



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 10:20 PM UTC

PDB ID : 8SES / pdb_00008ses
EMDB ID : EMD-40427
Title : Cryo-EM Structure of RyR1 + Adenine
Authors : Cholak, S.; Saville, J.W.; Zhu, X.; Berezuk, A.M.; Tuttle, K.S.; Haji-Ghassemi, O.; Van Petegem, F.; Subramaniam, S.
Deposited on : 2023-04-10
Resolution : 3.98 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

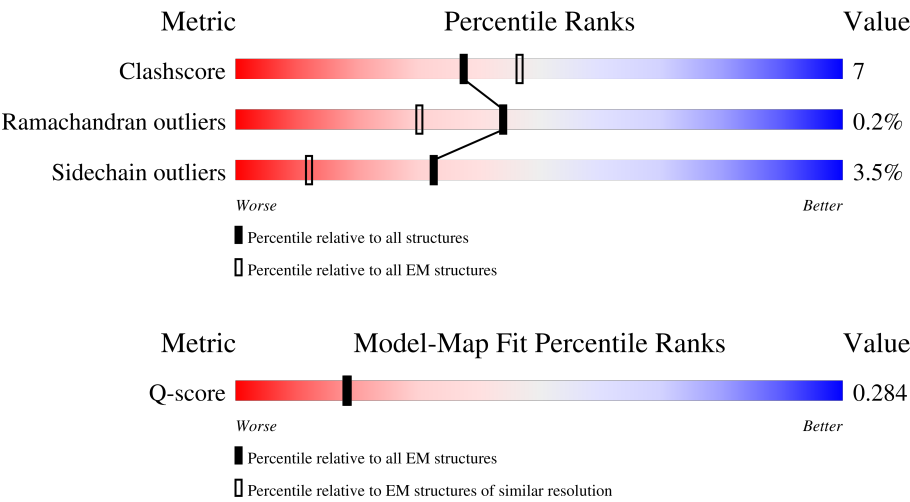
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.98 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7512 (3.48 - 4.48)

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

Mol	Chain	Length	Quality of chain
1	A	5037	12% 68% 18% • 13%
1	B	5037	12% 68% 18% • 13%
1	C	5037	12% 68% 18% • 13%
1	D	5037	12% 68% 18% • 13%

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Mol	Chain	Length	Quality of chain
2	E	350	21%9%69%
2	F	350	21%9%69%
2	G	350	22%9%69%
2	H	350	22%9%69%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 142940 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4377	Total	C	N	O	S	9	0
			34906	22208	6024	6438	236		
1	B	4377	Total	C	N	O	S	9	0
			34906	22208	6024	6438	236		
1	C	4377	Total	C	N	O	S	9	0
			34906	22208	6024	6438	236		
1	D	4377	Total	C	N	O	S	9	0
			34906	22208	6024	6438	236		

