA-CB-CG	5.55	119.35	113.80
1	A	98	HIS	CB-CG-CD2	-5.54	123.99	131.20
1	B	49	LEU	N-CA-C	5.54	118.59	109.72
1	C	1984	PHE	CA-CB-CG	5.54	119.34	113.80
1	D	949	ASN	CA-CB-CG	5.54	118.14	112.60
1	B	3292	PRO	CA-C-N	5.54	126.08	120.38
1	B	3292	PRO	C-N-CA	5.54	126.08	120.38
1	B	389	PHE	CA-CB-CG	5.54	119.34	113.80
1	B	2493	SER	N-CA-C	5.53	115.85	108.38
1	B	4224	GLU	CA-C-N	5.53	125.36	120.10
1	B	4224	GLU	C-N-CA	5.53	125.36	120.10
1	C	3154	ASP	CA-CB-CG	5.53	118.13	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3771	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	B	1736	VAL	N-CA-C	5.53	114.19	107.61
1	A	1772	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	B	1775	HIS	CB-CG-CD2	-5.53	124.02	131.20
1	B	3595	ARG	NE-CZ-NH2	5.53	124.17	119.20
1	B	2215	LEU	CA-C-N	5.52	126.11	119.98
1	B	2215	LEU	C-N-CA	5.52	126.11	119.98
1	A	943	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	2041	HIS	CB-CG-CD2	-5.52	124.03	131.20
1	A	2463	LEU	CA-C-N	5.51	127.67	120.28
1	A	2463	LEU	C-N-CA	5.51	127.67	120.28
1	D	2253	HIS	CA-CB-CG	-5.51	108.28	113.80
1	C	2630	VAL	CB-CA-C	-5.51	108.51	114.35
1	D	2319	PRO	CA-C-N	5.51	128.69	120.87
1	D	2319	PRO	C-N-CA	5.51	128.69	120.87
1	A	3876	ALA	CA-C-N	5.51	130.20	121.44
1	A	3876	ALA	C-N-CA	5.51	130.20	121.44
1	B	133	PHE	CA-CB-CG	5.50	119.31	113.80
1	C	49	LEU	N-CA-C	5.50	118.53	109.72
1	D	1444	GLU	CA-C-N	5.50	125.33	119.28
1	D	1444	GLU	C-N-CA	5.50	125.33	119.28
1	C	1444	GLU	CA-C-N	5.50	125.33	119.28
1	C	1444	GLU	C-N-CA	5.50	125.33	119.28
1	C	4775	TYR	CA-CB-CG	5.49	123.79	113.90
1	B	1772	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	B	1144	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	D	257	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	D	2575	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	D	2632	ILE	N-CA-C	5.49	116.26	110.72
1	B	4043	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	C	2799	GLU	N-CA-C	5.48	119.06	112.38
1	D	3160	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	3813	GLN	OE1-CD-NE2	-5.47	117.12	122.60
1	A	3901	ASN	N-CA-CB	-5.47	102.08	110.12
1	C	824	GLU	CA-C-N	5.47	125.47	119.89
1	C	824	GLU	C-N-CA	5.47	125.47	119.89
1	B	1218	GLY	CA-C-N	5.47	131.99	121.54
1	B	1218	GLY	C-N-CA	5.47	131.99	121.54
1	B	4563	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	D	3506	GLN	OE1-CD-NE2	-5.47	117.13	122.60
1	B	151	HIS	CB-CG-CD2	-5.46	124.10	131.20
1	B	4142	ASN	CA-CB-CG	-5.46	107.14	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2271	THR	N-CA-C	5.46	114.58	108.25
1	B	824	GLU	N-CA-CB	-5.46	105.37	111.10
1	D	48	PHE	N-CA-C	5.46	115.49	108.34
1	B	4958	CYS	CA-CB-SG	-5.46	101.85	114.40
1	A	4110	PHE	CA-CB-CG	5.45	119.25	113.80
1	A	4579	PHE	CA-CB-CG	-5.45	108.35	113.80
1	C	857	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	1769	THR	CA-CB-CG2	5.45	119.76	110.50
1	C	4125	PHE	N-CA-C	5.45	117.97	111.71
1	B	639	ASN	CA-CB-CG	5.44	118.04	112.60
1	B	270	SER	N-CA-C	5.44	122.39	110.80
1	B	3628	ARG	CA-C-N	5.44	127.57	120.28
1	B	3628	ARG	C-N-CA	5.44	127.57	120.28
1	C	1989	ALA	N-CA-C	5.44	117.96	111.71
1	B	3432	GLU	CB-CA-C	-5.44	101.77	110.79
1	C	3984	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	D	1976	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	C	4775	TYR	N-CA-CB	-5.43	102.14	110.12
1	C	3506	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	B	1036	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	B	3984	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	A	2292	GLU	N-CA-C	5.42	116.87	111.07
1	B	3350	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	D	1972	ASN	CA-CB-CG	-5.42	107.18	112.60
1	D	2498	HIS	CB-CG-CD2	-5.42	124.16	131.20
1	D	3436	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	C	579	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	A	2493	SER	N-CA-C	5.41	115.69	108.38
1	C	3348	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	B	243	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	B	4953	ASP	CA-CB-CG	-5.41	107.19	112.60
1	D	5022	PHE	CA-CB-CG	5.41	119.21	113.80
1	C	2215	LEU	CA-C-N	5.41	125.95	120.00
1	C	2215	LEU	C-N-CA	5.41	125.95	120.00
1	A	4679	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	C	681	HIS	CB-CG-CD2	-5.40	124.17	131.20
1	B	474	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	C	3728	ILE	N-CA-CB	-5.40	103.19	110.54
1	B	2498	HIS	CB-CG-CD2	-5.39	124.19	131.20
1	D	4993	MET	CB-CA-C	-5.39	101.84	110.79
1	A	392	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	D	172	VAL	N-CA-CB	-5.39	103.97	111.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2253	HIS	CA-CB-CG	-5.39	108.41	113.80
1	A	2191	PHE	CA-CB-CG	-5.39	108.41	113.80
1	B	3771	HIS	CB-CG-CD2	-5.39	124.20	131.20
1	A	3868	ARG	NE-CZ-NH2	5.38	124.05	119.20
1	C	3876	ALA	CA-C-N	5.38	130.01	121.18
1	C	3876	ALA	C-N-CA	5.38	130.01	121.18
1	C	728	ARG	CA-C-N	5.38	125.32	119.78
1	C	728	ARG	C-N-CA	5.38	125.32	119.78
1	B	17	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	1458	HIS	CB-CG-CD2	-5.38	124.21	131.20
1	C	2821	TRP	CA-CB-CG	5.38	123.81	113.60
1	A	2600	ARG	NE-CZ-NH2	5.37	124.04	119.20
1	A	4832	HIS	N-CA-C	5.37	119.70	113.20
1	C	2136	ARG	NE-CZ-NH2	5.37	124.04	119.20
1	B	2221	LYS	N-CA-C	5.37	117.46	110.43
1	A	1594	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	A	4775	TYR	CB-CA-C	5.37	120.98	110.67
1	C	3031	ALA	N-CA-C	5.37	117.46	110.43
1	B	2333	ASP	CA-CB-CG	5.37	117.97	112.60
1	C	164	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	A	2340	PHE	CA-CB-CG	5.36	119.16	113.80
1	C	3895	HIS	CB-CG-CD2	-5.36	124.23	131.20
1	C	266	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	B	2739	PRO	CA-C-N	5.36	127.80	120.35
1	B	2739	PRO	C-N-CA	5.36	127.80	120.35
1	A	818	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	B	48	PHE	N-CA-C	5.36	115.36	108.34
1	C	1594	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	A	2100	HIS	CA-CB-CG	5.35	119.15	113.80
1	C	1688	HIS	CB-CG-CD2	-5.35	124.24	131.20
2	H	70	GLN	OE1-CD-NE2	-5.35	117.25	122.60
1	A	3301	PRO	N-CA-CB	5.35	106.19	103.19
1	D	4142	ASN	CA-CB-CG	-5.35	107.25	112.60
1	D	4729	GLY	CA-C-N	5.35	128.44	120.31
1	D	4729	GLY	C-N-CA	5.35	128.44	120.31
2	E	76	ILE	N-CA-C	5.35	115.82	108.12
1	B	2294	ASP	CA-CB-CG	5.34	117.94	112.60
1	B	4658	ILE	CB-CA-C	-5.34	105.13	111.97
1	C	2100	HIS	CB-CG-CD2	-5.34	124.26	131.20
1	C	2600	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	D	1288	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	1422	ASP	CA-CB-CG	5.34	117.94	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4043	GLN	OE1-CD-NE2	-5.34	117.26	122.60
1	D	3934	TYR	N-CA-C	5.34	117.52	111.11
1	C	4192	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	D	3876	ALA	CA-C-N	5.34	129.93	121.44
1	D	3876	ALA	C-N-CA	5.34	129.93	121.44
1	D	2294	ASP	CA-CB-CG	5.33	117.94	112.60
1	B	3914	ASN	CA-CB-CG	-5.33	107.27	112.60
1	B	2136	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	A	426	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	D	4563	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	C	1558	HIS	CB-CG-CD2	-5.33	124.28	131.20
1	D	3868	ARG	CD-NE-CZ	5.33	131.86	124.40
1	A	2556	LEU	N-CA-CB	-5.32	103.51	110.59
1	D	49	LEU	N-CA-C	5.32	118.41	109.95
1	A	452	PHE	CA-CB-CG	-5.32	108.48	113.80
1	A	3436	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	C	113	HIS	CB-CG-CD2	-5.32	124.29	131.20
1	D	4958	CYS	CA-CB-SG	-5.32	102.17	114.40
1	A	1984	PHE	CA-CB-CG	5.31	119.11	113.80
1	D	203	ASN	CA-C-N	5.31	125.22	119.85
1	D	203	ASN	C-N-CA	5.31	125.22	119.85
1	B	2803	GLU	N-CA-C	5.31	117.48	111.11
1	C	3899	PHE	CA-CB-CG	-5.31	108.49	113.80
1	D	2788	HIS	CB-CG-CD2	-5.31	124.30	131.20
1	A	4163	PHE	CA-CB-CG	5.30	119.11	113.80
1	A	530	ILE	N-CA-CB	-5.30	106.02	112.33
1	A	1189	LEU	N-CA-C	5.30	114.39	108.25
1	B	5034	ASP	CA-CB-CG	5.30	117.90	112.60
1	D	4163	PHE	CA-CB-CG	5.29	119.09	113.80
1	B	98	HIS	CB-CG-CD2	-5.29	124.32	131.20
1	B	3877	ASP	CA-C-N	5.29	127.32	120.44
1	B	3877	ASP	C-N-CA	5.29	127.32	120.44
1	B	257	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	B	838	HIS	CB-CG-CD2	-5.29	124.32	131.20
1	C	4776	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	D	4065	PHE	CA-CB-CG	5.29	119.09	113.80
1	A	3728	ILE	N-CA-CB	-5.29	103.35	110.54
1	C	2716	ASP	N-CA-C	5.28	117.01	109.14
1	D	2126	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	C	3054	VAL	N-CA-C	5.28	118.46	111.17
1	A	4192	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	C	3927	GLN	OE1-CD-NE2	-5.28	117.32	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	579	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	A	1773	PRO	CA-C-N	5.27	125.27	119.89
1	A	1773	PRO	C-N-CA	5.27	125.27	119.89
1	A	3901	ASN	CA-CB-CG	5.27	117.87	112.60
1	C	4658	ILE	CB-CA-C	-5.27	105.22	111.97
1	A	1012	ASP	CA-CB-CG	5.27	117.87	112.60
1	B	1620	ALA	CA-C-N	5.27	129.40	120.86
1	B	1620	ALA	C-N-CA	5.27	129.40	120.86
1	D	579	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	A	1000	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	B	1444	GLU	CA-C-N	5.27	125.08	119.28
1	B	1444	GLU	C-N-CA	5.27	125.08	119.28
1	B	4217	PHE	CA-CB-CG	-5.27	108.53	113.80
1	A	197	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	D	4564	PHE	CA-CB-CG	-5.27	108.53	113.80
1	B	844	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	B	1141	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	B	2716	ASP	N-CA-C	5.26	117.19	109.24
1	B	197	GLN	OE1-CD-NE2	-5.26	117.34	122.60
1	A	1138	PRO	N-CA-C	5.26	119.74	111.38
1	D	4215	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	D	1702	HIS	CB-CG-CD2	-5.26	124.37	131.20
1	A	49	LEU	N-CA-C	5.25	118.12	109.72
1	A	1018	ASN	CA-C-N	5.25	126.41	119.84
1	A	1018	ASN	C-N-CA	5.25	126.41	119.84
1	C	2874	MET	CB-CA-C	5.25	121.09	110.38
1	C	1952	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	B	1758	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	A	812	HIS	CB-CG-CD2	-5.24	124.38	131.20
1	C	1036	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	D	151	HIS	CA-C-N	5.24	125.53	119.92
1	D	151	HIS	C-N-CA	5.24	125.53	119.92
1	A	2806	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	C	4944	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	C	838	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	B	579	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	B	2632	ILE	N-CA-C	5.23	116.01	110.72
1	C	4973	HIS	CB-CG-CD2	-5.23	124.39	131.20
1	C	98	HIS	CB-CG-CD2	-5.23	124.40	131.20
1	A	1028	ASP	CA-CB-CG	5.23	117.83	112.60
1	C	257	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	D	3031	ALA	N-CA-C	5.23	117.28	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4658	ILE	CB-CA-C	-5.23	105.28	111.97
1	A	838	HIS	CB-CG-CD2	-5.23	124.41	131.20
1	C	275	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	D	2548	LEU	N-CA-CB	-5.22	102.44	110.12
1	B	2221	LYS	CA-C-N	5.22	129.69	120.87
1	B	2221	LYS	C-N-CA	5.22	129.69	120.87
1	D	1777	PHE	CA-CB-CG	5.22	119.02	113.80
1	C	2260	ASN	CA-CB-CG	-5.22	107.38	112.60
1	B	350	HIS	CB-CG-CD2	-5.22	124.42	131.20
1	B	3144	PHE	CB-CA-C	5.22	119.72	110.85
1	C	2736	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	3426	GLU	CA-C-N	5.21	126.36	119.84
1	A	3426	GLU	C-N-CA	5.21	126.36	119.84
1	B	1594	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	C	1772	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	C	2333	ASP	CA-CB-CG	5.21	117.81	112.60
1	D	4753	HIS	N-CA-C	-5.21	104.51	111.24
1	C	2575	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	D	4973	HIS	CB-CG-CD2	-5.21	124.42	131.20
1	A	3526	ALA	CA-C-N	5.21	125.01	119.28
1	A	3526	ALA	C-N-CA	5.21	125.01	119.28
1	B	110	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	D	2333	ASP	CA-CB-CG	5.21	117.81	112.60
1	D	2360	LYS	CA-C-N	5.21	125.29	119.87
1	D	2360	LYS	C-N-CA	5.21	125.29	119.87
1	C	1721	GLU	N-CA-CB	-5.21	102.46	110.01
1	B	2794	TYR	N-CA-C	5.21	117.70	111.71
1	D	181	HIS	N-CA-C	5.21	118.23	109.95
1	A	2642	LYS	N-CA-CB	-5.20	102.47	110.01
1	B	3877	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	2333	ASP	CA-CB-CG	5.20	117.80	112.60
1	C	2104	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	A	181	HIS	N-CA-C	5.20	118.22	109.95
1	B	4994	TYR	N-CA-C	-5.20	105.50	111.07
1	D	2260	ASN	CB-CA-C	5.20	119.62	110.37
1	D	2794	TYR	N-CA-C	5.20	117.69	111.71
1	D	4547	GLN	OE1-CD-NE2	-5.20	117.40	122.60
2	E	70	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	D	530	ILE	N-CA-CB	-5.20	106.15	112.33
1	D	824	GLU	N-CA-CB	-5.20	105.64	111.10
1	B	1125	ASN	CA-CB-CG	5.19	117.79	112.60
1	A	2163	ARG	NE-CZ-NH2	5.19	123.87	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2100	HIS	CB-CG-CD2	-5.18	124.46	131.20
1	B	3010	PHE	CA-CB-CG	-5.18	108.62	113.80
1	D	4774	LYS	CA-C-N	5.17	127.22	120.28
1	D	4774	LYS	C-N-CA	5.17	127.22	120.28
1	A	105	HIS	N-CA-C	5.17	118.00	109.72
1	B	380	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	D	349	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	A	3207	GLU	CA-C-N	5.17	125.24	119.87
1	A	3207	GLU	C-N-CA	5.17	125.24	119.87
1	A	3622	LYS	N-CA-C	5.17	121.81	110.80
1	C	1543	GLU	N-CA-C	5.17	117.61	110.07
1	D	228	ASP	CA-CB-CG	5.17	117.77	112.60
1	D	98	HIS	CB-CG-CD2	-5.17	124.48	131.20
1	A	3621	HIS	CA-C-N	5.16	131.40	121.54
1	A	3621	HIS	C-N-CA	5.16	131.40	121.54
1	C	3159	ASP	CA-CB-CG	5.16	117.76	112.60
1	D	1656	ARG	CA-C-N	5.16	127.71	120.28
1	D	1656	ARG	C-N-CA	5.16	127.71	120.28
1	C	1972	ASN	CA-CB-CG	-5.16	107.44	112.60
1	C	4774	LYS	CA-C-N	5.16	127.19	120.28
1	C	4774	LYS	C-N-CA	5.16	127.19	120.28
1	D	1548	LEU	N-CA-C	5.16	117.09	108.99
1	B	226	HIS	CB-CG-CD2	-5.16	124.50	131.20
1	C	3951	PHE	CA-CB-CG	-5.16	108.64	113.80
1	D	151	HIS	CB-CG-CD2	-5.16	124.50	131.20
1	B	2629	ASP	CA-C-N	5.15	123.49	120.24
1	B	2629	ASP	C-N-CA	5.15	123.49	120.24
1	D	3292	PRO	N-CA-C	5.15	116.98	110.70
1	D	3595	ARG	NE-CZ-NH2	5.15	123.84	119.20
1	A	4991	PHE	CA-CB-CG	5.15	118.95	113.80
1	B	2041	HIS	CB-CG-CD2	-5.15	124.51	131.20
1	B	3613	TYR	CA-C-N	5.15	127.43	120.38
1	B	3613	TYR	C-N-CA	5.15	127.43	120.38
1	C	2021	CYS	N-CA-C	5.15	116.18	109.64
1	C	2691	TYR	N-CA-C	5.15	117.93	110.42
1	B	58	VAL	CA-C-N	5.14	123.36	119.66
1	B	58	VAL	C-N-CA	5.14	123.36	119.66
1	B	4076	ALA	CA-C-N	5.14	129.38	120.58
1	B	4076	ALA	C-N-CA	5.14	129.38	120.58
1	B	2330	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	A	3432	GLU	CA-CB-CG	5.14	124.38	114.10
1	D	460	GLN	OE1-CD-NE2	-5.14	117.46	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	918	ARG	NE-CZ-NH2	5.14	123.82	119.20
1	D	3247	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	2575	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	A	4658	ILE	CB-CA-C	-5.13	105.40	111.97
1	D	2224	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	A	4559	PHE	N-CA-C	5.13	116.56	111.07
1	A	4061	PHE	CA-CB-CG	5.13	118.93	113.80
1	B	2615	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	C	2044	ILE	N-CA-C	5.13	115.24	110.42
1	D	3432	GLU	CA-CB-CG	5.13	124.36	114.10
1	C	349	GLN	OE1-CD-NE2	-5.13	117.47	122.60
2	H	57	ARG	NE-CZ-NH2	5.13	123.81	119.20
1	B	4548	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	A	861	ILE	N-CA-C	5.12	115.23	107.75
1	B	2020	ASP	CA-CB-CG	5.12	117.72	112.60
1	D	1225	PRO	CA-C-N	5.12	127.66	120.28
1	D	1225	PRO	C-N-CA	5.12	127.66	120.28
1	B	4039	MET	CA-C-N	5.12	127.01	120.56
1	B	4039	MET	C-N-CA	5.12	127.01	120.56
1	D	17	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	918	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	C	1834	VAL	N-CA-C	5.12	115.84	110.62
1	C	2283	ASN	N-CA-C	5.12	117.75	108.69
1	A	3170	CYS	CB-CA-C	5.11	119.28	110.79
1	D	1964	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	C	4784	PHE	CA-CB-CG	5.11	118.91	113.80
1	B	2244	ARG	NE-CZ-NH2	5.11	123.80	119.20
2	H	76	ILE	N-CA-C	5.11	115.48	108.12
1	A	2452	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	D	402	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	B	4991	PHE	CA-CB-CG	5.10	118.90	113.80
1	A	5035	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	A	280	LEU	N-CA-C	5.10	116.59	108.79
1	A	3523	ASN	CA-CB-CG	5.10	117.70	112.60
1	A	4137	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	B	3876	ALA	CA-C-N	5.10	129.55	121.44
1	B	3876	ALA	C-N-CA	5.10	129.55	121.44
1	D	672	VAL	CA-C-N	5.10	124.76	119.56
1	D	672	VAL	C-N-CA	5.10	124.76	119.56
1	D	3526	ALA	CA-C-N	5.10	124.89	119.28
1	D	3526	ALA	C-N-CA	5.10	124.89	119.28
1	C	3357	HIS	CB-CG-CD2	-5.10	124.58	131.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3669	PHE	CA-C-N	5.10	127.06	120.44
1	D	3669	PHE	C-N-CA	5.10	127.06	120.44
1	B	1180	ARG	NE-CZ-NH2	5.09	123.79	119.20
1	D	426	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A	151	HIS	CA-CB-CG	5.09	118.89	113.80
1	A	4217	PHE	CA-CB-CG	-5.09	108.71	113.80
1	A	3503	TYR	N-CA-C	5.09	116.33	107.93
1	B	634	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	B	1575	LEU	N-CA-C	5.09	117.72	111.82
1	B	1809	ASP	CA-CB-CG	5.09	117.69	112.60
1	C	3586	ALA	N-CA-C	5.09	119.25	113.19
1	C	5035	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	D	3357	HIS	CB-CG-CD2	-5.09	124.58	131.20
2	F	42	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	D	553	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A	2716	ASP	N-CA-C	5.09	117.01	109.69
1	B	803	LEU	CA-C-N	5.09	125.62	120.38
1	B	803	LEU	C-N-CA	5.09	125.62	120.38
1	C	218	HIS	CA-CB-CG	-5.09	108.71	113.80
1	B	297	GLN	CA-C-N	5.08	126.09	121.31
1	B	297	GLN	C-N-CA	5.08	126.09	121.31
1	B	3666	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	2045	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	D	536	ASN	CA-CB-CG	5.08	117.68	112.60
1	A	3053	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	C	3432	GLU	CA-CB-CG	5.08	124.25	114.10
1	B	1062	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	C	1070	ASP	CA-CB-CG	5.07	117.67	112.60
1	C	4123	ILE	N-CA-C	5.07	115.58	108.17
1	D	3205	PHE	CA-CB-CG	5.07	118.87	113.80
1	B	203	ASN	CB-CA-C	5.07	117.63	109.41
1	A	336	PRO	CA-C-N	5.07	125.08	120.21
1	A	336	PRO	C-N-CA	5.07	125.08	120.21
1	A	3705	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	2330	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	B	540	PHE	CA-CB-CG	-5.07	108.73	113.80
1	B	808	TYR	CA-CB-CG	5.07	123.02	113.90
1	C	1296	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	C	3994	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	B	348	VAL	CB-CA-C	-5.07	104.63	110.91
2	E	38	SER	N-CA-C	5.07	116.29	107.93
1	C	3243	ILE	CA-C-N	5.06	126.17	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3243	ILE	C-N-CA	5.06	126.17	119.84
1	D	4217	PHE	CA-CB-CG	-5.06	108.74	113.80
1	D	3234	ASN	CA-C-N	5.06	127.90	120.71
1	D	3234	ASN	C-N-CA	5.06	127.90	120.71
1	D	2041	HIS	CB-CG-CD2	-5.06	124.63	131.20
1	A	68	THR	CB-CA-C	-5.05	100.28	109.38
1	A	1288	PHE	CA-CB-CG	5.05	118.85	113.80
1	C	270	SER	N-CA-C	5.05	120.34	113.37
1	B	4877	ASP	CA-C-N	5.05	131.19	121.54
1	B	4877	ASP	C-N-CA	5.05	131.19	121.54
1	C	2253	HIS	CA-CB-CG	-5.05	108.75	113.80
1	A	257	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	B	2104	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	C	530	ILE	N-CA-CB	-5.04	106.33	112.33
1	A	32	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	A	2788	HIS	CB-CG-CD2	-5.04	124.64	131.20
1	C	2574	HIS	CB-CG-CD2	-5.04	124.64	131.20
1	D	3672	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	D	2697	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	D	4043	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	B	2600	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	C	3906	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	D	2011	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	C	297	GLN	CA-C-N	5.04	126.04	121.31
1	C	297	GLN	C-N-CA	5.04	126.04	121.31
1	B	2452	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	D	3449	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	A	2763	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	A	4973	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	B	4886	HIS	CA-CB-CG	5.03	118.83	113.80
1	C	220	LEU	N-CA-C	5.03	115.94	108.60
1	C	4807	PHE	CA-CB-CG	-5.03	108.77	113.80
1	A	993	HIS	CB-CG-CD2	-5.03	124.67	131.20
1	C	1824	GLN	OE1-CD-NE2	-5.03	117.58	122.60
1	C	3914	ASN	CA-CB-CG	-5.02	107.58	112.60
1	A	1232	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	A	3771	HIS	CB-CG-CD2	-5.02	124.67	131.20
1	B	526	LEU	N-CA-CB	-5.02	102.74	110.12
1	B	2899	GLY	N-CA-C	5.02	117.37	110.69
1	C	4662	ASN	OD1-CG-ND2	-5.02	117.58	122.60
1	A	2883	HIS	CB-CG-CD2	-5.02	124.67	131.20
1	D	1144	GLN	OE1-CD-NE2	-5.02	117.58	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1972	ASN	CA-CB-CG	-5.02	107.58	112.60
1	B	111	HIS	CB-CG-CD2	-5.02	124.68	131.20
1	A	3180	ASN	CA-CB-CG	5.01	117.61	112.60
1	C	1542	VAL	N-CA-C	5.01	115.92	108.65
1	B	1101	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	C	2929	PHE	CB-CA-C	5.01	119.37	110.85
1	A	2688	HIS	N-CA-C	5.01	119.66	113.50
1	D	328	LYS	CA-C-N	5.01	128.18	120.82
1	D	328	LYS	C-N-CA	5.01	128.18	120.82
1	A	394	GLN	CB-CA-C	5.01	118.53	109.37
1	B	2655	TYR	N-CA-C	5.01	119.66	113.50
1	C	4100	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	B	3523	ASN	OD1-CG-ND2	-5.00	117.59	122.60
2	F	7	ILE	N-CA-C	-5.00	107.85	111.90
1	A	110	ARG	NE-CZ-NH2	5.00	123.70	119.20
1	A	3945	GLU	N-CA-C	5.00	116.42	111.07
1	B	3436	ARG	NE-CZ-NH2	5.00	123.70	119.20
1	A	1106	ARG	NE-CZ-NH2	5.00	123.70	119.20
1	B	502	HIS	CB-CG-CD2	-5.00	124.70	131.20
1	C	1089	TYR	N-CA-C	5.00	116.66	108.76

