



Full wwPDB EM Validation Report ⓘ

Nov 12, 2025 – 01:34 PM EST

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

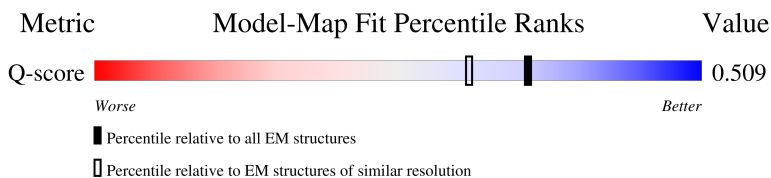
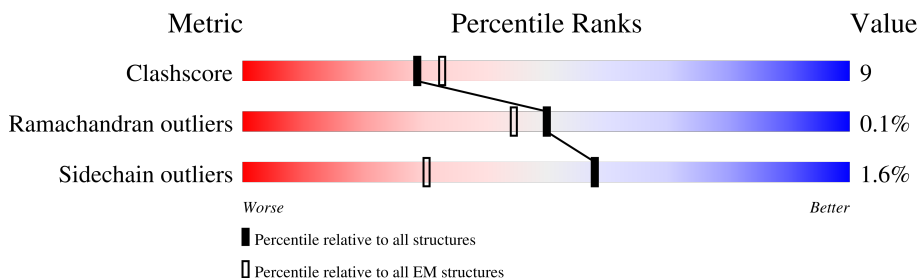
1 Overall quality at a glance

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		

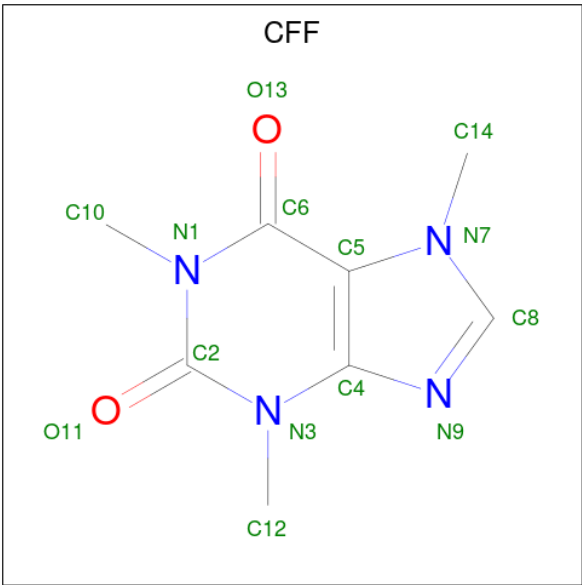
- Molecule 2 is a protein called Ryanodine receptor 1.

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).

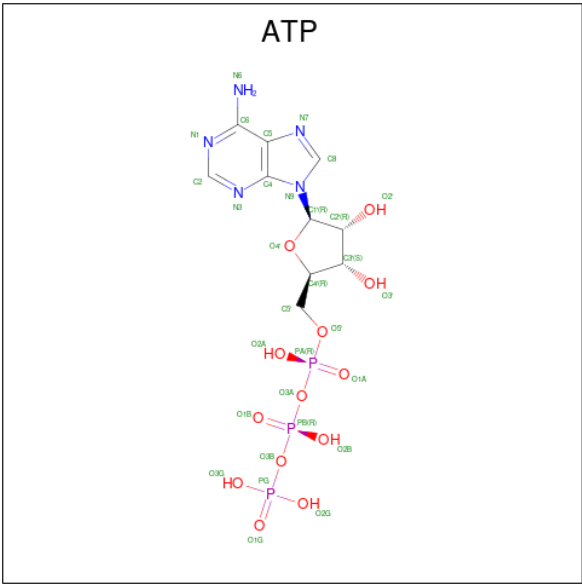
Mol	Chain	Residues	Atoms		AltConf
3	D	1	Total	Zn	0
			1	1	
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	

- 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).

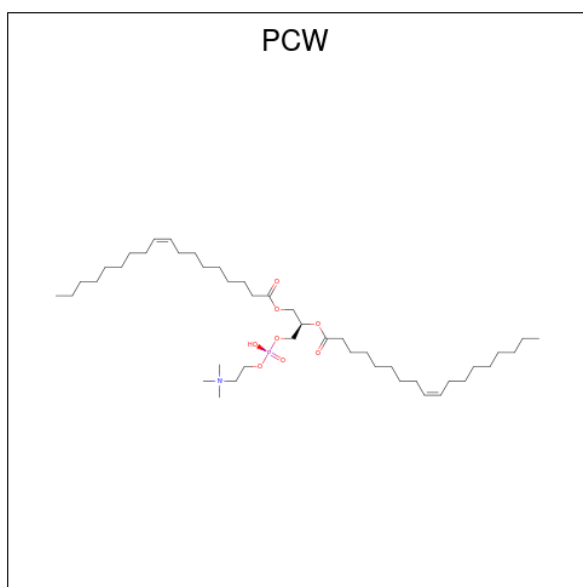


Mol	Chain	Residues	Atoms					AltConf
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10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

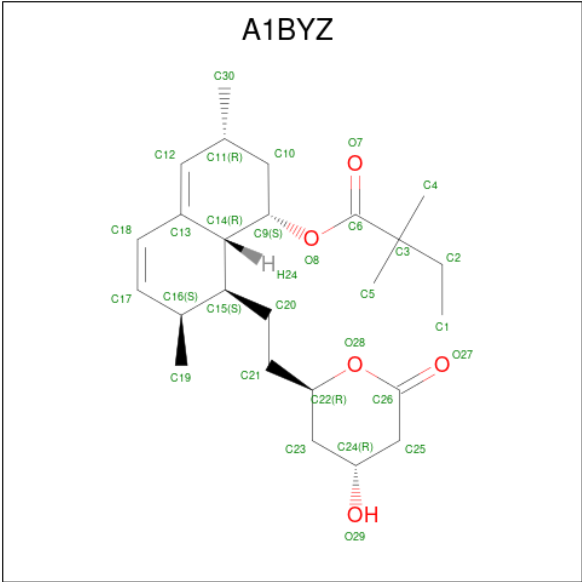
Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total	Ca	0
			1	1	
6	A	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	C	1	Total	Ca	0
			1	1	

- 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 Simvastatin (CCD ID: A1BYZ) (formula: $C_{25}H_{38}O_5$) (labeled as "Ligand of Interest" by depositor).




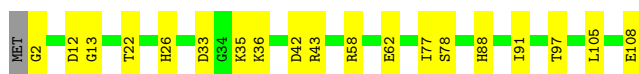
Mol	Chain	Residues	Atoms			AltConf
8	D	1	Total	C	O	0
			30	25	5	
8	D	1	Total	C	O	0
			30	25	5	
8	A	1	Total	C	O	0
			30	25	5	
8	A	1	Total	C	O	0
			30	25	5	
8	B	1	Total	C	O	0
			30	25	5	
8	B	1	Total	C	O	0
			30	25	5	
8	C	1	Total	C	O	0
			30	25	5	
8	C	1	Total	C	O	0
			30	25	5	

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: 




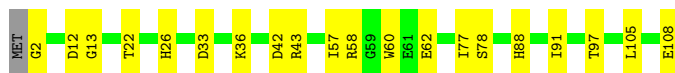
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F: 




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

Chain G: 



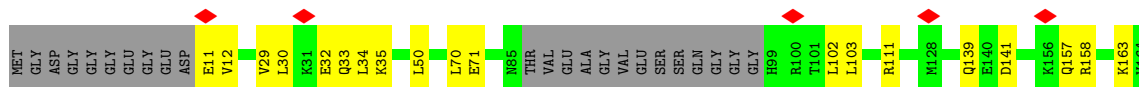
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain H: 



- Molecule 2: Ryanodine receptor 1

Chain D: 

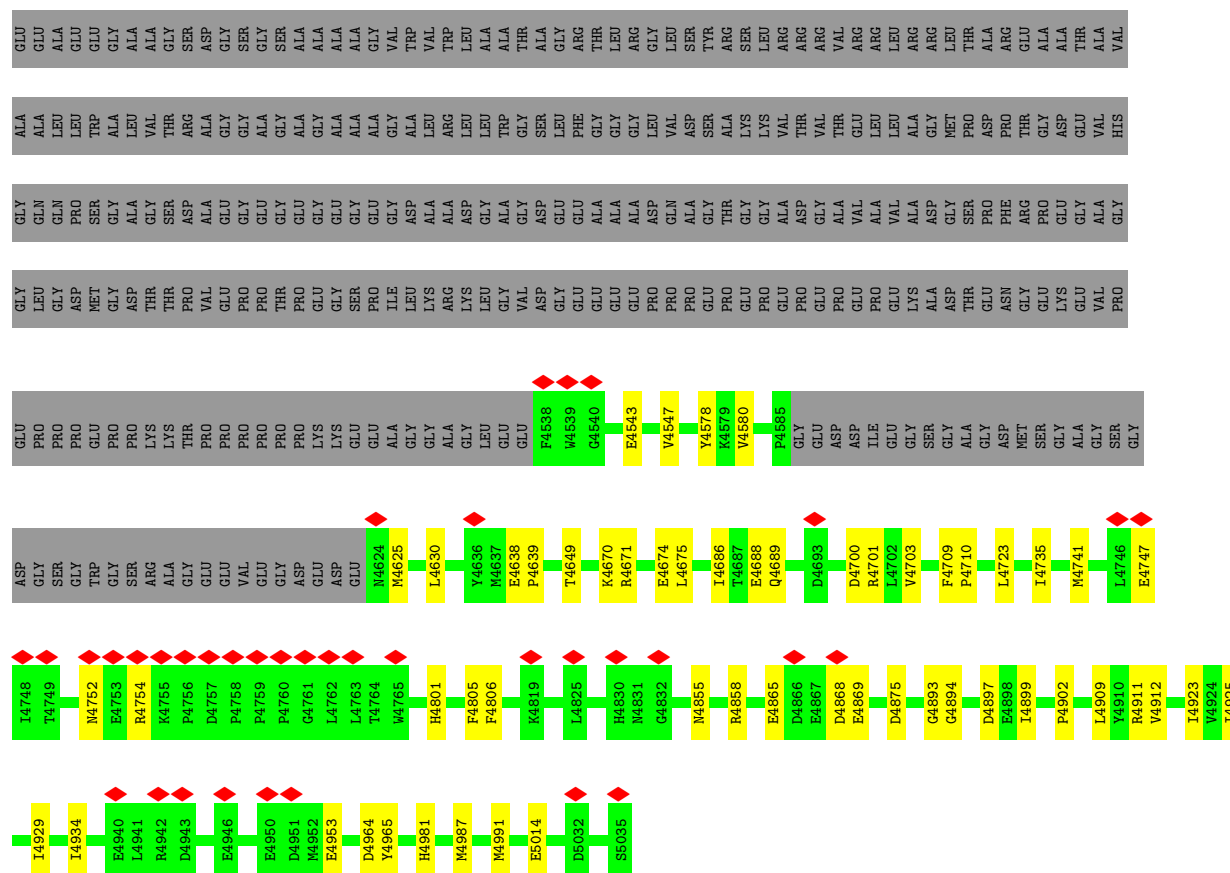




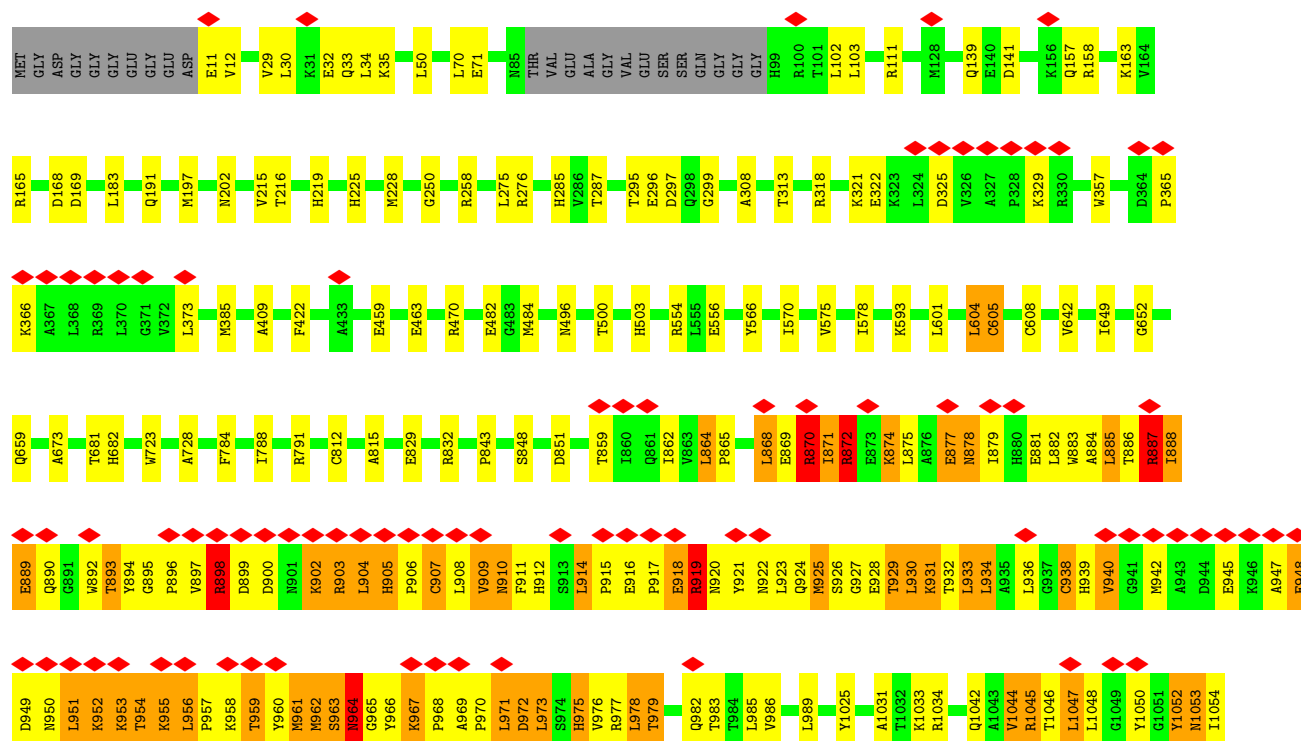




S4055	L3859	D3672	V3580	L3406	T3309	C3166	V3025	L2927	T2867	12747
S4056	G3860	E3683	F3581	L3409	S3310	L3170	L3026	L2928	L2868	12748
D4086	M3861	E3684	G3582	Y3410	D3311	G3177	G3027	K2929	W2808	P2749
F4087	N3862	Q3685	R3583	P3411	H3312	G3178	K3035	F2930	P2809	E2750
R4088	N3863	E3685	R3584	L3412	G3317	G3179	T3040	L2931	K2811	K2751
G4089	E3864	E3686	E3585	L3413	G3318	T3178	T3041	Q2932	E2812	L2752
L4090	E3865	E3687	E3586	L3414	N3319	T3179	T3041	M2933	K2813	D2753
D4095	D3865	E3688	E3587	R3415	R3322	N3181	V3055	N2934	E2814	S2754
F4096	T3867	E3689	A3587	E3434	I3323	N3182	S3056	G2935	K2815	F2755
M4100	V3868	E3690	D3588	L3435	I3324	Y3183	L3057	Y2936	A2816	L2756
E4122	V3691	V3591	Q3594	M3438	D3331	V3184	D3061	A2937	M2817	M2757
E4129	E3692	F3592	Q3595	V3439	G3337	L3195	A3062	V2938	L2818	K2758
M4133	E3693	I3593	T3598	G3440	K3337	L3198	P3063	T2939	A2819	F2759
N4133	L3711	R3595	S3509	F3443	V3341	L3198	D3077	R2940	W2820	A2760
I4142	T3712	R3596	L3515	L3444	P3203	M3202	R3079	G2941	E2821	E2761
D4160	E3713	V3597	M3518	Y3445	Q3344	P3203	T3080	L2942	W2822	Y2762
E3882	D3720	Q3598	N3524	W3446	V3204	V3220	V3081	K2943	T2823	T2763
I3884	H3735	V3603	M3525	S3449	V3347	R3226	M3082	D2944	W2824	H2764
C3895	L3736	L3607	T3529	K3453	L3354	R3226	K3083	M2945	E2825	E2765
E3896	E3737	T3610	D3530	R3454	L3355	L3230	I3088	E2946	K2826	K2766
F3902	G3612	H3612	Q3531	E3455	R3356	L3231	E3105	L2947	A2827	E2767
Y3940	T3613	T3613	D3532	E3456	S3357	E3237	R3106	D2948	R2828	A2768
K3943	Y3613	Y3613	L3533	N3463	I3360	E3238	M3107	T2949	E2829	F2769
D3944	Y3614	Y3614	L3534	E3464	P3361	E3239	V3108	K2892	K2890	D2770
V3945	Y3615	Y3615	L3535	T3465	L3366	E3240	N3109	K2893	E2831	K2771
K3962	Y3616	Y3616	L3536	N3466	V3373	C3241	N3110	Q2893	GLU	L2772
E3970	Y3617	Y3617	L3537	N3467	E3377	V3246	L3111	E2894	GLU	Q2773
Y3971	Y3618	Y3618	L3538	N3468	E3378	L3247	L3112	L2895	THR	W2774
I3972	Y3619	Y3619	L3539	N3469	Q3379	L3247	L3113	E2896	GLU	W2775
Q3973	Y3620	Y3620	L3540	F3470	E3379	M3267	GLY	A2897	LYS	W2776
G3974	Y3621	Y3621	L3541	L3471	L3380	P3268	LYS	Q2971	LYS	S2777
P3975	Y3622	Y3622	L3542	T3472	L3381	H3269	VAL	E2972	LYS	V2778
L3983	Y3623	Y3623	L3543	ALA	R3381	H3269	GLN	Q2973	THR	Y2779
F3989	Y3624	Y3624	L3544	ASP	R3382	H3269	ALA	E2974	ARG	G2780
K4005	Y3625	Y3625	L3545	LYS	R3383	H3269	ARG	E2975	LYS	E2781
D4009	Y3626	Y3626	L3546	LYS	E3384	H3269	THR	A2976	ILE	E2782
S4010	Y3627	Y3627	L3547	ASP	K3385	H3269	GLN	H2977	THR	D2783
L4019	Y3628	Y3628	L3548	LYS	A3386	H3269	VAL	E2978	ALA	E2784
D4021	Y3629	Y3629	L3549	LYS	A3387	H3269	VAL	E2979	GLN	E2785
ASP	Y3630	Y3630	L3550	LYS	E3388	H3269	VAL	E2980	THR	E2786
GLU	Y3631	Y3631	L3551	LYS	K3388	H3269	VAL	E2981	TYR	L2786
GLU	Y3632	Y3632	L3552	LYS	E3389	H3269	VAL	E2982	ASP	K2787
PRO	Y3633	Y3633	L3553	LYS	E3390	H3269	VAL	E2983	ARG	T2788
GLU	Y3634	Y3634	L3554	LYS	E3391	H3269	VAL	E2984	GLU	H2789
GLU	Y3635	Y3635	L3555	LYS	E3392	H3269	VAL	E2985	GLY	P2790
GLU	Y3636	Y3636	L3556	LYS	E3393	H3269	VAL	E2986	GLY	L2791
GLU	Y3637	Y3637	L3557	LYS	E3394	H3269	VAL	E2987	GLY	L2792
GLU	Y3638	Y3638	L3558	LYS	E3395	H3269	VAL	E2988	GLY	R2793
GLU	Y3639	Y3639	L3559	LYS	E3396	H3269	VAL	E2989	GLY	P2794
GLU	Y3640	Y3640	L3560	LYS	E3397	H3269	VAL	E2990	GLY	Y2795
GLU	Y3641	Y3641	L3561	LYS	E3398	H3269	VAL	E2991	GLY	K2796
GLU	Y3642	Y3642	L3562	LYS	E3399	H3269	VAL	E2992	GLY	T2797
GLU	Y3643	Y3643	L3563	LYS	E3400	H3269	VAL	E2993	GLY	F2798
GLU	Y3644	Y3644	L3564	LYS	E3401	H3269	VAL	E2994	GLY	S2799
GLU	Y3645	Y3645	L3565	LYS	E3402	H3269	VAL	E2995	GLY	E2800
GLU	Y3646	Y3646	L3566	LYS	E3403	H3269	VAL	E2996	GLY	K2801
GLU	Y3647	Y3647	L3567	LYS	E3404	H3269	VAL	E2997	GLY	D2802
GLU	Y3648	Y3648	L3568	LYS	E3405	H3269	VAL	E2998	GLY	K2803
GLU	Y3649	Y3649	L3569	LYS	E3406	H3269	VAL	E2999	GLY	E2804
GLU	Y3650	Y3650	L3570	LYS	E3407	H3269	VAL	E3000	GLY	Y2805
GLU	Y3651	Y3651	L3571	LYS	E3408	H3269	VAL	E3001	GLY	Y2806
GLU	Y3652	Y3652	L3572	LYS	E3409	H3269	VAL	E3002	GLY	Y2807
GLU	Y3653	Y3653	L3573	LYS	E3410	H3269	VAL	E3003	GLY	Y2808
GLU	Y3654	Y3654	L3574	LYS	E3411	H3269	VAL	E3004	GLY	Y2809
GLU	Y3655	Y3655	L3575	LYS	E3412	H3269	VAL	E3005	GLY	Y2810
GLU	Y3656	Y3656	L3576	LYS	E3413	H3269	VAL	E3006	GLY	Y2811
GLU	Y3657	Y3657	L3577	LYS	E3414	H3269	VAL	E3007	GLY	Y2812
GLU	Y3658	Y3658	L3578	LYS	E3415	H3269	VAL	E3008	GLY	Y2813
GLU	Y3659	Y3659	L3579	LYS	E3416	H3269	VAL	E3009	GLY	Y2814
GLU	Y3660	Y3660	L3580	LYS	E3417	H3269	VAL	E3010	GLY	Y2815
GLU	Y3661	Y3661	L3581	LYS	E3418	H3269	VAL	E3011	GLY	Y2816
GLU	Y3662	Y3662	L3582	LYS	E3419	H3269	VAL	E3012	GLY	Y2817
GLU	Y3663	Y3663	L3583	LYS	E3420	H3269	VAL	E3013	GLY	Y2818
GLU	Y3664	Y3664	L3584	LYS	E3421	H3269	VAL	E3014	GLY	Y2819
GLU	Y3665	Y3665	L3585	LYS	E3422	H3269	VAL	E3015	GLY	Y2820
GLU	Y3666	Y3666	L3586	LYS	E3423	H3269	VAL	E3016	GLY	Y2821
GLU	Y3667	Y3667	L3587	LYS	E3424	H3269	VAL	E3017	GLY	Y2822
GLU	Y3668	Y3668	L3588	LYS	E3425	H3269	VAL	E3018	GLY	Y2823
GLU	Y3669	Y3669	L3589	LYS	E3426	H3269	VAL	E3019	GLY	Y2824
GLU	Y3670	Y3670	L3590	LYS	E3427	H3269	VAL	E3020	GLY	Y2825
GLU	Y3671	Y3671	L3591	LYS	E3428	H3269	VAL	E3021	GLY	Y2826
GLU	Y3672	Y3672	L3592	LYS	E3429	H3269	VAL	E3022	GLY	Y2827
GLU	Y3673	Y3673	L3593	LYS	E3430	H3269	VAL	E3023	GLY	Y2828
GLU	Y3674	Y3674	L3594	LYS	E3431	H3269	VAL	E3024	GLY	Y2829
GLU	Y3675	Y3675	L3595	LYS	E3432	H3269	VAL	E3025	GLY	Y2830
GLU	Y3676	Y3676	L3596	LYS	E3433	H3269	VAL	E3026	GLY	Y2831
GLU	Y3677	Y3677	L3597	LYS	E3434	H3269	VAL	E3027	GLY	Y2832
GLU	Y3678	Y3678	L3598	LYS	E3435	H3269	VAL	E3028	GLY	Y2833
GLU	Y3679	Y3679	L3599	LYS	E3436	H3269	VAL	E3029	GLY	Y2834
GLU	Y3680	Y3680	L3600	LYS	E3437	H3269	VAL	E3030	GLY	Y2835
GLU	Y3681	Y3681	L3601	LYS	E3438	H3269	VAL	E3031	GLY	Y2836
GLU	Y3682	Y3682	L3602	LYS	E3439	H3269	VAL	E3032	GLY	Y2837
GLU	Y3683	Y3683	L3603	LYS	E3440	H3269	VAL	E3033	GLY	Y2838
GLU	Y3684	Y3684	L3604	LYS	E3441	H3269	VAL	E3034	GLY	Y2839
GLU	Y3685	Y3685	L3605	LYS	E3442	H3269	VAL	E3035	GLY	Y2840
GLU	Y3686	Y3686	L3606	LYS	E3443	H3269	VAL	E3036	GLY	Y2841
GLU	Y3687	Y3687	L3607	LYS	E3444	H3269	VAL	E3037	GLY	Y2842
GLU	Y3688	Y3688	L3608	LYS	E3445	H3269	VAL	E3038	GLY	Y2843
GLU	Y3689	Y3689	L3609	LYS	E3446	H3269	VAL	E3039	GLY	Y2844
GLU	Y3690	Y3690	L3610	LYS	E3447	H3269	VAL	E3040	GLY	Y2845
GLU	Y3691	Y3691	L3611	LYS	E3448	H3269	VAL	E3041	GLY	Y2846
GLU	Y3692	Y3692	L3612	LYS	E3449	H3269	VAL	E3042	GLY	Y2847
GLU	Y3693	Y3693	L3613	LYS	E3450	H3269	VAL	E3043	GLY	Y2848
GLU	Y3694	Y3694	L3614	LYS	E3451	H3269	VAL	E3044	GLY	Y2849
GLU	Y3695	Y3695	L3615	LYS	E3452	H3269	VAL	E3045	GLY	Y2850
GLU	Y3696	Y3696	L3616	LYS	E3453	H3269	VAL	E3046	GLY	Y2851
GLU	Y3697	Y3697	L3617	LYS	E3454	H3269	VAL	E3047	GLY	Y2852
GLU	Y3698	Y3698	L3618	LYS	E3455	H3269	VAL	E3048	GLY	Y2853
GLU	Y3699	Y3699	L3619	LYS	E3456	H3269	VAL	E3049	GLY	Y2854
GLU	Y3700	Y3700	L3620	LYS	E3457	H3269	VAL	E3050	GLY	Y2855
GLU	Y3701	Y3701	L3621	LYS	E3458	H3269	VAL	E3051	GLY	Y2856
GLU	Y3702	Y3702	L3622	LYS	E3459	H3269	VAL	E3052	GLY	Y2857
GLU	Y3703	Y3703	L3623	LYS	E3460	H3269	VAL	E3053	GLY	Y2858
GLU	Y3704	Y3704	L3624	LYS	E3461	H3269	VAL	E3054	GLY	Y2859
GLU	Y3705	Y3705	L3625	LYS	E3462	H3269	VAL	E3055	GLY	Y2860
GLU	Y3706	Y3706	L3626	LYS	E3463	H3269	VAL	E3056	GLY	Y2861
GLU	Y3707	Y3707	L3627	LYS	E3464	H3269	VAL	E3057	GLY	Y2862
GLU	Y3708	Y3708	L3628	LYS	E3465	H3269	VAL	E3058	GLY	Y2863
GLU	Y3709	Y3709	L3629	LYS	E3466	H3269	VAL	E3059	GLY	Y2864
GLU	Y3710	Y3710	L3630	LYS	E3467	H3269	VAL	E3060	GLY	Y2865
GLU	Y3711	Y3711	L3631	LYS	E3468	H3269	VAL	E3061	GLY	Y2866
GLU	Y3712	Y3712	L3632	LYS	E3469	H3269	VAL	E3062	GLY	Y2867
GLU	Y3713	Y3713	L3633	LYS	E3470	H3269	VAL	E3063	GLY	Y2868
GLU	Y3714	Y3714	L3634	LYS	E3471	H3269	VAL	E3064	GLY	Y2869
GLU	Y3715	Y3								