- Molecule 2 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-242	MET	-	expression tag	UNP P08515
E	-241	LYS	-	expression tag	UNP P08515
E	-240	SER	-	expression tag	UNP P08515
E	-239	SER	-	expression tag	UNP P08515
E	-238	HIS	-	expression tag	UNP P08515
E	-237	HIS	-	expression tag	UNP P08515
E	-236	HIS	-	expression tag	UNP P08515
E	-235	HIS	-	expression tag	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-234	HIS	-	expression tag	UNP P08515
E	-233	HIS	-	expression tag	UNP P08515
E	-232	GLY	-	expression tag	UNP P08515
E	-231	SER	-	expression tag	UNP P08515
E	-230	SER	-	expression tag	UNP P08515
E	-11	GLY	-	linker	UNP P08515
E	-10	ILE	-	linker	UNP P08515
E	-9	GLU	-	linker	UNP P08515
E	-8	GLU	-	linker	UNP P08515
E	-7	ASN	-	linker	UNP P08515
E	-6	LEU	-	linker	UNP P08515
E	-5	TYR	-	linker	UNP P08515
E	-4	PHE	-	linker	UNP P08515
E	-3	GLN	-	linker	UNP P08515
E	-2	SER	-	linker	UNP P08515
E	-1	ASN	-	linker	UNP P08515
E	0	ALA	-	linker	UNP P08515
F	-242	MET	-	expression tag	UNP P08515
F	-241	LYS	-	expression tag	UNP P08515
F	-240	SER	-	expression tag	UNP P08515
F	-239	SER	-	expression tag	UNP P08515
F	-238	HIS	-	expression tag	UNP P08515
F	-237	HIS	-	expression tag	UNP P08515
F	-236	HIS	-	expression tag	UNP P08515
F	-235	HIS	-	expression tag	UNP P08515
F	-234	HIS	-	expression tag	UNP P08515
F	-233	HIS	-	expression tag	UNP P08515
F	-232	GLY	-	expression tag	UNP P08515
F	-231	SER	-	expression tag	UNP P08515
F	-230	SER	-	expression tag	UNP P08515
F	-11	GLY	-	linker	UNP P08515
F	-10	ILE	-	linker	UNP P08515
F	-9	GLU	-	linker	UNP P08515
F	-8	GLU	-	linker	UNP P08515
F	-7	ASN	-	linker	UNP P08515
F	-6	LEU	-	linker	UNP P08515
F	-5	TYR	-	linker	UNP P08515
F	-4	PHE	-	linker	UNP P08515
F	-3	GLN	-	linker	UNP P08515
F	-2	SER	-	linker	UNP P08515
F	-1	ASN	-	linker	UNP P08515
F	0	ALA	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression tag	UNP P08515
G	-235	HIS	-	expression tag	UNP P08515
G	-234	HIS	-	expression tag	UNP P08515
G	-233	HIS	-	expression tag	UNP P08515
G	-232	GLY	-	expression tag	UNP P08515
G	-231	SER	-	expression tag	UNP P08515
G	-230	SER	-	expression tag	UNP P08515
G	-11	GLY	-	linker	UNP P08515
G	-10	ILE	-	linker	UNP P08515
G	-9	GLU	-	linker	UNP P08515
G	-8	GLU	-	linker	UNP P08515
G	-7	ASN	-	linker	UNP P08515
G	-6	LEU	-	linker	UNP P08515
G	-5	TYR	-	linker	UNP P08515
G	-4	PHE	-	linker	UNP P08515
G	-3	GLN	-	linker	UNP P08515
G	-2	SER	-	linker	UNP P08515
G	-1	ASN	-	linker	UNP P08515
G	0	ALA	-	linker	UNP P08515
H	-242	MET	-	expression tag	UNP P08515
H	-241	LYS	-	expression tag	UNP P08515
H	-240	SER	-	expression tag	UNP P08515
H	-239	SER	-	expression tag	UNP P08515
H	-238	HIS	-	expression tag	UNP P08515
H	-237	HIS	-	expression tag	UNP P08515
H	-236	HIS	-	expression tag	UNP P08515
H	-235	HIS	-	expression tag	UNP P08515
H	-234	HIS	-	expression tag	UNP P08515
H	-233	HIS	-	expression tag	UNP P08515
H	-232	GLY	-	expression tag	UNP P08515
H	-231	SER	-	expression tag	UNP P08515
H	-230	SER	-	expression tag	UNP P08515
H	-11	GLY	-	linker	UNP P08515
H	-10	ILE	-	linker	UNP P08515
H	-9	GLU	-	linker	UNP P08515
H	-8	GLU	-	linker	UNP P08515

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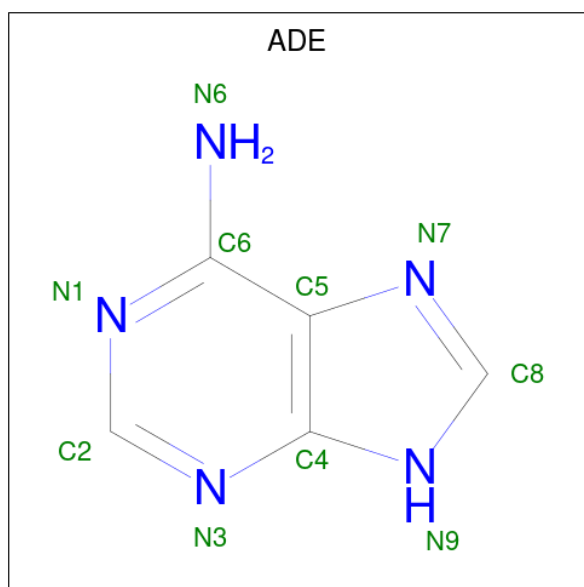
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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ASN	-	linker	UNP P08515
H	-6	LEU	-	linker	UNP P08515
H	-5	TYR	-	linker	UNP P08515
H	-4	PHE	-	linker	UNP P08515
H	-3	GLN	-	linker	UNP P08515
H	-2	SER	-	linker	UNP P08515
H	-1	ASN	-	linker	UNP P08515
H	0	ALA	-	linker	UNP P08515