There are no chirality outliers.

All (183) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1007	TYR	Sidechain
1	A	1020	ARG	Sidechain
1	A	1024	TYR	Sidechain
1	A	1122	TYR	Sidechain
1	A	1180	ARG	Sidechain
1	A	1434	TYR	Sidechain
1	A	1607	ARG	Sidechain
1	A	1661	ARG	Sidechain
1	A	178	ARG	Sidechain
1	A	1976	ARG	Sidechain
1	A	1994	ARG	Sidechain
1	A	2142	TYR	Sidechain
1	A	218	HIS	Sidechain
1	A	226	HIS	Sidechain
1	A	242	ARG	Sidechain
1	A	247	TYR	Sidechain
1	A	2650	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	2654	TYR	Sidechain
1	A	2673	HIS	Sidechain
1	A	2761	TYR	Sidechain
1	A	2794	TYR	Sidechain
1	A	341	TYR	Sidechain
1	A	3540	TYR	Sidechain
1	A	3577	ARG	Sidechain
1	A	3594	ARG	Sidechain
1	A	3595	ARG	Sidechain
1	A	3613	TYR	Sidechain
1	A	3722	TYR	Sidechain
1	A	3902	TYR	Sidechain
1	A	3934	TYR	Sidechain
1	A	3949	ARG	Sidechain
1	A	4080	TYR	Sidechain
1	A	4194	TYR	Sidechain
1	A	4560	TYR	Sidechain
1	A	4789	PHE	Sidechain
1	A	4791	TYR	Sidechain
1	A	4795	TYR	Sidechain
1	A	5032	TYR	Sidechain
1	A	506	TYR	Sidechain
1	A	523	TYR	Sidechain
1	A	714	TYR	Sidechain
1	A	757	PHE	Sidechain
1	A	76	ARG	Sidechain
1	A	808	TYR	Sidechain
1	B	1073	ARG	Sidechain
1	B	1122	TYR	Sidechain
1	B	1434	TYR	Sidechain
1	B	1661	ARG	Sidechain
1	B	178	ARG	Sidechain
1	B	1994	ARG	Sidechain
1	B	2028	ARG	Sidechain
1	B	2128	TYR	Sidechain
1	B	2142	TYR	Sidechain
1	B	218	HIS	Sidechain
1	B	2508	ARG	Sidechain
1	B	2650	ARG	Sidechain
1	B	275	ARG	Sidechain
1	B	2792	ARG	Sidechain
1	B	2794	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	3213	TYR	Sidechain
1	B	3219	TYR	Sidechain
1	B	3263	TYR	Sidechain
1	B	3283	ARG	Sidechain
1	B	3368	ARG	Sidechain
1	B	3613	TYR	Sidechain
1	B	3722	TYR	Sidechain
1	B	3937	TYR	Sidechain
1	B	3951	PHE	Sidechain
1	B	4077	PHE	Sidechain
1	B	4080	TYR	Sidechain
1	B	4194	TYR	Sidechain
1	B	4629	TYR	Sidechain
1	B	4630	TYR	Sidechain
1	B	4789	PHE	Sidechain
1	B	4791	TYR	Sidechain
1	B	4795	TYR	Sidechain
1	B	4892	ARG	Sidechain
1	B	497	TYR	Sidechain
1	B	5032	TYR	Sidechain
1	B	523	TYR	Sidechain
1	B	714	TYR	Sidechain
1	B	757	PHE	Sidechain
1	B	808	TYR	Sidechain
1	B	829	TYR	Sidechain
1	C	1073	ARG	Sidechain
1	C	1122	TYR	Sidechain
1	C	1180	ARG	Sidechain
1	C	1232	ARG	Sidechain
1	C	1259	ARG	Sidechain
1	C	1607	ARG	Sidechain
1	C	1661	ARG	Sidechain
1	C	2110	TYR	Sidechain
1	C	213	TYR	Sidechain
1	C	2142	TYR	Sidechain
1	C	218	HIS	Sidechain
1	C	2224	ARG	Sidechain
1	C	2359	ARG	Sidechain
1	C	2452	ARG	Sidechain
1	C	2650	ARG	Sidechain
1	C	2673	HIS	Sidechain
1	C	2691	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	3095	PHE	Sidechain
1	C	3213	TYR	Sidechain
1	C	341	TYR	Sidechain
1	C	3576	TYR	Sidechain
1	C	359	TYR	Sidechain
1	C	3594	ARG	Sidechain
1	C	3613	TYR	Sidechain
1	C	3722	TYR	Sidechain
1	C	3868	ARG	Sidechain
1	C	3902	TYR	Sidechain
1	C	3937	TYR	Sidechain
1	C	3951	PHE	Sidechain
1	C	4085	ARG	Sidechain
1	C	4194	TYR	Sidechain
1	C	4554	TYR	Sidechain
1	C	4711	PHE	Sidechain
1	C	4775	TYR	Sidechain
1	C	4789	PHE	Sidechain
1	C	4791	TYR	Sidechain
1	C	4795	TYR	Sidechain
1	C	4892	ARG	Sidechain
1	C	4994	TYR	Sidechain
1	C	5032	TYR	Sidechain
1	C	506	TYR	Sidechain
1	C	523	TYR	Sidechain
1	C	714	TYR	Sidechain
1	C	757	PHE	Sidechain
1	C	829	TYR	Sidechain
1	D	103	TYR	Sidechain
1	D	1051	TYR	Sidechain
1	D	110	ARG	Sidechain
1	D	1122	TYR	Sidechain
1	D	1259	ARG	Sidechain
1	D	1661	ARG	Sidechain
1	D	2028	ARG	Sidechain
1	D	2142	TYR	Sidechain
1	D	218	HIS	Sidechain
1	D	226	HIS	Sidechain
1	D	2369	ARG	Sidechain
1	D	2452	ARG	Sidechain
1	D	247	TYR	Sidechain
1	D	2508	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	2650	ARG	Sidechain
1	D	266	ARG	Sidechain
1	D	2673	HIS	Sidechain
1	D	2691	TYR	Sidechain
1	D	2697	ARG	Sidechain
1	D	2761	TYR	Sidechain
1	D	3095	PHE	Sidechain
1	D	3166	TYR	Sidechain
1	D	3213	TYR	Sidechain
1	D	3350	ARG	Sidechain
1	D	3409	TYR	Sidechain
1	D	341	TYR	Sidechain
1	D	3540	TYR	Sidechain
1	D	3550	ARG	Sidechain
1	D	3594	ARG	Sidechain
1	D	3613	TYR	Sidechain
1	D	3722	TYR	Sidechain
1	D	3829	PHE	Sidechain
1	D	3899	PHE	Sidechain
1	D	3902	TYR	Sidechain
1	D	3937	TYR	Sidechain
1	D	3949	ARG	Sidechain
1	D	3951	PHE	Sidechain
1	D	4085	ARG	Sidechain
1	D	4554	TYR	Sidechain
1	D	4629	TYR	Sidechain
1	D	4630	TYR	Sidechain
1	D	4711	PHE	Sidechain
1	D	4775	TYR	Sidechain
1	D	4789	PHE	Sidechain
1	D	4791	TYR	Sidechain
1	D	4795	TYR	Sidechain
1	D	497	TYR	Sidechain
1	D	506	TYR	Sidechain
1	D	523	TYR	Sidechain
1	D	714	TYR	Sidechain
1	D	757	PHE	Sidechain
1	D	830	ARG	Sidechain
2	E	42	ARG	Sidechain
2	F	42	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	35088	34740	34717	147	0
1	B	35088	34740	34717	148	0
1	C	35088	34740	34717	144	0
1	D	35088	34740	34717	157	0
2	E	832	829	831	2	0
2	F	832	829	831	1	0
2	G	832	829	831	2	0
2	H	832	829	831	0	0
All	All	143680	142276	142192	590	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 (590) 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:C:19:GLU:HG2	1:C:68:THR:HG23	1.70	0.74
1:B:3324:VAL:HG11	1:B:3361:THR:HG21	1.70	0.71
1:A:4199:GLU:CD	1:A:4199:GLU:H	2.04	0.64
1:B:1931:LEU:HD22	1:B:1931:LEU:H	1.64	0.63
1:C:19:GLU:CG	1:C:68:THR:HG23	2.29	0.62
1:D:4984:ASN:HD21	1:D:4986:ALA:HB3	1.64	0.62
1:C:1931:LEU:HD22	1:C:1931:LEU:H	1.65	0.62
1:A:4958:CYS:HG	1:A:4961:CYS:HG	1.48	0.61
1:A:1931:LEU:H	1:A:1931:LEU:HD22	1.67	0.60
1:C:3291:ALA:HB1	1:C:3292:PRO:HD2	1.84	0.60
1:A:3935:TRP:CH2	1:D:77:ALA:HB2	2.37	0.59
1:C:458:GLU:CD	1:C:458:GLU:H	2.11	0.59
1:A:4020:GLN:HA	1:A:4023:MET:HE3	1.84	0.59
1:D:458:GLU:CD	1:D:458:GLU:H	2.11	0.58
1:A:22:LEU:HD23	1:A:22:LEU:H	1.69	0.57
1:B:171:LEU:HD23	1:B:171:LEU:H	1.68	0.57
1:B:2282:ASP:HA	1:B:2341:VAL:HG13	1.87	0.57
1:A:1094:ALA:HB2	1:A:1143:TRP:CZ2	2.40	0.57
1:D:475:GLN:HE22	1:D:532:GLY:H	1.52	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1805:GLU:CD	1:D:1805:GLU:H	2.12	0.57
1:D:1651:LEU:C	1:D:1651:LEU:HD23	2.30	0.56
1:C:4985:LEU:HD23	1:C:4985:LEU:H	1.70	0.56
1:A:171:LEU:H	1:A:171:LEU:HD23	1.70	0.56
1:A:1805:GLU:CD	1:A:1805:GLU:H	2.14	0.56
1:C:4199:GLU:CD	1:C:4199:GLU:H	2.14	0.56
1:B:1805:GLU:CD	1:B:1805:GLU:H	2.14	0.56
1:A:458:GLU:CD	1:A:458:GLU:H	2.13	0.55
1:D:2282:ASP:HA	1:D:2341:VAL:HG13	1.89	0.55
1:B:597:HIS:CD2	1:B:1661:ARG:HH22	2.24	0.55
1:A:4194:TYR:CD1	1:A:4194:TYR:N	2.75	0.55
1:C:1805:GLU:H	1:C:1805:GLU:CD	2.14	0.55
1:B:458:GLU:CD	1:B:458:GLU:H	2.14	0.55
1:C:3288:GLY:O	1:C:3291:ALA:HB3	2.07	0.54
1:D:4115:SER:HB3	1:D:4128:PHE:CZ	2.42	0.54
1:B:4115:SER:HA	1:B:4128:PHE:CE1	2.42	0.54
1:C:2101:MET:SD	1:C:2105:TRP:CE2	3.01	0.54
1:D:597:HIS:CD2	1:D:1661:ARG:HH22	2.25	0.54
1:B:138:GLN:HG2	1:B:139:GLU:H	1.72	0.54
1:C:597:HIS:CD2	1:C:1661:ARG:HH22	2.26	0.54
1:A:475:GLN:HE22	1:A:532:GLY:H	1.56	0.54
1:C:4984:ASN:HD21	1:C:4986:ALA:HB3	1.73	0.54
1:D:1451:GLY:HA3	1:D:1494:MET:HG2	1.91	0.53
1:B:4199:GLU:H	1:B:4199:GLU:CD	2.17	0.53
1:D:3902:TYR:CD2	1:D:3906:GLN:HG3	2.43	0.53
1:A:4632:LEU:HD13	1:A:4632:LEU:H	1.74	0.53
1:C:4978:HIS:CE1	1:C:4983:HIS:CG	2.96	0.53
1:D:4194:TYR:N	1:D:4194:TYR:CD1	2.77	0.53
1:A:597:HIS:CD2	1:A:1661:ARG:HH22	2.27	0.53
1:A:2376:LEU:C	1:A:2376:LEU:HD23	2.34	0.52
1:C:17:ASP:O	1:C:68:THR:HG22	2.09	0.52
1:C:2879:ALA:HA	1:C:2882:TYR:CD2	2.44	0.52
1:A:213:TYR:CD1	1:A:340:LYS:HE3	2.44	0.52
1:B:213:TYR:CD1	1:B:340:LYS:HE3	2.45	0.52
1:B:3959:LYS:HA	1:B:3962:PHE:CD2	2.44	0.52
1:B:4194:TYR:CD1	1:B:4194:TYR:N	2.76	0.52
1:D:4199:GLU:H	1:D:4199:GLU:CD	2.17	0.52
1:A:4115:SER:HA	1:A:4128:PHE:CE1	2.44	0.52
1:A:3970:GLN:C	1:A:3972:PRO:HA	2.35	0.52
1:A:4984:ASN:HD21	1:A:4986:ALA:HB3	1.75	0.52
1:C:1715:LEU:C	1:C:1715:LEU:HD23	2.35	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1451:GLY:HA3	1:B:1494:MET:HG2	1.91	0.52
1:B:4989:MET:SD	1:B:4989:MET:C	2.93	0.52
1:D:4978:HIS:CE1	1:D:4983:HIS:CD2	2.98	0.52
1:C:4059:LEU:HA	1:C:4062:PHE:CE2	2.45	0.51
1:B:475:GLN:HE22	1:B:532:GLY:H	1.57	0.51
1:A:101:LEU:C	1:A:102:LEU:HD12	2.34	0.51
1:B:2340:PHE:CD2	1:B:2343:GLY:HA2	2.46	0.51
1:A:4059:LEU:HA	1:A:4062:PHE:CZ	2.46	0.51
1:B:4978:HIS:CE1	1:B:4983:HIS:CD2	2.98	0.51
1:B:1132:TRP:CE2	1:B:1136:SER:HB2	2.46	0.51
1:A:22:LEU:H	1:A:22:LEU:CD2	2.24	0.50
1:A:4989:MET:SD	1:A:4989:MET:C	2.94	0.50
1:D:4632:LEU:HD13	1:D:4632:LEU:H	1.76	0.50
1:D:4989:MET:SD	1:D:4989:MET:C	2.94	0.50
1:B:1715:LEU:HD23	1:B:1715:LEU:C	2.36	0.50
1:C:2417:HIS:CD2	1:C:2492:ALA:HB2	2.45	0.50
1:A:3902:TYR:CD2	1:A:3906:GLN:HG3	2.46	0.50
1:B:4978:HIS:CE1	1:B:4983:HIS:CG	2.99	0.50
1:D:4199:GLU:CD	1:D:4199:GLU:N	2.69	0.50
1:A:4978:HIS:CE1	1:A:4983:HIS:CD2	2.99	0.50
1:B:2879:ALA:HA	1:B:2882:TYR:CD2	2.47	0.50
1:B:4632:LEU:HD13	1:B:4632:LEU:H	1.77	0.50
1:C:4958:CYS:SG	1:C:4961:CYS:N	2.85	0.50
1:D:1132:TRP:CD2	1:D:1136:SER:HB3	2.47	0.50
1:D:3816:MET:HE1	1:D:3899:PHE:CD1	2.47	0.50
1:C:4989:MET:SD	1:C:4989:MET:C	2.94	0.50
1:A:4978:HIS:CE1	1:A:4983:HIS:CG	3.00	0.50
1:B:156:GLN:HA	1:C:226:HIS:CD2	2.47	0.50
1:D:1227:ALA:HA	1:D:1230:MET:HE2	1.92	0.50
1:D:1931:LEU:H	1:D:1931:LEU:HD22	1.77	0.49
1:B:3880:PHE:CD1	1:B:3880:PHE:C	2.89	0.49
1:B:4061:PHE:CE2	1:B:4062:PHE:CE1	3.00	0.49
1:C:2759:ALA:HB1	1:C:2806:ARG:HA	1.94	0.49
1:C:2908:TYR:CZ	1:C:2916:LYS:HE2	2.47	0.49
1:D:3829:PHE:HA	1:D:3832:ILE:HG12	1.94	0.49
1:A:1451:GLY:HA3	1:A:1494:MET:HG2	1.93	0.49
1:B:113:HIS:CG	1:B:114:SER:N	2.80	0.49
1:B:4245:MET:SD	1:B:4993:MET:HE3	2.52	0.49
1:C:3842:LEU:HD23	1:C:3843:ASP:H	1.76	0.49
1:D:2028:ARG:C	1:D:2032:GLN:HE21	2.21	0.49
1:A:150:MET:HE1	1:A:171:LEU:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3959:LYS:HA	1:D:3962:PHE:CD2	2.47	0.49
1:B:4987:ASN:HA	1:B:4990:PHE:CD2	2.48	0.49
1:B:3670:GLU:CD	1:B:3670:GLU:H	2.21	0.49
1:B:4984:ASN:HD21	1:B:4986:ALA:HB3	1.76	0.49
1:D:1243:PRO:HB3	1:D:1600:LEU:HD21	1.95	0.49
1:D:3670:GLU:CD	1:D:3670:GLU:H	2.21	0.49
1:D:4023:MET:SD	1:D:4023:MET:C	2.96	0.49
1:A:22:LEU:HB3	1:A:202:MET:HE1	1.94	0.49
1:A:4789:PHE:CD1	1:A:4789:PHE:C	2.90	0.49
1:A:4987:ASN:HA	1:A:4990:PHE:CD2	2.48	0.49
1:B:4199:GLU:CD	1:B:4199:GLU:N	2.70	0.49
1:C:4023:MET:SD	1:C:4023:MET:C	2.96	0.49
1:B:3829:PHE:HA	1:B:3832:ILE:HG12	1.95	0.48
1:C:3321:ARG:HE	1:C:3357:HIS:CE1	2.30	0.48
1:C:3933:PHE:CE1	1:C:3937:TYR:CD2	3.01	0.48
1:C:4199:GLU:CD	1:C:4199:GLU:N	2.71	0.48
1:A:1288:PHE:CZ	1:A:1460:HIS:HA	2.48	0.48
1:A:2028:ARG:C	1:A:2032:GLN:HE21	2.21	0.48
1:B:573:GLU:H	1:B:573:GLU:CD	2.22	0.48
1:C:461:HIS:CD2	1:C:465:GLN:HE21	2.32	0.48
1:C:1132:TRP:CE2	1:C:1136:SER:HB2	2.48	0.48
1:C:2290:LEU:HD23	1:C:2291:GLN:H	1.78	0.48
1:C:4987:ASN:HA	1:C:4990:PHE:CD2	2.48	0.48
1:A:882:TRP:CD1	1:A:921:ASN:HD21	2.31	0.48
1:A:4061:PHE:CD1	1:A:4061:PHE:C	2.92	0.48
