



Full wwPDB EM Validation Report ⓘ

Sep 29, 2025 – 12:06 PM EDT

PDB ID : 9NMP / pdb_00009nmp
EMDB ID : EMD-49536
Title : Structure of mouse RyR1 with simvastatin (Ca²⁺/CFF/ATP dataset; open pore)
Authors : Weninger, G.; Marks, A.R.
Deposited on : 2025-03-04
Resolution : 3.09 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

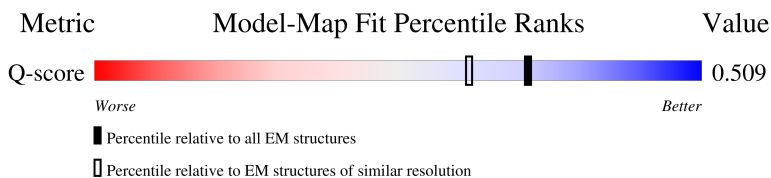
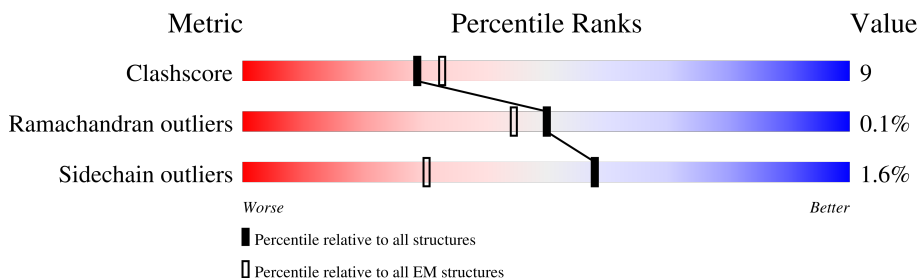
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.09 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14003 (2.59 - 3.59)

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	E	108	
1	F	108	
1	G	108	
1	H	108	

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Mol	Chain	Length	Quality of chain
2	A	5035	<div><div>10%</div><div><div></div><div>72%</div><div>14%</div><div>•</div><div>13%</div></div></div>
2	B	5035	<div><div>10%</div><div><div></div><div>72%</div><div>14%</div><div>•</div><div>13%</div></div></div>
2	C	5035	<div><div>10%</div><div><div></div><div>72%</div><div>14%</div><div>•</div><div>13%</div></div></div>
2	D	5035	<div><div>10%</div><div><div></div><div>72%</div><div>14%</div><div>•</div><div>13%</div></div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 143492 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	107	Total	C	N	O	S	0	0
			830	526	146	155	3		
1	F	107	Total	C	N	O	S	0	0
			830	526	146	155	3		
1	G	107	Total	C	N	O	S	0	0
			830	526	146	155	3		
1	H	107	Total	C	N	O	S	0	0
			830	526	146	155	3		

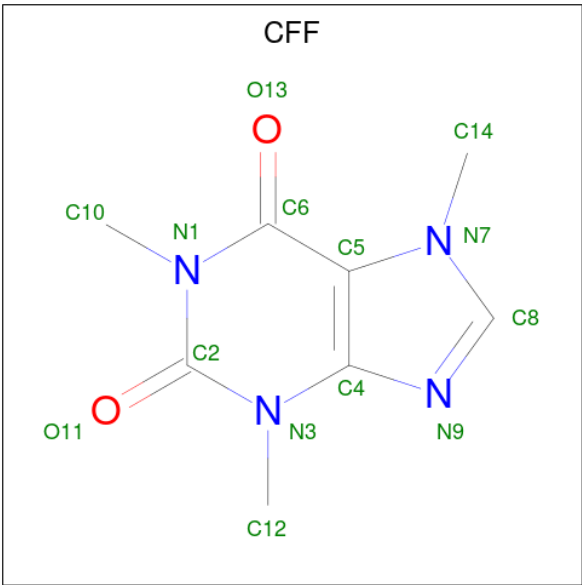
- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		
2	A	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		
2	B	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		
2	C	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

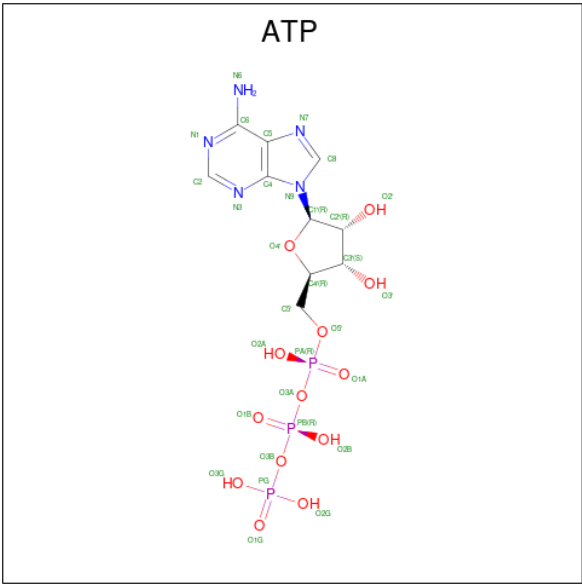
Mol	Chain	Residues	Atoms		AltConf
3	D	1	Total	Zn	0
			1	1	
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: C₈H₁₀N₄O₂).



Mol	Chain	Residues	Atoms				AltConf
4	D	1	Total	C	N	O	0
			14	8	4	2	
4	A	1	Total	C	N	O	0
			14	8	4	2	
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	C	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

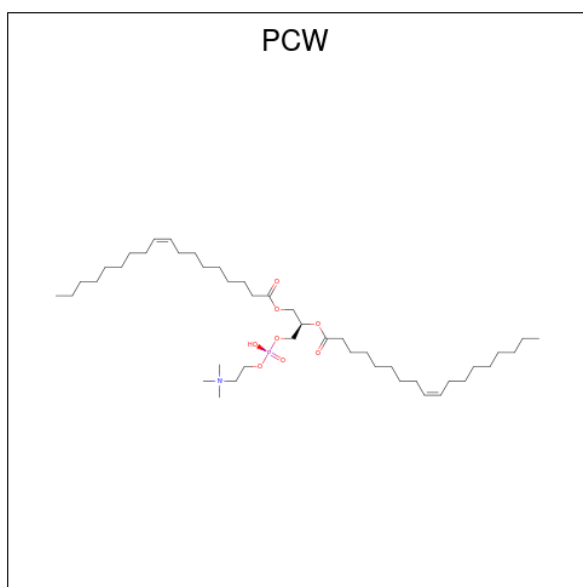


Mol	Chain	Residues	Atoms					AltConf
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

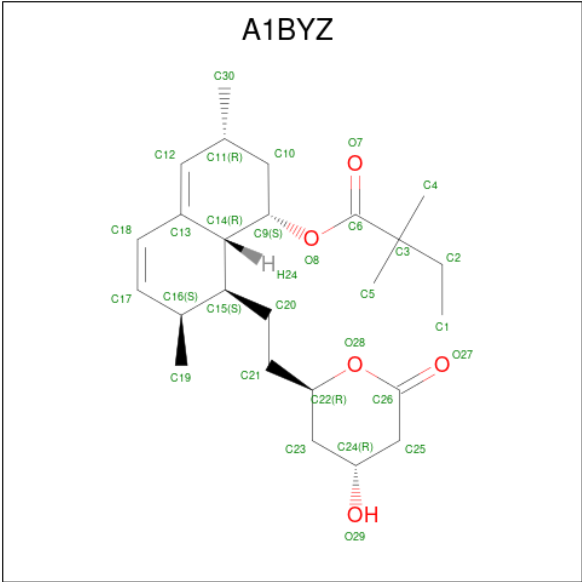
Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total	Ca	0
			1	1	
6	A	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	C	1	Total	Ca	0
			1	1	

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C₄₄H₈₅NO₈P).



Mol	Chain	Residues	Atoms					AltConf
7	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	C	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 8 is (1S,3R,7S,8S,8aR)-8-{2-[(2R,4R)-4-hydroxy-6-oxooxan-2-yl]ethyl}-3,7-dimethyl-1,2,3,7,8,8a-hexahydronaphthalen-1-yl 2,2-dimethylbutanoate (CCD ID: A1BYZ) (formula: C₂₅H₃₈O₅) (labeled as "Ligand of Interest" by depositor).




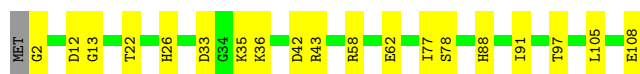
Mol	Chain	Residues	Atoms			AltConf
8	D	1	Total	C	O	0
			30	25	5	
8	D	1	Total	C	O	0
			30	25	5	
8	A	1	Total	C	O	0
			30	25	5	
8	A	1	Total	C	O	0
			30	25	5	
8	B	1	Total	C	O	0
			30	25	5	
8	B	1	Total	C	O	0
			30	25	5	
8	C	1	Total	C	O	0
			30	25	5	
8	C	1	Total	C	O	0
			30	25	5	

3 Residue-property plots [i](#)


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

- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain E: 




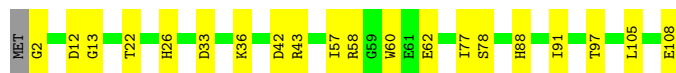
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F: 




- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain G: 




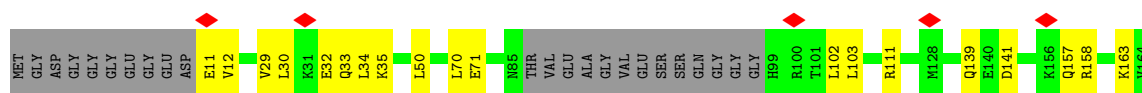
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

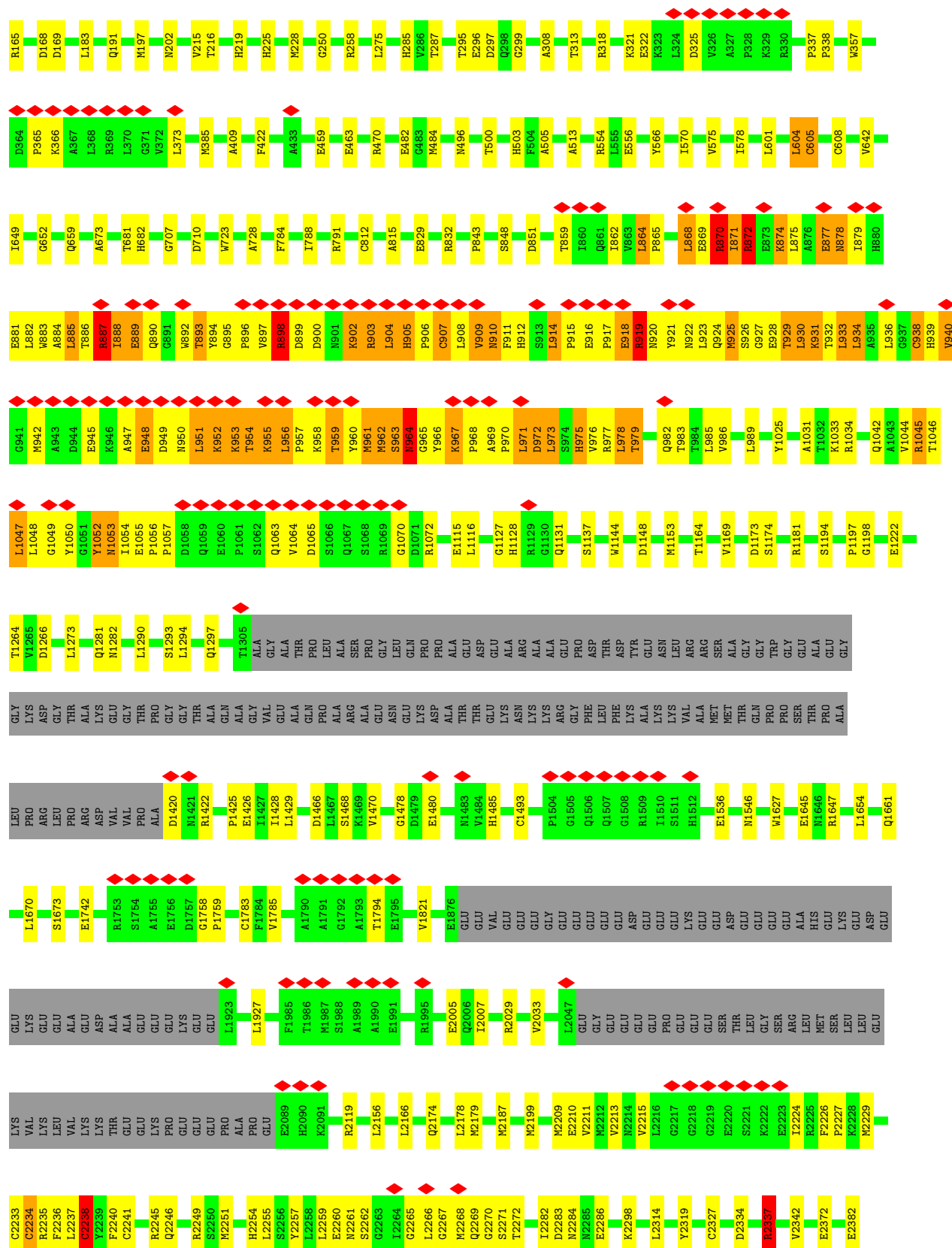
Chain H: 



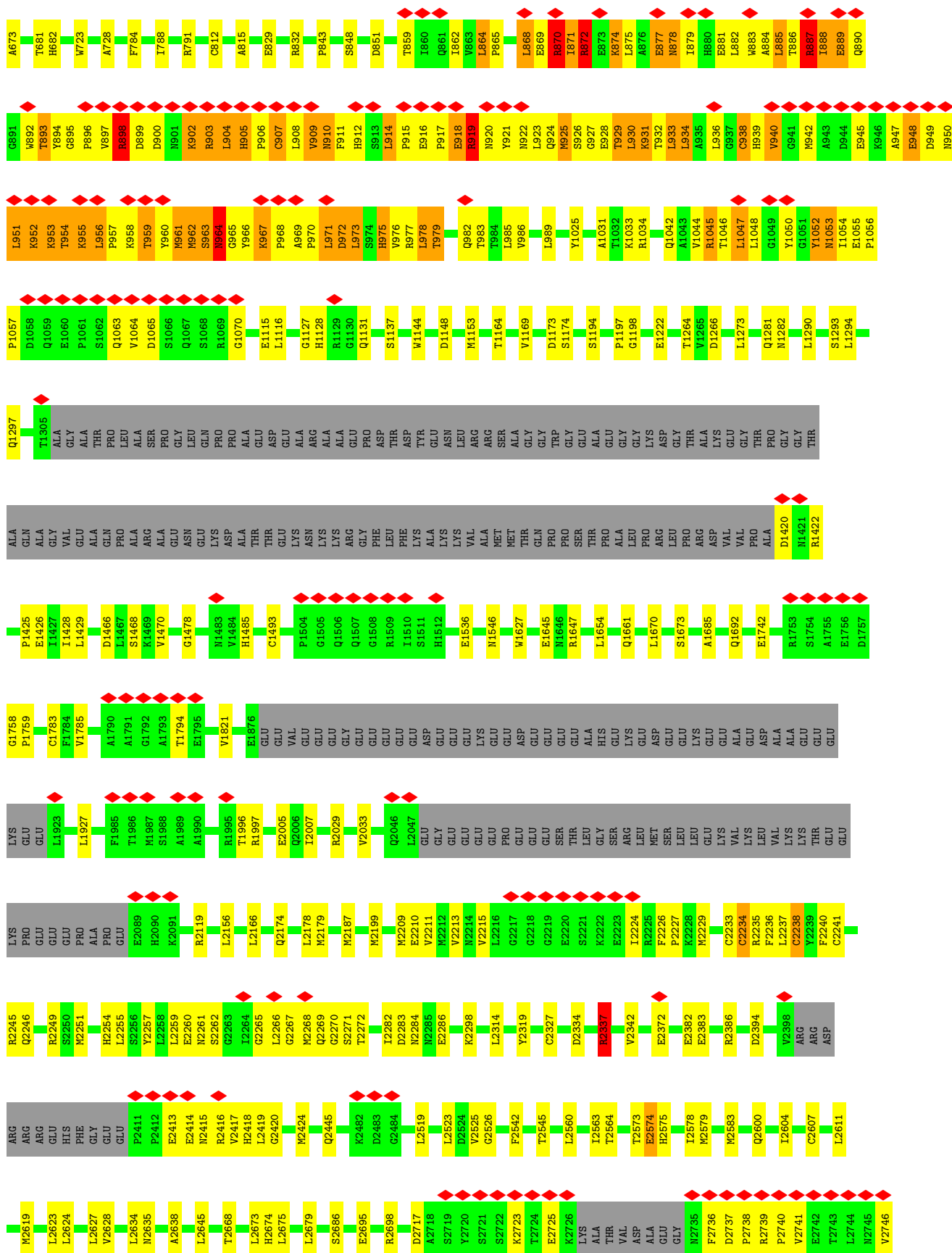
- Molecule 2: Ryanodine receptor 1

Chain D: 

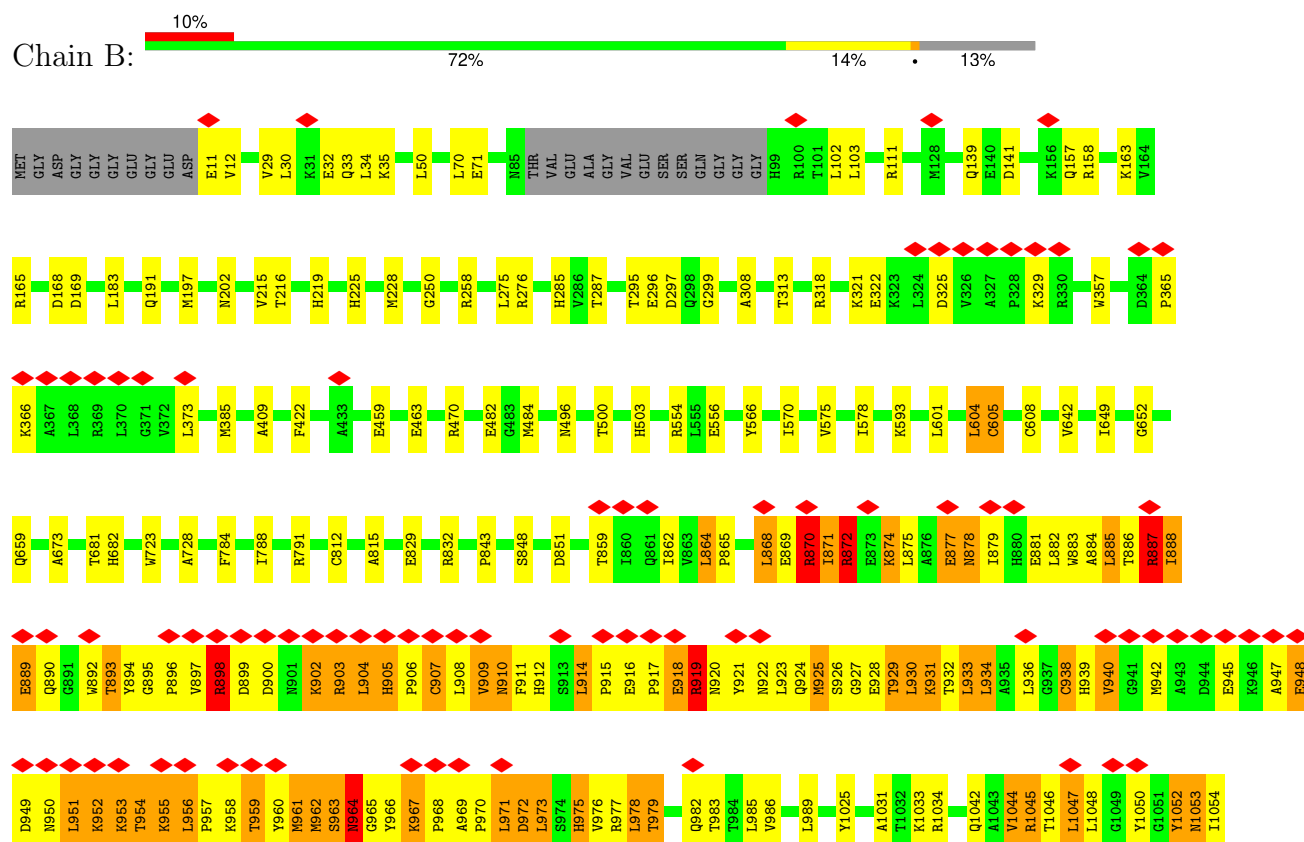








S4055	L3859	D3672	V3580	L3406	T3309	C3166	V3025	L2927	T2867	12747
S4056	G3860	E3683	F3581	L3409	S3310	L3170	L3026	L2928	L2868	12748
D4086	M3861	E3684	G3582	Y3410	D3311	L3177	G3027	K2929	W2808	P2749
F4087	N3862	Q3685	R3583	P3411	H3312	G3176	K3035	F2930	E2750	E2750
R4088	N3863	E3685	E3584	L3412	G3313	G3177	T3041	L2931	K2751	K2751
G4089	E3864	E3686	E3585	L3413	N3319	T3178	T3041	Q2932	L2752	D2753
L4090	E3865	E3687	E3586	L3414	N3319	T3179	T3041	M2933	D2753	D2753
D4095	D3865	E3688	E3587	R3415	R3322	N3181	V3055	N2934	S2754	S2754
F4096	T3867	E3689	A3587	E3434	I3323	N3182	S3056	G2935	F2755	F2755
M4100	V3868	E3690	D3588	L3435	I3324	Y3183	L3057	Y2936	K2815	K2815
E4122	I3869	V3691	E3591	M3438	D3331	V3184	D3061	A2937	M2817	M2817
E4129	N3870	E3692	F3592	V3439	K3337	L3195	A3062	V2938	L2818	L2818
N4133	R3871	E3693	I3593	G3440	K3337	L3198	P3063	T2939	W2758	W2758
I4142	Q3872	L3711	R3595	F3443	V3341	L3198	D3077	R2940	F2759	F2759
D3881	N3873	T3712	R3596	L3444	P3203	N3202	R3077	G2941	A2760	A2760
E3882	G3874	E3713	V3597	Y3445	Q3344	P3203	R3079	L2942	E2761	E2761
I3884	D3882	D3720	Q3598	W3446	V3204	V3204	T3080	K2943	Y2762	Y2762
E3885	E3882	H3735	M3518	S3449	V3347	Y3220	V3081	D2944	T2763	T2763
E3886	E3882	E3736	N3524	K3453	V3347	Y3220	M3082	M2945	H2764	H2764
E3887	E3882	E3737	M3525	R3454	L3354	R3226	K3083	E2946	E2765	E2765
E3888	E3882	E3737	T3529	R3454	L3355	R3226	I3088	L2947	K2766	K2766
E3889	E3882	E3737	D3530	E3455	R3356	R3226	E3105	D2948	A2768	A2768
E3890	E3882	E3737	Q3531	E3456	S3357	R3226	E3106	K2949	F2769	F2769
E3891	E3882	E3737	D3532	E3464	I3360	V3237	M3107	K2890	D2770	D2770
E3892	E3882	E3737	L3533	E3465	P3361	E3238	V3108	K2891	K2771	K2771
E3893	E3882	E3737	T3534	E3466	L3366	E3239	N3109	Q2893	L2772	L2772
E3894	E3882	E3737	Y3535	E3467	L3366	E3239	N3110	E2894	Q2773	Q2773
E3895	E3882	E3737	L3536	E3468	V3373	E3240	L3111	L2895	W2774	W2774
E3896	E3882	E3737	R3540	E3469	E3377	V3246	L3113	E2896	W2775	W2775
E3897	E3882	E3737	A3541	S3469	E3378	L3247	GLY	A2897	L2776	L2776
E3898	E3882	E3737	A3542	F3470	Q3379	L3247	LYS	K2897	S2777	S2777
E3899	E3882	E3737	L3543	L3471	L3380	M3267	VAL	Q2972	Y2778	Y2778
E3900	E3882	E3737	T3546	L3472	R3381	P3268	GLN	E2973	G2779	G2779
E3901	E3882	E3737	D3547	T3472	R3382	H3269	ALA	Q2974	L2780	L2780
E3902	E3882	E3737	R3551	ALA	R3383	R3284	ARG	L2975	E2781	E2781
E3903	E3882	E3737	E3552	ASP	E3384	M3265	THR	S2902	W2782	W2782
E3904	E3882	E3737	F3553	ASN	K3385	E3291	GLN	H2977	L2783	L2783
E3905	E3882	E3737	R3554	LYS	A3386	A3292	VAL	E2979	E2784	E2784
E3906	E3882	E3737	N3556	LYS	A3387	P3293	K3124	L2980	E2785	E2785
E3907	E3882	E3737	N3557	LYS	E3388	P3294	G3125	L2906	L2786	L2786
E3908	E3882	E3737	L3550	ALA	E3389	P3295	V3126	Y2907	L2787	L2787
E3909	E3882	E3737	Q3561	ALA	E3390	A3296	L3130	P2908	ASP	ASP
E3910	E3882	E3737	G3562	GLY	E3391	A3296	L3130	Y2909	K2787	K2787
E3911	E3882	E3737	K3563	ASP	G3391	L3297	T3133	D2910	T2788	T2788
E3912	E3882	E3737	V3564	VAL	E3392	P3298	T3133	Q2985	H2789	H2789
E3913	E3882	E3737	E3565	GLN	E3392	A3299	D3156	L2911	P2790	P2790
E3914	E3882	E3737	S3567	SER	E3393	G3300	V3164	R2986	L2791	L2791
E3915	E3882	E3737	L3570	GLY	V3395	A3301	D3160	V2987	L2792	L2792
E3916	E3882	E3737	M3574	GLY	R3396	A3301	V3164	E2988	R2793	R2793
E3917	E3882	E3737	E3574	ASP	F3399	A3301	S3165	K2989	P2794	P2794
E3918	E3882	E3737	E3574	GLN	C3403	T3306	S3165	E2990	Y2856	Y2856
E3919	E3882	E3737	E3574	GLU	E3403	T3306	S3165	E2990	N2857	N2857
E3920	E3882	E3737	E3574	GLU	E3403	T3306	S3165	E2990	Q2859	Q2859
E3921	E3882	E3737	E3574	GLU	E3403	T3306	S3165	E2990	P2860	P2860
E3922	E3882	E3737	E3574	GLU	E3403	T3306	S3165	E2990	P2861	P2861
E3923	E3882	E3737	E3574	GLU	E3403	T3306	S3165	E2990	D2862	D2862
E3924	E3882	E3737	E3574	GLU	E3403	T3306	S3165	E2990	L2863	L2863
E3925	E3882	E3737	E3574	GLU	E3403	T3306	S3165	E2990	F2798	F2798
E3926	E3882	E3737	E3574	GLU	E3403	T3306	S3165	E2990	S2799	S2799
E3927	E3882	E3737	E3574	GLU	E3403	T3306	S3165	E2990	E2800	E2800
E3928	E3882	E3737	E3574	GLU	E3403	T3306	S3165	E2990	K2801	K2801
E3929	E3882	E3737	E3574	GLU	E3403	T3306	S3165	E2990	D2802	D2802
E3930	E3882	E3737	E3574	GLU	E3403	T3306	S3165	E2990	K2803	K2803
E3931	E3882	E3737	E3574	GLU	E3403	T3306	S3165	E2990	E2804	E2804
E3932	E3882	E3737	E3574	GLU	E3403	T3306	S3165	E2990	E2805	E2805
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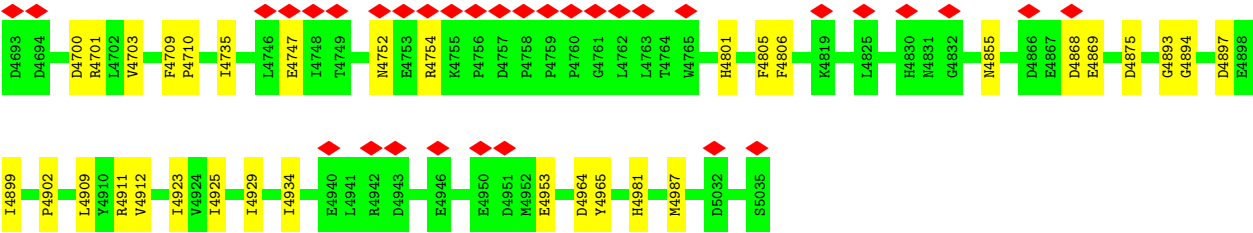


D2862	L2863	S2864	V2865	V2866	T2867	L2868	S2869	R2870	E2871	L2872	Q2873	A2874	N2875	A2876	E2877	Q2878	L2879	A2880	E2881	N2882	T2883	H2884	N2885	T2886	Q2887	Q2888	R2889	K2890	K2891	K2892	Q2893	E2894	L2895	E2896	A2897	K2898	G2899	G2900	G2901	S2902	H2903	P2904	L2905	L2906	V2907	P2908	Y2909	D2910	T2911	L2912	T2913	A2914	K2915	K2916	K2917	A2918	R2919	D2920	R2921																																																																																																																																																																																																																																																																																																																																																																																																																											
D2802	K2803	E2804	L2805	Y2806	L2807	L2808	P2809	L2810	K2811	E2812	S2813	L2814	K2815	A2816	M2817	L2818	A2819	W2820	E2821	W2822	T2823	V2824	E2825	K2826	A2827	R2828	E2829	G2830	E2831	GLU	GLU	LYS	THR	GLU	LYS	LYS	LYS	THR	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	THR	ASP	PRO	ARG	GLU	GLY	Y2856	N2857	P2858	Q2859	P2860	P2861																																																																																																																																																																																																																																																																																																																																																																																																																										
E2742	T2743	L2744	N2745	V2746	L2747	L2748	P2749	E2750	K2751	L2752	D2753	S2754	F2755	L2756	N2757	K2758	F2759	A2760	E2761	Y2762	T2763	H2764	E2765	K2766	Q2767	A2768	F2769	D2770	K2771	L2772	Q2773	N2774	N2775	W2776	S2777	Y2778	G2779	E2780	N2781	L2782	D2783	E2784	E2785	L2786	K2787	T2788	H2789	P2790	M2791	L2792	R2793	P2794	Y2795	K2796	T2797	F2798	S2799	K2800																																																																																																																																																																																																																																																																																																																																																																																																																												
L2604	C2607	L2611	M2619	L2623	L2624	L2627	V2628	L2634	N2635	A2638	L2645	T2668	L2673	H2674	L2675	L2679	S2686	E2695	R2698	D2717	A2718	S2719	Y2720	S2721	K2723	T2724	E2725	K2726	LYS	ALA	THR	VAL	ASP	ALA	GLU	GLY	N2735	F2736	D2737	P2738	R2739	P2740	V2741																																																																																																																																																																																																																																																																																																																																																																																																																																											
R2370	G2371	G2372	E2382	E2383	R2386	D2394	V2398	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	GLU	P2411	P2412	E2413	E2414	N2415	R2416	V2417	H2418	L2419	Q2445	D2483	G2484	L2519	L2523	V2525	G2526	L2560	I2563	T2564	T2573	E2574	H2575	M2583	Q2600																																																																																																																																																																																																																																																																																																																																																																																																																																											
K2228	M2229	C2233	C2234	R2235	F2236	L2237	C2238	F2239	F2240	C2241	R2245	Q2246	R2249	S2250	M2251	H2254	L2255	S2256	Y2257	L2258	L2259	E2260	N2261	S2262	G2263	T2264	L2266	Q2269	G2270	S2271	T2272	D2282	D2283	N2284	V2285	E2286	K2298	L2314	Y2319	C2327	D2334	V2337	V2342																																																																																																																																																																																																																																																																																																																																																																																																																																											
LYS	VAL	LEU	VAL	LYS	LYS	THR	GLU	GLU	LYS	PRO	GLU	GLU	PRO	ALA	PRO	GLU	E2089	H2090	K2091	R2119	L2156	L2166	Q2174	L2178	M2179	M2186	M2187	M2199	M2204	M2209	E2210	V2211	M2212	V2213	V2215	L2216	G2217	Q2218	G2219	E2220	S2221	K2222	E2223	R2225	F2226	P2227																																																																																																																																																																																																																																																																																																																																																																																																																																								
GLU	GLU	ALA	GLU	ASP	ALA	ALA	GLU	GLU	LYS	GLU	L1923	L1927	F1985	T1986	M1987	S1988	A1989	A1990	E1991	R1995	T1996	R1997	E2005	Q2006	I2007	R2029	V2033	L2047	GLU	GLY	GLU	GLU	GLU	GLU	PRO	GLU	GLU	SER	THR	LEU	GLY	SER	ARG	LEU	MET	SER	LEU	GLU	GLU																																																																																																																																																																																																																																																																																																																																																																																																																																					
ASP	VAL	VAL	PRO	ALA	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1469	V1470	G1478	D1479	E1480	N1483	V1484	H1485	C1493	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	E1536	N1546	E1584	W1627	E1645	R1647	L1654	Q1661	L1670	S1673																																																																																																																																																																																																																																																																																																																																																																																																																																													
LYS	GLU	GLY	THR	PRO	GLY	GLY	THR	ALA	GLY	VAL	GLU	ALA	THR	PRO	GLN	ALA	ALA	SER	PRO	GLY	ASN	GLU	LYS	ASP	PRO	ALA	THR	ASP	GLU	LYS	ALA	ASN	ARG	LYS	ALA	GLU	ARG	MET	GLY	THR	GLN	PRO	PRO	SER	THR	PRO	ALA	GLY	GLY	PRO	ARG	LEU	PRO	THR	ALA																																																																																																																																																																																																																																																																																																																																																																																																																															
Q1281	N1282	L1290	S1293	L1294	P1297	T1305	ALA	GLY	VAL	GLU	ALA	THR	PRO	LEU	ALA	ALA	SER	PRO	GLY	ASN	GLN	PRO	PRO	ALA	ALA	THR	ASP	GLU	LYS	ALA	ASN	ARG	LYS	ALA	GLU	TYR	ASP	THR	ASP	LEU	PHE	THR	PRO	TRP	GLY	GLY	GLU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY</









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25791	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 ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.628	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	424.448, 424.448, 424.448	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1BYZ, CA, PCW, CFF, ZN, ATP

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	E	0.24	0/848	0.40	0/1143
1	F	0.25	0/848	0.40	0/1143
1	G	0.25	0/848	0.41	0/1143
1	H	0.24	0/848	0.40	0/1143
2	A	0.29	0/35586	0.47	13/48203 (0.0%)
2	B	0.29	0/35586	0.47	14/48203 (0.0%)
2	C	0.29	0/35586	0.47	13/48203 (0.0%)
2	D	0.29	0/35586	0.47	13/48203 (0.0%)
All	All	0.29	0/145736	0.47	53/197384 (0.0%)

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
2	A	0	10
2	B	0	10
2	C	0	10
2	D	0	10
All	All	0	40

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2238	CYS	CA-CB-SG	9.57	136.40	114.40
2	B	2238	CYS	CA-CB-SG	9.57	136.40	114.40
2	C	2238	CYS	CA-CB-SG	9.57	136.40	114.40
2	A	2238	CYS	CA-CB-SG	9.55	136.37	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3241	CYS	CA-CB-SG	7.71	132.13	114.40
2	B	3241	CYS	CA-CB-SG	7.71	132.13	114.40
2	C	3241	CYS	CA-CB-SG	7.71	132.13	114.40
2	A	3241	CYS	CA-CB-SG	7.71	132.12	114.40
2	A	1052	TYR	N-CA-CB	7.00	120.27	109.85
2	B	1052	TYR	N-CA-CB	6.97	120.24	109.85
2	D	1052	TYR	N-CA-CB	6.96	120.22	109.85
2	C	1052	TYR	N-CA-CB	6.96	120.22	109.85
2	A	2233	CYS	CA-C-N	-6.61	108.92	121.54
2	A	2233	CYS	C-N-CA	-6.61	108.92	121.54
2	C	2233	CYS	CA-C-N	-6.60	108.93	121.54
2	C	2233	CYS	C-N-CA	-6.60	108.93	121.54
2	D	2233	CYS	CA-C-N	-6.60	108.93	121.54
2	D	2233	CYS	C-N-CA	-6.60	108.93	121.54
2	B	2233	CYS	CA-C-N	-6.60	108.93	121.54
2	B	2233	CYS	C-N-CA	-6.60	108.93	121.54
2	D	604	LEU	CA-C-N	-6.49	113.13	122.67
2	D	604	LEU	C-N-CA	-6.49	113.13	122.67
2	B	604	LEU	CA-C-N	-6.49	113.13	122.67
2	B	604	LEU	C-N-CA	-6.49	113.13	122.67
2	C	604	LEU	CA-C-N	-6.49	113.13	122.67
2	C	604	LEU	C-N-CA	-6.49	113.13	122.67
2	A	604	LEU	CA-C-N	-6.47	113.16	122.67
2	A	604	LEU	C-N-CA	-6.47	113.16	122.67
2	D	2234	CYS	N-CA-CB	6.40	121.31	110.49
2	C	2234	CYS	N-CA-CB	6.40	121.31	110.49
2	B	2234	CYS	N-CA-CB	6.39	121.28	110.49
2	A	2234	CYS	N-CA-CB	6.38	121.27	110.49
2	D	2238	CYS	CB-CA-C	6.11	119.82	109.55
2	B	2238	CYS	CB-CA-C	6.11	119.82	109.55
2	C	2238	CYS	CB-CA-C	6.11	119.82	109.55
2	A	2238	CYS	CB-CA-C	6.11	119.81	109.55
2	D	2234	CYS	CA-CB-SG	5.84	127.82	114.40
2	C	2234	CYS	CA-CB-SG	5.84	127.82	114.40
2	A	2234	CYS	CA-CB-SG	5.83	127.81	114.40
2	B	2234	CYS	CA-CB-SG	5.83	127.82	114.40
2	C	964	ASN	N-CA-C	-5.82	105.02	111.71
2	D	964	ASN	N-CA-C	-5.79	105.06	111.71
2	B	964	ASN	N-CA-C	-5.79	105.06	111.71
2	A	964	ASN	N-CA-C	-5.78	105.07	111.71
2	A	2238	CYS	N-CA-CB	-5.55	102.49	110.65
2	D	2238	CYS	N-CA-CB	-5.53	102.53	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2238	CYS	N-CA-CB	-5.53	102.53	110.65
2	B	2238	CYS	N-CA-CB	-5.50	102.56	110.65
2	B	2238	CYS	N-CA-C	-5.13	107.05	113.72
2	D	2238	CYS	N-CA-C	-5.12	107.06	113.72
2	A	2238	CYS	N-CA-C	-5.12	107.06	113.72
2	C	2238	CYS	N-CA-C	-5.12	107.06	113.72
2	B	1044	VAL	N-CA-C	-5.01	105.66	110.72

There are no chirality outliers.

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	1045	ARG	Sidechain
2	A	2238	CYS	Peptide
2	A	2337	ARG	Sidechain
2	A	605	CYS	Peptide
2	A	870	ARG	Sidechain
2	A	872	ARG	Sidechain
2	A	887	ARG	Sidechain
2	A	898	ARG	Sidechain
2	A	903	ARG	Sidechain
2	A	919	ARG	Sidechain
2	B	1045	ARG	Sidechain
2	B	2238	CYS	Peptide
2	B	2337	ARG	Sidechain
2	B	605	CYS	Peptide
2	B	870	ARG	Sidechain
2	B	872	ARG	Sidechain
2	B	887	ARG	Sidechain
2	B	898	ARG	Sidechain
2	B	903	ARG	Sidechain
2	B	919	ARG	Sidechain
2	C	1045	ARG	Sidechain
2	C	2238	CYS	Peptide
2	C	2337	ARG	Sidechain
2	C	605	CYS	Peptide
2	C	870	ARG	Sidechain
2	C	872	ARG	Sidechain
2	C	887	ARG	Sidechain
2	C	898	ARG	Sidechain
2	C	903	ARG	Sidechain
2	C	919	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	D	1045	ARG	Sidechain
2	D	2238	CYS	Peptide
2	D	2337	ARG	Sidechain
2	D	605	CYS	Peptide
2	D	870	ARG	Sidechain
2	D	872	ARG	Sidechain
2	D	887	ARG	Sidechain
2	D	898	ARG	Sidechain
2	D	903	ARG	Sidechain
2	D	919	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	E	830	0	828	16	0
1	F	830	0	828	15	0
1	G	830	0	828	16	0
1	H	830	0	828	16	0
2	A	34797	0	34382	638	0
2	B	34797	0	34382	643	0
2	C	34797	0	34382	644	0
2	D	34797	0	34382	642	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	14	0	10	0	0
4	B	14	0	10	0	0
4	C	14	0	10	0	0
4	D	14	0	10	0	0
5	A	62	0	24	1	0
5	B	62	0	24	1	0
5	C	62	0	24	1	0
5	D	62	0	24	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1	0	0	0	0
7	A	108	0	168	5	0
7	B	108	0	168	5	0
7	C	108	0	168	5	0
7	D	108	0	168	5	0
8	A	60	0	0	2	0
8	B	60	0	0	3	0
8	C	60	0	0	3	0
8	D	60	0	0	2	0
All	All	143492	0	141648	2626	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 9.