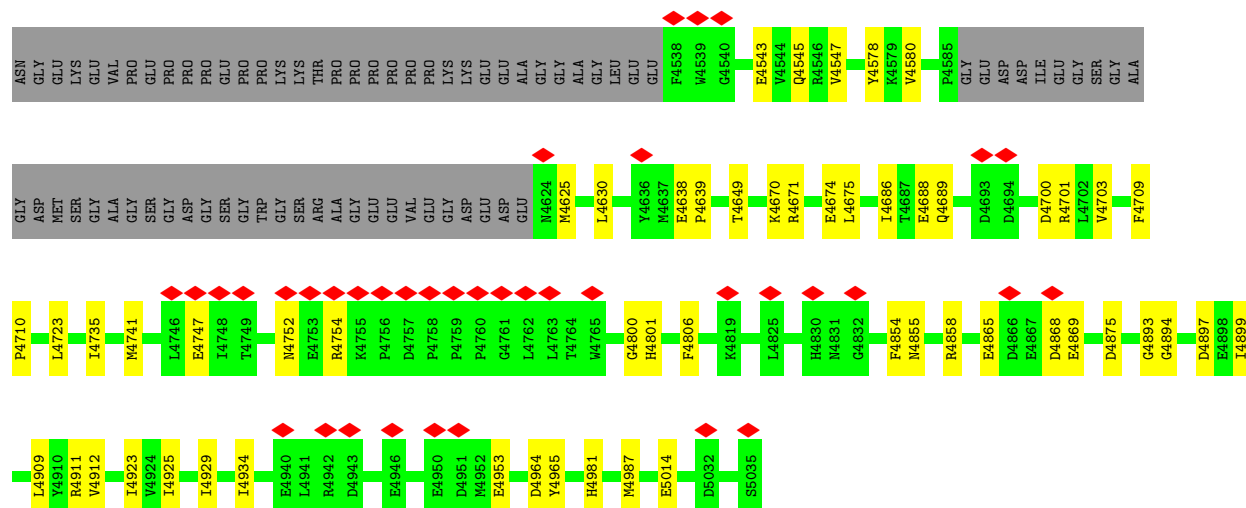


• Molecule 2: Ryanodine receptor 1

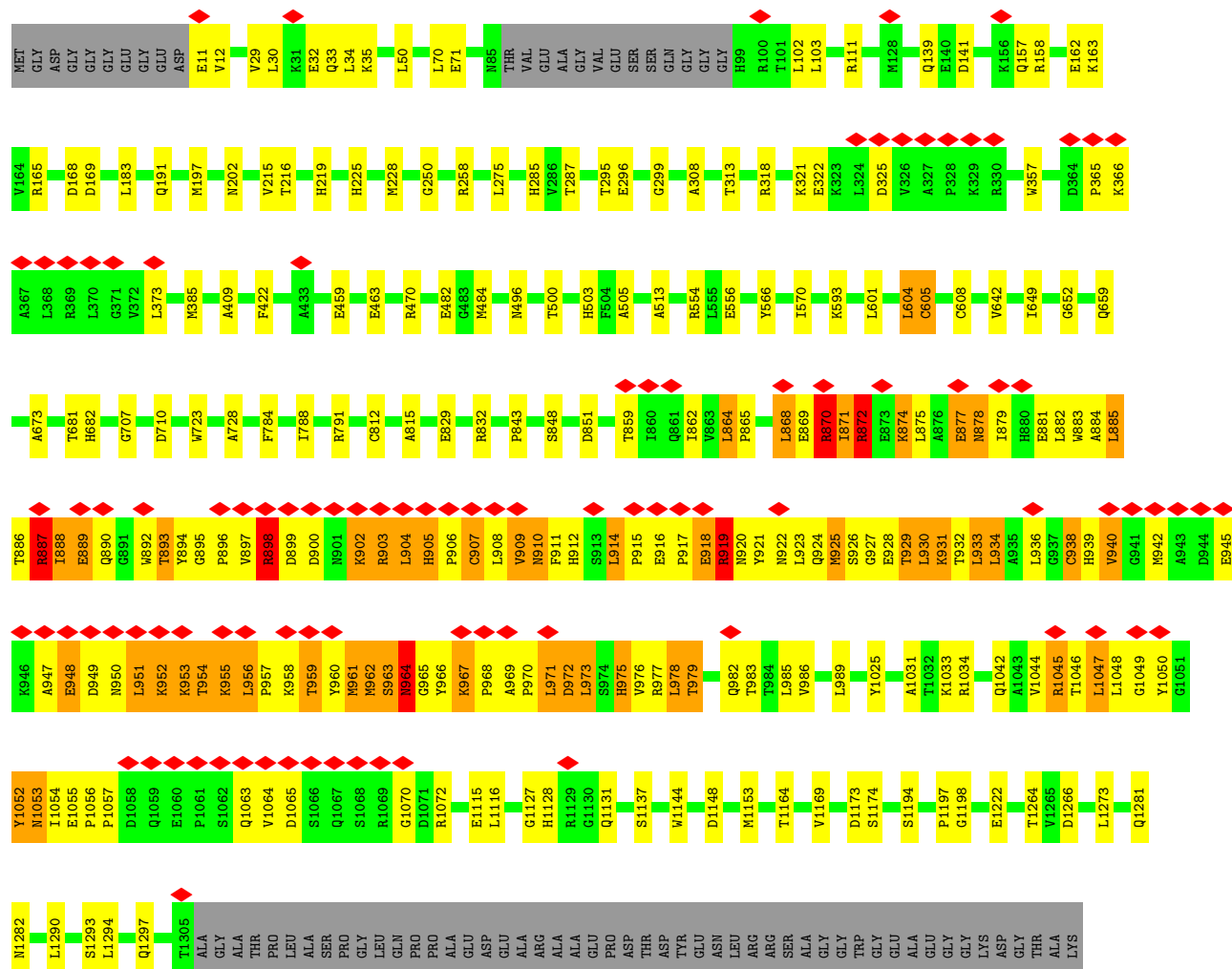


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D2802	K2803	E2804	L2805	Y2806	L2807	L2808	P2809	L2810	K2811	E2812	S2813	L2814	K2815	A2816	M2817	L2818	A2819	W2820	E2821	W2822	T2823	V2824	E2825	K2826	A2827	R2828	E2829	G2830	E2831	GLU	GLU	LYS	THR	GLU	LYS	LYS	THR	ARG	LYS	LYS	ILE	SER	GLN	THR	ALA	GLN	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	K2801																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
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																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
K2228	M2229	C2233	C2234	R2235	F2236	L2237	C2238	F2239	F2240	C2241	R2249	S2250	M2251	H2254	L2255	S2256	Y2257	L2258	L2259	E2260	N2261	S2262	G2263	T2264	L2266	Q2267	M2268	Q2269	S2270	S2271	T2272	L2282	D2283	N2284	V2285	E2286	K2298	L2314	Y2319	C2327	D2334	R2337	V2342																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
R2370	G2371	E2372	E2382	E2383	R2386	D2394	V2398	ARG	ASP	ARG	ARG	GLU	HIS	PHE	GLY	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																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
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																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
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	K2801																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
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	THR	ARG	LYS	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	THR	ASP	PRO	ARG	GLU	GLY	Y2856	N2857	P2858	Q2859	P2860	P2861																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
Q1281	N1282	L1290	S1293	L1294	Q1297	T1305	ALA	GLY	ALA	THR	GLN	PRO	LEU	ALA	SER	PRO	GLY	LEU	GLN	PRO	PRO	ALA	ASP	LYS	LYS	ARG	ALA	ALA	TYR	ASN	LEU	ARG	ALA	MET	GLU	THR	GLY	TRP	PRO	PRO	GLU	ALA	GLY	GLY	LYS	ASP	GLY	PRO	THR	ALA																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
ASP	VAL	VAL	PRO	ALA	D1420	R1422	P1425	E1426	I1427	I1428	L1429	D1466	L1467	K1468	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																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
E1742	R1753	S1754	A1755	D1756	E1757	G1758	P1759	P1781	P1782	C1783	F1784	V1785	A1790	A1791	G1792	A1793	T1794	E1795	V1821	E1876	GLU	GLU	VAL	GLU	GLU	GLY	GLY	GLU	GLU	GLU	GLU	ASP	GLU	GLU	GLY	LYS	GLU	ASP	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU



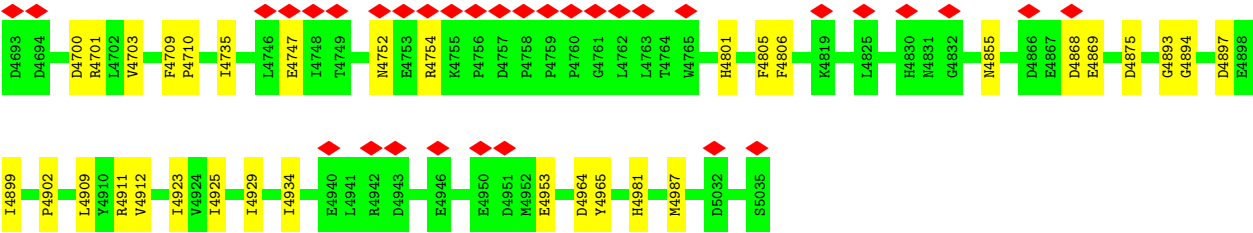


• Molecule 2: Ryanodine receptor 1









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: CA, PCW, CFF, ATP, A1BYZ, ZN

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	A1BYZ	C	8009	-	-	4/18/59/59	0/3/3/3
5	ATP	B	8007	-	-	8/18/38/38	0/3/3/3
5	ATP	D	8007	-	-	8/18/38/38	0/3/3/3
8	A1BYZ	C	8008	-	-	3/18/59/59	0/3/3/3
7	PCW	B	8005	-	-	25/57/57/57	-
8	A1BYZ	B	8009	-	-	4/18/59/59	0/3/3/3
4	CFF	A	8002	-	-	-	0/2/2/2
8	A1BYZ	D	8009	-	-	4/18/59/59	0/3/3/3
7	PCW	B	8006	-	-	29/57/57/57	-
8	A1BYZ	A	8009	-	-	4/18/59/59	0/3/3/3
5	ATP	A	8007	-	-	8/18/38/38	0/3/3/3
5	ATP	C	8007	-	-	8/18/38/38	0/3/3/3
4	CFF	D	8002	-	-	-	0/2/2/2
7	PCW	D	8006	-	-	29/57/57/57	-
7	PCW	A	8005	-	-	25/57/57/57	-
5	ATP	B	8003	-	-	9/18/38/38	0/3/3/3
5	ATP	C	8003	-	-	9/18/38/38	0/3/3/3
8	A1BYZ	A	8008	-	-	3/18/59/59	0/3/3/3
8	A1BYZ	B	8008	-	-	3/18/59/59	0/3/3/3
7	PCW	C	8006	-	-	29/57/57/57	-
5	ATP	D	8003	-	-	9/18/38/38	0/3/3/3
7	PCW	D	8005	-	-	25/57/57/57	-
8	A1BYZ	D	8008	-	-	3/18/59/59	0/3/3/3
5	ATP	A	8003	-	-	9/18/38/38	0/3/3/3
7	PCW	C	8005	-	-	25/57/57/57	-
4	CFF	B	8002	-	-	-	0/2/2/2
7	PCW	A	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
8	C	8009	A1BYZ	2	0
8	C	8008	A1BYZ	1	0