1:C:4194:TYR:CD1	1:C:4194:TYR:N	2.81	0.48
1:B:4061:PHE:CD1	1:B:4061:PHE:C	2.91	0.48
1:C:3965:LEU:HA	1:C:3968:TYR:CD2	2.49	0.48
1:D:213:TYR:CD2	1:D:340:LYS:HE3	2.49	0.48
1:C:2178:MET:SD	1:C:2178:MET:C	2.97	0.48
1:B:171:LEU:HD21	1:B:180:LEU:HB3	1.95	0.48
1:C:328:LYS:HE3	1:C:328:LYS:H	1.79	0.48
1:C:4061:PHE:CD1	1:C:4061:PHE:C	2.92	0.48
1:A:122:THR:HA	1:A:133:PHE:CE2	2.49	0.48
1:B:1451:GLY:CA	1:B:1494:MET:HG2	2.44	0.48
1:C:4160:LEU:HD11	1:C:4164:LEU:HD21	1.95	0.48
1:D:3965:LEU:HA	1:D:3968:TYR:CD2	2.48	0.48
1:B:2028:ARG:C	1:B:2032:GLN:HE21	2.22	0.48
1:D:1078:GLU:CD	1:D:1079:LYS:H	2.21	0.48
1:D:1954:ARG:HE	1:D:2041:HIS:CE1	2.32	0.48
1:D:2908:TYR:CZ	1:D:2916:LYS:HE3	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:573:GLU:CD	1:C:573:GLU:H	2.21	0.47
1:C:1288:PHE:CZ	1:C:1460:HIS:HA	2.49	0.47
1:D:2763:HIS:CE1	1:D:2791:LEU:HD13	2.48	0.47
1:D:4978:HIS:CE1	1:D:4983:HIS:CG	3.02	0.47
1:B:4023:MET:SD	1:B:4023:MET:C	2.97	0.47
1:C:1954:ARG:HE	1:C:2041:HIS:CE1	2.32	0.47
1:B:4072:VAL:HG23	1:B:4073:GLY:H	1.79	0.47
1:C:4861:LYS:HE3	1:C:4862:PHE:CE1	2.48	0.47
1:C:4978:HIS:CE1	1:C:4983:HIS:CD2	3.01	0.47
1:C:5017:ARG:HA	1:C:5019:TRP:CZ3	2.49	0.47
1:B:2545:GLU:CD	1:B:2545:GLU:H	2.23	0.47
1:B:4789:PHE:CD1	1:B:4789:PHE:C	2.90	0.47
1:D:3933:PHE:CD2	1:D:3937:TYR:CE2	3.02	0.47
1:A:1094:ALA:HB2	1:A:1143:TRP:CH2	2.50	0.47
1:C:1869:GLU:CD	1:C:1869:GLU:H	2.22	0.47
1:C:4632:LEU:H	1:C:4632:LEU:CD2	2.27	0.47
1:B:2178:MET:SD	1:B:2178:MET:C	2.97	0.47
1:C:4973:HIS:O	1:C:4977:THR:HG23	2.14	0.47
1:A:2897:LYS:HA	1:A:2897:LYS:HE2	1.95	0.47
1:A:4059:LEU:HA	1:A:4062:PHE:CE1	2.50	0.47
1:C:76:ARG:NH1	1:D:3935:TRP:H	2.12	0.47
1:C:4632:LEU:H	1:C:4632:LEU:HD22	1.79	0.47
1:D:138:GLN:HG2	1:D:139:GLU:H	1.80	0.47
1:A:4178:LEU:HD11	1:A:4194:TYR:HB3	1.96	0.47
1:D:1451:GLY:CA	1:D:1494:MET:HG2	2.44	0.47
1:D:4061:PHE:C	1:D:4061:PHE:CD1	2.92	0.47
1:A:1286:MET:SD	1:A:1286:MET:C	2.97	0.47
1:B:2094:LEU:HD23	1:B:2094:LEU:C	2.39	0.47
1:B:3965:LEU:HA	1:B:3968:TYR:CD2	2.49	0.47
1:D:67:PHE:CE1	1:D:111:HIS:HA	2.49	0.47
1:D:4061:PHE:CE2	1:D:4062:PHE:CE1	3.02	0.47
1:A:3829:PHE:HA	1:A:3832:ILE:HG12	1.97	0.47
1:B:913:LEU:HD12	1:B:914:PRO:HD2	1.97	0.47
1:B:3816:MET:HE1	1:B:3899:PHE:CD1	2.49	0.47
1:C:18:ASP:CG	1:C:206:CYS:H	2.23	0.47
1:A:4245:MET:SD	1:A:4993:MET:HE3	2.56	0.46
1:B:101:LEU:C	1:B:102:LEU:HD12	2.40	0.46
1:B:607:CYS:SG	1:B:617:ASN:HB2	2.56	0.46
1:A:4175:ARG:HB3	1:A:4176:PRO:HD3	1.98	0.46
1:C:1286:MET:SD	1:C:1286:MET:C	2.98	0.46
1:C:3334:TRP:CD1	1:C:3334:TRP:H	2.33	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4735:GLU:H	1:D:4735:GLU:CD	2.22	0.46
1:D:4987:ASN:HA	1:D:4990:PHE:CD2	2.49	0.46
1:A:2101:MET:SD	1:A:2105:TRP:CD2	3.08	0.46
1:A:2257:LEU:HD13	1:A:2257:LEU:C	2.40	0.46
1:D:1433:TYR:CD2	1:D:1573:MET:HB3	2.50	0.46
1:D:2577:ILE:HD12	1:D:2577:ILE:H	1.80	0.46
1:D:4160:LEU:HD12	1:D:4160:LEU:N	2.30	0.46
1:D:4789:PHE:CD1	1:D:4789:PHE:C	2.91	0.46
1:C:554:LEU:HD22	1:C:554:LEU:H	1.81	0.46
1:C:4245:MET:SD	1:C:4993:MET:HE3	2.55	0.46
1:D:113:HIS:CG	1:D:114:SER:N	2.82	0.46
1:D:462:GLU:CD	1:D:462:GLU:H	2.23	0.46
1:D:2897:LYS:HA	1:D:2897:LYS:HE2	1.95	0.46
1:D:3729:MET:HE3	1:D:3729:MET:HA	1.97	0.46
1:A:573:GLU:CD	1:A:573:GLU:H	2.23	0.46
1:A:3334:TRP:CD1	1:A:3334:TRP:H	2.31	0.46
1:B:1438:ARG:HH22	1:B:1513:ASP:HB2	1.80	0.46
1:D:1715:LEU:C	1:D:1715:LEU:HD23	2.40	0.46
1:A:546:TRP:CZ2	1:A:550:LYS:HE2	2.51	0.46
1:C:794:GLY:HA2	1:C:800:PHE:CE2	2.50	0.46
1:C:3291:ALA:HB1	1:C:3292:PRO:CD	2.44	0.46
1:D:882:TRP:CD1	1:D:921:ASN:HD21	2.33	0.46
1:D:3854:GLU:HA	1:D:3867:ASN:HD21	1.81	0.46
1:A:69:LEU:HD23	1:A:69:LEU:HA	1.82	0.46
1:A:731:THR:H	1:A:1476:MET:HE3	1.81	0.46
1:B:4735:GLU:H	1:B:4735:GLU:CD	2.24	0.46
1:D:3916:ILE:HD12	1:D:3968:TYR:CD2	2.50	0.46
1:C:3829:PHE:HA	1:C:3832:ILE:HG12	1.97	0.46
1:C:4789:PHE:CD1	1:C:4789:PHE:C	2.90	0.46
1:D:2094:LEU:HD23	1:D:2094:LEU:C	2.41	0.46
1:D:3758:MET:SD	1:D:3758:MET:C	2.99	0.46
1:D:3943:ILE:C	1:D:3943:ILE:HD12	2.41	0.46
1:A:171:LEU:HD21	1:A:180:LEU:HB3	1.97	0.46
1:A:1862:ILE:HA	1:A:1865:MET:SD	2.55	0.46
1:A:2316:LYS:HE2	1:A:2316:LYS:HA	1.98	0.46
1:B:3420:ARG:HA	1:B:3423:TRP:CE3	2.50	0.46
1:C:2094:LEU:C	1:C:2094:LEU:HD23	2.40	0.46
1:A:2290:LEU:HD23	1:A:2291:GLN:H	1.80	0.45
1:B:554:LEU:N	1:B:554:LEU:HD22	2.31	0.45
1:C:2282:ASP:HA	1:C:2341:VAL:HG13	1.97	0.45
1:C:4564:PHE:CE1	1:C:4568:PHE:CE1	3.04	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1715:LEU:C	1:A:1715:LEU:HD23	2.41	0.45
1:A:4958:CYS:CB	1:A:4961:CYS:HG	2.29	0.45
1:B:3757:GLU:HA	1:B:3760:LYS:HE3	1.98	0.45
2:E:29:MET:HB2	2:E:98:VAL:HG13	1.98	0.45
1:A:439:GLU:CD	1:A:439:GLU:H	2.25	0.45
1:A:4879:MET:HE1	1:B:4580:TYR:CA	2.46	0.45
1:D:4794:TRP:CD2	1:D:4798:MET:SD	3.09	0.45
2:G:97:LEU:HB3	2:G:99:PHE:CZ	2.51	0.45
1:A:3934:TYR:CG	1:A:3935:TRP:N	2.83	0.45
1:B:46:LEU:HD12	1:B:46:LEU:H	1.81	0.45
1:B:121:LEU:HD23	1:B:122:THR:H	1.82	0.45
1:C:1100:MET:SD	1:C:1198:GLN:HB3	2.56	0.45
1:D:573:GLU:CD	1:D:573:GLU:H	2.24	0.45
1:A:102:LEU:HG	1:A:162:LYS:HA	1.97	0.45
1:B:101:LEU:O	1:B:102:LEU:HD12	2.17	0.45
1:B:3933:PHE:CE2	1:B:3937:TYR:CE2	3.04	0.45
1:C:2577:ILE:HD12	1:C:2577:ILE:H	1.82	0.45
1:C:2792:ARG:HH12	1:C:2801:ASP:CG	2.25	0.45
1:D:316:PHE:CZ	1:D:390:LEU:HD11	2.52	0.45
1:B:2908:TYR:CD1	1:B:2908:TYR:C	2.94	0.45
1:C:475:GLN:HE22	1:C:532:GLY:H	1.65	0.45
1:A:856:VAL:HG22	1:A:857:ASP:H	1.82	0.45
1:A:1618:ARG:C	1:A:1626:TRP:CE3	2.95	0.45
1:B:2021:CYS:SG	1:B:2028:ARG:CZ	3.05	0.45
1:A:76:ARG:NH2	1:B:3935:TRP:H	2.14	0.45
1:A:101:LEU:O	1:A:102:LEU:HD12	2.16	0.45
1:A:1083:VAL:HG22	1:A:1188:PHE:O	2.17	0.45
1:A:2503:VAL:HG11	1:A:2557:ALA:HB1	1.99	0.45
1:A:4089:SER:HA	1:A:4122:MET:HA	1.99	0.45
1:C:1286:MET:SD	1:C:1288:PHE:CE2	3.10	0.45
1:C:2761:TYR:CE2	1:C:2765:LYS:HE3	2.52	0.45
1:C:5026:ASP:CG	1:C:5027:CYS:N	2.75	0.45
1:B:3758:MET:SD	1:B:3758:MET:C	3.00	0.45
1:D:67:PHE:CD1	1:D:111:HIS:HA	2.52	0.45
1:C:4879:MET:HE1	1:D:4580:TYR:CA	2.47	0.44
1:D:67:PHE:CD2	1:D:110:ARG:C	2.95	0.44
1:D:3696:ASP:CG	1:D:3773:ARG:HE	2.25	0.44
1:D:4985:LEU:H	1:D:4985:LEU:HD23	1.82	0.44
1:A:794:GLY:HA2	1:A:800:PHE:CE2	2.52	0.44
1:B:3902:TYR:CZ	1:B:3906:GLN:HG2	2.52	0.44
1:B:4181:ILE:C	1:B:4181:ILE:HD12	2.42	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:554:LEU:H	1:D:554:LEU:HD22	1.82	0.44
1:D:597:HIS:CG	1:D:1661:ARG:HH22	2.36	0.44
1:D:1579:MET:SD	1:D:1579:MET:N	2.91	0.44
1:A:3349:ALA:HB1	1:A:3353:LEU:HD11	1.97	0.44
1:A:3420:ARG:HA	1:A:3423:TRP:CE3	2.52	0.44
1:A:4160:LEU:N	1:A:4160:LEU:HD12	2.32	0.44
1:B:635:THR:HB	1:B:1637:MET:HE3	2.00	0.44
1:B:1277:TRP:CH2	1:B:1557:THR:HA	2.52	0.44
1:C:3959:LYS:HA	1:C:3962:PHE:CD2	2.52	0.44
1:C:4059:LEU:HA	1:C:4062:PHE:CZ	2.53	0.44
1:A:1286:MET:SD	1:A:1288:PHE:CE2	3.10	0.44
1:A:2770:LYS:HE2	1:A:2770:LYS:N	2.33	0.44
1:A:2775:TRP:HE1	1:D:1509:ILE:HG22	1.81	0.44
1:B:597:HIS:CG	1:B:1661:ARG:HH22	2.36	0.44
1:B:1083:VAL:HG22	1:B:1188:PHE:O	2.18	0.44
1:C:2517:PHE:CE1	1:C:2520:HIS:CD2	3.06	0.44
1:C:3842:LEU:CD2	1:C:3843:ASP:H	2.30	0.44
1:D:3842:LEU:HD23	1:D:3843:ASP:H	1.83	0.44
1:D:4181:ILE:HD12	1:D:4181:ILE:C	2.42	0.44
1:A:1451:GLY:CA	1:A:1494:MET:HG2	2.47	0.44
1:B:2215:LEU:N	1:B:2215:LEU:HD22	2.32	0.44
1:B:2661:TRP:CE3	1:B:2664:PHE:CE1	3.06	0.44
1:B:2908:TYR:CD2	1:B:2916:LYS:HE3	2.52	0.44
1:B:4794:TRP:CH2	1:B:4798:MET:HE2	2.53	0.44
1:A:137:LEU:HD22	1:A:137:LEU:N	2.33	0.44
1:A:1936:LYS:HZ1	1:A:2105:TRP:CD1	2.35	0.44
1:B:867:LEU:HA	1:B:870:ILE:HG22	2.00	0.44
1:B:2908:TYR:CE2	1:B:2916:LYS:CE	3.00	0.44
1:C:663:TYR:CE1	1:C:804:PRO:HB3	2.53	0.44
1:D:2290:LEU:HD23	1:D:2291:GLN:H	1.83	0.44
1:A:4095:LYS:HA	1:A:4095:LYS:HE2	1.99	0.44
1:A:4892:ARG:HH22	1:D:4899:ASP:CG	2.26	0.44
1:B:4958:CYS:SG	1:B:4960:ILE:HB	2.58	0.44
1:C:2816:MET:CG	1:C:2821:TRP:CZ3	3.01	0.44
1:D:2101:MET:SD	1:D:2105:TRP:CD2	3.11	0.44
1:D:2770:LYS:HE2	1:D:2770:LYS:N	2.32	0.44
1:D:4245:MET:SD	1:D:4993:MET:HE3	2.57	0.44
1:C:4115:SER:HB3	1:C:4128:PHE:CZ	2.53	0.44
1:D:2347:GLU:CD	1:D:2347:GLU:H	2.26	0.44
1:D:2538:THR:HG22	1:D:2541:PHE:CD2	2.52	0.44
1:D:5026:ASP:CG	1:D:5027:CYS:N	2.75	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1961:PHE:CG	1:A:2034:PHE:CZ	3.05	0.44
1:A:4063:ASP:CG	1:A:4064:MET:HE3	2.43	0.44
1:A:5021:PHE:CZ	1:A:5022:PHE:CD2	3.06	0.44
1:B:98:HIS:N	1:B:99:ARG:HE	2.16	0.44
1:B:3842:LEU:HD23	1:B:3843:ASP:H	1.83	0.44
1:C:546:TRP:CZ2	1:C:550:LYS:HE2	2.53	0.44
1:D:554:LEU:HD22	1:D:554:LEU:N	2.33	0.44
1:D:2425:PHE:CD1	1:D:2425:PHE:C	2.95	0.44
1:A:3696:ASP:CG	1:A:3773:ARG:HE	2.26	0.43
1:B:3670:GLU:CD	1:B:3670:GLU:N	2.75	0.43
1:C:4879:MET:HE1	1:D:4580:TYR:CB	2.47	0.43
1:D:1286:MET:C	1:D:1286:MET:SD	3.00	0.43
1:D:1933:GLU:N	1:D:1933:GLU:CD	2.76	0.43
1:D:2316:LYS:HE2	1:D:2316:LYS:HA	2.00	0.43
1:B:554:LEU:HD22	1:B:554:LEU:H	1.84	0.43
1:B:1763:PRO:HD3	1:B:1871:PHE:CE1	2.53	0.43
1:C:111:HIS:CE1	1:C:113:HIS:CG	3.06	0.43
1:C:144:GLU:C	1:C:146:CYS:SG	3.02	0.43
1:C:213:TYR:CD1	1:C:340:LYS:HE3	2.52	0.43
1:C:554:LEU:HD22	1:C:554:LEU:N	2.33	0.43
1:C:1288:PHE:CE2	1:C:1460:HIS:HA	2.53	0.43
1:A:4181:ILE:C	1:A:4181:ILE:HD12	2.43	0.43
1:A:4735:GLU:CD	1:A:4735:GLU:H	2.25	0.43
1:B:439:GLU:CD	1:B:439:GLU:H	2.26	0.43
1:B:3902:TYR:CZ	1:B:3906:GLN:CG	3.01	0.43
1:C:879:HIS:CD2	1:C:921:ASN:HD22	2.36	0.43
1:C:2425:PHE:CD1	1:C:2425:PHE:C	2.96	0.43
1:C:3696:ASP:CG	1:C:3773:ARG:HE	2.26	0.43
1:D:2234:ARG:HD3	1:D:2238:TYR:CE2	2.53	0.43
1:A:18:ASP:CG	1:A:206:CYS:H	2.26	0.43
1:B:67:PHE:CE1	1:B:111:HIS:HA	2.53	0.43
1:B:269:TRP:CZ3	1:B:333:GLY:HA2	2.53	0.43
1:B:1419:ASP:HA	1:B:1570:LYS:HE2	2.01	0.43
1:B:2101:MET:SD	1:B:2105:TRP:CD2	3.11	0.43
1:B:2131:LEU:H	1:B:2131:LEU:HD23	1.83	0.43
1:B:2290:LEU:HD23	1:B:2291:GLN:H	1.83	0.43
1:B:3696:ASP:CG	1:B:3773:ARG:HE	2.26	0.43
1:B:3810:ALA:HA	1:B:3813:GLN:CD	2.43	0.43
1:C:109:LEU:HD23	1:C:109:LEU:HA	1.93	0.43
1:C:3107:VAL:HG12	1:C:3175:LEU:HD21	1.99	0.43
1:C:3758:MET:SD	1:C:3758:MET:C	3.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4913:ARG:HB3	1:C:4913:ARG:CZ	2.48	0.43
1:D:1435:TYR:CE2	1:D:1518:CYS:HB2	2.53	0.43
1:D:2959:PHE:CZ	1:D:2963:LEU:HD11	2.53	0.43
2:F:97:LEU:HB3	2:F:99:PHE:CZ	2.53	0.43
1:A:3667:HIS:CG	1:A:3668:SER:N	2.86	0.43
1:B:67:PHE:CD2	1:B:110:ARG:C	2.96	0.43
1:C:2254:LEU:HD23	1:C:2254:LEU:C	2.43	0.43
1:A:4958:CYS:SG	1:A:4961:CYS:SG	3.04	0.43
1:B:150:MET:HE1	1:B:171:LEU:HB2	2.01	0.43
1:D:67:PHE:HB3	1:D:109:LEU:HD22	2.01	0.43
1:D:2517:PHE:CE1	1:D:2520:HIS:CD2	3.06	0.43
1:D:3670:GLU:CD	1:D:3670:GLU:N	2.76	0.43
1:D:4548:ARG:HA	1:D:4551:PHE:CE2	2.54	0.43
1:A:2577:ILE:H	1:A:2577:ILE:HD12	1.83	0.43
1:A:3758:MET:SD	1:A:3758:MET:C	3.02	0.43
1:B:67:PHE:CD1	1:B:111:HIS:HA	2.53	0.43