All (2626) 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)
2:B:899:ASP:HB3	2:B:902:LYS:HB2	1.30	1.10
2:A:899:ASP:HB3	2:A:902:LYS:HB2	1.30	1.09
2:D:899:ASP:HB3	2:D:902:LYS:HB2	1.30	1.08
2:C:899:ASP:HB3	2:C:902:LYS:HB2	1.30	1.08
1:H:2:GLY:N	1:H:78:SER:HG	1.55	1.03
1:F:2:GLY:N	1:F:78:SER:HG	1.53	1.03
2:C:2156:LEU:HD21	2:C:2199:MET:HE1	1.42	1.01
2:A:2156:LEU:HD21	2:A:2199:MET:HE1	1.42	0.99
2:B:879:ILE:HA	2:B:882:LEU:HD12	1.44	0.99
2:B:902:LYS:HB3	2:B:904:LEU:HG	1.45	0.99
2:C:879:ILE:HA	2:C:882:LEU:HD12	1.45	0.99
2:A:902:LYS:HB3	2:A:904:LEU:HG	1.45	0.98
2:B:2156:LEU:HD21	2:B:2199:MET:HE1	1.42	0.97
2:A:879:ILE:HA	2:A:882:LEU:HD12	1.45	0.97
2:C:902:LYS:HB3	2:C:904:LEU:HG	1.45	0.97
2:D:902:LYS:HB3	2:D:904:LEU:HG	1.45	0.97
2:D:2156:LEU:HD21	2:D:2199:MET:HE1	1.42	0.97
2:D:879:ILE:HA	2:D:882:LEU:HD12	1.44	0.97
2:D:3529:THR:HG23	2:D:3574:MET:HE3	1.47	0.97
2:B:2215:VAL:HG11	2:B:2229:MET:HE1	1.48	0.96
2:C:3529:THR:HG23	2:C:3574:MET:HE3	1.47	0.95
2:C:2215:VAL:HG11	2:C:2229:MET:HE1	1.48	0.95
2:A:3529:THR:HG23	2:A:3574:MET:HE3	1.47	0.95
2:A:2215:VAL:HG11	2:A:2229:MET:HE1	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2:GLY:N	1:G:78:SER:HG	1.64	0.94
2:B:3529:THR:HG23	2:B:3574:MET:HE3	1.47	0.93
2:D:2215:VAL:HG11	2:D:2229:MET:HE1	1.48	0.93
2:B:887:ARG:HG2	2:B:908:LEU:HD11	1.52	0.92
1:E:2:GLY:N	1:E:78:SER:HG	1.68	0.91
2:D:887:ARG:HG2	2:D:908:LEU:HD11	1.52	0.91
2:A:887:ARG:HG2	2:A:908:LEU:HD11	1.52	0.91
2:C:2766:LYS:NZ	2:C:2861:PRO:O	2.04	0.91
2:D:2912:LEU:O	2:D:2917:LYS:NZ	2.04	0.91
2:A:2766:LYS:NZ	2:A:2861:PRO:O	2.04	0.90
2:B:942:MET:HA	2:B:1052:TYR:HA	1.53	0.90
2:B:2766:LYS:NZ	2:B:2861:PRO:O	2.04	0.90
2:C:2912:LEU:O	2:C:2917:LYS:NZ	2.04	0.90
2:C:894:TYR:CG	2:C:964:ASN:HB3	2.07	0.90
2:C:887:ARG:HG2	2:C:908:LEU:HD11	1.52	0.90
2:D:2766:LYS:NZ	2:D:2861:PRO:O	2.04	0.89
2:A:2912:LEU:O	2:A:2917:LYS:NZ	2.04	0.89
2:B:902:LYS:HE3	2:B:904:LEU:HD21	1.55	0.89
2:A:942:MET:HA	2:A:1052:TYR:HA	1.53	0.89
2:B:2912:LEU:O	2:B:2917:LYS:NZ	2.04	0.89
2:D:894:TYR:CG	2:D:964:ASN:HB3	2.07	0.89
2:A:902:LYS:HE3	2:A:904:LEU:HD21	1.55	0.89
2:C:902:LYS:HE3	2:C:904:LEU:HD21	1.55	0.89
2:A:894:TYR:CG	2:A:964:ASN:HB3	2.07	0.88
2:B:894:TYR:CG	2:B:964:ASN:HB3	2.07	0.88
2:C:942:MET:HA	2:C:1052:TYR:HA	1.53	0.88
2:D:902:LYS:HE3	2:D:904:LEU:HD21	1.55	0.88
2:C:1131:GLN:NE2	2:C:1137:SER:OG	2.07	0.88
2:A:894:TYR:HB3	2:A:964:ASN:H	1.38	0.87
2:B:894:TYR:HB3	2:B:964:ASN:H	1.38	0.87
2:A:1131:GLN:NE2	2:A:1137:SER:OG	2.07	0.87
2:B:1131:GLN:NE2	2:B:1137:SER:OG	2.07	0.87
2:D:942:MET:HA	2:D:1052:TYR:HA	1.53	0.87
2:D:1131:GLN:NE2	2:D:1137:SER:OG	2.07	0.87
2:B:3525:MET:O	2:B:3596:ARG:NH2	2.09	0.86
2:C:3525:MET:O	2:C:3596:ARG:NH2	2.08	0.86
2:D:3525:MET:O	2:D:3596:ARG:NH2	2.09	0.85
2:A:956:LEU:HB2	2:A:967:LYS:HE2	1.59	0.85
2:C:894:TYR:HB3	2:C:964:ASN:H	1.38	0.85
2:D:894:TYR:HB3	2:D:964:ASN:H	1.38	0.85
2:B:956:LEU:HB2	2:B:967:LYS:HE2	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3525:MET:O	2:A:3596:ARG:NH2	2.09	0.85
2:D:829:GLU:OE2	2:D:832:ARG:NH1	2.11	0.84
2:B:3962:LYS:NZ	2:B:4021:ASP:OD2	2.11	0.84
2:D:956:LEU:HB2	2:D:967:LYS:HE2	1.59	0.84
2:C:956:LEU:HB2	2:C:967:LYS:HE2	1.59	0.84
2:D:2573:THR:O	2:D:2575:HIS:N	2.11	0.84
2:D:3962:LYS:NZ	2:D:4021:ASP:OD2	2.11	0.83
2:A:3962:LYS:NZ	2:A:4021:ASP:OD2	2.11	0.83
2:C:829:GLU:OE2	2:C:832:ARG:NH1	2.11	0.83
2:D:894:TYR:H	2:D:963:SER:H	1.26	0.83
2:A:2573:THR:O	2:A:2575:HIS:N	2.11	0.83
2:B:829:GLU:OE2	2:B:832:ARG:NH1	2.11	0.83
2:D:605:CYS:SG	2:D:1673:SER:OG	2.37	0.83
2:A:829:GLU:OE2	2:A:832:ARG:NH1	2.11	0.83
2:B:2573:THR:O	2:B:2575:HIS:N	2.11	0.83
2:C:2573:THR:O	2:C:2575:HIS:N	2.11	0.83
2:C:894:TYR:H	2:C:963:SER:H	1.26	0.83
2:C:3962:LYS:NZ	2:C:4021:ASP:OD2	2.11	0.83
2:A:605:CYS:SG	2:A:1673:SER:OG	2.37	0.83
2:C:3178:THR:O	2:C:3180:ARG:NH1	2.12	0.83
2:D:888:ILE:HD13	2:D:960:TYR:HA	1.60	0.83
2:D:1025:TYR:O	2:D:1033:LYS:NZ	2.12	0.83
2:A:888:ILE:HD13	2:A:960:TYR:HA	1.60	0.83
2:D:2209:MET:HE2	2:D:2251:MET:HE1	1.61	0.82
2:A:1025:TYR:O	2:A:1033:LYS:NZ	2.12	0.82
2:C:2209:MET:HE2	2:C:2251:MET:HE1	1.61	0.82
2:B:3178:THR:O	2:B:3180:ARG:NH1	2.12	0.82
2:A:2209:MET:HE2	2:A:2251:MET:HE1	1.61	0.82
2:C:605:CYS:SG	2:C:1673:SER:OG	2.37	0.82
2:A:3178:THR:O	2:A:3180:ARG:NH1	2.12	0.82
2:C:888:ILE:HD13	2:C:960:TYR:HA	1.60	0.82
2:B:605:CYS:SG	2:B:1673:SER:OG	2.37	0.82
2:C:2723:LYS:NZ	2:C:2725:GLU:OE1	2.13	0.82
2:D:3178:THR:O	2:D:3180:ARG:NH1	2.12	0.81
2:B:888:ILE:HD13	2:B:960:TYR:HA	1.60	0.81
2:D:2723:LYS:NZ	2:D:2725:GLU:OE1	2.13	0.81
2:C:1025:TYR:O	2:C:1033:LYS:NZ	2.12	0.81
2:A:2234:CYS:O	2:A:2235:ARG:C	2.23	0.81
2:B:894:TYR:H	2:B:963:SER:H	1.26	0.81
2:A:894:TYR:H	2:A:963:SER:H	1.26	0.81
2:B:1025:TYR:O	2:B:1033:LYS:NZ	2.12	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2209:MET:HE2	2:B:2251:MET:HE1	1.61	0.81
2:D:2234:CYS:O	2:D:2235:ARG:C	2.23	0.81
2:B:2723:LYS:NZ	2:B:2725:GLU:OE1	2.13	0.81
2:A:2723:LYS:NZ	2:A:2725:GLU:OE1	2.13	0.81
2:A:496:ASN:OD1	2:A:554:ARG:NH1	2.15	0.80
2:C:496:ASN:OD1	2:C:554:ARG:NH1	2.15	0.80
2:C:956:LEU:HD13	2:C:960:TYR:HB3	1.64	0.80
2:D:496:ASN:OD1	2:D:554:ARG:NH1	2.15	0.80
2:C:2234:CYS:O	2:C:2235:ARG:C	2.23	0.80
2:D:956:LEU:HD13	2:D:960:TYR:HB3	1.64	0.80
2:A:956:LEU:HD13	2:A:960:TYR:HB3	1.64	0.80
2:B:496:ASN:OD1	2:B:554:ARG:NH1	2.15	0.79
2:D:899:ASP:HB3	2:D:902:LYS:CB	2.12	0.79
2:B:956:LEU:HD13	2:B:960:TYR:HB3	1.64	0.79
2:B:2234:CYS:O	2:B:2235:ARG:C	2.23	0.79
2:C:899:ASP:HB3	2:C:902:LYS:CB	2.12	0.79
2:C:961:MET:HG3	2:C:965:GLY:HA2	1.65	0.79
2:D:961:MET:HG3	2:D:965:GLY:HA2	1.65	0.79
2:A:903:ARG:HH21	2:A:903:ARG:HA	1.47	0.79
2:B:961:MET:HG3	2:B:965:GLY:HA2	1.65	0.79
2:B:903:ARG:HA	2:B:903:ARG:HH21	1.47	0.79
2:B:894:TYR:HB2	2:B:962:MET:HB3	1.65	0.79
2:A:961:MET:HG3	2:A:965:GLY:HA2	1.65	0.78
2:A:899:ASP:HB3	2:A:902:LYS:CB	2.12	0.78
2:C:894:TYR:HB2	2:C:962:MET:HB3	1.65	0.78
2:A:894:TYR:HB2	2:A:962:MET:HB3	1.65	0.78
2:D:903:ARG:HA	2:D:903:ARG:HH21	1.47	0.78
2:A:2372:GLU:HG2	2:B:197:MET:HE1	1.66	0.78
2:A:2234:CYS:O	2:A:2236:PHE:N	2.17	0.78
2:C:903:ARG:HH21	2:C:903:ARG:HA	1.47	0.77
2:D:2234:CYS:O	2:D:2236:PHE:N	2.17	0.77
2:D:2372:GLU:HG2	2:A:197:MET:HE1	1.67	0.77
2:D:894:TYR:HB2	2:D:962:MET:HB3	1.65	0.77
2:B:899:ASP:HB3	2:B:902:LYS:CB	2.12	0.77
2:B:2234:CYS:O	2:B:2236:PHE:N	2.17	0.77
2:D:197:MET:HE1	2:C:2372:GLU:HG2	1.67	0.76
2:B:2372:GLU:HG2	2:C:197:MET:HE1	1.67	0.76
2:B:865:PRO:HD2	2:B:868:LEU:HB2	1.68	0.76
2:A:951:LEU:HD23	2:A:975:HIS:CE1	2.21	0.76
2:B:871:ILE:HG13	2:B:1050:TYR:CD2	2.21	0.76
2:A:865:PRO:HD2	2:A:868:LEU:HB2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:871:ILE:HG13	2:C:1050:TYR:CD2	2.21	0.76
2:C:2234:CYS:O	2:C:2236:PHE:N	2.17	0.76
2:D:865:PRO:HD2	2:D:868:LEU:HB2	1.68	0.75
2:D:951:LEU:HD23	2:D:975:HIS:CE1	2.21	0.75
2:A:871:ILE:HG13	2:A:1050:TYR:CD2	2.21	0.75
2:B:951:LEU:HD23	2:B:975:HIS:CE1	2.21	0.75
2:B:951:LEU:HD23	2:B:975:HIS:HE1	1.51	0.75
2:C:865:PRO:HD2	2:C:868:LEU:HB2	1.68	0.75
2:D:871:ILE:HG13	2:D:1050:TYR:CD2	2.21	0.75
2:A:951:LEU:HD23	2:A:975:HIS:HE1	1.51	0.74
2:B:859:THR:HA	2:B:862:ILE:HD12	1.69	0.74
2:C:951:LEU:HD23	2:C:975:HIS:CE1	2.21	0.74
2:B:3309:THR:OG1	2:B:3311:ASP:OD1	2.06	0.74
2:D:888:ILE:HG12	2:D:960:TYR:CG	2.23	0.74
2:B:956:LEU:HD12	2:B:968:PRO:HD2	1.70	0.74
2:A:859:THR:HA	2:A:862:ILE:HD12	1.69	0.74
7:D:8006:PCW:H482	7:A:8005:PCW:H271	1.70	0.74
2:C:859:THR:HA	2:C:862:ILE:HD12	1.69	0.74
2:A:888:ILE:HG12	2:A:960:TYR:CG	2.23	0.73
2:A:3309:THR:OG1	2:A:3311:ASP:OD1	2.06	0.73
2:A:3859:LEU:HD11	2:A:3871:ARG:HH22	1.52	0.73
2:D:956:LEU:HD12	2:D:968:PRO:HD2	1.70	0.73
2:C:888:ILE:HG12	2:C:960:TYR:CG	2.23	0.73
2:C:3309:THR:OG1	2:C:3311:ASP:OD1	2.06	0.73
2:B:3859:LEU:HD11	2:B:3871:ARG:HH22	1.53	0.73
2:C:951:LEU:HD23	2:C:975:HIS:HE1	1.51	0.73
2:D:864:LEU:HD11	2:D:930:LEU:HB2	1.70	0.73
2:C:3859:LEU:HD11	2:C:3871:ARG:HH22	1.52	0.73
2:C:956:LEU:HD12	2:C:968:PRO:HD2	1.70	0.73
2:D:898:ARG:HB3	2:D:906:PRO:HD2	1.71	0.73
2:C:898:ARG:HB3	2:C:906:PRO:HD2	1.71	0.73
2:D:951:LEU:HD23	2:D:975:HIS:HE1	1.51	0.72
2:B:864:LEU:HD11	2:B:930:LEU:HB2	1.70	0.72
2:D:859:THR:HA	2:D:862:ILE:HD12	1.69	0.72
2:D:3309:THR:OG1	2:D:3311:ASP:OD1	2.06	0.72
2:D:3859:LEU:HD11	2:D:3871:ARG:HH22	1.52	0.72
2:B:888:ILE:HG12	2:B:960:TYR:CG	2.23	0.72
2:B:3881:ASP:OD2	2:B:3882:GLU:N	2.23	0.72
2:A:3881:ASP:OD2	2:A:3882:GLU:N	2.23	0.72
7:B:8006:PCW:H482	7:C:8005:PCW:H271	1.72	0.72
7:D:8005:PCW:H271	7:C:8006:PCW:H482	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:956:LEU:HD12	2:A:968:PRO:HD2	1.70	0.72
2:C:864:LEU:HD11	2:C:930:LEU:HB2	1.70	0.72
2:C:2824:VAL:HG22	2:C:2938:VAL:HG23	1.72	0.72
2:D:3881:ASP:OD2	2:D:3882:GLU:N	2.23	0.71
2:B:898:ARG:HB3	2:B:906:PRO:HD2	1.71	0.71
2:D:953:LYS:HA	2:D:971:LEU:HA	1.72	0.71
2:A:898:ARG:HB3	2:A:906:PRO:HD2	1.71	0.71
2:C:953:LYS:HA	2:C:971:LEU:HA	1.72	0.71
2:C:3881:ASP:OD2	2:C:3882:GLU:N	2.23	0.71
2:A:864:LEU:HD11	2:A:930:LEU:HB2	1.70	0.71
2:A:914:LEU:HD21	2:A:919:ARG:HA	1.73	0.71
2:C:3107:MET:O	2:C:3111:LEU:HD23	1.91	0.71
2:C:2949:THR:O	2:C:2954:LYS:NZ	2.25	0.70
2:D:2824:VAL:HG22	2:D:2938:VAL:HG23	1.72	0.70
2:A:953:LYS:HA	2:A:971:LEU:HA	1.72	0.70
2:B:2949:THR:O	2:B:2954:LYS:NZ	2.25	0.70
2:D:2949:THR:O	2:D:2954:LYS:NZ	2.25	0.70
2:A:2824:VAL:HG22	2:A:2938:VAL:HG23	1.72	0.70
2:B:953:LYS:HA	2:B:971:LEU:HA	1.72	0.70
2:B:3870:ASN:O	2:B:3872:GLN:NE2	2.25	0.70
2:D:973:LEU:HB2	2:D:976:VAL:HG23	1.74	0.70
2:A:3870:ASN:O	2:A:3872:GLN:NE2	2.25	0.70
2:B:973:LEU:HB2	2:B:976:VAL:HG23	1.74	0.70
2:D:3107:MET:O	2:D:3111:LEU:HD23	1.91	0.69
2:A:973:LEU:HB2	2:A:976:VAL:HG23	1.74	0.69
2:A:3107:MET:O	2:A:3111:LEU:HD23	1.91	0.69
2:C:973:LEU:HB2	2:C:976:VAL:HG23	1.74	0.69
1:H:88:HIS:ND1	1:H:91:ILE:HD13	2.08	0.69
2:B:914:LEU:HD21	2:B:919:ARG:HA	1.73	0.69
2:B:3107:MET:O	2:B:3111:LEU:HD23	1.91	0.69
2:C:914:LEU:HD21	2:C:919:ARG:HA	1.73	0.69
1:E:88:HIS:ND1	1:E:91:ILE:HD13	2.08	0.69
1:G:88:HIS:ND1	1:G:91:ILE:HD13	2.08	0.69
2:A:2949:THR:O	2:A:2954:LYS:NZ	2.25	0.69
2:B:885:LEU:O	2:B:888:ILE:HG23	1.93	0.69
2:B:2824:VAL:HG22	2:B:2938:VAL:HG23	1.72	0.69
1:F:88:HIS:ND1	1:F:91:ILE:HD13	2.08	0.69
2:A:1466:ASP:OD2	2:A:1468:SER:OG	2.11	0.69
2:C:2414:GLU:O	2:C:2418:HIS:NE2	2.26	0.69
2:A:894:TYR:CB	2:A:964:ASN:H	2.06	0.68
2:B:894:TYR:CB	2:B:964:ASN:H	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:885:LEU:O	2:C:888:ILE:HG23	1.93	0.68
2:B:2414:GLU:O	2:B:2418:HIS:NE2	2.26	0.68
2:C:3870:ASN:O	2:C:3872:GLN:NE2	2.25	0.68
2:B:2948:ASP:O	2:B:2949:THR:OG1	2.10	0.68
2:C:250:GLY:H	2:C:373:LEU:HD11	1.58	0.68
2:D:894:TYR:CB	2:D:964:ASN:H	2.07	0.68
2:D:914:LEU:HD21	2:D:919:ARG:HA	1.73	0.68
2:A:2414:GLU:O	2:A:2418:HIS:NE2	2.26	0.68
2:B:911:PHE:CZ	2:B:922:ASN:HB2	2.29	0.68
2:C:894:TYR:CB	2:C:964:ASN:H	2.07	0.68
2:A:885:LEU:O	2:A:888:ILE:HG23	1.93	0.68
2:D:914:LEU:HD12	2:D:915:PRO:HD2	1.75	0.68
2:A:911:PHE:CZ	2:A:922:ASN:HB2	2.29	0.68
2:B:1222:GLU:N	2:B:1222:GLU:OE1	2.27	0.68
2:C:914:LEU:HD12	2:C:915:PRO:HD2	1.75	0.68
1:G:12:ASP:OD1	1:G:13:GLY:N	2.26	0.68
1:H:12:ASP:OD1	1:H:13:GLY:N	2.27	0.68
2:D:250:GLY:H	2:D:373:LEU:HD11	1.58	0.68
2:D:885:LEU:O	2:D:888:ILE:HG23	1.93	0.68
2:D:3870:ASN:O	2:D:3872:GLN:NE2	2.25	0.68
2:D:872:ARG:HG3	2:D:927:GLY:HA2	1.76	0.68
2:A:1222:GLU:OE1	2:A:1222:GLU:N	2.27	0.68
2:B:911:PHE:HA	2:B:914:LEU:HD23	1.76	0.67
2:C:911:PHE:CZ	2:C:922:ASN:HB2	2.29	0.67
2:D:2414:GLU:O	2:D:2418:HIS:NE2	2.26	0.67
2:A:914:LEU:HD12	2:A:915:PRO:HD2	1.75	0.67
2:B:914:LEU:HD12	2:B:915:PRO:HD2	1.74	0.67
2:C:911:PHE:HA	2:C:914:LEU:HD23	1.76	0.67
2:D:898:ARG:CB	2:D:906:PRO:HD2	2.24	0.67
2:D:911:PHE:HZ	2:D:922:ASN:HB2	1.59	0.67
2:A:250:GLY:H	2:A:373:LEU:HD11	1.58	0.67
2:B:872:ARG:HG3	2:B:927:GLY:HA2	1.76	0.67
2:A:898:ARG:CB	2:A:906:PRO:HD2	2.24	0.67
2:C:865:PRO:HD2	2:C:868:LEU:CB	2.25	0.67
2:C:982:GLN:HA	2:C:985:LEU:HD12	1.76	0.67
2:D:911:PHE:CZ	2:D:922:ASN:HB2	2.29	0.67
2:D:1222:GLU:OE1	2:D:1222:GLU:N	2.27	0.67
2:A:911:PHE:HA	2:A:914:LEU:HD23	1.76	0.67
2:B:250:GLY:H	2:B:373:LEU:HD11	1.58	0.67
2:B:871:ILE:HA	2:B:874:LYS:HD3	1.77	0.67
2:C:898:ARG:CB	2:C:906:PRO:HD2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:ASP:OD1	1:E:13:GLY:N	2.28	0.67
2:D:911:PHE:HA	2:D:914:LEU:HD23	1.76	0.67
2:B:1466:ASP:OD2	2:B:1468:SER:OG	2.11	0.67
2:A:2749:PRO:HD2	2:A:2752:LEU:HD12	1.77	0.67
2:C:872:ARG:HG3	2:C:927:GLY:HA2	1.76	0.67
1:F:12:ASP:OD1	1:F:13:GLY:N	2.28	0.67
2:D:865:PRO:HD2	2:D:868:LEU:CB	2.25	0.67
2:C:1466:ASP:OD2	2:C:1468:SER:OG	2.11	0.67
2:C:911:PHE:HZ	2:C:922:ASN:HB2	1.59	0.66
2:D:2948:ASP:O	2:D:2949:THR:OG1	2.10	0.66
2:A:3377:GLU:OE1	2:A:3449:SER:OG	2.12	0.66
2:A:872:ARG:HG3	2:A:927:GLY:HA2	1.76	0.66
2:B:982:GLN:HA	2:B:985:LEU:HD12	1.76	0.66
2:C:1222:GLU:OE1	2:C:1222:GLU:N	2.27	0.66
2:D:3377:GLU:OE1	2:D:3449:SER:OG	2.12	0.66
2:A:911:PHE:HZ	2:A:922:ASN:HB2	1.59	0.66
2:B:898:ARG:CB	2:B:906:PRO:HD2	2.24	0.66
2:D:871:ILE:HA	2:D:874:LYS:HD3	1.77	0.66
2:B:2564:THR:HG22	2:B:2607:CYS:HA	1.78	0.66
2:D:982:GLN:HA	2:D:985:LEU:HD12	1.76	0.66
2:C:2749:PRO:HD2	2:C:2752:LEU:HD12	1.77	0.66
2:A:859:THR:HB	2:A:931:LYS:HB3	1.78	0.66
2:A:865:PRO:HD2	2:A:868:LEU:CB	2.25	0.66
2:B:865:PRO:HD2	2:B:868:LEU:CB	2.25	0.66
2:C:2564:THR:HG22	2:C:2607:CYS:HA	1.78	0.66
2:B:859:THR:HB	2:B:931:LYS:HB3	1.78	0.66
2:D:986:VAL:HG22	2:D:1044:VAL:HG21	1.78	0.66
2:A:871:ILE:HA	2:A:874:LYS:HD3	1.77	0.66
2:B:2749:PRO:HD2	2:B:2752:LEU:HD12	1.77	0.66
2:C:4048:VAL:HG11	2:C:4160:ASP:OD2	1.96	0.66
2:A:887:ARG:HG3	2:A:892:TRP:CD1	2.32	0.65
2:B:911:PHE:HZ	2:B:922:ASN:HB2	1.59	0.65
2:D:887:ARG:HG3	2:D:892:TRP:CD1	2.32	0.65
2:B:4048:VAL:HG11	2:B:4160:ASP:OD2	1.96	0.65
2:C:887:ARG:HG3	2:C:892:TRP:CD1	2.32	0.65
1:F:62:GLU:N	1:F:62:GLU:OE1	2.29	0.65
1:H:62:GLU:OE1	1:H:62:GLU:N	2.30	0.65
2:D:868:LEU:HD13	2:D:930:LEU:HB3	1.79	0.65
2:B:894:TYR:CD2	2:B:964:ASN:HB3	2.31	0.65
2:C:940:VAL:HA	2:C:1053:ASN:O	1.96	0.65
1:E:36:LYS:NZ	1:E:42:ASP:OD2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:982:GLN:HA	2:A:985:LEU:HD12	1.76	0.65
2:B:887:ARG:HG3	2:B:892:TRP:CD1	2.32	0.65
2:B:940:VAL:HA	2:B:1053:ASN:O	1.96	0.65
2:B:1420:ASP:OD1	2:B:1422:ARG:NH1	2.30	0.65
2:A:2564:THR:HG22	2:A:2607:CYS:HA	1.78	0.65
2:D:1420:ASP:OD1	2:D:1422:ARG:NH1	2.30	0.65
2:D:1466:ASP:OD2	2:D:1468:SER:OG	2.11	0.65
2:D:4048:VAL:HG11	2:D:4160:ASP:OD2	1.96	0.65
2:B:2560:LEU:O	2:B:2564:THR:HG23	1.97	0.65
2:C:1420:ASP:OD1	2:C:1422:ARG:NH1	2.30	0.65
2:A:940:VAL:HA	2:A:1053:ASN:O	1.96	0.65
2:C:986:VAL:HG22	2:C:1044:VAL:HG21	1.78	0.65
1:H:36:LYS:NZ	1:H:42:ASP:OD2	2.29	0.65
2:D:914:LEU:HD21	2:D:919:ARG:HB2	1.79	0.65
2:C:894:TYR:CD2	2:C:964:ASN:HB3	2.31	0.65
2:A:894:TYR:CD2	2:A:964:ASN:HB3	2.31	0.65
2:D:2564:THR:HG22	2:D:2607:CYS:HA	1.78	0.65
2:D:2749:PRO:HD2	2:D:2752:LEU:HD12	1.77	0.65
2:A:919:ARG:HA	2:A:922:ASN:ND2	2.12	0.65
2:C:871:ILE:HA	2:C:874:LYS:HD3	1.77	0.65
2:B:4925:ILE:O	2:B:4929:ILE:HD12	1.97	0.64
2:C:914:LEU:HD21	2:C:919:ARG:HB2	1.79	0.64
2:D:859:THR:HB	2:D:931:LYS:HB3	1.78	0.64
2:A:2560:LEU:O	2:A:2564:THR:HG23	1.97	0.64
1:F:36:LYS:NZ	1:F:42:ASP:OD2	2.30	0.64
2:D:894:TYR:CD2	2:D:964:ASN:HB3	2.31	0.64
2:D:919:ARG:HA	2:D:922:ASN:ND2	2.12	0.64
2:D:2866:VAL:HG12	2:D:2933:MET:HE3	1.79	0.64
2:A:986:VAL:HG22	2:A:1044:VAL:HG21	1.78	0.64
2:B:986:VAL:HG22	2:B:1044:VAL:HG21	1.78	0.64
2:C:859:THR:HB	2:C:931:LYS:HB3	1.78	0.64
2:C:868:LEU:HD13	2:C:930:LEU:HB3	1.79	0.64
2:C:2245:ARG:NH2	2:C:2284:ASN:OD1	2.31	0.64
1:G:36:LYS:NZ	1:G:42:ASP:OD1	2.30	0.64
2:D:940:VAL:HA	2:D:1053:ASN:O	1.96	0.64
2:D:4925:ILE:O	2:D:4929:ILE:HD12	1.97	0.64
2:A:868:LEU:HD13	2:A:930:LEU:HB3	1.79	0.64
2:D:2245:ARG:NH2	2:D:2284:ASN:OD1	2.31	0.64
2:A:914:LEU:HD21	2:A:919:ARG:HB2	1.79	0.64
2:A:2245:ARG:NH2	2:A:2284:ASN:OD1	2.31	0.64
7:A:8006:PCW:H482	7:B:8005:PCW:H271	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:GLU:OE1	1:E:62:GLU:N	2.31	0.64
2:D:2560:LEU:O	2:D:2564:THR:HG23	1.97	0.64
2:D:3529:THR:HG23	2:D:3574:MET:CE	2.25	0.64
2:A:1042:GLN:O	2:A:1046:THR:HG23	1.98	0.64
2:B:3972:ILE:HG21	2:B:3983:LEU:HD12	1.80	0.64
2:A:3392:GLU:OE2	2:A:3396:ARG:NE	2.30	0.64
2:A:4925:ILE:O	2:A:4929:ILE:HD12	1.97	0.64
1:G:62:GLU:OE1	1:G:62:GLU:N	2.30	0.64
2:C:919:ARG:HA	2:C:922:ASN:ND2	2.12	0.64
2:C:2866:VAL:HG12	2:C:2933:MET:HE3	1.79	0.64
2:A:4048:VAL:HG11	2:A:4160:ASP:OD2	1.96	0.64
2:B:1042:GLN:O	2:B:1046:THR:HG23	1.98	0.64
2:B:919:ARG:HA	2:B:922:ASN:ND2	2.12	0.64
2:C:3377:GLU:OE1	2:C:3449:SER:OG	2.12	0.64
2:C:3392:GLU:OE2	2:C:3396:ARG:NE	2.30	0.64
2:D:3392:GLU:OE2	2:D:3396:ARG:NE	2.30	0.63
2:A:3506:VAL:O	2:A:3509:SER:OG	2.13	0.63
2:A:4752:ASN:OD1	2:A:4754:ARG:NH2	2.31	0.63
2:B:1070:GLY:N	2:B:1115:GLU:OE1	2.32	0.63
2:C:2560:LEU:O	2:C:2564:THR:HG23	1.97	0.63
2:C:4752:ASN:OD1	2:C:4754:ARG:NH2	2.31	0.63
2:A:1420:ASP:OD1	2:A:1422:ARG:NH1	2.30	0.63
2:B:2245:ARG:NH2	2:B:2284:ASN:OD1	2.31	0.63
2:B:3392:GLU:OE2	2:B:3396:ARG:NE	2.30	0.63
2:D:1042:GLN:O	2:D:1046:THR:HG23	1.98	0.63
2:A:2779:GLY:N	2:A:2789:HIS:O	2.31	0.63
2:A:3972:ILE:HG21	2:A:3983:LEU:HD12	1.80	0.63
2:B:318:ARG:NH2	2:B:322:GLU:O	2.32	0.63
2:B:868:LEU:HD13	2:B:930:LEU:HB3	1.79	0.63
2:A:2866:VAL:HG12	2:A:2933:MET:HE3	1.79	0.63
2:B:914:LEU:HD21	2:B:919:ARG:HB2	1.79	0.63
2:B:4752:ASN:OD1	2:B:4754:ARG:NH2	2.31	0.63
2:C:1042:GLN:O	2:C:1046:THR:HG23	1.98	0.63
2:D:1070:GLY:N	2:D:1115:GLU:OE1	2.32	0.63
2:D:4752:ASN:OD1	2:D:4754:ARG:NH2	2.31	0.63
2:B:2866:VAL:HG12	2:B:2933:MET:HE3	1.79	0.63
2:C:952:LYS:HZ2	2:C:952:LYS:H	1.47	0.63
2:C:4925:ILE:O	2:C:4929:ILE:HD12	1.97	0.63
2:A:3529:THR:HG23	2:A:3574:MET:CE	2.25	0.63
2:C:882:LEU:HG	2:C:970:PRO:HB3	1.81	0.63
2:D:894:TYR:HB3	2:D:964:ASN:N	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3972:ILE:HG21	2:D:3983:LEU:HD12	1.80	0.62
2:C:2259:LEU:O	2:C:2262:SER:OG	2.16	0.62
2:C:3972:ILE:HG21	2:C:3983:LEU:HD12	1.80	0.62
2:A:2259:LEU:O	2:A:2262:SER:OG	2.16	0.62
2:C:1070:GLY:N	2:C:1115:GLU:OE1	2.32	0.62
2:B:952:LYS:HZ2	2:B:952:LYS:H	1.47	0.62
2:B:3529:THR:HG23	2:B:3574:MET:CE	2.25	0.62
2:A:894:TYR:HB3	2:A:964:ASN:N	2.13	0.62
2:B:882:LEU:HG	2:B:970:PRO:HB3	1.81	0.62
2:C:2779:GLY:N	2:C:2789:HIS:O	2.31	0.62
2:A:1070:GLY:N	2:A:1115:GLU:OE1	2.32	0.62
2:D:318:ARG:NH2	2:D:322:GLU:O	2.32	0.62
2:A:882:LEU:HG	2:A:970:PRO:HB3	1.81	0.62
2:A:1794:THR:HG22	2:A:2174:GLN:OE1	2.00	0.62
2:B:1794:THR:HG22	2:B:2174:GLN:OE1	2.00	0.62
2:C:940:VAL:HB	2:C:1054:ILE:HG13	1.81	0.62
2:A:318:ARG:NH2	2:A:322:GLU:O	2.32	0.62
2:A:952:LYS:HZ2	2:A:952:LYS:H	1.47	0.62
2:C:3529:THR:HG23	2:C:3574:MET:CE	2.25	0.62
2:A:2156:LEU:CD2	2:A:2199:MET:HE1	2.24	0.62
2:C:3541:TYR:OH	2:C:3598:GLN:NE2	2.31	0.62
2:D:882:LEU:HG	2:D:970:PRO:HB3	1.81	0.61
2:D:2259:LEU:O	2:D:2262:SER:OG	2.16	0.61
2:D:1794:THR:HG22	2:D:2174:GLN:OE1	2.00	0.61
2:A:940:VAL:HB	2:A:1054:ILE:HG13	1.81	0.61
2:C:2817:MET:HE1	2:C:2931:LEU:HD11	1.82	0.61
2:B:169:ASP:OD1	2:B:202:ASN:ND2	2.32	0.61
2:B:973:LEU:HA	2:B:975:HIS:CE1	2.36	0.61
2:B:2740:PRO:HG3	2:B:2886:THR:HG22	1.83	0.61
2:C:894:TYR:HB3	2:C:964:ASN:N	2.13	0.61
2:C:973:LEU:HB2	2:C:976:VAL:CG2	2.31	0.61
2:C:1794:THR:HG22	2:C:2174:GLN:OE1	2.00	0.61
2:A:2674:HIS:ND1	2:A:2717:ASP:OD2	2.34	0.61
2:A:2817:MET:HE1	2:A:2931:LEU:HD11	1.82	0.61
2:B:940:VAL:HB	2:B:1054:ILE:HG13	1.81	0.61
2:C:3435:LEU:HD23	2:C:3518:MET:HE2	1.82	0.61
2:A:932:THR:O	2:A:936:LEU:HG	2.01	0.61
2:A:3435:LEU:HD23	2:A:3518:MET:HE2	1.82	0.61
2:D:2740:PRO:HG3	2:D:2886:THR:HG22	1.83	0.61
2:B:318:ARG:NH1	2:B:325:ASP:OD2	2.34	0.61
2:B:973:LEU:HB2	2:B:976:VAL:CG2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2779:GLY:N	2:B:2789:HIS:O	2.31	0.61
2:D:2968:MET:O	2:D:2971:SER:OG	2.17	0.61
2:A:169:ASP:OD1	2:A:202:ASN:ND2	2.32	0.61
2:B:2674:HIS:ND1	2:B:2717:ASP:OD2	2.34	0.61
2:C:318:ARG:NH1	2:C:325:ASP:OD2	2.34	0.61
2:D:318:ARG:NH1	2:D:325:ASP:OD2	2.34	0.61
2:D:928:GLU:O	2:D:932:THR:HG22	2.01	0.61
2:C:870:ARG:HH21	2:C:874:LYS:HD3	1.66	0.61
2:D:2674:HIS:ND1	2:D:2717:ASP:OD2	2.34	0.61
2:D:2817:MET:HE1	2:D:2931:LEU:HD11	1.82	0.61
2:A:2740:PRO:HG3	2:A:2886:THR:HG22	1.83	0.61
2:B:898:ARG:HA	2:B:904:LEU:O	2.01	0.61
2:B:902:LYS:HB3	2:B:904:LEU:CG	2.28	0.61
2:C:318:ARG:NH2	2:C:322:GLU:O	2.32	0.61
2:B:932:THR:O	2:B:936:LEU:HG	2.01	0.60
2:B:3435:LEU:HD23	2:B:3518:MET:HE2	1.82	0.60
2:C:936:LEU:HB2	2:C:938:CYS:SG	2.41	0.60
2:C:2674:HIS:ND1	2:C:2717:ASP:OD2	2.34	0.60
2:D:898:ARG:HA	2:D:904:LEU:O	2.01	0.60
2:D:1264:THR:OG1	2:D:1266:ASP:OD1	2.20	0.60
2:A:973:LEU:HA	2:A:975:HIS:CE1	2.36	0.60
2:C:898:ARG:HA	2:C:904:LEU:O	2.01	0.60
2:D:169:ASP:OD1	2:D:202:ASN:ND2	2.32	0.60
2:D:936:LEU:HB2	2:D:938:CYS:SG	2.41	0.60
2:D:2779:GLY:N	2:D:2789:HIS:O	2.31	0.60
2:A:895:GLY:CA	2:A:904:LEU:HB2	2.31	0.60
2:C:2156:LEU:CD2	2:C:2199:MET:HE1	2.24	0.60
2:D:932:THR:O	2:D:936:LEU:HG	2.01	0.60
2:A:649:ILE:HG23	2:A:815:ALA:HB3	1.84	0.60
2:A:898:ARG:HA	2:A:904:LEU:O	2.01	0.60
2:A:936:LEU:HB2	2:A:938:CYS:SG	2.41	0.60
2:B:2817:MET:HE1	2:B:2931:LEU:HD11	1.82	0.60
2:B:4129:GLU:OE2	2:B:4133:ASN:ND2	2.35	0.60
2:C:169:ASP:OD1	2:C:202:ASN:ND2	2.32	0.60
2:C:884:ALA:HB1	2:C:968:PRO:HG3	1.83	0.60
2:C:1264:THR:OG1	2:C:1266:ASP:OD1	2.20	0.60
2:C:2740:PRO:HG3	2:C:2886:THR:HG22	1.83	0.60
2:D:870:ARG:HH21	2:D:874:LYS:HD3	1.66	0.60
2:D:973:LEU:HA	2:D:975:HIS:CE1	2.36	0.60
2:A:928:GLU:O	2:A:932:THR:HG22	2.01	0.60
2:B:928:GLU:O	2:B:932:THR:HG22	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2156:LEU:CD2	2:B:2199:MET:HE1	2.24	0.60
2:B:2259:LEU:O	2:B:2262:SER:OG	2.16	0.60
2:C:932:THR:O	2:C:936:LEU:HG	2.01	0.60
2:A:884:ALA:HB1	2:A:968:PRO:HG3	1.83	0.60
2:B:2246:GLN:N	2:B:2246:GLN:OE1	2.35	0.60
2:D:2383:GLU:HA	2:D:2386:ARG:NH2	2.17	0.60
2:A:318:ARG:NH1	2:A:325:ASP:OD2	2.34	0.60
2:A:4129:GLU:OE2	2:A:4133:ASN:ND2	2.35	0.60
2:C:928:GLU:O	2:C:932:THR:HG22	2.01	0.60
2:C:2948:ASP:O	2:C:2949:THR:OG1	2.10	0.60
2:D:884:ALA:HB1	2:D:968:PRO:HG3	1.83	0.60
2:D:895:GLY:CA	2:D:904:LEU:HB2	2.31	0.60
2:D:940:VAL:HB	2:D:1054:ILE:HG13	1.81	0.60
2:D:973:LEU:HB2	2:D:976:VAL:CG2	2.31	0.60
2:D:3435:LEU:HD23	2:D:3518:MET:HE2	1.82	0.60
2:A:3541:TYR:OH	2:A:3598:GLN:NE2	2.31	0.60
2:C:973:LEU:HA	2:C:975:HIS:CE1	2.36	0.60
2:B:883:TRP:HH2	2:B:907:CYS:HB3	1.67	0.60
2:B:3506:VAL:O	2:B:3509:SER:OG	2.13	0.60
2:A:973:LEU:HB2	2:A:976:VAL:CG2	2.31	0.59
2:B:2383:GLU:HA	2:B:2386:ARG:NH2	2.17	0.59
2:C:881:GLU:HB3	2:C:969:ALA:H	1.67	0.59
2:C:985:LEU:HD21	2:C:1057:PRO:HD2	1.84	0.59
2:A:3754:VAL:HG13	2:A:3758:GLU:OE2	2.02	0.59
2:B:936:LEU:HB2	2:B:938:CYS:SG	2.41	0.59
2:B:2968:MET:O	2:B:2971:SER:OG	2.17	0.59
2:B:3754:VAL:HG13	2:B:3758:GLU:OE2	2.02	0.59
2:B:3856:ALA:HB1	2:B:3871:ARG:NE	2.17	0.59
2:C:895:GLY:CA	2:C:904:LEU:HB2	2.31	0.59
2:C:3506:VAL:O	2:C:3509:SER:OG	2.13	0.59
2:C:3962:LYS:NZ	2:C:4025:ASP:OD1	2.36	0.59
2:D:2156:LEU:CD2	2:D:2199:MET:HE1	2.24	0.59
2:B:884:ALA:HB1	2:B:968:PRO:HG3	1.83	0.59
2:B:3962:LYS:NZ	2:B:4025:ASP:OD1	2.36	0.59
2:A:881:GLU:HB3	2:A:969:ALA:H	1.67	0.59
2:B:895:GLY:CA	2:B:904:LEU:HB2	2.31	0.59
2:B:919:ARG:HA	2:B:922:ASN:HD22	1.67	0.59
2:B:985:LEU:HD21	2:B:1057:PRO:HD2	1.84	0.59
2:D:3524:ASN:O	2:D:3583:ARG:NH2	2.36	0.59
2:D:3541:TYR:OH	2:D:3598:GLN:NE2	2.31	0.59
2:B:3524:ASN:O	2:B:3583:ARG:NH2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:649:ILE:HG23	2:C:815:ALA:HB3	1.84	0.59
2:C:3828:GLU:OE1	2:C:3828:GLU:N	2.33	0.59
2:D:3440:GLY:O	2:D:3444:ILE:HG13	2.02	0.59
2:B:870:ARG:HH21	2:B:874:LYS:HD3	1.66	0.59
2:B:929:THR:HA	2:B:932:THR:HG22	1.85	0.59
2:C:3856:ALA:HB1	2:C:3871:ARG:NE	2.17	0.59
2:D:3856:ALA:HB1	2:D:3871:ARG:NE	2.17	0.59
2:A:912:HIS:HA	2:A:919:ARG:NH1	2.17	0.59
2:A:2383:GLU:HA	2:A:2386:ARG:NH2	2.17	0.59
2:B:649:ILE:HG23	2:B:815:ALA:HB3	1.84	0.59
2:B:3440:GLY:O	2:B:3444:ILE:HG13	2.02	0.59
2:C:929:THR:HA	2:C:932:THR:HG22	1.85	0.59
2:C:4129:GLU:OE2	2:C:4133:ASN:ND2	2.35	0.59
2:D:3754:VAL:HG13	2:D:3758:GLU:OE2	2.02	0.59
2:A:870:ARG:HH21	2:A:874:LYS:HD3	1.66	0.59
2:A:3524:ASN:O	2:A:3583:ARG:NH2	2.36	0.59
2:C:883:TRP:HH2	2:C:907:CYS:HB3	1.67	0.59
2:C:2246:GLN:OE1	2:C:2246:GLN:N	2.35	0.59
2:C:2383:GLU:HA	2:C:2386:ARG:NH2	2.17	0.59
2:C:3344:GLN:OE1	2:C:3415:ARG:NH2	2.36	0.59
2:D:912:HIS:HA	2:D:919:ARG:NH1	2.18	0.59
2:A:1173:ASP:OD1	2:A:1174:SER:N	2.36	0.59
2:A:3856:ALA:HB1	2:A:3871:ARG:NE	2.17	0.59
2:B:912:HIS:HA	2:B:919:ARG:NH1	2.18	0.59
2:C:1173:ASP:OD1	2:C:1174:SER:N	2.36	0.59
2:C:2249:ARG:NH2	2:C:2286:GLU:OE2	2.36	0.59
2:D:649:ILE:HG23	2:D:815:ALA:HB3	1.84	0.59
2:D:929:THR:HA	2:D:932:THR:HG22	1.85	0.59
2:D:4129:GLU:OE2	2:D:4133:ASN:ND2	2.35	0.59
2:A:902:LYS:HB3	2:A:904:LEU:CG	2.28	0.59
2:A:985:LEU:HD21	2:A:1057:PRO:HD2	1.84	0.59
2:B:1173:ASP:OD1	2:B:1174:SER:N	2.36	0.59
2:C:912:HIS:HA	2:C:919:ARG:NH1	2.18	0.59
2:C:2863:LEU:HD12	2:C:2926:GLU:OE1	2.03	0.59
2:D:895:GLY:HA3	2:D:904:LEU:HB2	1.84	0.58
2:D:898:ARG:HH12	2:D:907:CYS:HB2	1.68	0.58
2:D:985:LEU:HD21	2:D:1057:PRO:HD2	1.84	0.58
2:B:1264:THR:OG1	2:B:1266:ASP:OD1	2.20	0.58
2:C:3754:VAL:HG13	2:C:3758:GLU:OE2	2.02	0.58
2:A:919:ARG:HA	2:A:922:ASN:HD22	1.67	0.58
2:A:3344:GLN:OE1	2:A:3415:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:163:LYS:O	2:C:165:ARG:NH1	2.36	0.58
2:C:877:GLU:HA	2:C:911:PHE:CD2	2.39	0.58
2:C:3440:GLY:O	2:C:3444:ILE:HG13	2.02	0.58
2:D:883:TRP:HH2	2:D:907:CYS:HB3	1.67	0.58
2:D:2863:LEU:HD12	2:D:2926:GLU:OE1	2.03	0.58
2:A:895:GLY:HA3	2:A:904:LEU:HB2	1.84	0.58
2:A:929:THR:HA	2:A:932:THR:HG22	1.85	0.58
2:A:2863:LEU:HD12	2:A:2926:GLU:OE1	2.03	0.58
2:C:914:LEU:HD21	2:C:919:ARG:CA	2.33	0.58
2:C:3761:MET:HE3	2:C:3761:MET:HA	1.85	0.58
2:D:3962:LYS:NZ	2:D:4025:ASP:OD1	2.36	0.58
2:A:888:ILE:CD1	2:A:960:TYR:HA	2.32	0.58
2:A:3962:LYS:NZ	2:A:4025:ASP:OD1	2.36	0.58
2:A:4868:ASP:OD1	2:A:4869:GLU:N	2.36	0.58
2:B:881:GLU:HB3	2:B:969:ALA:H	1.67	0.58
2:B:2249:ARG:NH2	2:B:2286:GLU:OE2	2.36	0.58
2:C:2695:GLU:OE1	2:C:2698:ARG:NH2	2.37	0.58
2:A:898:ARG:HH12	2:A:907:CYS:HB2	1.69	0.58
2:A:2249:ARG:NH2	2:A:2286:GLU:OE2	2.36	0.58
2:D:287:THR:HG21	2:D:482:GLU:OE2	2.04	0.58
2:D:877:GLU:HA	2:D:911:PHE:CD2	2.39	0.58
2:D:1173:ASP:OD1	2:D:1174:SER:N	2.36	0.58
2:D:2249:ARG:NH2	2:D:2286:GLU:OE2	2.36	0.58
2:D:3761:MET:HA	2:D:3761:MET:HE3	1.85	0.58
2:A:3440:GLY:O	2:A:3444:ILE:HG13	2.02	0.58
2:B:163:LYS:O	2:B:165:ARG:NH1	2.36	0.58
2:B:877:GLU:HA	2:B:911:PHE:CD2	2.39	0.58
2:B:3943:LYS:O	2:B:4005:LYS:NZ	2.36	0.58
2:B:4868:ASP:OD1	2:B:4869:GLU:N	2.37	0.58
2:C:914:LEU:CD2	2:C:919:ARG:HB2	2.34	0.58
2:C:919:ARG:HA	2:C:922:ASN:HD22	1.67	0.58
2:C:919:ARG:HG2	2:C:920:ASN:N	2.18	0.58
2:D:881:GLU:HB3	2:D:969:ALA:H	1.67	0.58
2:B:2863:LEU:HD12	2:B:2926:GLU:OE1	2.03	0.58
2:C:888:ILE:CD1	2:C:960:TYR:HA	2.32	0.58
2:D:4868:ASP:OD1	2:D:4869:GLU:N	2.37	0.58
2:A:877:GLU:HA	2:A:911:PHE:CD2	2.39	0.58
2:A:1264:THR:OG1	2:A:1266:ASP:OD1	2.20	0.58
2:A:2265:GLY:HA2	2:A:2268:MET:HE1	1.86	0.58
2:B:895:GLY:HA3	2:B:904:LEU:HB2	1.84	0.58
2:B:914:LEU:CD2	2:B:919:ARG:HB2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3170:LEU:HD12	2:B:3195:LEU:HD11	1.86	0.58
2:C:225:HIS:O	2:C:228:MET:HE2	2.04	0.58
2:D:2695:GLU:OE1	2:D:2698:ARG:NH2	2.37	0.58
2:D:3344:GLN:OE1	2:D:3415:ARG:NH2	2.36	0.58
2:A:50:LEU:HD11	2:A:183:LEU:HD13	1.86	0.58
2:A:287:THR:HG21	2:A:482:GLU:OE2	2.04	0.58
2:A:914:LEU:CD2	2:A:919:ARG:HB2	2.34	0.58
2:A:2948:ASP:O	2:A:2949:THR:OG1	2.10	0.58
2:B:914:LEU:HD21	2:B:919:ARG:CA	2.33	0.58
2:B:3344:GLN:OE1	2:B:3415:ARG:NH2	2.36	0.58
2:D:888:ILE:HG12	2:D:960:TYR:CD2	2.39	0.58
2:D:914:LEU:HD21	2:D:919:ARG:CA	2.33	0.58
2:A:914:LEU:HD21	2:A:919:ARG:CA	2.33	0.58
2:A:1654:LEU:O	2:A:1661:GLN:NE2	2.36	0.58
2:B:225:HIS:O	2:B:228:MET:HE2	2.04	0.58
2:C:895:GLY:HA3	2:C:904:LEU:HB2	1.84	0.58
2:C:898:ARG:HH12	2:C:907:CYS:HB2	1.68	0.58
2:C:2265:GLY:HA2	2:C:2268:MET:HE1	1.86	0.58
2:D:225:HIS:O	2:D:228:MET:HE2	2.04	0.57
2:D:905:HIS:CE1	2:D:907:CYS:HB2	2.39	0.57
2:A:2246:GLN:OE1	2:A:2246:GLN:N	2.35	0.57
2:A:2695:GLU:OE1	2:A:2698:ARG:NH2	2.36	0.57
2:B:894:TYR:HB3	2:B:964:ASN:N	2.13	0.57
2:D:919:ARG:HA	2:D:922:ASN:HD22	1.67	0.57
2:D:3111:LEU:HD13	2:D:3183:TYR:CE2	2.40	0.57
2:A:883:TRP:HH2	2:A:907:CYS:HB3	1.67	0.57
2:C:3111:LEU:HD13	2:C:3183:TYR:CE2	2.40	0.57
2:C:3524:ASN:O	2:C:3583:ARG:NH2	2.36	0.57
2:C:3524:ASN:O	2:C:3583:ARG:NH1	2.37	0.57
2:D:163:LYS:O	2:D:165:ARG:NH1	2.36	0.57
2:A:29:VAL:HG12	2:A:30:LEU:HG	1.86	0.57
2:C:888:ILE:HG12	2:C:960:TYR:CD2	2.39	0.57
2:C:2968:MET:O	2:C:2971:SER:OG	2.17	0.57
2:C:3170:LEU:HD12	2:C:3195:LEU:HD11	1.86	0.57
2:D:50:LEU:HD11	2:D:183:LEU:HD13	1.86	0.57
2:A:919:ARG:HG2	2:A:920:ASN:N	2.18	0.57
2:B:3366:LEU:HD11	2:B:3409:LEU:HD12	1.87	0.57
2:B:3384:ALA:O	2:B:3388:ALA:N	2.36	0.57
2:C:905:HIS:CE1	2:C:907:CYS:HB2	2.39	0.57
2:C:2209:MET:HE1	2:C:2254:HIS:ND1	2.20	0.57
2:C:3366:LEU:HD11	2:C:3409:LEU:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4868:ASP:OD1	2:C:4869:GLU:N	2.37	0.57
2:D:3943:LYS:O	2:D:4005:LYS:NZ	2.36	0.57
2:A:163:LYS:O	2:A:165:ARG:NH1	2.36	0.57
2:B:898:ARG:HH12	2:B:907:CYS:HB2	1.68	0.57
2:B:2265:GLY:HA2	2:B:2268:MET:HE1	1.86	0.57
2:B:3828:GLU:OE1	2:B:3828:GLU:N	2.33	0.57
2:C:29:VAL:HG12	2:C:30:LEU:HG	1.86	0.57
2:D:919:ARG:HG2	2:D:920:ASN:N	2.18	0.57
2:D:2246:GLN:OE1	2:D:2246:GLN:N	2.35	0.57
2:D:3170:LEU:HD12	2:D:3195:LEU:HD11	1.86	0.57
2:A:929:THR:HA	2:A:932:THR:CG2	2.35	0.57
2:A:957:PRO:HG2	2:A:960:TYR:CD1	2.40	0.57
2:C:50:LEU:HD11	2:C:183:LEU:HD13	1.86	0.57
2:D:2209:MET:HE1	2:D:2254:HIS:ND1	2.20	0.57
2:A:225:HIS:O	2:A:228:MET:HE2	2.04	0.57
2:A:3111:LEU:HD13	2:A:3183:TYR:CE2	2.40	0.57
2:B:892:TRP:HA	2:B:903:ARG:HE	1.70	0.57
2:C:3943:LYS:O	2:C:4005:LYS:NZ	2.36	0.57
2:D:29:VAL:HG12	2:D:30:LEU:HG	1.86	0.57
2:D:914:LEU:CD2	2:D:919:ARG:HB2	2.34	0.57
2:A:1281:GLN:O	2:A:1282:ASN:OD1	2.23	0.57
2:B:50:LEU:HD11	2:B:183:LEU:HD13	1.86	0.57
2:B:287:THR:HG21	2:B:482:GLU:OE2	2.04	0.57
2:B:2695:GLU:OE1	2:B:2698:ARG:NH2	2.37	0.57
2:C:287:THR:HG21	2:C:482:GLU:OE2	2.04	0.57
2:C:892:TRP:HA	2:C:903:ARG:HE	1.70	0.57
2:A:892:TRP:HA	2:A:903:ARG:HE	1.70	0.57
2:A:2968:MET:O	2:A:2971:SER:OG	2.17	0.57
2:A:3170:LEU:HD12	2:A:3195:LEU:HD11	1.86	0.57
2:A:3761:MET:HA	2:A:3761:MET:HE3	1.85	0.57
1:H:22:THR:N	1:H:108:GLU:O	2.37	0.57
2:D:2768:ALA:HB3	2:D:2858:PRO:HB3	1.87	0.57
2:B:3856:ALA:HB1	2:B:3871:ARG:HE	1.70	0.57
2:C:1281:GLN:O	2:C:1282:ASN:OD1	2.23	0.57
2:C:4675:LEU:HD23	2:C:4709:PHE:HE1	1.70	0.57
1:E:22:THR:N	1:E:108:GLU:O	2.38	0.56
2:D:929:THR:HA	2:D:932:THR:CG2	2.35	0.56
2:D:2166:LEU:HD21	2:D:2178:LEU:HD23	1.87	0.56
8:D:8009:A1BYZ:C5	8:D:8009:A1BYZ:C9	2.83	0.56
2:A:3524:ASN:O	2:A:3583:ARG:NH1	2.37	0.56
2:B:2209:MET:HE1	2:B:2254:HIS:ND1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4675:LEU:HD23	2:B:4709:PHE:HE1	1.70	0.56
2:C:3856:ALA:HB1	2:C:3871:ARG:HE	1.70	0.56
2:D:902:LYS:HB3	2:D:904:LEU:CG	2.28	0.56
2:D:2265:GLY:HA2	2:D:2268:MET:HE1	1.86	0.56
2:D:2877:GLU:OE2	2:D:2921:ARG:NE	2.38	0.56
2:D:3366:LEU:HD11	2:D:3409:LEU:HD12	1.87	0.56
2:D:3894:LEU:HB3	2:D:3902:PHE:CE2	2.41	0.56
2:A:3943:LYS:O	2:A:4005:LYS:NZ	2.36	0.56
2:B:2166:LEU:HD21	2:B:2178:LEU:HD23	1.87	0.56
2:B:3761:MET:HA	2:B:3761:MET:HE3	1.85	0.56
8:B:8009:A1BYZ:C5	8:B:8009:A1BYZ:C9	2.83	0.56
1:G:22:THR:N	1:G:108:GLU:O	2.38	0.56
2:D:3856:ALA:HB1	2:D:3871:ARG:HE	1.70	0.56
2:A:888:ILE:HG12	2:A:960:TYR:CD2	2.39	0.56
2:A:2166:LEU:HD21	2:A:2178:LEU:HD23	1.87	0.56
2:A:2209:MET:HE1	2:A:2254:HIS:ND1	2.20	0.56
2:A:2746:VAL:HG21	2:A:2818:ILE:HG22	1.87	0.56
2:A:3366:LEU:HD11	2:A:3409:LEU:HD12	1.87	0.56
2:A:3894:LEU:HB3	2:A:3902:PHE:CE2	2.41	0.56
2:B:888:ILE:HG12	2:B:960:TYR:CD2	2.39	0.56
2:B:888:ILE:CD1	2:B:960:TYR:HA	2.32	0.56
2:C:250:GLY:N	2:C:373:LEU:HD11	2.21	0.56
1:G:60:TRP:CZ2	2:C:1785:VAL:HG11	2.41	0.56
2:D:957:PRO:HG2	2:D:960:TYR:CD1	2.40	0.56
2:D:3384:ALA:O	2:D:3388:ALA:N	2.36	0.56
2:A:905:HIS:CE1	2:A:907:CYS:HB2	2.39	0.56
2:A:3384:ALA:O	2:A:3388:ALA:N	2.36	0.56
2:A:3856:ALA:HB1	2:A:3871:ARG:HE	1.70	0.56
2:B:905:HIS:CE1	2:B:907:CYS:HB2	2.39	0.56
2:B:914:LEU:HD11	2:B:919:ARG:N	2.21	0.56
2:B:929:THR:HA	2:B:932:THR:CG2	2.35	0.56
2:B:1281:GLN:O	2:B:1282:ASN:OD1	2.23	0.56
2:B:3111:LEU:HD13	2:B:3183:TYR:CE2	2.40	0.56
2:C:929:THR:HA	2:C:932:THR:CG2	2.35	0.56
2:C:2166:LEU:HD21	2:C:2178:LEU:HD23	1.87	0.56
2:C:2768:ALA:HB3	2:C:2858:PRO:HB3	1.87	0.56
8:C:8009:A1BYZ:C5	8:C:8009:A1BYZ:C9	2.83	0.56
2:D:892:TRP:HA	2:D:903:ARG:HE	1.70	0.56
2:B:2971:SER:HA	2:B:2974:PHE:CE1	2.41	0.56
1:F:22:THR:N	1:F:108:GLU:O	2.38	0.56
2:D:899:ASP:CB	2:D:902:LYS:HB2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3557:ASN:HB3	2:D:3560:LEU:HD12	1.88	0.56
2:A:2971:SER:HA	2:A:2974:PHE:CE1	2.41	0.56
2:B:29:VAL:HG12	2:B:30:LEU:HG	1.86	0.56
2:B:919:ARG:HG2	2:B:920:ASN:N	2.18	0.56
2:B:2746:VAL:HG21	2:B:2818:ILE:HG22	1.87	0.56
2:C:2234:CYS:SG	2:C:2271:SER:HB3	2.46	0.56
2:C:2971:SER:HA	2:C:2974:PHE:CE1	2.41	0.56
2:C:3384:ALA:O	2:C:3388:ALA:N	2.36	0.56
2:D:250:GLY:N	2:D:373:LEU:HD11	2.21	0.56
2:A:554:ARG:NE	2:A:556:GLU:OE2	2.39	0.56
2:A:881:GLU:HB3	2:A:969:ALA:N	2.21	0.56
2:B:957:PRO:HG2	2:B:960:TYR:CD1	2.40	0.56
2:B:3111:LEU:HD13	2:B:3183:TYR:HE2	1.71	0.56
2:B:3347:VAL:HG11	2:B:3415:ARG:HB2	1.88	0.56
2:D:914:LEU:HD11	2:D:919:ARG:N	2.21	0.56
2:A:250:GLY:N	2:A:373:LEU:HD11	2.21	0.56
2:C:914:LEU:HD11	2:C:919:ARG:N	2.21	0.56
2:C:2746:VAL:HG21	2:C:2818:ILE:HG22	1.87	0.56
2:C:3347:VAL:HG11	2:C:3415:ARG:HB2	1.88	0.56
2:D:888:ILE:CD1	2:D:960:TYR:HA	2.32	0.56
2:A:914:LEU:HD11	2:A:919:ARG:N	2.21	0.56
2:A:2877:GLU:OE2	2:A:2921:ARG:NE	2.38	0.56
2:A:4675:LEU:HD23	2:A:4709:PHE:HE1	1.70	0.56
8:A:8009:A1BYZ:C5	8:A:8009:A1BYZ:C9	2.83	0.56
2:B:3894:LEU:HB3	2:B:3902:PHE:CE2	2.41	0.56
2:C:902:LYS:HB3	2:C:904:LEU:CG	2.28	0.56
2:C:3686:GLU:OE1	2:C:3686:GLU:N	2.39	0.56
2:D:881:GLU:HB3	2:D:969:ALA:N	2.21	0.55
2:D:1281:GLN:O	2:D:1282:ASN:OD1	2.23	0.55
2:D:2234:CYS:SG	2:D:2271:SER:HB3	2.46	0.55
2:D:3111:LEU:HD13	2:D:3183:TYR:HE2	1.71	0.55
2:A:916:GLU:HA	2:A:919:ARG:NE	2.21	0.55
2:A:2234:CYS:SG	2:A:2271:SER:HB3	2.46	0.55
2:A:3686:GLU:OE1	2:A:3686:GLU:N	2.39	0.55
2:B:2234:CYS:SG	2:B:2271:SER:HB3	2.46	0.55
2:B:2947:LEU:O	2:B:2954:LYS:NZ	2.39	0.55
2:C:881:GLU:HB3	2:C:969:ALA:N	2.21	0.55
2:C:957:PRO:HG2	2:C:960:TYR:CD1	2.40	0.55
2:B:3377:GLU:OE1	2:B:3449:SER:OG	2.12	0.55
2:C:3894:LEU:HB3	2:C:3902:PHE:CE2	2.41	0.55
2:D:554:ARG:NE	2:D:556:GLU:OE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3828:GLU:OE1	2:D:3828:GLU:N	2.33	0.55
2:B:554:ARG:NE	2:B:556:GLU:OE2	2.39	0.55
2:B:2768:ALA:HB3	2:B:2858:PRO:HB3	1.87	0.55
2:C:1654:LEU:O	2:C:1661:GLN:NE2	2.36	0.55
2:D:2746:VAL:HG21	2:D:2818:ILE:HG22	1.87	0.55
2:B:881:GLU:O	2:B:968:PRO:HB3	2.07	0.55
2:C:2947:LEU:O	2:C:2954:LYS:NZ	2.39	0.55
2:D:4675:LEU:HD23	2:D:4709:PHE:HE1	1.70	0.55
2:A:881:GLU:O	2:A:968:PRO:HB3	2.07	0.55
2:A:2768:ALA:HB3	2:A:2858:PRO:HB3	1.87	0.55
2:B:916:GLU:HA	2:B:919:ARG:NE	2.21	0.55
2:C:554:ARG:NE	2:C:556:GLU:OE2	2.39	0.55
2:C:2877:GLU:OE2	2:C:2921:ARG:NE	2.38	0.55
2:D:881:GLU:O	2:D:968:PRO:HB3	2.07	0.55
2:D:3531:GLN:HA	2:D:3534:ILE:HD12	1.89	0.55
2:D:3686:GLU:N	2:D:3686:GLU:OE1	2.39	0.55
2:B:409:ALA:HB2	2:B:484:MET:HE1	1.89	0.55
2:B:3166:CYS:HB3	2:B:3202:MET:HE1	1.89	0.55
2:C:864:LEU:HD11	2:C:930:LEU:CB	2.37	0.55
2:D:952:LYS:HZ2	2:D:952:LYS:H	1.55	0.55
2:D:2971:SER:HA	2:D:2974:PHE:CE1	2.41	0.55
2:A:884:ALA:CB	2:A:968:PRO:HG3	2.37	0.55
2:B:881:GLU:HB3	2:B:969:ALA:N	2.21	0.55
2:B:899:ASP:CB	2:B:902:LYS:HB2	2.21	0.55
2:C:884:ALA:CB	2:C:968:PRO:HG3	2.37	0.55
2:C:3111:LEU:HD13	2:C:3183:TYR:HE2	1.71	0.55
2:A:3531:GLN:HA	2:A:3534:ILE:HD12	1.89	0.55
2:A:3557:ASN:HB3	2:A:3560:LEU:HD12	1.88	0.55
2:B:914:LEU:HD21	2:B:919:ARG:CB	2.37	0.55
2:B:3524:ASN:O	2:B:3583:ARG:NH1	2.37	0.55
2:C:1425:PRO:O	2:C:1429:LEU:HD23	2.07	0.55
2:C:2628:VAL:HG21	2:C:2675:LEU:HG	1.89	0.55
2:D:3524:ASN:O	2:D:3583:ARG:NH1	2.37	0.55
2:B:2257:TYR:O	2:B:2261:ASN:ND2	2.40	0.55
2:C:601:LEU:HD23	2:C:604:LEU:HD12	1.89	0.55
2:D:409:ALA:HB2	2:D:484:MET:HE1	1.89	0.55
2:D:916:GLU:HA	2:D:919:ARG:NE	2.21	0.55
2:A:3347:VAL:HG11	2:A:3415:ARG:HB2	1.88	0.55
2:C:916:GLU:HA	2:C:919:ARG:NE	2.21	0.55
2:C:942:MET:HE2	2:C:1052:TYR:CE1	2.42	0.55
2:C:3166:CYS:HB3	2:C:3202:MET:HE1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:942:MET:HE2	2:D:1052:TYR:CE1	2.42	0.54
2:D:2257:TYR:O	2:D:2261:ASN:ND2	2.40	0.54
2:D:2928:LEU:HA	2:D:2931:LEU:HD12	1.89	0.54
2:D:2947:LEU:O	2:D:2954:LYS:NZ	2.39	0.54
2:A:2928:LEU:HA	2:A:2931:LEU:HD12	1.89	0.54
2:A:3111:LEU:HD13	2:A:3183:TYR:HE2	1.71	0.54
2:A:3166:CYS:HB3	2:A:3202:MET:HE1	1.89	0.54
2:B:864:LEU:HD11	2:B:930:LEU:CB	2.37	0.54
2:D:3166:CYS:HB3	2:D:3202:MET:HE1	1.89	0.54
2:C:409:ALA:HB2	2:C:484:MET:HE1	1.89	0.54
2:C:2260:GLU:OE2	2:C:2298:LYS:NZ	2.41	0.54
2:D:601:LEU:HD23	2:D:604:LEU:HD12	1.89	0.54
2:D:2628:VAL:HG21	2:D:2675:LEU:HG	1.89	0.54
2:D:3506:VAL:O	2:D:3509:SER:OG	2.13	0.54
2:A:956:LEU:HD13	2:A:960:TYR:CB	2.36	0.54
2:B:884:ALA:CB	2:B:968:PRO:HG3	2.37	0.54
2:B:2628:VAL:HG21	2:B:2675:LEU:HG	1.89	0.54
2:B:3531:GLN:HA	2:B:3534:ILE:HD12	1.89	0.54
2:C:881:GLU:O	2:C:968:PRO:HB3	2.07	0.54
2:D:956:LEU:HD13	2:D:960:TYR:CB	2.36	0.54
2:D:3347:VAL:HG11	2:D:3415:ARG:HB2	1.88	0.54
2:A:942:MET:HE2	2:A:1052:TYR:CE1	2.42	0.54
2:A:3828:GLU:N	2:A:3828:GLU:OE1	2.33	0.54
2:B:3557:ASN:HB3	2:B:3560:LEU:HD12	1.88	0.54
2:C:2257:TYR:O	2:C:2261:ASN:ND2	2.40	0.54
1:G:26:HIS:CE1	1:G:105:LEU:HD11	2.43	0.54
2:A:409:ALA:HB2	2:A:484:MET:HE1	1.89	0.54
2:B:2877:GLU:OE2	2:B:2921:ARG:NE	2.38	0.54
2:B:3686:GLU:OE1	2:B:3686:GLU:N	2.39	0.54
2:C:914:LEU:HD21	2:C:919:ARG:CB	2.37	0.54
2:A:3077:ASP:O	2:A:3081:VAL:HG23	2.08	0.54
2:B:1425:PRO:O	2:B:1429:LEU:HD23	2.07	0.54
2:B:2260:GLU:OE2	2:B:2298:LYS:NZ	2.41	0.54
2:D:884:ALA:CB	2:D:968:PRO:HG3	2.37	0.54
2:A:3443:PHE:CG	2:A:3515:LEU:HD22	2.43	0.54
2:C:139:GLN:NE2	2:C:141:ASP:O	2.41	0.54
2:B:884:ALA:HB3	2:B:968:PRO:HB3	1.90	0.54
2:C:3531:GLN:HA	2:C:3534:ILE:HD12	1.89	0.54
1:H:26:HIS:CE1	1:H:105:LEU:HD11	2.43	0.54
2:D:139:GLN:NE2	2:D:141:ASP:O	2.41	0.54
2:D:1425:PRO:O	2:D:1429:LEU:HD23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3443:PHE:CG	2:D:3515:LEU:HD22	2.43	0.54
8:D:8009:A1BYZ:C9	8:D:8009:A1BYZ:C4	2.86	0.54
2:A:874:LYS:HB2	2:A:874:LYS:NZ	2.23	0.54
2:A:914:LEU:HD21	2:A:919:ARG:CB	2.37	0.54
2:A:2260:GLU:OE2	2:A:2298:LYS:NZ	2.41	0.54
2:A:2947:LEU:O	2:A:2954:LYS:NZ	2.39	0.54
2:B:250:GLY:N	2:B:373:LEU:HD11	2.21	0.54
2:B:942:MET:HE2	2:B:1052:TYR:CE1	2.42	0.54
2:B:2928:LEU:HA	2:B:2931:LEU:HD12	1.89	0.54
2:B:3541:TYR:OH	2:B:3598:GLN:NE2	2.31	0.54
2:C:1821:VAL:HG22	2:C:1927:LEU:HD21	1.90	0.54
2:C:3388:ALA:O	2:C:3392:GLU:N	2.39	0.54
2:A:139:GLN:NE2	2:A:141:ASP:O	2.41	0.54
2:B:139:GLN:NE2	2:B:141:ASP:O	2.41	0.54
2:B:2878:GLN:OE1	2:B:2940:ARG:NH1	2.41	0.54
2:B:3443:PHE:CG	2:B:3515:LEU:HD22	2.43	0.54
2:C:2382:GLU:C	2:C:2386:ARG:HH12	2.16	0.54
2:D:215:VAL:HG12	2:D:275:LEU:HD12	1.90	0.53
2:D:905:HIS:ND1	2:D:907:CYS:HB2	2.23	0.53
2:D:1821:VAL:HG22	2:D:1927:LEU:HD21	1.90	0.53
2:A:1425:PRO:O	2:A:1429:LEU:HD23	2.07	0.53
2:A:2878:GLN:OE1	2:A:2940:ARG:NH1	2.41	0.53
8:A:8009:A1BYZ:C9	8:A:8009:A1BYZ:C4	2.86	0.53
2:B:2802:ASP:OD1	2:B:2803:LYS:N	2.41	0.53
2:C:956:LEU:HD13	2:C:960:TYR:CB	2.36	0.53
2:C:2878:GLN:OE1	2:C:2940:ARG:NH1	2.41	0.53
1:E:58:ARG:O	1:E:62:GLU:OE1	2.26	0.53
2:D:2878:GLN:OE1	2:D:2940:ARG:NH1	2.41	0.53
2:D:3672:ASP:OD1	2:D:3735:HIS:NE2	2.36	0.53
2:A:884:ALA:HB3	2:A:968:PRO:HB3	1.90	0.53
2:B:872:ARG:HH12	2:B:923:LEU:HD22	1.72	0.53
2:B:2314:LEU:HD11	2:B:2417:VAL:HG11	1.90	0.53
2:C:942:MET:HB2	2:C:1052:TYR:CE1	2.43	0.53
1:F:26:HIS:CE1	1:F:105:LEU:HD11	2.43	0.53
2:D:872:ARG:HH12	2:D:923:LEU:HD22	1.72	0.53
2:A:864:LEU:HD11	2:A:930:LEU:CB	2.37	0.53
2:A:2628:VAL:HG21	2:A:2675:LEU:HG	1.89	0.53
2:A:3108:VAL:HG12	2:A:3176:LEU:HD12	1.91	0.53