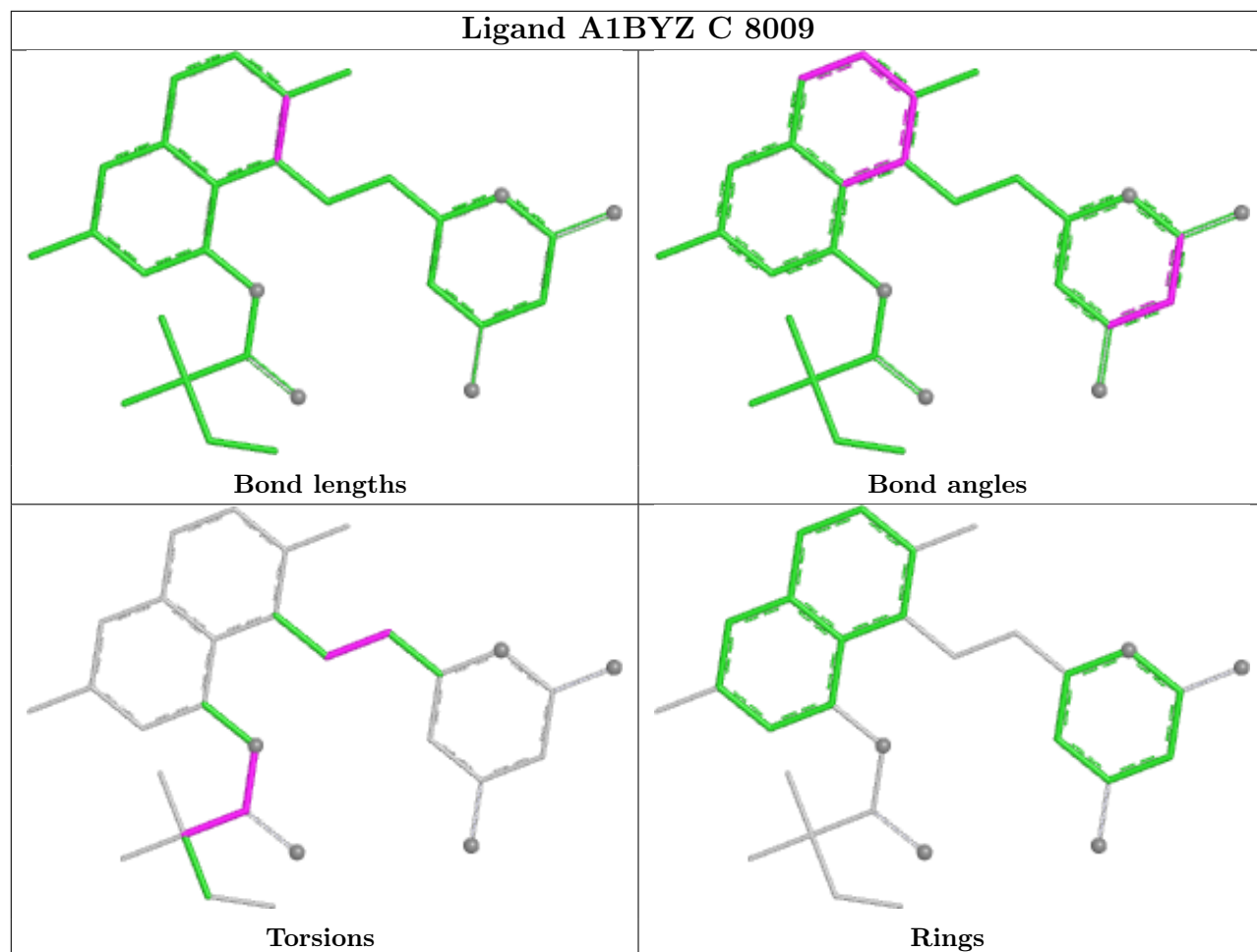
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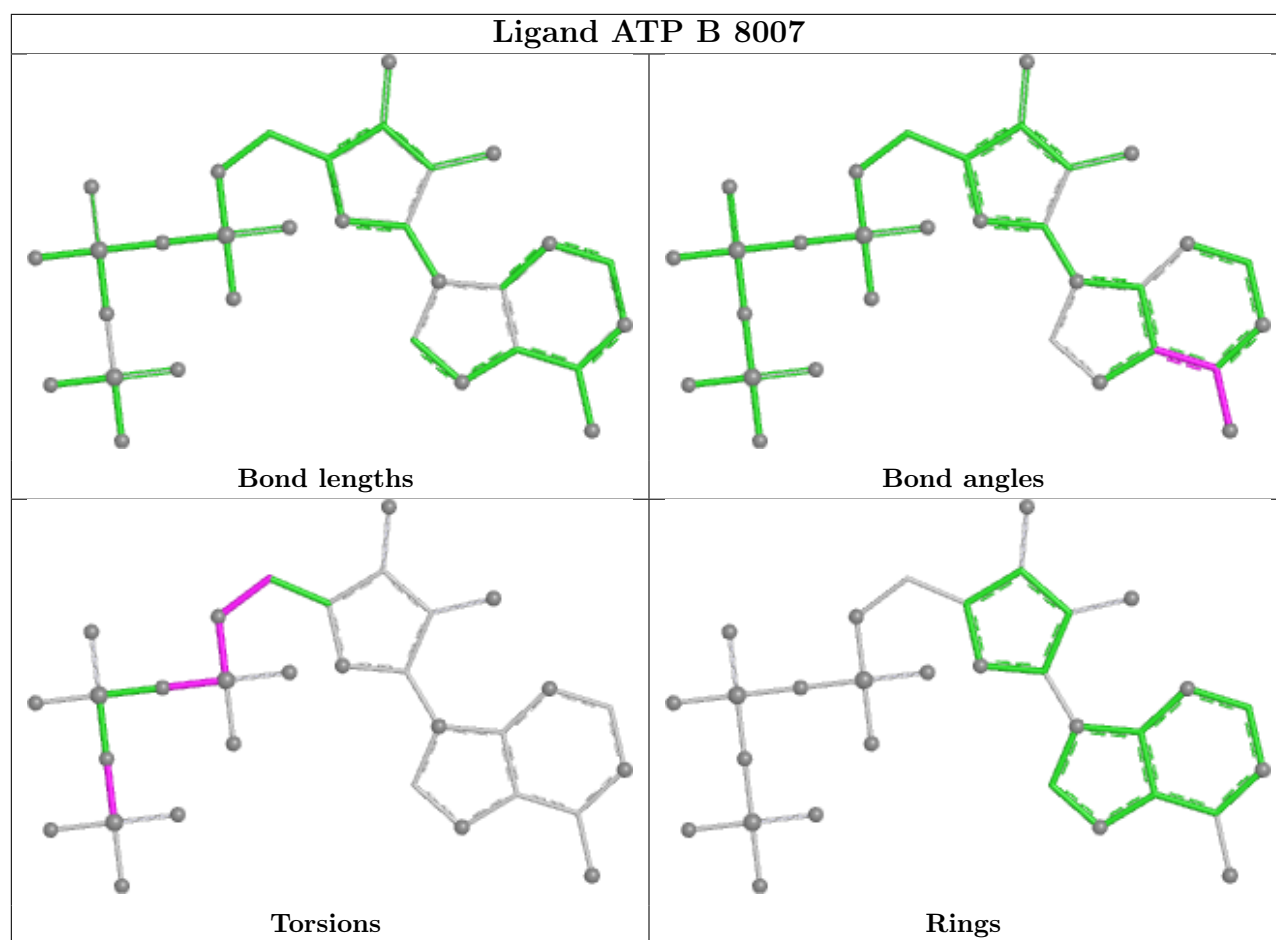
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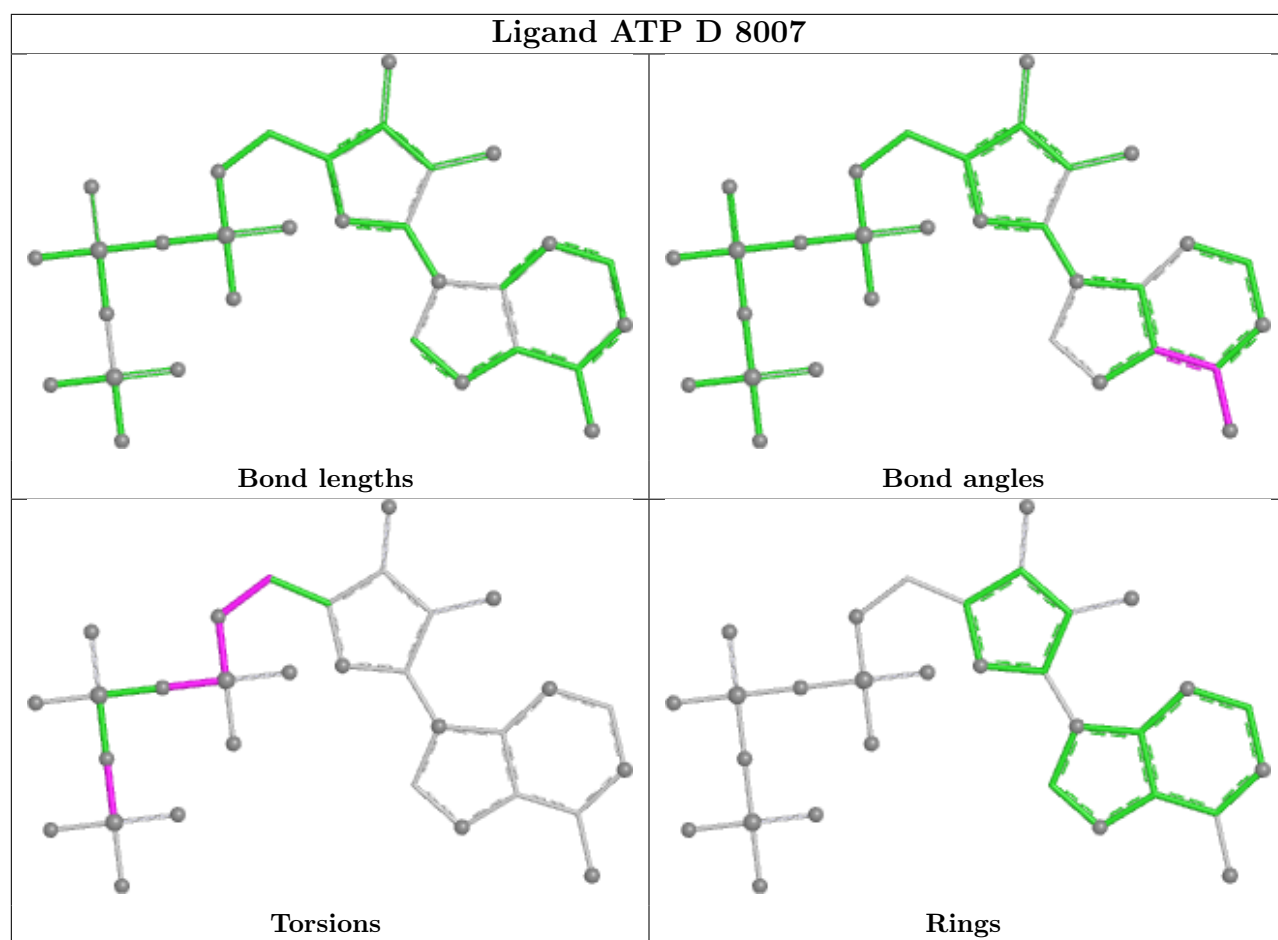
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	8005	PCW	2	0
8	B	8009	A1BYZ	2	0
8	D	8009	A1BYZ	2	0
7	B	8006	PCW	3	0
8	A	8009	A1BYZ	2	0
7	D	8006	PCW	3	0
7	A	8005	PCW	2	0
5	B	8003	ATP	1	0
5	C	8003	ATP	1	0
8	B	8008	A1BYZ	1	0
7	C	8006	PCW	3	0
5	D	8003	ATP	1	0
7	D	8005	PCW	2	0
5	A	8003	ATP	1	0
7	C	8005	PCW	2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

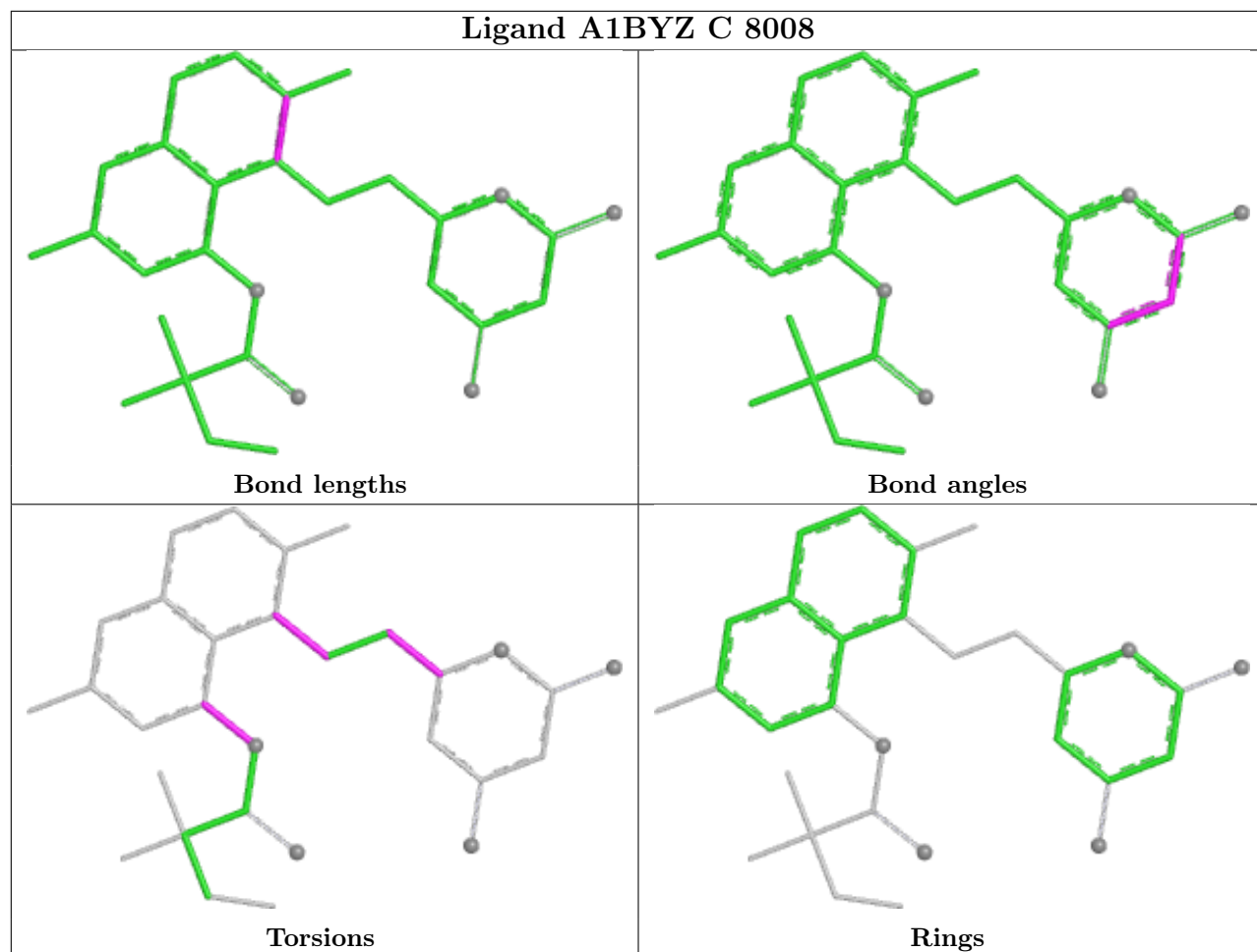
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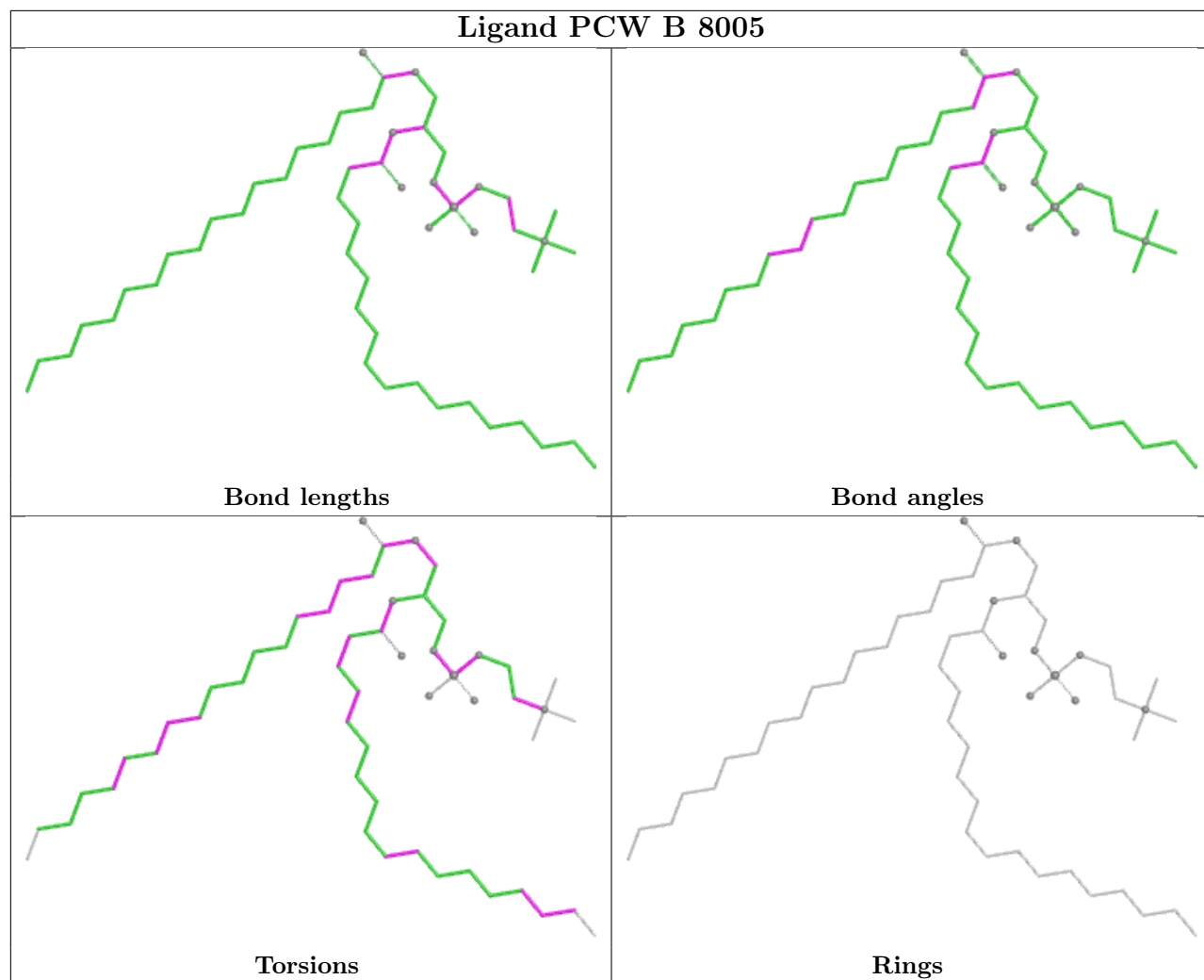