1:C:148:TRP:CE3	1:C:171:LEU:HD21	2.54	0.43
1:C:3765:TYR:CE2	1:C:4753:HIS:CG	3.07	0.43
1:C:4735:GLU:CD	1:C:4735:GLU:H	2.25	0.43
1:D:2228:MET:SD	1:D:2229:VAL:N	2.92	0.43
1:D:2348:GLU:CD	1:D:2348:GLU:H	2.27	0.43
1:D:3933:PHE:CE2	1:D:3937:TYR:CE2	3.07	0.43
1:B:1805:GLU:CD	1:B:1805:GLU:N	2.76	0.43
1:C:4134:GLU:HG3	1:C:4135:PRO:HD3	2.01	0.43
1:D:110:ARG:HH21	1:D:115:ARG:HB3	1.84	0.43
1:D:3940:LYS:HG2	1:D:3941:ASP:H	1.83	0.43
1:D:4115:SER:HA	1:D:4128:PHE:CE1	2.53	0.43
1:A:2131:LEU:HD23	1:A:2131:LEU:H	1.84	0.43
1:B:2908:TYR:CE2	1:B:2916:LYS:HE3	2.54	0.43
1:C:597:HIS:CG	1:C:1661:ARG:HH22	2.37	0.43
1:C:2442:LEU:HD22	1:C:2442:LEU:H	1.84	0.43
1:A:1805:GLU:CD	1:A:1805:GLU:N	2.77	0.43
1:B:3106:MET:SD	1:B:3106:MET:C	3.02	0.43
1:D:171:LEU:HD21	1:D:180:LEU:HB3	2.01	0.43
1:D:1274:HIS:CG	1:D:1277:TRP:HA	2.54	0.43
1:D:3817:LEU:HD11	1:D:3902:TYR:CE2	2.54	0.43
1:D:4958:CYS:SG	1:D:4960:ILE:HB	2.59	0.43
1:A:1094:ALA:HB2	1:A:1143:TRP:CE2	2.53	0.42
1:B:3540:TYR:CE2	1:B:3601:ALA:HA	2.54	0.42
1:B:3653:PHE:CD1	1:B:3653:PHE:C	2.95	0.42
1:C:19:GLU:HA	1:C:67:PHE:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2816:MET:HG3	1:A:2821:TRP:CZ3	2.54	0.42
1:B:1122:TYR:CD2	1:B:1122:TYR:N	2.87	0.42
1:B:4971:THR:HG23	1:B:4972:PRO:HD2	2.02	0.42
1:D:2312:MET:SD	1:D:2312:MET:N	2.92	0.42
1:A:169:LEU:HD12	1:A:169:LEU:C	2.45	0.42
1:A:342:GLY:C	1:A:389:PHE:CZ	2.97	0.42
1:A:3670:GLU:CD	1:A:3670:GLU:H	2.27	0.42
1:A:4688:ILE:HD12	1:A:4688:ILE:N	2.34	0.42
1:B:1159:THR:HG22	1:B:1180:ARG:HA	2.00	0.42
1:B:3933:PHE:CD2	1:B:3937:TYR:CE2	3.08	0.42
1:C:736:HIS:CE1	1:C:739:ALA:HB3	2.54	0.42
1:D:1205:GLY:C	1:D:1207:ASP:H	2.27	0.42
1:D:2908:TYR:CE2	1:D:2916:LYS:HE3	2.54	0.42
1:D:3420:ARG:HA	1:D:3423:TRP:CE3	2.54	0.42
1:B:3943:ILE:C	1:B:3943:ILE:HD12	2.44	0.42
1:C:5000:GLU:HA	1:C:5003:HIS:CD2	2.55	0.42
1:D:2138:LEU:N	1:D:2139:PRO:CD	2.83	0.42
1:D:2174:GLU:N	1:D:2174:GLU:CD	2.78	0.42
1:B:144:GLU:C	1:B:146:CYS:SG	3.02	0.42
1:B:2312:MET:SD	1:B:2312:MET:N	2.92	0.42
1:C:65:CYS:HG	1:C:66:CYS:HG	1.67	0.42
1:C:137:LEU:N	1:C:137:LEU:HD22	2.34	0.42
1:C:439:GLU:CD	1:C:439:GLU:H	2.27	0.42
1:C:3729:MET:HE3	1:C:3729:MET:O	2.19	0.42
1:C:3916:ILE:HD12	1:C:3968:TYR:CD2	2.54	0.42
1:D:171:LEU:H	1:D:171:LEU:HD23	1.84	0.42
1:D:2417:HIS:CD2	1:D:2492:ALA:HB2	2.55	0.42
1:D:2700:MET:HB2	1:D:2701:PRO:HD3	2.02	0.42
1:A:35:LEU:HD23	1:A:51:PRO:HA	2.02	0.42
1:A:3324:VAL:CG1	1:A:3361:THR:HG22	2.50	0.42
1:A:3942:VAL:C	1:A:3943:ILE:HD12	2.45	0.42
1:B:546:TRP:CZ2	1:B:550:LYS:HE2	2.54	0.42
1:B:5021:PHE:CZ	1:B:5022:PHE:CD2	3.07	0.42
1:D:137:LEU:N	1:D:137:LEU:HD22	2.34	0.42
1:D:3752:SER:H	1:D:3755:GLU:CD	2.28	0.42
1:D:3816:MET:SD	1:D:3817:LEU:N	2.93	0.42
1:A:3934:TYR:CE2	1:A:3935:TRP:CE2	3.07	0.42
1:B:220:LEU:CD1	1:B:220:LEU:C	2.93	0.42
1:B:3816:MET:SD	1:B:3817:LEU:N	2.93	0.42
1:B:4837:LEU:HD23	1:B:4837:LEU:C	2.45	0.42
1:D:3754:GLU:C	1:D:3754:GLU:CD	2.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:THR:C	1:A:199:LEU:HD12	2.45	0.42
1:A:901:LYS:HG3	1:A:903:LEU:HD21	2.00	0.42
1:A:2254:LEU:HD23	1:A:2254:LEU:C	2.45	0.42
1:C:2228:MET:SD	1:C:2229:VAL:N	2.93	0.42
1:A:4023:MET:SD	1:A:4023:MET:C	3.03	0.42
1:B:277:GLY:HA2	1:B:316:PHE:H	1.85	0.42
1:B:739:ALA:HB1	1:B:740:PRO:HD2	2.01	0.42
1:C:1705:GLY:HA3	1:C:1836:PHE:CD2	2.54	0.42
1:D:13:PHE:CD1	1:D:162:LYS:HB3	2.55	0.42
1:D:4986:ALA:HB1	1:D:4990:PHE:CZ	2.55	0.42
1:A:2425:PHE:CD1	1:A:2425:PHE:C	2.97	0.42
1:A:2603:ILE:HA	1:A:2606:CYS:SG	2.60	0.42
1:B:1933:GLU:N	1:B:1933:GLU:CD	2.78	0.42
1:B:2908:TYR:CE2	1:B:2916:LYS:HE2	2.55	0.42
1:B:3540:TYR:HB3	1:B:3604:TYR:CD2	2.54	0.42
1:B:3970:GLN:C	1:B:3972:PRO:HA	2.45	0.42
1:C:1933:GLU:CD	1:C:1933:GLU:N	2.78	0.42
1:D:102:LEU:HD21	1:D:105:HIS:CE1	2.55	0.42
1:D:2224:ARG:H	1:D:2224:ARG:HD3	1.85	0.42
1:D:2254:LEU:C	1:D:2254:LEU:HD23	2.45	0.42
1:D:4160:LEU:N	1:D:4160:LEU:CD1	2.83	0.42
1:A:554:LEU:N	1:A:554:LEU:HD22	2.35	0.41
1:A:581:ASN:ND2	1:A:581:ASN:H	2.18	0.41
1:A:1775:HIS:C	1:A:1776:HIS:CG	2.98	0.41
1:B:2228:MET:SD	1:B:2229:VAL:N	2.93	0.41
1:B:2778:GLY:H	1:B:2787:THR:HG21	1.84	0.41
1:B:3289:PRO:HG2	1:B:3308:THR:HG22	2.02	0.41
1:B:3754:GLU:CD	1:B:3754:GLU:C	2.88	0.41
1:C:111:HIS:O	1:C:115:ARG:HA	2.20	0.41
1:C:582:HIS:CD2	1:C:582:HIS:N	2.88	0.41
1:C:2138:LEU:N	1:C:2139:PRO:CD	2.83	0.41
1:C:4899:ASP:CG	1:D:4892:ARG:HH22	2.28	0.41
1:C:4958:CYS:CB	1:C:4961:CYS:HG	2.33	0.41
1:D:3810:ALA:HA	1:D:3813:GLN:CD	2.45	0.41
1:D:4965:SER:HB2	1:D:4975:PHE:CG	2.55	0.41
1:D:5021:PHE:CE2	1:D:5022:PHE:CG	3.08	0.41
1:A:1214:PHE:CE2	1:A:1219:LEU:HD13	2.54	0.41
1:A:1291:LEU:HD12	1:A:1550:PRO:HG2	2.03	0.41
1:A:3817:LEU:HD11	1:A:3902:TYR:CE2	2.54	0.41
1:B:150:MET:HE1	1:B:171:LEU:CB	2.50	0.41
1:B:716:PHE:CZ	1:B:718:GLY:CA	3.04	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3449:HIS:CE1	1:B:3453:ARG:HH22	2.38	0.41
1:B:4995:LEU:CD1	1:B:5011:TRP:HB2	2.51	0.41
1:B:5017:ARG:HA	1:B:5019:TRP:CZ3	2.55	0.41
1:C:4995:LEU:CD1	1:C:5011:TRP:HB2	2.50	0.41
1:D:122:THR:HA	1:D:133:PHE:CE2	2.55	0.41
1:D:686:TRP:CE2	1:D:748:LEU:HB2	2.55	0.41
1:D:4063:ASP:CG	1:D:4064:MET:HE3	2.45	0.41
1:B:2138:LEU:N	1:B:2139:PRO:CD	2.83	0.41
1:D:121:LEU:HD23	1:D:122:THR:H	1.85	0.41
1:A:144:GLU:C	1:A:146:CYS:SG	3.03	0.41
1:A:4064:MET:HE2	1:A:4064:MET:HA	2.01	0.41
1:B:1618:ARG:C	1:B:1626:TRP:CE3	2.98	0.41
1:B:2517:PHE:CE1	1:B:2520:HIS:CD2	3.08	0.41
1:C:1618:ARG:C	1:C:1626:TRP:CE3	2.98	0.41
1:C:1805:GLU:CD	1:C:1805:GLU:N	2.77	0.41
1:C:2700:MET:HB2	1:C:2701:PRO:HD3	2.01	0.41
1:D:4879:MET:HE3	1:D:4879:MET:HB3	1.92	0.41
1:A:1078:GLU:HB3	1:A:1081:TYR:CE2	2.55	0.41
1:C:46:LEU:H	1:C:46:LEU:CD1	2.34	0.41
1:C:601:ASP:HA	1:C:604:CYS:SG	2.61	0.41
1:C:1961:PHE:CG	1:C:2034:PHE:CE1	3.08	0.41
1:C:2348:GLU:H	1:C:2348:GLU:CD	2.29	0.41
1:C:3940:LYS:HG2	1:C:3941:ASP:H	1.84	0.41
1:A:2228:MET:SD	1:A:2229:VAL:N	2.93	0.41
1:A:2970:SER:HA	1:A:2973:PHE:CE2	2.56	0.41
1:A:4141:PHE:CD1	1:A:4141:PHE:C	2.99	0.41
1:A:4243:PHE:CD1	1:A:4671:PHE:CD2	3.08	0.41
1:C:2312:MET:SD	1:C:2312:MET:N	2.94	0.41
1:C:4879:MET:HE3	1:C:4879:MET:HB3	1.97	0.41
1:D:349:GLN:HE21	1:D:354:GLY:HA2	1.85	0.41
1:D:3706:SER:HB2	1:D:3778:MET:HG2	2.02	0.41
1:D:4688:ILE:HD12	1:D:4688:ILE:N	2.36	0.41
1:A:1933:GLU:N	1:A:1933:GLU:CD	2.79	0.41
1:C:3933:PHE:CD2	1:C:3951:PHE:CZ	3.09	0.41
1:D:32:GLN:CD	1:D:32:GLN:H	2.29	0.41
1:A:2228:MET:SD	1:A:2228:MET:C	3.04	0.41
1:A:5026:ASP:CG	1:A:5027:CYS:N	2.78	0.41
1:B:601:ASP:HA	1:B:604:CYS:SG	2.61	0.41
1:B:3891:LEU:HB3	1:B:3899:PHE:CZ	2.56	0.41
1:C:581:ASN:H	1:C:581:ASN:ND2	2.18	0.41
1:C:2282:ASP:H	1:C:2341:VAL:HG22	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4632:LEU:HD22	1:C:4632:LEU:N	2.35	0.41
1:D:246:TYR:CZ	1:D:373:LYS:HE3	2.56	0.41
2:G:26:TYR:CD1	2:G:26:TYR:C	2.97	0.41
1:A:139:GLU:CD	1:A:139:GLU:H	2.29	0.41
1:A:1435:TYR:CE1	1:A:1518:CYS:HB2	2.55	0.41
1:A:2155:LEU:HD23	1:A:2156:LEU:N	2.36	0.41
1:A:2661:TRP:CE3	1:A:2664:PHE:CE1	3.09	0.41
1:A:3729:MET:HE3	1:A:3729:MET:O	2.20	0.41
1:A:3964:SER:HA	1:A:3967:GLU:HG2	2.03	0.41
1:A:4219:PHE:CD2	1:A:4219:PHE:C	2.99	0.41
1:B:2254:LEU:HD23	1:B:2255:SER:N	2.35	0.41
1:B:2738:ARG:HA	1:B:2739:PRO:HD2	1.99	0.41
1:B:3539:ARG:HG2	1:B:3539:ARG:HH21	1.85	0.41
1:B:3722:TYR:CZ	1:B:3782:MET:HE2	2.56	0.41
1:B:4063:ASP:CG	1:B:4064:MET:HE3	2.45	0.41
1:B:4095:LYS:CA	1:B:4095:LYS:HE2	2.51	0.41
1:B:4715:TYR:HA	1:B:4716:TRP:CE3	2.56	0.41
1:C:1297:PHE:CZ	1:C:1544:PRO:HA	2.55	0.41
1:D:3653:PHE:CD1	1:D:3653:PHE:C	2.98	0.41
1:D:3906:GLN:H	1:D:3906:GLN:CD	2.28	0.41
2:E:83:GLY:HA2	2:E:94:HIS:CE1	2.56	0.41
1:A:597:HIS:CG	1:A:1661:ARG:HH22	2.39	0.41
1:A:2138:LEU:N	1:A:2139:PRO:CD	2.84	0.41
1:A:2517:PHE:CE1	1:A:2520:HIS:CD2	3.08	0.41
1:B:346:CYS:SG	1:B:347:PHE:N	2.94	0.41
1:B:4857:ASN:HB3	1:B:4858:PHE:CZ	2.56	0.41
1:B:4861:LYS:HE3	1:B:4862:PHE:CZ	2.56	0.41
1:C:2882:TYR:CE2	1:C:2922:LYS:HB3	2.56	0.41
1:C:4879:MET:HE1	1:D:4580:TYR:HB3	2.03	0.41
1:D:554:LEU:H	1:D:554:LEU:CD2	2.34	0.41
1:D:2018:GLU:CD	1:D:2021:CYS:H	2.29	0.41
1:D:4141:PHE:CD1	1:D:4141:PHE:C	2.98	0.41
1:A:1599:MET:HG2	1:A:1601:MET:SD	2.61	0.40
1:A:2211:MET:SD	1:A:2211:MET:C	3.04	0.40
1:A:2316:LYS:HA	1:A:2316:LYS:CE	2.52	0.40
1:C:323:LEU:HD13	1:C:325:THR:H	1.86	0.40
1:C:510:GLU:CD	1:C:510:GLU:H	2.28	0.40
1:C:607:CYS:SG	1:C:617:ASN:HB2	2.61	0.40
1:C:2316:LYS:HA	1:C:2316:LYS:CE	2.51	0.40
1:C:3419:ASN:HB2	1:C:3423:TRP:CZ2	2.56	0.40
1:D:2131:LEU:H	1:D:2131:LEU:CD2	2.34	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2735:PHE:CD2	1:D:2737:PRO:HD3	2.56	0.40
1:D:5000:GLU:HA	1:D:5003:HIS:CD2	2.55	0.40
1:A:1701:ALA:C	1:A:1702:HIS:CG	2.99	0.40
1:A:2742:THR:O	1:A:2814:LYS:HE2	2.20	0.40
1:B:3752:SER:H	1:B:3755:GLU:CD	2.29	0.40
1:B:3793:MET:SD	1:B:3793:MET:N	2.94	0.40
1:C:686:TRP:CE2	1:C:748:LEU:HB2	2.56	0.40
1:C:1078:GLU:CD	1:C:1079:LYS:H	2.29	0.40
1:D:3897:ASN:HA	1:D:3900:GLN:NE2	2.37	0.40
1:D:4217:PHE:CD1	1:D:4237:PHE:CD1	3.09	0.40
1:A:913:LEU:HD12	1:A:914:PRO:HD2	2.04	0.40
1:A:1274:HIS:CG	1:A:1277:TRP:HA	2.57	0.40
1:A:3106:MET:C	1:A:3106:MET:SD	3.04	0.40
1:A:3409:TYR:N	1:A:3410:PRO:HD2	2.37	0.40
1:A:3754:GLU:CD	1:A:3754:GLU:C	2.89	0.40
1:B:1297:PHE:CZ	1:B:1544:PRO:HA	2.56	0.40
1:B:2174:GLU:H	1:B:2174:GLU:CD	2.28	0.40
1:D:109:LEU:HD23	1:D:109:LEU:HA	1.93	0.40
1:D:213:TYR:CD1	1:D:340:LYS:HG2	2.56	0.40
1:A:582:HIS:CD2	1:A:582:HIS:N	2.87	0.40
1:B:109:LEU:HD23	1:B:109:LEU:HA	1.96	0.40
1:B:4088:ILE:C	1:B:4122:MET:SD	3.04	0.40
1:B:4715:TYR:CG	1:B:4716:TRP:N	2.90	0.40
1:C:2347:GLU:H	1:C:2347:GLU:CD	2.30	0.40
1:C:3754:GLU:CD	1:C:3754:GLU:C	2.89	0.40
1:D:1618:ARG:C	1:D:1626:TRP:CE3	3.00	0.40
1:D:2224:ARG:C	1:D:2226:PRO:HD3	2.46	0.40
1:D:3937:TYR:CD2	1:D:3937:TYR:N	2.89	0.40
1:D:4089:SER:HA	1:D:4122:MET:HA	2.04	0.40
1:D:4548:ARG:HA	1:D:4551:PHE:CZ	2.56	0.40
1:A:1121:ALA:C	1:A:1122:TYR:CD1	3.00	0.40
1:C:346:CYS:SG	1:C:347:PHE:N	2.94	0.40
1:C:1110:ARG:HE	1:C:1112:ASP:CG	2.30	0.40
1:C:2661:TRP:CE3	1:C:2664:PHE:CE1	3.10	0.40
1:C:3793:MET:N	1:C:3793:MET:SD	2.94	0.40
1:D:144:GLU:C	1:D:146:CYS:SG	3.04	0.40
1:D:2603:ILE:HA	1:D:2606:CYS:SG	2.62	0.40
1:D:4242:ILE:HG13	1:D:4989:MET:HE1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4376/5037 (87%)	3991 (91%)	331 (8%)	54 (1%)	10	44
1	B	4376/5037 (87%)	3973 (91%)	345 (8%)	58 (1%)	9	42
1	C	4376/5037 (87%)	3976 (91%)	343 (8%)	57 (1%)	9	42
1	D	4376/5037 (87%)	3980 (91%)	332 (8%)	64 (2%)	8	40
2	E	105/108 (97%)	92 (88%)	11 (10%)	2 (2%)	6	32
2	F	105/108 (97%)	96 (91%)	8 (8%)	1 (1%)	12	48
2	G	105/108 (97%)	93 (89%)	11 (10%)	1 (1%)	12	48
2	H	105/108 (97%)	92 (88%)	10 (10%)	3 (3%)	3	23
All	All	17924/20580 (87%)	16293 (91%)	1391 (8%)	240 (1%)	12	42