2:B:942:MET:HB2	2:B:1052:TYR:CE1	2.43	0.53
2:C:215:VAL:HG12	2:C:275:LEU:HD12	1.90	0.53
2:C:872:ARG:HH12	2:C:923:LEU:HD22	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3557:ASN:HB3	2:C:3560:LEU:HD12	1.88	0.53
8:C:8009:A1BYZ:C9	8:C:8009:A1BYZ:C4	2.86	0.53
2:D:884:ALA:HB3	2:D:968:PRO:HB3	1.90	0.53
2:D:2260:GLU:OE2	2:D:2298:LYS:NZ	2.41	0.53
2:D:2314:LEU:HD11	2:D:2417:VAL:HG11	1.90	0.53
2:D:2802:ASP:OD1	2:D:2803:LYS:N	2.41	0.53
2:B:903:ARG:HA	2:B:903:ARG:NH2	2.21	0.53
2:B:3108:VAL:HG12	2:B:3176:LEU:HD12	1.91	0.53
2:B:3515:LEU:HD21	2:B:3603:VAL:HG13	1.91	0.53
8:B:8009:A1BYZ:C9	8:B:8009:A1BYZ:C4	2.86	0.53
2:C:905:HIS:ND1	2:C:907:CYS:HB2	2.24	0.53
2:C:2913:THR:HG23	2:C:2916:GLU:OE1	2.08	0.53
2:C:2928:LEU:HA	2:C:2931:LEU:HD12	1.89	0.53
2:A:601:LEU:HD23	2:A:604:LEU:HD12	1.89	0.53
2:A:2802:ASP:OD1	2:A:2803:LYS:N	2.41	0.53
2:B:1654:LEU:O	2:B:1661:GLN:NE2	2.36	0.53
2:B:3672:ASP:OD1	2:B:3735:HIS:NE2	2.36	0.53
2:C:3077:ASP:O	2:C:3081:VAL:HG23	2.08	0.53
2:C:3443:PHE:CG	2:C:3515:LEU:HD22	2.43	0.53
2:D:914:LEU:HD21	2:D:919:ARG:CB	2.37	0.53
2:D:1654:LEU:O	2:D:1661:GLN:NE2	2.36	0.53
2:D:2382:GLU:C	2:D:2386:ARG:HH12	2.16	0.53
2:A:215:VAL:HG12	2:A:275:LEU:HD12	1.90	0.53
2:A:3380:LEU:HD21	2:A:3395:VAL:HG21	1.91	0.53
2:B:905:HIS:ND1	2:B:907:CYS:HB2	2.23	0.53
2:B:958:LYS:HA	2:B:961:MET:HE3	1.91	0.53
2:B:1821:VAL:HG22	2:B:1927:LEU:HD21	1.90	0.53
2:C:958:LYS:HA	2:C:961:MET:HE3	1.91	0.53
2:D:864:LEU:HD11	2:D:930:LEU:CB	2.37	0.53
2:A:899:ASP:CB	2:A:902:LYS:HB2	2.21	0.53
2:A:3344:GLN:O	2:A:3347:VAL:HG12	2.09	0.53
2:B:3077:ASP:O	2:B:3081:VAL:HG23	2.08	0.53
2:C:2802:ASP:OD1	2:C:2803:LYS:N	2.41	0.53
2:C:3311:ASP:OD1	2:C:3312:HIS:N	2.42	0.53
2:C:3515:LEU:HD21	2:C:3603:VAL:HG13	1.91	0.53
2:D:168:ASP:OD1	2:C:385:MET:HE1	2.09	0.53
2:D:898:ARG:HH11	2:D:906:PRO:HD2	1.74	0.53
2:A:1758:GLY:N	2:A:1759:PRO:CD	2.72	0.53
2:A:2913:THR:HG23	2:A:2916:GLU:OE1	2.08	0.53
2:C:2314:LEU:HD11	2:C:2417:VAL:HG11	1.90	0.53
2:C:3380:LEU:HD21	2:C:3395:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:58:ARG:O	1:H:62:GLU:OE1	2.27	0.53
2:A:385:MET:HE1	2:B:168:ASP:OD1	2.09	0.53
2:B:2382:GLU:C	2:B:2386:ARG:HH12	2.16	0.53
1:E:26:HIS:CE1	1:E:105:LEU:HD11	2.44	0.53
1:G:58:ARG:O	1:G:62:GLU:OE1	2.26	0.53
2:D:32:GLU:OE2	2:D:33:GLN:N	2.42	0.53
2:D:942:MET:HB2	2:D:1052:TYR:CE1	2.43	0.53
2:D:2913:THR:HG23	2:D:2916:GLU:OE1	2.08	0.53
2:D:3344:GLN:O	2:D:3347:VAL:HG12	2.09	0.53
2:D:3380:LEU:HD21	2:D:3395:VAL:HG21	1.91	0.53
2:A:872:ARG:HH12	2:A:923:LEU:HD22	1.72	0.53
2:A:905:HIS:ND1	2:A:907:CYS:HB2	2.24	0.53
2:B:3344:GLN:O	2:B:3347:VAL:HG12	2.09	0.53
2:B:3380:LEU:HD21	2:B:3395:VAL:HG21	1.91	0.53
2:B:4675:LEU:HD23	2:B:4709:PHE:CE1	2.44	0.53
2:C:3108:VAL:HG12	2:C:3176:LEU:HD12	1.91	0.53
2:D:874:LYS:NZ	2:D:874:LYS:HB2	2.23	0.52
2:D:3077:ASP:O	2:D:3081:VAL:HG23	2.08	0.52
2:A:32:GLU:OE2	2:A:33:GLN:N	2.42	0.52
2:A:912:HIS:HA	2:A:919:ARG:CZ	2.39	0.52
2:A:2382:GLU:C	2:A:2386:ARG:HH12	2.16	0.52
2:B:32:GLU:OE2	2:B:33:GLN:N	2.42	0.52
2:B:956:LEU:HD13	2:B:960:TYR:CB	2.36	0.52
2:B:1758:GLY:N	2:B:1759:PRO:CD	2.72	0.52
2:C:874:LYS:HB2	2:C:874:LYS:NZ	2.23	0.52
2:D:912:HIS:HA	2:D:919:ARG:CZ	2.40	0.52
2:A:2382:GLU:O	2:A:2386:ARG:NH1	2.42	0.52
2:A:3515:LEU:HD21	2:A:3603:VAL:HG13	1.91	0.52
2:B:874:LYS:HB2	2:B:874:LYS:NZ	2.23	0.52
2:C:32:GLU:OE2	2:C:33:GLN:N	2.42	0.52
2:D:2382:GLU:O	2:D:2386:ARG:NH1	2.42	0.52
2:A:942:MET:HB2	2:A:1052:TYR:CE1	2.43	0.52
2:A:2257:TYR:O	2:A:2261:ASN:ND2	2.40	0.52
2:B:215:VAL:HG12	2:B:275:LEU:HD12	1.90	0.52
2:B:601:LEU:HD23	2:B:604:LEU:HD12	1.89	0.52
2:B:912:HIS:HA	2:B:919:ARG:CZ	2.40	0.52
2:B:2913:THR:HG23	2:B:2916:GLU:OE1	2.08	0.52
2:C:2382:GLU:O	2:C:2386:ARG:NH1	2.42	0.52
2:C:3672:ASP:OD1	2:C:3735:HIS:NE2	2.36	0.52
2:D:979:THR:O	2:D:983:THR:HG23	2.10	0.52
2:D:2737:ASP:OD1	2:D:2739:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3108:VAL:HG12	2:D:3176:LEU:HD12	1.91	0.52
2:D:3515:LEU:HD21	2:D:3603:VAL:HG13	1.91	0.52
2:B:898:ARG:HH11	2:B:906:PRO:HD2	1.74	0.52
2:C:884:ALA:HB3	2:C:968:PRO:HB3	1.90	0.52
2:D:2005:GLU:N	2:D:2005:GLU:OE1	2.43	0.52
2:A:3584:GLU:OE1	2:A:3584:GLU:N	2.37	0.52
2:B:2005:GLU:OE1	2:B:2005:GLU:N	2.43	0.52
2:C:912:HIS:HA	2:C:919:ARG:CZ	2.40	0.52
2:C:979:THR:O	2:C:983:THR:HG23	2.10	0.52
2:C:1758:GLY:N	2:C:1759:PRO:CD	2.72	0.52
2:C:2737:ASP:OD1	2:C:2739:ARG:NH1	2.43	0.52
2:C:3344:GLN:O	2:C:3347:VAL:HG12	2.09	0.52
2:D:3311:ASP:OD1	2:D:3312:HIS:N	2.42	0.52
2:A:898:ARG:HH11	2:A:906:PRO:HD2	1.74	0.52
2:A:1821:VAL:HG22	2:A:1927:LEU:HD21	1.90	0.52
2:A:2737:ASP:OD1	2:A:2739:ARG:NH1	2.43	0.52
2:A:3311:ASP:OD1	2:A:3312:HIS:N	2.42	0.52
2:B:385:MET:HE1	2:C:168:ASP:OD1	2.09	0.52
2:B:2382:GLU:O	2:B:2386:ARG:NH1	2.42	0.52
2:B:3079:ARG:NH1	2:B:3156:ASP:OD2	2.43	0.52
2:C:3584:GLU:OE1	2:C:3584:GLU:N	2.37	0.52
2:A:2314:LEU:HD11	2:A:2417:VAL:HG11	1.90	0.52
2:C:898:ARG:HH11	2:C:906:PRO:HD2	1.74	0.52
2:C:2213:VAL:HG11	2:C:2257:TYR:OH	2.10	0.52
2:C:3079:ARG:NH1	2:C:3156:ASP:OD2	2.43	0.52
2:C:4981:HIS:O	5:C:8003:ATP:N6	2.43	0.52
2:D:1758:GLY:N	2:D:1759:PRO:CD	2.72	0.52
2:D:2741:VAL:HG11	2:D:2820:TRP:NE1	2.25	0.52
2:A:958:LYS:HA	2:A:961:MET:HE3	1.91	0.52
2:A:1164:THR:HG22	2:A:1169:VAL:HA	1.92	0.52
2:A:2741:VAL:HG11	2:A:2820:TRP:NE1	2.25	0.52
2:B:2226:PHE:N	2:B:2227:PRO:HD3	2.25	0.52
2:C:71:GLU:OE1	2:C:111:ARG:NH2	2.42	0.52
2:C:2226:PHE:N	2:C:2227:PRO:HD3	2.25	0.52
2:D:958:LYS:HA	2:D:961:MET:HE3	1.91	0.52
2:A:2213:VAL:HG11	2:A:2257:TYR:OH	2.10	0.52
2:A:2226:PHE:N	2:A:2227:PRO:HD3	2.25	0.52
2:B:605:CYS:SG	2:B:1670:LEU:HD12	2.50	0.52
2:D:103:LEU:HD23	2:D:163:LYS:HA	1.92	0.52
2:D:868:LEU:HD13	2:D:930:LEU:HG	1.92	0.52
2:A:868:LEU:HD13	2:A:930:LEU:HG	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2005:GLU:N	2:A:2005:GLU:OE1	2.43	0.52
2:A:4675:LEU:HD23	2:A:4709:PHE:CE1	2.44	0.52
2:B:103:LEU:HD23	2:B:163:LYS:HA	1.92	0.52
2:B:2863:LEU:HD22	2:B:2929:LYS:HB3	1.93	0.52
2:B:3311:ASP:OD1	2:B:3312:HIS:N	2.42	0.52
2:C:4675:LEU:HD23	2:C:4709:PHE:CE1	2.44	0.52
2:D:2007:ILE:HD11	2:D:3642:LEU:HD21	1.93	0.51
2:A:605:CYS:SG	2:A:1670:LEU:HD12	2.50	0.51
2:B:979:THR:O	2:B:983:THR:HG23	2.10	0.51
2:B:2737:ASP:OD1	2:B:2739:ARG:NH1	2.43	0.51
2:C:2005:GLU:OE1	2:C:2005:GLU:N	2.43	0.51
2:D:71:GLU:OE1	2:D:111:ARG:NH2	2.42	0.51
2:D:4675:LEU:HD23	2:D:4709:PHE:CE1	2.44	0.51
2:D:4981:HIS:O	5:D:8003:ATP:N6	2.43	0.51
2:A:898:ARG:O	2:A:898:ARG:HG2	2.11	0.51
2:A:2007:ILE:HD11	2:A:3642:LEU:HD21	1.92	0.51
2:B:608:CYS:SG	2:B:1673:SER:OG	2.69	0.51
2:C:1164:THR:HG22	2:C:1169:VAL:HA	1.92	0.51
2:C:2741:VAL:HG11	2:C:2820:TRP:NE1	2.25	0.51
2:D:1164:THR:HG22	2:D:1169:VAL:HA	1.92	0.51
2:D:2226:PHE:N	2:D:2227:PRO:HD3	2.25	0.51
2:D:3337:LYS:O	2:D:3341:VAL:HG23	2.11	0.51
2:A:2542:PHE:O	2:A:2545:THR:OG1	2.28	0.51
2:B:1164:THR:HG22	2:B:1169:VAL:HA	1.92	0.51
2:B:2741:VAL:HG11	2:B:2820:TRP:NE1	2.25	0.51
2:C:2007:ILE:HD11	2:C:3642:LEU:HD21	1.93	0.51
2:C:4953:GLU:N	2:C:4953:GLU:OE2	2.44	0.51
1:F:58:ARG:O	1:F:62:GLU:OE1	2.28	0.51
2:D:2213:VAL:HG11	2:D:2257:TYR:OH	2.10	0.51
2:A:2863:LEU:HD22	2:A:2929:LYS:HB3	1.93	0.51
2:A:4964:ASP:OD1	2:A:4965:TYR:N	2.44	0.51
2:B:942:MET:HB2	2:B:1052:TYR:CD1	2.46	0.51
2:B:2213:VAL:HG11	2:B:2257:TYR:OH	2.10	0.51
2:B:4981:HIS:O	5:B:8003:ATP:N6	2.43	0.51
2:D:1063:GLN:OE1	2:D:1063:GLN:N	2.44	0.51
2:D:4964:ASP:OD1	2:D:4965:TYR:N	2.44	0.51
2:A:1063:GLN:OE1	2:A:1063:GLN:N	2.44	0.51
2:C:605:CYS:SG	2:C:1670:LEU:HD12	2.50	0.51
2:C:4964:ASP:OD1	2:C:4965:TYR:N	2.44	0.51
2:D:605:CYS:SG	2:D:1670:LEU:HD12	2.50	0.51
2:D:1116:LEU:HD12	2:D:1194:SER:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3079:ARG:NH1	2:D:3156:ASP:OD2	2.43	0.51
2:A:3515:LEU:HD23	2:A:3607:LEU:HD21	1.93	0.51
2:B:909:VAL:HG21	2:B:914:LEU:HA	1.93	0.51
2:B:4964:ASP:OD1	2:B:4965:TYR:N	2.44	0.51
2:D:1297:GLN:NE2	2:D:1546:ASN:OD1	2.44	0.51
2:D:3515:LEU:HD23	2:D:3607:LEU:HD21	1.93	0.51
2:D:4953:GLU:N	2:D:4953:GLU:OE2	2.44	0.51
2:A:885:LEU:HD12	2:A:960:TYR:HE2	1.76	0.51
2:A:979:THR:O	2:A:983:THR:HG23	2.10	0.51
2:B:2007:ILE:HD11	2:B:3642:LEU:HD21	1.93	0.51
2:B:3861:MET:N	2:B:3861:MET:SD	2.84	0.51
2:B:4953:GLU:N	2:B:4953:GLU:OE2	2.44	0.51
2:C:942:MET:HB2	2:C:1052:TYR:CD1	2.46	0.51
2:D:385:MET:HE1	2:A:168:ASP:OD1	2.11	0.51
2:A:3079:ARG:NH1	2:A:3156:ASP:OD2	2.43	0.51
2:A:4953:GLU:N	2:A:4953:GLU:OE2	2.44	0.51
2:B:868:LEU:HD13	2:B:930:LEU:HG	1.92	0.51
2:C:883:TRP:CH2	2:C:907:CYS:HB3	2.46	0.51
2:C:909:VAL:HG21	2:C:914:LEU:HA	1.93	0.51
2:D:887:ARG:HA	2:D:890:GLN:CD	2.36	0.51
2:D:3354:LEU:HA	2:D:3357:SER:OG	2.11	0.51
7:D:8005:PCW:H442	7:D:8005:PCW:H20	1.93	0.51
2:B:2882:ASN:O	2:B:2886:THR:HG23	2.11	0.51
2:C:885:LEU:HD12	2:C:960:TYR:HE2	1.76	0.51
2:C:887:ARG:HA	2:C:890:GLN:CD	2.36	0.51
2:C:898:ARG:O	2:C:898:ARG:HG2	2.11	0.51
2:C:909:VAL:HG23	2:C:914:LEU:HB2	1.93	0.51
2:C:1116:LEU:HD12	2:C:1194:SER:HB3	1.93	0.51
2:D:2873:GLN:O	2:D:2877:GLU:HG2	2.11	0.51
2:A:903:ARG:HA	2:A:903:ARG:NH2	2.21	0.51
2:A:3337:LYS:O	2:A:3341:VAL:HG23	2.11	0.51
2:A:4981:HIS:O	5:A:8003:ATP:N6	2.43	0.51
2:B:887:ARG:HA	2:B:890:GLN:CD	2.36	0.51
2:B:1063:GLN:OE1	2:B:1063:GLN:N	2.44	0.51
2:B:1645:GLU:OE1	2:B:1647:ARG:NH2	2.43	0.51
2:D:843:PRO:O	2:D:1198:GLY:N	2.38	0.50
2:A:887:ARG:HA	2:A:890:GLN:CD	2.36	0.50
2:A:942:MET:HB2	2:A:1052:TYR:CD1	2.46	0.50
2:A:3861:MET:N	2:A:3861:MET:SD	2.84	0.50
2:B:885:LEU:HD12	2:B:960:TYR:HE2	1.76	0.50
2:B:3354:LEU:HA	2:B:3357:SER:OG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:883:TRP:CH2	2:D:907:CYS:HB3	2.46	0.50
2:D:3861:MET:N	2:D:3861:MET:SD	2.84	0.50
2:B:1116:LEU:HD12	2:B:1194:SER:HB3	1.93	0.50
2:C:868:LEU:HD13	2:C:930:LEU:HG	1.92	0.50
2:C:2863:LEU:HD22	2:C:2929:LYS:HB3	1.92	0.50
2:C:3861:MET:SD	2:C:3861:MET:N	2.84	0.50
2:D:885:LEU:HD12	2:D:960:TYR:HE2	1.76	0.50
2:A:103:LEU:HD23	2:A:163:LYS:HA	1.92	0.50
2:A:1116:LEU:HD12	2:A:1194:SER:HB3	1.92	0.50
2:B:953:LYS:HE3	2:B:969:ALA:HB1	1.93	0.50
2:C:2882:ASN:O	2:C:2886:THR:HG23	2.11	0.50
2:C:3337:LYS:O	2:C:3341:VAL:HG23	2.11	0.50
2:D:985:LEU:HD21	2:D:1057:PRO:CD	2.42	0.50
2:D:2961:LEU:HD21	2:D:3040:ILE:HD13	1.94	0.50
2:A:3645:LEU:HD21	2:A:3653:MET:HE3	1.93	0.50
2:B:2961:LEU:HD21	2:B:3040:ILE:HD13	1.94	0.50
2:B:3388:ALA:O	2:B:3392:GLU:N	2.39	0.50
2:D:71:GLU:OE1	2:D:111:ARG:NE	2.44	0.50
2:D:2882:ASN:O	2:D:2886:THR:HG23	2.11	0.50
2:D:3645:LEU:HD21	2:D:3653:MET:HE3	1.93	0.50
2:B:848:SER:N	2:B:851:ASP:OD1	2.43	0.50
2:B:898:ARG:HB2	2:B:905:HIS:CD2	2.47	0.50
2:B:902:LYS:HG3	2:B:904:LEU:HD11	1.93	0.50
2:B:3534:ILE:HG13	2:B:3597:VAL:HG23	1.94	0.50
7:C:8005:PCW:H442	7:C:8005:PCW:H20	1.93	0.50
2:D:2372:GLU:HG2	2:A:197:MET:CE	2.39	0.50
2:D:2600:GLN:O	2:D:2604:ILE:HG12	2.12	0.50
2:D:3584:GLU:OE1	2:D:3584:GLU:N	2.37	0.50
2:B:3515:LEU:HD23	2:B:3607:LEU:HD21	1.93	0.50
2:C:2600:GLN:O	2:C:2604:ILE:HG12	2.12	0.50
2:D:898:ARG:O	2:D:898:ARG:HG2	2.11	0.50
2:D:942:MET:HB2	2:D:1052:TYR:CD1	2.46	0.50
2:D:2863:LEU:HD22	2:D:2929:LYS:HB3	1.93	0.50
2:A:883:TRP:CH2	2:A:907:CYS:HB3	2.46	0.50
2:A:3354:LEU:HA	2:A:3357:SER:OG	2.11	0.50
2:B:2600:GLN:O	2:B:2604:ILE:HG12	2.12	0.50
2:B:2873:GLN:O	2:B:2877:GLU:HG2	2.11	0.50
2:B:2877:GLU:OE1	2:B:2909:TYR:OH	2.21	0.50
2:B:3025:VAL:HG23	2:B:3025:VAL:O	2.12	0.50
2:C:976:VAL:HG11	2:C:1045:ARG:O	2.12	0.50
2:C:1063:GLN:N	2:C:1063:GLN:OE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3354:LEU:HA	2:C:3357:SER:OG	2.11	0.50
2:D:3025:VAL:HG23	2:D:3025:VAL:O	2.12	0.50
2:D:4875:ASP:O	2:C:4580:VAL:HG12	2.12	0.50
2:A:898:ARG:HB2	2:A:905:HIS:CD2	2.47	0.50
2:B:877:GLU:HG3	2:B:911:PHE:CG	2.47	0.50
2:C:953:LYS:HE3	2:C:969:ALA:HB1	1.93	0.50
2:C:985:LEU:HD21	2:C:1057:PRO:CD	2.42	0.50
2:C:2873:GLN:O	2:C:2877:GLU:HG2	2.11	0.50
2:C:3025:VAL:HG23	2:C:3025:VAL:O	2.12	0.50
2:C:3515:LEU:HD23	2:C:3607:LEU:HD21	1.93	0.50
2:D:953:LYS:HE3	2:D:969:ALA:HB1	1.93	0.50
2:A:909:VAL:HG21	2:A:914:LEU:HA	1.93	0.50
2:A:3534:ILE:HG13	2:A:3597:VAL:HG23	1.94	0.50
2:B:3337:LYS:O	2:B:3341:VAL:HG23	2.11	0.50
2:C:3645:LEU:HD21	2:C:3653:MET:HE3	1.93	0.50
2:C:3691:VAL:HG12	2:C:3693:GLU:H	1.77	0.50
2:D:909:VAL:HG23	2:D:914:LEU:HB2	1.93	0.49
2:A:1758:GLY:N	2:A:1759:PRO:HD2	2.27	0.49
7:A:8005:PCW:H442	7:A:8005:PCW:H20	1.93	0.49
2:B:258:ARG:O	2:B:285:HIS:NE2	2.42	0.49
2:B:976:VAL:HG11	2:B:1045:ARG:O	2.12	0.49
2:B:3591:GLU:O	2:B:3594:VAL:HG12	2.12	0.49
2:D:902:LYS:HG3	2:D:904:LEU:HD11	1.93	0.49
2:A:976:VAL:HG11	2:A:1045:ARG:O	2.12	0.49
2:A:985:LEU:HD21	2:A:1057:PRO:CD	2.42	0.49
2:A:2600:GLN:O	2:A:2604:ILE:HG12	2.12	0.49
2:A:2873:GLN:O	2:A:2877:GLU:HG2	2.12	0.49
2:A:2961:LEU:HD21	2:A:3040:ILE:HD13	1.94	0.49
2:A:3691:VAL:HG12	2:A:3693:GLU:H	1.77	0.49
2:C:898:ARG:HB2	2:C:905:HIS:CD2	2.47	0.49
2:C:1758:GLY:N	2:C:1759:PRO:HD2	2.27	0.49
2:D:898:ARG:HB2	2:D:905:HIS:CD2	2.47	0.49
2:D:976:VAL:HG11	2:D:1045:ARG:O	2.12	0.49
2:B:898:ARG:O	2:B:898:ARG:HG2	2.11	0.49
2:B:985:LEU:HD21	2:B:1057:PRO:CD	2.42	0.49
2:C:4122:GLU:OE1	2:C:4122:GLU:N	2.44	0.49
2:D:909:VAL:HG21	2:D:914:LEU:HA	1.93	0.49
2:A:608:CYS:SG	2:A:1673:SER:OG	2.69	0.49
2:A:877:GLU:HG3	2:A:911:PHE:CG	2.47	0.49
2:A:909:VAL:HG23	2:A:914:LEU:HB2	1.93	0.49
2:A:2882:ASN:O	2:A:2886:THR:HG23	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:909:VAL:HG23	2:B:914:LEU:HB2	1.93	0.49
2:B:2234:CYS:O	2:B:2237:LEU:N	2.46	0.49
2:B:2875:MET:HB3	2:B:2940:ARG:HB2	1.94	0.49
2:B:3220:TYR:CD1	2:B:3237:VAL:HG12	2.48	0.49
2:C:3591:GLU:O	2:C:3594:VAL:HG12	2.12	0.49
2:D:1758:GLY:N	2:D:1759:PRO:HD2	2.27	0.49
2:D:3534:ILE:HG13	2:D:3597:VAL:HG23	1.94	0.49
2:D:3691:VAL:HG12	2:D:3693:GLU:H	1.77	0.49
2:A:902:LYS:HG3	2:A:904:LEU:HD11	1.93	0.49
2:A:1645:GLU:OE1	2:A:1647:ARG:NH2	2.43	0.49
2:A:2875:MET:HB3	2:A:2940:ARG:HB2	1.94	0.49
2:C:103:LEU:HD23	2:C:163:LYS:HA	1.92	0.49
2:A:1297:GLN:NE2	2:A:1546:ASN:OD1	2.44	0.49
2:C:902:LYS:HG3	2:C:904:LEU:HD11	1.93	0.49
2:C:903:ARG:HA	2:C:903:ARG:NH2	2.21	0.49
2:C:2234:CYS:O	2:C:2237:LEU:N	2.46	0.49
2:C:3220:TYR:CD1	2:C:3237:VAL:HG12	2.48	0.49
2:D:500:THR:HG23	2:D:503:HIS:H	1.77	0.49
2:D:877:GLU:HG3	2:D:911:PHE:CG	2.47	0.49
2:D:3317:LEU:HD23	2:D:3354:LEU:CD2	2.43	0.49
2:A:71:GLU:OE1	2:A:111:ARG:NH2	2.42	0.49
2:A:3025:VAL:HG23	2:A:3025:VAL:O	2.12	0.49
2:A:3230:ILE:HG13	2:A:3231:LEU:HD12	1.95	0.49
2:C:848:SER:N	2:C:851:ASP:OD1	2.43	0.49
2:C:3230:ILE:HG13	2:C:3231:LEU:HD12	1.95	0.49
2:D:3176:LEU:HD23	2:D:3176:LEU:C	2.38	0.49
2:C:673:ALA:O	2:C:681:THR:OG1	2.31	0.49
2:C:877:GLU:HG3	2:C:911:PHE:CG	2.47	0.49
2:C:2961:LEU:HD21	2:C:3040:ILE:HD13	1.94	0.49
2:D:1536:GLU:OE1	2:D:1536:GLU:N	2.46	0.49
2:D:2246:GLN:NE2	2:D:3867:THR:O	2.46	0.49
2:D:3230:ILE:HG13	2:D:3231:LEU:HD12	1.95	0.49
2:A:940:VAL:HG23	2:A:1052:TYR:HB3	1.95	0.49
2:A:3317:LEU:HD23	2:A:3354:LEU:CD2	2.43	0.49
2:B:883:TRP:CH2	2:B:907:CYS:HB3	2.46	0.49
2:B:940:VAL:HG23	2:B:1052:TYR:HB3	1.95	0.49
7:B:8005:PCW:H442	7:B:8005:PCW:H20	1.93	0.49
2:C:258:ARG:O	2:C:285:HIS:NE2	2.42	0.49
2:C:500:THR:HG23	2:C:503:HIS:H	1.77	0.49
2:C:2415:ASN:O	2:C:2415:ASN:ND2	2.46	0.49
2:C:3176:LEU:HD23	2:C:3176:LEU:C	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4747:GLU:OE2	2:A:4747:GLU:HA	2.13	0.49
2:B:295:THR:O	2:B:299:GLY:N	2.46	0.49
2:B:673:ALA:O	2:B:681:THR:OG1	2.30	0.49
2:B:957:PRO:HB2	2:B:959:THR:HG23	1.95	0.49
2:B:3230:ILE:HG13	2:B:3231:LEU:HD12	1.95	0.49
2:B:3317:LEU:HD23	2:B:3354:LEU:CD2	2.43	0.49
2:C:2246:GLN:NE2	2:C:3867:THR:O	2.46	0.49
2:C:3435:LEU:CD2	2:C:3518:MET:HE2	2.42	0.49
2:D:2583:MET:HE3	2:D:2611:LEU:HD23	1.95	0.48
2:A:953:LYS:HE3	2:A:969:ALA:HB1	1.93	0.48
2:A:2246:GLN:NE2	2:A:3867:THR:O	2.46	0.48
2:B:2394:ASP:OD2	2:B:2419:LEU:N	2.46	0.48
2:B:4054:SER:O	2:B:4056:SER:N	2.46	0.48
2:C:2875:MET:HB3	2:C:2940:ARG:HB2	1.94	0.48
2:C:3317:LEU:HD23	2:C:3354:LEU:CD2	2.43	0.48
2:C:3556:ASN:OD1	2:C:3557:ASN:N	2.46	0.48
2:D:1783:CYS:SG	2:D:1785:VAL:HG22	2.53	0.48
2:D:2746:VAL:HG22	2:D:2747:ILE:N	2.28	0.48
2:D:4855:ASN:CG	7:C:8006:PCW:H341	2.38	0.48
2:A:1536:GLU:OE1	2:A:1536:GLU:N	2.46	0.48
2:A:2895:LEU:HD22	2:A:2901:GLY:O	2.13	0.48
2:B:500:THR:HG23	2:B:503:HIS:H	1.77	0.48
2:B:1758:GLY:N	2:B:1759:PRO:HD2	2.27	0.48
2:B:2415:ASN:O	2:B:2415:ASN:ND2	2.46	0.48
2:B:3645:LEU:HD21	2:B:3653:MET:HE3	1.93	0.48
2:B:3691:VAL:HG12	2:B:3693:GLU:H	1.77	0.48
2:C:843:PRO:O	2:C:1198:GLY:N	2.38	0.48
2:C:4747:GLU:HA	2:C:4747:GLU:OE2	2.13	0.48
2:D:608:CYS:SG	2:D:1673:SER:OG	2.69	0.48
2:D:3556:ASN:OD1	2:D:3557:ASN:N	2.46	0.48
2:A:500:THR:HG23	2:A:503:HIS:H	1.77	0.48
2:A:1783:CYS:SG	2:A:1785:VAL:HG22	2.53	0.48
2:A:2234:CYS:O	2:A:2237:LEU:N	2.46	0.48
2:A:4054:SER:O	2:A:4056:SER:N	2.46	0.48
2:C:2394:ASP:OD2	2:C:2419:LEU:N	2.47	0.48
2:D:951:LEU:HD22	2:D:973:LEU:HB3	1.95	0.48
2:D:2007:ILE:CD1	2:D:3642:LEU:HD21	2.44	0.48
2:D:2415:ASN:ND2	2:D:2415:ASN:O	2.46	0.48
2:D:4054:SER:O	2:D:4056:SER:N	2.46	0.48
2:D:4122:GLU:OE1	2:D:4122:GLU:N	2.44	0.48
2:A:888:ILE:HG13	2:A:889:GLU:N	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:957:PRO:HB2	2:A:959:THR:HG23	1.95	0.48
2:A:2007:ILE:CD1	2:A:3642:LEU:HD21	2.44	0.48
2:A:2415:ASN:O	2:A:2415:ASN:ND2	2.46	0.48
2:A:3176:LEU:HD23	2:A:3176:LEU:C	2.38	0.48
2:A:3591:GLU:O	2:A:3594:VAL:HG12	2.12	0.48
2:B:71:GLU:OE1	2:B:111:ARG:NE	2.44	0.48
2:B:2372:GLU:HG2	2:C:197:MET:CE	2.41	0.48
2:C:1536:GLU:OE1	2:C:1536:GLU:N	2.46	0.48
2:C:4054:SER:O	2:C:4056:SER:N	2.46	0.48
2:D:872:ARG:CG	2:D:927:GLY:HA2	2.43	0.48
2:D:877:GLU:O	2:D:881:GLU:HG2	2.13	0.48
2:D:903:ARG:HA	2:D:903:ARG:NH2	2.21	0.48
2:D:3220:TYR:CD1	2:D:3237:VAL:HG12	2.48	0.48
2:D:4747:GLU:HA	2:D:4747:GLU:OE2	2.13	0.48
2:A:3246:VAL:HG12	2:A:3247:LEU:N	2.29	0.48
2:A:3435:LEU:CD2	2:A:3518:MET:HE2	2.42	0.48
2:A:3556:ASN:OD1	2:A:3557:ASN:N	2.46	0.48
2:B:3410:TYR:O	2:B:3413:LEU:N	2.47	0.48
2:C:2542:PHE:O	2:C:2545:THR:OG1	2.28	0.48
2:D:2234:CYS:O	2:D:2237:LEU:N	2.46	0.48
2:D:2394:ASP:OD2	2:D:2419:LEU:N	2.46	0.48
2:D:2875:MET:HB3	2:D:2940:ARG:HB2	1.94	0.48
2:A:3220:TYR:CD1	2:A:3237:VAL:HG12	2.48	0.48
2:B:890:GLN:HB2	2:B:892:TRP:HD1	1.79	0.48
2:B:2746:VAL:HG22	2:B:2747:ILE:N	2.28	0.48
2:B:3435:LEU:CD2	2:B:3518:MET:HE2	2.42	0.48
2:B:4747:GLU:HA	2:B:4747:GLU:OE2	2.13	0.48
2:C:888:ILE:HG13	2:C:889:GLU:N	2.26	0.48
2:C:957:PRO:HB2	2:C:959:THR:HG23	1.95	0.48
2:C:3246:VAL:HG12	2:C:3247:LEU:N	2.29	0.48
2:D:890:GLN:HB2	2:D:892:TRP:HD1	1.79	0.48
2:A:2746:VAL:HG22	2:A:2747:ILE:N	2.28	0.48
2:B:3176:LEU:C	2:B:3176:LEU:HD23	2.38	0.48
2:B:3246:VAL:HG12	2:B:3247:LEU:N	2.29	0.48
2:B:4122:GLU:OE1	2:B:4122:GLU:N	2.44	0.48
2:B:4580:VAL:HG12	2:C:4875:ASP:O	2.12	0.48
2:C:158:ARG:CZ	2:C:165:ARG:HH21	2.27	0.48
2:C:951:LEU:HD22	2:C:973:LEU:HB3	1.95	0.48
2:D:898:ARG:NH1	2:D:907:CYS:HB2	2.29	0.48
2:D:940:VAL:HG23	2:D:1052:TYR:HB3	1.95	0.48
2:D:1645:GLU:OE1	2:D:1647:ARG:NH2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3246:VAL:HG12	2:D:3247:LEU:N	2.29	0.48
2:A:877:GLU:O	2:A:881:GLU:HG2	2.14	0.48
2:A:940:VAL:HB	2:A:1054:ILE:CG1	2.43	0.48
2:B:1536:GLU:OE1	2:B:1536:GLU:N	2.46	0.48
2:B:2007:ILE:CD1	2:B:3642:LEU:HD21	2.44	0.48
2:B:2583:MET:HE3	2:B:2611:LEU:HD23	1.95	0.48
2:C:877:GLU:O	2:C:881:GLU:HG2	2.13	0.48
2:C:890:GLN:HB2	2:C:892:TRP:HD1	1.79	0.48
2:C:955:LYS:HE3	2:C:955:LYS:HB3	1.61	0.48
2:C:1783:CYS:SG	2:C:1785:VAL:HG22	2.53	0.48
2:C:3168:ARG:O	2:C:3172:SER:OG	2.27	0.48
2:D:158:ARG:CZ	2:D:165:ARG:HH21	2.27	0.48
2:D:295:THR:O	2:D:299:GLY:N	2.46	0.48
2:D:940:VAL:HB	2:D:1054:ILE:CG1	2.43	0.48
2:D:957:PRO:HB2	2:D:959:THR:HG23	1.95	0.48
2:D:2634:LEU:HD12	2:D:2686:SER:HB3	1.96	0.48
2:A:890:GLN:HB2	2:A:892:TRP:HD1	1.79	0.48
2:A:2372:GLU:HG2	2:B:197:MET:CE	2.41	0.48
2:A:3864:GLU:O	2:A:3868:VAL:HG23	2.14	0.48
2:B:902:LYS:HD2	2:B:902:LYS:HA	1.55	0.48
2:B:1783:CYS:SG	2:B:1785:VAL:HG22	2.53	0.48
2:B:2234:CYS:HB3	2:B:2238:CYS:HB3	1.55	0.48
2:B:3556:ASN:OD1	2:B:3557:ASN:N	2.46	0.48
2:C:2007:ILE:CD1	2:C:3642:LEU:HD21	2.44	0.48
2:C:3534:ILE:HG13	2:C:3597:VAL:HG23	1.94	0.48
1:E:2:GLY:N	1:E:78:SER:OG	2.42	0.48
2:A:258:ARG:O	2:A:285:HIS:NE2	2.42	0.48
2:A:295:THR:O	2:A:299:GLY:N	2.46	0.48
2:A:898:ARG:NH1	2:A:907:CYS:HB2	2.29	0.48
2:B:871:ILE:HG13	2:B:1050:TYR:CE2	2.49	0.48
2:B:872:ARG:CG	2:B:927:GLY:HA2	2.43	0.48
2:B:888:ILE:HG13	2:B:889:GLU:N	2.26	0.48
2:B:2863:LEU:HD13	2:B:2929:LYS:HB2	1.96	0.48
2:B:2895:LEU:HD22	2:B:2901:GLY:O	2.14	0.48
2:C:872:ARG:CG	2:C:927:GLY:HA2	2.43	0.48
2:C:3864:GLU:O	2:C:3868:VAL:HG23	2.14	0.48
2:D:859:THR:CG2	2:D:932:THR:HA	2.44	0.47
2:D:955:LYS:HB3	2:D:955:LYS:HE3	1.61	0.47
2:D:3435:LEU:CD2	2:D:3518:MET:HE2	2.42	0.47
2:D:3864:GLU:O	2:D:3868:VAL:HG23	2.14	0.47
2:A:158:ARG:CZ	2:A:165:ARG:HH21	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:859:THR:CG2	2:A:932:THR:HA	2.44	0.47
2:A:3388:ALA:O	2:A:3392:GLU:N	2.39	0.47
2:B:158:ARG:CZ	2:B:165:ARG:HH21	2.27	0.47
2:B:877:GLU:O	2:B:881:GLU:HG2	2.13	0.47
2:B:951:LEU:HD22	2:B:973:LEU:HB3	1.95	0.47
7:B:8006:PCW:H341	2:C:4855:ASN:CG	2.39	0.47
2:C:940:VAL:HG23	2:C:1052:TYR:HB3	1.95	0.47
2:C:2119:ARG:NH2	2:C:3720:ASP:OD1	2.47	0.47
2:C:2746:VAL:HG22	2:C:2747:ILE:N	2.28	0.47
2:C:3410:TYR:O	2:C:3413:LEU:N	2.47	0.47
2:C:4088:ARG:NH1	2:C:4090:LEU:HD12	2.29	0.47
1:F:33:ASP:OD2	1:F:35:LYS:HG3	2.14	0.47
2:A:920:ASN:HA	2:A:923:LEU:HD12	1.97	0.47
2:A:2265:GLY:O	2:A:2267:GLY:N	2.45	0.47
2:A:3410:TYR:O	2:A:3413:LEU:N	2.47	0.47
2:A:4122:GLU:OE1	2:A:4122:GLU:N	2.44	0.47
2:B:157:GLN:OE1	2:B:158:ARG:NH1	2.47	0.47
2:B:2246:GLN:NE2	2:B:3867:THR:O	2.46	0.47
2:B:3088:ILE:HD12	2:B:3088:ILE:H	1.79	0.47
2:C:295:THR:O	2:C:299:GLY:N	2.46	0.47
2:C:886:THR:O	2:C:890:GLN:HG3	2.14	0.47
2:C:898:ARG:NH1	2:C:907:CYS:HB2	2.29	0.47
2:C:2624:LEU:O	2:C:2628:VAL:HG23	2.14	0.47
2:C:4670:LYS:O	2:C:4674:GLU:HG2	2.15	0.47
2:D:871:ILE:HG13	2:D:1050:TYR:CE2	2.49	0.47
2:B:4670:LYS:O	2:B:4674:GLU:HG2	2.15	0.47
2:C:871:ILE:HG13	2:C:1050:TYR:CE2	2.49	0.47
2:C:2583:MET:HE3	2:C:2611:LEU:HD23	1.95	0.47
2:C:2863:LEU:HD13	2:C:2929:LYS:HB2	1.96	0.47
2:C:2889:ARG:O	2:C:2893:GLN:OE1	2.32	0.47
2:D:888:ILE:HG13	2:D:889:GLU:N	2.26	0.47
2:D:2895:LEU:HD22	2:D:2901:GLY:O	2.14	0.47
2:D:3088:ILE:H	2:D:3088:ILE:HD12	1.79	0.47
2:D:3591:GLU:O	2:D:3594:VAL:HG12	2.12	0.47
2:D:3859:LEU:C	2:D:3859:LEU:HD12	2.39	0.47
2:A:2394:ASP:OD2	2:A:2419:LEU:N	2.46	0.47
2:A:3182:PRO:O	2:A:3185:GLU:HG3	2.15	0.47
2:B:931:LYS:HA	2:B:934:LEU:HD22	1.95	0.47
2:C:1116:LEU:HD12	2:C:1194:SER:CB	2.45	0.47
2:D:2624:LEU:O	2:D:2628:VAL:HG23	2.14	0.47
2:D:3322:ARG:HA	2:D:3325:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:848:SER:N	2:A:851:ASP:OD1	2.43	0.47
2:A:971:LEU:CD1	2:A:973:LEU:HD21	2.45	0.47
2:A:2583:MET:HE3	2:A:2611:LEU:HD23	1.95	0.47
2:A:2624:LEU:O	2:A:2628:VAL:HG23	2.14	0.47
2:A:3088:ILE:H	2:A:3088:ILE:HD12	1.79	0.47
2:B:649:ILE:HD13	2:B:812:CYS:HB3	1.96	0.47
2:C:916:GLU:HA	2:C:919:ARG:CD	2.44	0.47
2:C:971:LEU:CD1	2:C:973:LEU:HD21	2.45	0.47
2:C:2634:LEU:HD12	2:C:2686:SER:HB3	1.96	0.47
2:C:2895:LEU:HD22	2:C:2901:GLY:O	2.14	0.47
2:D:157:GLN:OE1	2:D:158:ARG:NH1	2.47	0.47
2:D:916:GLU:HA	2:D:919:ARG:CD	2.44	0.47
2:D:1127:GLY:O	2:D:1128:HIS:C	2.58	0.47
2:D:2265:GLY:O	2:D:2267:GLY:N	2.45	0.47
2:A:157:GLN:OE1	2:A:158:ARG:NH1	2.47	0.47
2:A:942:MET:HG3	2:A:1052:TYR:CD2	2.50	0.47
2:A:2863:LEU:HD13	2:A:2929:LYS:HB2	1.96	0.47
2:A:2942:LEU:HD21	2:A:2945:MET:HB2	1.97	0.47
2:C:608:CYS:SG	2:C:1673:SER:C	2.98	0.47
2:C:608:CYS:SG	2:C:1673:SER:OG	2.69	0.47
2:C:859:THR:CG2	2:C:932:THR:HA	2.44	0.47
2:C:3088:ILE:H	2:C:3088:ILE:HD12	1.79	0.47
2:D:608:CYS:SG	2:D:1673:SER:C	2.98	0.47
2:D:673:ALA:O	2:D:681:THR:OG1	2.31	0.47
2:D:886:THR:O	2:D:890:GLN:HG3	2.14	0.47
2:D:942:MET:HG3	2:D:1052:TYR:CD2	2.50	0.47
2:D:2746:VAL:HG22	2:D:2747:ILE:H	1.79	0.47
2:D:3410:TYR:O	2:D:3413:LEU:N	2.47	0.47
2:D:4638:GLU:HB3	2:D:4639:PRO:HD3	1.97	0.47
2:D:4670:LYS:O	2:D:4674:GLU:HG2	2.15	0.47
2:A:885:LEU:HD12	2:A:960:TYR:CE2	2.50	0.47
2:A:951:LEU:HD22	2:A:973:LEU:HB3	1.95	0.47
2:A:1127:GLY:O	2:A:1128:HIS:C	2.58	0.47
2:A:2574:GLU:H	2:A:2619:MET:HE1	1.80	0.47
2:A:2746:VAL:HG22	2:A:2747:ILE:H	1.79	0.47
2:A:3220:TYR:CE1	2:A:3237:VAL:HG12	2.50	0.47
2:A:4088:ARG:NH1	2:A:4090:LEU:HD12	2.29	0.47
2:B:296:GLU:OE1	2:B:296:GLU:N	2.37	0.47
2:B:859:THR:CG2	2:B:932:THR:HA	2.44	0.47
2:B:916:GLU:HA	2:B:919:ARG:CD	2.44	0.47
2:B:940:VAL:HB	2:B:1054:ILE:CG1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:971:LEU:CD1	2:B:973:LEU:HD21	2.45	0.47
2:B:3062:ALA:HB3	2:B:3063:PRO:HD3	1.97	0.47
2:B:3182:PRO:O	2:B:3185:GLU:HG3	2.15	0.47
2:B:3864:GLU:O	2:B:3868:VAL:HG23	2.14	0.47
2:C:920:ASN:HA	2:C:923:LEU:HD12	1.97	0.47
2:C:940:VAL:HB	2:C:1054:ILE:CG1	2.43	0.47
2:C:985:LEU:HD11	2:C:1056:PRO:HB3	1.97	0.47
2:C:2942:LEU:HD21	2:C:2945:MET:HB2	1.97	0.47
2:C:3062:ALA:HB3	2:C:3063:PRO:HD3	1.97	0.47
2:C:3182:PRO:O	2:C:3185:GLU:HG3	2.15	0.47
2:C:3220:TYR:CE1	2:C:3237:VAL:HG12	2.50	0.47
2:C:3859:LEU:C	2:C:3859:LEU:HD12	2.39	0.47
2:D:931:LYS:HA	2:D:934:LEU:HD22	1.95	0.47
2:D:2574:GLU:H	2:D:2619:MET:HE1	1.80	0.47
2:A:608:CYS:SG	2:A:1673:SER:C	2.98	0.47
2:B:70:LEU:HD13	2:B:102:LEU:HD11	1.97	0.47
2:B:71:GLU:OE1	2:B:111:ARG:NH2	2.42	0.47
2:C:2179:MET:HE2	2:C:2211:VAL:HG11	1.97	0.47
2:D:885:LEU:HD12	2:D:960:TYR:CE2	2.50	0.47
2:D:1116:LEU:HD12	2:D:1194:SER:CB	2.45	0.47
2:D:2210:GLU:OE1	2:D:2210:GLU:HA	2.15	0.47
2:D:2942:LEU:HD21	2:D:2945:MET:HB2	1.97	0.47
2:D:3062:ALA:HB3	2:D:3063:PRO:HD3	1.97	0.47
2:A:896:PRO:HD2	2:A:904:LEU:HD13	1.97	0.47
2:A:916:GLU:HA	2:A:919:ARG:CD	2.45	0.47
2:A:3062:ALA:HB3	2:A:3063:PRO:HD3	1.97	0.47
2:B:920:ASN:HA	2:B:923:LEU:HD12	1.97	0.47
2:B:985:LEU:HD11	2:B:1056:PRO:HB3	1.97	0.47
2:B:2283:ASP:HA	2:B:2342:VAL:HG13	1.97	0.47
2:B:2624:LEU:O	2:B:2628:VAL:HG23	2.14	0.47
2:B:2634:LEU:HD12	2:B:2686:SER:HB3	1.96	0.47
2:B:3859:LEU:C	2:B:3859:LEU:HD12	2.39	0.47
2:B:4088:ARG:NH1	2:B:4090:LEU:HD12	2.29	0.47
2:C:157:GLN:OE1	2:C:158:ARG:NH1	2.47	0.47
2:C:942:MET:HG3	2:C:1052:TYR:CD2	2.50	0.47
2:C:2746:VAL:HG22	2:C:2747:ILE:H	1.79	0.47
2:C:3322:ARG:HA	2:C:3325:VAL:HG12	1.97	0.47
2:D:926:SER:O	2:D:930:LEU:HD22	2.15	0.47
2:D:952:LYS:O	2:D:972:ASP:HB3	2.15	0.47
2:D:2863:LEU:HD13	2:D:2929:LYS:HB2	1.96	0.47
2:A:71:GLU:OE1	2:A:111:ARG:NE	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:886:THR:O	2:A:890:GLN:HG3	2.14	0.47
2:A:952:LYS:O	2:A:972:ASP:HB3	2.15	0.47
2:A:2889:ARG:O	2:A:2893:GLN:OE1	2.32	0.47
2:B:886:THR:O	2:B:890:GLN:HG3	2.14	0.47
2:C:885:LEU:HD12	2:C:960:TYR:CE2	2.50	0.47
2:C:3434:GLU:O	2:C:3438:MET:HG3	2.15	0.47
1:H:33:ASP:OD2	1:H:35:LYS:HG3	2.14	0.46
2:D:649:ILE:HD13	2:D:812:CYS:HB3	1.96	0.46
2:A:843:PRO:O	2:A:1198:GLY:N	2.38	0.46
2:A:921:TYR:O	2:A:924:GLN:HG3	2.15	0.46
2:A:926:SER:O	2:A:930:LEU:HD22	2.15	0.46
2:A:2179:MET:HE2	2:A:2211:VAL:HG11	1.97	0.46
2:A:3322:ARG:HA	2:A:3325:VAL:HG12	1.97	0.46
2:B:608:CYS:SG	2:B:1673:SER:C	2.98	0.46
2:B:885:LEU:HD12	2:B:960:TYR:CE2	2.50	0.46
2:B:896:PRO:HD2	2:B:904:LEU:HD13	1.97	0.46
2:B:2179:MET:HE2	2:B:2211:VAL:HG11	1.97	0.46
2:B:2746:VAL:HG22	2:B:2747:ILE:H	1.79	0.46
2:B:2756:ILE:HG23	2:B:2810:ILE:HB	1.97	0.46
2:B:4638:GLU:HB3	2:B:4639:PRO:HD3	1.97	0.46
2:C:910:ASN:O	2:C:911:PHE:C	2.58	0.46
2:D:921:TYR:O	2:D:924:GLN:HG3	2.16	0.46
2:D:971:LEU:CD1	2:D:973:LEU:HD21	2.45	0.46
2:D:2756:ILE:HG23	2:D:2810:ILE:HB	1.97	0.46
2:D:3220:TYR:CE1	2:D:3237:VAL:HG12	2.50	0.46
2:D:4709:PHE:HB3	2:D:4710:PRO:HD3	1.98	0.46
2:A:2756:ILE:HG23	2:A:2810:ILE:HB	1.97	0.46
2:A:4638:GLU:HB3	2:A:4639:PRO:HD3	1.97	0.46
2:A:4670:LYS:O	2:A:4674:GLU:HG2	2.14	0.46
2:B:652:GLY:N	2:B:659:GLN:OE1	2.46	0.46
2:B:1297:GLN:NE2	2:B:1546:ASN:OD1	2.44	0.46
2:B:2334:ASP:O	2:B:2337:ARG:HG2	2.15	0.46
2:B:2942:LEU:HD21	2:B:2945:MET:HB2	1.97	0.46
2:B:3220:TYR:CE1	2:B:3237:VAL:HG12	2.50	0.46
2:C:1297:GLN:NE2	2:C:1546:ASN:OD1	2.44	0.46
2:C:1645:GLU:OE1	2:C:1647:ARG:NH2	2.43	0.46
1:E:33:ASP:OD2	1:E:35:LYS:HG3	2.14	0.46
2:D:2889:ARG:O	2:D:2893:GLN:OE1	2.32	0.46
2:A:649:ILE:HD13	2:A:812:CYS:HB3	1.96	0.46
2:A:871:ILE:HG13	2:A:1050:TYR:CE2	2.49	0.46
2:A:1116:LEU:HD12	2:A:1194:SER:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2210:GLU:OE1	2:A:2210:GLU:HA	2.15	0.46
2:A:3859:LEU:HD12	2:A:3859:LEU:C	2.39	0.46
2:B:2265:GLY:O	2:B:2267:GLY:N	2.45	0.46
2:B:3434:GLU:O	2:B:3438:MET:HG3	2.15	0.46
2:C:2334:ASP:O	2:C:2337:ARG:HG2	2.15	0.46
2:C:2756:ILE:HG23	2:C:2810:ILE:HB	1.97	0.46
2:D:2179:MET:HE2	2:D:2211:VAL:HG11	1.97	0.46
2:D:3182:PRO:O	2:D:3185:GLU:HG3	2.15	0.46
2:D:4088:ARG:NH1	2:D:4090:LEU:HD12	2.29	0.46
2:A:931:LYS:HA	2:A:934:LEU:HD22	1.96	0.46
2:A:2334:ASP:O	2:A:2337:ARG:HG2	2.15	0.46
2:A:2634:LEU:HD12	2:A:2686:SER:HB3	1.96	0.46
2:B:942:MET:HG3	2:B:1052:TYR:CD2	2.50	0.46
2:B:2210:GLU:OE1	2:B:2210:GLU:HA	2.15	0.46
2:C:931:LYS:HA	2:C:934:LEU:HD22	1.95	0.46
2:C:2210:GLU:OE1	2:C:2210:GLU:HA	2.15	0.46
2:C:4709:PHE:HB3	2:C:4710:PRO:HD3	1.98	0.46
2:D:896:PRO:HD2	2:D:904:LEU:HD13	1.97	0.46
2:D:2334:ASP:O	2:D:2337:ARG:HG2	2.15	0.46
2:A:872:ARG:CG	2:A:927:GLY:HA2	2.43	0.46
2:A:911:PHE:CE1	2:A:923:LEU:HG	2.51	0.46
2:B:898:ARG:NH1	2:B:907:CYS:HB2	2.29	0.46
2:B:1116:LEU:HD12	2:B:1194:SER:CB	2.45	0.46
2:C:649:ILE:HD13	2:C:812:CYS:HB3	1.96	0.46
2:C:652:GLY:N	2:C:659:GLN:OE1	2.46	0.46
2:C:911:PHE:CE1	2:C:923:LEU:HG	2.51	0.46
2:C:1127:GLY:O	2:C:1128:HIS:C	2.58	0.46
2:C:2234:CYS:C	2:C:2236:PHE:N	2.74	0.46
2:D:848:SER:N	2:D:851:ASP:OD1	2.43	0.46
2:D:911:PHE:CE1	2:D:923:LEU:HG	2.51	0.46
2:D:4096:PHE:CZ	2:D:4100:MET:HE2	2.51	0.46
2:A:673:ALA:O	2:A:681:THR:OG1	2.31	0.46
2:A:3672:ASP:OD1	2:A:3735:HIS:NE2	2.36	0.46
2:A:4096:PHE:CZ	2:A:4100:MET:HE2	2.51	0.46
2:B:914:LEU:HD11	2:B:918:GLU:C	2.41	0.46
2:B:952:LYS:O	2:B:972:ASP:HB3	2.15	0.46
2:B:2889:ARG:O	2:B:2893:GLN:OE1	2.32	0.46
2:B:3322:ARG:HA	2:B:3325:VAL:HG12	1.97	0.46
2:B:3373:VAL:HG12	2:B:3399:PHE:CZ	2.51	0.46
2:B:3645:LEU:HD21	2:B:3653:MET:CE	2.46	0.46
2:B:4220:PHE:CE1	2:B:4224:VAL:HG21	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:896:PRO:HD2	2:C:904:LEU:HD13	1.97	0.46
2:C:2283:ASP:HA	2:C:2342:VAL:HG13	1.97	0.46
2:C:3645:LEU:HD21	2:C:3653:MET:CE	2.46	0.46
1:E:43:ARG:HA	2:A:1692:GLN:HE21	1.81	0.46
2:D:70:LEU:HD13	2:D:102:LEU:HD11	1.97	0.46
2:D:914:LEU:HD11	2:D:918:GLU:C	2.41	0.46
2:D:931:LYS:O	2:D:934:LEU:HB2	2.16	0.46
2:D:1293:SER:OG	2:D:1294:LEU:HD12	2.16	0.46
2:D:3645:LEU:HD21	2:D:3653:MET:CE	2.46	0.46
2:A:70:LEU:HD13	2:A:102:LEU:HD11	1.97	0.46
2:B:183:LEU:HD12	2:B:191:GLN:O	2.16	0.46
2:B:910:ASN:O	2:B:911:PHE:C	2.58	0.46
2:C:70:LEU:HD13	2:C:102:LEU:HD11	1.97	0.46
2:C:183:LEU:HD12	2:C:191:GLN:O	2.16	0.46
2:C:470:ARG:NE	2:C:3713:GLU:OE1	2.42	0.46
2:C:952:LYS:O	2:C:972:ASP:HB3	2.15	0.46
2:C:2802:ASP:OD1	2:C:2802:ASP:C	2.59	0.46
2:C:3373:VAL:HG12	2:C:3399:PHE:CZ	2.51	0.46
2:C:4009:ASP:OD1	2:C:4010:SER:N	2.49	0.46
2:D:258:ARG:O	2:D:285:HIS:NE2	2.42	0.46
2:D:2799:SER:O	2:D:2802:ASP:OD1	2.34	0.46
2:D:3373:VAL:HG12	2:D:3399:PHE:CZ	2.51	0.46
2:D:3944:ASP:OD2	2:D:3945:VAL:N	2.49	0.46
2:A:365:PRO:O	2:A:366:LYS:HB3	2.16	0.46
2:A:868:LEU:CD1	2:A:930:LEU:HB3	2.45	0.46
2:A:911:PHE:O	2:A:914:LEU:HD23	2.16	0.46
2:A:2215:VAL:HG21	2:A:2229:MET:CE	2.46	0.46
2:A:2224:ILE:HD11	2:A:2268:MET:SD	2.56	0.46
2:A:2799:SER:O	2:A:2802:ASP:OD1	2.34	0.46
2:A:2871:GLU:HG2	2:A:2940:ARG:HB3	1.98	0.46
2:B:642:VAL:HG21	2:B:682:HIS:HD1	1.81	0.46
2:B:921:TYR:O	2:B:924:GLN:HG3	2.16	0.46
2:B:1426:GLU:OE1	2:B:1426:GLU:N	2.41	0.46
2:B:2215:VAL:HG21	2:B:2229:MET:CE	2.46	0.46
2:C:870:ARG:NH2	2:C:871:ILE:HB	2.31	0.46
2:C:911:PHE:O	2:C:914:LEU:HD23	2.16	0.46
2:C:914:LEU:HD11	2:C:918:GLU:C	2.41	0.46
2:C:921:TYR:O	2:C:924:GLN:HG3	2.16	0.46
2:C:3041:THR:OG1	2:C:3081:VAL:HG21	2.16	0.46
2:C:4220:PHE:CE1	2:C:4224:VAL:HG21	2.51	0.46
2:C:4638:GLU:HB3	2:C:4639:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:365:PRO:O	2:D:366:LYS:HB3	2.16	0.46
2:D:868:LEU:CD1	2:D:930:LEU:HB3	2.45	0.46
2:D:985:LEU:HD11	2:D:1056:PRO:HB3	1.97	0.46
2:D:2119:ARG:NH2	2:D:3720:ASP:OD1	2.47	0.46
2:D:2283:ASP:HA	2:D:2342:VAL:HG13	1.97	0.46
2:D:3004:LEU:HB2	2:D:3005:PRO:HD3	1.97	0.46
2:D:4009:ASP:OD1	2:D:4010:SER:N	2.49	0.46
2:D:4893:GLY:N	2:D:4897:ASP:OD2	2.47	0.46
2:A:931:LYS:O	2:A:934:LEU:HB2	2.16	0.46
2:A:2283:ASP:HA	2:A:2342:VAL:HG13	1.97	0.46
2:B:1127:GLY:O	2:B:1128:HIS:C	2.58	0.46
2:B:2574:GLU:H	2:B:2619:MET:HE1	1.80	0.46
2:B:4009:ASP:OD1	2:B:4010:SER:N	2.49	0.46
2:C:926:SER:O	2:C:930:LEU:HD22	2.15	0.46
2:C:2265:GLY:O	2:C:2267:GLY:N	2.45	0.46
2:C:4096:PHE:CZ	2:C:4100:MET:HE2	2.51	0.46
1:G:26:HIS:ND1	1:G:105:LEU:HD11	2.31	0.46
2:D:870:ARG:NH2	2:D:871:ILE:HB	2.31	0.46
2:D:2224:ILE:HD11	2:D:2268:MET:SD	2.56	0.46
2:D:3388:ALA:O	2:D:3392:GLU:N	2.39	0.46
2:D:3434:GLU:O	2:D:3438:MET:HG3	2.15	0.46
2:A:985:LEU:HD11	2:A:1056:PRO:HB3	1.97	0.46
2:A:2525:VAL:HG23	2:A:2526:GLY:N	2.31	0.46
2:A:3373:VAL:HG12	2:A:3399:PHE:CZ	2.51	0.46
2:A:3645:LEU:HD21	2:A:3653:MET:CE	2.46	0.46
2:A:3944:ASP:OD2	2:A:3945:VAL:N	2.49	0.46
2:B:926:SER:O	2:B:930:LEU:HD22	2.15	0.46
2:B:931:LYS:O	2:B:934:LEU:HB2	2.16	0.46
2:B:2224:ILE:HD11	2:B:2268:MET:SD	2.56	0.46
2:B:3181:ASN:OD1	2:B:3183:TYR:CD1	2.69	0.46
2:B:3324:ILE:CG2	2:B:3409:LEU:HD21	2.46	0.46
2:C:1293:SER:OG	2:C:1294:LEU:HD12	2.16	0.46
2:C:2907:VAL:HG23	2:C:2912:LEU:HG	1.98	0.46
2:C:3004:LEU:HB2	2:C:3005:PRO:HD3	1.97	0.46
2:D:197:MET:CE	2:C:2372:GLU:HG2	2.41	0.45
2:D:2907:VAL:HG23	2:D:2912:LEU:HG	1.98	0.45
2:D:3041:THR:OG1	2:D:3081:VAL:HG21	2.16	0.45
2:A:914:LEU:HD11	2:A:918:GLU:C	2.41	0.45
2:A:955:LYS:HE3	2:A:955:LYS:HB3	1.61	0.45
2:A:2119:ARG:NH2	2:A:3720:ASP:OD1	2.47	0.45
2:A:2645:LEU:HD13	2:A:2679:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3324:ILE:CG2	2:A:3409:LEU:HD21	2.46	0.45
2:B:870:ARG:NH2	2:B:874:LYS:HD3	2.31	0.45
2:B:911:PHE:CE1	2:B:923:LEU:HG	2.51	0.45
2:B:2119:ARG:NH2	2:B:3720:ASP:OD1	2.47	0.45
2:B:2871:GLU:HG2	2:B:2940:ARG:HB3	1.98	0.45
2:B:4054:SER:O	2:B:4055:SER:C	2.59	0.45
2:C:71:GLU:OE1	2:C:111:ARG:NE	2.44	0.45
2:C:2645:LEU:HD13	2:C:2679:LEU:HD21	1.99	0.45
2:C:2794:PRO:O	2:C:2798:PHE:N	2.41	0.45
2:C:3324:ILE:CG2	2:C:3409:LEU:HD21	2.46	0.45
2:D:920:ASN:HA	2:D:923:LEU:HD12	1.97	0.45
2:D:3894:LEU:HD13	2:D:3902:PHE:CZ	2.52	0.45
2:D:4054:SER:O	2:D:4055:SER:C	2.59	0.45
2:D:4248:MET:HE1	2:D:4987:MET:HE1	1.98	0.45
2:A:3894:LEU:HD13	2:A:3902:PHE:CZ	2.52	0.45
2:A:4709:PHE:HB3	2:A:4710:PRO:HD3	1.98	0.45
2:B:956:LEU:HD12	2:B:968:PRO:CD	2.44	0.45
2:B:2799:SER:O	2:B:2802:ASP:OD1	2.34	0.45
2:B:3584:GLU:OE1	2:B:3584:GLU:N	2.37	0.45
2:C:3203:PRO:HA	2:C:3284:ARG:NH2	2.31	0.45
2:C:3536:LEU:CD2	2:C:3560:LEU:HD13	2.46	0.45
2:D:893:THR:O	2:D:904:LEU:HA	2.16	0.45
2:D:2525:VAL:HG23	2:D:2526:GLY:N	2.31	0.45
2:D:2802:ASP:OD1	2:D:2802:ASP:C	2.59	0.45
2:A:642:VAL:HG21	2:A:682:HIS:HD1	1.81	0.45
2:A:870:ARG:NH2	2:A:871:ILE:HB	2.31	0.45
2:A:3181:ASN:OD1	2:A:3183:TYR:CD1	2.69	0.45
2:B:868:LEU:CD1	2:B:930:LEU:HB3	2.45	0.45
2:B:2525:VAL:HG23	2:B:2526:GLY:N	2.31	0.45
2:B:3004:LEU:HB2	2:B:3005:PRO:HD3	1.97	0.45
2:B:4096:PHE:CZ	2:B:4100:MET:HE2	2.51	0.45
2:B:4248:MET:HE1	2:B:4987:MET:HE1	1.98	0.45
2:C:2574:GLU:H	2:C:2619:MET:HE1	1.80	0.45
2:C:2799:SER:O	2:C:2802:ASP:OD1	2.34	0.45
1:H:26:HIS:ND1	1:H:105:LEU:HD11	2.31	0.45
2:D:911:PHE:O	2:D:914:LEU:HD23	2.16	0.45
2:D:2215:VAL:HG21	2:D:2229:MET:CE	2.46	0.45
2:D:2645:LEU:HD13	2:D:2679:LEU:HD21	1.99	0.45
2:A:2907:VAL:HG23	2:A:2912:LEU:HG	1.98	0.45
2:A:4054:SER:O	2:A:4055:SER:C	2.59	0.45
2:B:365:PRO:O	2:B:366:LYS:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:870:ARG:NH2	2:B:871:ILE:HB	2.31	0.45
2:B:879:ILE:CA	2:B:882:LEU:HD12	2.33	0.45
2:B:911:PHE:O	2:B:914:LEU:HD23	2.16	0.45
2:B:978:LEU:HD13	2:B:982:GLN:HB3	1.98	0.45
2:B:2234:CYS:C	2:B:2236:PHE:N	2.74	0.45
2:B:2645:LEU:HD13	2:B:2679:LEU:HD21	1.99	0.45
2:B:2816:ALA:HB1	2:B:2882:ASN:ND2	2.32	0.45
2:B:2907:VAL:HG23	2:B:2912:LEU:HG	1.98	0.45
2:B:3756:PHE:HA	2:B:3759:LYS:HZ2	1.82	0.45
2:C:642:VAL:HG21	2:C:682:HIS:HD1	1.81	0.45
2:C:3944:ASP:OD2	2:C:3945:VAL:N	2.49	0.45
2:C:4248:MET:HE1	2:C:4987:MET:HE1	1.98	0.45
2:A:183:LEU:HD12	2:A:191:GLN:O	2.16	0.45
2:A:4009:ASP:OD1	2:A:4010:SER:N	2.49	0.45
2:B:422:PHE:CD1	2:B:422:PHE:C	2.95	0.45
2:B:4709:PHE:HB3	2:B:4710:PRO:HD3	1.98	0.45
1:F:26:HIS:ND1	1:F:105:LEU:HD11	2.31	0.45
2:D:862:ILE:HG22	2:D:931:LYS:HG2	1.99	0.45
2:D:888:ILE:CG1	2:D:960:TYR:HA	2.47	0.45
2:D:954:THR:HG22	2:D:972:ASP:HB2	1.98	0.45
2:D:4220:PHE:CE1	2:D:4224:VAL:HG21	2.51	0.45
2:B:321:LYS:HZ1	2:B:357:TRP:CG	2.35	0.45
2:B:1293:SER:OG	2:B:1294:LEU:HD12	2.16	0.45
2:B:3203:PRO:HA	2:B:3284:ARG:NH2	2.31	0.45
2:B:4686:ILE:HD12	2:B:4735:ILE:CD1	2.47	0.45
2:C:843:PRO:O	2:C:1197:PRO:HA	2.17	0.45
2:C:2215:VAL:HG21	2:C:2229:MET:CE	2.46	0.45
2:C:2866:VAL:CG1	2:C:2933:MET:HE3	2.45	0.45
2:C:2875:MET:HB3	2:C:2940:ARG:HD2	1.99	0.45
2:D:183:LEU:HD12	2:D:191:GLN:O	2.16	0.45
2:D:2862:ASP:O	2:D:2865:VAL:HG12	2.17	0.45
2:D:2871:GLU:HG2	2:D:2940:ARG:HB3	1.98	0.45
2:D:4066:ASP:OD1	2:D:4172:SER:OG	2.26	0.45
2:A:910:ASN:O	2:A:911:PHE:C	2.58	0.45
2:A:954:THR:HG22	2:A:972:ASP:HB2	1.98	0.45
2:A:3434:GLU:O	2:A:3438:MET:HG3	2.15	0.45
2:A:3536:LEU:CD2	2:A:3560:LEU:HD13	2.46	0.45
2:A:4686:ILE:HD12	2:A:4735:ILE:CD1	2.47	0.45
2:B:843:PRO:O	2:B:1197:PRO:HA	2.17	0.45
2:B:893:THR:O	2:B:904:LEU:HA	2.16	0.45
2:B:2187:MET:HE2	2:B:2236:PHE:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:296:GLU:OE1	2:C:296:GLU:N	2.37	0.45
2:C:931:LYS:O	2:C:934:LEU:HB2	2.16	0.45
2:C:978:LEU:HD13	2:C:982:GLN:HB3	1.98	0.45
2:C:2187:MET:HE2	2:C:2236:PHE:HA	1.99	0.45
2:D:910:ASN:O	2:D:911:PHE:C	2.58	0.45
2:D:978:LEU:HD22	2:D:978:LEU:HA	1.78	0.45
2:D:3324:ILE:CG2	2:D:3409:LEU:HD21	2.46	0.45
2:A:898:ARG:HB2	2:A:905:HIS:HA	1.99	0.45
2:A:1293:SER:OG	2:A:1294:LEU:HD12	2.16	0.45
2:A:3004:LEU:HB2	2:A:3005:PRO:HD3	1.97	0.45
2:B:888:ILE:CG1	2:B:960:TYR:HA	2.47	0.45
2:B:898:ARG:HB2	2:B:905:HIS:HA	1.99	0.45
2:B:2753:ASP:HA	2:B:2756:ILE:HD12	1.99	0.45
2:B:3041:THR:OG1	2:B:3081:VAL:HG21	2.16	0.45
2:C:893:THR:O	2:C:904:LEU:HA	2.16	0.45
2:C:2224:ILE:HD11	2:C:2268:MET:SD	2.56	0.45
2:C:4054:SER:O	2:C:4055:SER:C	2.59	0.45
2:C:4686:ILE:HD12	2:C:4735:ILE:CD1	2.47	0.45
2:D:422:PHE:C	2:D:422:PHE:CD1	2.95	0.45
2:D:642:VAL:HG21	2:D:682:HIS:HD1	1.81	0.45
2:D:843:PRO:O	2:D:1197:PRO:HA	2.17	0.45
2:D:898:ARG:HB2	2:D:905:HIS:HA	1.99	0.45
2:D:978:LEU:HD13	2:D:982:GLN:HB3	1.98	0.45
2:D:3198:LEU:HD11	2:D:3202:MET:CE	2.47	0.45
2:D:4580:VAL:HG12	2:A:4875:ASP:O	2.17	0.45
2:A:956:LEU:HD12	2:A:968:PRO:CD	2.44	0.45
2:A:961:MET:CG	2:A:965:GLY:HA2	2.43	0.45
2:A:3203:PRO:HA	2:A:3284:ARG:NH2	2.31	0.45
2:A:4086:ASP:OD2	2:A:4088:ARG:NH2	2.50	0.45
2:A:4220:PHE:CE1	2:A:4224:VAL:HG21	2.51	0.45
2:B:2802:ASP:OD1	2:B:2802:ASP:C	2.59	0.45
2:B:3177:GLY:C	2:B:3269:HIS:ND1	2.75	0.45
2:B:3536:LEU:CD2	2:B:3560:LEU:HD13	2.46	0.45
2:C:459:GLU:H	2:C:459:GLU:CD	2.25	0.45
2:C:3177:GLY:C	2:C:3269:HIS:ND1	2.75	0.45
2:D:3108:VAL:HA	2:D:3176:LEU:HD12	1.99	0.45
2:D:3181:ASN:OD1	2:D:3183:TYR:CD1	2.69	0.45
2:D:3226:ARG:CZ	2:D:3226:ARG:HB3	2.47	0.45
2:A:879:ILE:CA	2:A:882:LEU:HD12	2.33	0.45
2:A:3177:GLY:C	2:A:3269:HIS:ND1	2.75	0.45
2:B:843:PRO:O	2:B:1198:GLY:N	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2255:LEU:C	2:B:2255:LEU:HD23	2.42	0.45
2:C:321:LYS:HZ1	2:C:357:TRP:CG	2.35	0.45
2:C:898:ARG:HB2	2:C:905:HIS:HA	1.99	0.45
2:C:2862:ASP:O	2:C:2865:VAL:HG12	2.17	0.45
2:C:2871:GLU:HG2	2:C:2940:ARG:HB3	1.98	0.45
2:C:3756:PHE:HA	2:C:3759:LYS:HZ2	1.81	0.45
2:C:4066:ASP:OD1	2:C:4172:SER:OG	2.26	0.45
2:D:1426:GLU:OE1	2:D:1426:GLU:N	2.41	0.44
2:D:3177:GLY:C	2:D:3269:HIS:ND1	2.75	0.44
2:D:3820:LEU:HD13	2:D:3902:PHE:HD1	1.81	0.44
2:A:470:ARG:NE	2:A:3713:GLU:OE1	2.42	0.44
2:A:862:ILE:HG22	2:A:931:LYS:HG2	1.99	0.44
2:A:893:THR:O	2:A:904:LEU:HA	2.16	0.44
2:C:899:ASP:CB	2:C:902:LYS:HB2	2.21	0.44
2:C:954:THR:HG22	2:C:972:ASP:HB2	1.98	0.44