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

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

- Molecule 4 is ADENINE (CCD ID: ADE) (formula: C₅H₅N₅) (labeled as "Ligand of Interest" by depositor).

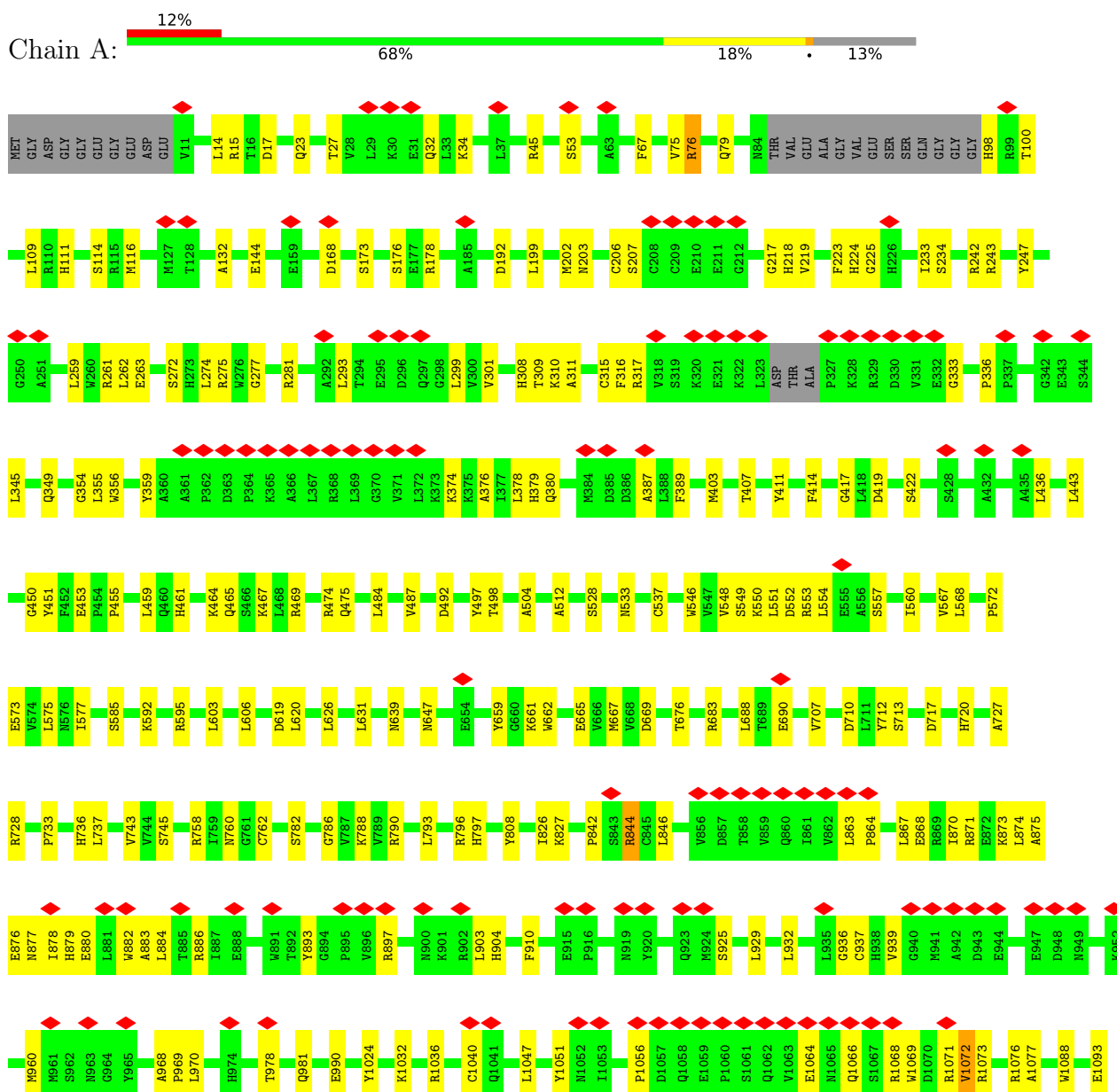


Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total 10	C 5	N 5	0
4	B	1	Total 10	C 5	N 5	0
4	C	1	Total 10	C 5	N 5	0
4	D	1	Total 10	C 5	N 5	0