All (240) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	ALA
1	A	126	SER
1	A	285	VAL
1	A	329	ARG
1	A	4072	VAL
1	A	4227	GLU
1	A	5028	PHE
1	B	153	ALA
1	B	276	TRP
1	B	285	VAL
1	B	740	PRO
1	B	4155	PRO
1	B	4227	GLU
1	B	4691	GLN
1	C	46	LEU
1	C	153	ALA
1	C	285	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2989	SER
1	C	3239	MET
1	C	4072	VAL
1	C	4227	GLU
1	C	5028	PHE
1	D	153	ALA
1	D	285	VAL
1	D	3614	LYS
1	D	3687	GLU
1	D	4227	GLU
1	D	5028	PHE
1	A	16	THR
1	A	386	ASP
1	A	1019	PRO
1	A	3478	MET
1	A	3622	LYS
1	A	3870	ASN
1	B	269	TRP
1	B	270	SER
1	B	308	HIS
1	B	386	ASP
1	B	632	LEU
1	B	817	PRO
1	B	2109	ASP
1	B	2372	GLY
1	B	3623	LEU
1	B	3735	LEU
1	B	4072	VAL
1	C	11	VAL
1	C	272	SER
1	C	373	LYS
1	C	555	GLU
1	C	632	LEU
1	C	1064	GLU
1	C	1792	ALA
1	C	1925	GLY
1	C	2020	ASP
1	C	3327	LEU
1	C	4905	ALA
1	C	5020	ASP
1	D	64	ILE
1	D	555	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	632	LEU
1	D	949	ASN
1	D	2225	PHE
1	D	2741	GLU
1	D	3735	LEU
1	D	4762	PRO
2	E	94	HIS
2	H	94	HIS
1	A	43	GLY
1	A	176	SER
1	A	309	THR
1	A	372	LEU
1	A	632	LEU
1	A	731	THR
1	A	858	THR
1	A	1785	ALA
1	A	1803	PRO
1	A	2669	GLU
1	A	3053	ARG
1	A	3427	PRO
1	A	3687	GLU
1	A	4909	TYR
1	B	176	SER
1	B	372	LEU
1	B	555	GLU
1	B	804	PRO
1	B	2092	GLN
1	B	2774	ASN
1	B	2990	PRO
1	B	3177	THR
1	B	3687	GLU
1	B	4909	TYR
1	B	5020	ASP
1	C	103	TYR
1	C	112	ALA
1	C	146	CYS
1	C	309	THR
1	C	334	MET
1	C	734	GLY
1	C	1009	ALA
1	C	1218	GLY
1	C	2570	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2990	PRO
1	C	3022	ALA
1	C	3030	HIS
1	C	3687	GLU
1	D	155	LYS
1	D	386	ASP
1	D	1064	GLU
1	D	1218	GLY
1	D	1803	PRO
1	D	2342	ASN
1	D	2750	LYS
1	D	2858	GLN
1	D	3030	HIS
1	D	3158	LEU
1	D	3615	SER
1	D	3870	ASN
1	D	4909	TYR
2	F	94	HIS
2	G	94	HIS
1	A	146	CYS
1	A	555	GLU
1	A	1134	LEU
1	A	3151	GLN
1	A	4710	SER
1	B	146	CYS
1	B	224	HIS
1	B	228	ASP
1	B	272	SER
1	B	334	MET
1	B	1219	LEU
1	B	2225	PHE
1	B	2669	GLU
1	B	2736	ASP
1	B	3286	GLU
1	B	3788	GLY
1	B	3870	ASN
1	B	4960	ILE
1	C	16	THR
1	C	213	TYR
1	C	224	HIS
1	C	1134	LEU
1	C	1536	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1803	PRO
1	C	2669	GLU
1	C	3735	LEU
1	C	4086	GLY
1	D	43	GLY
1	D	177	GLU
1	D	195	PHE
1	D	213	TYR
1	D	817	PRO
1	D	1061	SER
1	D	1277	TRP
1	D	1784	ALA
1	D	2220	THR
1	D	2411	PRO
1	D	2669	GLU
1	D	2990	PRO
1	D	3022	ALA
1	D	3053	ARG
1	D	3787	LYS
1	D	4036	VAL
1	D	4086	GLY
1	D	4121	GLU
1	D	4960	ILE
2	H	81	ALA
1	A	195	PHE
1	A	675	LEU
1	A	2741	GLU
1	A	2774	ASN
1	A	2947	ASP
1	A	2990	PRO
1	A	3735	LEU
1	A	4960	ILE
1	B	16	THR
1	B	733	PRO
1	B	1478	ASP
1	B	1481	GLY
1	B	2220	THR
1	B	3204	ALA
1	B	3226	GLU
1	B	3427	PRO
1	B	4121	GLU
1	C	210	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1181	GLU
1	C	3227	ARG
1	C	3623	LEU
1	C	3941	ASP
1	C	4960	ILE
1	D	372	LEU
1	D	951	LYS
1	D	1140	GLY
1	D	2513	GLU
1	D	2989	SER
1	D	3427	PRO
1	A	1545	ASN
1	A	2220	THR
1	A	2411	PRO
1	A	4905	ALA
1	B	1785	ALA
1	B	3293	PRO
1	C	675	LEU
1	C	2784	GLU
1	C	3787	LYS
1	D	825	PRO
1	D	858	THR
1	D	1544	PRO
1	D	2748	PRO
1	D	4155	PRO
1	D	4905	ALA
1	D	4906	GLY
1	A	267	ILE
1	A	1544	PRO
1	A	1754	GLY
1	A	3026	GLY
1	A	3788	GLY
1	C	4155	PRO
1	B	43	GLY
1	B	4906	GLY
1	D	3611	HIS
1	A	707	VAL
1	A	1704	PRO
1	A	3054	VAL
1	C	1544	PRO
1	C	3788	GLY
1	D	4135	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	56	ILE
1	A	4906	GLY
1	B	1509	ILE
1	B	2989	SER
1	B	4972	PRO
1	C	1129	GLY
1	D	842	PRO
1	D	2372	GLY
1	D	2864	GLY
2	H	88	PRO
1	A	2989	SER
1	C	1787	PRO
1	C	3427	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3827/4276 (90%)	3527 (92%)	300 (8%)	11	32
1	B	3827/4276 (90%)	3537 (92%)	290 (8%)	12	33
1	C	3827/4276 (90%)	3552 (93%)	275 (7%)	13	35
1	D	3827/4276 (90%)	3536 (92%)	291 (8%)	12	33
2	E	89/90 (99%)	84 (94%)	5 (6%)	19	40
2	F	89/90 (99%)	84 (94%)	5 (6%)	19	40
2	G	89/90 (99%)	81 (91%)	8 (9%)	9	27
2	H	89/90 (99%)	83 (93%)	6 (7%)	15	36
All	All	15664/17464 (90%)	14484 (92%)	1180 (8%)	14	33