2:D:459:GLU:CD	2:D:459:GLU:H	2.25	0.44
2:D:2816:ALA:HB1	2:D:2882:ASN:ND2	2.32	0.44
2:D:2866:VAL:CG1	2:D:2933:MET:HE3	2.45	0.44
2:D:4628:TYR:OH	2:A:4858:ARG:NH1	2.49	0.44
2:A:888:ILE:CG1	2:A:960:TYR:HA	2.47	0.44
2:A:978:LEU:HD22	2:A:978:LEU:HA	1.78	0.44
2:A:3108:VAL:HA	2:A:3176:LEU:HD12	1.99	0.44
2:B:723:TRP:CZ2	2:B:728:ALA:HB2	2.53	0.44
2:B:954:THR:HG22	2:B:972:ASP:HB2	1.98	0.44
2:B:3944:ASP:OD2	2:B:3945:VAL:N	2.49	0.44
2:B:4671:ARG:NH1	2:B:4700:ASP:OD1	2.51	0.44
2:C:3226:ARG:HB3	2:C:3226:ARG:CZ	2.47	0.44
2:C:3820:LEU:HD13	2:C:3902:PHE:HD1	1.81	0.44
2:C:4893:GLY:N	2:C:4897:ASP:OD2	2.47	0.44
2:D:947:ALA:HA	2:D:950:ASN:ND2	2.32	0.44
2:D:2753:ASP:HA	2:D:2756:ILE:HD12	1.99	0.44
2:D:2875:MET:HB3	2:D:2940:ARG:HD2	1.99	0.44
2:D:4024:LYS:N	2:D:4142:ILE:HD13	2.33	0.44
2:D:4088:ARG:HH12	2:D:4090:LEU:HD12	1.82	0.44
2:D:4686:ILE:HD12	2:D:4735:ILE:CD1	2.47	0.44
2:A:978:LEU:HD13	2:A:982:GLN:HB3	1.98	0.44
2:A:2237:LEU:O	2:A:2240:PHE:HB3	2.18	0.44
2:A:2802:ASP:OD1	2:A:2802:ASP:C	2.59	0.44
2:B:872:ARG:HH12	2:B:923:LEU:HB3	1.82	0.44
2:B:978:LEU:HD11	2:B:1044:VAL:HG11	1.99	0.44
2:B:978:LEU:HD21	2:B:1044:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2413:GLU:HG3	2:B:2413:GLU:O	2.17	0.44
2:C:422:PHE:CD1	2:C:422:PHE:C	2.95	0.44
2:C:978:LEU:HD21	2:C:1044:VAL:HG12	1.99	0.44
2:C:2255:LEU:HD23	2:C:2255:LEU:C	2.42	0.44
2:C:2816:ALA:HB1	2:C:2882:ASN:ND2	2.32	0.44
2:C:3181:ASN:OD1	2:C:3183:TYR:CD1	2.69	0.44
2:C:3198:LEU:HD11	2:C:3202:MET:CE	2.47	0.44
1:E:33:ASP:OD2	1:E:33:ASP:C	2.60	0.44
2:D:956:LEU:HD12	2:D:968:PRO:CD	2.44	0.44
2:D:1478:GLY:HA2	2:D:1485:HIS:H	1.83	0.44
2:D:2234:CYS:HB3	2:D:2238:CYS:HB3	1.55	0.44
2:D:3203:PRO:HA	2:D:3284:ARG:NH2	2.31	0.44
2:D:4671:ARG:NH1	2:D:4700:ASP:OD1	2.51	0.44
2:A:723:TRP:CZ2	2:A:728:ALA:HB2	2.53	0.44
2:A:1478:GLY:HA2	2:A:1485:HIS:H	1.83	0.44
2:A:2862:ASP:O	2:A:2865:VAL:HG12	2.17	0.44
2:A:3446:TRP:HZ3	2:A:3610:THR:HG22	1.83	0.44
2:A:4248:MET:HE1	2:A:4987:MET:HE1	1.99	0.44
2:A:4689:GLN:OE1	2:A:4701:ARG:NH2	2.51	0.44
2:B:34:LEU:HD23	2:B:35:LYS:N	2.33	0.44
2:B:2237:LEU:O	2:B:2240:PHE:HB3	2.18	0.44
2:B:3108:VAL:HA	2:B:3176:LEU:HD12	1.99	0.44
2:B:3294:PRO:HB2	2:B:3297:LEU:HB3	1.99	0.44
2:C:365:PRO:O	2:C:366:LYS:HB3	2.16	0.44
2:C:865:PRO:CD	2:C:868:LEU:HB2	2.44	0.44
2:C:2525:VAL:HG23	2:C:2526:GLY:N	2.31	0.44
2:C:2753:ASP:HA	2:C:2756:ILE:HD12	1.99	0.44
2:C:4086:ASP:OD2	2:C:4088:ARG:NH2	2.50	0.44
2:D:2237:LEU:O	2:D:2240:PHE:HB3	2.18	0.44
2:D:2413:GLU:HG3	2:D:2413:GLU:O	2.17	0.44
2:D:3859:LEU:HD11	2:D:3871:ARG:NH2	2.29	0.44
2:A:843:PRO:O	2:A:1197:PRO:HA	2.17	0.44
2:A:862:ILE:HD13	2:A:931:LYS:O	2.18	0.44
2:A:2255:LEU:HD23	2:A:2255:LEU:C	2.42	0.44
2:A:2816:ALA:HB1	2:A:2882:ASN:ND2	2.32	0.44
2:B:3226:ARG:HB3	2:B:3226:ARG:CZ	2.47	0.44
2:C:947:ALA:HA	2:C:950:ASN:ND2	2.32	0.44
2:C:2237:LEU:O	2:C:2240:PHE:HB3	2.18	0.44
2:C:3580:VAL:HB	2:C:3583:ARG:HD3	2.00	0.44
2:C:3894:LEU:HD13	2:C:3902:PHE:CZ	2.52	0.44
2:D:463:GLU:HG3	2:D:3711:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2255:LEU:HD23	2:D:2255:LEU:C	2.42	0.44
2:A:872:ARG:HH12	2:A:923:LEU:HB3	1.82	0.44
2:A:1426:GLU:OE1	2:A:1426:GLU:N	2.41	0.44
2:A:2972:GLN:O	2:A:2975:ILE:HG22	2.18	0.44
2:B:459:GLU:H	2:B:459:GLU:CD	2.25	0.44
2:B:2862:ASP:O	2:B:2865:VAL:HG12	2.17	0.44
2:B:3446:TRP:HZ3	2:B:3610:THR:HG22	1.83	0.44
2:B:4869:GLU:OE1	2:B:4869:GLU:HA	2.18	0.44
2:C:868:LEU:CD1	2:C:930:LEU:HB3	2.45	0.44
2:C:2972:GLN:O	2:C:2975:ILE:HG22	2.18	0.44
2:C:3108:VAL:HA	2:C:3176:LEU:HD12	1.99	0.44
2:C:4088:ARG:HH12	2:C:4090:LEU:HD12	1.82	0.44
2:C:4689:GLN:OE1	2:C:4701:ARG:NH2	2.51	0.44
2:D:321:LYS:HZ1	2:D:357:TRP:CG	2.35	0.44
2:D:932:THR:HG23	2:D:989:LEU:HD22	2.00	0.44
2:D:978:LEU:HD11	2:D:1044:VAL:HG11	1.99	0.44
2:D:3446:TRP:HZ3	2:D:3610:THR:HG22	1.83	0.44
2:D:3580:VAL:HB	2:D:3583:ARG:HD3	2.00	0.44
2:D:4543:GLU:O	2:D:4547:VAL:HG23	2.18	0.44
2:D:4869:GLU:OE1	2:D:4869:GLU:HA	2.18	0.44
2:A:422:PHE:C	2:A:422:PHE:CD1	2.95	0.44
2:A:947:ALA:HA	2:A:950:ASN:ND2	2.32	0.44
2:A:971:LEU:H	2:A:971:LEU:HG	1.58	0.44
2:A:3293:PRO:O	2:A:3295:PRO:CD	2.66	0.44
2:A:3546:THR:HG22	2:A:3547:ASP:N	2.33	0.44
2:A:4088:ARG:HH12	2:A:4090:LEU:HD12	1.82	0.44
2:B:973:LEU:CB	2:B:976:VAL:HG23	2.46	0.44
2:B:1047:LEU:HA	2:B:1050:TYR:CD2	2.53	0.44
2:B:2866:VAL:CG1	2:B:2933:MET:HE3	2.45	0.44
2:B:4086:ASP:OD2	2:B:4088:ARG:NH2	2.50	0.44
2:C:34:LEU:HD23	2:C:35:LYS:N	2.33	0.44
2:C:862:ILE:HG22	2:C:931:LYS:HG2	1.99	0.44
2:C:1478:GLY:HA2	2:C:1485:HIS:H	1.82	0.44
2:D:2254:HIS:O	2:D:2255:LEU:C	2.60	0.44
2:D:3536:LEU:CD2	2:D:3560:LEU:HD13	2.46	0.44
2:A:870:ARG:NH2	2:A:874:LYS:HD3	2.31	0.44
2:A:1047:LEU:HA	2:A:1050:TYR:CD2	2.53	0.44
2:A:2383:GLU:OE1	2:A:2386:ARG:NH2	2.51	0.44
2:A:3198:LEU:HD11	2:A:3202:MET:CE	2.47	0.44
2:B:470:ARG:NE	2:B:3713:GLU:OE1	2.42	0.44
2:B:862:ILE:HD13	2:B:931:LYS:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:884:ALA:HA	2:B:908:LEU:HD22	2.00	0.44
2:B:2314:LEU:HD12	2:B:2319:TYR:CG	2.53	0.44
2:B:3868:VAL:HG12	2:B:3870:ASN:H	1.83	0.44
2:B:4024:LYS:N	2:B:4142:ILE:HD13	2.33	0.44
2:C:723:TRP:CZ2	2:C:728:ALA:HB2	2.53	0.44
2:C:2413:GLU:O	2:C:2413:GLU:HG3	2.17	0.44
2:C:4543:GLU:O	2:C:4547:VAL:HG23	2.18	0.44
1:E:26:HIS:ND1	1:E:105:LEU:HD11	2.32	0.44
2:D:723:TRP:CZ2	2:D:728:ALA:HB2	2.53	0.44
2:D:862:ILE:HD13	2:D:931:LYS:O	2.18	0.44
2:D:1047:LEU:HA	2:D:1050:TYR:CD2	2.53	0.44
2:D:3377:GLU:O	2:D:3380:LEU:HG	2.18	0.44
2:D:3453:LYS:O	2:D:3456:GLU:HG3	2.18	0.44
2:D:4689:GLN:OE1	2:D:4701:ARG:NH2	2.51	0.44
7:D:8006:PCW:H341	2:A:4855:ASN:CG	2.43	0.44
2:A:321:LYS:HZ1	2:A:357:TRP:CG	2.35	0.44
2:A:2866:VAL:CG1	2:A:2933:MET:HE3	2.45	0.44
2:A:3868:VAL:HG12	2:A:3870:ASN:H	1.83	0.44
2:B:463:GLU:HG3	2:B:3711:LEU:HD13	2.00	0.44
2:B:933:LEU:HD22	2:B:1054:ILE:HG21	2.00	0.44
2:B:947:ALA:HA	2:B:950:ASN:ND2	2.32	0.44
2:B:3377:GLU:O	2:B:3380:LEU:HG	2.18	0.44
2:B:4689:GLN:OE1	2:B:4701:ARG:NH2	2.51	0.44
2:C:463:GLU:HG3	2:C:3711:LEU:HD13	2.00	0.44
2:C:884:ALA:HA	2:C:908:LEU:HD22	2.00	0.44
2:C:2383:GLU:OE1	2:C:2386:ARG:NH2	2.51	0.44
2:D:2972:GLN:O	2:D:2975:ILE:HG22	2.18	0.43
2:A:459:GLU:CD	2:A:459:GLU:H	2.25	0.43
2:A:463:GLU:HG3	2:A:3711:LEU:HD13	2.00	0.43
2:A:2187:MET:HE2	2:A:2236:PHE:HA	1.99	0.43
2:A:3041:THR:OG1	2:A:3081:VAL:HG21	2.16	0.43
2:A:4024:LYS:N	2:A:4142:ILE:HD13	2.33	0.43
2:B:862:ILE:HG22	2:B:931:LYS:HG2	1.99	0.43
2:B:865:PRO:CD	2:B:868:LEU:HB2	2.44	0.43
2:B:2972:GLN:O	2:B:2975:ILE:HG22	2.18	0.43
2:B:3105:GLU:HA	2:B:3108:VAL:HG22	2.00	0.43
2:B:3293:PRO:O	2:B:3295:PRO:CD	2.66	0.43
2:B:3894:LEU:HD13	2:B:3902:PHE:CZ	2.52	0.43
2:B:4543:GLU:O	2:B:4547:VAL:HG23	2.18	0.43
2:C:888:ILE:CG1	2:C:960:TYR:HA	2.47	0.43
2:C:973:LEU:CB	2:C:976:VAL:HG23	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1047:LEU:HA	2:C:1050:TYR:CD2	2.53	0.43
2:C:3267:MET:HG3	2:C:3267:MET:O	2.18	0.43
2:C:3294:PRO:HB2	2:C:3297:LEU:HB3	1.99	0.43
2:C:3868:VAL:HG12	2:C:3870:ASN:H	1.83	0.43
2:C:4869:GLU:OE1	2:C:4869:GLU:HA	2.18	0.43
2:D:34:LEU:HD23	2:D:35:LYS:N	2.33	0.43
2:D:902:LYS:HA	2:D:902:LYS:HD2	1.55	0.43
2:D:2187:MET:HE2	2:D:2236:PHE:HA	1.99	0.43
2:A:875:LEU:HD12	2:A:878:ASN:HD22	1.83	0.43
2:A:978:LEU:HD11	2:A:1044:VAL:HG11	1.99	0.43
2:A:1742:GLU:OE1	2:A:1742:GLU:N	2.45	0.43
2:A:3226:ARG:HB3	2:A:3226:ARG:CZ	2.48	0.43
2:A:3294:PRO:HB2	2:A:3297:LEU:HB3	1.99	0.43
2:A:3820:LEU:HD13	2:A:3902:PHE:HD1	1.81	0.43
2:B:308:ALA:HB1	2:B:313:THR:HG21	2.01	0.43
2:B:2782:ILE:O	2:B:2783:ASP:C	2.61	0.43
2:B:3546:THR:HG22	2:B:3547:ASP:N	2.33	0.43
2:B:3820:LEU:HD13	2:B:3902:PHE:HD1	1.81	0.43
2:B:4854:PHE:O	2:B:4858:ARG:NH1	2.50	0.43
2:C:707:GLY:N	2:C:710:ASP:OD2	2.44	0.43
2:C:930:LEU:O	2:C:934:LEU:HD22	2.18	0.43
2:C:2254:HIS:O	2:C:2255:LEU:C	2.60	0.43
2:C:3291:GLU:OE2	2:C:3310:SER:N	2.38	0.43
2:C:3546:THR:HG22	2:C:3547:ASP:N	2.33	0.43
2:C:3594:VAL:O	2:C:3597:VAL:HG12	2.19	0.43
2:D:884:ALA:HA	2:D:908:LEU:HD22	2.00	0.43
2:D:3267:MET:HG3	2:D:3267:MET:O	2.18	0.43
2:D:4086:ASP:OD2	2:D:4088:ARG:NH2	2.50	0.43
2:A:652:GLY:N	2:A:659:GLN:OE1	2.46	0.43
2:A:884:ALA:HA	2:A:908:LEU:HD22	2.00	0.43
2:A:2753:ASP:HA	2:A:2756:ILE:HD12	1.99	0.43
2:B:4214:LYS:O	2:B:4218:ARG:HG3	2.18	0.43
2:C:11:GLU:OE1	2:C:12:VAL:N	2.52	0.43
2:C:894:TYR:CB	2:C:964:ASN:HB3	2.48	0.43
2:C:2314:LEU:HD12	2:C:2319:TYR:CG	2.53	0.43
2:C:3377:GLU:O	2:C:3380:LEU:HG	2.18	0.43
2:C:3453:LYS:O	2:C:3456:GLU:HG3	2.18	0.43
2:D:3294:PRO:HB2	2:D:3297:LEU:HB3	1.99	0.43
2:A:296:GLU:OE1	2:A:296:GLU:N	2.37	0.43
2:A:308:ALA:HB1	2:A:313:THR:HG21	2.00	0.43
2:A:952:LYS:HZ3	2:A:952:LYS:HG2	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3130:LEU:O	2:A:3133:THR:OG1	2.36	0.43
7:A:8006:PCW:H341	2:B:4855:ASN:CG	2.44	0.43
2:B:3198:LEU:HD11	2:B:3202:MET:CE	2.47	0.43
2:B:4187:MET:HE3	2:B:4191:ARG:HA	2.00	0.43
2:C:605:CYS:HB2	2:C:608:CYS:H	1.84	0.43
2:C:2241:CYS:SG	2:C:2251:MET:HG3	2.59	0.43
2:C:4024:LYS:N	2:C:4142:ILE:HD13	2.33	0.43
2:D:470:ARG:NE	2:D:3713:GLU:OE1	2.42	0.43
2:D:875:LEU:HD12	2:D:878:ASN:HD22	1.83	0.43
2:D:877:GLU:HA	2:D:911:PHE:CE2	2.54	0.43
2:A:11:GLU:OE1	2:A:12:VAL:N	2.52	0.43
2:A:930:LEU:O	2:A:934:LEU:HD22	2.18	0.43
2:A:3267:MET:HG3	2:A:3267:MET:O	2.18	0.43
2:B:953:LYS:HE2	2:B:953:LYS:HB2	1.84	0.43
2:B:1478:GLY:HA2	2:B:1485:HIS:H	1.82	0.43
2:B:3267:MET:O	2:B:3267:MET:HG3	2.18	0.43
2:C:933:LEU:HD22	2:C:1054:ILE:HG21	2.00	0.43
2:C:2234:CYS:HB3	2:C:2238:CYS:HB3	1.55	0.43
2:C:3105:GLU:HA	2:C:3108:VAL:HG22	2.00	0.43
2:C:3446:TRP:HZ3	2:C:3610:THR:HG22	1.83	0.43
2:D:2241:CYS:SG	2:D:2251:MET:HG3	2.59	0.43
2:D:3868:VAL:HG12	2:D:3870:ASN:H	1.83	0.43
2:A:297:ASP:N	2:A:297:ASP:OD1	2.52	0.43
2:A:978:LEU:HD21	2:A:1044:VAL:HG12	1.99	0.43
2:A:2254:HIS:O	2:A:2255:LEU:C	2.60	0.43
2:A:2314:LEU:HD12	2:A:2319:TYR:CG	2.53	0.43
2:A:2413:GLU:HG3	2:A:2413:GLU:O	2.17	0.43
2:A:2875:MET:HB3	2:A:2940:ARG:HD2	1.99	0.43
2:A:3105:GLU:HA	2:A:3108:VAL:HG22	2.00	0.43
2:A:3319:ASN:O	2:A:3323:ILE:HG12	2.19	0.43
2:A:3546:THR:HG22	2:A:3547:ASP:H	1.83	0.43
2:A:3580:VAL:HB	2:A:3583:ARG:HD3	2.00	0.43
2:B:930:LEU:O	2:B:934:LEU:HD22	2.18	0.43
2:B:3108:VAL:HG12	2:B:3176:LEU:CD1	2.49	0.43
2:C:862:ILE:HD13	2:C:931:LYS:O	2.18	0.43
2:C:3293:PRO:O	2:C:3295:PRO:CD	2.66	0.43
2:C:4214:LYS:O	2:C:4218:ARG:HG3	2.18	0.43
2:D:916:GLU:N	2:D:917:PRO:CD	2.82	0.43
2:D:930:LEU:O	2:D:934:LEU:HD22	2.18	0.43
2:D:2782:ILE:O	2:D:2783:ASP:C	2.61	0.43
2:D:3587:ALA:O	2:D:3593:ILE:HD11	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:956:LEU:HD22	2:A:957:PRO:HD2	2.01	0.43
2:A:3377:GLU:O	2:A:3380:LEU:HG	2.18	0.43
2:A:3894:LEU:CB	2:A:3902:PHE:CE2	3.02	0.43
2:A:4671:ARG:NH1	2:A:4700:ASP:OD1	2.51	0.43
2:B:2914:ALA:O	2:B:2917:LYS:HB2	2.19	0.43
2:B:4543:GLU:OE1	2:B:4543:GLU:HA	2.19	0.43
2:C:2914:ALA:O	2:C:2917:LYS:HB2	2.19	0.43
2:C:3324:ILE:HG21	2:C:3409:LEU:HD21	2.01	0.43
2:C:4688:GLU:O	2:C:4689:GLN:NE2	2.52	0.43
2:D:870:ARG:NH2	2:D:874:LYS:HD3	2.31	0.43
2:D:2872:LEU:O	2:D:2875:MET:HG2	2.19	0.43
2:D:3546:THR:HG22	2:D:3547:ASP:N	2.33	0.43
2:D:3594:VAL:O	2:D:3597:VAL:HG12	2.19	0.43
2:D:3756:PHE:HA	2:D:3759:LYS:HZ2	1.83	0.43
2:A:872:ARG:HH22	2:A:923:LEU:HD23	1.84	0.43
2:A:877:GLU:HA	2:A:911:PHE:CE2	2.54	0.43
2:A:894:TYR:CB	2:A:964:ASN:HB3	2.48	0.43
2:A:916:GLU:N	2:A:917:PRO:CD	2.82	0.43
2:A:933:LEU:HD22	2:A:1054:ILE:HG21	2.00	0.43
2:A:2872:LEU:O	2:A:2875:MET:HG2	2.19	0.43
2:B:1273:LEU:HD22	2:B:1290:LEU:HD11	2.01	0.43
2:B:2875:MET:HB3	2:B:2940:ARG:HD2	1.99	0.43
2:B:3324:ILE:HG21	2:B:3409:LEU:HD21	2.01	0.43
2:B:4088:ARG:HH12	2:B:4090:LEU:HD12	1.82	0.43
2:C:952:LYS:HZ3	2:C:952:LYS:HG2	1.66	0.43
2:C:956:LEU:HD12	2:C:968:PRO:CD	2.44	0.43
1:H:33:ASP:OD2	1:H:33:ASP:C	2.60	0.43
2:D:11:GLU:OE1	2:D:12:VAL:N	2.52	0.43
2:D:605:CYS:HB2	2:D:608:CYS:H	1.84	0.43
2:D:916:GLU:HA	2:D:919:ARG:HD2	2.01	0.43
2:D:1031:ALA:O	2:D:1034:ARG:HG2	2.19	0.43
2:D:2269:GLN:HG3	2:D:2269:GLN:O	2.19	0.43
2:D:2314:LEU:HD12	2:D:2319:TYR:CG	2.53	0.43
2:D:2914:ALA:O	2:D:2917:LYS:HB2	2.19	0.43
2:D:3546:THR:HG22	2:D:3547:ASP:H	1.84	0.43
2:A:916:GLU:HA	2:A:919:ARG:HD2	2.01	0.43
2:A:2782:ILE:O	2:A:2783:ASP:C	2.61	0.43
2:A:3453:LYS:O	2:A:3456:GLU:HG3	2.18	0.43
2:A:4869:GLU:OE1	2:A:4869:GLU:HA	2.18	0.43
2:B:877:GLU:HA	2:B:911:PHE:CE2	2.54	0.43
2:B:881:GLU:HB3	2:B:970:PRO:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:308:ALA:HB1	2:C:313:THR:HG21	2.00	0.43
2:C:978:LEU:HD11	2:C:1044:VAL:HG11	1.99	0.43
2:C:2519:LEU:O	2:C:2523:LEU:HD13	2.19	0.43
2:C:2782:ILE:O	2:C:2783:ASP:C	2.61	0.43
2:C:4187:MET:HE3	2:C:4191:ARG:HA	2.00	0.43
1:G:77:ILE:O	1:G:97:THR:HG23	2.19	0.43
2:D:791:ARG:HA	2:D:1627:TRP:O	2.19	0.43
2:D:872:ARG:HH12	2:D:923:LEU:HB3	1.82	0.43
2:D:973:LEU:CB	2:D:976:VAL:HG23	2.46	0.43
2:D:2519:LEU:O	2:D:2523:LEU:HD13	2.19	0.43
2:D:3108:VAL:HG12	2:D:3176:LEU:CD1	2.49	0.43
2:D:3324:ILE:HG21	2:D:3409:LEU:HD21	2.01	0.43
2:D:3399:PHE:HB2	2:D:3455:GLU:HG3	2.01	0.43
2:A:3756:PHE:HA	2:A:3759:LYS:HZ2	1.83	0.43
2:B:952:LYS:HZ3	2:B:952:LYS:HG2	1.65	0.43
2:B:1155:ASP:OD1	2:B:1157:THR:OG1	2.32	0.43
2:B:2768:ALA:HA	2:B:2771:LYS:HE3	2.01	0.43
2:B:3556:ASN:OD1	2:B:3556:ASN:C	2.62	0.43
2:C:872:ARG:HH12	2:C:923:LEU:HB3	1.82	0.43
2:C:1273:LEU:HD22	2:C:1290:LEU:HD11	2.01	0.43
2:D:707:GLY:N	2:D:710:ASP:OD2	2.44	0.42
2:D:978:LEU:HD21	2:D:1044:VAL:HG12	1.99	0.42
2:D:3293:PRO:O	2:D:3295:PRO:CD	2.66	0.42
2:A:34:LEU:HD23	2:A:35:LYS:N	2.33	0.42
2:A:2241:CYS:SG	2:A:2251:MET:HG3	2.59	0.42
2:A:2519:LEU:O	2:A:2523:LEU:HD13	2.19	0.42
2:A:3285:TRP:HB3	2:A:3306:THR:HG21	2.01	0.42
2:A:4543:GLU:OE1	2:A:4543:GLU:HA	2.19	0.42
2:B:875:LEU:HD12	2:B:878:ASN:HD22	1.83	0.42
2:B:932:THR:HG23	2:B:989:LEU:HD22	2.00	0.42
2:B:2519:LEU:O	2:B:2523:LEU:HD13	2.19	0.42
2:B:2794:PRO:O	2:B:2798:PHE:N	2.41	0.42
2:B:3453:LYS:O	2:B:3456:GLU:HG3	2.18	0.42
2:B:4625:MET:HA	2:B:4625:MET:HE2	2.01	0.42
2:C:791:ARG:HA	2:C:1627:TRP:O	2.19	0.42
2:C:875:LEU:HD12	2:C:878:ASN:HD22	1.83	0.42
2:C:932:THR:HG23	2:C:989:LEU:HD22	2.00	0.42
2:C:1857:SER:OG	2:C:1860:ASP:OD1	2.35	0.42
2:C:4671:ARG:NH1	2:C:4700:ASP:OD1	2.51	0.42
1:F:33:ASP:OD2	1:F:33:ASP:C	2.60	0.42
2:D:3366:LEU:HD13	2:D:3406:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4214:LYS:O	2:D:4218:ARG:HG3	2.18	0.42
2:A:3110:ASN:ND2	2:A:3126:VAL:HG13	2.34	0.42
2:A:4214:LYS:O	2:A:4218:ARG:HG3	2.18	0.42
2:B:948:GLU:HG2	2:B:1050:TYR:HA	2.01	0.42
2:B:2563:ILE:HG22	2:B:2611:LEU:HD11	2.01	0.42
2:B:3110:ASN:ND2	2:B:3126:VAL:HG13	2.34	0.42
2:B:3160:ASP:O	2:B:3164:VAL:HG23	2.19	0.42
2:B:3594:VAL:O	2:B:3597:VAL:HG12	2.19	0.42
2:C:216:THR:OG1	2:C:219:HIS:CD2	2.73	0.42
2:C:877:GLU:HA	2:C:911:PHE:CE2	2.54	0.42
2:C:881:GLU:HB3	2:C:970:PRO:N	2.34	0.42
2:C:3108:VAL:HG12	2:C:3176:LEU:CD1	2.49	0.42
2:C:3110:ASN:ND2	2:C:3126:VAL:HG13	2.34	0.42
2:C:3410:TYR:N	2:C:3411:PRO:HD2	2.34	0.42
2:C:3962:LYS:HG3	2:C:4025:ASP:OD1	2.20	0.42
2:D:872:ARG:HH22	2:D:923:LEU:HD23	1.84	0.42
2:D:956:LEU:HD22	2:D:957:PRO:HD2	2.01	0.42
2:D:3055:VAL:HG23	2:D:3062:ALA:HB1	2.02	0.42
2:D:3105:GLU:HA	2:D:3108:VAL:HG22	2.00	0.42
2:D:3130:LEU:O	2:D:3133:THR:OG1	2.36	0.42
2:D:3894:LEU:CB	2:D:3902:PHE:CE2	3.02	0.42
2:D:4625:MET:HE2	2:D:4625:MET:HA	2.01	0.42
2:A:3587:ALA:O	2:A:3593:ILE:HD11	2.19	0.42
2:B:11:GLU:OE1	2:B:12:VAL:N	2.52	0.42
2:B:894:TYR:CB	2:B:964:ASN:HB3	2.48	0.42
2:B:2254:HIS:O	2:B:2255:LEU:C	2.60	0.42
2:B:2269:GLN:O	2:B:2269:GLN:HG3	2.19	0.42
2:B:3962:LYS:HG3	2:B:4025:ASP:OD1	2.20	0.42
2:C:859:THR:HG21	2:C:932:THR:HA	2.01	0.42
2:C:925:MET:O	2:C:929:THR:HG23	2.20	0.42
2:C:2768:ALA:HA	2:C:2771:LYS:HE3	2.01	0.42
2:C:3160:ASP:O	2:C:3164:VAL:HG23	2.19	0.42
2:C:3366:LEU:HD13	2:C:3406:LEU:HD23	2.01	0.42
2:D:652:GLY:N	2:D:659:GLN:OE1	2.46	0.42
2:D:881:GLU:HB3	2:D:970:PRO:N	2.34	0.42
2:D:894:TYR:CB	2:D:964:ASN:HB3	2.48	0.42
2:D:1480:GLU:OE1	2:D:1480:GLU:N	2.43	0.42
2:D:1742:GLU:OE1	2:D:1742:GLU:N	2.45	0.42
2:D:3110:ASN:ND2	2:D:3126:VAL:HG13	2.34	0.42
2:D:3285:TRP:HB3	2:D:3306:THR:HG21	2.02	0.42
2:D:3319:ASN:O	2:D:3323:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:875:LEU:HD12	2:A:875:LEU:O	2.19	0.42
2:A:2314:LEU:HD11	2:A:2417:VAL:CG1	2.50	0.42
2:A:3055:VAL:HG23	2:A:3062:ALA:HB1	2.01	0.42
2:A:3594:VAL:O	2:A:3597:VAL:HG12	2.19	0.42
2:A:4543:GLU:O	2:A:4547:VAL:HG23	2.18	0.42
2:B:605:CYS:HB2	2:B:608:CYS:H	1.84	0.42
2:B:875:LEU:HD12	2:B:875:LEU:O	2.19	0.42
2:B:951:LEU:H	2:B:951:LEU:HG	1.70	0.42
2:B:961:MET:CG	2:B:965:GLY:HA2	2.43	0.42
2:B:1031:ALA:O	2:B:1034:ARG:HG2	2.19	0.42
2:B:2241:CYS:SG	2:B:2251:MET:HG3	2.59	0.42
2:C:902:LYS:HA	2:C:902:LYS:HD2	1.55	0.42
2:C:916:GLU:N	2:C:917:PRO:CD	2.82	0.42
2:C:3285:TRP:HB3	2:C:3306:THR:HG21	2.02	0.42
2:C:3587:ALA:O	2:C:3593:ILE:HD11	2.19	0.42
1:G:57:ILE:CG1	1:G:60:TRP:HD1	2.32	0.42
2:D:308:ALA:HB1	2:D:313:THR:HG21	2.01	0.42
2:D:933:LEU:HD22	2:D:1054:ILE:HG21	2.00	0.42
2:D:4649:THR:OG1	2:D:4801:HIS:CD2	2.73	0.42
2:A:902:LYS:CE	2:A:904:LEU:HD21	2.39	0.42
2:A:2623:LEU:O	2:A:2627:LEU:HD13	2.19	0.42
2:A:4625:MET:HE2	2:A:4625:MET:HA	2.01	0.42
2:B:859:THR:HG21	2:B:932:THR:HA	2.01	0.42
2:B:872:ARG:HH22	2:B:923:LEU:HD23	1.84	0.42
2:B:3580:VAL:HB	2:B:3583:ARG:HD3	2.00	0.42
2:C:1031:ALA:O	2:C:1034:ARG:HG2	2.19	0.42
2:C:2269:GLN:HG3	2:C:2269:GLN:O	2.19	0.42
2:C:3319:ASN:O	2:C:3323:ILE:HG12	2.19	0.42
1:F:80:ASP:OD2	1:F:81:TYR:CD1	2.73	0.42
2:D:3410:TYR:N	2:D:3411:PRO:HD2	2.34	0.42
2:A:1153:MET:HE1	2:A:1164:THR:HG23	2.02	0.42
2:A:2269:GLN:HG3	2:A:2269:GLN:O	2.19	0.42
2:A:2768:ALA:HA	2:A:2771:LYS:HE3	2.01	0.42
2:A:2794:PRO:O	2:A:2798:PHE:N	2.41	0.42
2:A:3324:ILE:HG21	2:A:3409:LEU:HD21	2.01	0.42
2:A:4649:THR:OG1	2:A:4801:HIS:CD2	2.73	0.42
2:A:4893:GLY:N	2:A:4897:ASP:OD2	2.47	0.42
2:B:2383:GLU:OE1	2:B:2386:ARG:NH2	2.51	0.42
2:B:2623:LEU:O	2:B:2627:LEU:HD13	2.19	0.42
2:C:978:LEU:HD22	2:C:978:LEU:HA	1.78	0.42
2:C:2270:GLY:O	2:C:2272:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4543:GLU:OE1	2:C:4543:GLU:HA	2.19	0.42
1:E:77:ILE:O	1:E:97:THR:HG23	2.19	0.42
2:D:216:THR:OG1	2:D:219:HIS:CD2	2.73	0.42
2:D:1428:ILE:HG23	2:D:1429:LEU:HD22	2.01	0.42
2:D:2314:LEU:HD11	2:D:2417:VAL:CG1	2.50	0.42
2:D:3962:LYS:HG3	2:D:4025:ASP:OD1	2.20	0.42
2:A:791:ARG:HA	2:A:1627:TRP:O	2.19	0.42
2:A:881:GLU:HB3	2:A:970:PRO:N	2.34	0.42
2:A:948:GLU:HG2	2:A:1050:TYR:HA	2.02	0.42
2:A:973:LEU:CB	2:A:976:VAL:HG23	2.46	0.42
2:A:1031:ALA:O	2:A:1034:ARG:HG2	2.19	0.42
2:A:2563:ILE:HG22	2:A:2611:LEU:HD11	2.01	0.42
2:A:3108:VAL:HG12	2:A:3176:LEU:CD1	2.49	0.42
2:A:3160:ASP:O	2:A:3164:VAL:HG23	2.20	0.42
2:A:3366:LEU:HD13	2:A:3406:LEU:HD23	2.01	0.42
2:B:1153:MET:HE1	2:B:1164:THR:HG23	2.02	0.42
2:B:3285:TRP:HB3	2:B:3306:THR:HG21	2.02	0.42
2:B:3443:PHE:CD2	2:B:3515:LEU:HD22	2.55	0.42
2:B:4688:GLU:O	2:B:4689:GLN:NE2	2.52	0.42
2:C:872:ARG:HH22	2:C:923:LEU:HD23	1.84	0.42
2:C:956:LEU:HD22	2:C:957:PRO:HD2	2.01	0.42
2:C:3999:PHE:HD1	2:C:4019:LEU:HD11	1.85	0.42
2:D:925:MET:O	2:D:929:THR:HG23	2.20	0.42
2:D:2623:LEU:O	2:D:2627:LEU:HD13	2.19	0.42
2:D:3160:ASP:O	2:D:3164:VAL:HG23	2.19	0.42
2:D:3556:ASN:OD1	2:D:3556:ASN:C	2.62	0.42
2:D:4688:GLU:O	2:D:4689:GLN:NE2	2.52	0.42
2:A:859:THR:HG21	2:A:932:THR:HA	2.01	0.42
2:A:1273:LEU:HD22	2:A:1290:LEU:HD11	2.01	0.42
2:B:955:LYS:HB3	2:B:955:LYS:HE3	1.61	0.42
2:B:2270:GLY:O	2:B:2272:THR:HG23	2.20	0.42
2:B:2413:GLU:O	2:B:2416:ARG:N	2.53	0.42
2:B:2922:GLU:HA	2:B:2925:GLN:HG2	2.02	0.42
2:B:3410:TYR:N	2:B:3411:PRO:HD2	2.34	0.42
2:C:875:LEU:HD12	2:C:875:LEU:O	2.19	0.42
2:C:3055:VAL:HG23	2:C:3062:ALA:HB1	2.02	0.42
2:C:3360:ILE:HB	2:C:3361:PRO:HD3	2.02	0.42
2:C:3392:GLU:O	2:C:3396:ARG:HG2	2.20	0.42
2:C:3974:GLY:N	2:C:3975:PRO:HA	2.35	0.42
1:H:77:ILE:O	1:H:97:THR:HG23	2.20	0.42
1:H:80:ASP:OD2	1:H:81:TYR:CD1	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:784:PHE:CG	2:D:788:ILE:HD11	2.55	0.42
2:D:870:ARG:HD3	2:D:1052:TYR:OH	2.20	0.42
2:D:2270:GLY:O	2:D:2272:THR:HG23	2.20	0.42
2:D:2876:ALA:HB1	2:D:2921:ARG:NH1	2.35	0.42
2:A:784:PHE:CG	2:A:788:ILE:HD11	2.55	0.42
2:A:932:THR:HG23	2:A:989:LEU:HD22	2.00	0.42
2:A:1144:TRP:HB2	2:A:1148:ASP:HB2	2.02	0.42
2:A:1428:ILE:HG23	2:A:1429:LEU:HD22	2.01	0.42
2:A:2876:ALA:HB1	2:A:2921:ARG:NH1	2.35	0.42
2:A:2914:ALA:O	2:A:2917:LYS:HB2	2.19	0.42
2:A:3399:PHE:HB2	2:A:3455:GLU:HG3	2.01	0.42
2:A:3403:CYS:SG	2:A:3456:GLU:HA	2.60	0.42
2:A:3859:LEU:HD11	2:A:3871:ARG:NH2	2.29	0.42
2:A:3999:PHE:HD1	2:A:4019:LEU:HD11	1.85	0.42
2:A:4187:MET:HE3	2:A:4191:ARG:HA	2.00	0.42
2:B:784:PHE:CG	2:B:788:ILE:HD11	2.55	0.42
2:B:874:LYS:HE3	2:B:875:LEU:N	2.35	0.42
2:B:1064:VAL:HG13	2:B:1065:ASP:N	2.35	0.42
2:B:1546:ASN:OD1	2:B:1546:ASN:O	2.38	0.42
2:B:3130:LEU:O	2:B:3133:THR:OG1	2.36	0.42
2:B:3587:ALA:O	2:B:3593:ILE:HD11	2.19	0.42
2:C:2623:LEU:O	2:C:2627:LEU:HD13	2.19	0.42
2:C:3546:THR:HG22	2:C:3547:ASP:H	1.84	0.42
2:D:337:PRO:HA	2:D:338:PRO:HD3	1.92	0.42
2:D:859:THR:HG21	2:D:932:THR:HA	2.01	0.42
2:D:931:LYS:HB3	2:D:931:LYS:HE3	1.79	0.42
2:D:1127:GLY:HA3	2:D:1144:TRP:CE3	2.55	0.42
2:D:2635:ASN:OD1	2:D:2638:ALA:N	2.53	0.42
2:D:2762:TYR:CZ	2:D:2863:LEU:HG	2.55	0.42
2:D:2771:LYS:HB3	2:D:2776:TRP:HB2	2.02	0.42
2:D:4187:MET:HE3	2:D:4191:ARG:HA	2.00	0.42
2:D:4543:GLU:OE1	2:D:4543:GLU:HA	2.19	0.42
2:A:605:CYS:HB2	2:A:608:CYS:H	1.84	0.42
2:A:925:MET:O	2:A:929:THR:HG23	2.20	0.42
2:A:3198:LEU:HD12	2:A:3198:LEU:O	2.20	0.42
2:A:3556:ASN:OD1	2:A:3556:ASN:C	2.62	0.42
2:A:4703:VAL:O	2:A:4703:VAL:HG22	2.20	0.42
2:B:216:THR:OG1	2:B:219:HIS:CD2	2.73	0.42
2:B:297:ASP:OD1	2:B:297:ASP:N	2.52	0.42
2:B:791:ARG:HA	2:B:1627:TRP:O	2.19	0.42
2:B:3267:MET:O	2:B:3267:MET:CG	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3319:ASN:O	2:B:3323:ILE:HG12	2.19	0.42
2:B:3360:ILE:HB	2:B:3361:PRO:HD3	2.02	0.42
2:B:3974:GLY:N	2:B:3975:PRO:HA	2.35	0.42
2:B:3999:PHE:HD1	2:B:4019:LEU:HD11	1.85	0.42
2:B:4893:GLY:N	2:B:4897:ASP:OD2	2.47	0.42
2:C:784:PHE:CG	2:C:788:ILE:HD11	2.55	0.42
2:C:874:LYS:HE3	2:C:875:LEU:N	2.35	0.42
2:C:1064:VAL:HG13	2:C:1065:ASP:N	2.35	0.42
2:C:2563:ILE:HG22	2:C:2611:LEU:HD11	2.01	0.42
2:C:3367:ARG:NH1	2:C:3441:GLU:OE1	2.42	0.42
2:C:4625:MET:HE2	2:C:4625:MET:HA	2.01	0.42
1:E:91:ILE:N	1:E:91:ILE:HD12	2.35	0.41
2:D:1273:LEU:HD22	2:D:1290:LEU:HD11	2.01	0.41
2:D:3850:PHE:CZ	2:D:3940:TYR:OH	2.73	0.41
2:D:3999:PHE:HD1	2:D:4019:LEU:HD11	1.85	0.41
2:D:4854:PHE:O	2:D:4858:ARG:NH1	2.50	0.41
2:A:1546:ASN:OD1	2:A:1546:ASN:O	2.38	0.41
2:A:2779:GLY:HA3	2:A:2788:THR:HB	2.01	0.41
2:A:3392:GLU:O	2:A:3396:ARG:HG2	2.20	0.41
2:A:3443:PHE:CD2	2:A:3515:LEU:HD22	2.55	0.41
2:B:916:GLU:HA	2:B:919:ARG:HD2	2.01	0.41
2:B:916:GLU:N	2:B:917:PRO:CD	2.82	0.41
2:B:1127:GLY:HA3	2:B:1144:TRP:CE3	2.55	0.41
2:B:3177:GLY:HA3	2:B:3269:HIS:CE1	2.55	0.41
2:B:3198:LEU:HD12	2:B:3198:LEU:O	2.20	0.41
2:B:3366:LEU:HD13	2:B:3406:LEU:HD23	2.01	0.41
2:B:3399:PHE:HB2	2:B:3455:GLU:HG3	2.01	0.41
2:B:3403:CYS:SG	2:B:3456:GLU:HA	2.60	0.41
2:B:4578:TYR:HE1	2:B:4630:LEU:HD21	1.85	0.41
2:B:4909:LEU:HA	2:B:4912:VAL:HG22	2.02	0.41
2:C:843:PRO:HG2	2:C:1072:ARG:O	2.20	0.41
2:C:967:LYS:HZ1	2:C:969:ALA:HB2	1.84	0.41
2:C:1428:ILE:HG23	2:C:1429:LEU:HD22	2.01	0.41
2:C:3399:PHE:HB2	2:C:3455:GLU:HG3	2.01	0.41
2:C:4649:THR:OG1	2:C:4801:HIS:CD2	2.73	0.41
1:E:91:ILE:HD11	2:A:1685:ALA:HA	2.01	0.41
1:G:2:GLY:N	1:G:78:SER:OG	2.41	0.41
2:D:297:ASP:OD1	2:D:297:ASP:N	2.52	0.41
2:D:2334:ASP:HA	2:D:2337:ARG:HD3	2.02	0.41
2:D:2383:GLU:OE1	2:D:2386:ARG:NH2	2.51	0.41
2:D:3360:ILE:HB	2:D:3361:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1470:VAL:HG13	2:A:1493:CYS:HB3	2.03	0.41
2:A:3177:GLY:HA3	2:A:3269:HIS:CE1	2.55	0.41
2:A:3850:PHE:CZ	2:A:3940:TYR:OH	2.73	0.41
2:A:3962:LYS:HG3	2:A:4025:ASP:OD1	2.20	0.41
2:B:1996:THR:O	2:B:1997:ARG:C	2.63	0.41
2:B:2876:ALA:HB1	2:B:2921:ARG:NH1	2.35	0.41
2:B:3239:GLU:O	2:B:3240:MET:C	2.63	0.41
2:B:3546:THR:HG22	2:B:3547:ASP:H	1.84	0.41
2:B:4703:VAL:HG22	2:B:4703:VAL:O	2.20	0.41
8:B:8008:A1BYZ:O7	8:B:8008:A1BYZ:C10	2.68	0.41
2:C:1996:THR:O	2:C:1997:ARG:C	2.63	0.41
2:C:2234:CYS:O	2:C:2236:PHE:C	2.63	0.41
2:C:2746:VAL:O	2:C:2815:LYS:HE2	2.20	0.41
2:C:3202:MET:HG3	2:C:3204:VAL:H	1.85	0.41
2:D:2768:ALA:HA	2:D:2771:LYS:HE3	2.01	0.41
2:D:3198:LEU:HD12	2:D:3198:LEU:O	2.20	0.41
2:D:3443:PHE:CD2	2:D:3515:LEU:HD22	2.55	0.41
2:A:216:THR:OG1	2:A:219:HIS:CD2	2.73	0.41
2:A:870:ARG:HD3	2:A:1052:TYR:OH	2.20	0.41
2:A:2266:LEU:HD13	2:A:2327:CYS:HB3	2.02	0.41
2:A:2771:LYS:HB3	2:A:2776:TRP:HB2	2.02	0.41
2:A:3079:ARG:O	2:A:3083:LYS:HG2	2.21	0.41
2:A:3410:TYR:N	2:A:3411:PRO:HD2	2.34	0.41
2:B:956:LEU:HD22	2:B:957:PRO:HD2	2.01	0.41
2:B:1144:TRP:HB2	2:B:1148:ASP:HB2	2.02	0.41
2:B:2234:CYS:O	2:B:2236:PHE:C	2.63	0.41
2:B:2266:LEU:HD13	2:B:2327:CYS:HB3	2.03	0.41
2:B:2314:LEU:HD11	2:B:2417:VAL:CG1	2.50	0.41
2:B:2872:LEU:O	2:B:2875:MET:HG2	2.19	0.41
2:B:3850:PHE:CZ	2:B:3940:TYR:OH	2.73	0.41
2:C:2872:LEU:O	2:C:2875:MET:HG2	2.19	0.41
2:C:3894:LEU:CB	2:C:3902:PHE:CE2	3.02	0.41
2:C:4909:LEU:HA	2:C:4912:VAL:HG22	2.02	0.41
1:F:91:ILE:HD12	1:F:91:ILE:N	2.35	0.41
2:D:566:TYR:O	2:D:570:ILE:HG12	2.20	0.41
2:D:2234:CYS:O	2:D:2236:PHE:C	2.63	0.41
2:D:2563:ILE:HG22	2:D:2611:LEU:HD11	2.01	0.41
2:D:3008:ASN:OD1	2:D:3008:ASN:C	2.63	0.41
2:A:874:LYS:HE3	2:A:875:LEU:N	2.35	0.41
2:A:1996:THR:O	2:A:1997:ARG:C	2.63	0.41
2:A:4580:VAL:HG12	2:B:4875:ASP:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4865:GLU:HA	2:A:4865:GLU:OE2	2.21	0.41
2:A:4899:ILE:HG13	2:A:4911:ARG:NH2	2.35	0.41
2:B:843:PRO:HG2	2:B:1072:ARG:O	2.20	0.41
2:B:967:LYS:HZ1	2:B:969:ALA:HB2	1.85	0.41
2:B:2975:ILE:HD11	2:B:3057:LEU:HD22	2.02	0.41
2:B:3055:VAL:HG23	2:B:3062:ALA:HB1	2.02	0.41
2:C:870:ARG:NH2	2:C:874:LYS:HD3	2.31	0.41
2:C:870:ARG:HD3	2:C:1052:TYR:OH	2.20	0.41
2:C:2334:ASP:HA	2:C:2337:ARG:HD3	2.03	0.41
2:C:2876:ALA:HB1	2:C:2921:ARG:NH1	2.35	0.41
2:C:2922:GLU:HA	2:C:2925:GLN:HG2	2.02	0.41
2:C:3008:ASN:OD1	2:C:3008:ASN:C	2.63	0.41
2:D:902:LYS:CE	2:D:904:LEU:HD21	2.39	0.41
2:D:1144:TRP:HB2	2:D:1148:ASP:HB2	2.02	0.41
2:D:1546:ASN:OD1	2:D:1546:ASN:O	2.38	0.41
2:D:3267:MET:O	2:D:3267:MET:CG	2.68	0.41
2:D:4703:VAL:HG22	2:D:4703:VAL:O	2.20	0.41
2:A:951:LEU:H	2:A:951:LEU:HG	1.70	0.41
2:A:1127:GLY:HA3	2:A:1144:TRP:CE3	2.55	0.41
2:A:4578:TYR:HE1	2:A:4630:LEU:HD21	1.85	0.41
2:B:925:MET:O	2:B:929:THR:HG23	2.20	0.41
2:B:1781:PRO:HA	2:B:1782:PRO:HD3	1.97	0.41
2:B:3567:SER:HB3	2:B:3570:LEU:HD13	2.03	0.41
2:B:4934:ILE:H	2:B:4934:ILE:HD12	1.86	0.41
2:C:916:GLU:HA	2:C:919:ARG:HD2	2.01	0.41
2:C:1127:GLY:H	2:C:1144:TRP:HZ3	1.68	0.41
2:C:3079:ARG:O	2:C:3083:LYS:HG2	2.21	0.41
2:C:3403:CYS:SG	2:C:3456:GLU:HA	2.60	0.41
2:C:3443:PHE:CD2	2:C:3515:LEU:HD22	2.55	0.41
2:C:4578:TYR:HE1	2:C:4630:LEU:HD21	1.85	0.41
8:C:8008:A1BYZ:O7	8:C:8008:A1BYZ:C10	2.68	0.41
1:G:91:ILE:HD12	1:G:91:ILE:N	2.35	0.41
2:D:875:LEU:HD12	2:D:875:LEU:O	2.19	0.41
2:D:1064:VAL:HG13	2:D:1065:ASP:N	2.35	0.41
2:D:2975:ILE:HD11	2:D:3057:LEU:HD22	2.02	0.41
2:D:3567:SER:HB3	2:D:3570:LEU:HD13	2.03	0.41
2:A:1064:VAL:HG13	2:A:1065:ASP:N	2.35	0.41
2:A:2029:ARG:O	2:A:2033:VAL:HG23	2.21	0.41
2:A:2234:CYS:O	2:A:2236:PHE:C	2.63	0.41
2:A:2874:ALA:O	2:A:2878:GLN:OE1	2.39	0.41
2:A:2978:LEU:HA	2:A:2981:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3360:ILE:HB	2:A:3361:PRO:HD3	2.02	0.41
2:A:3567:SER:HB3	2:A:3570:LEU:HD13	2.03	0.41
2:A:3896:GLU:HA	2:A:3970:GLU:OE1	2.21	0.41
2:B:566:TYR:O	2:B:570:ILE:HG12	2.20	0.41
2:B:859:THR:HG21	2:B:932:THR:CA	2.51	0.41
2:B:1428:ILE:HG23	2:B:1429:LEU:HD22	2.01	0.41
2:B:1470:VAL:HG13	2:B:1493:CYS:HB3	2.03	0.41
2:B:2635:ASN:OD1	2:B:2638:ALA:N	2.53	0.41
2:B:2762:TYR:CZ	2:B:2863:LEU:HG	2.55	0.41
2:C:859:THR:HG21	2:C:932:THR:CA	2.51	0.41
2:C:902:LYS:CE	2:C:904:LEU:HD21	2.39	0.41
2:C:948:GLU:HG2	2:C:1050:TYR:HA	2.01	0.41
2:C:1144:TRP:HB2	2:C:1148:ASP:HB2	2.02	0.41
2:C:2413:GLU:O	2:C:2416:ARG:N	2.53	0.41
2:C:3239:GLU:O	2:C:3240:MET:C	2.63	0.41
2:D:1153:MET:HE1	2:D:1164:THR:HG23	2.02	0.41
2:D:1470:VAL:HG13	2:D:1493:CYS:HB3	2.03	0.41
2:D:2413:GLU:O	2:D:2416:ARG:N	2.53	0.41
2:D:2779:GLY:HA3	2:D:2788:THR:HB	2.02	0.41
2:D:2782:ILE:O	2:D:2783:ASP:OD1	2.39	0.41
2:D:3177:GLY:HA3	2:D:3269:HIS:CE1	2.55	0.41
2:D:3202:MET:HG3	2:D:3204:VAL:H	1.85	0.41
2:D:3291:GLU:OE2	2:D:3310:SER:N	2.38	0.41
2:D:3392:GLU:O	2:D:3396:ARG:HG2	2.20	0.41
2:D:3403:CYS:SG	2:D:3456:GLU:HA	2.60	0.41
2:D:3936:PHE:CE2	2:D:3940:TYR:CE2	3.09	0.41
2:D:3974:GLY:N	2:D:3975:PRO:HA	2.35	0.41
2:A:2782:ILE:O	2:A:2783:ASP:OD1	2.39	0.41
2:A:2975:ILE:HD11	2:A:3057:LEU:HD22	2.02	0.41
2:A:3057:LEU:HD23	2:A:3057:LEU:C	2.45	0.41
2:B:2370:ARG:NH1	2:B:2373:GLY:O	2.54	0.41
2:B:2779:GLY:HA3	2:B:2788:THR:HB	2.02	0.41
2:B:3079:ARG:O	2:B:3083:LYS:HG2	2.21	0.41
2:B:3170:LEU:CD1	2:B:3195:LEU:HD11	2.50	0.41
2:B:4649:THR:OG1	2:B:4801:HIS:CD2	2.73	0.41
2:C:2779:GLY:HA3	2:C:2788:THR:HB	2.02	0.41
2:C:3556:ASN:OD1	2:C:3556:ASN:C	2.62	0.41
2:C:3687:GLU:O	2:C:3688:GLU:HB3	2.21	0.41
2:C:4934:ILE:H	2:C:4934:ILE:HD12	1.86	0.41
2:D:296:GLU:OE1	2:D:296:GLU:N	2.37	0.41
2:D:575:VAL:HA	2:D:578:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:874:LYS:HE3	2:D:875:LEU:N	2.35	0.41
2:D:1127:GLY:H	2:D:1144:TRP:HZ3	1.68	0.41
2:D:2922:GLU:HA	2:D:2925:GLN:HG2	2.02	0.41
2:D:3367:ARG:NH1	2:D:3441:GLU:OE1	2.42	0.41
2:D:4934:ILE:H	2:D:4934:ILE:HD12	1.86	0.41
2:A:865:PRO:CD	2:A:868:LEU:HB2	2.44	0.41
2:A:2635:ASN:OD1	2:A:2638:ALA:N	2.53	0.41
2:A:3239:GLU:O	2:A:3240:MET:C	2.63	0.41
2:A:3291:GLU:OE2	2:A:3310:SER:N	2.38	0.41
2:A:4173:ILE:H	2:A:4173:ILE:HD12	1.86	0.41
2:A:4688:GLU:O	2:A:4689:GLN:NE2	2.52	0.41
2:B:2186:ILE:HG21	2:B:2204:MET:HE1	2.03	0.41
2:B:3894:LEU:CB	2:B:3902:PHE:CE2	3.02	0.41
2:B:3896:GLU:HA	2:B:3970:GLU:OE1	2.21	0.41
2:B:5014:GLU:OE2	2:B:5014:GLU:HA	2.21	0.41
2:C:2771:LYS:HB3	2:C:2776:TRP:HB2	2.02	0.41
2:C:2874:ALA:O	2:C:2878:GLN:OE1	2.39	0.41
2:C:3177:GLY:HA3	2:C:3269:HIS:CE1	2.55	0.41
2:C:3567:SER:HB3	2:C:3570:LEU:HD13	2.03	0.41
2:C:4899:ILE:HG13	2:C:4911:ARG:NH2	2.35	0.41
1:H:91:ILE:N	1:H:91:ILE:HD12	2.35	0.41
2:D:892:TRP:CZ3	2:D:905:HIS:HD2	2.39	0.41
2:D:948:GLU:HG2	2:D:1050:TYR:HA	2.01	0.41
2:D:956:LEU:HD22	2:D:956:LEU:HA	1.84	0.41
2:D:2029:ARG:O	2:D:2033:VAL:HG23	2.21	0.41
2:D:2578:ILE:HG23	2:D:2579:MET:N	2.36	0.41
2:D:2746:VAL:O	2:D:2815:LYS:HE2	2.20	0.41
2:D:2978:LEU:O	2:D:2982:VAL:HG23	2.21	0.41
2:D:3057:LEU:HD23	2:D:3057:LEU:C	2.45	0.41
2:D:3170:LEU:CD1	2:D:3195:LEU:HD11	2.50	0.41
2:D:3553:PHE:O	2:D:3556:ASN:OD1	2.39	0.41
2:D:4173:ILE:H	2:D:4173:ILE:HD12	1.86	0.41
2:D:4800:GLY:HA2	2:D:4806:PHE:HB2	2.03	0.41
2:D:4865:GLU:HA	2:D:4865:GLU:OE2	2.21	0.41
2:A:276:ARG:HE	2:A:329:LYS:HD3	1.86	0.41
2:A:2270:GLY:O	2:A:2272:THR:HG23	2.20	0.41
2:A:2668:THR:HG21	2:A:2673:LEU:HD21	2.03	0.41
2:A:2798:PHE:O	2:A:2803:LYS:HD2	2.21	0.41
2:A:2922:GLU:HA	2:A:2925:GLN:HG2	2.02	0.41
2:A:3202:MET:HG3	2:A:3204:VAL:H	1.85	0.41
2:A:3534:ILE:CG1	2:A:3597:VAL:HG23	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3553:PHE:O	2:A:3556:ASN:OD1	2.39	0.41
2:A:3687:GLU:O	2:A:3688:GLU:HB3	2.21	0.41
2:A:3974:GLY:N	2:A:3975:PRO:HA	2.35	0.41
2:A:4894:GLY:HA2	2:A:4923:ILE:HD11	2.03	0.41
2:A:4902:PRO:HB3	2:A:4911:ARG:HG2	2.03	0.41
2:A:4909:LEU:HA	2:A:4912:VAL:HG22	2.02	0.41
2:A:4934:ILE:HD12	2:A:4934:ILE:H	1.86	0.41
2:B:575:VAL:HA	2:B:578:ILE:HG12	2.02	0.41
2:B:870:ARG:HD3	2:B:1052:TYR:OH	2.20	0.41
2:B:898:ARG:HH12	2:B:907:CYS:CB	2.34	0.41
2:B:971:LEU:H	2:B:971:LEU:HG	1.57	0.41
2:B:1127:GLY:H	2:B:1144:TRP:HZ3	1.68	0.41
2:B:1742:GLU:OE1	2:B:1742:GLU:N	2.45	0.41
2:B:2029:ARG:O	2:B:2033:VAL:HG23	2.21	0.41
2:B:2746:VAL:O	2:B:2815:LYS:HE2	2.20	0.41
2:B:3057:LEU:HD23	2:B:3057:LEU:C	2.45	0.41
2:B:3291:GLU:OE2	2:B:3310:SER:N	2.38	0.41
2:B:3553:PHE:O	2:B:3556:ASN:OD1	2.39	0.41
2:B:3987:ARG:NH2	2:C:162:GLU:HA	2.36	0.41
2:B:4723:LEU:HD22	2:B:4741:MET:HE2	2.03	0.41
2:B:4899:ILE:HG13	2:B:4911:ARG:NH2	2.35	0.41
2:C:505:ALA:HB2	2:C:513:ALA:HB2	2.03	0.41
2:C:1127:GLY:HA3	2:C:1144:TRP:CE3	2.55	0.41
2:C:1153:MET:HE1	2:C:1164:THR:HG23	2.02	0.41
2:C:1546:ASN:OD1	2:C:1546:ASN:O	2.38	0.41
2:C:2314:LEU:HD11	2:C:2417:VAL:CG1	2.50	0.41
2:C:2370:ARG:NH1	2:C:2373:GLY:O	2.54	0.41
2:C:2420:GLY:O	2:C:2424:MET:HE3	2.21	0.41
2:C:2578:ILE:HG23	2:C:2579:MET:N	2.36	0.41
2:C:2635:ASN:OD1	2:C:2638:ALA:N	2.53	0.41
2:C:2975:ILE:HD11	2:C:3057:LEU:HD22	2.02	0.41
2:C:3198:LEU:HD12	2:C:3198:LEU:O	2.20	0.41
2:C:3267:MET:O	2:C:3267:MET:CG	2.68	0.41
2:C:3553:PHE:O	2:C:3556:ASN:OD1	2.39	0.41
2:C:3894:LEU:HD13	2:C:3902:PHE:HZ	1.86	0.41
2:C:4703:VAL:HG22	2:C:4703:VAL:O	2.20	0.41
2:C:4806:PHE:HA	7:C:8006:PCW:H39	2.03	0.41
2:D:862:ILE:CG2	2:D:934:LEU:HD23	2.51	0.41
2:D:961:MET:CG	2:D:965:GLY:HA2	2.43	0.41
2:D:2266:LEU:HD13	2:D:2327:CYS:HB3	2.03	0.41
2:D:2420:GLY:O	2:D:2424:MET:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2748:ILE:O	2:D:2748:ILE:HG23	2.21	0.41
2:D:2863:LEU:O	2:D:2929:LYS:HD2	2.21	0.41
2:D:2978:LEU:HA	2:D:2981:VAL:HG22	2.03	0.41
2:D:3837:ALA:O	2:D:3841:THR:HG23	2.21	0.41
2:A:958:LYS:HA	2:A:961:MET:HB3	2.03	0.41
2:A:2420:GLY:O	2:A:2424:MET:HE3	2.21	0.41
2:A:2762:TYR:CZ	2:A:2863:LEU:HG	2.55	0.41
2:A:2881:GLU:OE1	2:A:2909:TYR:HB2	2.21	0.41
2:A:4806:PHE:HA	7:A:8006:PCW:H39	2.03	0.41
2:B:459:GLU:OE2	2:B:459:GLU:N	2.54	0.41
2:B:2771:LYS:HB3	2:B:2776:TRP:HB2	2.02	0.41
2:B:2978:LEU:HA	2:B:2981:VAL:HG22	2.03	0.41
2:B:3540:ARG:HD2	2:B:3543:LEU:HD12	2.03	0.41
2:B:3687:GLU:O	2:B:3688:GLU:HB3	2.21	0.41
2:B:4806:PHE:HA	7:B:8006:PCW:H39	2.03	0.41
2:B:4865:GLU:HA	2:B:4865:GLU:OE2	2.21	0.41
2:C:566:TYR:O	2:C:570:ILE:HG12	2.20	0.41
2:C:899:ASP:HB3	2:C:902:LYS:CG	2.51	0.41
2:C:951:LEU:H	2:C:951:LEU:HG	1.70	0.41
2:C:2863:LEU:O	2:C:2929:LYS:HD2	2.21	0.41
2:C:4173:ILE:H	2:C:4173:ILE:HD12	1.86	0.41
2:C:4545:GLN:OE1	2:C:4545:GLN:HA	2.21	0.41
1:F:77:ILE:O	1:F:97:THR:HG23	2.20	0.40
1:G:33:ASP:OD1	1:G:33:ASP:N	2.55	0.40
1:H:2:GLY:N	1:H:78:SER:OG	2.35	0.40
2:D:951:LEU:HD21	2:D:1049:GLY:CA	2.51	0.40
2:D:985:LEU:HD11	2:D:1056:PRO:CB	2.51	0.40
2:D:2874:ALA:O	2:D:2878:GLN:OE1	2.39	0.40
2:D:3079:ARG:O	2:D:3083:LYS:HG2	2.21	0.40
2:D:4578:TYR:HE1	2:D:4630:LEU:HD21	1.85	0.40
2:D:4899:ILE:HG13	2:D:4911:ARG:NH2	2.35	0.40
2:A:575:VAL:HA	2:A:578:ILE:HG12	2.03	0.40
2:A:1127:GLY:H	2:A:1144:TRP:HZ3	1.68	0.40
2:A:2334:ASP:HA	2:A:2337:ARG:HD3	2.03	0.40
2:A:2413:GLU:O	2:A:2416:ARG:N	2.53	0.40
2:A:2746:VAL:O	2:A:2815:LYS:HE2	2.20	0.40
2:B:276:ARG:HE	2:B:329:LYS:HD3	1.86	0.40
2:B:898:ARG:NH1	2:B:906:PRO:HD2	2.36	0.40
2:B:958:LYS:HA	2:B:961:MET:HB3	2.03	0.40
2:B:985:LEU:HD11	2:B:1056:PRO:HA	2.03	0.40
2:B:2445:GLN:OE1	2:B:2445:GLN:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2668:THR:HG21	2:B:2673:LEU:HD21	2.02	0.40
2:B:3202:MET:HG3	2:B:3204:VAL:H	1.85	0.40
2:B:3710:ALA:HB2	2:B:3785:MET:HE2	2.03	0.40
2:B:3894:LEU:HD13	2:B:3902:PHE:HZ	1.86	0.40
2:B:4800:GLY:HA2	2:B:4806:PHE:HB2	2.03	0.40
2:C:1470:VAL:HG13	2:C:1493:CYS:HB3	2.03	0.40
2:C:2668:THR:HG21	2:C:2673:LEU:HD21	2.03	0.40
2:C:2762:TYR:CZ	2:C:2863:LEU:HG	2.55	0.40
2:C:2978:LEU:O	2:C:2982:VAL:HG23	2.21	0.40
2:C:3057:LEU:HD23	2:C:3057:LEU:C	2.45	0.40
1:F:80:ASP:OD2	1:F:80:ASP:C	2.65	0.40
2:D:843:PRO:HG2	2:D:1072:ARG:O	2.20	0.40
2:D:952:LYS:HZ3	2:D:952:LYS:HG2	1.57	0.40
2:D:2736:PHE:O	2:D:2738:PRO:HD3	2.21	0.40
2:D:2958:PHE:HE1	2:D:3035:LYS:HG2	1.86	0.40
2:D:3534:ILE:CG1	2:D:3597:VAL:HG23	2.51	0.40
2:D:4909:LEU:HA	2:D:4912:VAL:HG22	2.02	0.40
2:A:862:ILE:CG2	2:A:934:LEU:HD23	2.51	0.40
2:A:892:TRP:CZ3	2:A:905:HIS:HD2	2.39	0.40
2:A:2958:PHE:HE1	2:A:3035:LYS:HG2	1.87	0.40
2:A:2990:SER:O	2:A:2993:GLU:N	2.52	0.40
2:A:3170:LEU:CD1	2:A:3195:LEU:HD11	2.50	0.40
2:A:3683:GLU:HB3	2:A:3686:GLU:HB2	2.04	0.40
2:A:3837:ALA:O	2:A:3841:THR:HG23	2.22	0.40
2:A:4723:LEU:HD22	2:A:4741:MET:HE2	2.03	0.40
2:A:5014:GLU:OE2	2:A:5014:GLU:HA	2.21	0.40
2:B:2782:ILE:O	2:B:2783:ASP:OD1	2.39	0.40
2:B:2798:PHE:O	2:B:2803:LYS:HD2	2.21	0.40
2:B:3392:GLU:O	2:B:3396:ARG:HG2	2.20	0.40
2:B:3936:PHE:CE2	2:B:3940:TYR:CE2	3.09	0.40
2:B:4545:GLN:OE1	2:B:4545:GLN:HA	2.21	0.40
2:C:593:LYS:NZ	2:C:1584:GLU:OE2	2.39	0.40
2:C:879:ILE:CA	2:C:882:LEU:HD12	2.33	0.40
2:C:898:ARG:NH1	2:C:906:PRO:HD2	2.36	0.40
2:C:953:LYS:HE2	2:C:953:LYS:HB2	1.84	0.40
2:C:2266:LEU:HD13	2:C:2327:CYS:HB3	2.03	0.40
2:C:2445:GLN:OE1	2:C:2445:GLN:HA	2.22	0.40
2:C:2782:ILE:O	2:C:2783:ASP:OD1	2.39	0.40
2:C:3896:GLU:HA	2:C:3970:GLU:OE1	2.21	0.40
2:C:4894:GLY:HA2	2:C:4923:ILE:HD11	2.03	0.40
2:C:4902:PRO:HB3	2:C:4911:ARG:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:ARG:HA	2:C:1692:GLN:HE21	1.86	0.40
1:H:80:ASP:OD2	1:H:80:ASP:C	2.64	0.40
2:D:4806:PHE:HA	7:D:8006:PCW:H39	2.03	0.40
2:D:4894:GLY:HA2	2:D:4923:ILE:HD11	2.03	0.40
2:A:566:TYR:O	2:A:570:ILE:HG12	2.20	0.40
2:A:967:LYS:HZ1	2:A:969:ALA:HB2	1.86	0.40
2:A:4578:TYR:HD2	2:A:4805:PHE:CZ	2.40	0.40
2:B:862:ILE:CG2	2:B:934:LEU:HD23	2.51	0.40
2:B:2874:ALA:O	2:B:2878:GLN:OE1	2.39	0.40
2:B:2958:PHE:HE1	2:B:3035:LYS:HG2	1.86	0.40
2:B:4042:MET:HE2	2:B:4045:ARG:NH2	2.37	0.40
2:B:4894:GLY:HA2	2:B:4923:ILE:HD11	2.03	0.40
2:C:951:LEU:HD21	2:C:1049:GLY:CA	2.51	0.40
2:C:956:LEU:HD22	2:C:956:LEU:HA	1.84	0.40
2:C:985:LEU:HD11	2:C:1056:PRO:CB	2.51	0.40
2:C:985:LEU:HD11	2:C:1056:PRO:HA	2.03	0.40
2:C:2736:PHE:O	2:C:2738:PRO:HD3	2.21	0.40
2:C:2958:PHE:HE1	2:C:3035:LYS:HG2	1.86	0.40
2:C:3524:ASN:OD1	2:C:3583:ARG:NH1	2.54	0.40
2:C:3683:GLU:HB3	2:C:3686:GLU:HB2	2.04	0.40
2:C:3710:ALA:HB2	2:C:3785:MET:HE2	2.03	0.40
2:C:3936:PHE:CE2	2:C:3940:TYR:CE2	3.09	0.40
2:D:505:ALA:HB2	2:D:513:ALA:HB2	2.03	0.40
2:D:859:THR:HG21	2:D:932:THR:CA	2.51	0.40
2:D:899:ASP:HB3	2:D:902:LYS:CG	2.51	0.40
2:D:2668:THR:HG21	2:D:2673:LEU:HD21	2.03	0.40
2:D:3239:GLU:O	2:D:3240:MET:C	2.63	0.40
2:D:3894:LEU:HD13	2:D:3902:PHE:HZ	1.86	0.40
2:D:3896:GLU:HA	2:D:3970:GLU:OE1	2.21	0.40
2:D:4042:MET:HE2	2:D:4045:ARG:NH2	2.37	0.40
2:D:5014:GLU:OE2	2:D:5014:GLU:HA	2.21	0.40
2:A:859:THR:HG21	2:A:932:THR:CA	2.51	0.40
2:A:2445:GLN:OE1	2:A:2445:GLN:HA	2.22	0.40
2:A:3008:ASN:C	2:A:3008:ASN:OD1	2.63	0.40
2:A:3540:ARG:HD2	2:A:3543:LEU:HD12	2.04	0.40
2:A:4987:MET:O	2:A:4991:MET:HG3	2.22	0.40
2:B:593:LYS:NZ	2:B:1584:GLU:OE2	2.39	0.40
2:B:4173:ILE:HD12	2:B:4173:ILE:H	1.86	0.40
2:C:862:ILE:CG2	2:C:934:LEU:HD23	2.51	0.40
2:C:3909:GLN:O	2:C:3915:THR:HG22	2.22	0.40
2:D:216:THR:OG1	2:D:219:HIS:NE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1181:ARG:HB2	2:D:1181:ARG:CZ	2.52	0.40
2:D:2881:GLU:OE1	2:D:2909:TYR:HB2	2.21	0.40
2:D:3687:GLU:O	2:D:3688:GLU:HB3	2.21	0.40
2:D:4578:TYR:HD2	2:D:4805:PHE:CZ	2.40	0.40
2:D:4987:MET:O	2:D:4991:MET:HG3	2.22	0.40
2:A:2578:ILE:HG23	2:A:2579:MET:N	2.36	0.40
2:A:2736:PHE:O	2:A:2738:PRO:HD3	2.21	0.40
2:A:3894:LEU:HD13	2:A:3902:PHE:HZ	1.86	0.40
2:A:4686:ILE:HD12	2:A:4735:ILE:HD13	2.04	0.40
2:B:985:LEU:HD11	2:B:1056:PRO:CB	2.51	0.40
2:B:2334:ASP:HA	2:B:2337:ARG:HD3	2.03	0.40
2:B:2736:PHE:O	2:B:2738:PRO:HD3	2.21	0.40
2:B:2875:MET:HE1	2:B:2938:VAL:HG22	2.04	0.40
2:C:874:LYS:H	2:C:874:LYS:HG3	1.57	0.40
2:C:2875:MET:HE1	2:C:2938:VAL:HG22	2.04	0.40
2:C:2881:GLU:OE1	2:C:2909:TYR:HB2	2.21	0.40
2:C:3534:ILE:CG1	2:C:3597:VAL:HG23	2.51	0.40
2:C:3837:ALA:O	2:C:3841:THR:HG23	2.21	0.40
2:C:4578:TYR:HD2	2:C:4805:PHE:CZ	2.40	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	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
1	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
1	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
1	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	A	4345/5035 (86%)	4228 (97%)	114 (3%)	3 (0%)	48	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	4345/5035 (86%)	4227 (97%)	115 (3%)	3 (0%)	48	79
2	C	4345/5035 (86%)	4227 (97%)	115 (3%)	3 (0%)	48	79
2	D	4345/5035 (86%)	4228 (97%)	114 (3%)	3 (0%)	48	79
All	All	17800/20572 (86%)	17318 (97%)	470 (3%)	12 (0%)	50	79