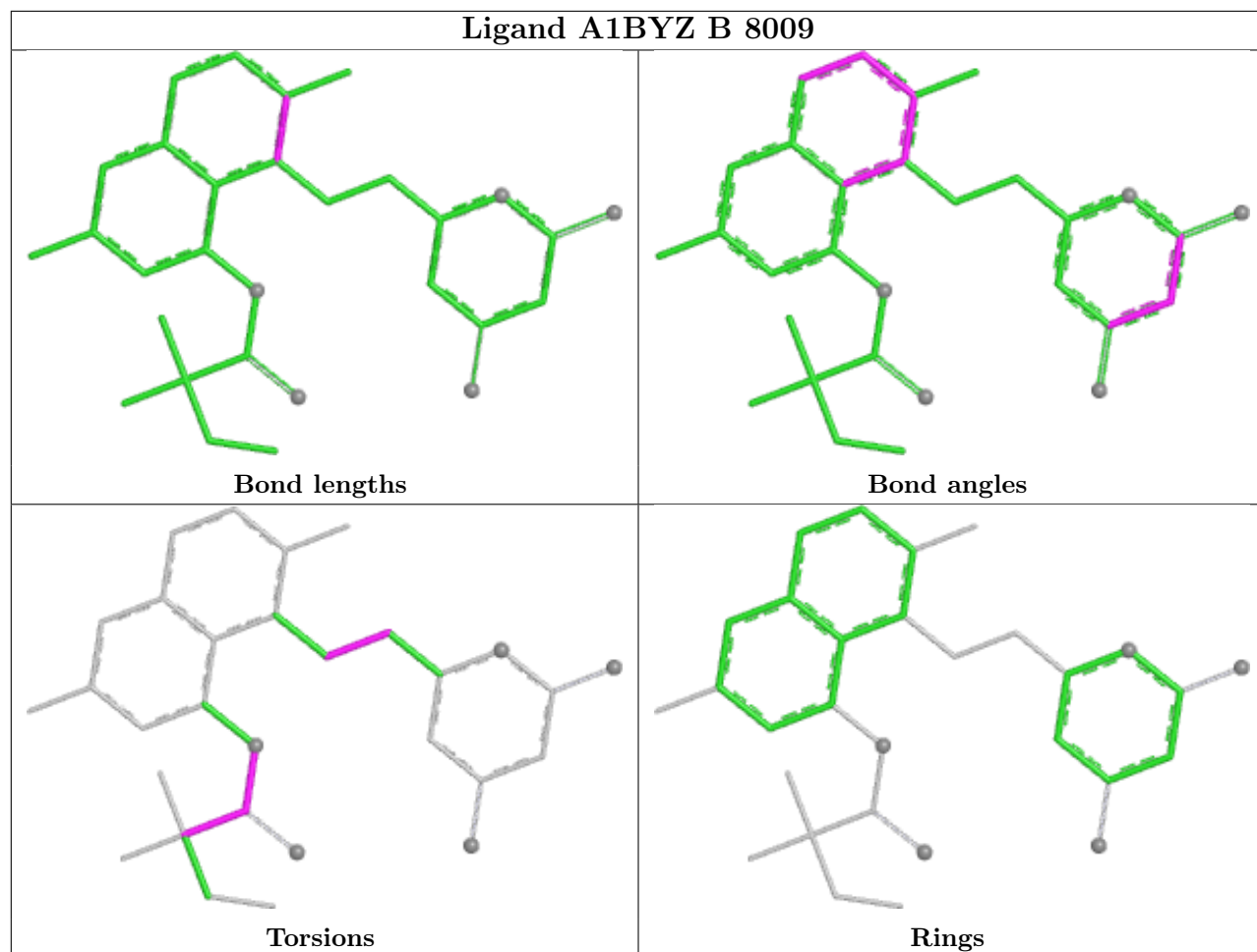




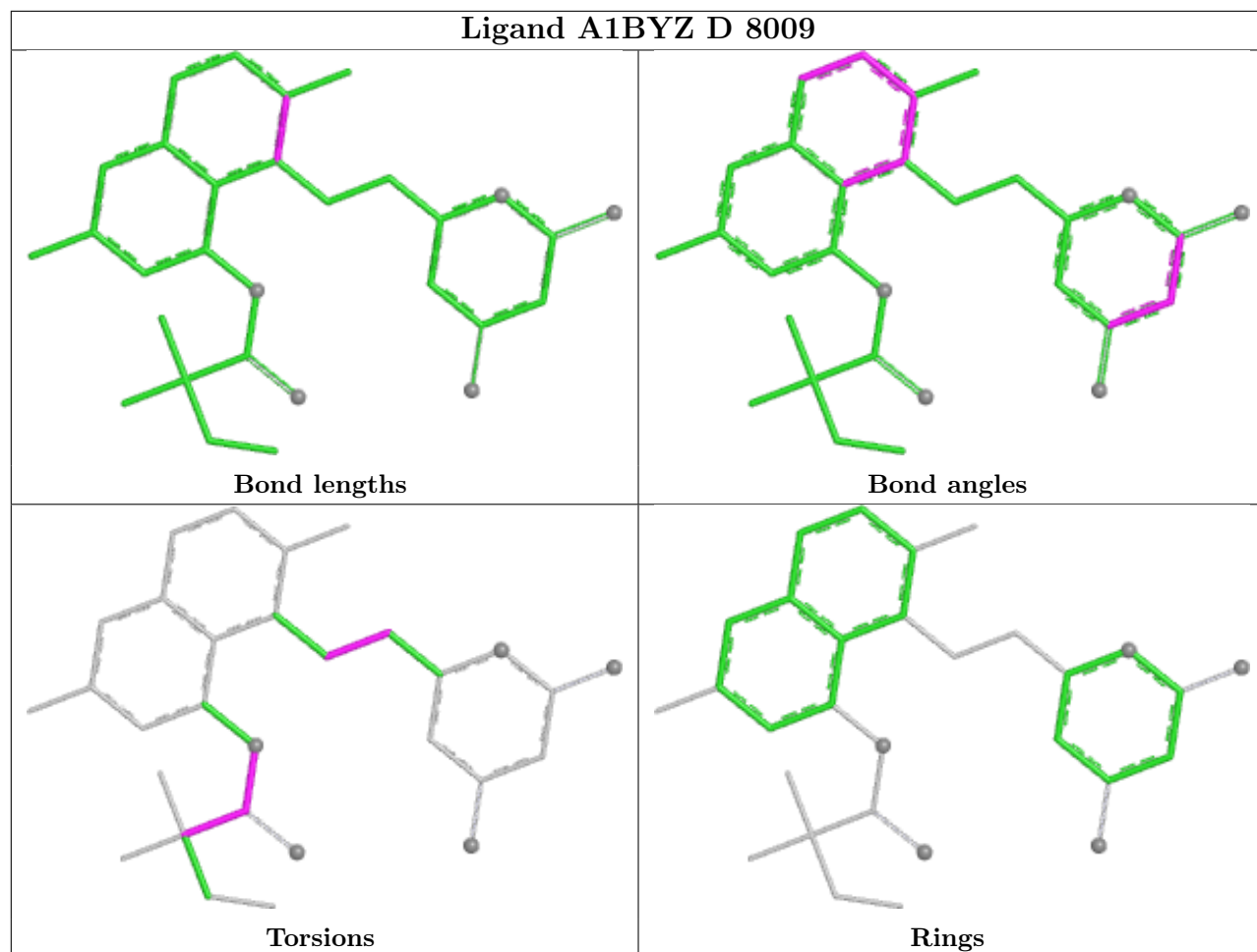
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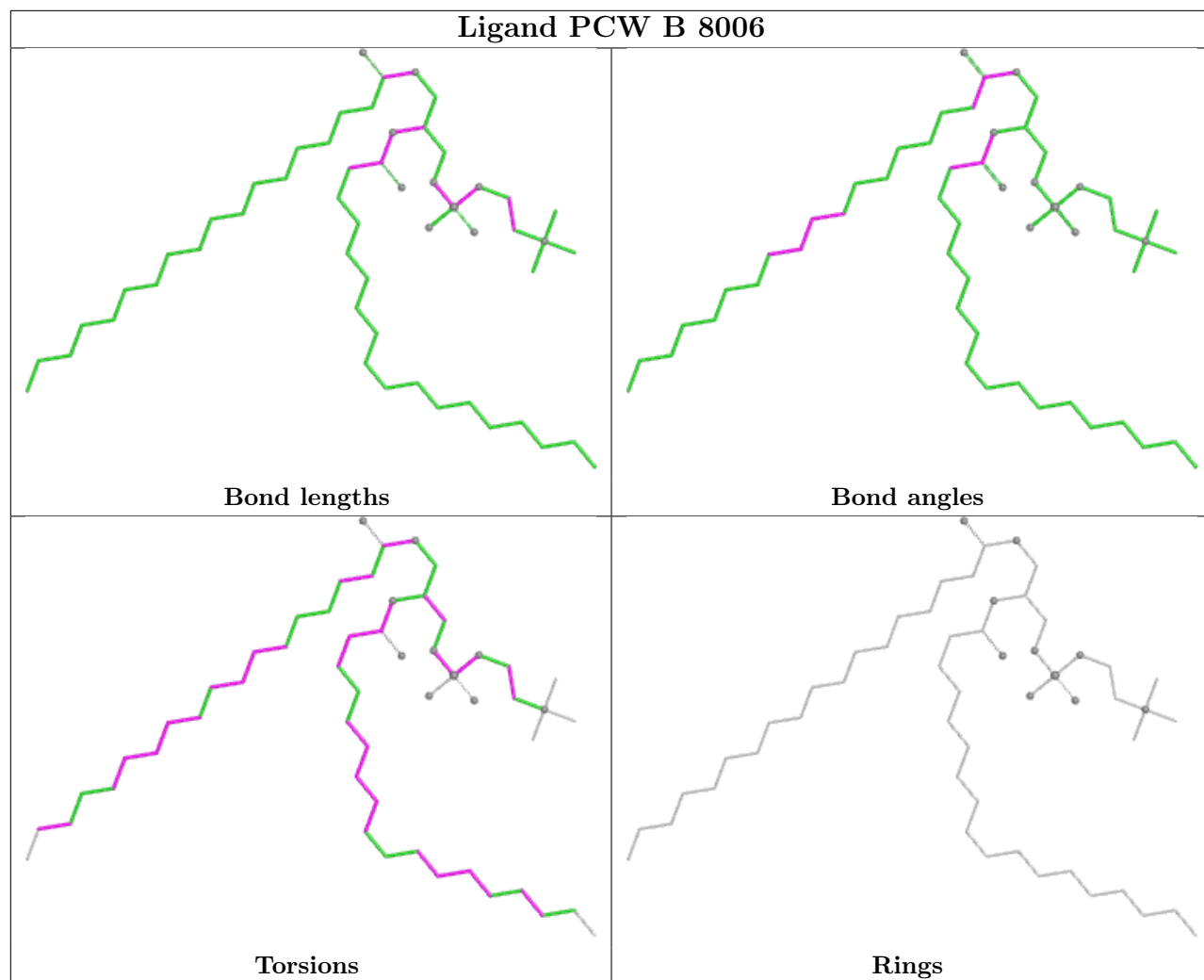




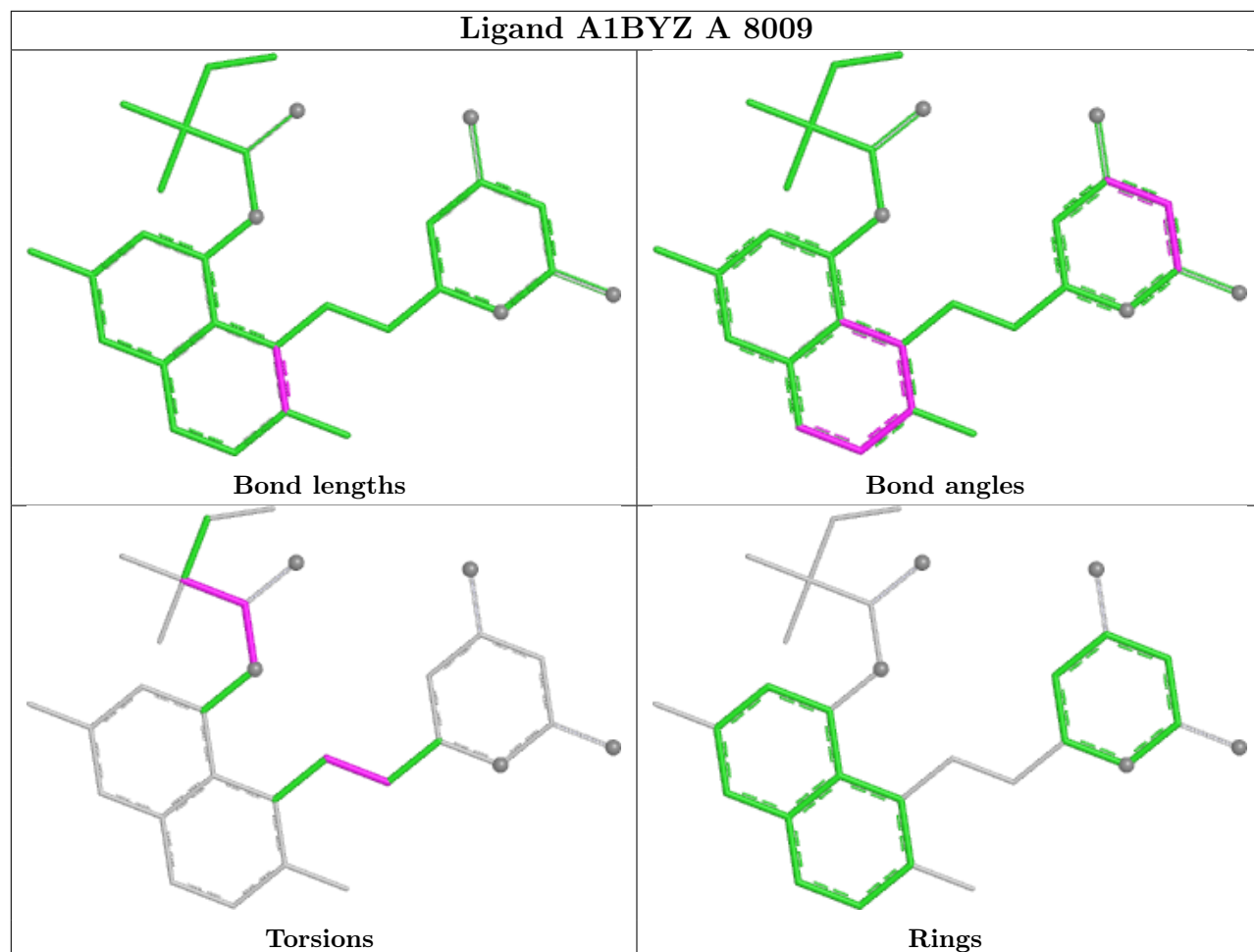


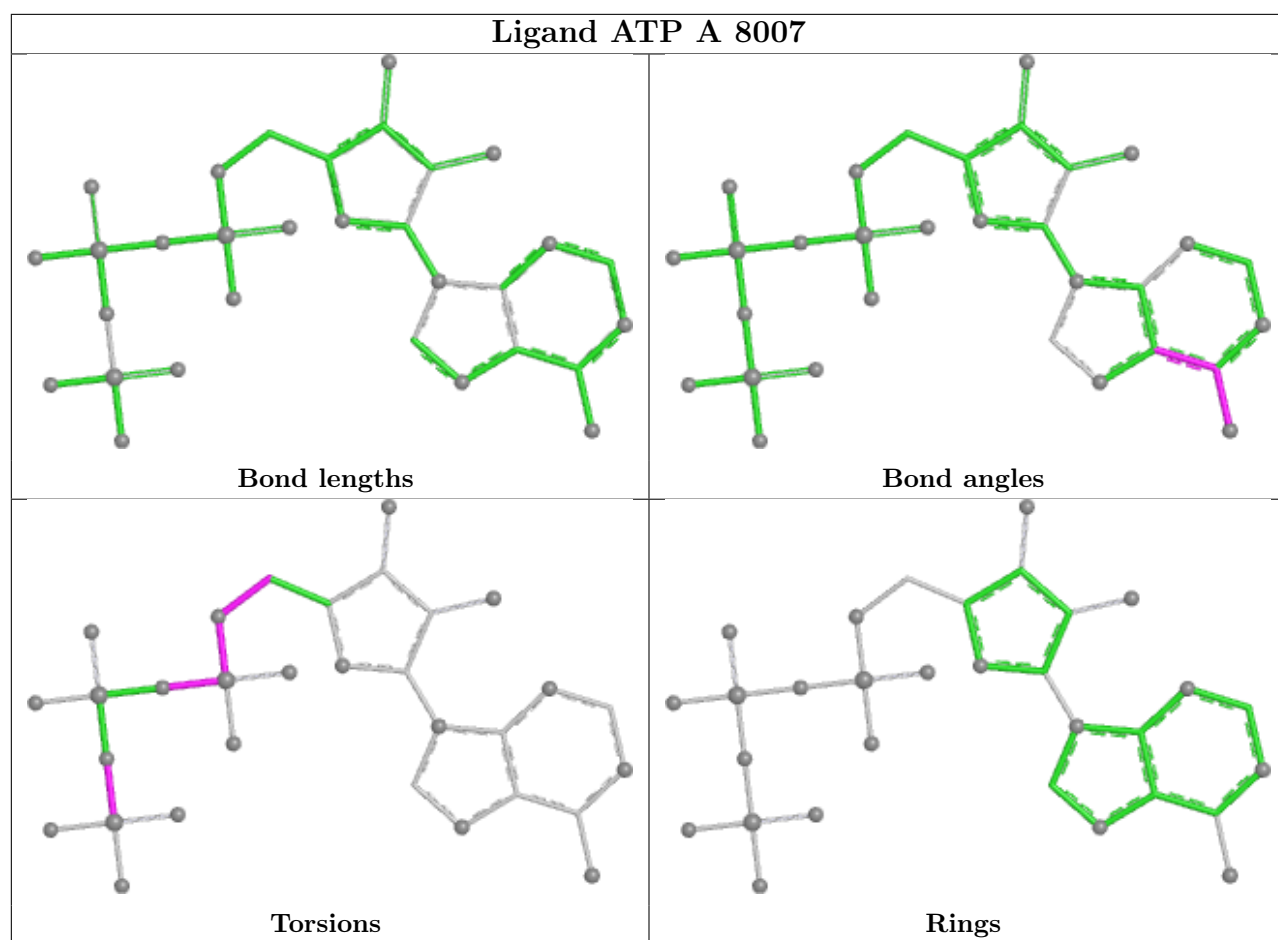
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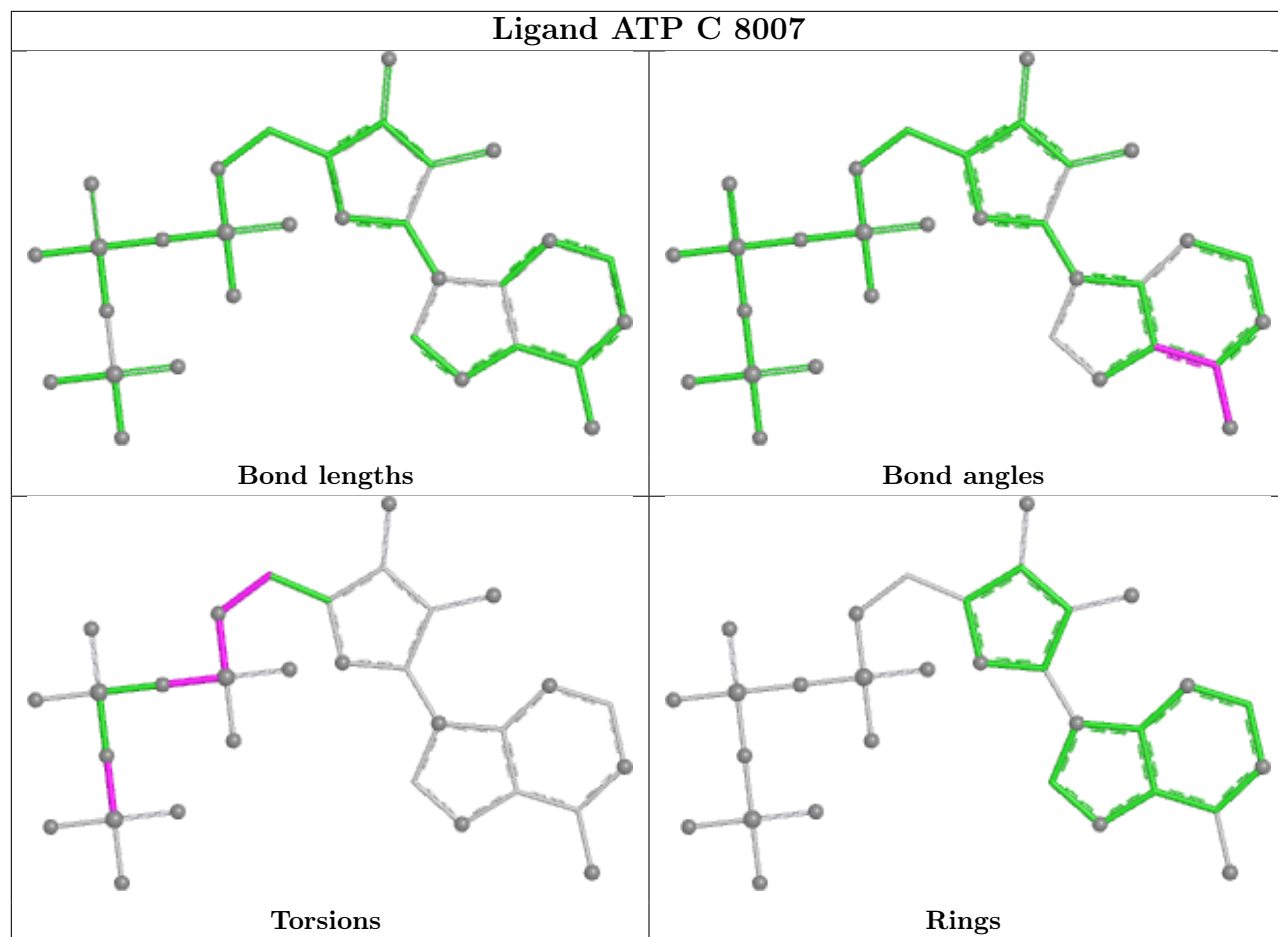