All (1180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	22	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	28	VAL
1	A	29	LEU
1	A	32	GLN
1	A	46	LEU
1	A	67	PHE
1	A	78	LEU
1	A	110	ARG
1	A	121	LEU
1	A	139	GLU
1	A	173	SER
1	A	191	VAL
1	A	192	ASP
1	A	211	GLU
1	A	220	LEU
1	A	223	PHE
1	A	233	ILE
1	A	244	LEU
1	A	267	ILE
1	A	270	SER
1	A	274	LEU
1	A	276	TRP
1	A	278	GLN
1	A	280	LEU
1	A	296	ASP
1	A	303	ASP
1	A	310	LYS
1	A	322	LYS
1	A	323	LEU
1	A	325	THR
1	A	328	LYS
1	A	334	MET
1	A	346	CYS
1	A	359	TYR
1	A	363	ASP
1	A	367	LEU
1	A	372	LEU
1	A	381	GLU
1	A	386	ASP
1	A	389	PHE
1	A	395	GLN
1	A	396	GLU
1	A	414	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	439	GLU
1	A	445	LEU
1	A	452	PHE
1	A	460	GLN
1	A	495	ASN
1	A	510	GLU
1	A	513	GLU
1	A	514	SER
1	A	525	LEU
1	A	536	ASN
1	A	554	LEU
1	A	555	GLU
1	A	576	ASN
1	A	577	ILE
1	A	581	ASN
1	A	607	CYS
1	A	630	GLU
1	A	631	LEU
1	A	639	ASN
1	A	649	PHE
1	A	682	LEU
1	A	688	LEU
1	A	736	HIS
1	A	765	GLN
1	A	808	TYR
1	A	812	HIS
1	A	813	GLU
1	A	819	GLU
1	A	846	LEU
1	A	859	VAL
1	A	863	LEU
1	A	884	LEU
1	A	911	HIS
1	A	957	LYS
1	A	961	MET
1	A	963	ASN
1	A	998	ARG
1	A	1000	ARG
1	A	1011	GLN
1	A	1012	ASP
1	A	1017	ARG
1	A	1036	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1151	CYS
1	A	1154	ASP
1	A	1161	ILE
1	A	1184	ILE
1	A	1188	PHE
1	A	1226	PHE
1	A	1244	GLN
1	A	1254	HIS
1	A	1291	LEU
1	A	1301	PHE
1	A	1422	ASP
1	A	1446	SER
1	A	1458	HIS
1	A	1514	LEU
1	A	1526	LEU
1	A	1527	MET
1	A	1545	ASN
1	A	1579	MET
1	A	1616	GLU
1	A	1622	GLU
1	A	1628	VAL
1	A	1641	ILE
1	A	1651	LEU
1	A	1660	GLN
1	A	1674	CYS
1	A	1712	TYR
1	A	1739	THR
1	A	1752	ARG
1	A	1756	ASN
1	A	1758	ARG
1	A	1799	SER
1	A	1805	GLU
1	A	1808	ARG
1	A	1812	LEU
1	A	1857	GLU
1	A	1858	ASP
1	A	1926	LEU
1	A	1931	LEU
1	A	1933	GLU
1	A	1939	MET
1	A	1946	PHE
1	A	1950	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1951	LEU
1	A	1953	HIS
1	A	1984	PHE
1	A	1996	ARG
1	A	2004	GLU
1	A	2012	PHE
1	A	2018	GLU
1	A	2131	LEU
1	A	2150	GLU
1	A	2155	LEU
1	A	2170	MET
1	A	2177	LEU
1	A	2180	GLN
1	A	2219	GLU
1	A	2221	LYS
1	A	2250	MET
1	A	2257	LEU
1	A	2271	THR
1	A	2274	ASP
1	A	2280	VAL
1	A	2290	LEU
1	A	2291	GLN
1	A	2293	GLN
1	A	2307	LEU
1	A	2312	MET
1	A	2357	LEU
1	A	2369	ARG
1	A	2464	ASP
1	A	2491	SER
1	A	2497	ASP
1	A	2503	VAL
1	A	2513	GLU
1	A	2518	LEU
1	A	2523	ASP
1	A	2531	ARG
1	A	2537	ASP
1	A	2538	THR
1	A	2561	LEU
1	A	2615	ARG
1	A	2623	LEU
1	A	2624	ARG
1	A	2666	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2688	HIS
1	A	2690	LYS
1	A	2697	ARG
1	A	2744	ASN
1	A	2766	TRP
1	A	2813	LEU
1	A	2821	TRP
1	A	2869	ARG
1	A	2880	GLU
1	A	2894	LEU
1	A	2926	LEU
1	A	2927	LEU
1	A	2928	LYS
1	A	2933	ASN
1	A	2939	ARG
1	A	2977	LEU
1	A	2981	VAL
1	A	2998	PHE
1	A	3030	HIS
1	A	3051	ARG
1	A	3053	ARG
1	A	3096	PHE
1	A	3154	ASP
1	A	3173	TYR
1	A	3203	VAL
1	A	3263	TYR
1	A	3276	MET
1	A	3329	ILE
1	A	3350	ARG
1	A	3366	ARG
1	A	3372	VAL
1	A	3376	GLU
1	A	3378	GLN
1	A	3518	LEU
1	A	3535	LEU
1	A	3542	LEU
1	A	3575	LEU
1	A	3607	GLU
1	A	3613	TYR
1	A	3653	PHE
1	A	3669	PHE
1	A	3670	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3683	GLN
1	A	3696	ASP
1	A	3725	TYR
1	A	3728	ILE
1	A	3754	GLU
1	A	3793	MET
1	A	3837	GLN
1	A	3843	ASP
1	A	3856	LEU
1	A	3860	ASN
1	A	3870	ASN
1	A	3879	GLU
1	A	3883	ASP
1	A	3884	LEU
1	A	3895	HIS
1	A	3921	ASP
1	A	3923	LEU
1	A	3934	TYR
1	A	3949	ARG
1	A	3953	LYS
1	A	3978	GLN
1	A	3992	PHE
1	A	4003	LEU
1	A	4010	ILE
1	A	4026	MET
1	A	4040	ILE
1	A	4044	MET
1	A	4047	MET
1	A	4061	PHE
1	A	4062	PHE
1	A	4063	ASP
1	A	4064	MET
1	A	4069	LYS
1	A	4072	VAL
1	A	4092	ASP
1	A	4094	GLN
1	A	4095	LYS
1	A	4104	THR
1	A	4107	GLU
1	A	4127	GLU
1	A	4138	ASP
1	A	4141	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	4161	ARG
1	A	4168	GLU
1	A	4194	TYR
1	A	4199	GLU
1	A	4215	ARG
1	A	4232	GLU
1	A	4240	ASP
1	A	4244	GLU
1	A	4552	LEU
1	A	4559	PHE
1	A	4575	PHE
1	A	4580	TYR
1	A	4584	ASP
1	A	4632	LEU
1	A	4636	THR
1	A	4639	MET
1	A	4662	ASN
1	A	4671	PHE
1	A	4676	GLU
1	A	4677	LEU
1	A	4705	VAL
1	A	4720	VAL
1	A	4722	ARG
1	A	4735	GLU
1	A	4740	LEU
1	A	4775	TYR
1	A	4783	ILE
1	A	4788	SER
1	A	4789	PHE
1	A	4798	MET
1	A	4844	LEU
1	A	4865	LYS
1	A	4880	MET
1	A	4884	LEU
1	A	4901	ILE
1	A	4908	GLU
1	A	4928	LEU
1	A	4949	GLN
1	A	4966	ASP
1	A	4968	PHE
1	A	4971	THR
1	A	4976	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	4989	MET
1	A	4997	ASN
1	A	5035	GLN
1	A	5036	LEU
1	B	17	ASP
1	B	29	LEU
1	B	32	GLN
1	B	35	LEU
1	B	58	VAL
1	B	67	PHE
1	B	68	THR
1	B	76	ARG
1	B	78	LEU
1	B	109	LEU
1	B	113	HIS
1	B	121	LEU
1	B	125	ARG
1	B	133	PHE
1	B	144	GLU
1	B	169	LEU
1	B	191	VAL
1	B	192	ASP
1	B	220	LEU
1	B	227	MET
1	B	233	ILE
1	B	237	ASP
1	B	244	LEU
1	B	266	ARG
1	B	275	ARG
1	B	296	ASP
1	B	303	ASP
1	B	322	LYS
1	B	323	LEU
1	B	325	THR
1	B	328	LYS
1	B	359	TYR
1	B	367	LEU
1	B	374	LYS
1	B	381	GLU
1	B	386	ASP
1	B	389	PHE
1	B	395	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	439	GLU
1	B	460	GLN
1	B	495	ASN
1	B	513	GLU
1	B	536	ASN
1	B	554	LEU
1	B	555	GLU
1	B	577	ILE
1	B	591	ASP
1	B	630	GLU
1	B	631	LEU
1	B	634	GLN
1	B	649	PHE
1	B	654	GLU
1	B	656	SER
1	B	682	LEU
1	B	719	LEU
1	B	745	SER
1	B	757	PHE
1	B	765	GLN
1	B	778	PHE
1	B	808	TYR
1	B	818	ARG
1	B	829	TYR
1	B	846	LEU
1	B	854	CYS
1	B	876	GLU
1	B	884	LEU
1	B	922	LEU
1	B	957	LYS
1	B	961	MET
1	B	963	ASN
1	B	999	ASP
1	B	1016	ARG
1	B	1054	GLU
1	B	1066	GLN
1	B	1079	LYS
1	B	1089	TYR
1	B	1125	ASN
1	B	1139	PHE
1	B	1144	GLN
1	B	1154	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1167	GLU
1	B	1223	PHE
1	B	1238	PHE
1	B	1244	GLN
1	B	1254	HIS
1	B	1285	GLU
1	B	1446	SER
1	B	1506	GLN
1	B	1514	LEU
1	B	1527	MET
1	B	1532	ASN
1	B	1537	ASN
1	B	1539	PHE
1	B	1583	GLU
1	B	1590	GLN
1	B	1607	ARG
1	B	1616	GLU
1	B	1622	GLU
1	B	1628	VAL
1	B	1673	VAL
1	B	1690	ASP
1	B	1707	LEU
1	B	1712	TYR
1	B	1739	THR
1	B	1769	THR
1	B	1799	SER
1	B	1805	GLU
1	B	1808	ARG
1	B	1856	ASP
1	B	1858	ASP
1	B	1866	ILE
1	B	1872	THR
1	B	1874	GLU
1	B	1931	LEU
1	B	1933	GLU
1	B	1939	MET
1	B	1946	PHE
1	B	1950	GLU
1	B	1951	LEU
1	B	1953	HIS
1	B	1979	LEU
1	B	1984	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1997	GLU
1	B	2018	GLU
1	B	2097	LEU
1	B	2116	LEU
1	B	2131	LEU
1	B	2150	GLU
1	B	2155	LEU
1	B	2170	MET
1	B	2177	LEU
1	B	2180	GLN
1	B	2219	GLU
1	B	2223	ILE
1	B	2245	GLN
1	B	2250	MET
1	B	2259	GLU
1	B	2267	MET
1	B	2271	THR
1	B	2274	ASP
1	B	2290	LEU
1	B	2294	ASP
1	B	2307	LEU
1	B	2312	MET
1	B	2333	ASP
1	B	2340	PHE
1	B	2357	LEU
1	B	2371	GLU
1	B	2439	GLU
1	B	2452	ARG
1	B	2487	GLN
1	B	2490	MET
1	B	2503	VAL
1	B	2513	GLU
1	B	2518	LEU
1	B	2523	ASP
1	B	2545	GLU
1	B	2561	LEU
1	B	2575	ARG
1	B	2607	LEU
1	B	2608	MET
1	B	2620	GLN
1	B	2666	VAL
1	B	2700	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2713	ASP
1	B	2734	ASN
1	B	2740	VAL
1	B	2825	LYS
1	B	2877	GLN
1	B	2880	GLU
1	B	2881	ASN
1	B	2886	TRP
1	B	2897	LYS
1	B	2908	TYR
1	B	2911	LEU
1	B	2926	LEU
1	B	2933	ASN
1	B	2938	THR
1	B	2981	VAL
1	B	2998	PHE
1	B	3007	ASN
1	B	3020	THR
1	B	3092	LEU
1	B	3107	VAL
1	B	3154	ASP
1	B	3160	ASP
1	B	3173	TYR
1	B	3230	LEU
1	B	3265	GLU
1	B	3266	MET
1	B	3276	MET
1	B	3310	ASP
1	B	3371	LYS
1	B	3381	LEU
1	B	3539	ARG
1	B	3542	LEU
1	B	3546	ASP
1	B	3549	VAL
1	B	3575	LEU
1	B	3613	TYR
1	B	3653	PHE
1	B	3657	TYR
1	B	3663	LEU
1	B	3669	PHE
1	B	3670	GLU
1	B	3683	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	3690	VAL
1	B	3696	ASP
1	B	3733	CYS
1	B	3754	GLU
1	B	3793	MET
1	B	3833	GLN
1	B	3842	LEU
1	B	3843	ASP
1	B	3860	ASN
1	B	3864	THR
1	B	3870	ASN
1	B	3879	GLU
1	B	3880	PHE
1	B	3883	ASP
1	B	3884	LEU
1	B	3895	HIS
1	B	3900	GLN
1	B	3923	LEU
1	B	3927	GLN
1	B	3935	TRP
1	B	3949	ARG
1	B	3953	LYS
1	B	3978	GLN
1	B	4003	LEU
1	B	4010	ILE
1	B	4019	LEU
1	B	4036	VAL
1	B	4040	ILE
1	B	4044	MET
1	B	4047	MET
1	B	4061	PHE
1	B	4063	ASP
1	B	4064	MET
1	B	4069	LYS
1	B	4071	ILE
1	B	4075	GLU
1	B	4089	SER
1	B	4092	ASP
1	B	4095	LYS
1	B	4104	THR
1	B	4115	SER
1	B	4120	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	4127	GLU
1	B	4138	ASP
1	B	4183	ILE
1	B	4199	GLU
1	B	4232	GLU
1	B	4240	ASP
1	B	4244	GLU
1	B	4552	LEU
1	B	4554	TYR
1	B	4559	PHE
1	B	4580	TYR
1	B	4632	LEU
1	B	4633	GLU
1	B	4662	ASN
1	B	4671	PHE
1	B	4702	ASP
1	B	4725	LEU
1	B	4735	GLU
1	B	4740	LEU
1	B	4783	ILE
1	B	4788	SER
1	B	4789	PHE
1	B	4798	MET
1	B	4844	LEU
1	B	4856	PHE
1	B	4863	TYR
1	B	4865	LYS
1	B	4877	ASP
1	B	4880	MET
1	B	4884	LEU
1	B	4908	GLU
1	B	4918	ILE
1	B	4949	GLN
1	B	4952	GLU
1	B	4957	LYS
1	B	4966	ASP
1	B	4968	PHE
1	B	4989	MET
1	B	4997	ASN
1	B	5019	TRP
1	B	5022	PHE
1	B	5036	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	17	ASP
1	C	28	VAL
1	C	29	LEU
1	C	32	GLN
1	C	67	PHE
1	C	68	THR
1	C	78	LEU
1	C	109	LEU
1	C	110	ARG
1	C	113	HIS
1	C	121	LEU
1	C	125	ARG
1	C	137	LEU
1	C	139	GLU
1	C	171	LEU
1	C	180	LEU
1	C	192	ASP
1	C	214	VAL
1	C	220	LEU
1	C	227	MET
1	C	233	ILE
1	C	241	GLN
1	C	273	HIS
1	C	275	ARG
1	C	280	LEU
1	C	296	ASP
1	C	303	ASP
1	C	310	LYS
1	C	328	LYS
1	C	334	MET
1	C	363	ASP
1	C	374	LYS
1	C	381	GLU
1	C	386	ASP
1	C	389	PHE
1	C	395	GLN
1	C	414	PHE
1	C	439	GLU
1	C	445	LEU
1	C	465	GLN
1	C	483	MET
1	C	495	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	510	GLU
1	C	513	GLU
1	C	514	SER
1	C	555	GLU
1	C	577	ILE
1	C	581	ASN
1	C	610	ASN
1	C	630	GLU
1	C	631	LEU
1	C	634	GLN
1	C	636	ASN
1	C	639	ASN
1	C	663	TYR
1	C	682	LEU
1	C	736	HIS
1	C	741	GLU
1	C	764	VAL
1	C	819	GLU
1	C	846	LEU
1	C	872	GLU
1	C	911	HIS
1	C	922	LEU
1	C	927	GLU
1	C	957	LYS
1	C	961	MET
1	C	999	ASP
1	C	1016	ARG
1	C	1079	LYS
1	C	1139	PHE
1	C	1144	GLN
1	C	1151	CYS
1	C	1152	MET
1	C	1154	ASP
1	C	1158	ASN
1	C	1177	THR
1	C	1238	PHE
1	C	1244	GLN
1	C	1255	TYR
1	C	1285	GLU
1	C	1446	SER
1	C	1514	LEU
1	C	1519	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1573	MET
1	C	1590	GLN
1	C	1608	MET
1	C	1622	GLU
1	C	1628	VAL
1	C	1644	GLU
1	C	1660	GLN
1	C	1673	VAL
1	C	1695	LEU
1	C	1698	LEU
1	C	1714	LEU
1	C	1739	THR
1	C	1767	VAL
1	C	1805	GLU
1	C	1808	ARG
1	C	1856	ASP
1	C	1858	ASP
1	C	1869	GLU
1	C	1872	THR
1	C	1874	GLU
1	C	1926	LEU
1	C	1931	LEU
1	C	1933	GLU
1	C	1939	MET
1	C	1944	GLU
1	C	1950	GLU
1	C	1951	LEU
1	C	1953	HIS
1	C	2018	GLU
1	C	2097	LEU
1	C	2150	GLU
1	C	2155	LEU
1	C	2170	MET
1	C	2177	LEU
1	C	2180	GLN
1	C	2190	VAL
1	C	2219	GLU
1	C	2221	LYS
1	C	2243	SER
1	C	2248	ARG
1	C	2250	MET
1	C	2271	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2274	ASP
1	C	2290	LEU
1	C	2294	ASP
1	C	2307	LEU
1	C	2312	MET
1	C	2316	LYS
1	C	2333	ASP
1	C	2341	VAL
1	C	2357	LEU
1	C	2369	ARG
1	C	2377	LEU
1	C	2415	ARG
1	C	2475	GLN
1	C	2491	SER
1	C	2503	VAL
1	C	2513	GLU
1	C	2518	LEU
1	C	2523	ASP
1	C	2531	ARG
1	C	2537	ASP
1	C	2545	GLU
1	C	2559	LEU
1	C	2561	LEU
1	C	2615	ARG
1	C	2620	GLN
1	C	2623	LEU
1	C	2666	VAL
1	C	2734	ASN
1	C	2744	ASN
1	C	2780	ASN
1	C	2874	MET
1	C	2877	GLN
1	C	2881	ASN
1	C	2897	LYS
1	C	2948	THR
1	C	2955	PHE
1	C	2961	GLN
1	C	2981	VAL
1	C	2998	PHE
1	C	3051	ARG
1	C	3227	ARG
1	C	3243	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	3263	TYR
1	C	3276	MET
1	C	3287	ARG
1	C	3305	THR
1	C	3310	ASP
1	C	3324	VAL
1	C	3378	GLN
1	C	3381	LEU
1	C	3467	MET
1	C	3518	LEU
1	C	3522	LEU
1	C	3539	ARG
1	C	3542	LEU
1	C	3575	LEU
1	C	3607	GLU
1	C	3613	TYR
1	C	3653	PHE
1	C	3657	TYR
1	C	3663	LEU
1	C	3669	PHE
1	C	3683	GLN
1	C	3696	ASP
1	C	3725	TYR
1	C	3728	ILE
1	C	3733	CYS
1	C	3754	GLU
1	C	3789	GLU
1	C	3793	MET
1	C	3833	GLN
1	C	3842	LEU
1	C	3856	LEU
1	C	3860	ASN
1	C	3869	GLN
1	C	3879	GLU
1	C	3884	LEU
1	C	3902	TYR
1	C	3921	ASP
1	C	3923	LEU
1	C	3927	GLN
1	C	3978	GLN
1	C	3992	PHE
1	C	4003	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	4010	ILE
1	C	4011	GLU
1	C	4015	GLU
1	C	4040	ILE
1	C	4044	MET
1	C	4047	MET
1	C	4061	PHE
1	C	4062	PHE
1	C	4063	ASP
1	C	4064	MET
1	C	4067	LYS
1	C	4068	LEU
1	C	4069	LYS
1	C	4089	SER
1	C	4092	ASP
1	C	4093	PHE
1	C	4094	GLN
1	C	4095	LYS
1	C	4104	THR
1	C	4123	ILE
1	C	4125	PHE
1	C	4128	PHE
1	C	4138	ASP
1	C	4141	PHE
1	C	4172	GLU
1	C	4199	GLU
1	C	4240	ASP
1	C	4244	GLU
1	C	4540	PHE
1	C	4548	ARG
1	C	4552	LEU
1	C	4554	TYR
1	C	4557	ARG
1	C	4559	PHE
1	C	4580	TYR
1	C	4627	MET
1	C	4632	LEU
1	C	4633	GLU
1	C	4662	ASN
1	C	4679	ARG
1	C	4705	VAL
1	C	4725	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	4735	GLU
1	C	4783	ILE
1	C	4788	SER
1	C	4789	PHE
1	C	4798	MET
1	C	4844	LEU
1	C	4860	ARG
1	C	4865	LYS
1	C	4870	ASP
1	C	4880	MET
1	C	4884	LEU
1	C	4889	VAL
1	C	4908	GLU
1	C	4918	ILE
1	C	4949	GLN
1	C	4966	ASP
1	C	4971	THR
1	C	4985	LEU
1	C	4989	MET
1	C	4997	ASN
1	C	5006	GLN
1	C	5035	GLN
1	C	5036	LEU
1	D	17	ASP
1	D	28	VAL
1	D	29	LEU
1	D	32	GLN
1	D	35	LEU
1	D	46	LEU
1	D	67	PHE
1	D	68	THR
1	D	70	GLU
1	D	100	THR
1	D	103	TYR
1	D	108	LEU
1	D	109	LEU
1	D	113	HIS
1	D	121	LEU
1	D	125	ARG
1	D	137	LEU
1	D	139	GLU
1	D	149	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	190	GLN
1	D	192	ASP
1	D	214	VAL
1	D	220	LEU
1	D	233	ILE
1	D	241	GLN
1	D	278	GLN
1	D	296	ASP
1	D	303	ASP
1	D	322	LYS
1	D	323	LEU
1	D	325	THR
1	D	328	LYS
1	D	359	TYR
1	D	367	LEU
1	D	374	LYS
1	D	381	GLU
1	D	386	ASP
1	D	389	PHE
1	D	395	GLN
1	D	396	GLU
1	D	439	GLU
1	D	460	GLN
1	D	462	GLU
1	D	495	ASN
1	D	513	GLU
1	D	536	ASN
1	D	554	LEU
1	D	555	GLU
1	D	576	ASN
1	D	577	ILE
1	D	581	ASN
1	D	591	ASP
1	D	630	GLU
1	D	631	LEU
1	D	636	ASN
1	D	639	ASN
1	D	640	TYR
1	D	647	ASN
1	D	663	TYR
1	D	719	LEU
1	D	745	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	819	GLU
1	D	838	HIS
1	D	846	LEU
1	D	852	VAL
1	D	870	ILE
1	D	884	LEU
1	D	922	LEU
1	D	947	GLU
1	D	950	LEU
1	D	957	LYS
1	D	961	MET
1	D	963	ASN
1	D	999	ASP
1	D	1016	ARG
1	D	1021	LEU
1	D	1139	PHE
1	D	1144	GLN
1	D	1151	CYS
1	D	1154	ASP
1	D	1158	ASN
1	D	1161	ILE
1	D	1177	THR
1	D	1182	ILE
1	D	1231	GLN
1	D	1232	ARG
1	D	1235	THR
1	D	1244	GLN
1	D	1254	HIS
1	D	1446	SER
1	D	1478	ASP
1	D	1514	LEU
1	D	1543	GLU
1	D	1570	LYS
1	D	1573	MET
1	D	1579	MET
1	D	1590	GLN
1	D	1616	GLU
1	D	1622	GLU
1	D	1623	ARG
1	D	1651	LEU
1	D	1660	GLN
1	D	1685	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1699	GLU
1	D	1712	TYR
1	D	1721	GLU
1	D	1739	THR
1	D	1747	LEU
1	D	1768	THR
1	D	1802	ILE
1	D	1803	PRO
1	D	1805	GLU
1	D	1808	ARG
1	D	1858	ASP
1	D	1872	THR
1	D	1874	GLU
1	D	1929	MET
1	D	1931	LEU
1	D	1933	GLU
1	D	1939	MET
1	D	1941	ASN
1	D	1950	GLU
1	D	1951	LEU
1	D	1953	HIS
1	D	1979	LEU
1	D	1997	GLU
1	D	2097	LEU
1	D	2104	ARG
1	D	2150	GLU
1	D	2155	LEU
1	D	2170	MET
1	D	2177	LEU
1	D	2180	GLN
1	D	2190	VAL
1	D	2219	GLU
1	D	2245	GLN
1	D	2250	MET
1	D	2259	GLU
1	D	2271	THR
1	D	2274	ASP
1	D	2280	VAL
1	D	2290	LEU
1	D	2294	ASP
1	D	2307	LEU
1	D	2312	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	2316	LYS
1	D	2342	ASN
1	D	2357	LEU
1	D	2377	LEU
1	D	2491	SER
1	D	2503	VAL
1	D	2513	GLU
1	D	2518	LEU
1	D	2523	ASP
1	D	2531	ARG
1	D	2537	ASP
1	D	2538	THR
1	D	2561	LEU
1	D	2620	GLN
1	D	2666	VAL
1	D	2734	ASN
1	D	2751	LEU
1	D	2766	TRP
1	D	2773	ASN
1	D	2803	GLU
1	D	2809	ILE
1	D	2819	TRP
1	D	2820	GLU
1	D	2886	TRP
1	D	2961	GLN
1	D	2977	LEU
1	D	2981	VAL
1	D	2998	PHE
1	D	3016	TYR
1	D	3092	LEU
1	D	3096	PHE
1	D	3154	ASP
1	D	3160	ASP
1	D	3164	SER
1	D	3192	GLU
1	D	3247	ASP
1	D	3264	THR
1	D	3268	HIS
1	D	3276	MET
1	D	3280	TYR
1	D	3283	ARG
1	D	3296	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	3310	ASP
1	D	3324	VAL
1	D	3366	ARG
1	D	3378	GLN
1	D	3381	LEU
1	D	3467	MET
1	D	3501	ASP
1	D	3535	LEU
1	D	3542	LEU
1	D	3550	ARG
1	D	3566	SER
1	D	3575	LEU
1	D	3613	TYR
1	D	3622	LYS
1	D	3653	PHE
1	D	3657	TYR
1	D	3663	LEU
1	D	3669	PHE
1	D	3670	GLU
1	D	3683	GLN
1	D	3696	ASP
1	D	3701	LEU
1	D	3713	LYS
1	D	3754	GLU
1	D	3789	GLU
1	D	3824	LYS
1	D	3825	GLU
1	D	3833	GLN
1	D	3837	GLN
1	D	3842	LEU
1	D	3843	ASP
1	D	3856	LEU
1	D	3860	ASN
1	D	3864	THR
1	D	3870	ASN
1	D	3879	GLU
1	D	3884	LEU
1	D	3923	LEU
1	D	3927	GLN
1	D	3943	ILE
1	D	3949	ARG
1	D	3987	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	3989	VAL
1	D	4003	LEU
1	D	4010	ILE
1	D	4040	ILE
1	D	4044	MET
1	D	4047	MET
1	D	4061	PHE
1	D	4063	ASP
1	D	4064	MET
1	D	4069	LYS
1	D	4071	ILE
1	D	4089	SER
1	D	4092	ASP
1	D	4095	LYS
1	D	4104	THR
1	D	4122	MET
1	D	4123	ILE
1	D	4125	PHE
1	D	4127	GLU
1	D	4138	ASP
1	D	4139	ILE
1	D	4161	ARG
1	D	4168	GLU
1	D	4199	GLU
1	D	4200	THR
1	D	4232	GLU
1	D	4244	GLU
1	D	4544	LEU
1	D	4548	ARG
1	D	4554	TYR
1	D	4559	PHE
1	D	4575	PHE
1	D	4580	TYR
1	D	4632	LEU
1	D	4662	ASN
1	D	4671	PHE
1	D	4679	ARG
1	D	4705	VAL
1	D	4725	LEU
1	D	4735	GLU
1	D	4768	LEU
1	D	4783	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	4788	SER
1	D	4789	PHE
1	D	4798	MET
1	D	4844	LEU
1	D	4865	LYS
1	D	4880	MET
1	D	4884	LEU
1	D	4901	ILE
1	D	4908	GLU
1	D	4928	LEU
1	D	4929	LEU
1	D	4949	GLN
1	D	4952	GLU
1	D	4954	MET
1	D	4968	PHE
1	D	4985	LEU
1	D	4989	MET
1	D	5022	PHE
1	D	5035	GLN
1	D	5036	LEU
2	E	13	ARG
2	E	26	TYR
2	E	36	PHE
2	E	41	ASP
2	E	80	TYR
2	F	13	ARG
2	F	26	TYR
2	F	34	LYS
2	F	36	PHE
2	F	91	ILE
2	G	11	ASP
2	G	13	ARG
2	G	26	TYR
2	G	30	LEU
2	G	39	SER
2	G	85	THR
2	G	96	THR
2	G	106	LEU
2	H	13	ARG
2	H	26	TYR
2	H	34	LYS
2	H	39	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	52	LYS
2	H	91	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (190) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	151	HIS
1	A	255	HIS
1	A	461	HIS
1	A	576	ASN
1	A	877	ASN
1	A	921	ASN
1	A	993	HIS
1	A	1035	ASN
1	A	1127	HIS
1	A	1130	GLN
1	A	1133	HIS
1	A	1420	ASN
1	A	1480	GLN
1	A	1611	HIS
1	A	1660	GLN
1	A	1702	HIS
1	A	1952	GLN
1	A	2032	GLN
1	A	2095	GLN
1	A	2107	GLN
1	A	2184	ASN
1	A	2193	GLN
1	A	2291	GLN
1	A	2342	ASN
1	A	2417	HIS
1	A	2520	HIS
1	A	2647	HIS
1	A	2756	ASN
1	A	2763	HIS
1	A	2780	ASN
1	A	3128	ASN
1	A	3146	HIS
1	A	3418	ASN
1	A	3611	HIS
1	A	3667	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3896	ASN
1	A	3927	GLN
1	A	4054	ASN
1	A	4149	ASN
1	A	4204	GLN
1	A	4209	GLN
1	A	4754	ASN
1	B	23	GLN
1	B	57	ASN
1	B	151	HIS
1	B	203	ASN
1	B	576	ASN
1	B	678	GLN
1	B	1003	GLN
1	B	1158	ASN
1	B	1558	HIS
1	B	1560	ASN
1	B	1590	GLN
1	B	1611	HIS
1	B	1825	HIS
1	B	2032	GLN
1	B	2092	GLN
1	B	2095	GLN
1	B	2125	HIS
1	B	2184	ASN
1	B	2193	GLN
1	B	2291	GLN
1	B	2417	HIS
1	B	2475	GLN
1	B	2520	HIS
1	B	2574	HIS
1	B	2621	HIS
1	B	2646	ASN
1	B	2647	HIS
1	B	2763	HIS
1	B	2883	HIS
1	B	2892	GLN
1	B	2924	GLN
1	B	2961	GLN
1	B	2993	GLN
1	B	3008	GLN
1	B	3146	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	3149	GLN
1	B	3422	HIS
1	B	3430	ASN
1	B	3523	ASN
1	B	3572	GLN
1	B	3647	HIS
1	B	3734	HIS
1	B	3761	GLN
1	B	3830	GLN
1	B	3837	GLN
1	B	3860	ASN
1	B	3960	GLN
1	B	3963	ASN
1	B	4078	GLN
1	B	4130	ASN
1	B	4149	ASN
1	B	4162	ASN
1	B	5035	GLN
1	C	226	HIS
1	C	461	HIS
1	C	465	GLN
1	C	489	ASN
1	C	921	ASN
1	C	949	ASN
1	C	1041	GLN
1	C	1125	ASN
1	C	1133	HIS
1	C	1206	GLN
1	C	1511	HIS
1	C	1590	GLN
1	C	1611	HIS
1	C	1660	GLN
1	C	1825	HIS
1	C	1941	ASN
1	C	2029	GLN
1	C	2032	GLN
1	C	2095	GLN
1	C	2184	ASN
1	C	2193	GLN
1	C	2245	GLN
1	C	2291	GLN
1	C	2417	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2520	HIS
1	C	2647	HIS
1	C	2673	HIS
1	C	2872	GLN
1	C	2924	GLN
1	C	2931	GLN
1	C	2933	ASN
1	C	3008	GLN
1	C	3033	ASN
1	C	3127	GLN
1	C	3146	HIS
1	C	3326	ASN
1	C	3466	ASN
1	C	3667	HIS
1	C	3761	GLN
1	C	3837	GLN
1	C	3889	GLN
1	C	3927	GLN
1	C	3994	HIS
1	C	4034	ASN
1	C	4149	ASN
1	C	4209	GLN
1	D	12	GLN
1	D	32	GLN
1	D	203	ASN
1	D	593	HIS
1	D	678	GLN
1	D	838	HIS
1	D	911	HIS
1	D	921	ASN
1	D	949	ASN
1	D	1133	HIS
1	D	1220	GLN
1	D	1611	HIS
1	D	1663	HIS
1	D	1760	HIS
1	D	1861	GLN
1	D	2032	GLN
1	D	2095	GLN
1	D	2125	HIS
1	D	2173	GLN
1	D	2184	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	2193	GLN
1	D	2284	ASN
1	D	2291	GLN
1	D	2417	HIS
1	D	2520	HIS
1	D	2763	HIS
1	D	2892	GLN
1	D	2933	ASN
1	D	2993	GLN
1	D	3033	ASN
1	D	3109	ASN
1	D	3127	GLN
1	D	3146	HIS
1	D	3430	ASN
1	D	3466	ASN
1	D	3523	ASN
1	D	3647	HIS
1	D	3667	HIS
1	D	3734	HIS
1	D	3761	GLN
1	D	3830	GLN
1	D	4149	ASN
1	D	4209	GLN
2	E	25	HIS
2	E	65	GLN
2	F	65	GLN
2	F	94	HIS
2	H	65	GLN