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	2574	GLU
2	D	4055	SER
2	A	2574	GLU
2	A	4055	SER
2	B	2574	GLU
2	B	4055	SER
2	C	2574	GLU
2	C	4055	SER
2	D	3357	SER
2	A	3357	SER
2	B	3357	SER
2	C	3357	SER

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	E	89/90 (99%)	89 (100%)	0	100	100
1	F	89/90 (99%)	89 (100%)	0	100	100
1	G	89/90 (99%)	89 (100%)	0	100	100
1	H	89/90 (99%)	89 (100%)	0	100	100
2	A	3806/4296 (89%)	3742 (98%)	64 (2%)	56	78
2	B	3806/4296 (89%)	3742 (98%)	64 (2%)	56	78
2	C	3806/4296 (89%)	3742 (98%)	64 (2%)	56	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	3806/4296 (89%)	3742 (98%)	64 (2%)	56	78
All	All	15580/17544 (89%)	15324 (98%)	256 (2%)	58	79

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	864	LEU
2	D	868	LEU
2	D	869	GLU
2	D	870	ARG
2	D	871	ILE
2	D	872	ARG
2	D	874	LYS
2	D	877	GLU
2	D	878	ASN
2	D	885	LEU
2	D	887	ARG
2	D	888	ILE
2	D	889	GLU
2	D	893	THR
2	D	897	VAL
2	D	898	ARG
2	D	900	ASP
2	D	902	LYS
2	D	904	LEU
2	D	905	HIS
2	D	907	CYS
2	D	909	VAL
2	D	910	ASN
2	D	914	LEU
2	D	918	GLU
2	D	919	ARG
2	D	925	MET
2	D	929	THR
2	D	930	LEU
2	D	931	LYS
2	D	933	LEU
2	D	934	LEU
2	D	938	CYS
2	D	939	HIS
2	D	940	VAL
2	D	945	GLU

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Mol	Chain	Res	Type
2	D	948	GLU
2	D	949	ASP
2	D	951	LEU
2	D	952	LYS
2	D	953	LYS
2	D	954	THR
2	D	955	LYS
2	D	956	LEU
2	D	959	THR
2	D	961	MET
2	D	962	MET
2	D	963	SER
2	D	964	ASN
2	D	966	TYR
2	D	967	LYS
2	D	971	LEU
2	D	972	ASP
2	D	973	LEU
2	D	975	HIS
2	D	977	ARG
2	D	978	LEU
2	D	979	THR
2	D	1047	LEU
2	D	1048	LEU
2	D	1053	ASN
2	D	1055	GLU
2	D	2282	ILE
2	D	2337	ARG
2	A	864	LEU
2	A	868	LEU
2	A	869	GLU
2	A	870	ARG
2	A	871	ILE
2	A	872	ARG
2	A	874	LYS
2	A	877	GLU
2	A	878	ASN
2	A	885	LEU
2	A	887	ARG
2	A	888	ILE
2	A	889	GLU
2	A	893	THR

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Mol	Chain	Res	Type
2	A	897	VAL
2	A	898	ARG
2	A	900	ASP
2	A	902	LYS
2	A	904	LEU
2	A	905	HIS
2	A	907	CYS
2	A	909	VAL
2	A	910	ASN
2	A	914	LEU
2	A	918	GLU
2	A	919	ARG
2	A	925	MET
2	A	929	THR
2	A	930	LEU
2	A	931	LYS
2	A	933	LEU
2	A	934	LEU
2	A	938	CYS
2	A	939	HIS
2	A	940	VAL
2	A	945	GLU
2	A	948	GLU
2	A	949	ASP
2	A	951	LEU
2	A	952	LYS
2	A	953	LYS
2	A	954	THR
2	A	955	LYS
2	A	956	LEU
2	A	959	THR
2	A	961	MET
2	A	962	MET
2	A	963	SER
2	A	964	ASN
2	A	966	TYR
2	A	967	LYS
2	A	971	LEU
2	A	972	ASP
2	A	973	LEU
2	A	975	HIS
2	A	977	ARG

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Mol	Chain	Res	Type
2	A	978	LEU
2	A	979	THR
2	A	1047	LEU
2	A	1048	LEU
2	A	1053	ASN
2	A	1055	GLU
2	A	2282	ILE
2	A	2337	ARG
2	B	864	LEU
2	B	868	LEU
2	B	869	GLU
2	B	870	ARG
2	B	871	ILE
2	B	872	ARG
2	B	874	LYS
2	B	877	GLU
2	B	878	ASN
2	B	885	LEU
2	B	887	ARG
2	B	888	ILE
2	B	889	GLU
2	B	893	THR
2	B	897	VAL
2	B	898	ARG
2	B	900	ASP
2	B	902	LYS
2	B	904	LEU
2	B	905	HIS
2	B	907	CYS
2	B	909	VAL
2	B	910	ASN
2	B	914	LEU
2	B	918	GLU
2	B	919	ARG
2	B	925	MET
2	B	929	THR
2	B	930	LEU
2	B	931	LYS
2	B	933	LEU
2	B	934	LEU
2	B	938	CYS
2	B	939	HIS

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Mol	Chain	Res	Type
2	B	940	VAL
2	B	945	GLU
2	B	948	GLU
2	B	949	ASP
2	B	951	LEU
2	B	952	LYS
2	B	953	LYS
2	B	954	THR
2	B	955	LYS
2	B	956	LEU
2	B	959	THR
2	B	961	MET
2	B	962	MET
2	B	963	SER
2	B	964	ASN
2	B	966	TYR
2	B	967	LYS
2	B	971	LEU
2	B	972	ASP
2	B	973	LEU
2	B	975	HIS
2	B	977	ARG
2	B	978	LEU
2	B	979	THR
2	B	1047	LEU
2	B	1048	LEU
2	B	1053	ASN
2	B	1055	GLU
2	B	2282	ILE
2	B	2337	ARG
2	C	864	LEU
2	C	868	LEU
2	C	869	GLU
2	C	870	ARG
2	C	871	ILE
2	C	872	ARG
2	C	874	LYS
2	C	877	GLU
2	C	878	ASN
2	C	885	LEU
2	C	887	ARG
2	C	888	ILE

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Mol	Chain	Res	Type
2	C	889	GLU
2	C	893	THR
2	C	897	VAL
2	C	898	ARG
2	C	900	ASP
2	C	902	LYS
2	C	904	LEU
2	C	905	HIS
2	C	907	CYS
2	C	909	VAL
2	C	910	ASN
2	C	914	LEU
2	C	918	GLU
2	C	919	ARG
2	C	925	MET
2	C	929	THR
2	C	930	LEU
2	C	931	LYS
2	C	933	LEU
2	C	934	LEU
2	C	938	CYS
2	C	939	HIS
2	C	940	VAL
2	C	945	GLU
2	C	948	GLU
2	C	949	ASP
2	C	951	LEU
2	C	952	LYS
2	C	953	LYS
2	C	954	THR
2	C	955	LYS
2	C	956	LEU
2	C	959	THR
2	C	961	MET
2	C	962	MET
2	C	963	SER
2	C	964	ASN
2	C	966	TYR
2	C	967	LYS
2	C	971	LEU
2	C	972	ASP
2	C	973	LEU

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Mol	Chain	Res	Type
2	C	975	HIS
2	C	977	ARG
2	C	978	LEU
2	C	979	THR
2	C	1047	LEU
2	C	1048	LEU
2	C	1053	ASN
2	C	1055	GLU
2	C	2282	ILE
2	C	2337	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	21	GLN
2	D	106	HIS
2	D	380	HIS
2	D	594	HIS
2	D	905	HIS
2	D	950	ASN
2	D	995	ASN
2	D	1085	GLN
2	D	1131	GLN
2	D	1202	HIS
2	D	1299	HIS
2	D	1485	HIS
2	D	1570	GLN
2	D	1591	GLN
2	D	1612	HIS
2	D	1632	GLN
2	D	1641	HIS
2	D	1762	HIS
2	D	2773	GLN
2	D	2774	ASN
2	D	2932	GLN
2	D	2992	HIS
2	D	3110	ASN
2	D	3423	HIS
2	D	3598	GLN
2	D	3612	HIS
2	D	3885	GLN
2	D	3917	ASN

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Mol	Chain	Res	Type
2	D	3930	GLN
2	D	4001	HIS
2	D	4156	HIS
2	D	4834	GLN
2	D	5004	GLN
2	A	380	HIS
2	A	594	HIS
2	A	905	HIS
2	A	950	ASN
2	A	995	ASN
2	A	1085	GLN
2	A	1131	GLN
2	A	1202	HIS
2	A	1299	HIS
2	A	1430	ASN
2	A	1485	HIS
2	A	1570	GLN
2	A	1591	GLN
2	A	1632	GLN
2	A	1641	HIS
2	A	1762	HIS
2	A	1939	GLN
2	A	1973	ASN
2	A	2004	GLN
2	A	2764	HIS
2	A	2773	GLN
2	A	2774	ASN
2	A	2992	HIS
2	A	3110	ASN
2	A	3423	HIS
2	A	3612	HIS
2	A	3885	GLN
2	A	3917	ASN
2	A	3930	GLN
2	A	4037	ASN
2	A	4057	ASN
2	A	4156	HIS
2	A	4834	GLN
2	B	380	HIS
2	B	594	HIS
2	B	905	HIS
2	B	950	ASN