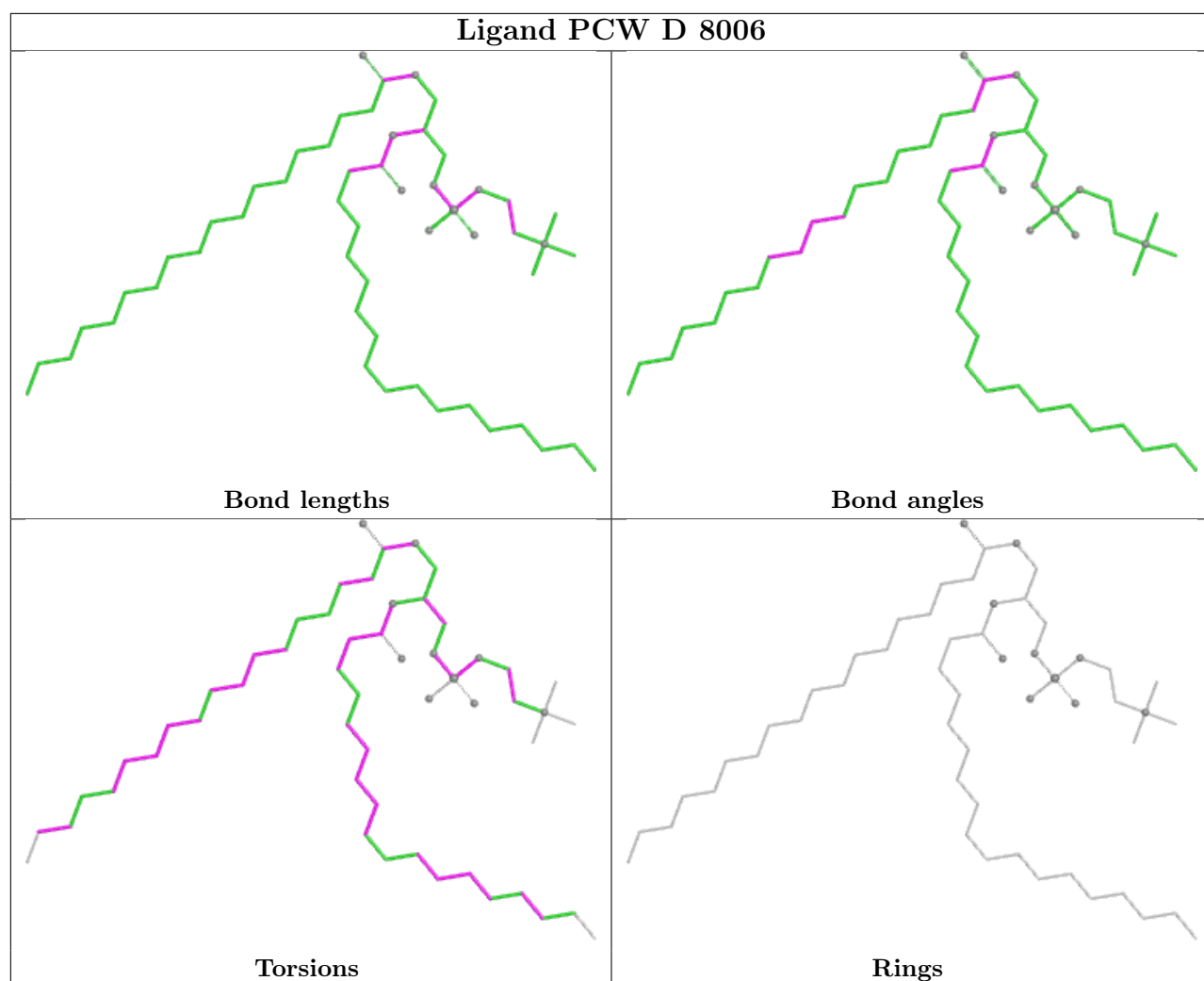


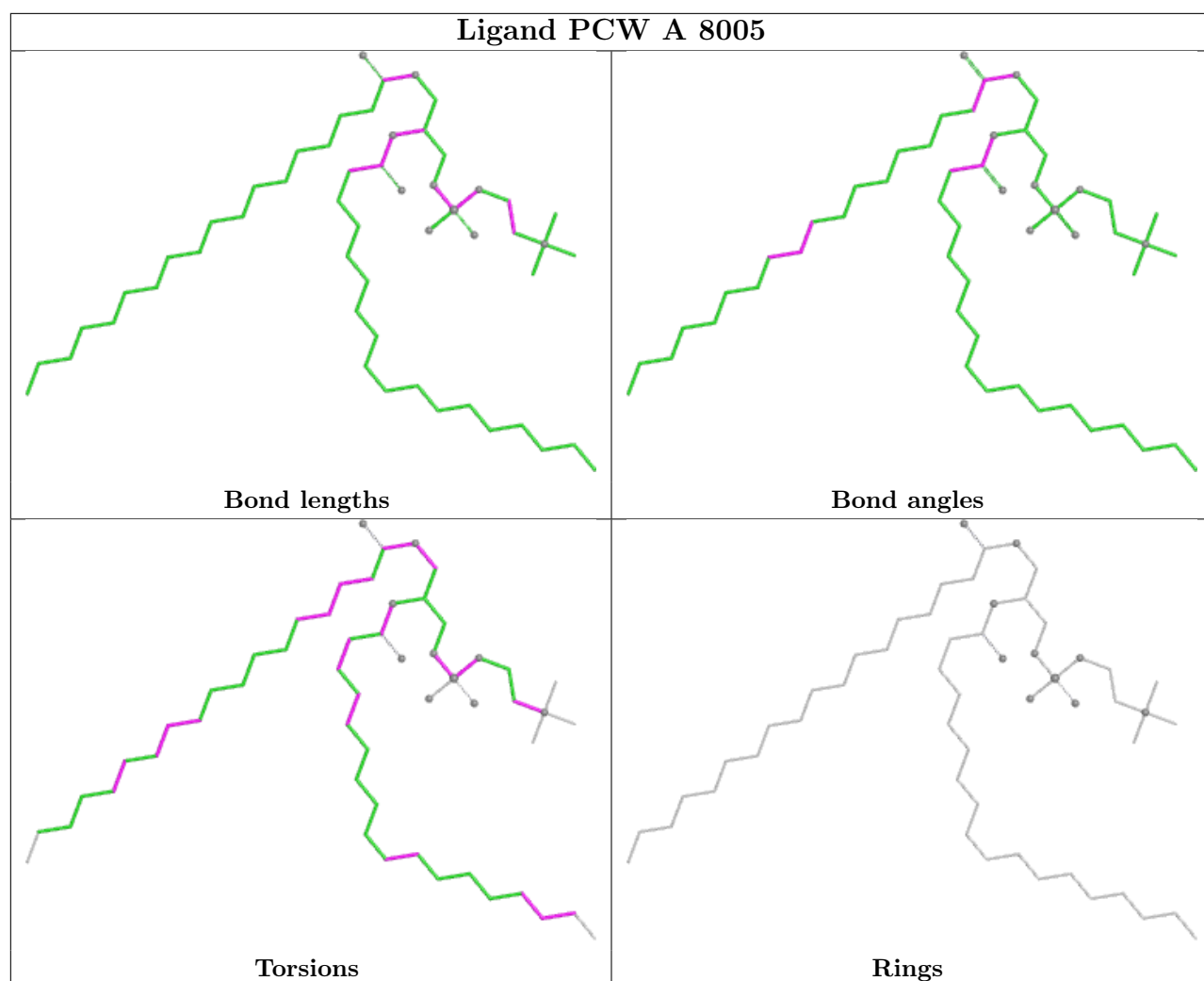
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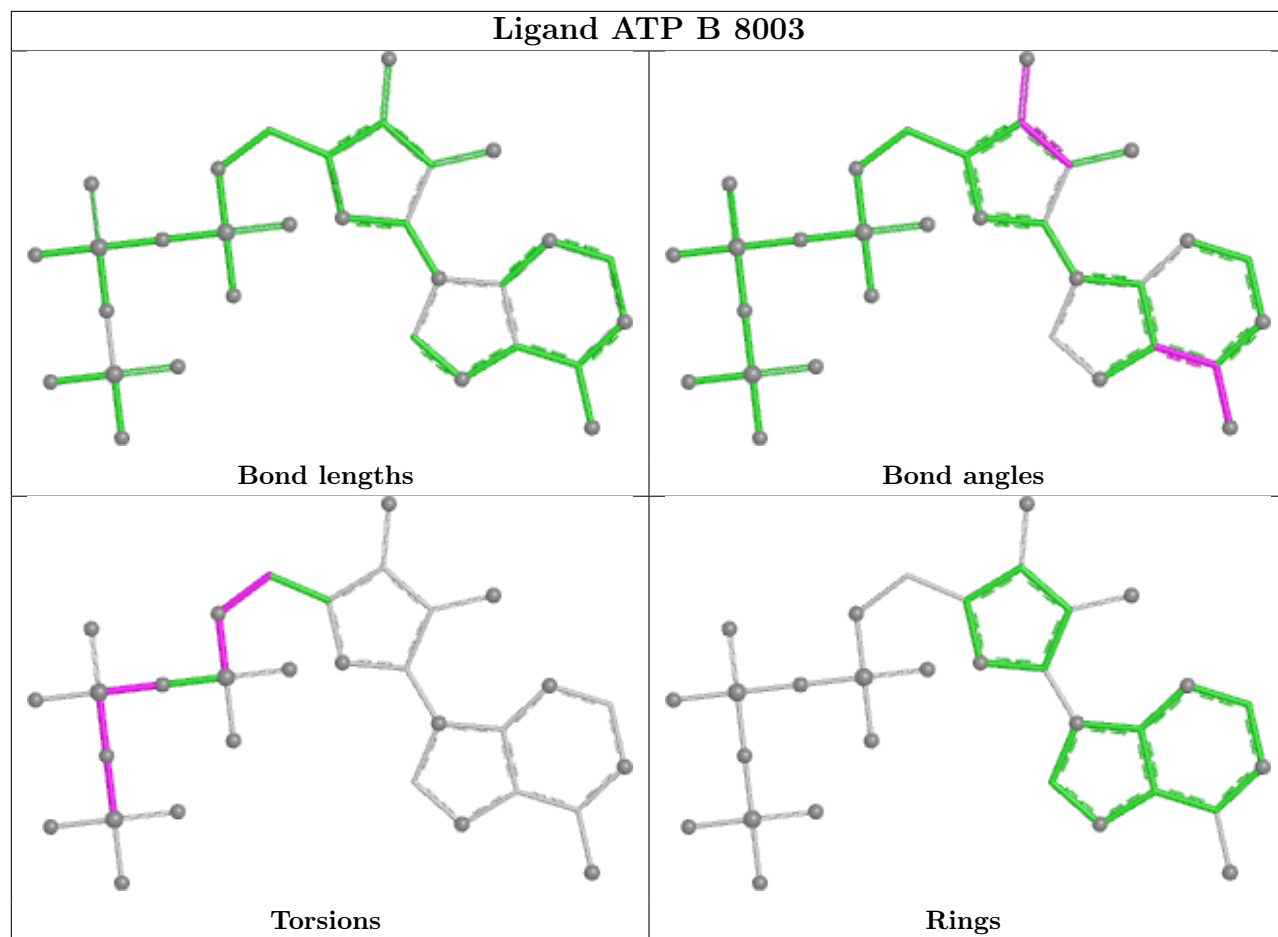