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 oligosaccharides 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

There are no chain breaks in this entry.

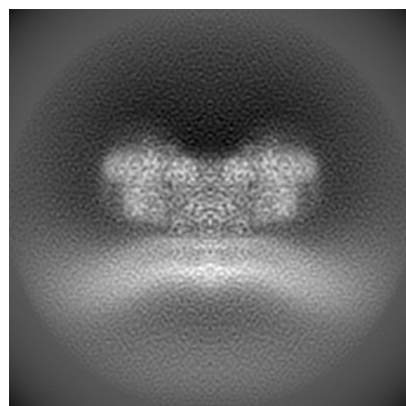
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54595. These allow visual inspection of the internal detail of the map and identification of artifacts.

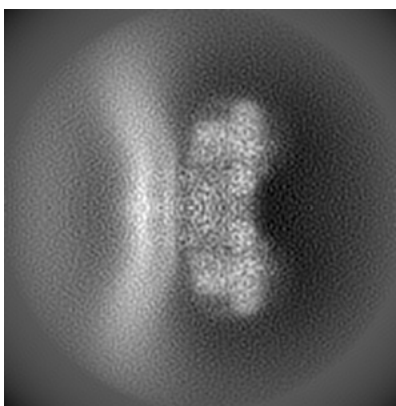
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

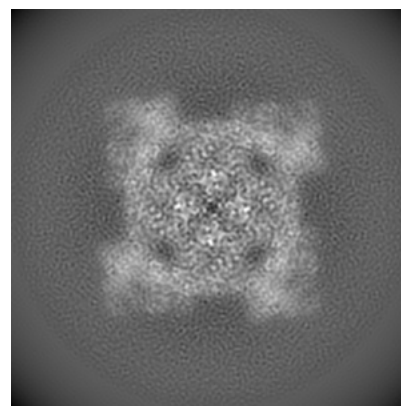
6.1.1 Primary map



X

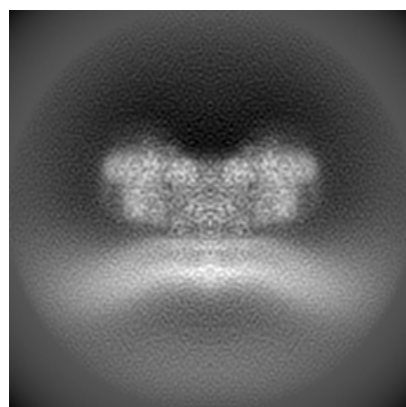


Y

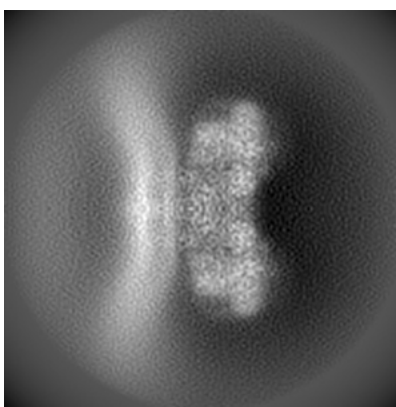


Z

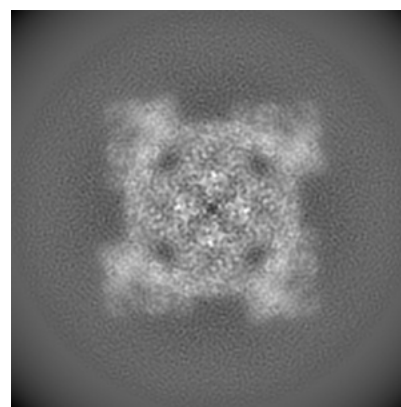
6.1.2 Raw map



X



Y

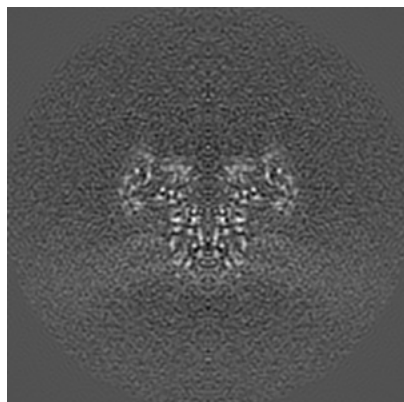


Z

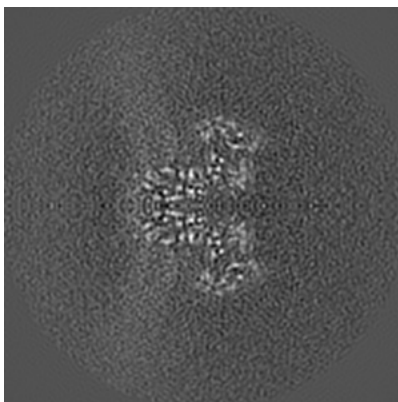
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

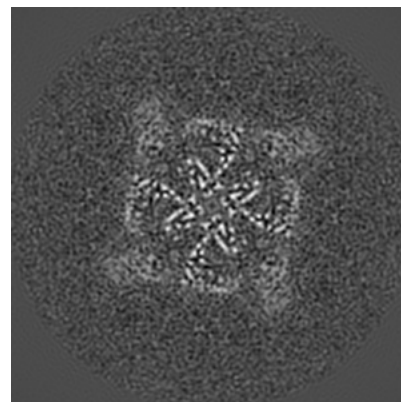
6.2.1 Primary map



X Index: 85

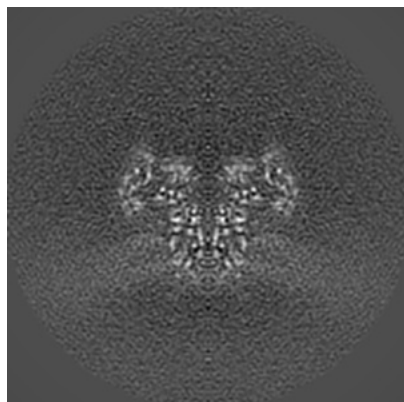


Y Index: 85

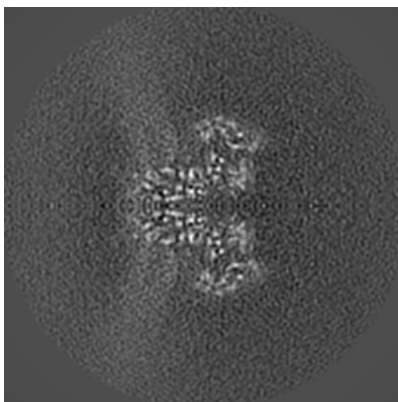


Z Index: 85

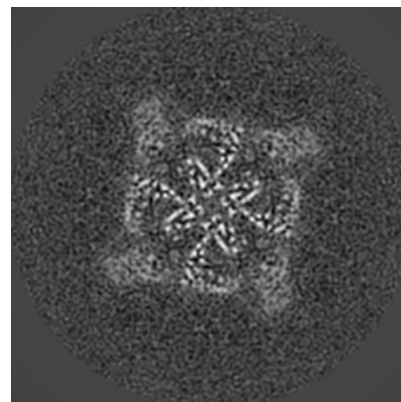
6.2.2 Raw map



X Index: 85



Y Index: 85

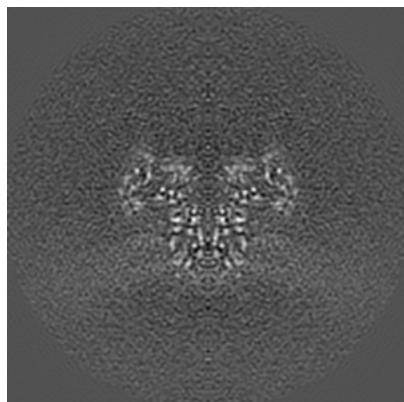


Z Index: 85

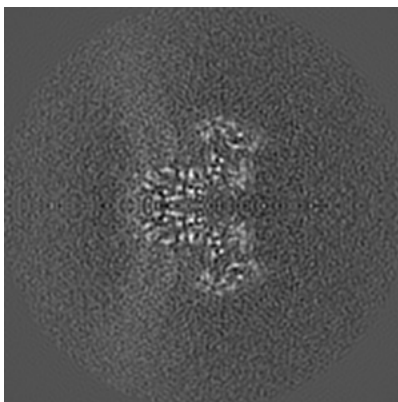
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

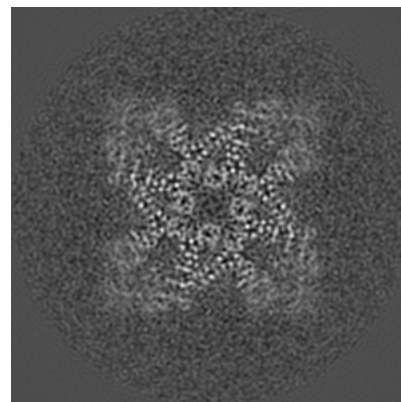
6.3.1 Primary map



X Index: 85

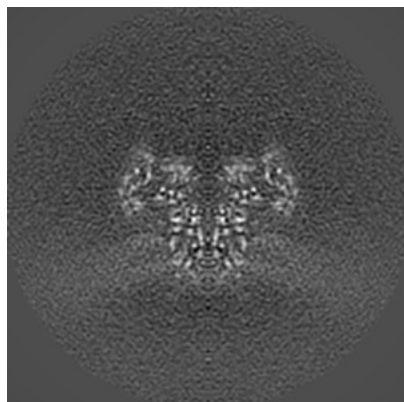


Y Index: 85

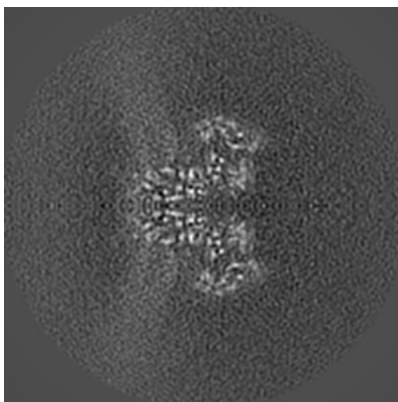


Z Index: 100

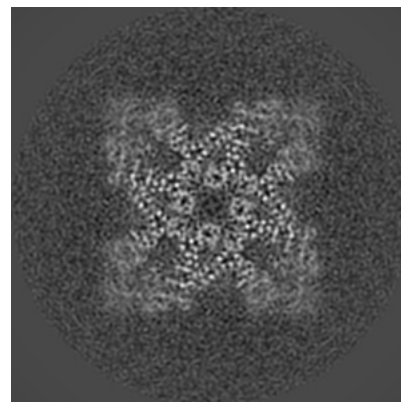
6.3.2 Raw map



X Index: 85



Y Index: 85

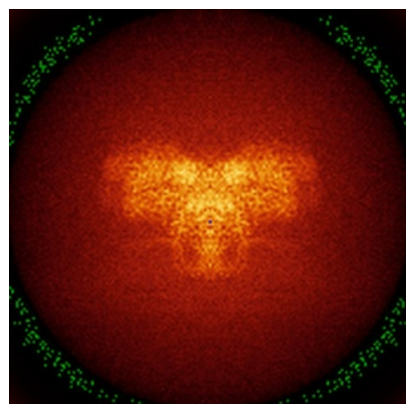


Z Index: 100

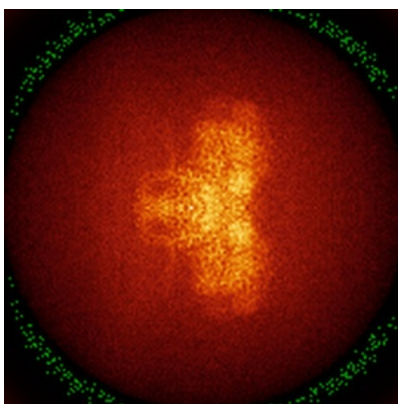
The images above show the largest variance slices of the map in three orthogonal directions.

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

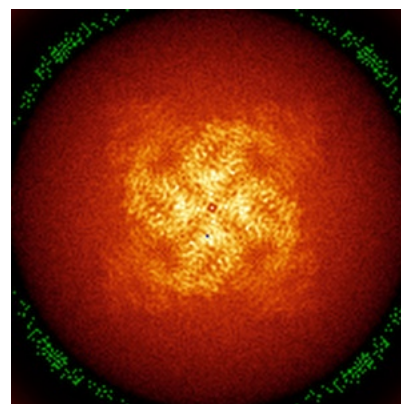
6.4.1 Primary map



X

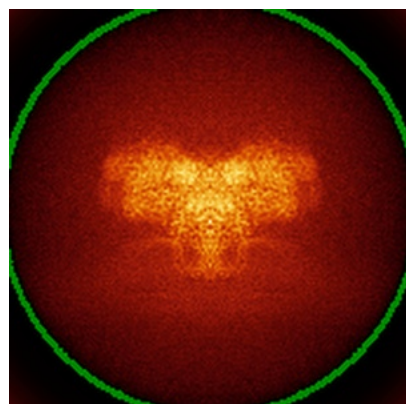


Y

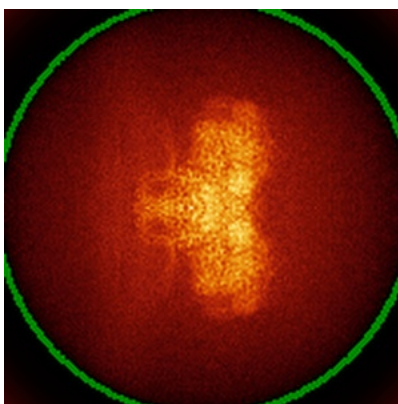


Z

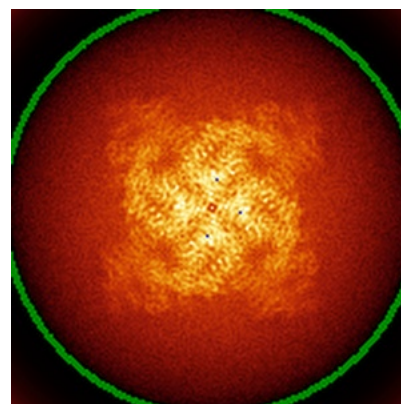
6.4.2 Raw map



X



Y

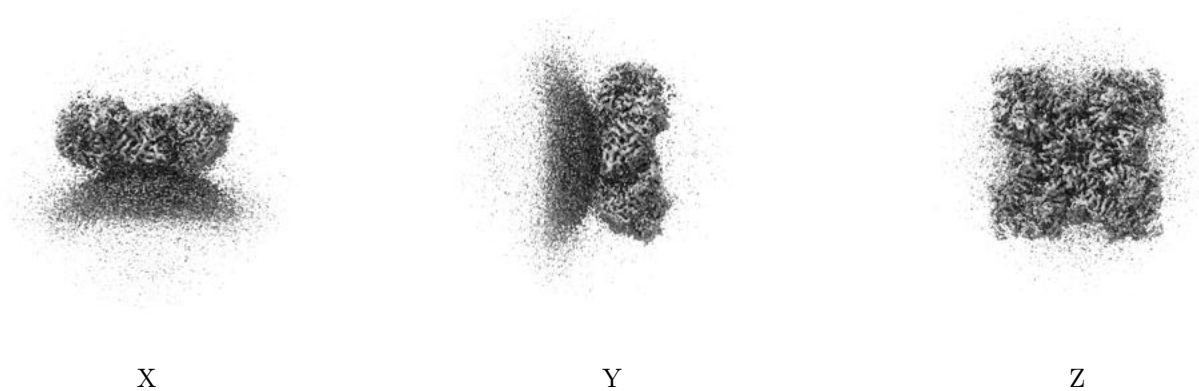


Z

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

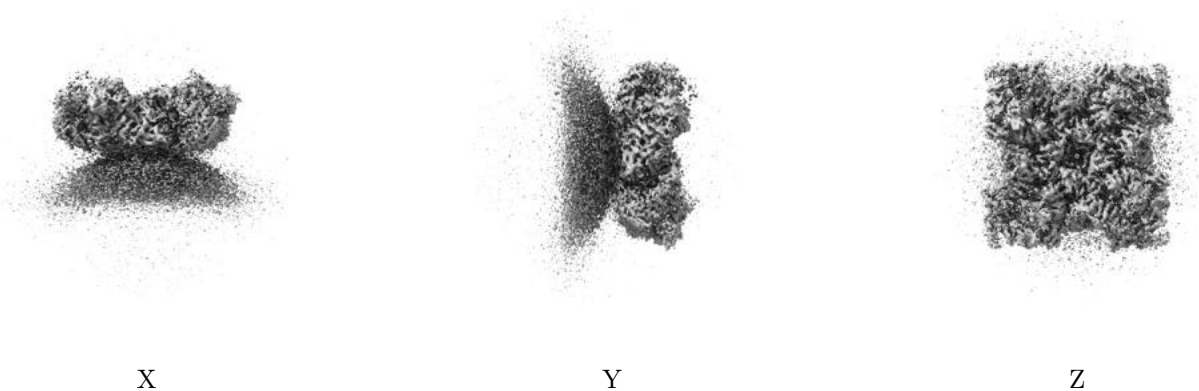
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.105. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

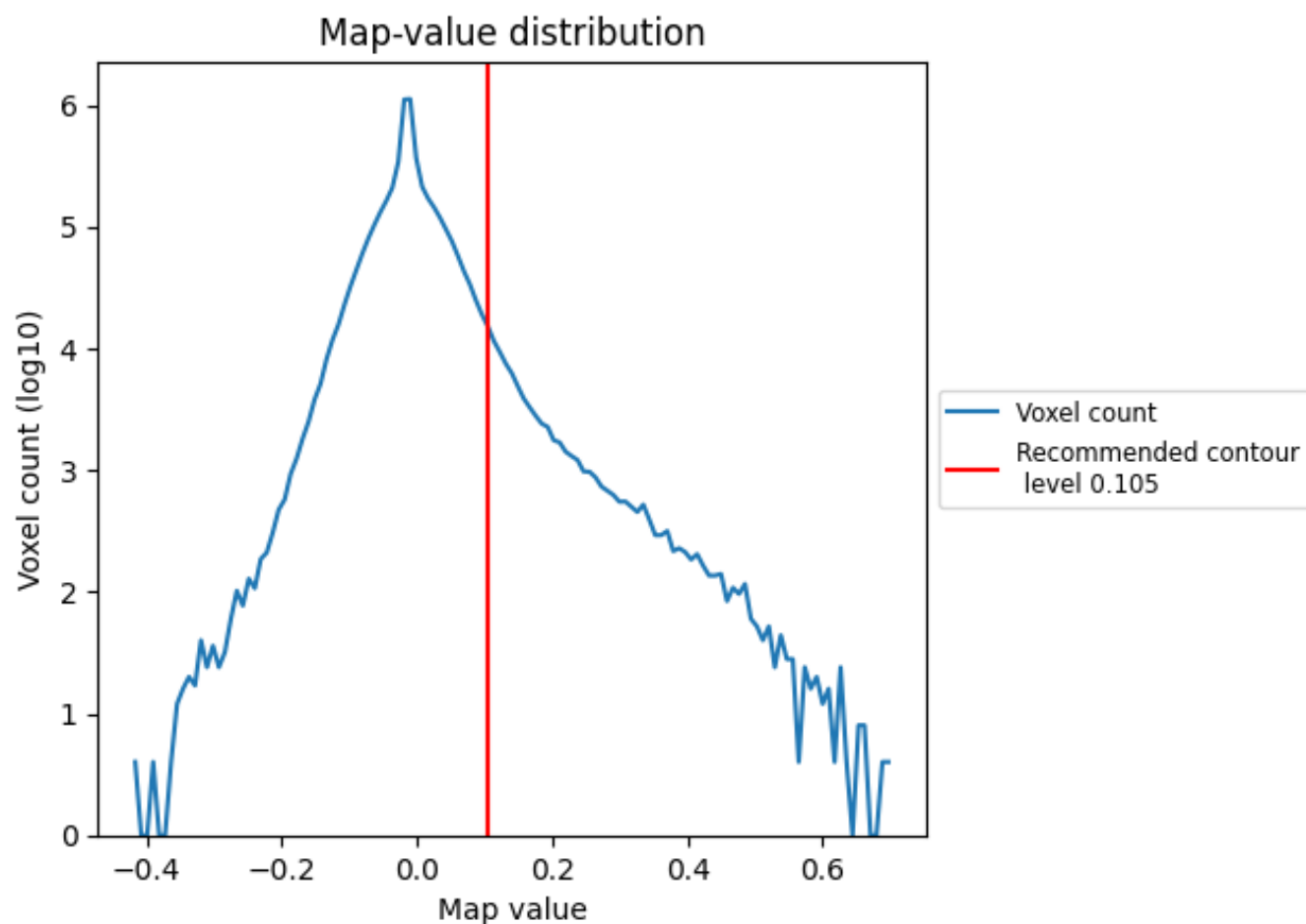
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