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Mol	Chain	Res	Type
2	B	995	ASN
2	B	1085	GLN
2	B	1131	GLN
2	B	1202	HIS
2	B	1485	HIS
2	B	1570	GLN
2	B	1591	GLN
2	B	1612	HIS
2	B	1632	GLN
2	B	1641	HIS
2	B	1720	HIS
2	B	1762	HIS
2	B	2037	GLN
2	B	2773	GLN
2	B	2774	ASN
2	B	2932	GLN
2	B	2992	HIS
2	B	3110	ASN
2	B	3423	HIS
2	B	3612	HIS
2	B	3885	GLN
2	B	3917	ASN
2	B	3930	GLN
2	B	4156	HIS
2	B	4834	GLN
2	B	5004	GLN
2	C	106	HIS
2	C	380	HIS
2	C	594	HIS
2	C	905	HIS
2	C	950	ASN
2	C	995	ASN
2	C	1085	GLN
2	C	1131	GLN
2	C	1202	HIS
2	C	1485	HIS
2	C	1570	GLN
2	C	1591	GLN
2	C	1612	HIS
2	C	1632	GLN
2	C	1641	HIS
2	C	1720	HIS

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Mol	Chain	Res	Type
2	C	1762	HIS
2	C	1973	ASN
2	C	2004	GLN
2	C	2037	GLN
2	C	2773	GLN
2	C	2774	ASN
2	C	2932	GLN
2	C	2992	HIS
2	C	3110	ASN
2	C	3423	HIS
2	C	3612	HIS
2	C	3885	GLN
2	C	3917	ASN
2	C	3930	GLN
2	C	4156	HIS
2	C	4834	GLN
2	C	5004	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 8 are monoatomic - leaving 28 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PCW	B	8005	-	53,53,53	1.25	7 (13%)	59,61,61	1.12	3 (5%)
8	A1BYZ	B	8008	-	32,32,32	0.68	1 (3%)	40,47,47	0.85	1 (2%)
7	PCW	A	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.19	4 (6%)
5	ATP	D	8007	-	28,33,33	0.61	0	34,52,52	0.88	1 (2%)
7	PCW	B	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.19	4 (6%)
4	CFF	D	8002	-	8,15,15	2.14	3 (37%)	8,23,23	1.49	1 (12%)
8	A1BYZ	B	8009	-	32,32,32	0.60	1 (3%)	40,47,47	1.19	4 (10%)
7	PCW	C	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.19	4 (6%)
8	A1BYZ	A	8009	-	32,32,32	0.60	1 (3%)	40,47,47	1.19	4 (10%)
8	A1BYZ	D	8008	-	32,32,32	0.68	1 (3%)	40,47,47	0.85	1 (2%)
5	ATP	D	8003	-	28,33,33	0.66	0	34,52,52	0.89	2 (5%)
5	ATP	A	8003	-	28,33,33	0.66	0	34,52,52	0.89	2 (5%)
4	CFF	C	8002	-	8,15,15	2.14	3 (37%)	8,23,23	1.49	1 (12%)
8	A1BYZ	A	8008	-	32,32,32	0.67	1 (3%)	40,47,47	0.85	1 (2%)
8	A1BYZ	C	8009	-	32,32,32	0.60	1 (3%)	40,47,47	1.19	4 (10%)
5	ATP	A	8007	-	28,33,33	0.60	0	34,52,52	0.88	1 (2%)
5	ATP	B	8007	-	28,33,33	0.61	0	34,52,52	0.88	1 (2%)
8	A1BYZ	C	8008	-	32,32,32	0.68	1 (3%)	40,47,47	0.85	1 (2%)
7	PCW	C	8005	-	53,53,53	1.25	7 (13%)	59,61,61	1.12	3 (5%)
5	ATP	C	8003	-	28,33,33	0.66	0	34,52,52	0.90	2 (5%)
4	CFF	A	8002	-	8,15,15	2.14	3 (37%)	8,23,23	1.49	1 (12%)
8	A1BYZ	D	8009	-	32,32,32	0.60	1 (3%)	40,47,47	1.19	4 (10%)
4	CFF	B	8002	-	8,15,15	2.14	3 (37%)	8,23,23	1.49	1 (12%)
5	ATP	B	8003	-	28,33,33	0.66	0	34,52,52	0.89	2 (5%)
7	PCW	D	8005	-	53,53,53	1.26	7 (13%)	59,61,61	1.12	3 (5%)
5	ATP	C	8007	-	28,33,33	0.61	0	34,52,52	0.88	1 (2%)
7	PCW	A	8005	-	53,53,53	1.26	7 (13%)	59,61,61	1.12	3 (5%)
7	PCW	D	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.19	4 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PCW	B	8005	-	-	25/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	A1BYZ	B	8008	-	-	3/18/59/59	0/3/3/3
7	PCW	A	8006	-	-	29/57/57/57	-
5	ATP	D	8007	-	-	8/18/38/38	0/3/3/3
7	PCW	B	8006	-	-	29/57/57/57	-
4	CFF	D	8002	-	-	-	0/2/2/2
8	A1BYZ	B	8009	-	-	4/18/59/59	0/3/3/3
7	PCW	C	8006	-	-	29/57/57/57	-
8	A1BYZ	A	8009	-	-	4/18/59/59	0/3/3/3
8	A1BYZ	D	8008	-	-	3/18/59/59	0/3/3/3
5	ATP	D	8003	-	-	9/18/38/38	0/3/3/3
5	ATP	A	8003	-	-	9/18/38/38	0/3/3/3
4	CFF	C	8002	-	-	-	0/2/2/2
8	A1BYZ	A	8008	-	-	3/18/59/59	0/3/3/3
8	A1BYZ	C	8009	-	-	4/18/59/59	0/3/3/3
5	ATP	A	8007	-	-	8/18/38/38	0/3/3/3
5	ATP	B	8007	-	-	8/18/38/38	0/3/3/3
8	A1BYZ	C	8008	-	-	3/18/59/59	0/3/3/3
7	PCW	C	8005	-	-	25/57/57/57	-
5	ATP	C	8003	-	-	9/18/38/38	0/3/3/3
4	CFF	A	8002	-	-	-	0/2/2/2
8	A1BYZ	D	8009	-	-	4/18/59/59	0/3/3/3
5	ATP	B	8003	-	-	9/18/38/38	0/3/3/3
4	CFF	B	8002	-	-	-	0/2/2/2
7	PCW	D	8005	-	-	25/57/57/57	-
5	ATP	C	8007	-	-	8/18/38/38	0/3/3/3
7	PCW	A	8005	-	-	25/57/57/57	-
7	PCW	D	8006	-	-	29/57/57/57	-

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8002	CFF	C5-C4	-3.52	1.33	1.39
4	A	8002	CFF	C5-C4	-3.49	1.33	1.39
4	D	8002	CFF	C5-C4	-3.49	1.33	1.39
4	C	8002	CFF	C5-C4	-3.49	1.33	1.39
4	D	8002	CFF	C6-N1	-3.34	1.32	1.38
4	A	8002	CFF	C6-N1	-3.34	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8002	CFF	C6-N1	-3.34	1.32	1.38
4	C	8002	CFF	C6-N1	-3.34	1.32	1.38
8	D	8008	A1BYZ	C16-C15	-3.34	1.51	1.54
8	B	8008	A1BYZ	C16-C15	-3.34	1.51	1.54
8	C	8008	A1BYZ	C16-C15	-3.34	1.51	1.54
8	A	8008	A1BYZ	C16-C15	-3.32	1.51	1.54
7	D	8006	PCW	O3-C11	3.03	1.42	1.33
7	B	8006	PCW	O3-C11	3.03	1.42	1.33
7	C	8006	PCW	O3-C11	3.03	1.42	1.33
7	A	8006	PCW	O3-C11	3.02	1.42	1.33
7	A	8005	PCW	O3-C11	3.00	1.42	1.33
7	D	8005	PCW	O3-C11	3.00	1.42	1.33
7	B	8005	PCW	O3-C11	3.00	1.42	1.33
7	C	8005	PCW	O3-C11	3.00	1.42	1.33
8	D	8009	A1BYZ	C16-C15	-2.98	1.51	1.54
8	A	8009	A1BYZ	C16-C15	-2.98	1.51	1.54
8	B	8009	A1BYZ	C16-C15	-2.98	1.51	1.54
8	C	8009	A1BYZ	C16-C15	-2.98	1.51	1.54
7	A	8005	PCW	O2-C31	2.96	1.42	1.34
7	D	8005	PCW	O2-C31	2.96	1.42	1.34
7	C	8005	PCW	O2-C31	2.96	1.42	1.34
7	B	8005	PCW	O2-C31	2.94	1.42	1.34
7	A	8006	PCW	O2-C31	2.70	1.41	1.34
7	D	8006	PCW	O2-C31	2.69	1.41	1.34
7	B	8006	PCW	O2-C31	2.69	1.41	1.34
7	C	8006	PCW	O2-C31	2.69	1.41	1.34
7	D	8005	PCW	P-O4P	2.64	1.69	1.59
7	B	8005	PCW	P-O4P	2.64	1.69	1.59
7	C	8005	PCW	P-O4P	2.64	1.69	1.59
7	A	8005	PCW	P-O4P	2.63	1.69	1.59
4	C	8002	CFF	O13-C6	-2.60	1.18	1.24
4	D	8002	CFF	O13-C6	-2.60	1.18	1.24
4	A	8002	CFF	O13-C6	-2.60	1.18	1.24
4	B	8002	CFF	O13-C6	-2.60	1.18	1.24
7	A	8006	PCW	P-O4P	2.54	1.69	1.59
7	D	8006	PCW	P-O4P	2.52	1.69	1.59
7	B	8006	PCW	P-O4P	2.52	1.69	1.59
7	C	8006	PCW	P-O4P	2.52	1.69	1.59
7	A	8006	PCW	O2-C2	-2.39	1.41	1.46
7	D	8005	PCW	C5-C4	2.39	1.58	1.51
7	B	8005	PCW	C5-C4	2.39	1.58	1.51
7	C	8005	PCW	C5-C4	2.39	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	8006	PCW	O2-C2	-2.38	1.41	1.46
7	B	8006	PCW	O2-C2	-2.38	1.41	1.46
7	C	8006	PCW	O2-C2	-2.38	1.41	1.46
7	A	8005	PCW	C5-C4	2.37	1.58	1.51
7	D	8005	PCW	C32-C31	2.36	1.57	1.50
7	B	8005	PCW	C32-C31	2.36	1.57	1.50
7	C	8005	PCW	C32-C31	2.35	1.57	1.50
7	A	8005	PCW	C32-C31	2.33	1.57	1.50
7	A	8005	PCW	O2-C2	-2.30	1.41	1.46
7	A	8005	PCW	P-O3P	2.29	1.68	1.59
7	D	8005	PCW	P-O3P	2.29	1.68	1.59
7	B	8005	PCW	P-O3P	2.29	1.68	1.59
7	C	8005	PCW	P-O3P	2.29	1.68	1.59
7	D	8005	PCW	O2-C2	-2.28	1.41	1.46
7	B	8005	PCW	O2-C2	-2.28	1.41	1.46
7	C	8005	PCW	O2-C2	-2.28	1.41	1.46
7	A	8006	PCW	C5-C4	2.23	1.58	1.51
7	D	8006	PCW	C5-C4	2.23	1.58	1.51
7	B	8006	PCW	C5-C4	2.23	1.58	1.51
7	C	8006	PCW	C5-C4	2.21	1.58	1.51
7	A	8006	PCW	P-O3P	2.16	1.67	1.59
7	D	8006	PCW	P-O3P	2.15	1.67	1.59
7	B	8006	PCW	P-O3P	2.15	1.67	1.59
7	C	8006	PCW	P-O3P	2.15	1.67	1.59
7	A	8006	PCW	C32-C31	2.06	1.56	1.50
7	D	8006	PCW	C32-C31	2.04	1.56	1.50
7	B	8006	PCW	C32-C31	2.04	1.56	1.50
7	C	8006	PCW	C32-C31	2.04	1.56	1.50

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	8006	PCW	O2-C31-C32	4.14	120.43	111.48
7	B	8006	PCW	O2-C31-C32	4.14	120.43	111.48
7	C	8006	PCW	O2-C31-C32	4.14	120.43	111.48
7	A	8006	PCW	O2-C31-C32	4.13	120.41	111.48
7	C	8005	PCW	O2-C31-C32	3.98	120.09	111.48
7	D	8005	PCW	O2-C31-C32	3.98	120.09	111.48
7	A	8006	PCW	C21-C20-C19	3.97	154.60	124.83
7	A	8005	PCW	O2-C31-C32	3.97	120.08	111.48
7	D	8006	PCW	C21-C20-C19	3.97	154.60	124.83
7	B	8006	PCW	C21-C20-C19	3.97	154.60	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	8006	PCW	C21-C20-C19	3.97	154.60	124.83
7	B	8005	PCW	O2-C31-C32	3.97	120.06	111.48
7	A	8005	PCW	C21-C20-C19	3.78	153.19	124.83
7	D	8005	PCW	C21-C20-C19	3.78	153.15	124.83
7	B	8005	PCW	C21-C20-C19	3.78	153.15	124.83
7	C	8005	PCW	C21-C20-C19	3.78	153.15	124.83
8	A	8009	A1BYZ	C15-C16-C17	-3.57	108.70	110.88
8	D	8009	A1BYZ	C15-C16-C17	-3.56	108.70	110.88
8	B	8009	A1BYZ	C15-C16-C17	-3.56	108.70	110.88
8	D	8009	A1BYZ	C14-C15-C16	3.52	112.57	110.70
8	B	8009	A1BYZ	C14-C15-C16	3.52	112.57	110.70
8	C	8009	A1BYZ	C14-C15-C16	3.52	112.57	110.70
8	C	8009	A1BYZ	C15-C16-C17	-3.52	108.73	110.88
8	A	8009	A1BYZ	C14-C15-C16	3.50	112.56	110.70
8	D	8008	A1BYZ	C24-C25-C26	-3.01	111.36	116.30
8	B	8008	A1BYZ	C24-C25-C26	-3.01	111.36	116.30
8	C	8008	A1BYZ	C24-C25-C26	-3.01	111.36	116.30
8	A	8008	A1BYZ	C24-C25-C26	-2.98	111.41	116.30
4	B	8002	CFF	C14-N7-C8	-2.95	111.22	125.43
4	D	8002	CFF	C14-N7-C8	-2.95	111.25	125.43
4	A	8002	CFF	C14-N7-C8	-2.95	111.25	125.43
4	C	8002	CFF	C14-N7-C8	-2.94	111.28	125.43
8	A	8009	A1BYZ	C24-C25-C26	-2.94	111.48	116.30
8	D	8009	A1BYZ	C24-C25-C26	-2.93	111.49	116.30
8	B	8009	A1BYZ	C24-C25-C26	-2.93	111.49	116.30
8	C	8009	A1BYZ	C24-C25-C26	-2.93	111.49	116.30
7	A	8005	PCW	O3-C11-C12	2.81	120.41	111.83
7	D	8005	PCW	O3-C11-C12	2.81	120.40	111.83
7	B	8005	PCW	O3-C11-C12	2.81	120.40	111.83
7	C	8005	PCW	O3-C11-C12	2.81	120.40	111.83
7	A	8006	PCW	C18-C19-C20	2.71	145.15	124.83
7	C	8006	PCW	C18-C19-C20	2.71	145.15	124.83
7	D	8006	PCW	C18-C19-C20	2.71	145.14	124.83
7	B	8006	PCW	C18-C19-C20	2.71	145.11	124.83
7	A	8006	PCW	O3-C11-C12	2.59	119.74	111.83
7	D	8006	PCW	O3-C11-C12	2.59	119.72	111.83
7	B	8006	PCW	O3-C11-C12	2.59	119.72	111.83
7	C	8006	PCW	O3-C11-C12	2.59	119.72	111.83
5	A	8007	ATP	C5-C6-N6	2.30	123.81	120.31
8	C	8009	A1BYZ	C16-C17-C18	-2.29	121.23	123.59
5	D	8003	ATP	C5-C6-N6	2.29	123.81	120.31
5	B	8003	ATP	C5-C6-N6	2.29	123.81	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	8003	ATP	C5-C6-N6	2.29	123.81	120.31
8	A	8009	A1BYZ	C16-C17-C18	-2.29	121.23	123.59
5	D	8007	ATP	C5-C6-N6	2.29	123.79	120.31
5	B	8007	ATP	C5-C6-N6	2.29	123.79	120.31
5	C	8007	ATP	C5-C6-N6	2.29	123.79	120.31
5	A	8003	ATP	C5-C6-N6	2.28	123.78	120.31
8	D	8009	A1BYZ	C16-C17-C18	-2.26	121.26	123.59
8	B	8009	A1BYZ	C16-C17-C18	-2.26	121.26	123.59
5	D	8003	ATP	O3'-C3'-C2'	-2.01	105.36	111.82
5	B	8003	ATP	O3'-C3'-C2'	-2.01	105.36	111.82
5	C	8003	ATP	O3'-C3'-C2'	-2.01	105.36	111.82
5	A	8003	ATP	O3'-C3'-C2'	-2.01	105.38	111.82

There are no chirality outliers.

All (312) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	8003	ATP	C5'-O5'-PA-O1A
5	D	8003	ATP	C5'-O5'-PA-O2A
5	D	8003	ATP	C5'-O5'-PA-O3A
5	D	8007	ATP	PB-O3B-PG-O3G
5	D	8007	ATP	C5'-O5'-PA-O2A
5	A	8003	ATP	C5'-O5'-PA-O1A
5	A	8003	ATP	C5'-O5'-PA-O2A
5	A	8003	ATP	C5'-O5'-PA-O3A
5	A	8007	ATP	PB-O3B-PG-O3G
5	A	8007	ATP	C5'-O5'-PA-O2A
5	B	8003	ATP	C5'-O5'-PA-O1A
5	B	8003	ATP	C5'-O5'-PA-O2A
5	B	8003	ATP	C5'-O5'-PA-O3A
5	B	8007	ATP	PB-O3B-PG-O3G
5	B	8007	ATP	C5'-O5'-PA-O2A
5	C	8003	ATP	C5'-O5'-PA-O1A
5	C	8003	ATP	C5'-O5'-PA-O2A
5	C	8003	ATP	C5'-O5'-PA-O3A
5	C	8007	ATP	PB-O3B-PG-O3G
5	C	8007	ATP	C5'-O5'-PA-O2A
7	D	8005	PCW	C32-C31-O2-C2
7	D	8005	PCW	O31-C31-O2-C2
7	D	8005	PCW	C1-O3P-P-O2P
7	D	8005	PCW	C1-O3P-P-O4P
7	D	8005	PCW	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
7	D	8006	PCW	C1-O3P-P-O2P
7	A	8005	PCW	C32-C31-O2-C2
7	A	8005	PCW	O31-C31-O2-C2
7	A	8005	PCW	C1-O3P-P-O2P
7	A	8005	PCW	C1-O3P-P-O4P
7	A	8005	PCW	C4-O4P-P-O2P
7	A	8006	PCW	C1-O3P-P-O2P
7	B	8005	PCW	C32-C31-O2-C2
7	B	8005	PCW	O31-C31-O2-C2
7	B	8005	PCW	C1-O3P-P-O2P
7	B	8005	PCW	C1-O3P-P-O4P
7	B	8005	PCW	C4-O4P-P-O2P
7	B	8006	PCW	C1-O3P-P-O2P
7	C	8005	PCW	C32-C31-O2-C2
7	C	8005	PCW	O31-C31-O2-C2
7	C	8005	PCW	C1-O3P-P-O2P
7	C	8005	PCW	C1-O3P-P-O4P
7	C	8005	PCW	C4-O4P-P-O2P
7	C	8006	PCW	C1-O3P-P-O2P
8	D	8009	A1BYZ	C3-C6-O8-C9
8	D	8009	A1BYZ	O7-C6-O8-C9
8	A	8009	A1BYZ	C3-C6-O8-C9
8	A	8009	A1BYZ	O7-C6-O8-C9
8	B	8009	A1BYZ	C3-C6-O8-C9
8	B	8009	A1BYZ	O7-C6-O8-C9
8	C	8009	A1BYZ	C3-C6-O8-C9
8	C	8009	A1BYZ	O7-C6-O8-C9
8	D	8008	A1BYZ	C10-C9-O8-C6
8	A	8008	A1BYZ	C10-C9-O8-C6
8	B	8008	A1BYZ	C10-C9-O8-C6
8	C	8008	A1BYZ	C10-C9-O8-C6
7	D	8006	PCW	O11-C11-O3-C3
7	A	8006	PCW	O11-C11-O3-C3
7	B	8006	PCW	O11-C11-O3-C3
7	C	8006	PCW	O11-C11-O3-C3
7	D	8006	PCW	C32-C31-O2-C2
7	A	8006	PCW	C32-C31-O2-C2
7	B	8006	PCW	C32-C31-O2-C2
7	C	8006	PCW	C32-C31-O2-C2
7	D	8006	PCW	C12-C11-O3-C3
7	A	8006	PCW	C12-C11-O3-C3
7	B	8006	PCW	C12-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
7	C	8006	PCW	C12-C11-O3-C3
7	D	8006	PCW	O31-C31-O2-C2
7	A	8006	PCW	O31-C31-O2-C2
7	B	8006	PCW	O31-C31-O2-C2
7	C	8006	PCW	O31-C31-O2-C2
7	D	8006	PCW	C21-C22-C23-C24
7	A	8006	PCW	C21-C22-C23-C24
7	B	8006	PCW	C21-C22-C23-C24
7	C	8006	PCW	C21-C22-C23-C24
7	D	8005	PCW	C22-C23-C24-C25
7	B	8005	PCW	C22-C23-C24-C25
7	C	8005	PCW	C22-C23-C24-C25
7	A	8005	PCW	C22-C23-C24-C25
8	D	8009	A1BYZ	C15-C20-C21-C22
8	A	8009	A1BYZ	C15-C20-C21-C22
8	B	8009	A1BYZ	C15-C20-C21-C22
8	C	8009	A1BYZ	C15-C20-C21-C22
7	D	8005	PCW	C4-C5-N-C6
7	A	8005	PCW	C4-C5-N-C6
7	B	8005	PCW	C4-C5-N-C6
7	C	8005	PCW	C4-C5-N-C6
7	D	8005	PCW	C31-C32-C33-C34
7	A	8005	PCW	C31-C32-C33-C34
7	B	8005	PCW	C31-C32-C33-C34
7	C	8005	PCW	C31-C32-C33-C34
7	D	8005	PCW	C4-C5-N-C8
7	A	8005	PCW	C4-C5-N-C8
7	B	8005	PCW	C4-C5-N-C8
7	C	8005	PCW	C4-C5-N-C8
7	A	8006	PCW	C35-C36-C37-C38
7	D	8006	PCW	C35-C36-C37-C38
7	B	8006	PCW	C35-C36-C37-C38
7	C	8006	PCW	C35-C36-C37-C38
7	D	8005	PCW	C33-C34-C35-C36
7	A	8005	PCW	C33-C34-C35-C36
7	B	8005	PCW	C33-C34-C35-C36
7	C	8005	PCW	C33-C34-C35-C36
7	D	8006	PCW	C11-C12-C13-C14
7	A	8006	PCW	C11-C12-C13-C14
7	B	8006	PCW	C11-C12-C13-C14
7	C	8006	PCW	C11-C12-C13-C14
7	D	8005	PCW	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
7	A	8005	PCW	C11-C12-C13-C14
7	B	8005	PCW	C11-C12-C13-C14
7	C	8005	PCW	C11-C12-C13-C14
7	D	8006	PCW	C22-C23-C24-C25
7	D	8006	PCW	C34-C35-C36-C37
7	A	8006	PCW	C22-C23-C24-C25
7	A	8006	PCW	C34-C35-C36-C37
7	B	8006	PCW	C22-C23-C24-C25
7	B	8006	PCW	C34-C35-C36-C37
7	C	8006	PCW	C22-C23-C24-C25
7	C	8006	PCW	C34-C35-C36-C37
7	D	8005	PCW	C12-C11-O3-C3
7	A	8005	PCW	C12-C11-O3-C3
7	B	8005	PCW	C12-C11-O3-C3
7	C	8005	PCW	C12-C11-O3-C3
7	D	8005	PCW	C4-C5-N-C7
7	A	8005	PCW	C4-C5-N-C7
7	B	8005	PCW	C4-C5-N-C7
7	C	8005	PCW	C4-C5-N-C7
7	D	8005	PCW	C13-C14-C15-C16
7	B	8005	PCW	C13-C14-C15-C16
7	A	8005	PCW	C13-C14-C15-C16
7	C	8005	PCW	C13-C14-C15-C16
7	D	8005	PCW	C20-C21-C22-C23
7	A	8005	PCW	C20-C21-C22-C23
7	B	8005	PCW	C20-C21-C22-C23
7	C	8005	PCW	C20-C21-C22-C23
7	A	8005	PCW	C44-C45-C46-C47
7	C	8005	PCW	C44-C45-C46-C47
7	D	8005	PCW	C44-C45-C46-C47
7	B	8005	PCW	C44-C45-C46-C47
7	D	8005	PCW	C2-C3-O3-C11
7	A	8005	PCW	C2-C3-O3-C11
7	B	8005	PCW	C2-C3-O3-C11
7	C	8005	PCW	C2-C3-O3-C11
7	A	8005	PCW	O11-C11-O3-C3
7	D	8005	PCW	O11-C11-O3-C3
7	B	8005	PCW	O11-C11-O3-C3
7	C	8005	PCW	O11-C11-O3-C3
7	D	8006	PCW	C15-C16-C17-C18
7	A	8006	PCW	C15-C16-C17-C18
7	B	8006	PCW	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
7	C	8006	PCW	C15-C16-C17-C18
5	D	8003	ATP	PB-O3B-PG-O1G
5	A	8003	ATP	PB-O3B-PG-O1G
5	B	8003	ATP	PB-O3B-PG-O1G
5	C	8003	ATP	PB-O3B-PG-O1G
8	D	8008	A1BYZ	C20-C21-C22-C23
8	A	8008	A1BYZ	C20-C21-C22-C23
8	B	8008	A1BYZ	C20-C21-C22-C23
8	C	8008	A1BYZ	C20-C21-C22-C23
7	D	8006	PCW	C20-C21-C22-C23
7	A	8006	PCW	C20-C21-C22-C23
7	B	8006	PCW	C20-C21-C22-C23
7	C	8006	PCW	C20-C21-C22-C23
7	D	8006	PCW	C42-C43-C44-C45
7	A	8006	PCW	C42-C43-C44-C45
7	B	8006	PCW	C42-C43-C44-C45
7	C	8006	PCW	C42-C43-C44-C45
5	D	8003	ATP	PA-O3A-PB-O1B
5	A	8003	ATP	PA-O3A-PB-O1B
5	B	8003	ATP	PA-O3A-PB-O1B
5	C	8003	ATP	PA-O3A-PB-O1B
5	D	8003	ATP	C4'-C5'-O5'-PA
5	A	8003	ATP	C4'-C5'-O5'-PA
5	B	8003	ATP	C4'-C5'-O5'-PA
5	C	8003	ATP	C4'-C5'-O5'-PA
7	D	8005	PCW	C12-C13-C14-C15
7	A	8005	PCW	C12-C13-C14-C15
7	B	8005	PCW	C12-C13-C14-C15
7	C	8005	PCW	C12-C13-C14-C15
7	D	8006	PCW	C31-C32-C33-C34
7	A	8006	PCW	C31-C32-C33-C34
7	B	8006	PCW	C31-C32-C33-C34
7	C	8006	PCW	C31-C32-C33-C34
7	D	8006	PCW	O3P-C1-C2-O2
7	A	8006	PCW	O3P-C1-C2-O2
7	B	8006	PCW	O3P-C1-C2-O2
7	C	8006	PCW	O3P-C1-C2-O2
8	D	8008	A1BYZ	C16-C15-C20-C21
8	A	8008	A1BYZ	C16-C15-C20-C21
8	B	8008	A1BYZ	C16-C15-C20-C21
8	C	8008	A1BYZ	C16-C15-C20-C21
7	B	8006	PCW	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
7	D	8006	PCW	C44-C45-C46-C47
7	A	8006	PCW	C44-C45-C46-C47
7	C	8006	PCW	C44-C45-C46-C47
7	D	8006	PCW	C40-C41-C42-C43
7	A	8006	PCW	C40-C41-C42-C43
7	B	8006	PCW	C40-C41-C42-C43
7	C	8006	PCW	C40-C41-C42-C43
7	D	8006	PCW	O3P-C1-C2-C3
7	A	8006	PCW	O3P-C1-C2-C3
7	B	8006	PCW	O3P-C1-C2-C3
7	C	8006	PCW	O3P-C1-C2-C3
5	D	8003	ATP	PB-O3B-PG-O3G
5	A	8003	ATP	PB-O3B-PG-O3G
5	B	8003	ATP	PB-O3B-PG-O3G
5	C	8003	ATP	PB-O3B-PG-O3G
7	D	8006	PCW	C41-C42-C43-C44
7	A	8006	PCW	C41-C42-C43-C44
7	B	8006	PCW	C41-C42-C43-C44
7	C	8006	PCW	C41-C42-C43-C44
7	C	8005	PCW	C45-C46-C47-C48
7	D	8005	PCW	C45-C46-C47-C48
7	A	8005	PCW	C45-C46-C47-C48
7	B	8005	PCW	C45-C46-C47-C48
7	D	8006	PCW	O4P-C4-C5-N
7	A	8006	PCW	O4P-C4-C5-N
7	B	8006	PCW	O4P-C4-C5-N
7	C	8006	PCW	O4P-C4-C5-N
5	D	8007	ATP	C5'-O5'-PA-O1A
5	D	8007	ATP	C5'-O5'-PA-O3A
5	A	8007	ATP	C5'-O5'-PA-O1A
5	A	8007	ATP	C5'-O5'-PA-O3A
5	B	8007	ATP	C5'-O5'-PA-O1A
5	B	8007	ATP	C5'-O5'-PA-O3A
5	C	8007	ATP	C5'-O5'-PA-O1A
5	C	8007	ATP	C5'-O5'-PA-O3A
7	D	8005	PCW	C1-O3P-P-O1P
7	D	8005	PCW	C4-O4P-P-O1P
7	D	8005	PCW	C4-O4P-P-O3P
7	D	8006	PCW	C4-O4P-P-O2P
7	A	8005	PCW	C1-O3P-P-O1P
7	A	8005	PCW	C4-O4P-P-O1P
7	A	8005	PCW	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
7	A	8006	PCW	C4-O4P-P-O2P
7	B	8005	PCW	C1-O3P-P-O1P
7	B	8005	PCW	C4-O4P-P-O1P
7	B	8005	PCW	C4-O4P-P-O3P
7	B	8006	PCW	C4-O4P-P-O2P
7	C	8005	PCW	C1-O3P-P-O1P
7	C	8005	PCW	C4-O4P-P-O1P
7	C	8005	PCW	C4-O4P-P-O3P
7	C	8006	PCW	C4-O4P-P-O2P
7	D	8005	PCW	C19-C20-C21-C22
7	A	8005	PCW	C19-C20-C21-C22
7	B	8005	PCW	C19-C20-C21-C22
7	C	8005	PCW	C19-C20-C21-C22
7	D	8006	PCW	C37-C38-C39-C40
7	A	8006	PCW	C37-C38-C39-C40
7	B	8006	PCW	C37-C38-C39-C40
7	C	8006	PCW	C37-C38-C39-C40
7	D	8006	PCW	C19-C20-C21-C22
7	A	8006	PCW	C19-C20-C21-C22
7	B	8006	PCW	C19-C20-C21-C22
7	C	8006	PCW	C19-C20-C21-C22
7	D	8006	PCW	C36-C37-C38-C39
7	B	8006	PCW	C36-C37-C38-C39
7	C	8006	PCW	C36-C37-C38-C39
8	D	8009	A1BYZ	C2-C3-C6-O7
8	A	8009	A1BYZ	C2-C3-C6-O7
8	B	8009	A1BYZ	C2-C3-C6-O7
8	C	8009	A1BYZ	C2-C3-C6-O7
5	D	8007	ATP	PB-O3A-PA-O1A
5	A	8007	ATP	PB-O3A-PA-O1A
5	B	8007	ATP	PB-O3A-PA-O1A
5	C	8007	ATP	PB-O3A-PA-O1A
7	A	8006	PCW	C36-C37-C38-C39
7	A	8006	PCW	C25-C26-C27-C28
5	D	8007	ATP	C4'-C5'-O5'-PA
5	A	8007	ATP	C4'-C5'-O5'-PA
5	B	8007	ATP	C4'-C5'-O5'-PA
5	C	8007	ATP	C4'-C5'-O5'-PA
7	D	8006	PCW	C25-C26-C27-C28
7	B	8006	PCW	C25-C26-C27-C28
7	C	8006	PCW	C25-C26-C27-C28
7	D	8005	PCW	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
7	D	8006	PCW	C17-C18-C19-C20
7	A	8005	PCW	C39-C40-C41-C42
7	A	8006	PCW	C17-C18-C19-C20
7	B	8005	PCW	C39-C40-C41-C42
7	B	8006	PCW	C17-C18-C19-C20
7	C	8005	PCW	C39-C40-C41-C42
7	C	8006	PCW	C17-C18-C19-C20
5	D	8007	ATP	PB-O3B-PG-O1G
5	A	8007	ATP	PB-O3B-PG-O1G
5	B	8007	ATP	PB-O3B-PG-O1G
5	C	8007	ATP	PB-O3B-PG-O1G
5	D	8003	ATP	PG-O3B-PB-O1B
5	D	8003	ATP	PG-O3B-PB-O2B
5	A	8003	ATP	PG-O3B-PB-O1B
5	A	8003	ATP	PG-O3B-PB-O2B
5	B	8003	ATP	PG-O3B-PB-O1B
5	B	8003	ATP	PG-O3B-PB-O2B
5	C	8003	ATP	PG-O3B-PB-O1B
5	C	8003	ATP	PG-O3B-PB-O2B
7	D	8006	PCW	O2-C31-C32-C33
7	A	8006	PCW	O2-C31-C32-C33
7	B	8006	PCW	O2-C31-C32-C33
7	C	8006	PCW	O2-C31-C32-C33
7	D	8006	PCW	C16-C17-C18-C19
7	A	8006	PCW	C16-C17-C18-C19
7	B	8006	PCW	C16-C17-C18-C19
7	C	8006	PCW	C16-C17-C18-C19
7	D	8006	PCW	O31-C31-C32-C33
7	B	8006	PCW	O31-C31-C32-C33
7	A	8006	PCW	O31-C31-C32-C33
7	C	8006	PCW	O31-C31-C32-C33
5	D	8007	ATP	PB-O3A-PA-O2A
5	A	8007	ATP	PB-O3A-PA-O2A
5	B	8007	ATP	PB-O3A-PA-O2A
5	C	8007	ATP	PB-O3A-PA-O2A

There are no ring outliers.

18 monomers are involved in 30 short contacts:

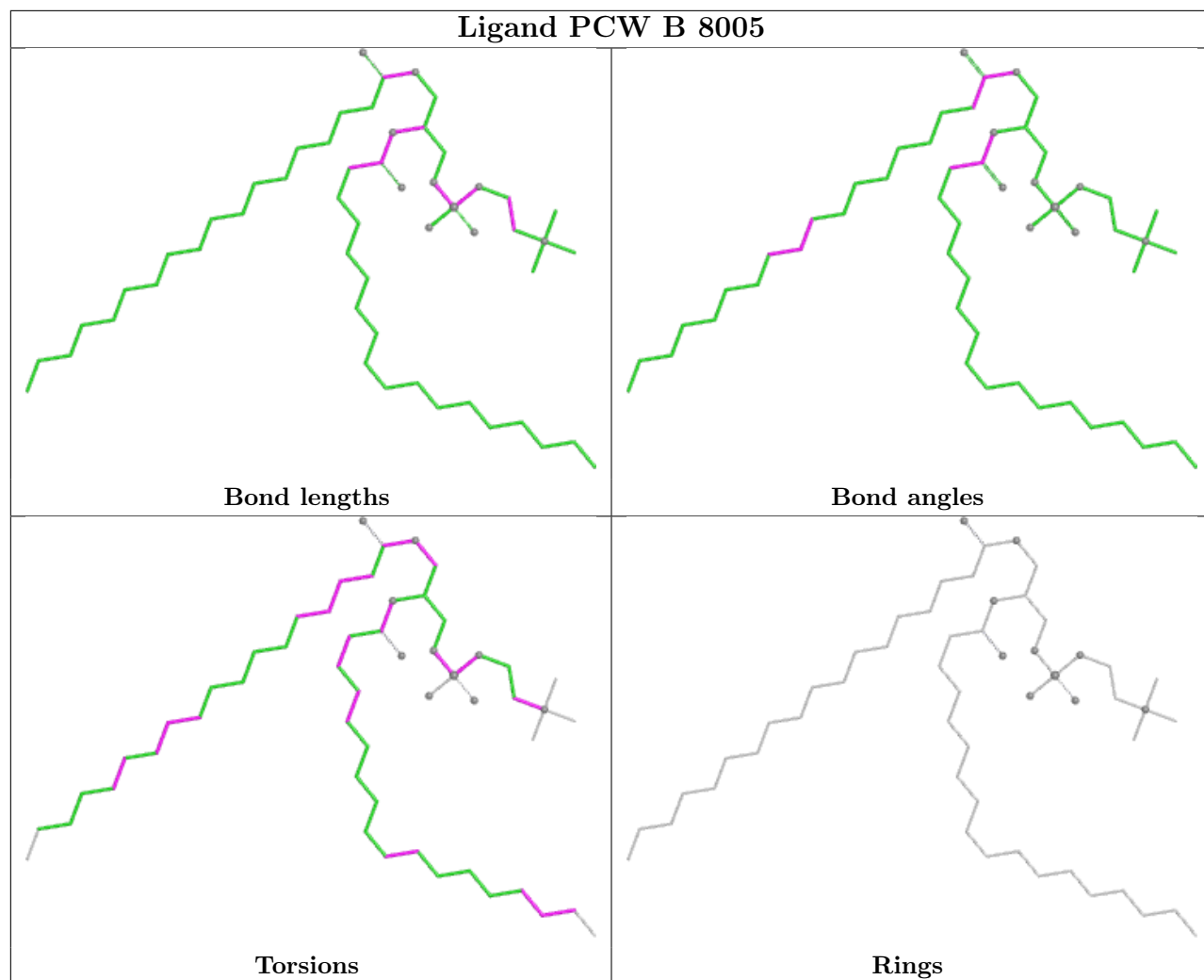
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	8005	PCW	2	0
8	B	8008	A1BYZ	1	0

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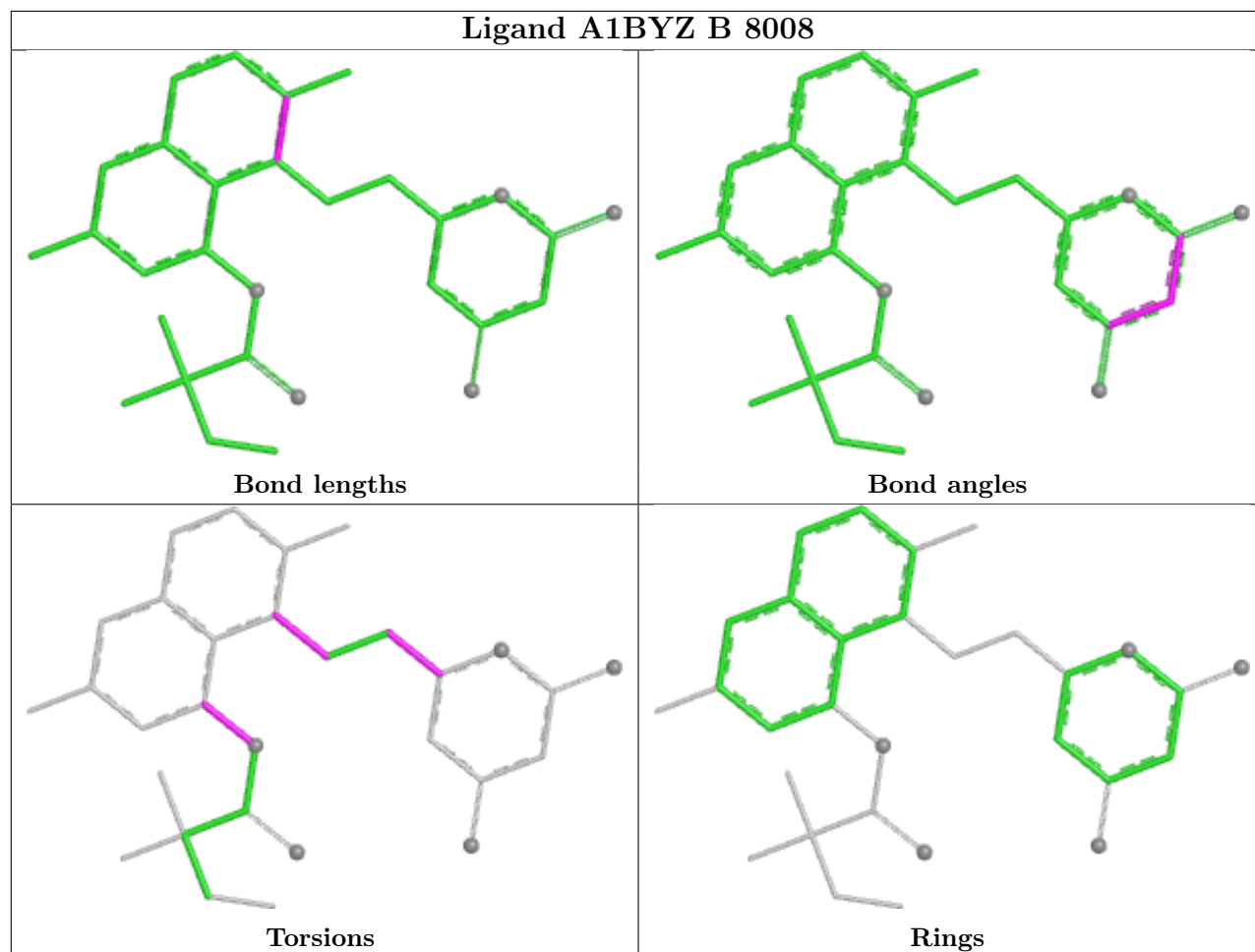
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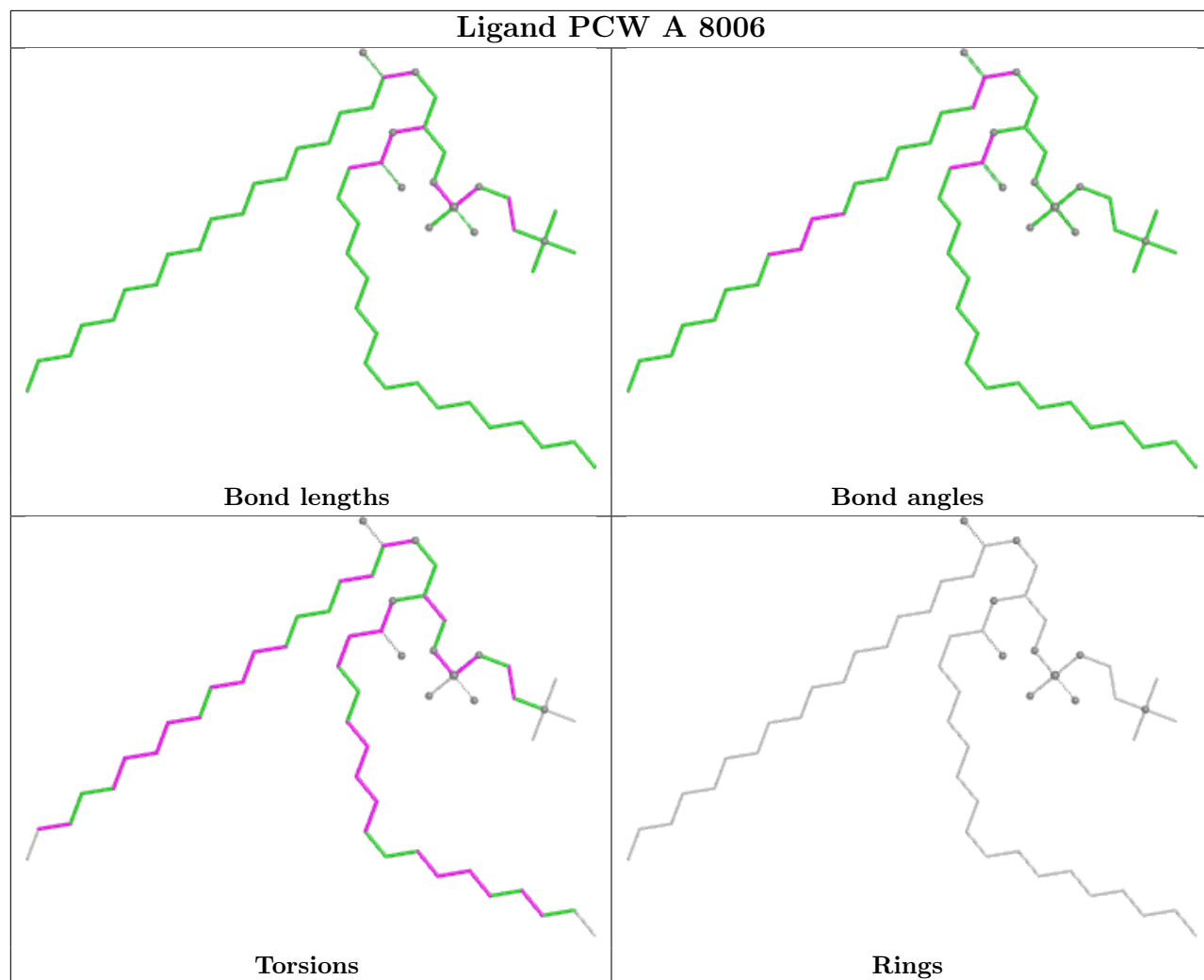
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	8006	PCW	3	0
7	B	8006	PCW	3	0
8	B	8009	A1BYZ	2	0
7	C	8006	PCW	3	0
8	A	8009	A1BYZ	2	0
5	D	8003	ATP	1	0
5	A	8003	ATP	1	0
8	C	8009	A1BYZ	2	0
8	C	8008	A1BYZ	1	0
7	C	8005	PCW	2	0
5	C	8003	ATP	1	0
8	D	8009	A1BYZ	2	0
5	B	8003	ATP	1	0
7	D	8005	PCW	2	0
7	A	8005	PCW	2	0
7	D	8006	PCW	3	0

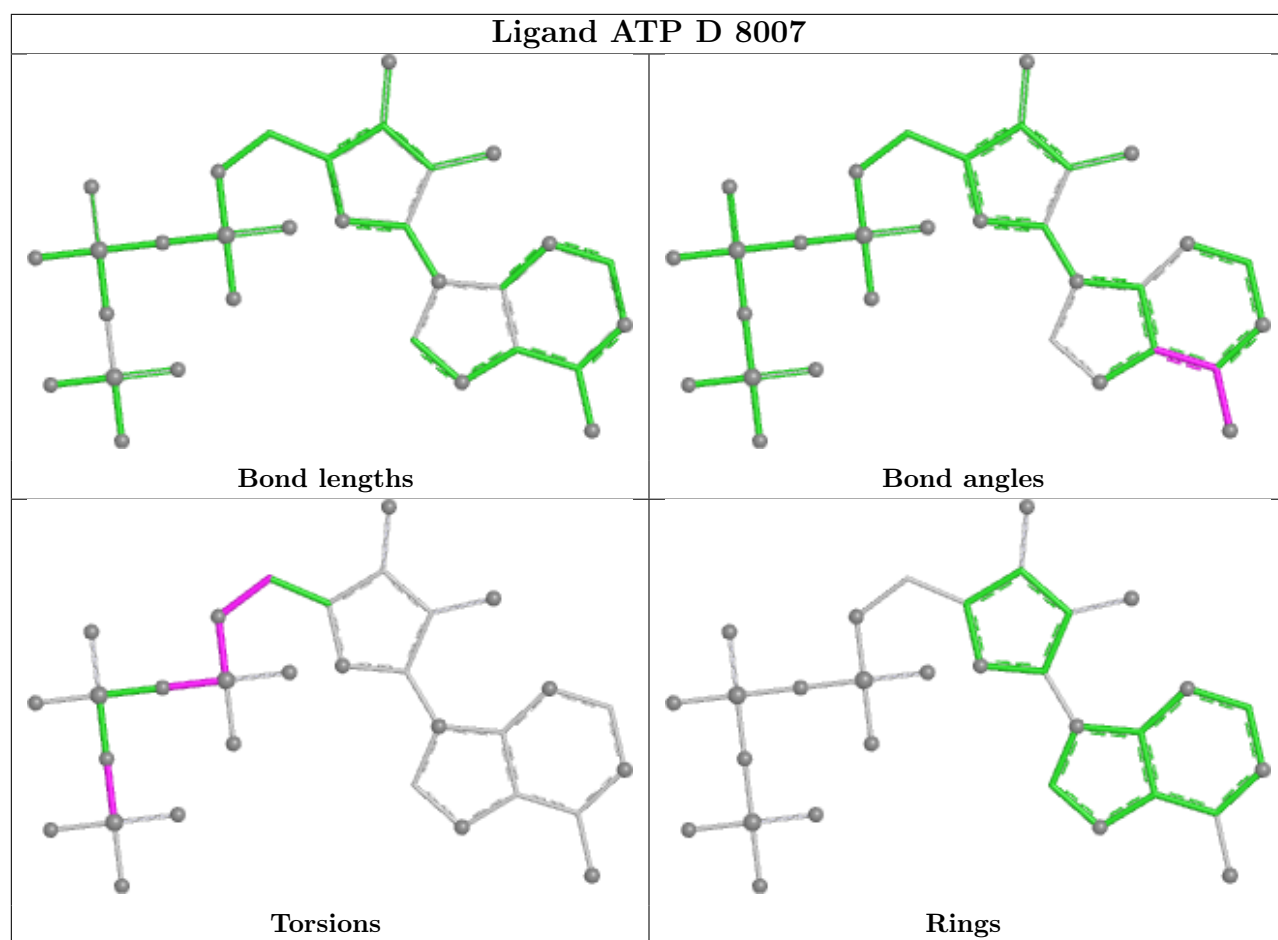
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