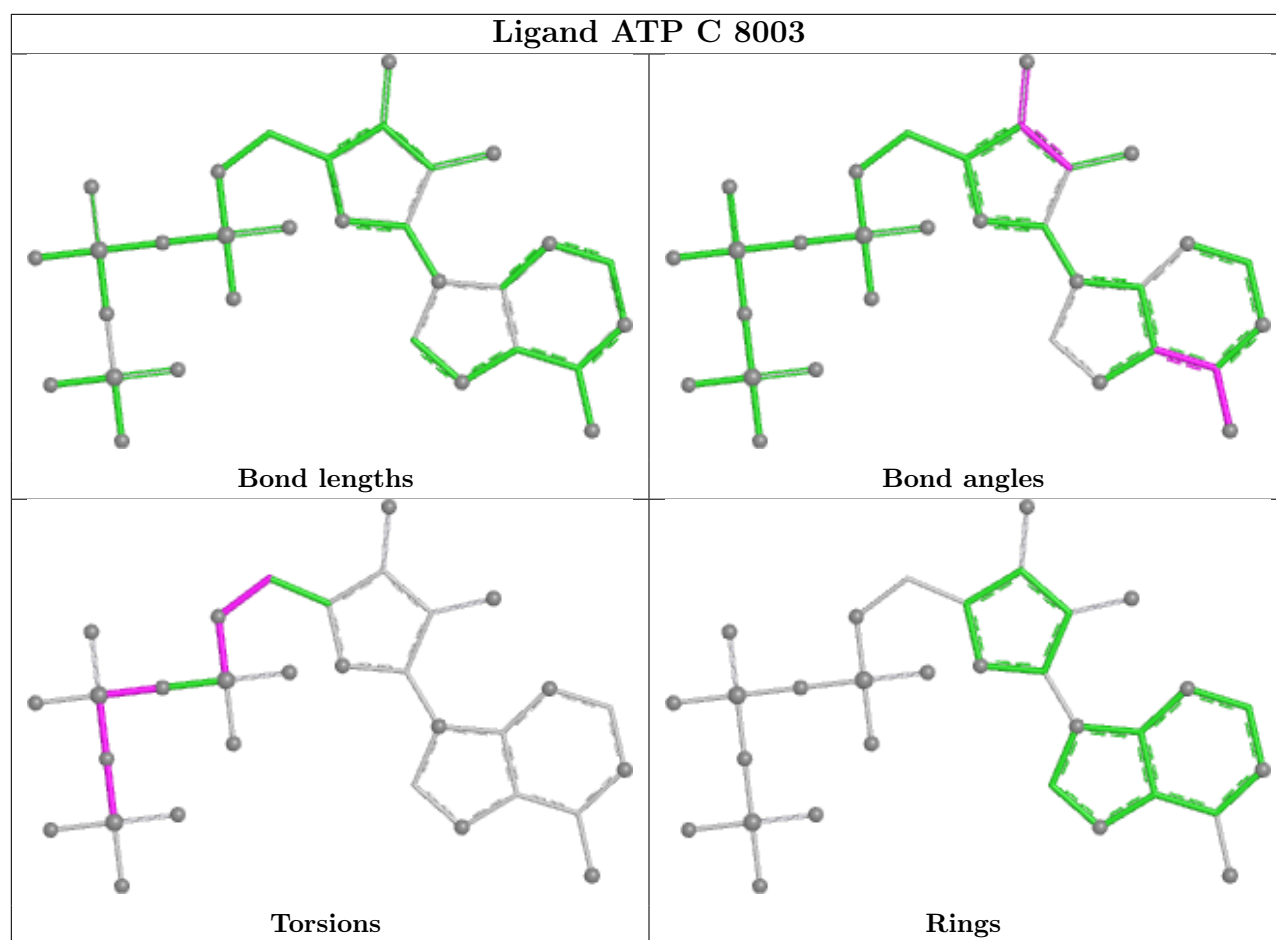




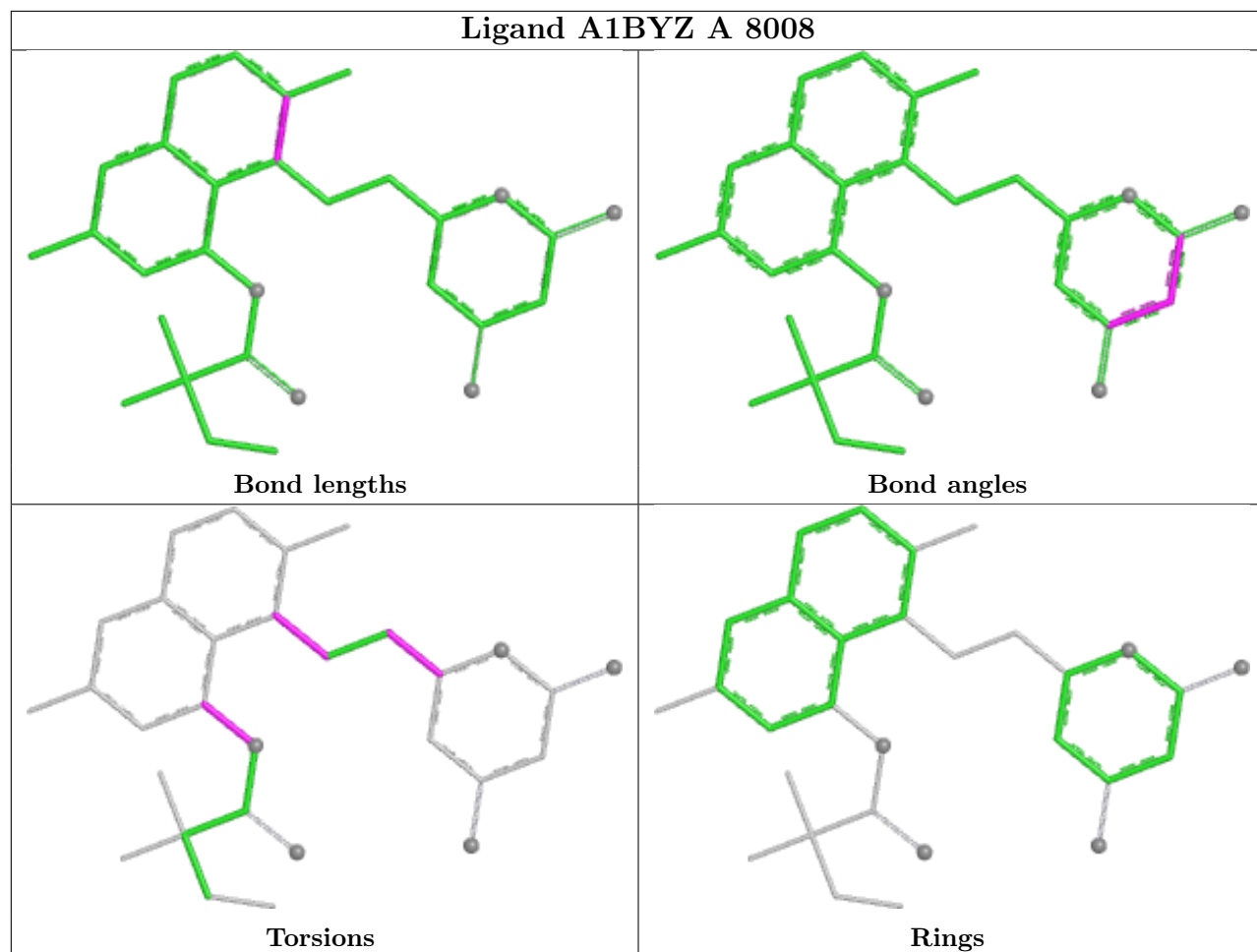




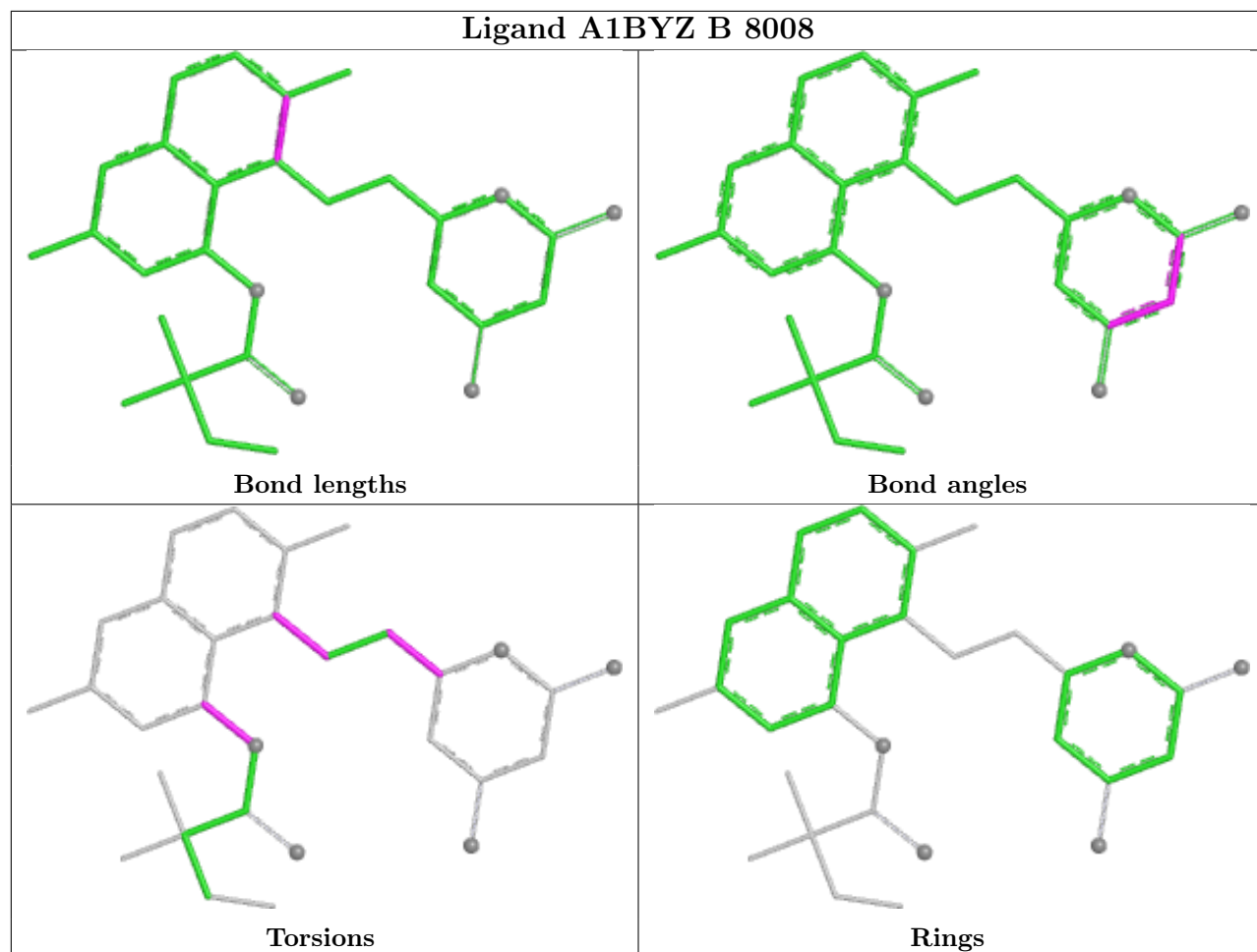


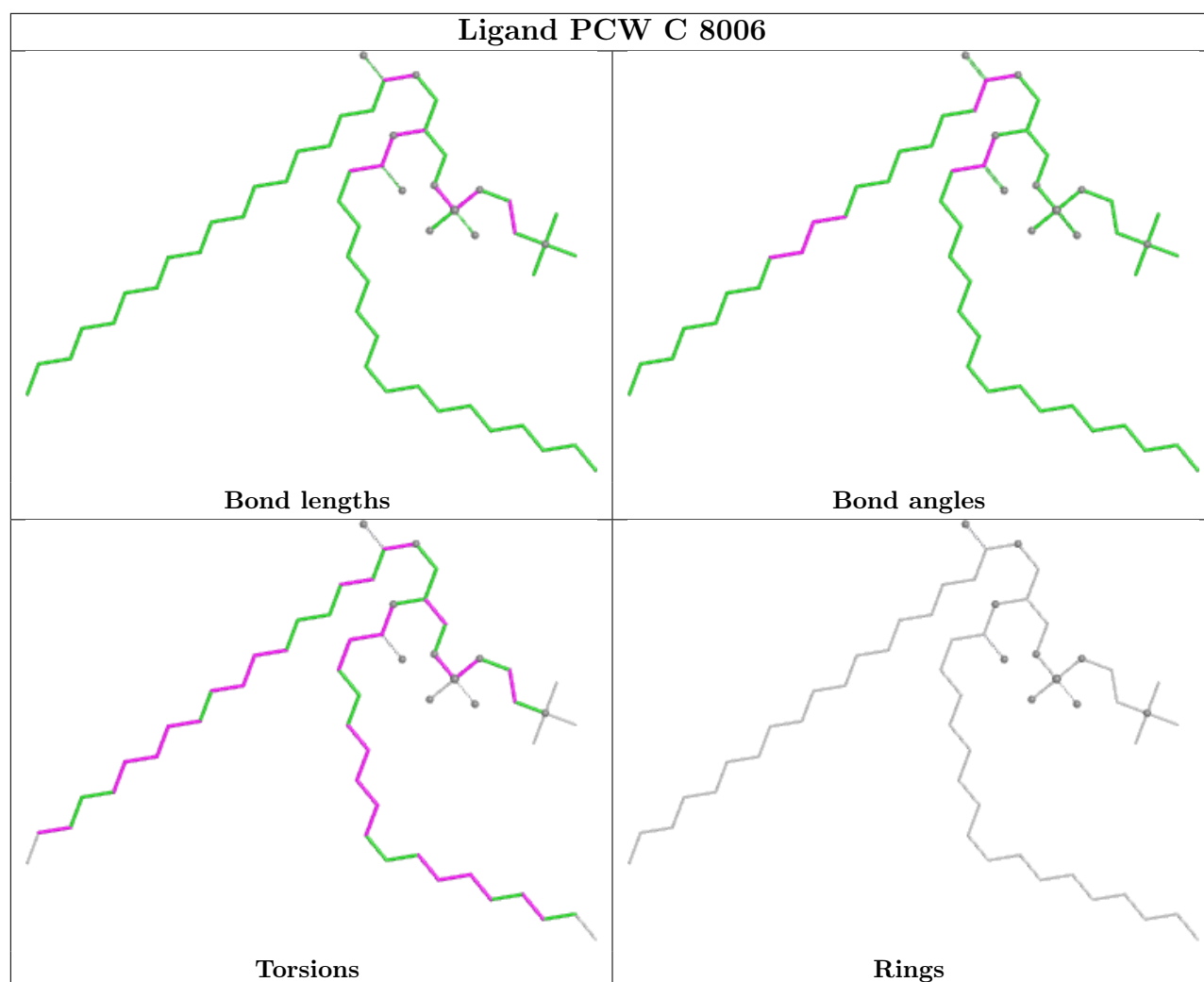


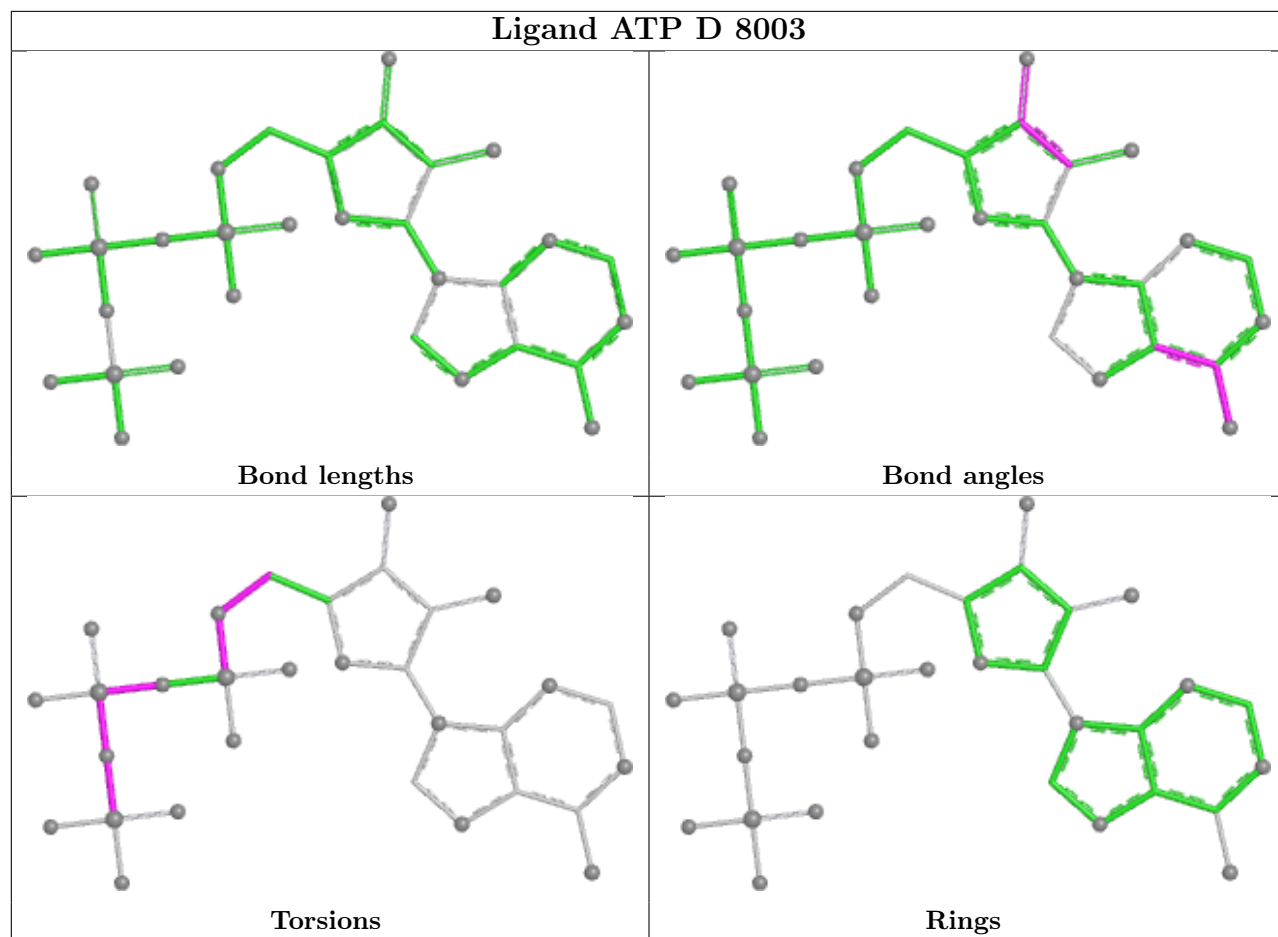
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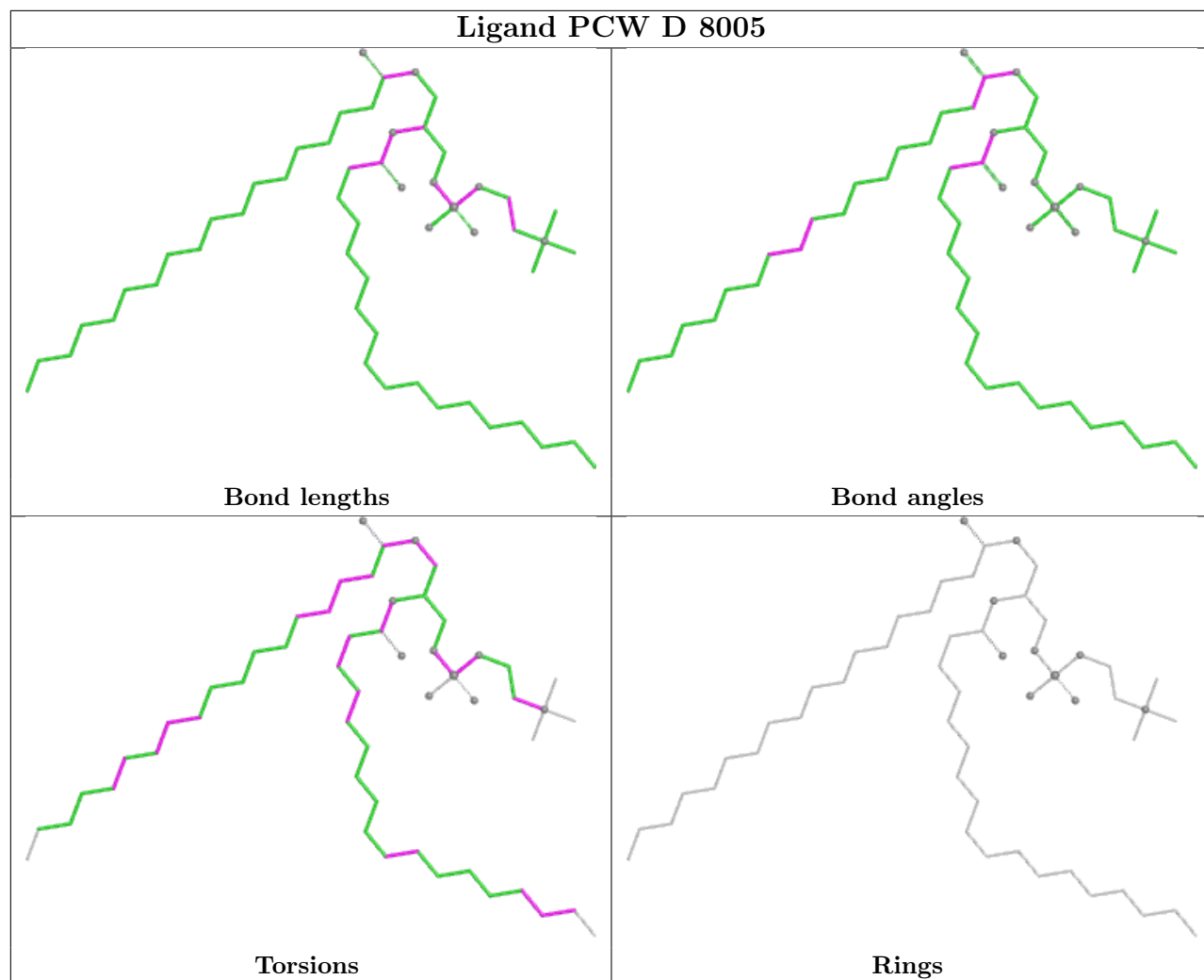


Ligand A1BYZ B 8008

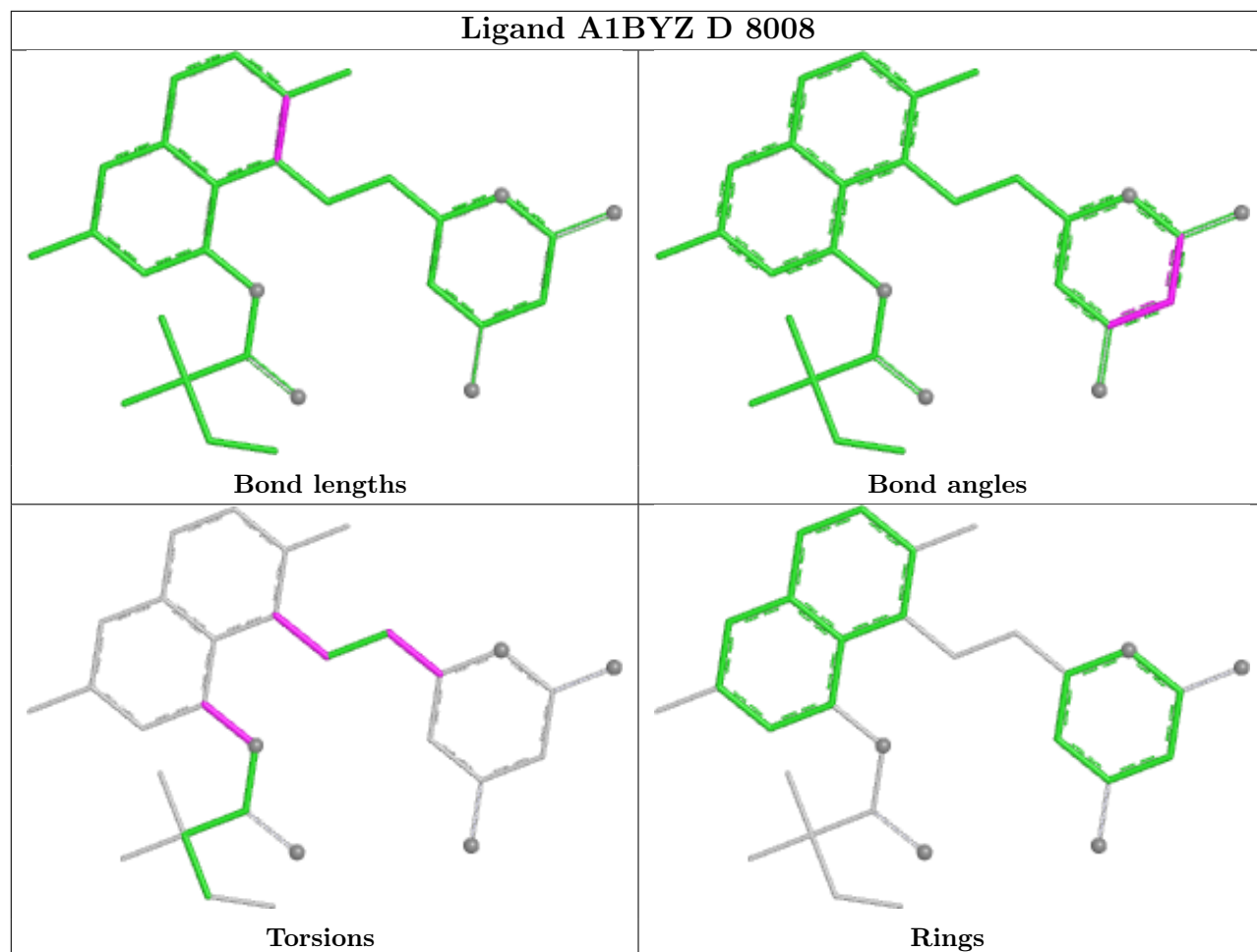


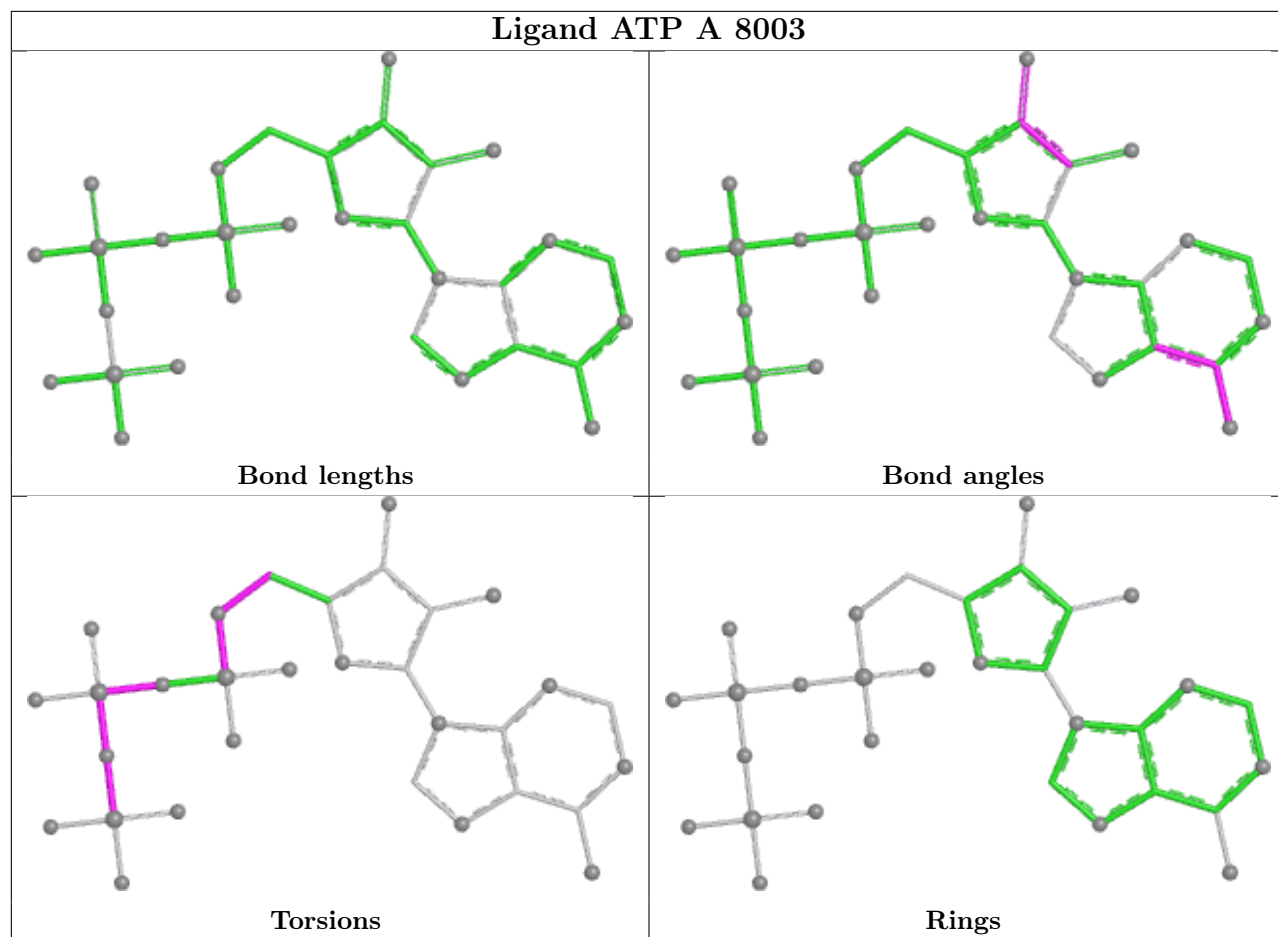


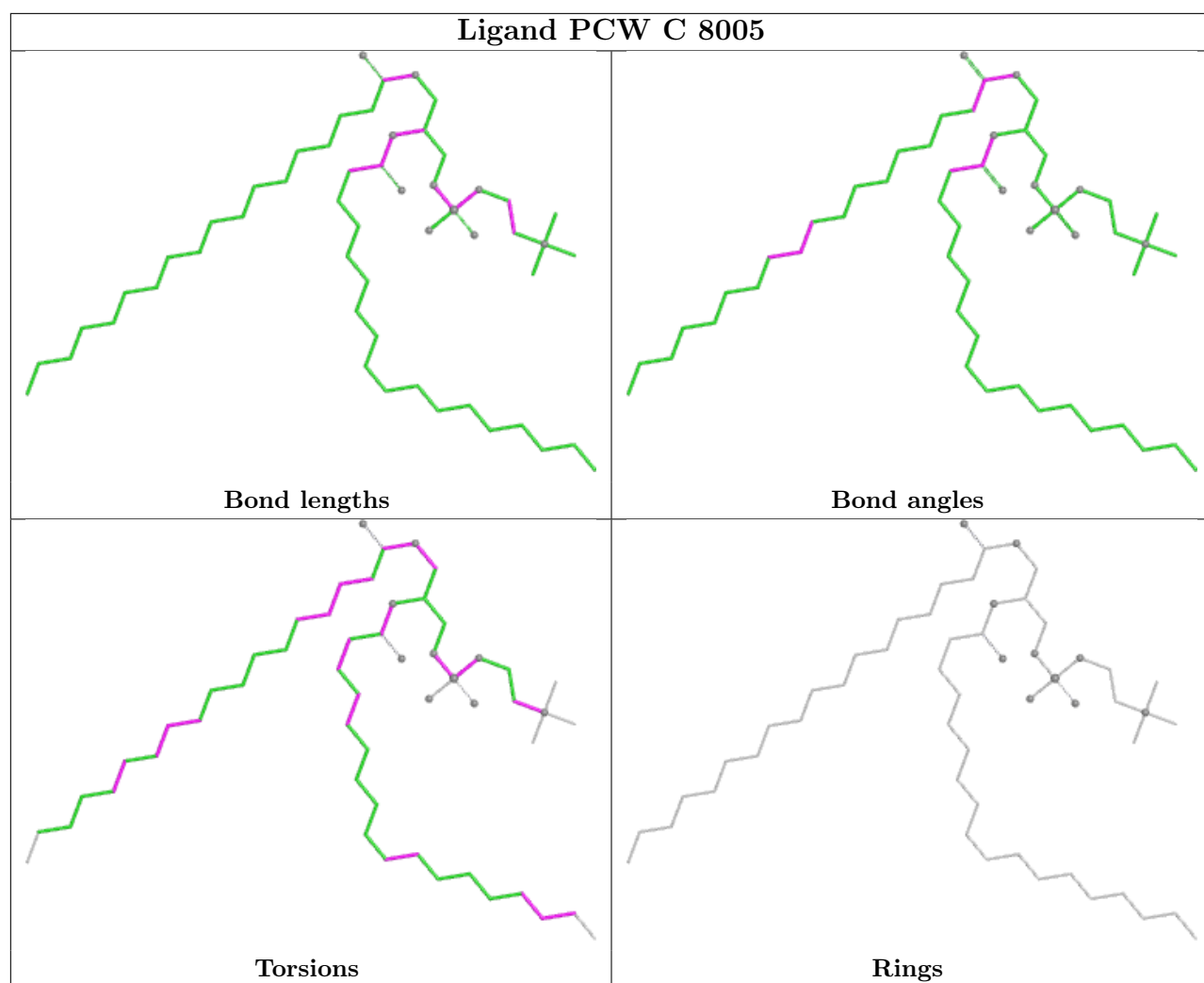


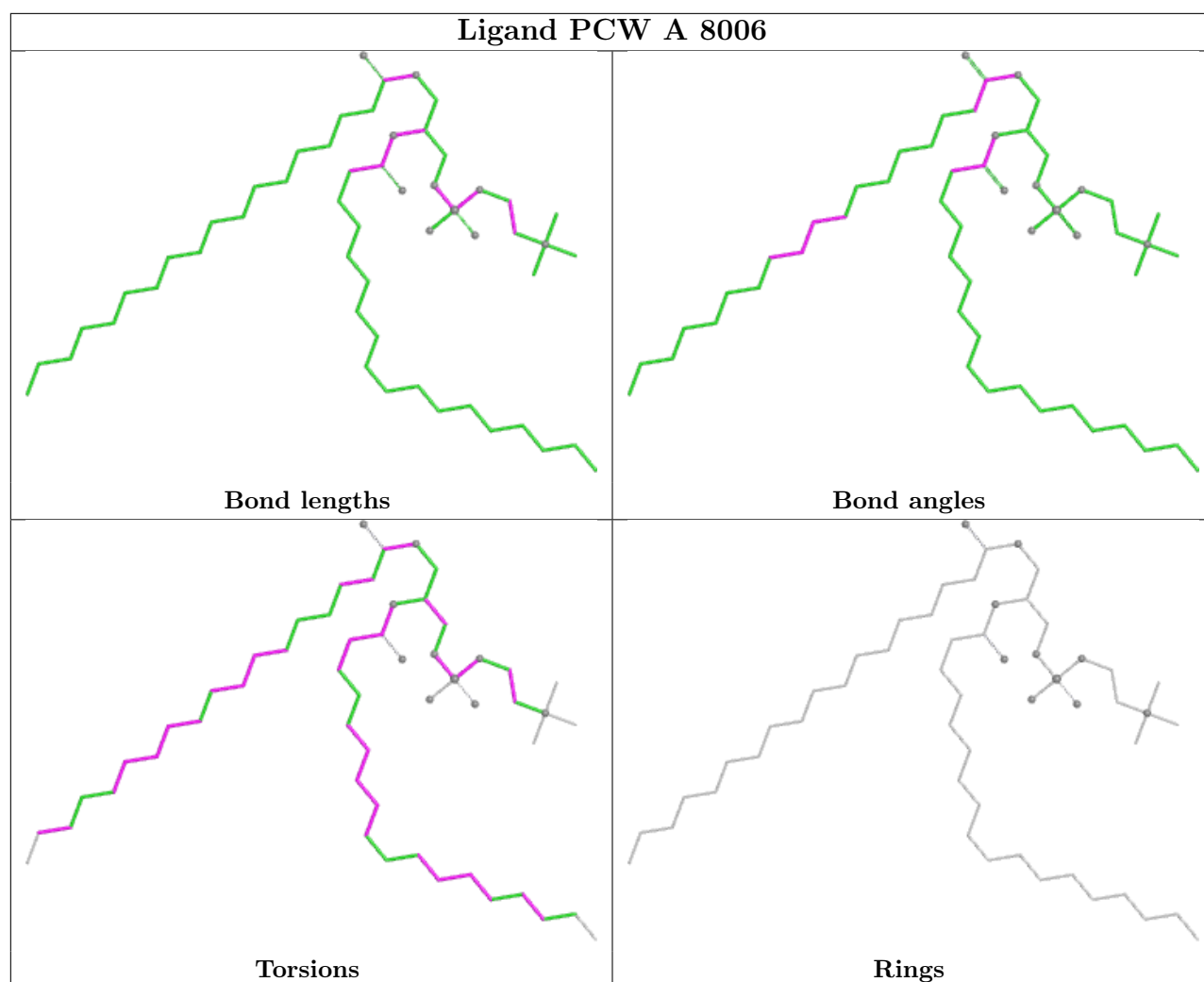


Ligand A1BYZ D 8008









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.