3 Residue-property plots

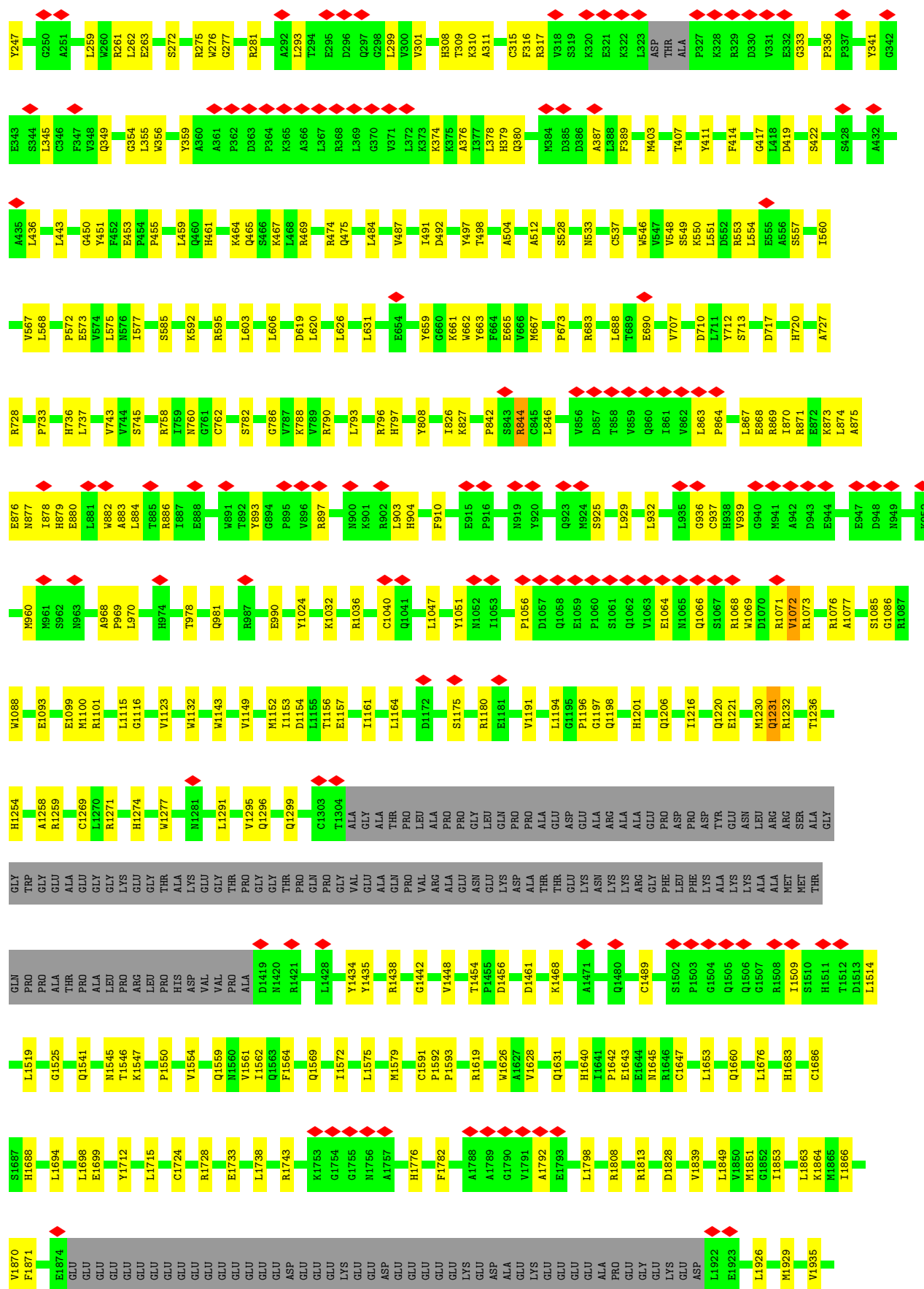
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Ryanodine receptor 1