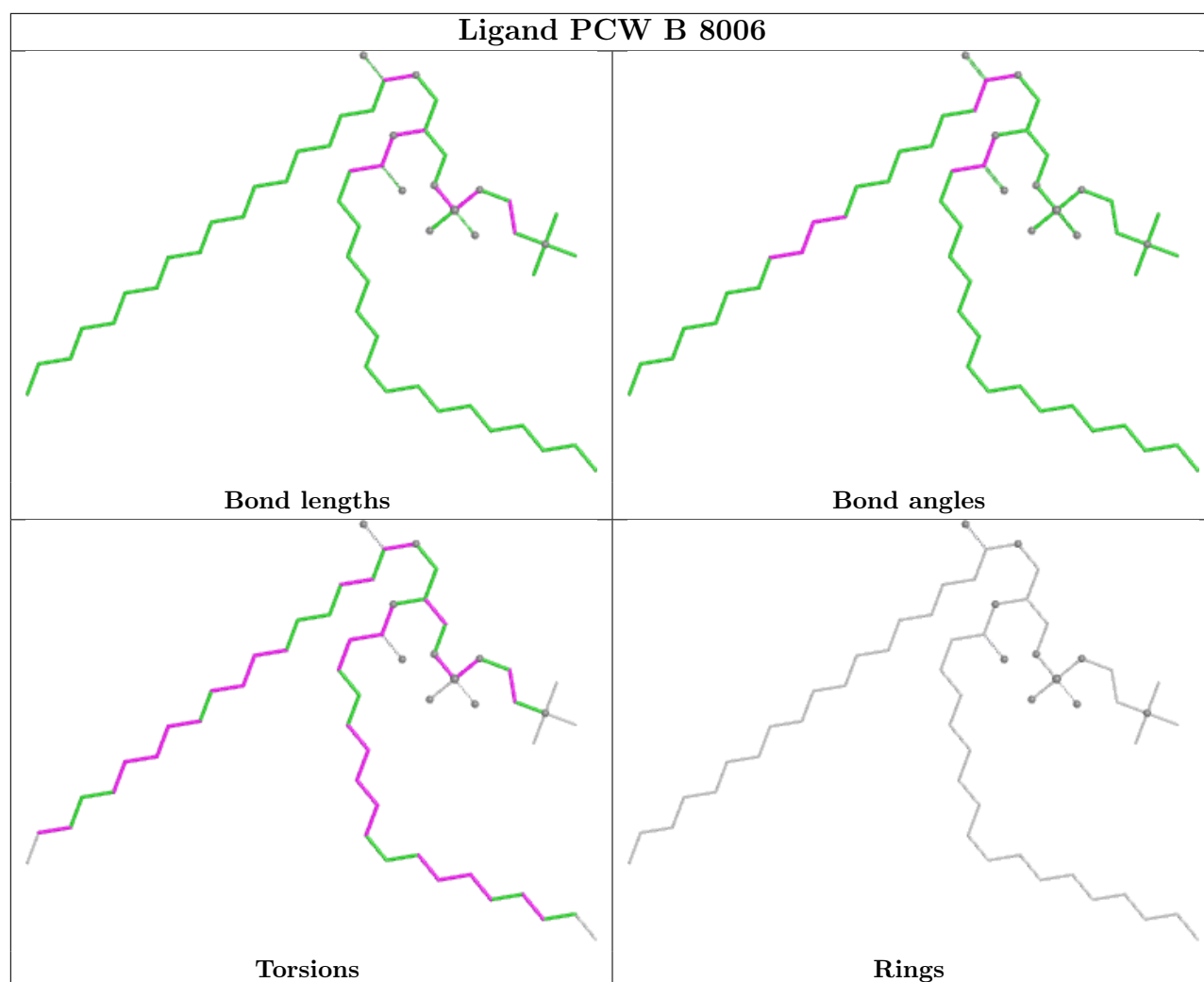


Ligand A1BYZ B 8008

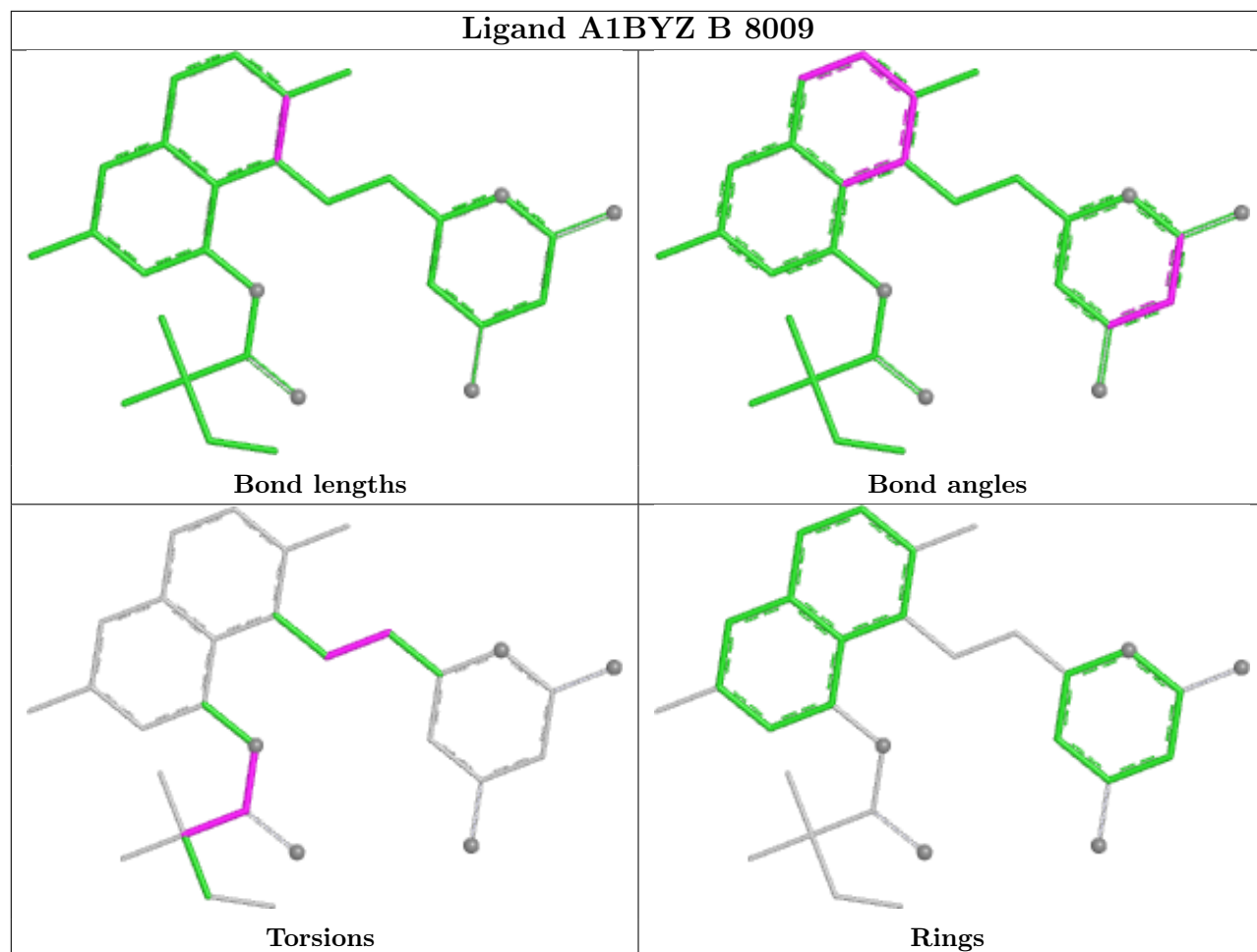


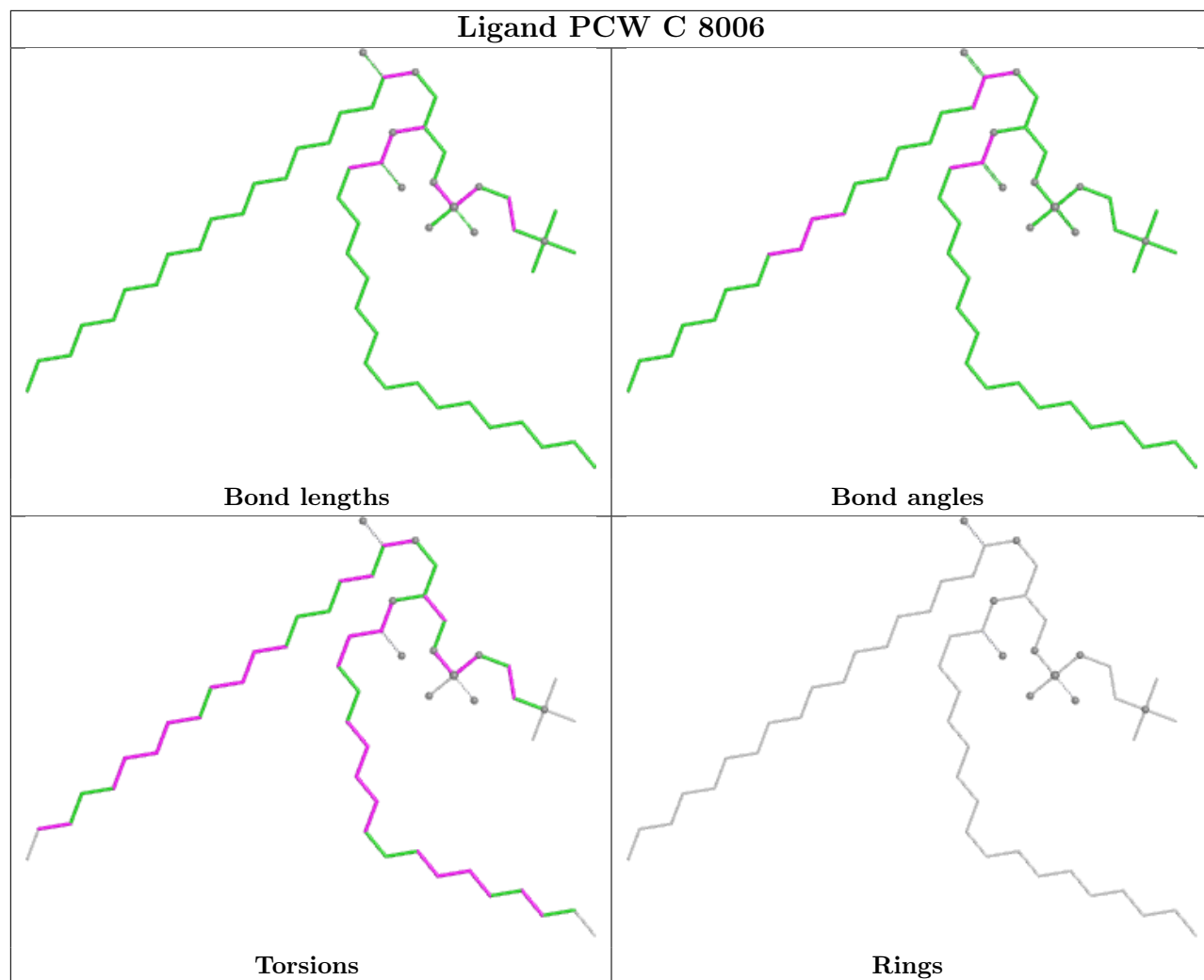




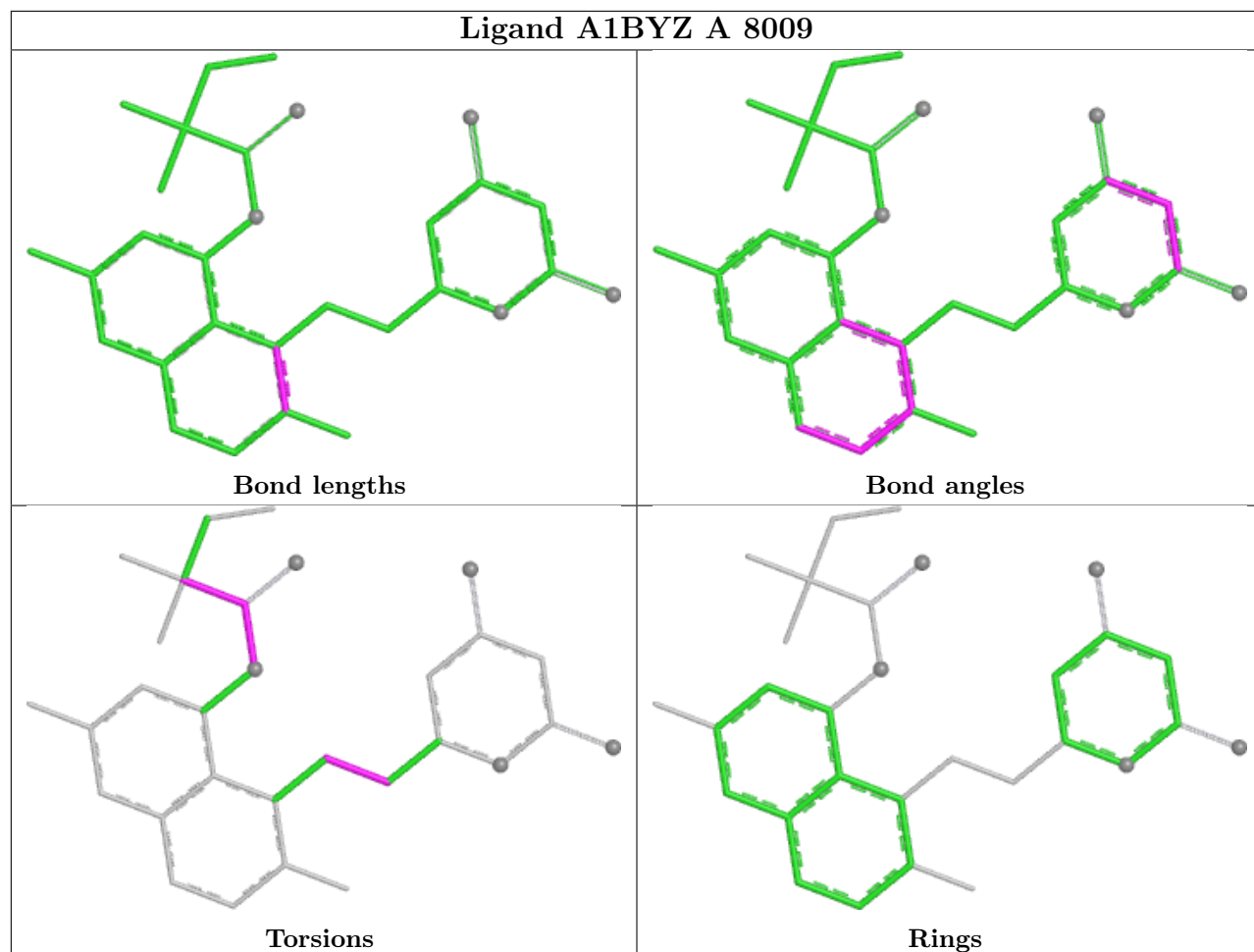


Ligand A1BYZ B 8009

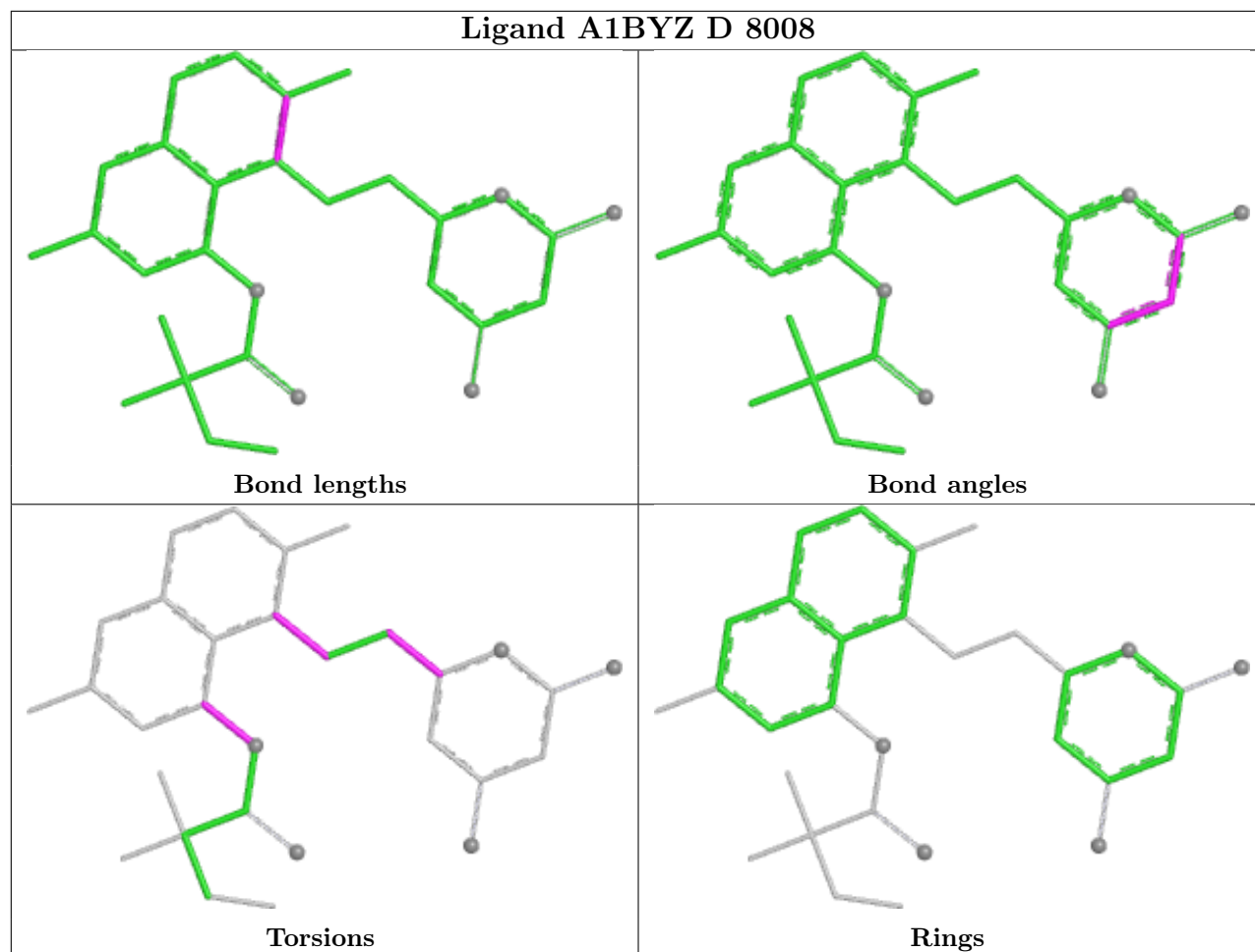


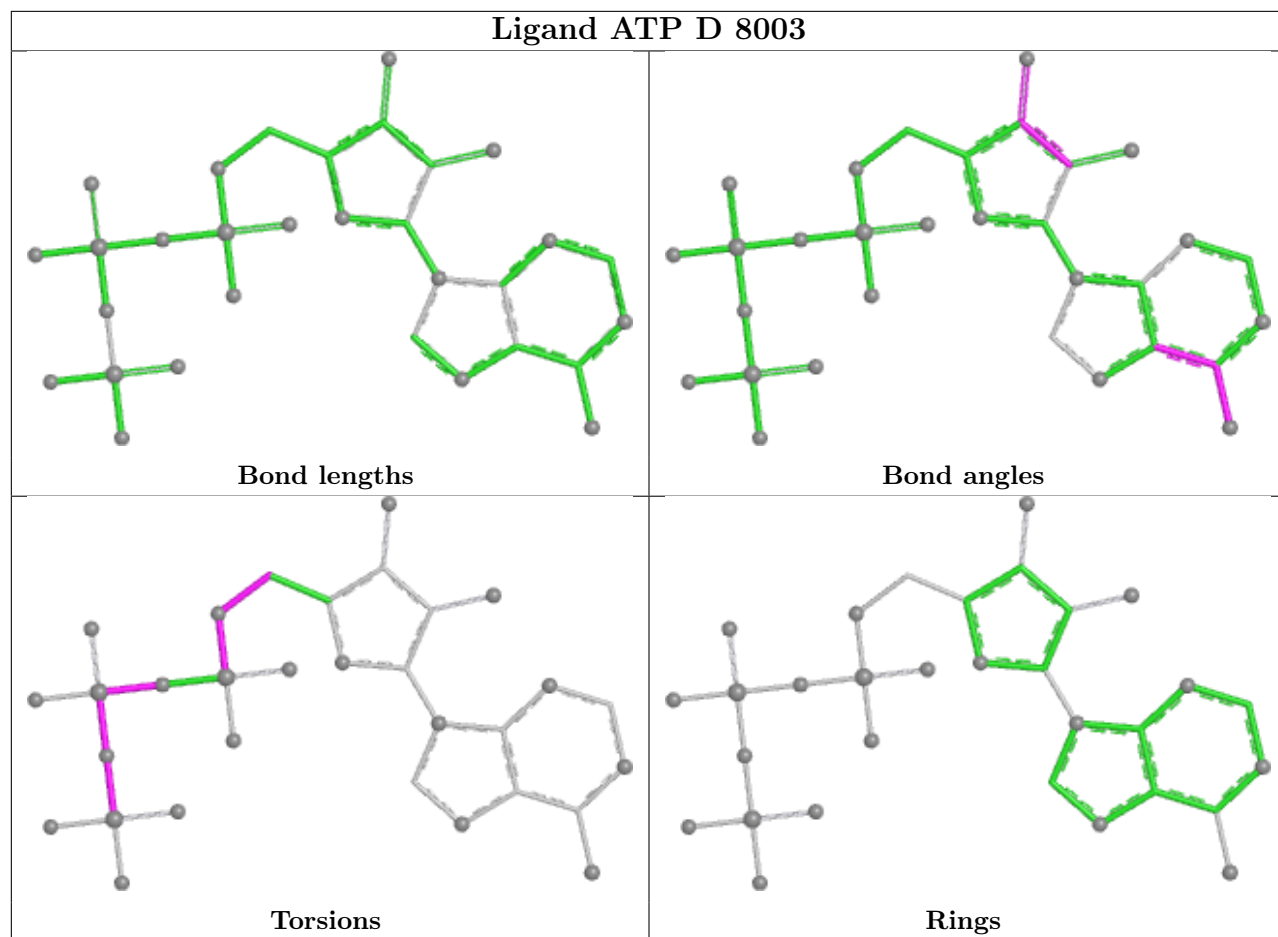


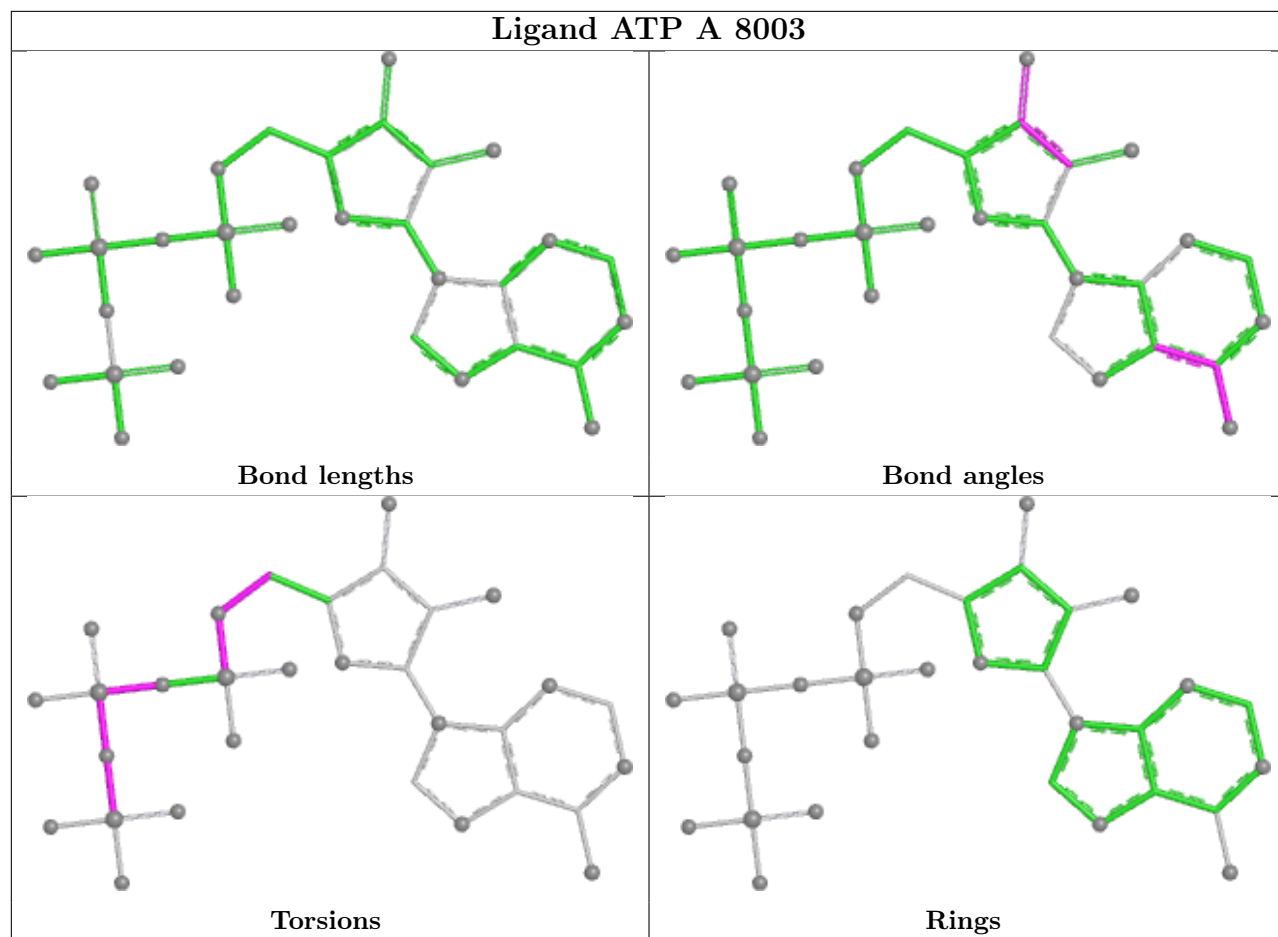
Ligand A1BYZ A 8009



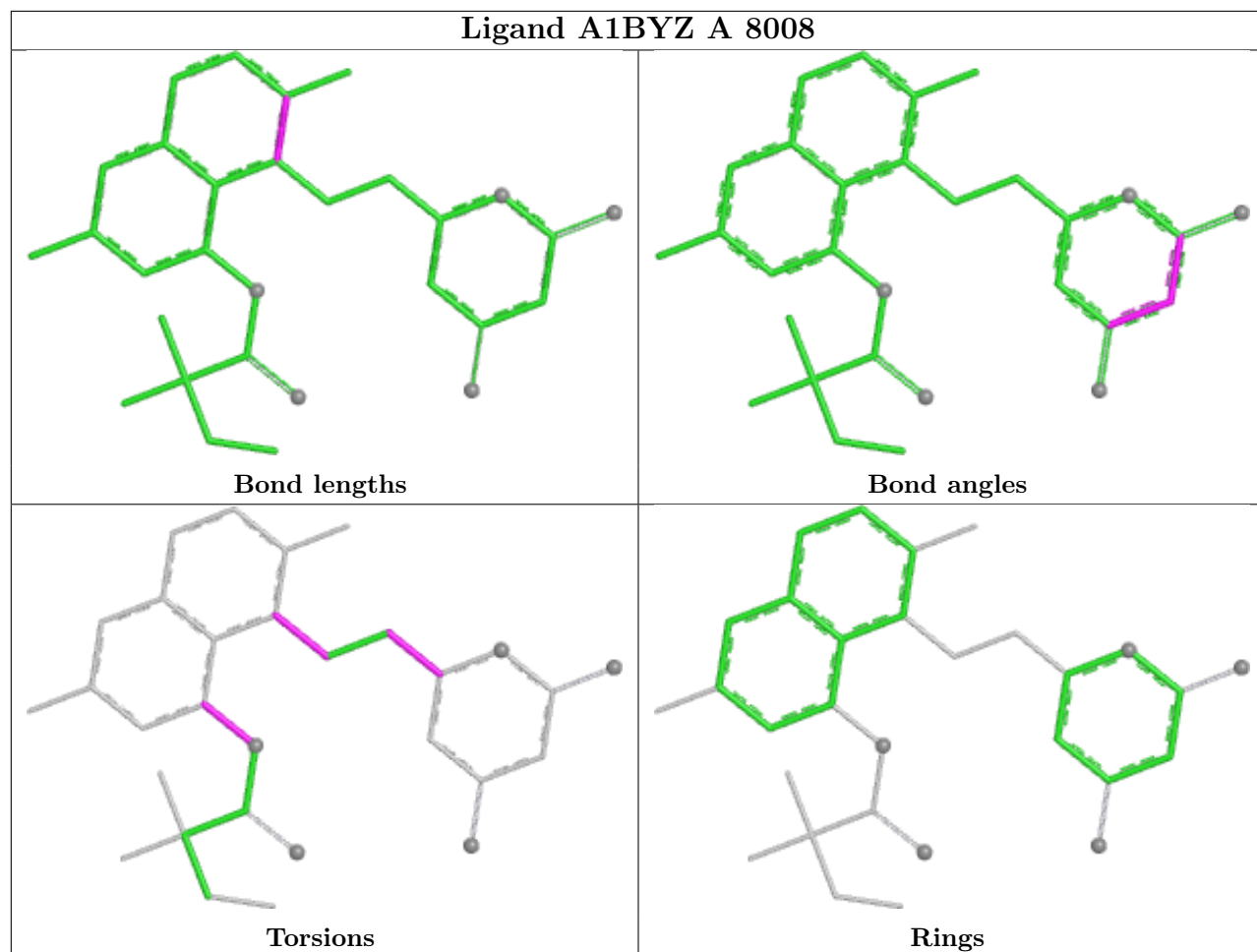
Ligand A1BYZ D 8008



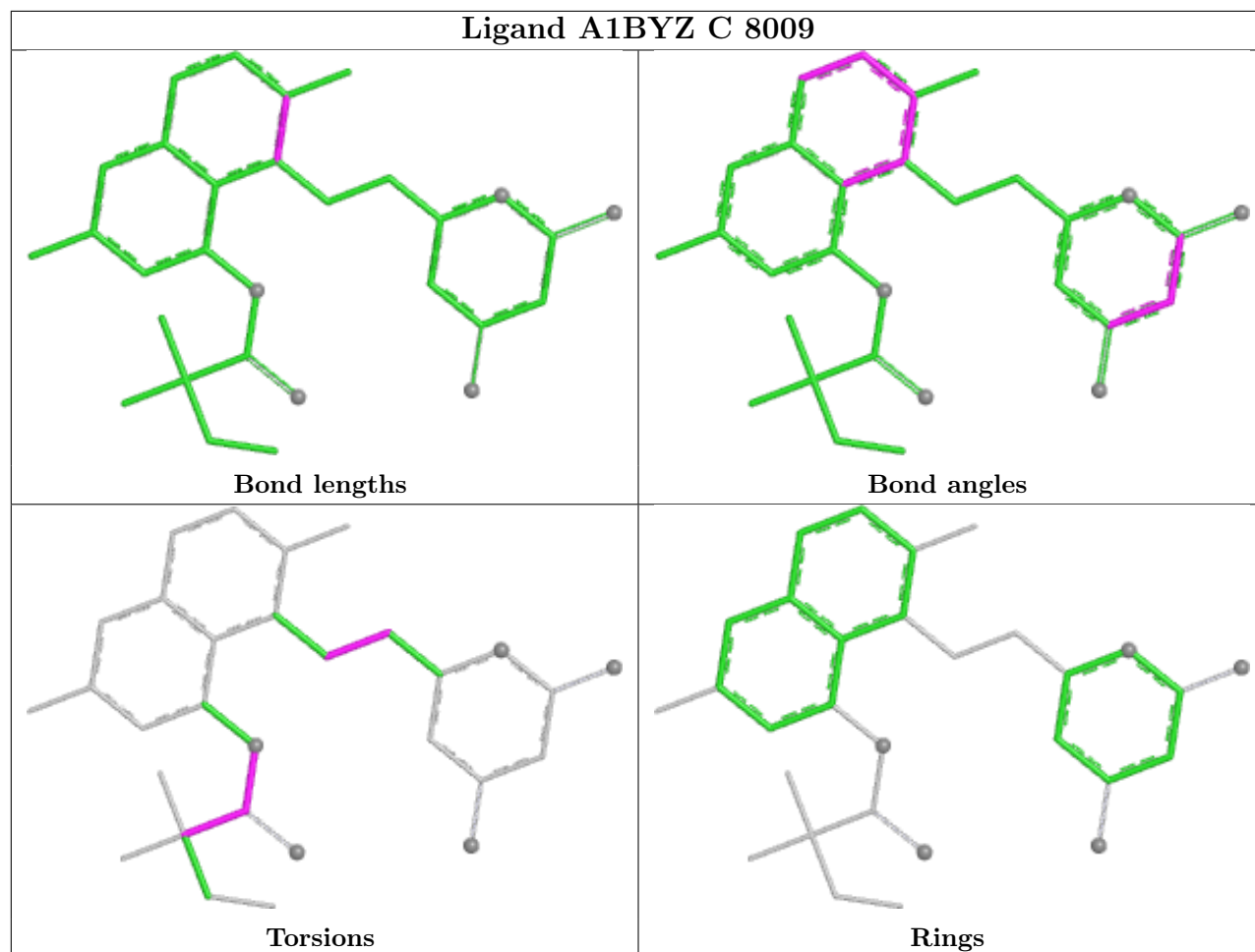


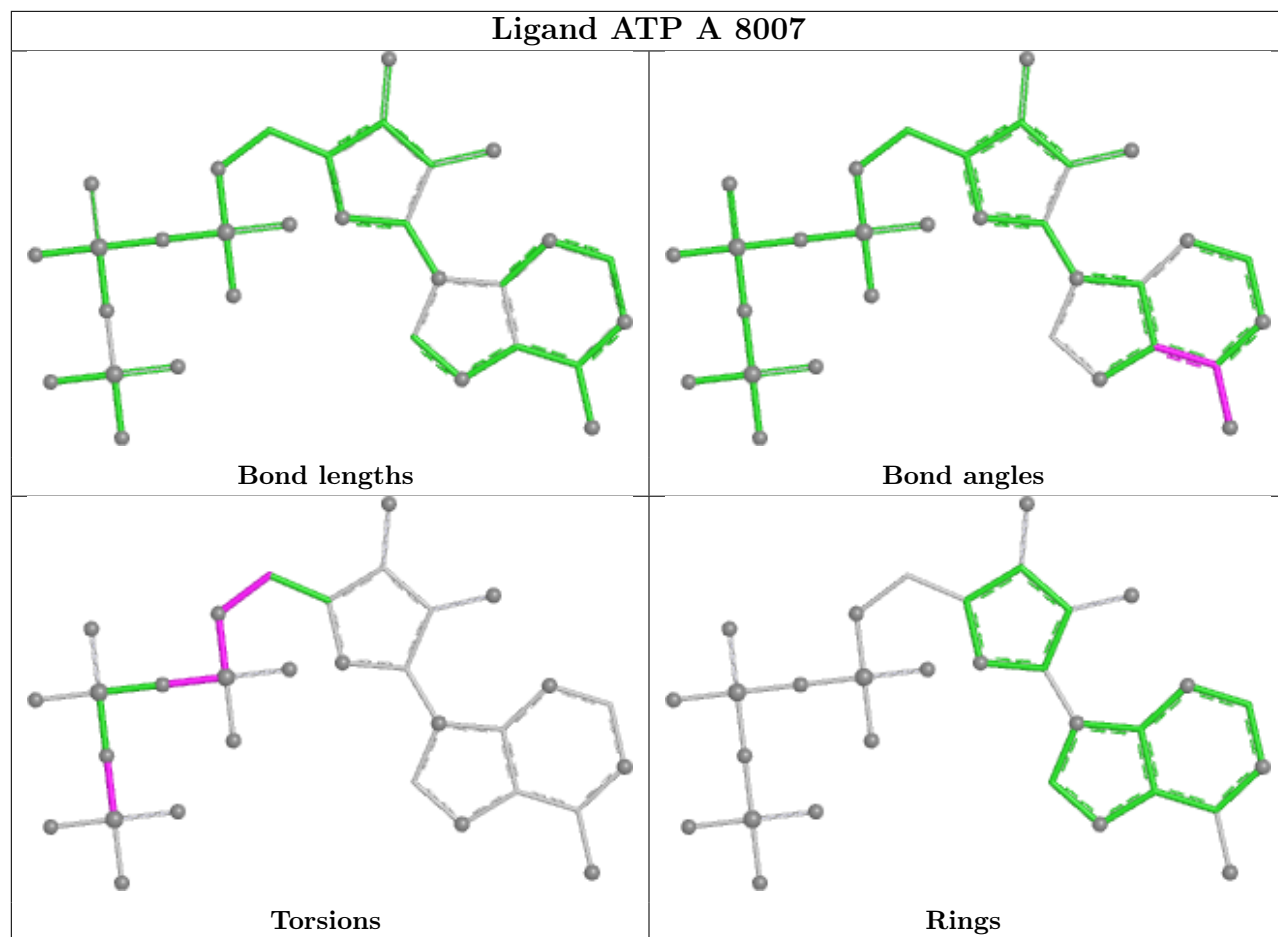


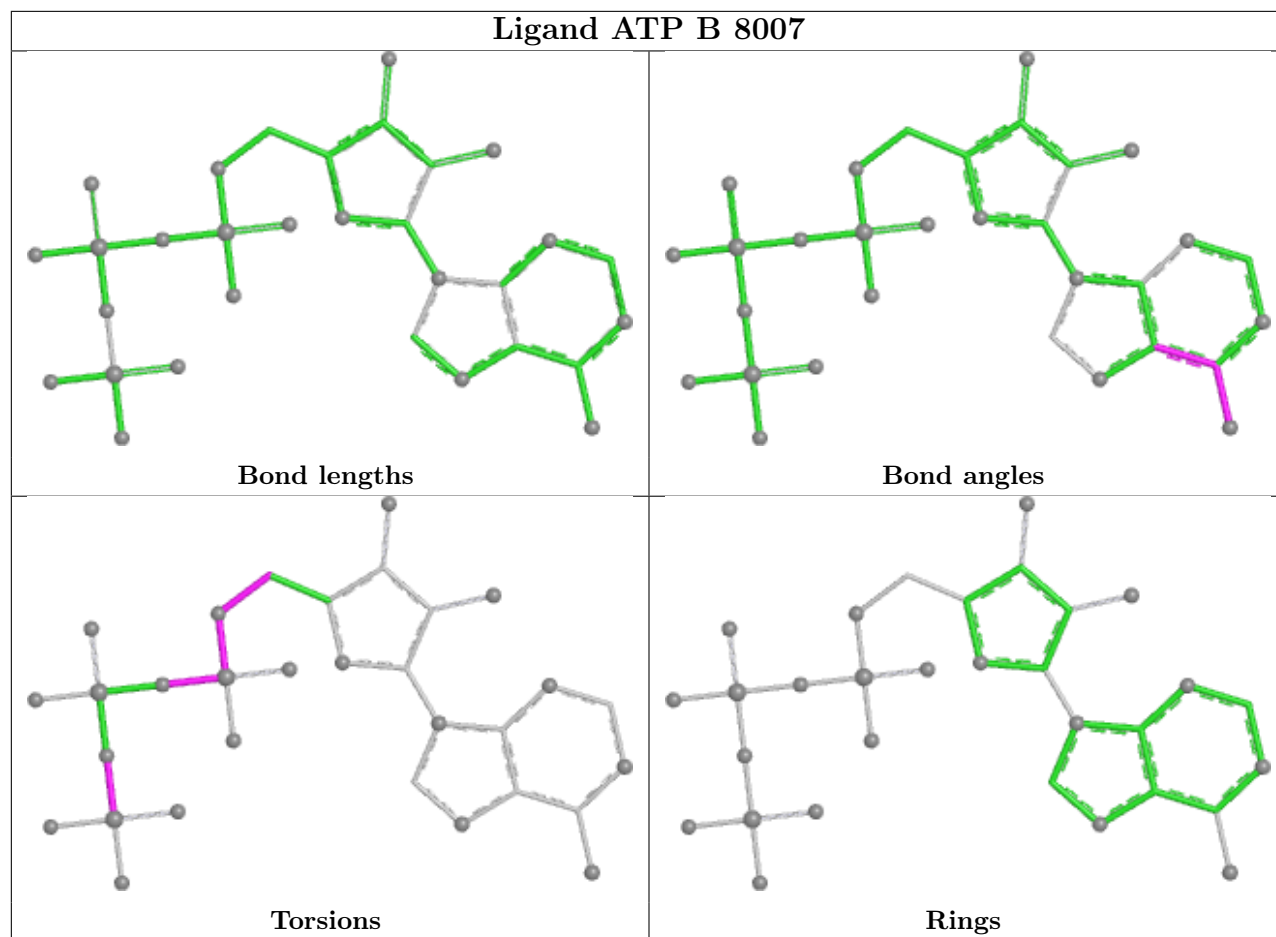
Ligand A1BYZ A 8008



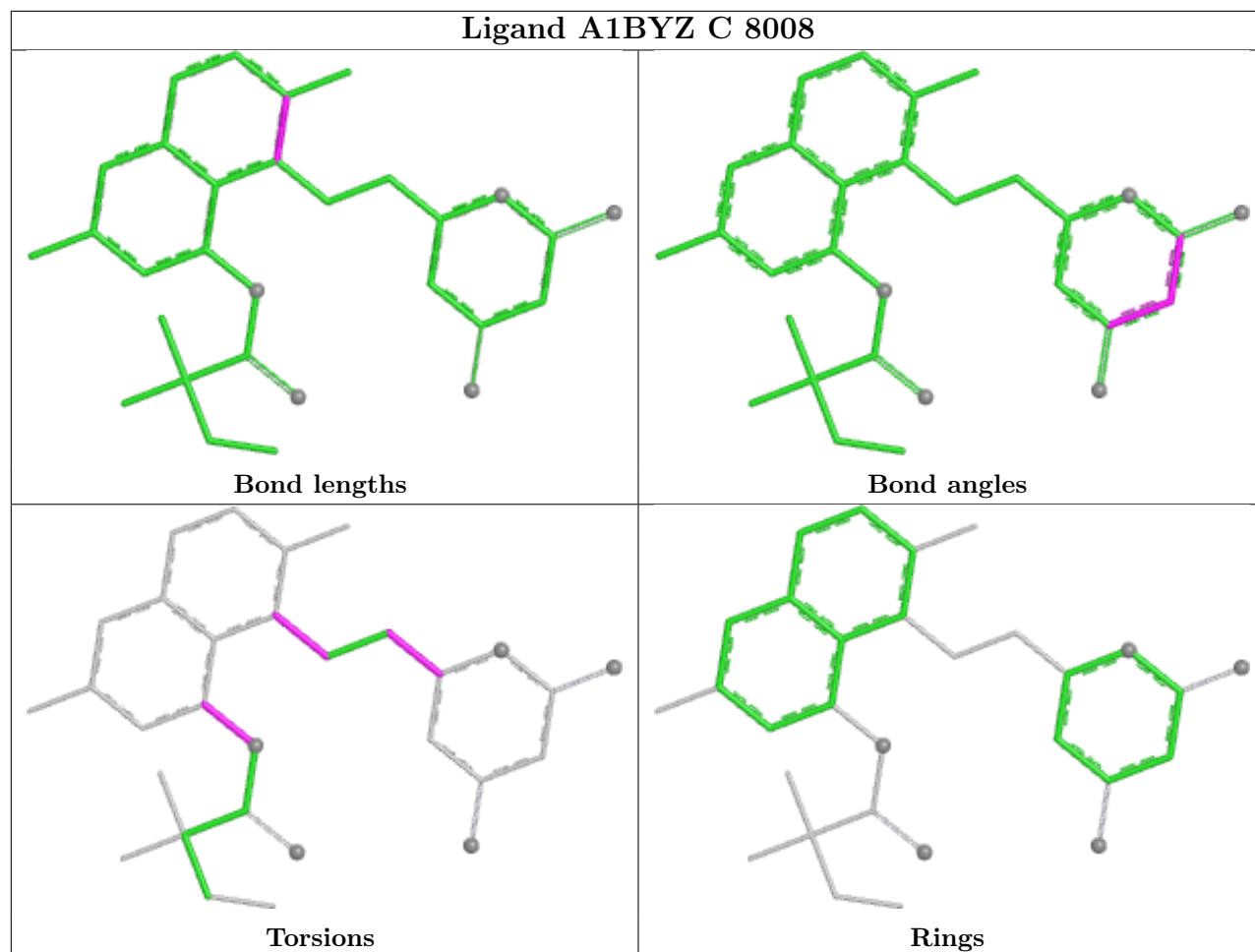
Ligand A1BYZ C 8009

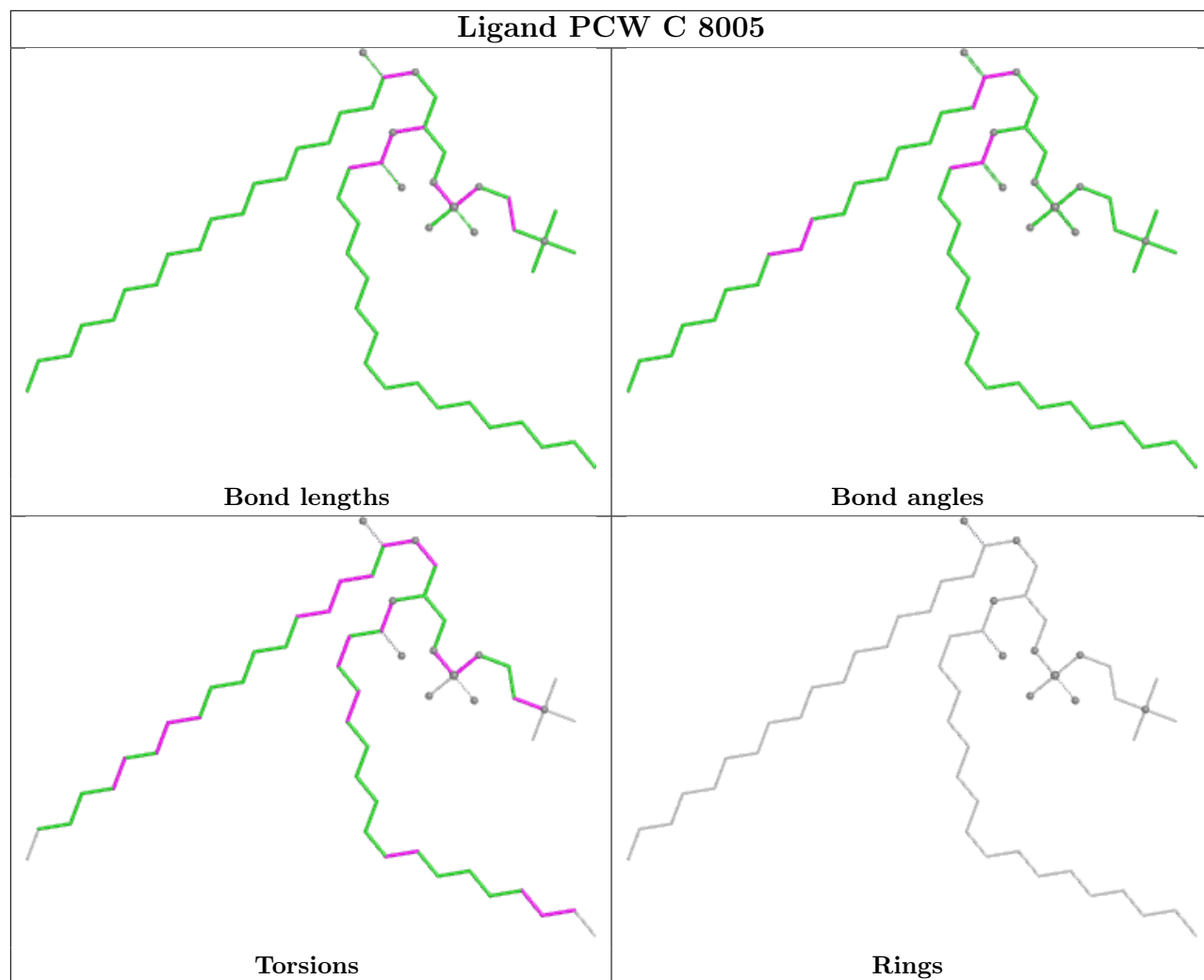


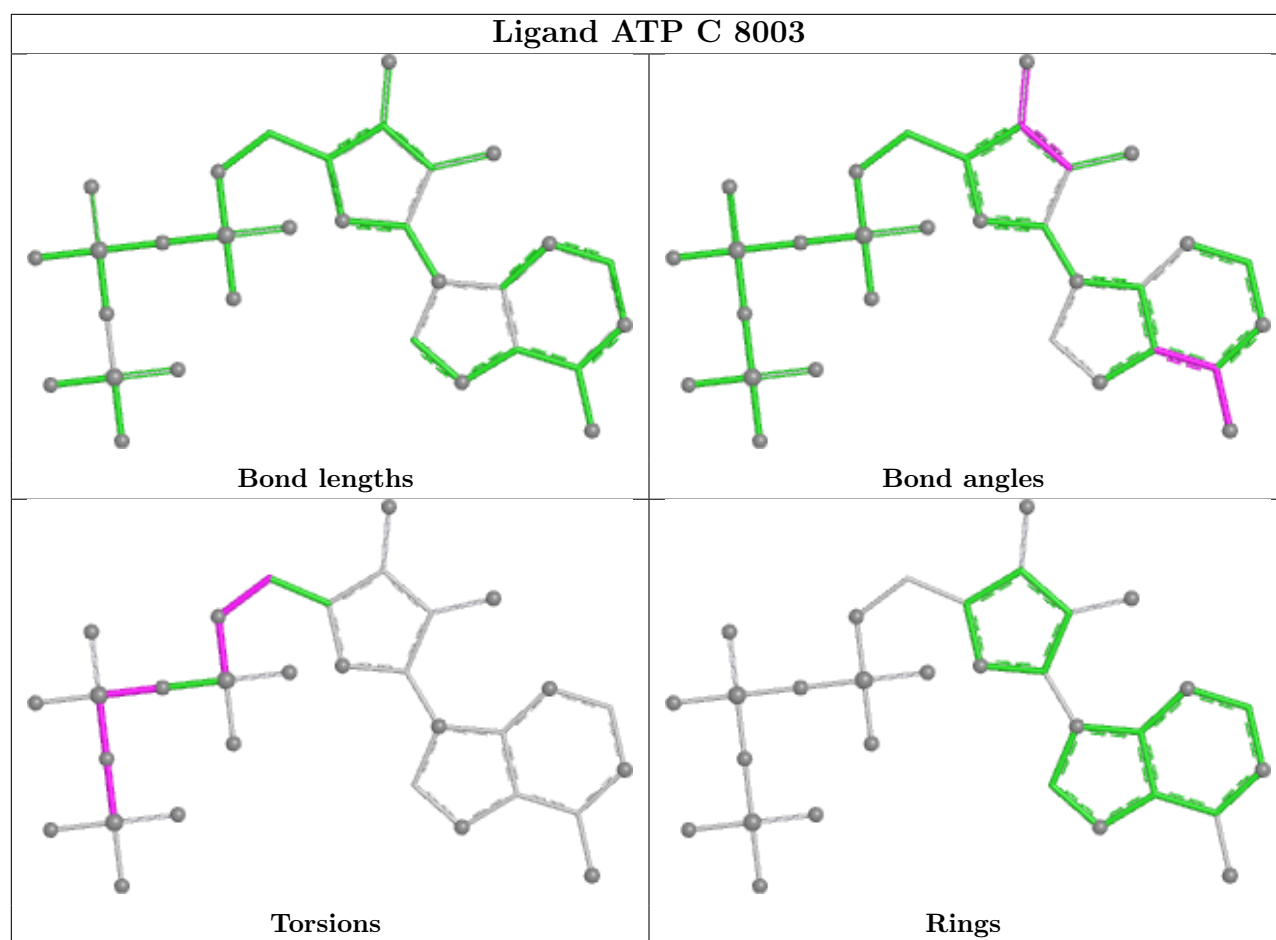




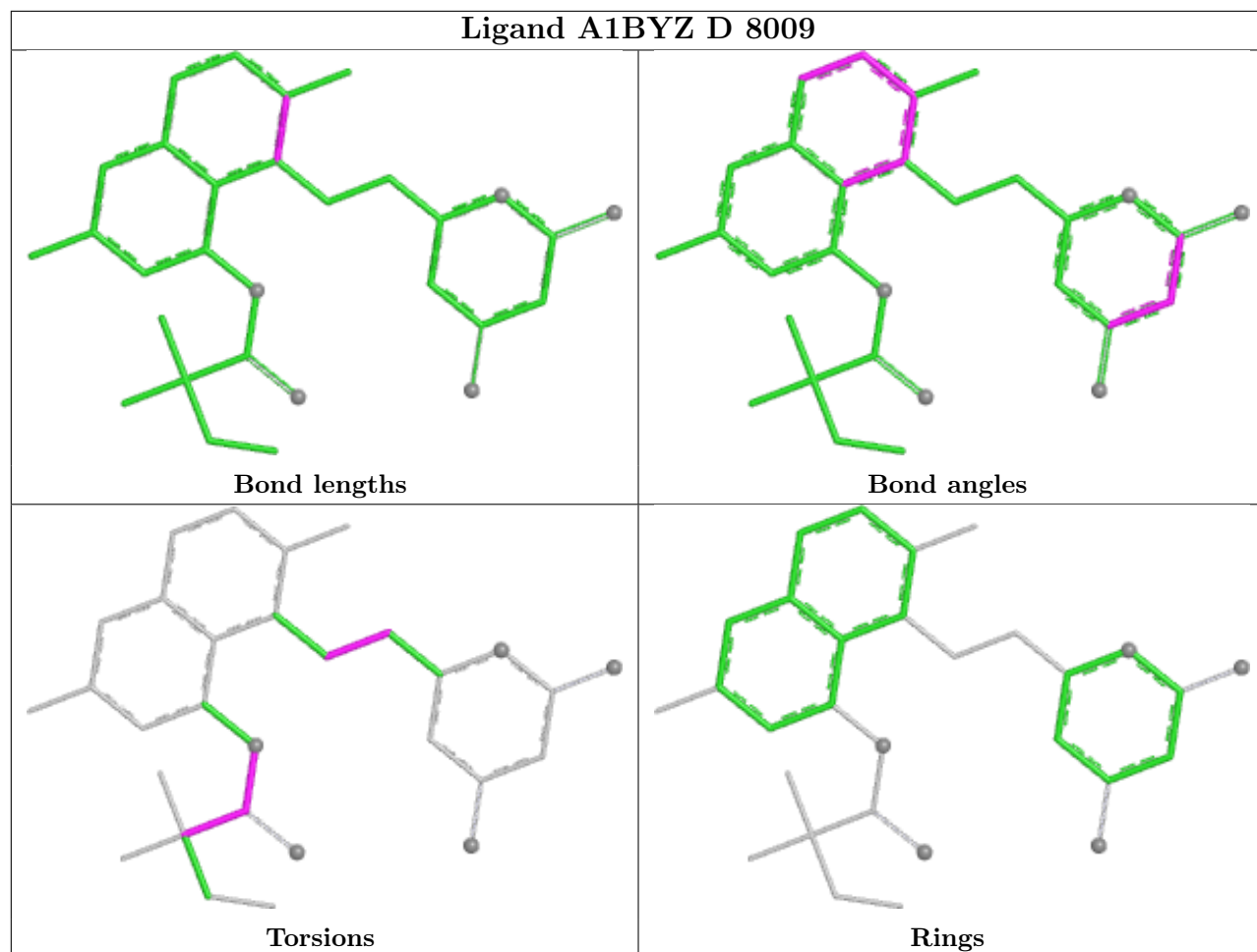
Ligand A1BYZ C 8008

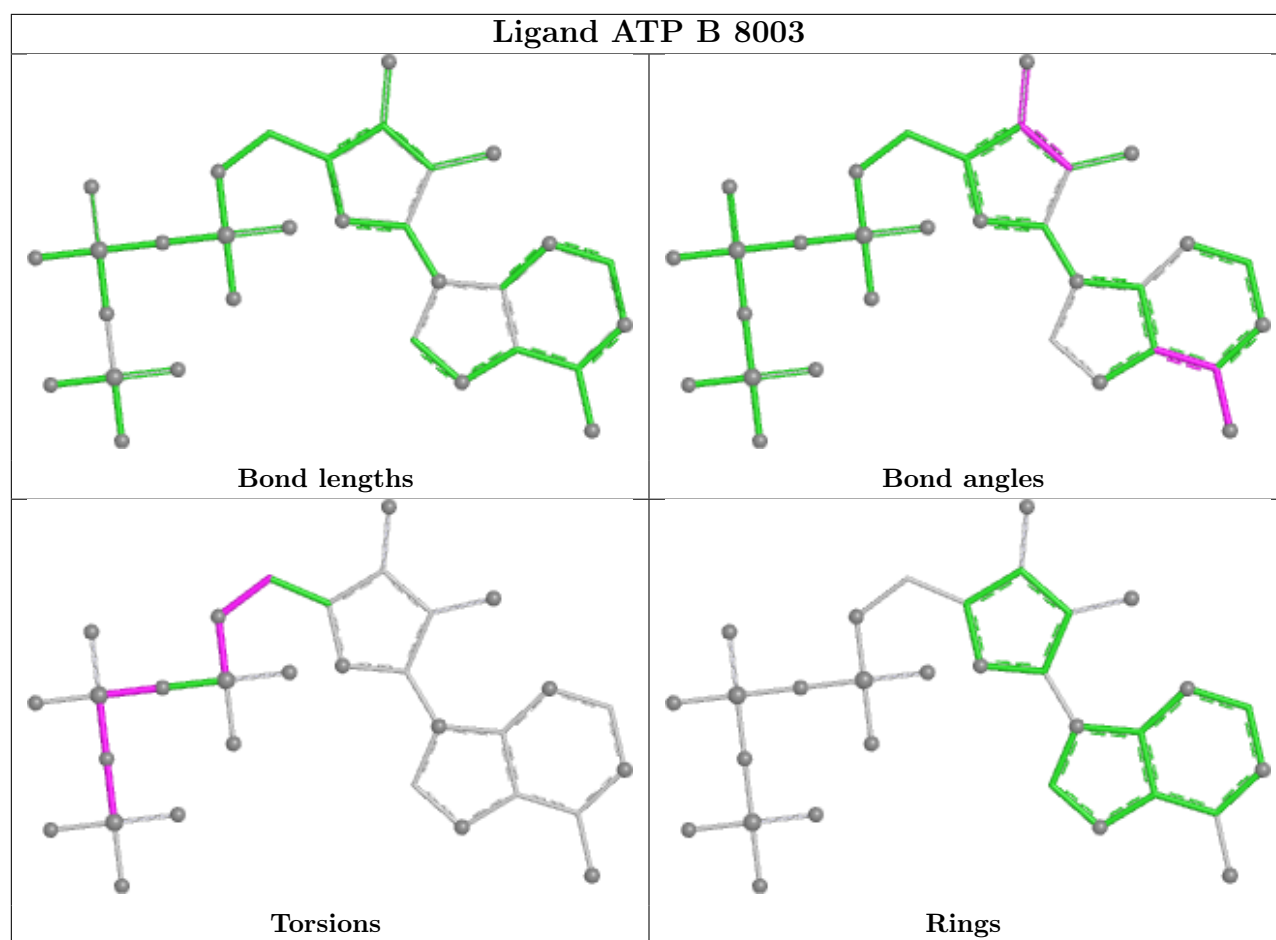


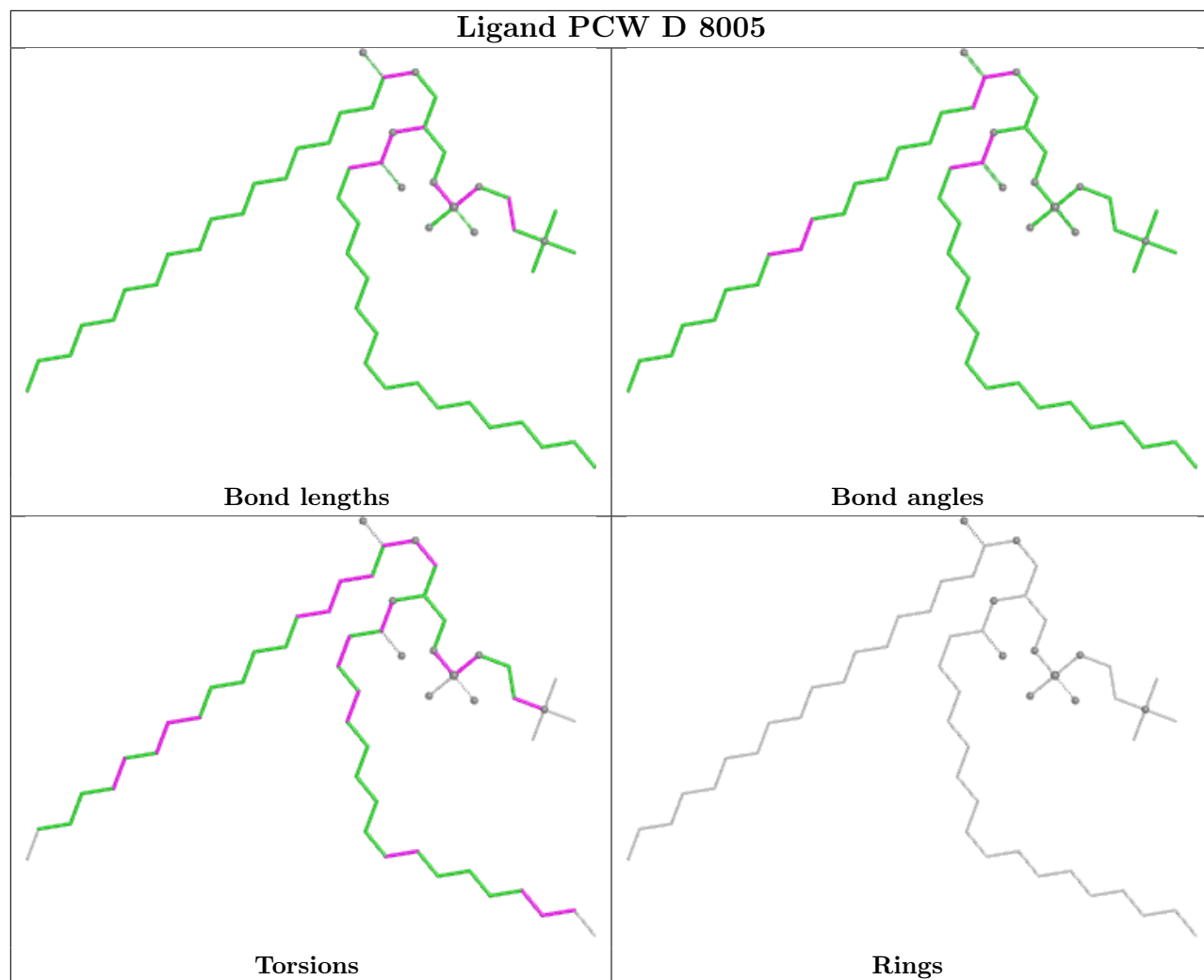


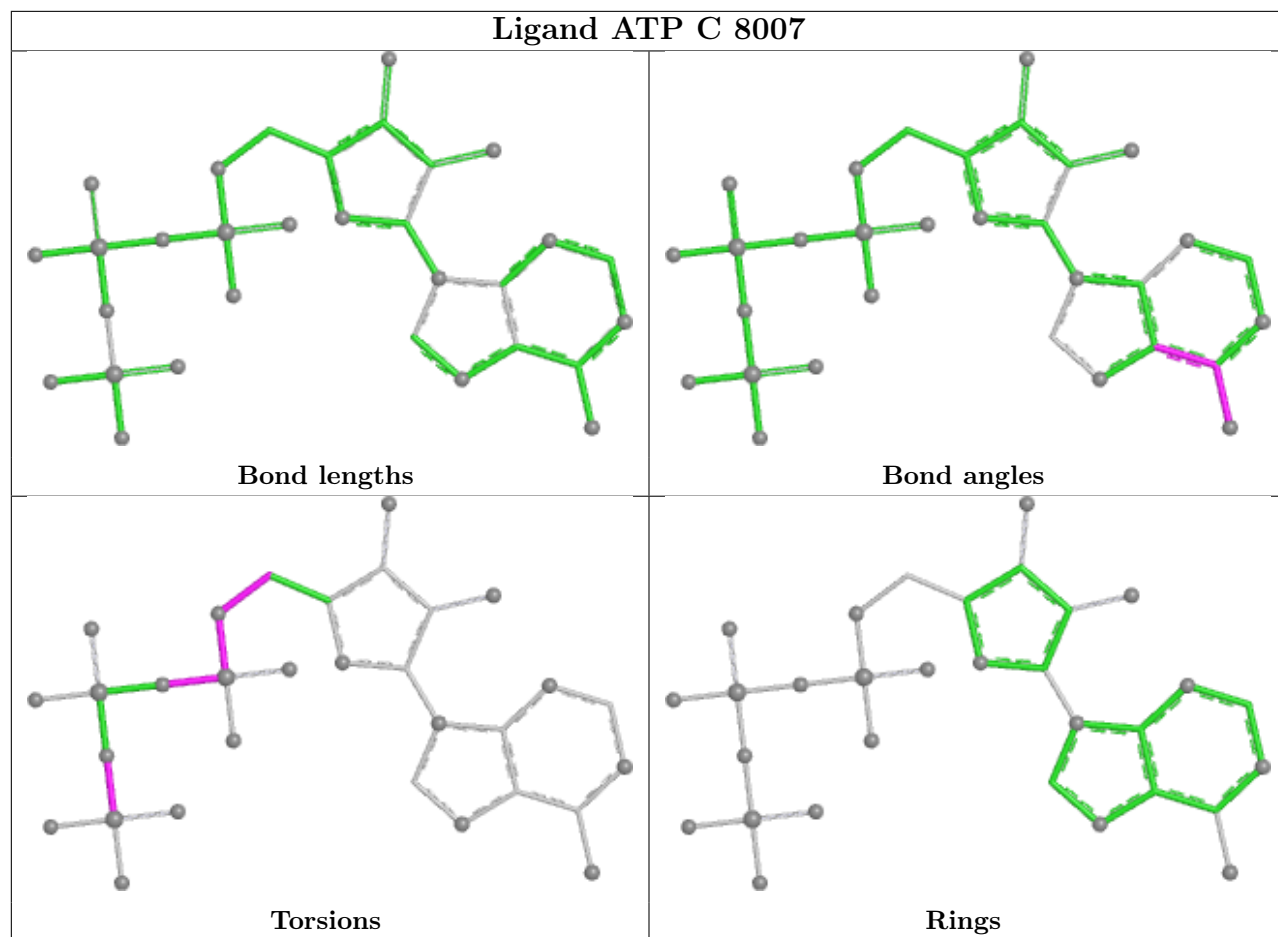


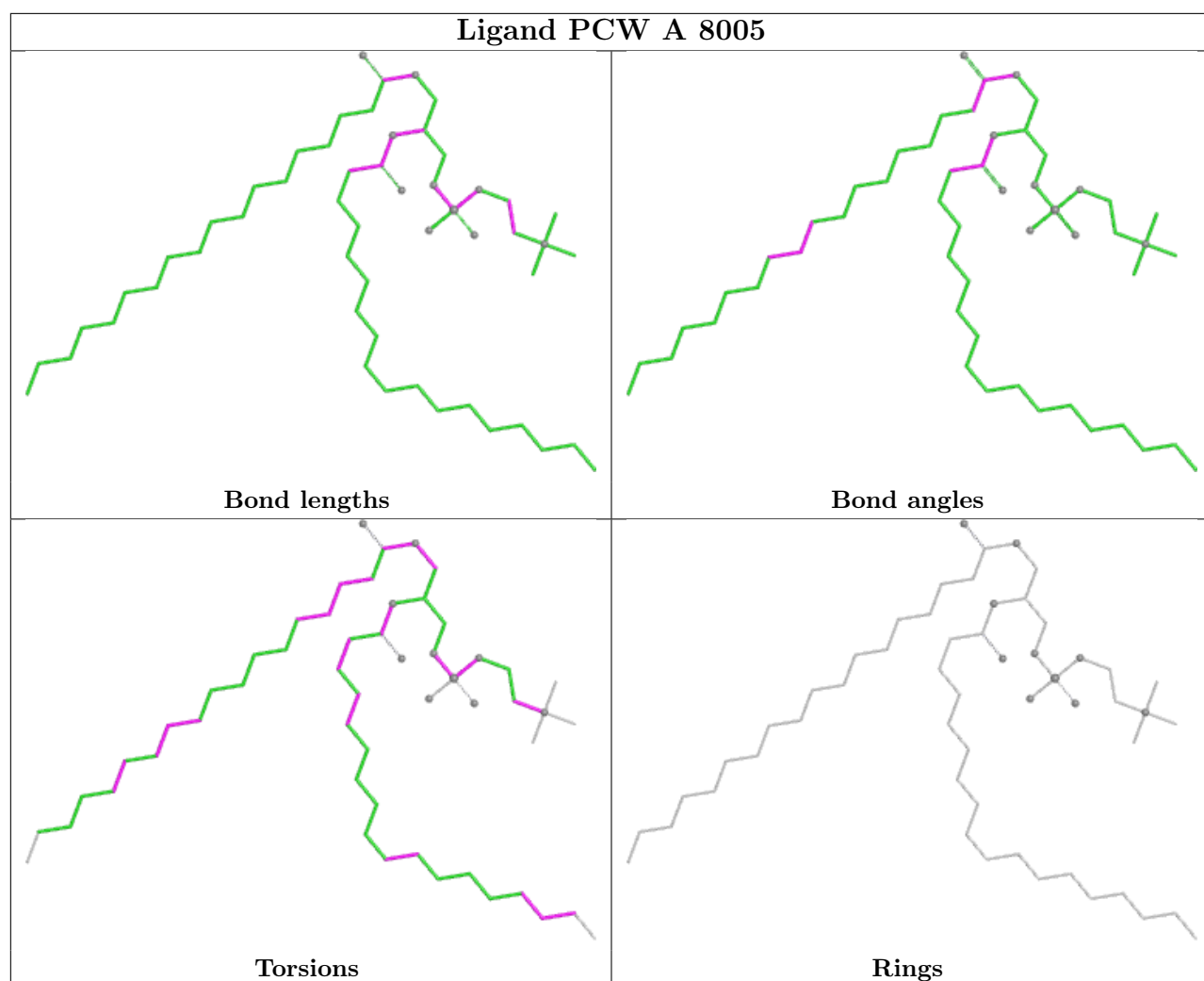
Ligand A1BYZ D 8009

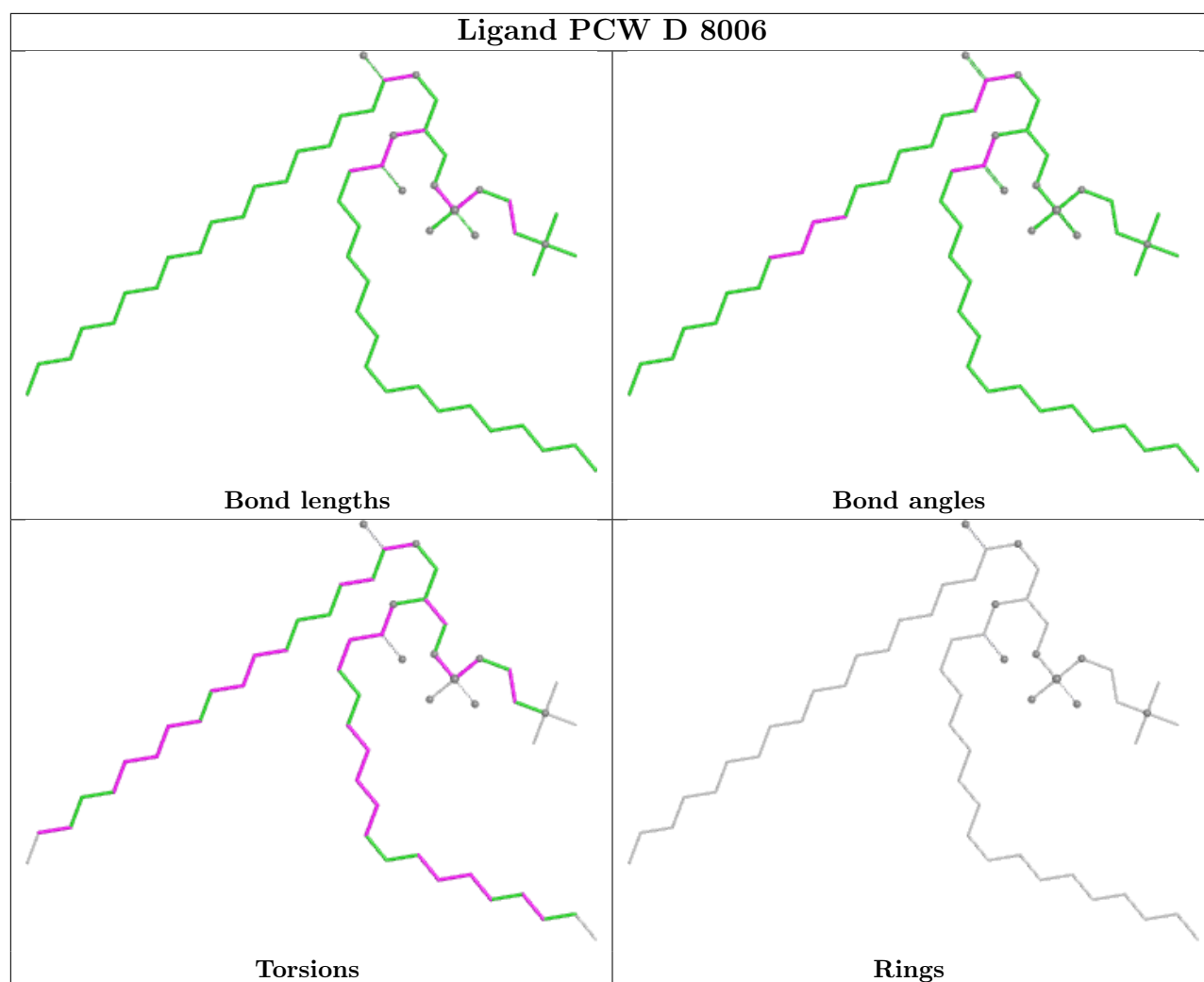












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

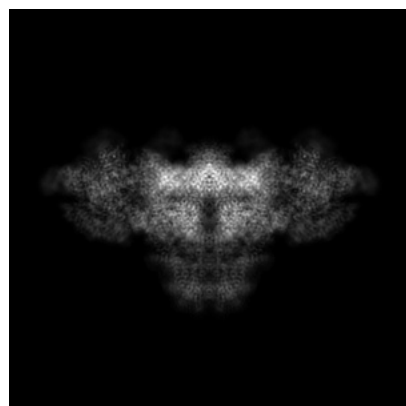
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49536. These allow visual inspection of the internal detail of the map and identification of artifacts.

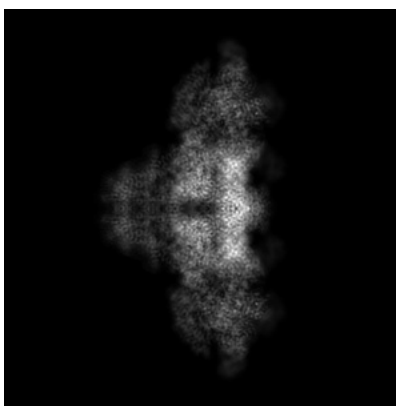
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

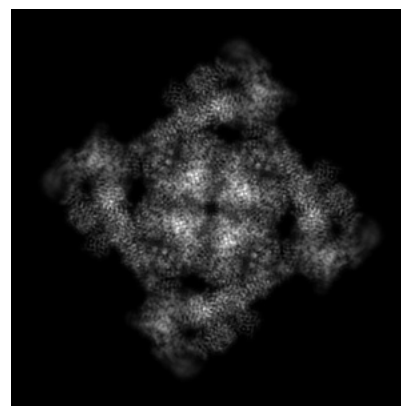
6.1.1 Primary map



X

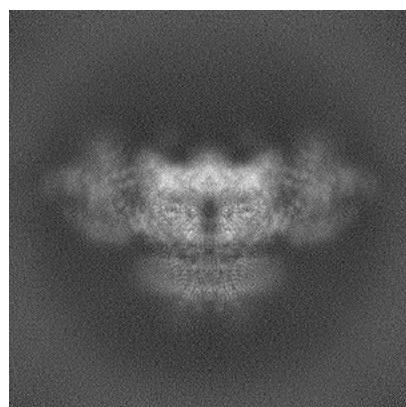


Y

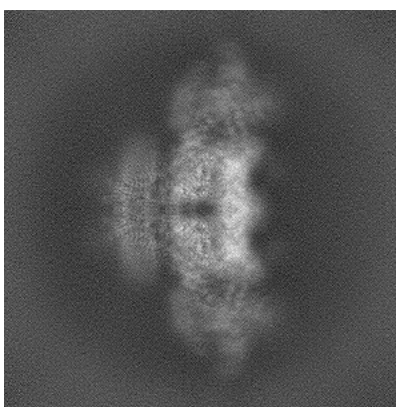


Z

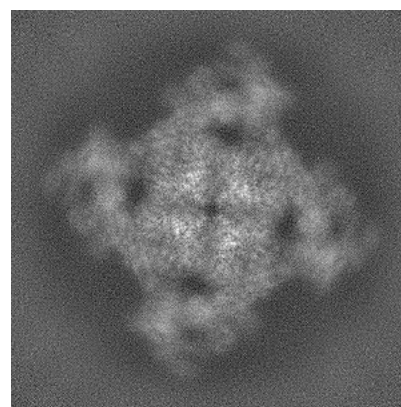
6.1.2 Raw map



X



Y



Z

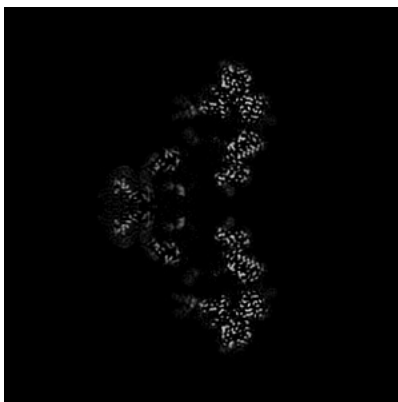
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

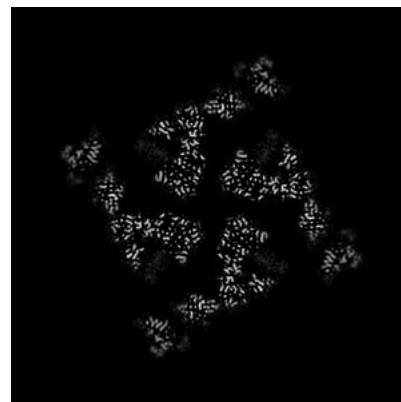
6.2.1 Primary map



X Index: 256



Y Index: 256

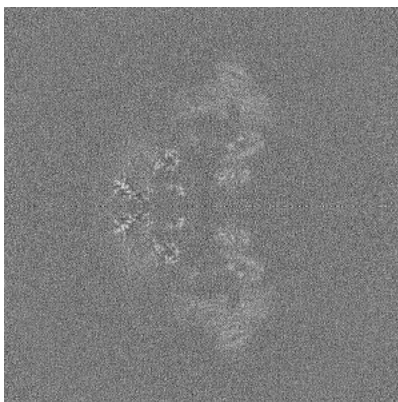


Z Index: 256

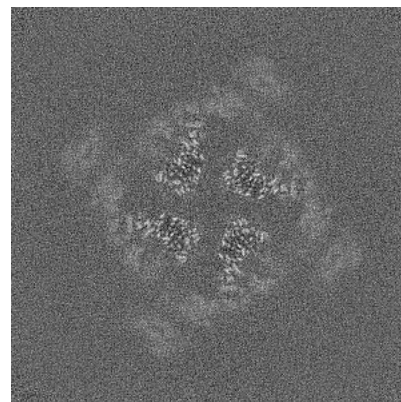
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

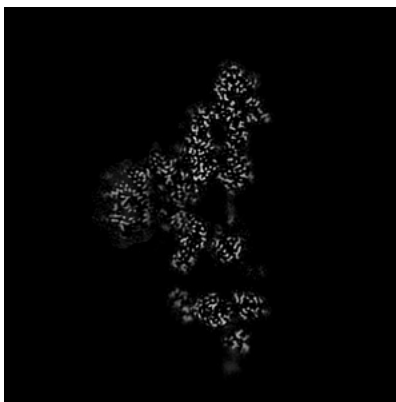
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

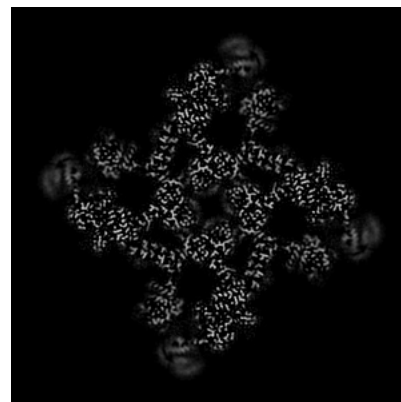
6.3.1 Primary map



X Index: 238

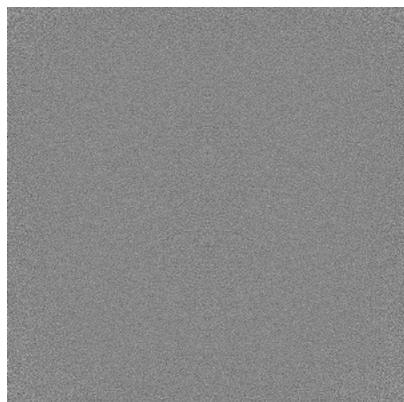


Y Index: 274

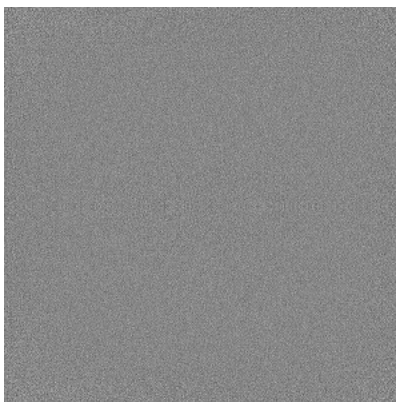


Z Index: 287

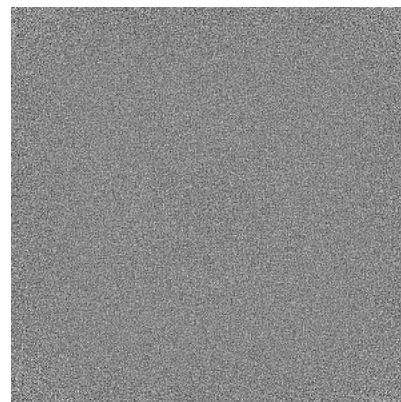
6.3.2 Raw map



X Index: 0



Y Index: 0

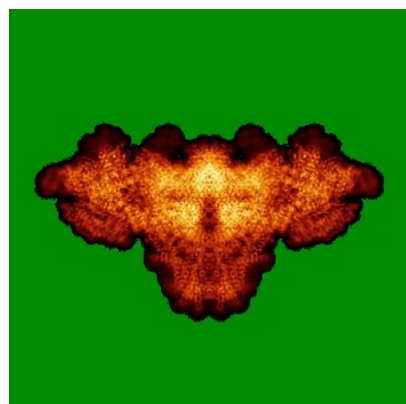


Z Index: 0

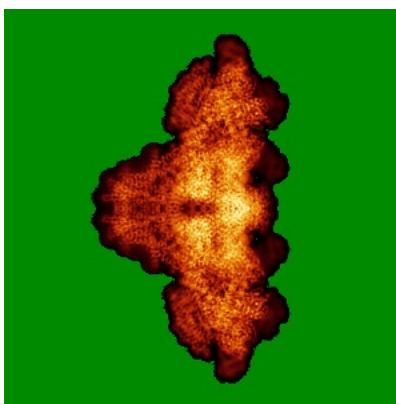