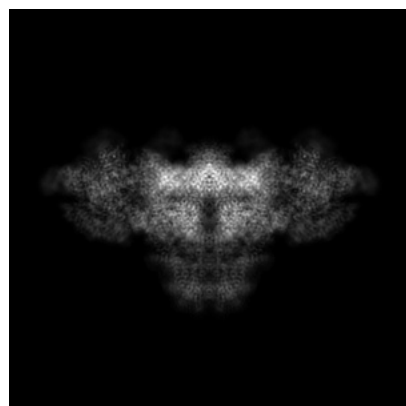
6 Map visualisation [i](#)

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.

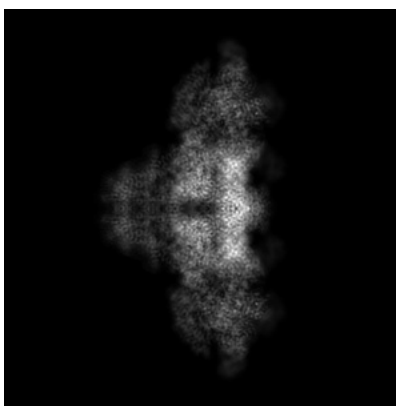
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

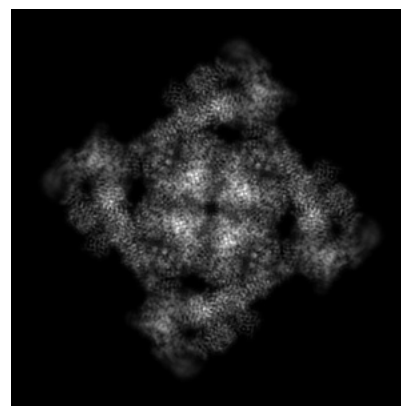
6.1.1 Primary map



X

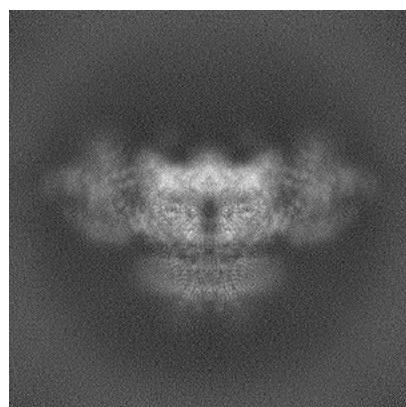


Y

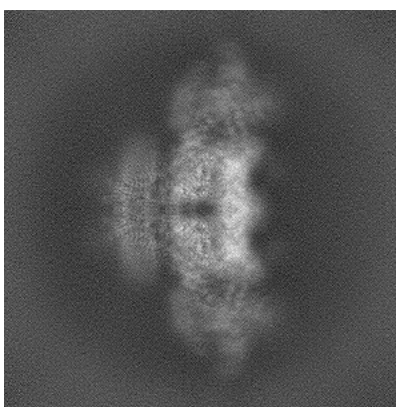


Z

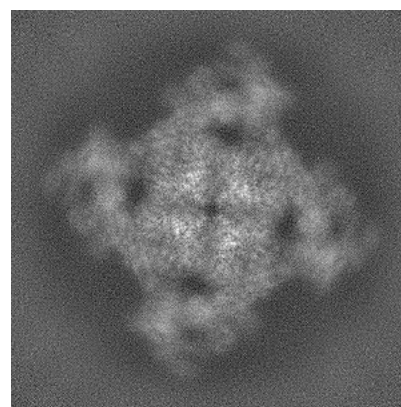
6.1.2 Raw map



X



Y



Z

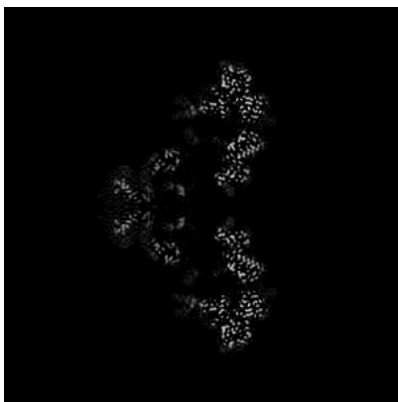
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

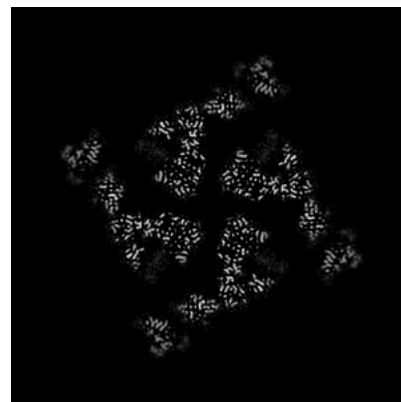
6.2.1 Primary map



X Index: 256



Y Index: 256

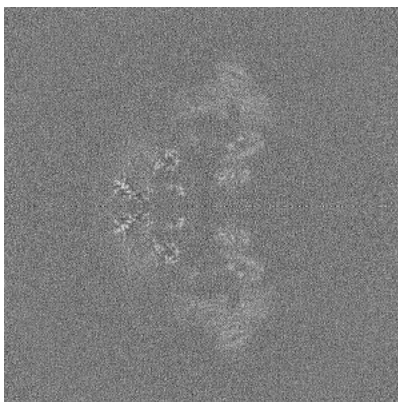


Z Index: 256

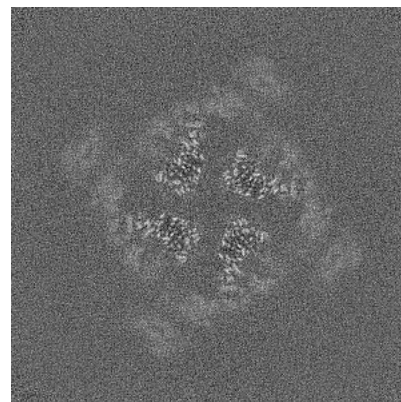
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

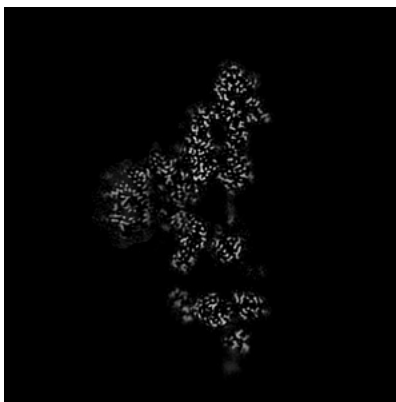
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

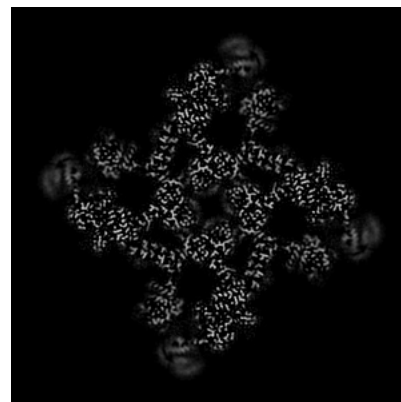
6.3.1 Primary map



X Index: 238

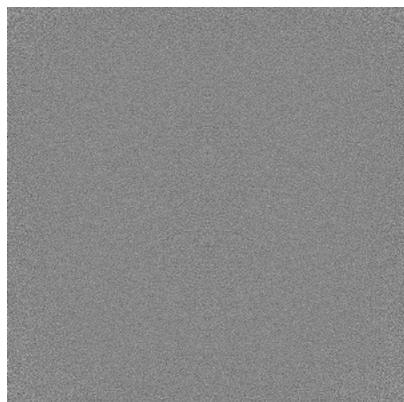


Y Index: 274

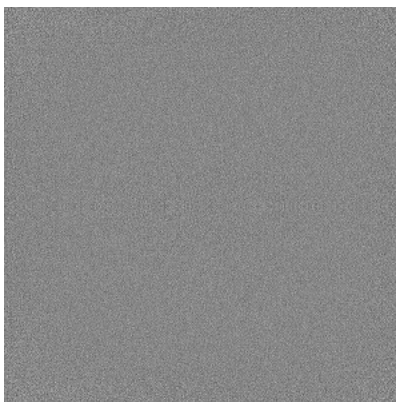


Z Index: 287

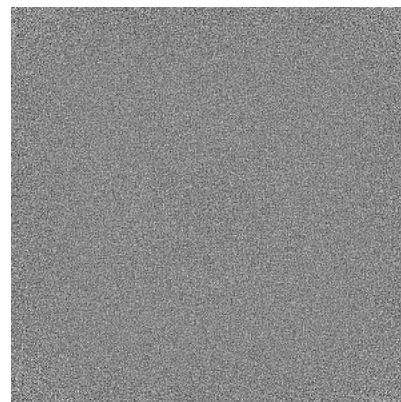
6.3.2 Raw map



X Index: 0



Y Index: 0

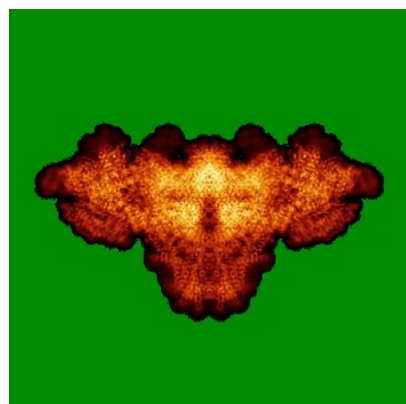


Z Index: 0

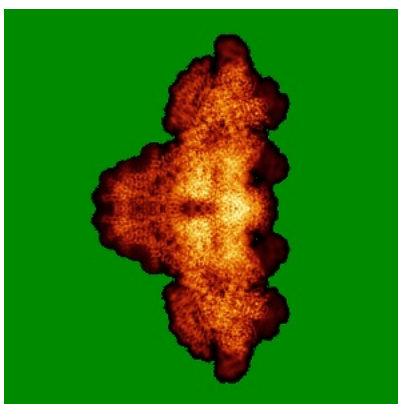
The images above show the largest variance slices of the map in three orthogonal directions.

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

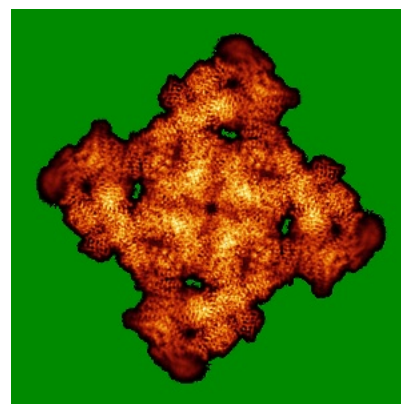
6.4.1 Primary map



X

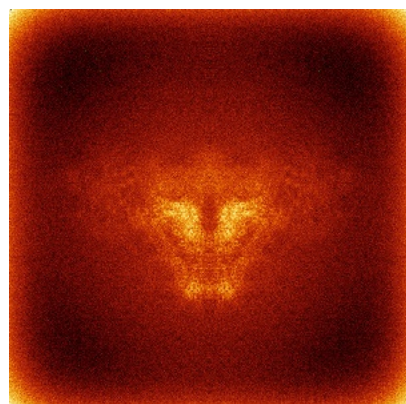


Y

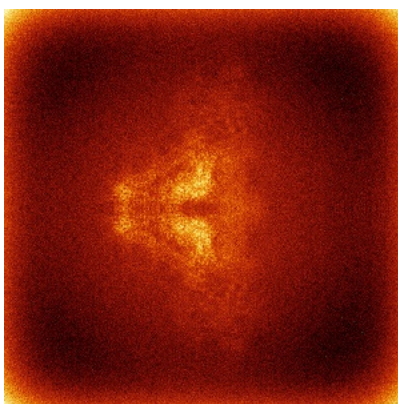


Z

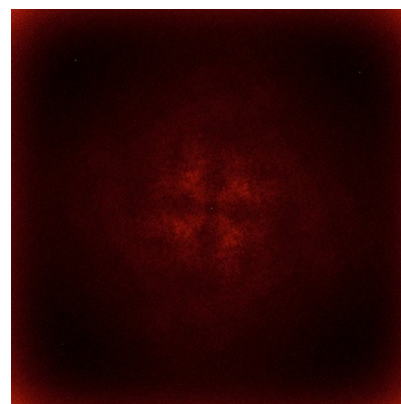
6.4.2 Raw map



X



Y

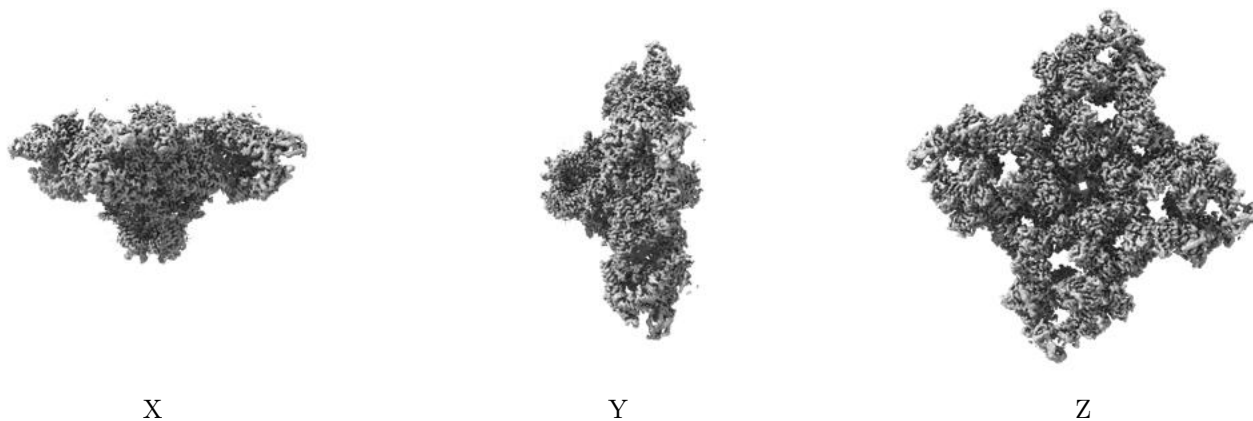


Z

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.

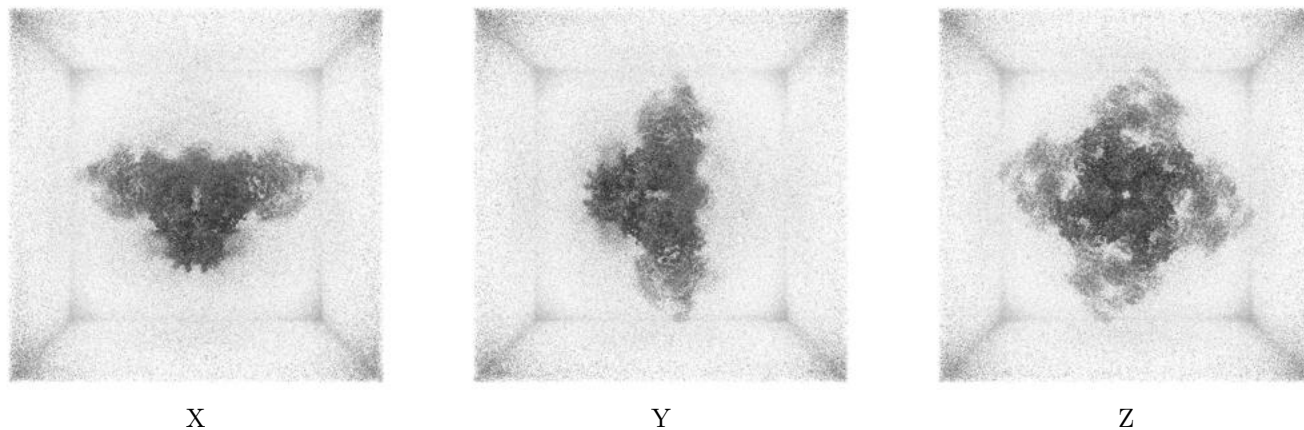
6.5 Orthogonal surface views [i](#)

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.

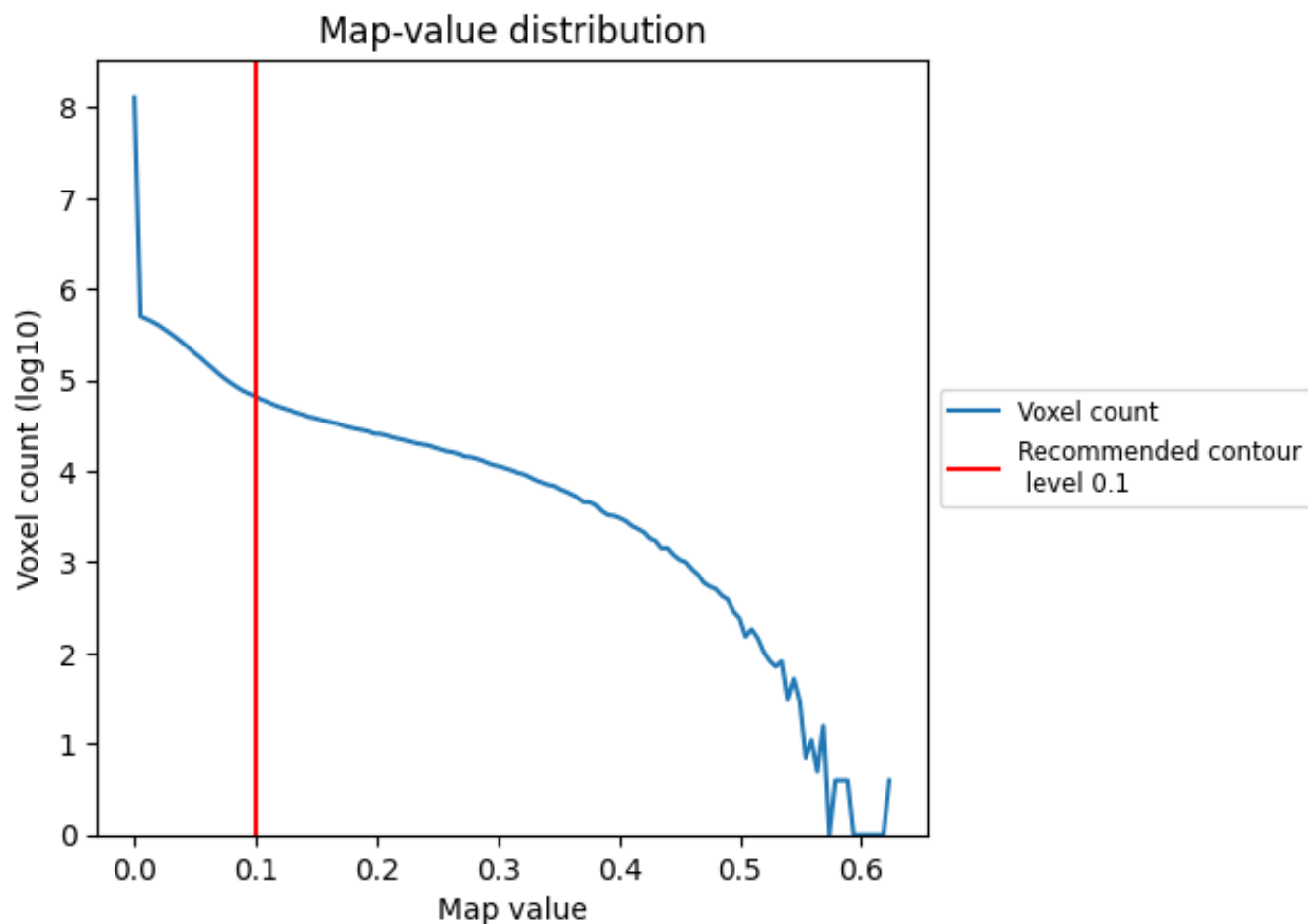
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