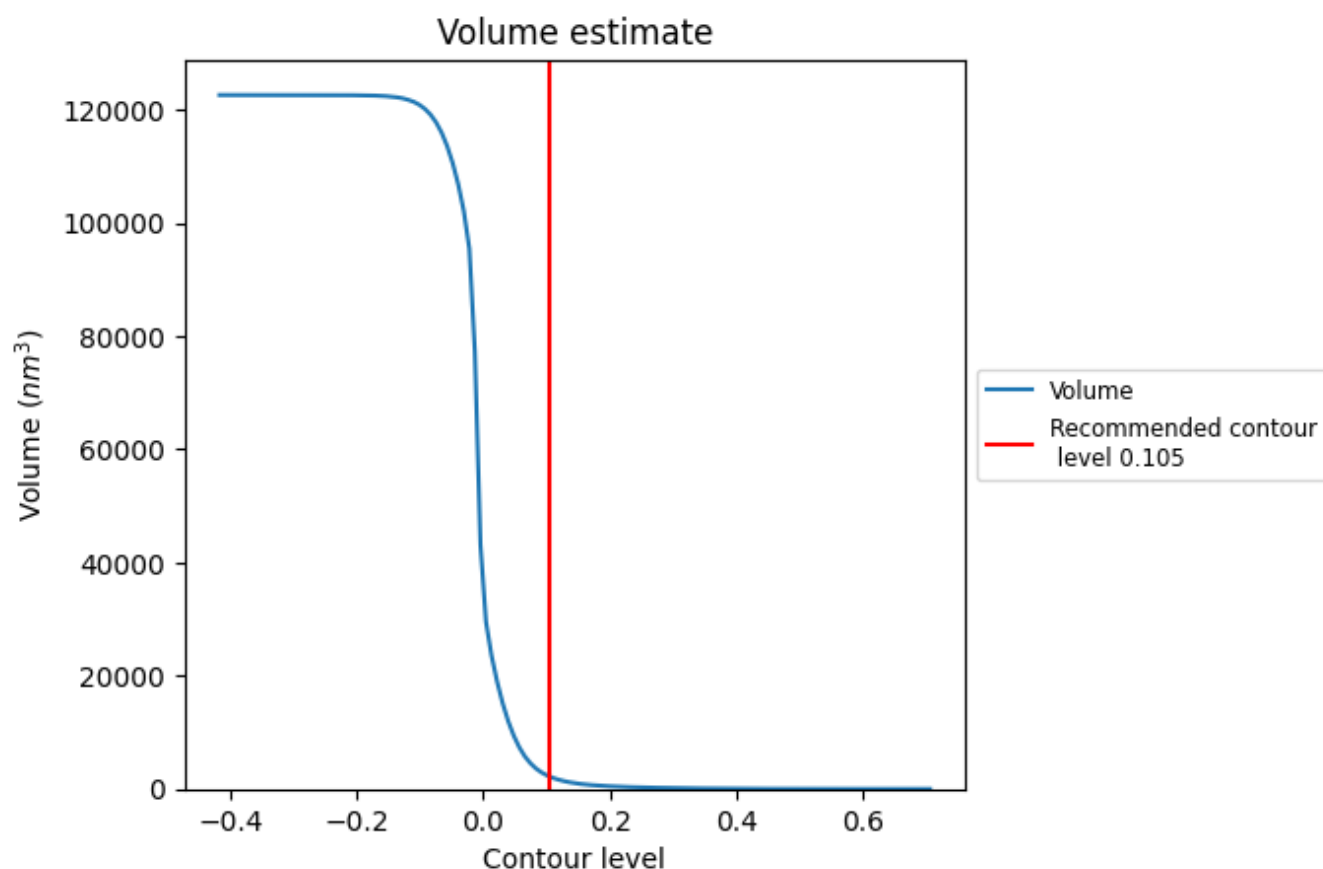
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

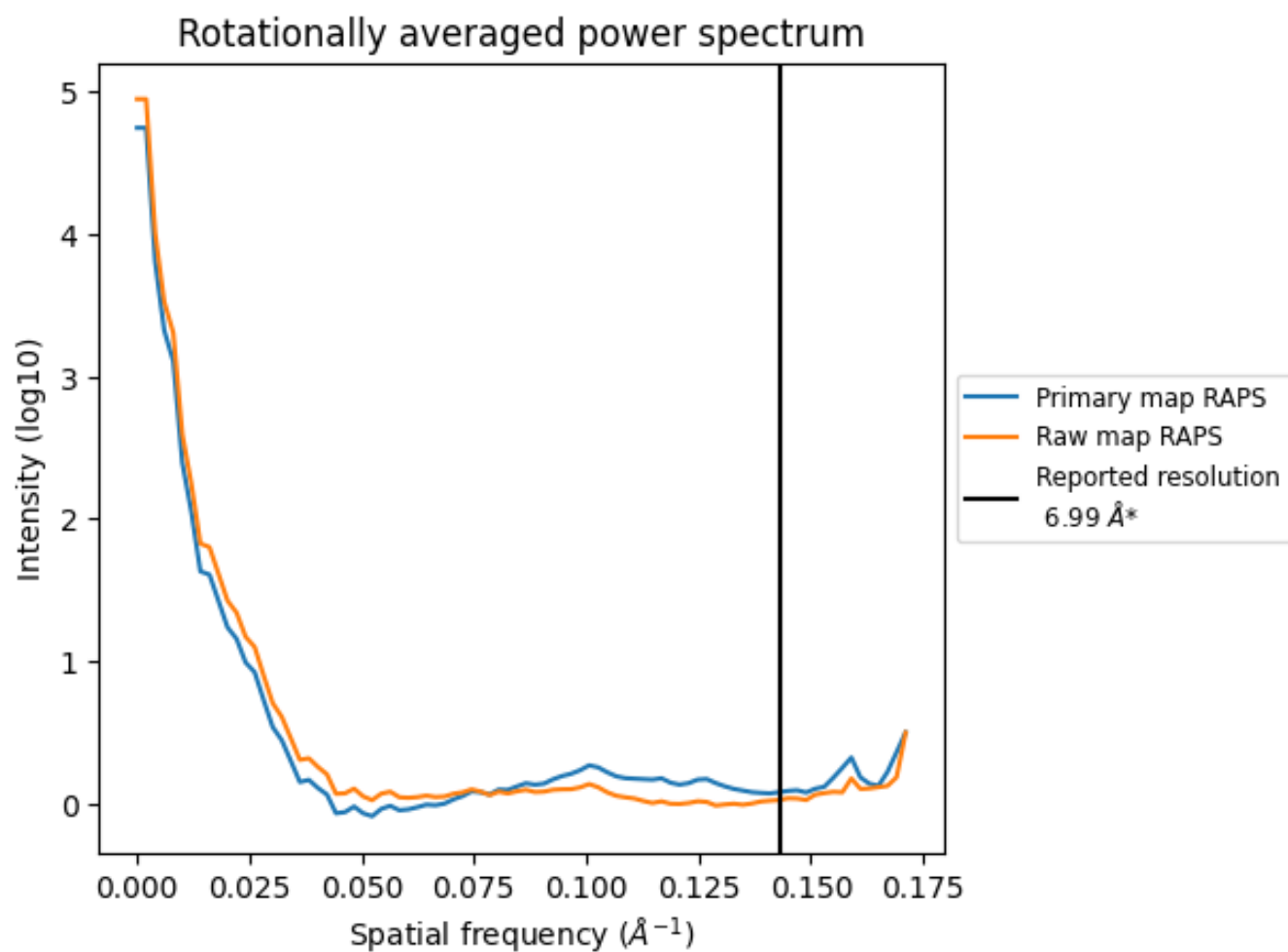
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2199 nm³; this corresponds to an approximate mass of 1987 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

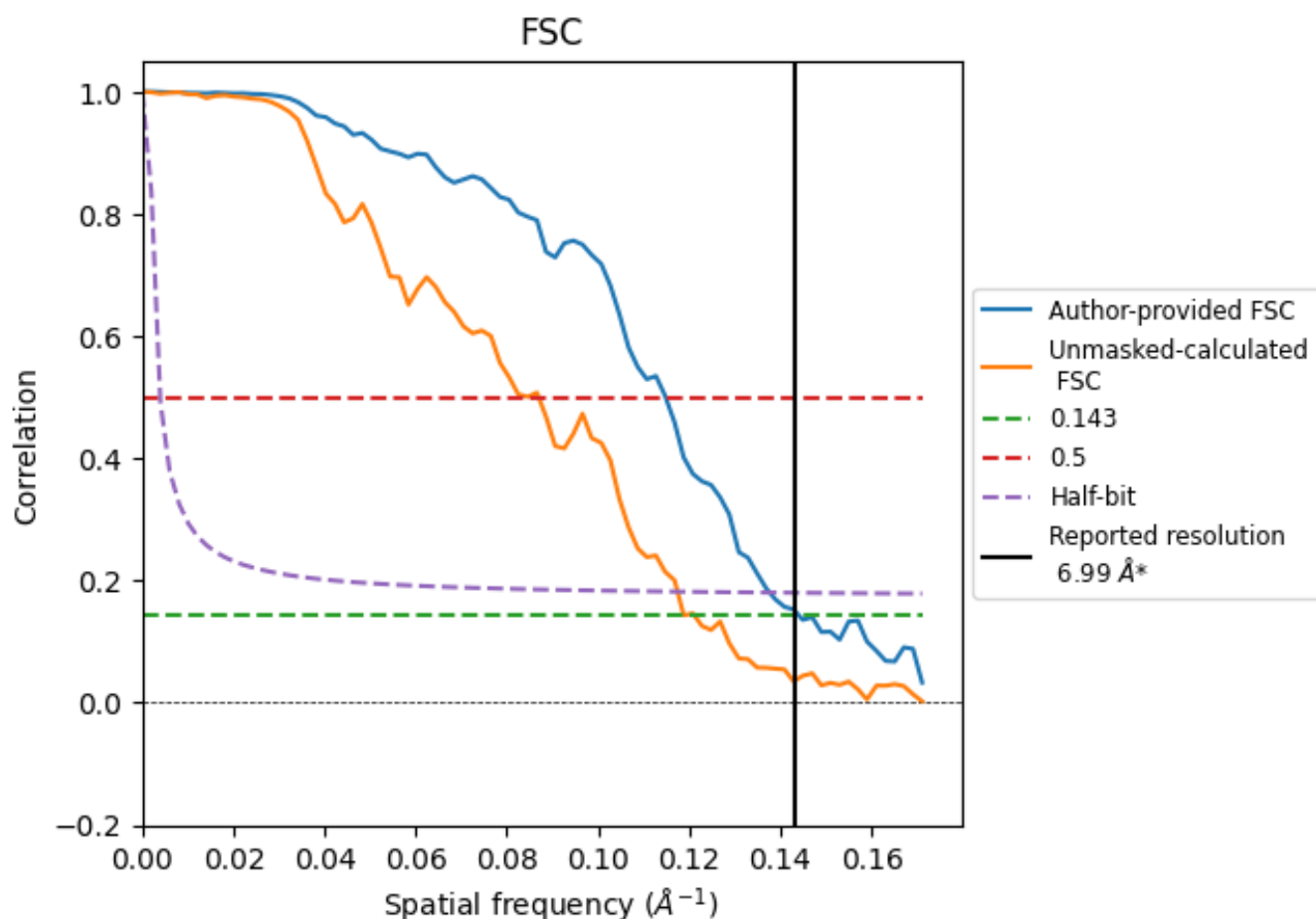


*Reported resolution corresponds to spatial frequency of 0.143 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.143 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

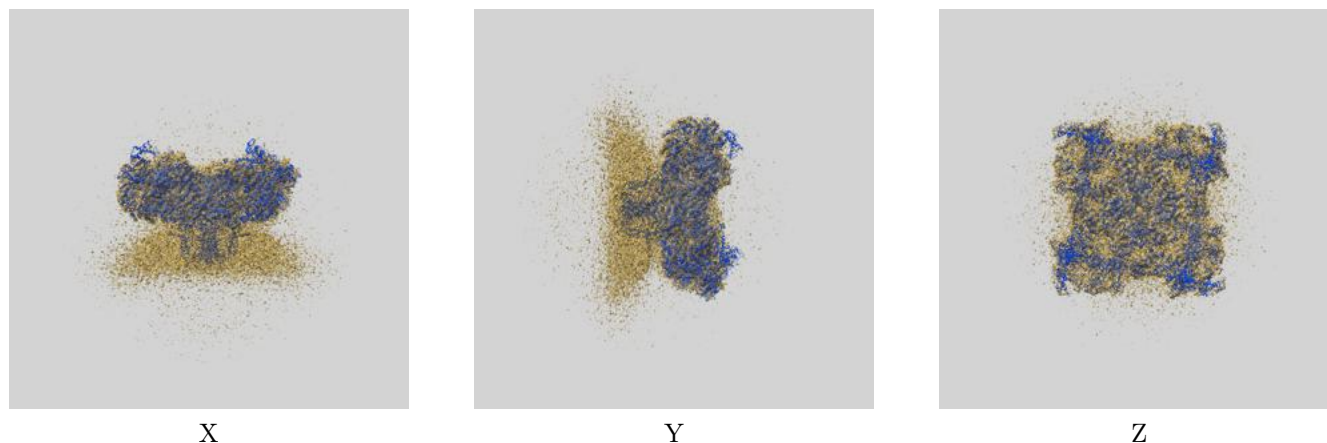
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.99	-	-
Author-provided FSC curve	6.94	8.70	7.26
Unmasked-calculated*	8.42	11.51	8.52

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.42 differs from the reported value 6.99 by more than 10 %

9 Map-model fit [i](#)

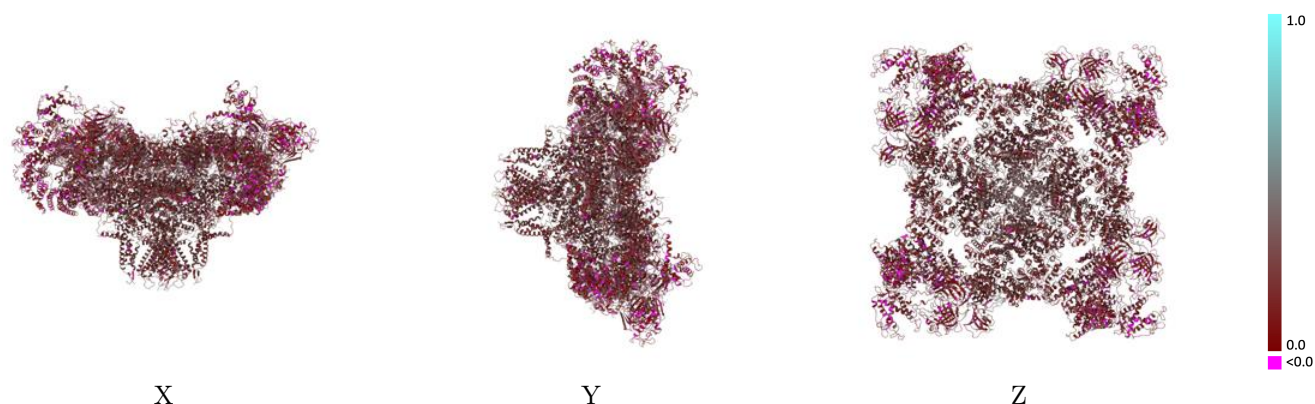
This section contains information regarding the fit between EMDB map EMD-54595 and PDB model 9S5E. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



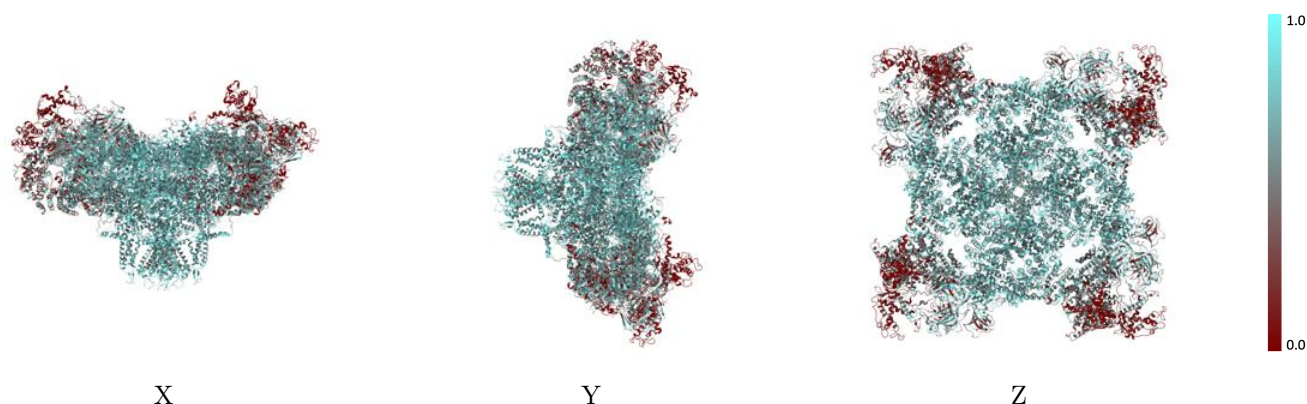
The images above show the 3D surface view of the map at the recommended contour level 0.105 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



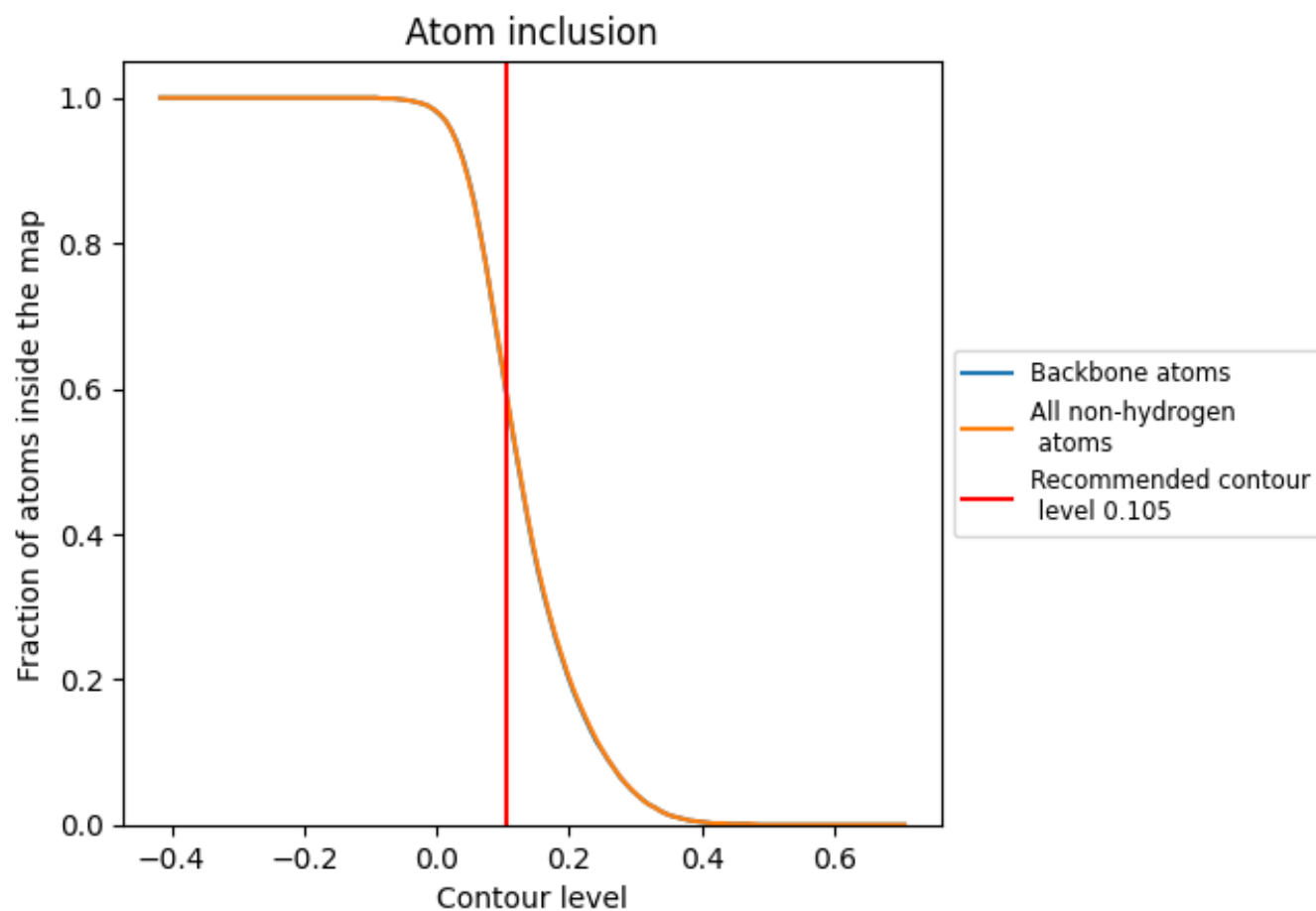
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.105).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 60% 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 (0.105) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5960	0.2300
A	0.6050	0.2310
B	0.6070	0.2300
C	0.6080	0.2300
D	0.6080	0.2310
E	0.4820	0.2010
F	0.4750	0.1990
G	0.4860	0.1990
H	0.4680	0.2020