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

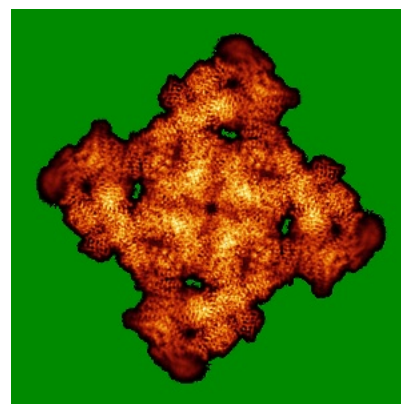
6.4.1 Primary map



X

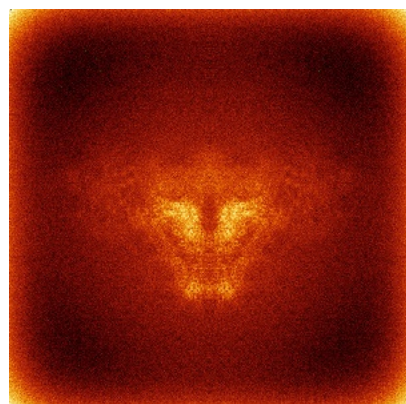


Y

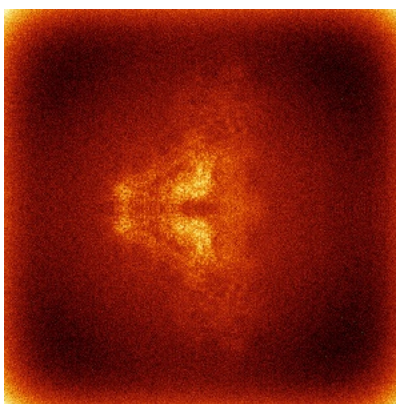


Z

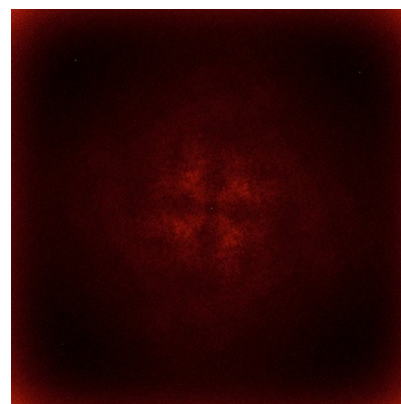
6.4.2 Raw map



X



Y

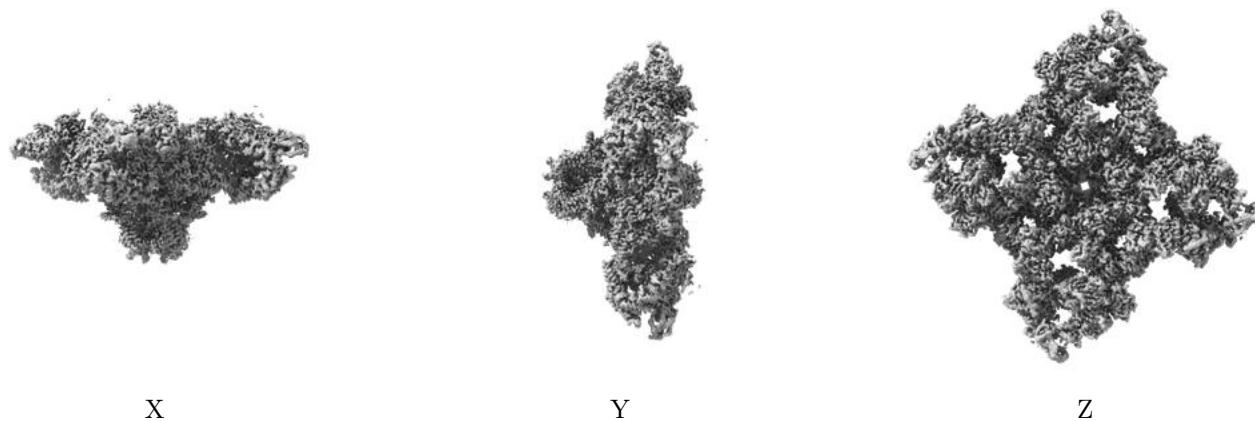


Z

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.

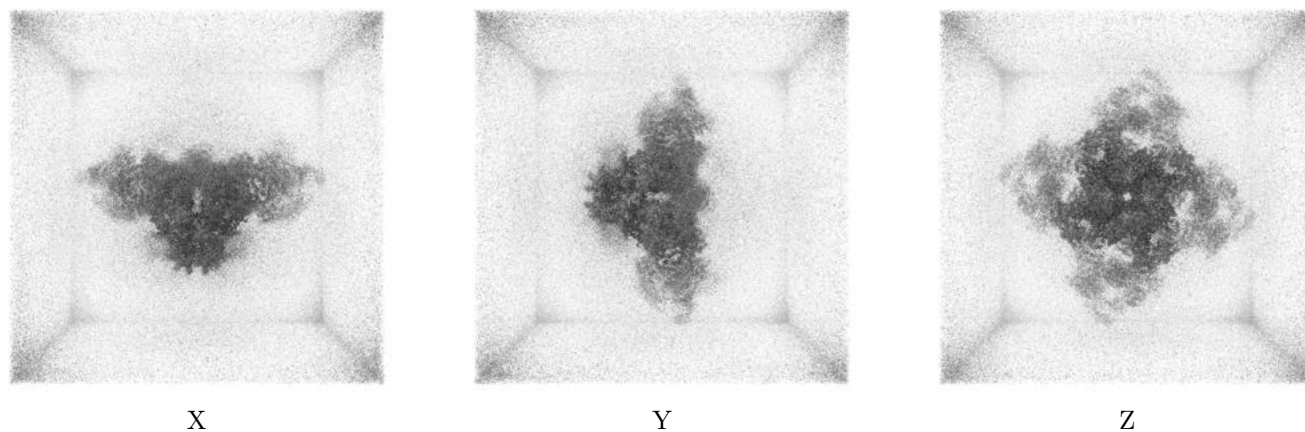
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

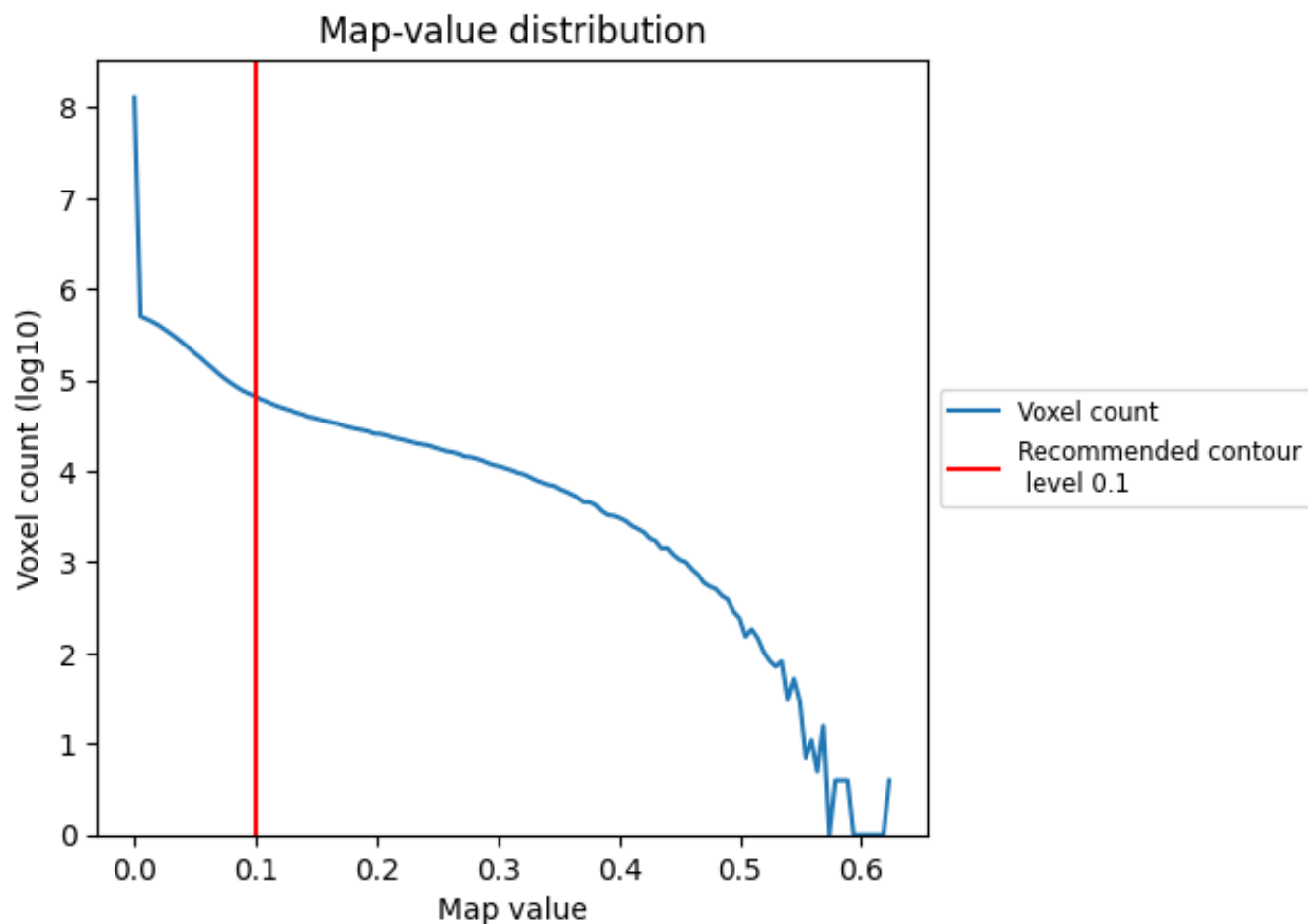
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

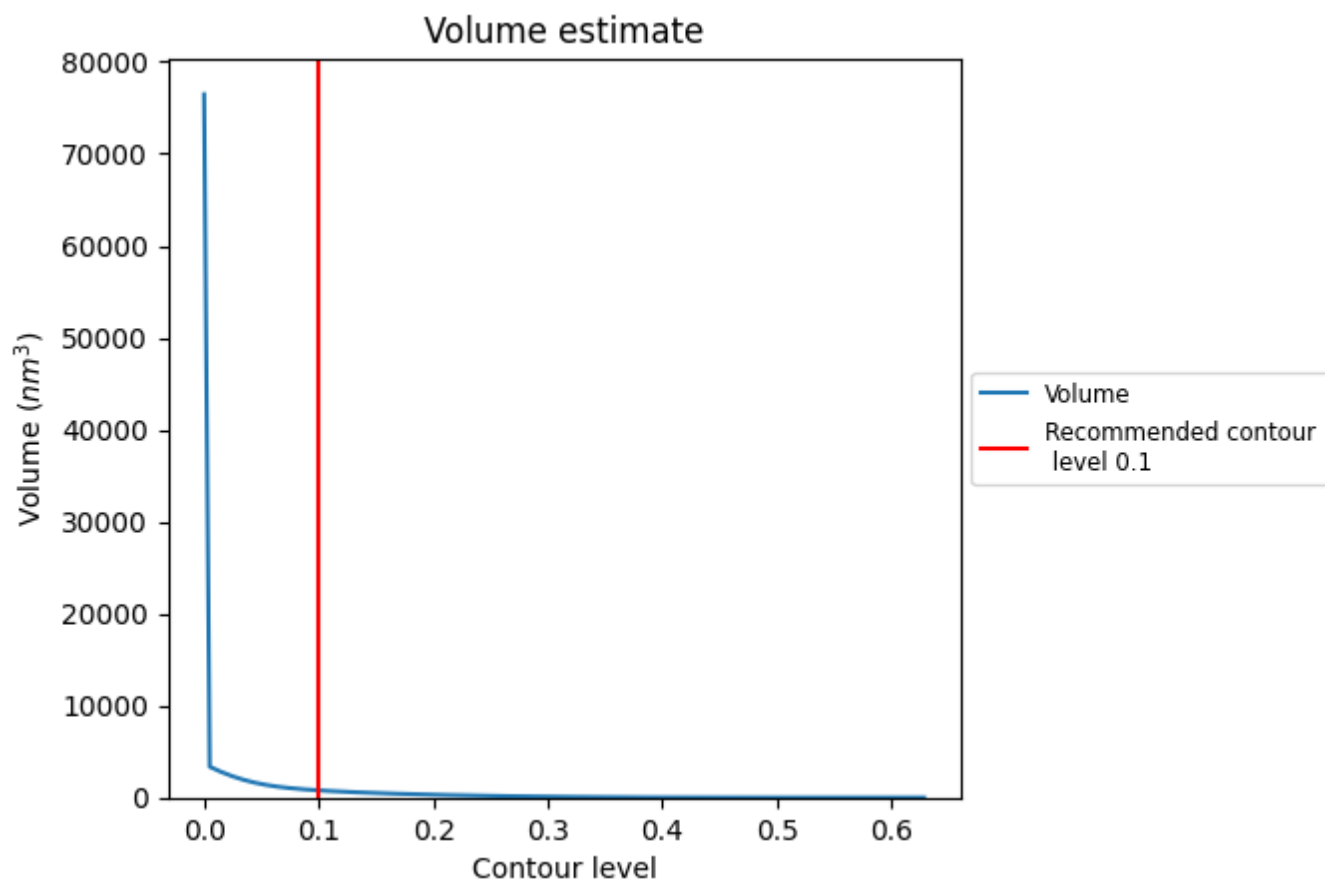
This section contains the results of statistical analysis of the map.

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.

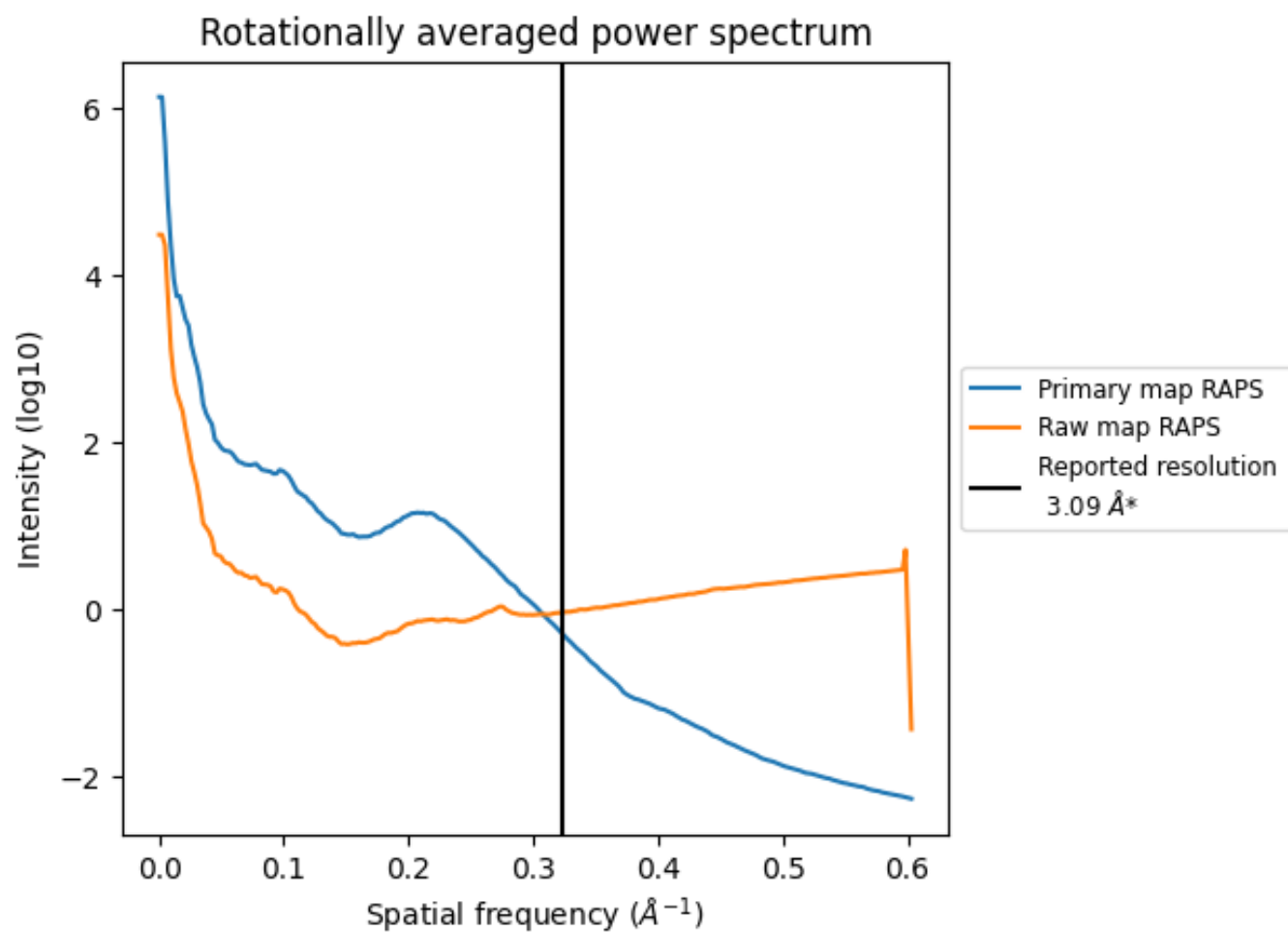
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 783 nm³; this corresponds to an approximate mass of 707 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 ⓘ

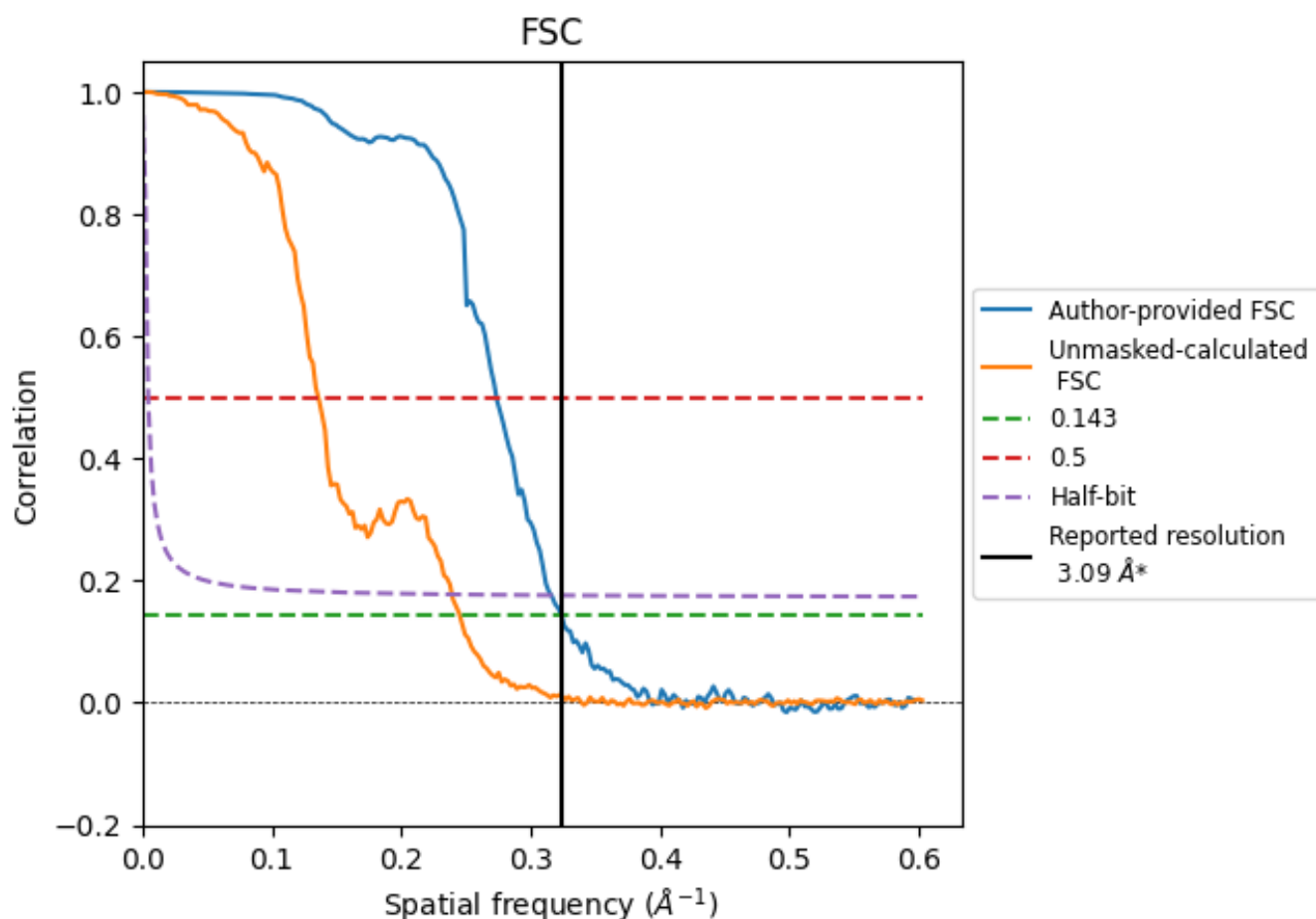


*Reported resolution corresponds to spatial frequency of 0.324 \AA^{-1}

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 0.324 \AA^{-1}

8.2 Resolution estimates [i](#)

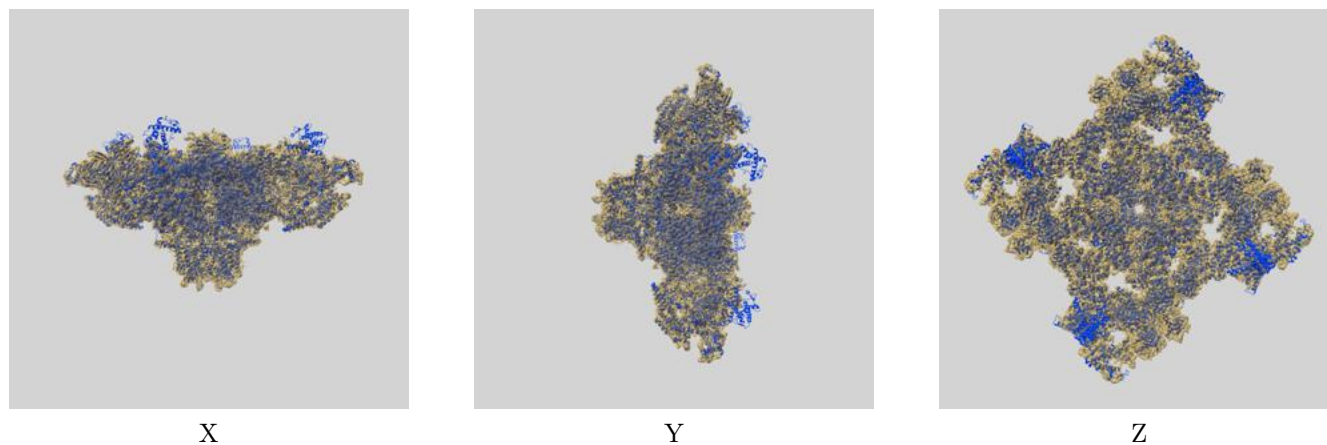
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	3.09	3.65	3.16
Unmasked-calculated*	4.08	7.35	4.18

*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 4.08 differs from the reported value 3.09 by more than 10 %

9 Map-model fit [i](#)

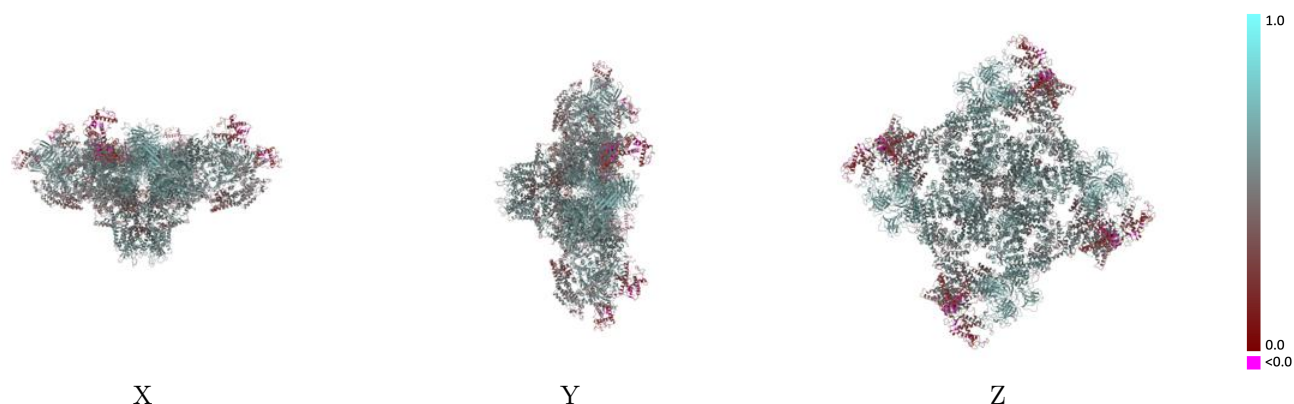
This section contains information regarding the fit between EMDB map EMD-49536 and PDB model 9NMP. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



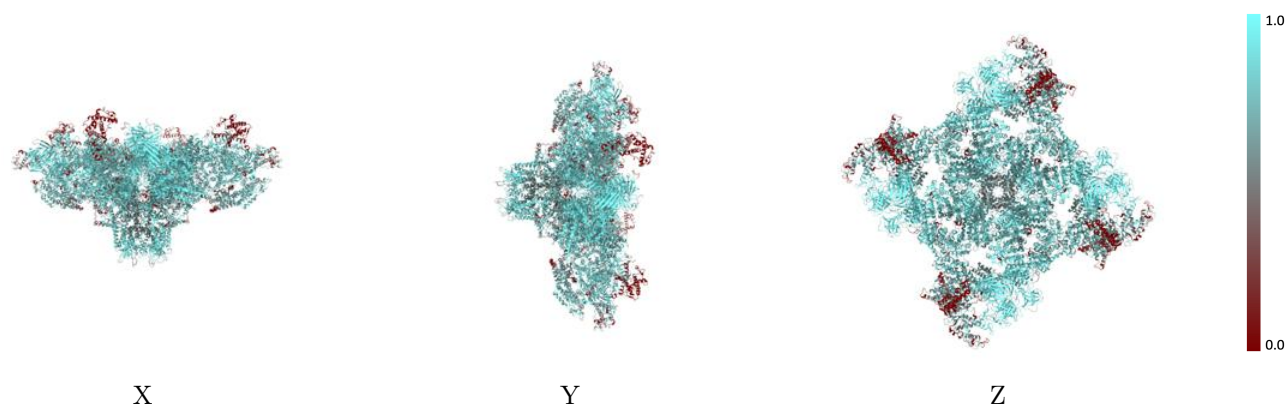
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



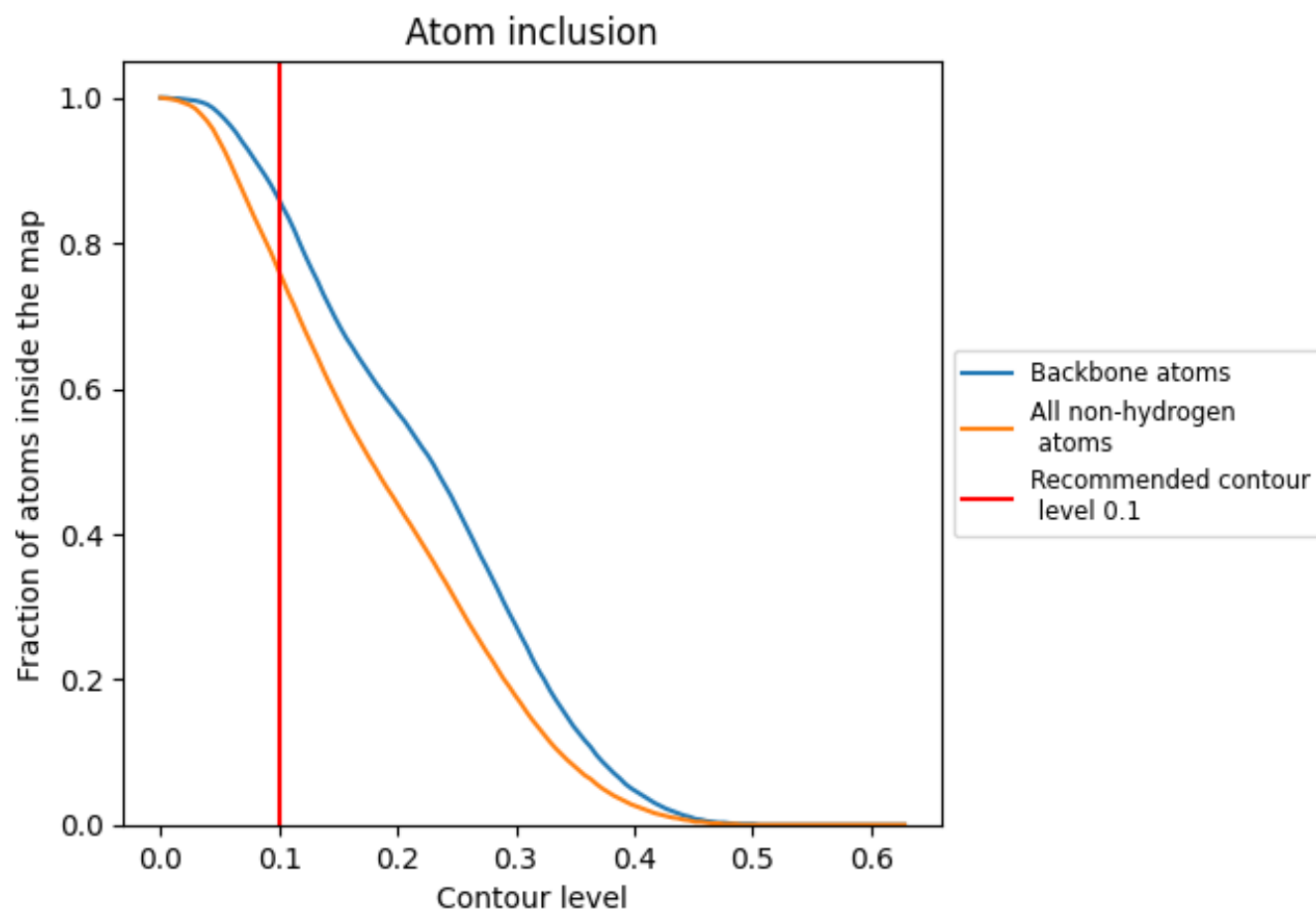
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 76% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.7610</div>	<div><div></div>0.5090</div>
A	<div><div></div>0.7600</div>	<div><div></div>0.5080</div>
B	<div><div></div>0.7580</div>	<div><div></div>0.5070</div>
C	<div><div></div>0.7580</div>	<div><div></div>0.5070</div>
D	<div><div></div>0.7580</div>	<div><div></div>0.5070</div>
E	<div><div></div>0.8810</div>	<div><div></div>0.5870</div>
F	<div><div></div>0.8840</div>	<div><div></div>0.5890</div>
G	<div><div></div>0.8770</div>	<div><div></div>0.5850</div>
H	<div><div></div>0.8840</div>	<div><div></div>0.5910</div>

1.0

0.0

<0.0