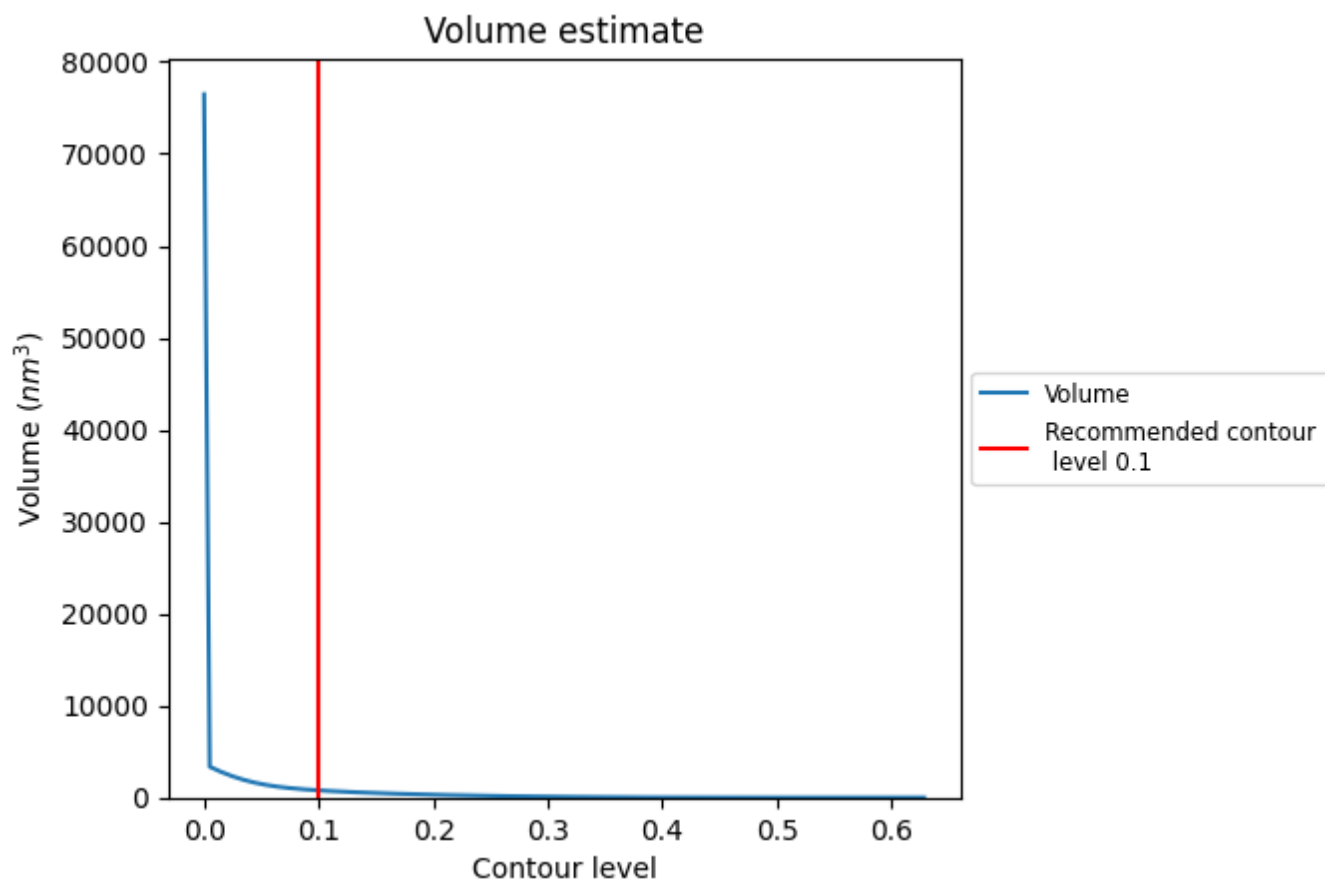
This section contains the results of statistical analysis of the map.

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.

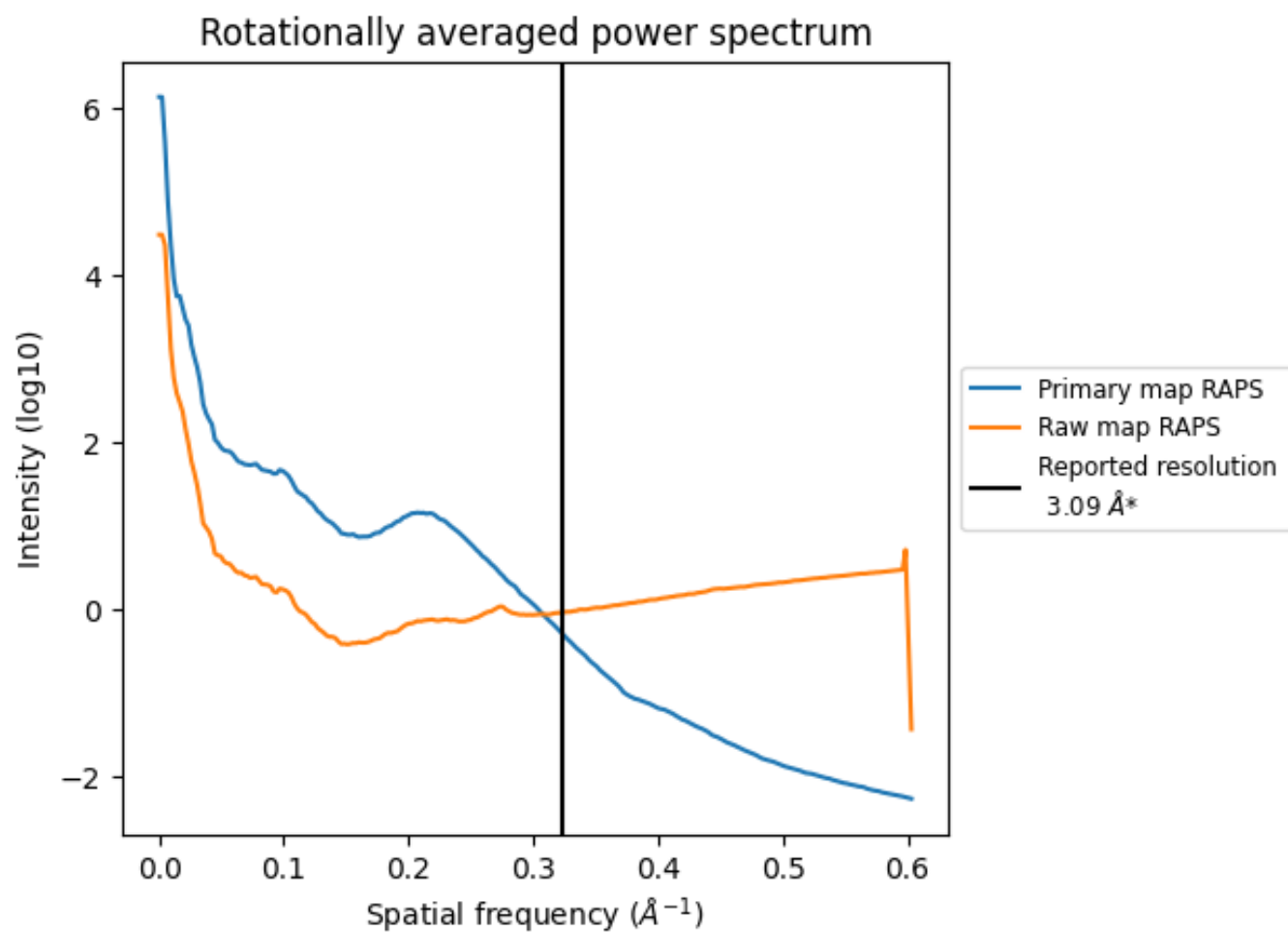
7.2 Volume estimate [i](#)



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 ⓘ

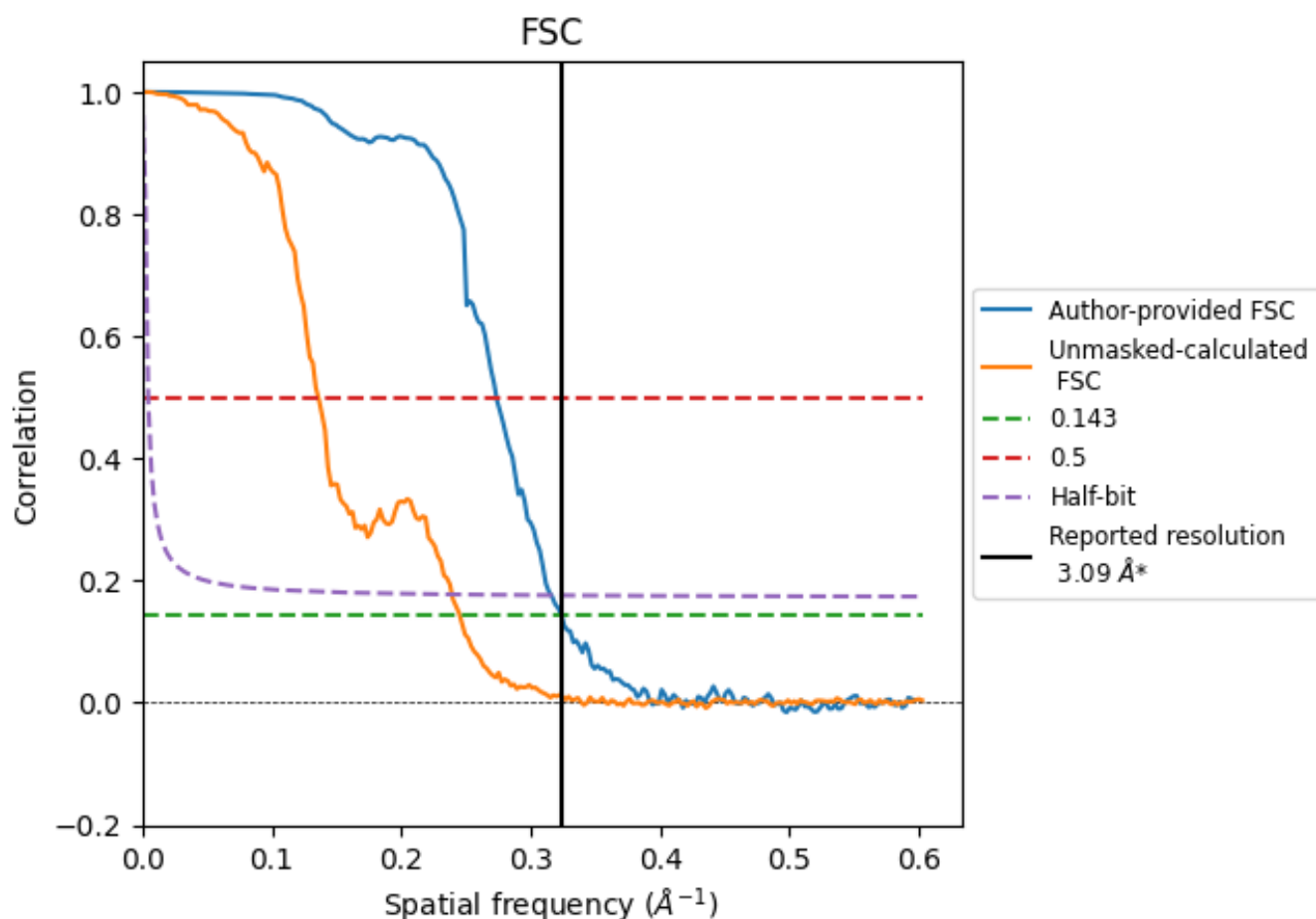


*Reported resolution corresponds to spatial frequency of 0.324 \AA^{-1}

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](#)

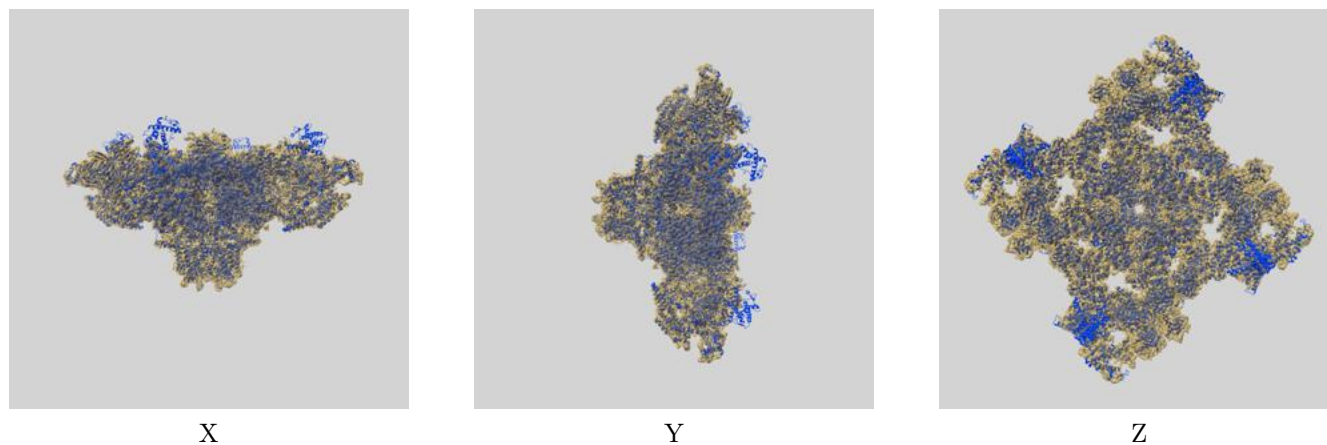
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	3.09	3.65	3.16
Unmasked-calculated*	4.08	7.35	4.18

*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](#)

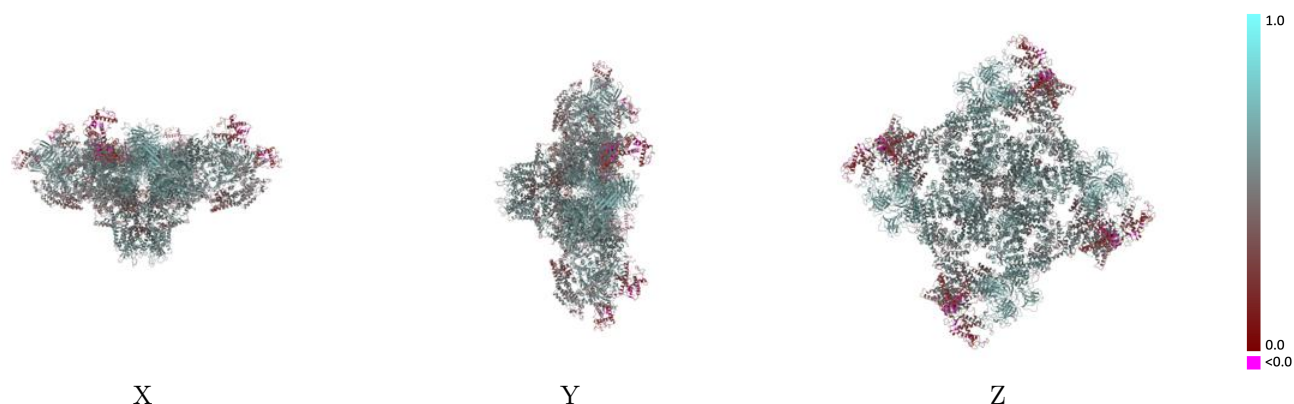
This section contains information regarding the fit between EMDB map EMD-49536 and PDB model 9NMP. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



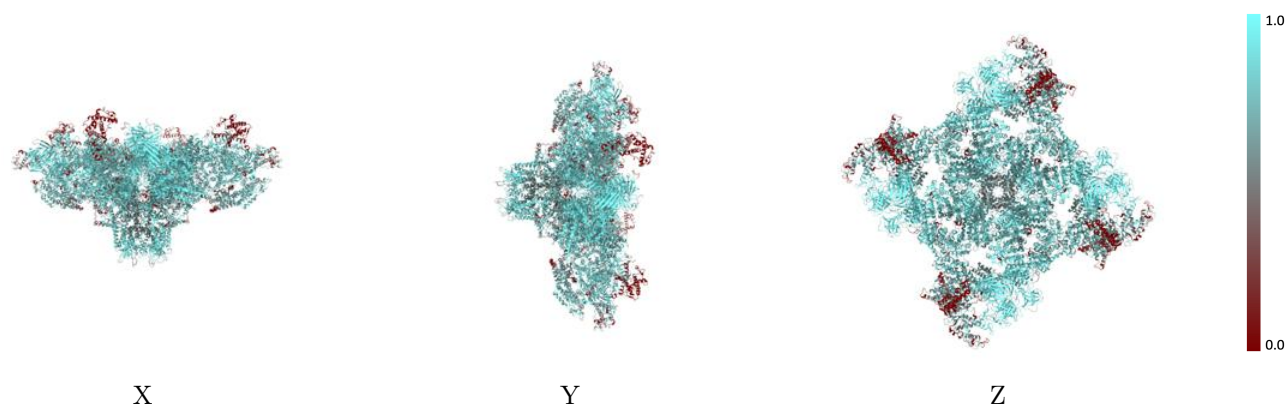
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



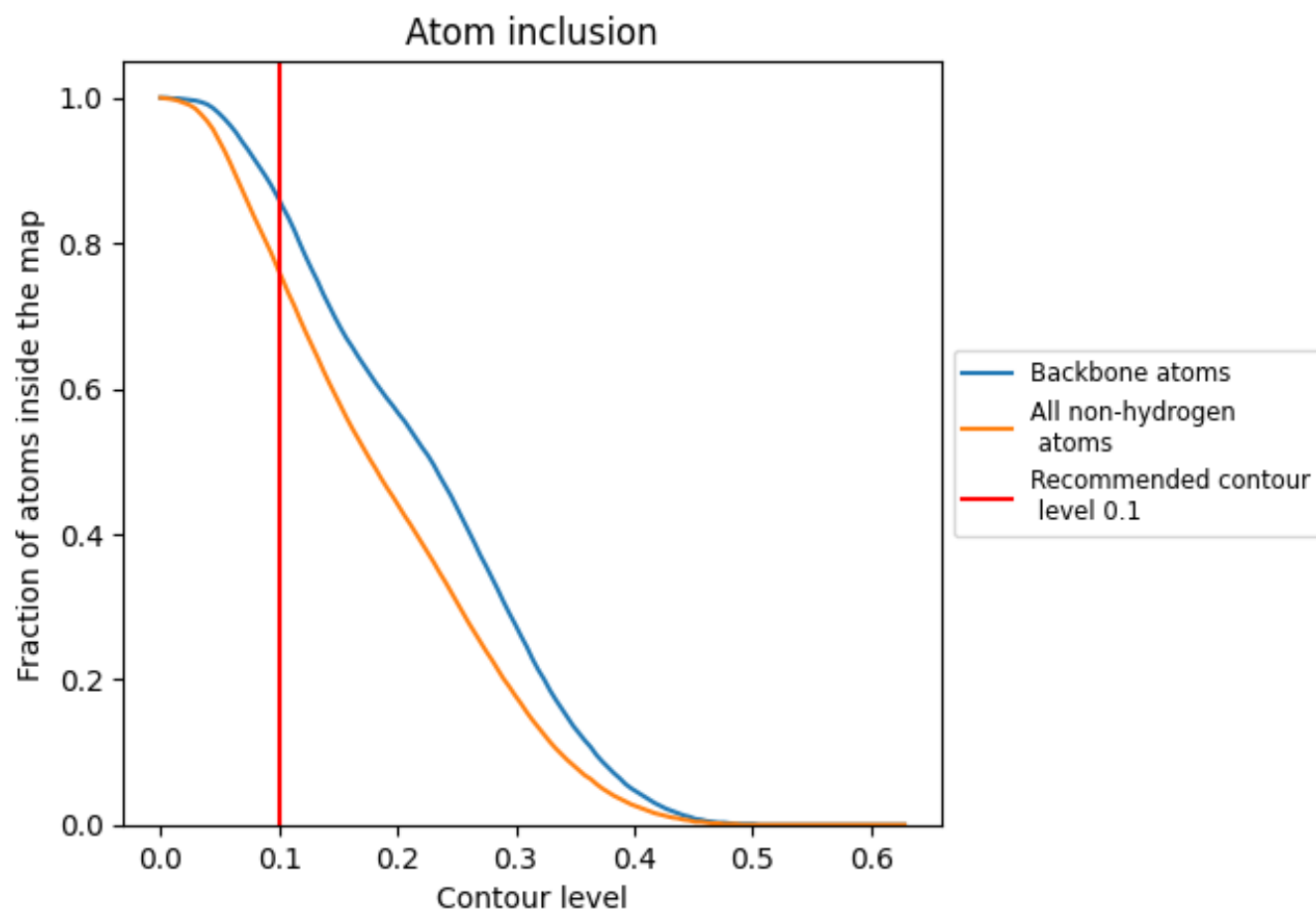
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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></div> 0.7610	<div><div></div></div> 0.5090
A	<div><div></div></div> 0.7600	<div><div></div></div> 0.5080
B	<div><div></div></div> 0.7580	<div><div></div></div> 0.5070
C	<div><div></div></div> 0.7580	<div><div></div></div> 0.5070
D	<div><div></div></div> 0.7580	<div><div></div></div> 0.5070
E	<div><div></div></div> 0.8810	<div><div></div></div> 0.5870
F	<div><div></div></div> 0.8840	<div><div></div></div> 0.5890
G	<div><div></div></div> 0.8770	<div><div></div></div> 0.5850
H	<div><div></div></div> 0.8840	<div><div></div></div> 0.5910

1.0

0.0

<0.0