Q3927	G3786	Y3576	S3474	R3366	R2682	T3157	R3051	L2963	A2896	LYS	S2776
Q3928	K3787	L3579	K3475	E3377	E3265	L3158	H3052	M2967	K2897	LYS	Y2777
S3929	G3788	P3580	S3476	G3380	M3266	D3159	R3053	Q2970	G2898	THR	G2778
D3932	T3797	G3581	K3477	R3380	E3271	D3160	L3056	Q2970	G2899	ARG	E2779
W3935	L3800	R3582	M3478	L3381	E3271	D3162	V3064	E2972	G2900	LYS	N2780
G3939	L3805	E3583	A3479	E3382	P3275	S3171	L3075	F2973	T2901	ILE	N2781
E3944	N3809	D3584	LYS	A3383	M3276	G3174	M3081	E2978	D2902	GLN	D2782
E3945	E3810	D3585	ALA	K3384	E3290	S3174	G3084	A2979	P2903	THR	E2783
Q3946	E3811	A3586	GLY	A3385	A3291	R3187	E3085	G2979	L2904	ALA	E2784
G3947	V3812	A3587	ALA	E3386	P3292	P3188	E3086	S2982	L2905	GLN	L2785
L3948	V3812	E3588	GLN	A3387	P3293	G3191	E3104	S2983	V2906	THR	K2786
L3949	K3823	E3589	ASP	E3388	P3294	L3194	E3105	S2984	P2907	ASP	T2787
L3965	E3824	S3600	GLY	E3389	A3295	R3187	K3105	S2985	D2908	ARG	H2788
T3966	V3826	L3603	ALA	E3390	L3296	P3188	M3106	G2986	Y2909	THR	L2789
G3827	G3827	Y3604	GLN	L3392	P3297	G3191	V3107	V2986	T2910	THR	K2786
F3829	F3829	H3605	ARG	L3393	A3298	K3201	R3111	E2987	L2911	THR	L2791
Q3830	Q3830	L3606	THR	V3394	G3299	P3202	G3112	K2988	T2912	GLY	D2792
L3835	L3835	T3609	LYS	R3395	A3300	A3204	G3113	S2989	A2913	GLY	P2793
V3869	V3869	E3610	LYS	R3403	P3301	P3208	G3114	P2990	K2914	GLY	Y2794
V3990	V3990	E3611	LYS	Y3406	P3302	N3211	V3115	H2991	E2915	GLY	K2795
G3991	G3991	H3611	LYS	R3414	P3303	N3211	G3116	E2992	K2916	GLY	T2796
F3992	F3992	P3612	LYS	Y3415	C3304	N3211	GLN	Q2993	D2861	GLY	F2797
V3995	V3995	K3613	LYS	V3416	S3309	N3211	ALA	K2996	L2862	GLY	S2798
M3999	M3999	S3615	LYS	N3419	N3318	A3215	ARG	F2997	S2863	GLY	E2799
M4000	M4000	K3616	LYS	R3420	N3318	C3216	THR	F2998	G2864	GLY	K2800
M4001	M4001	G3617	LYS	A3421	L3320	S3217	GLN	T3001	V2865	GLY	D2801
Q4009	Q4009	A3618	LYS	H3422	R3321	V3218	VAL	L3002	T2866	GLY	K2802
Q4020	Q4020	K3619	LYS	V3423	I3322	T3221	K3123	N3007	A2923	GLY	E2803
M4023	M4023	T3620	LYS	T3424	N3326	K3222	G3124	Q3008	Q2924	GLY	L2804
M4026	M4026	H3621	LYS	E3426	N3326	S3223	N3128	Q3009	E2925	GLY	Y2805
L4030	L4030	K3622	LYS	P3427	N3326	P3224	L3129	F3010	L2926	GLY	K2806
L4040	L4040	L3434	LYS	L3434	L3329	R3225	T3130	T3011	L2927	GLY	W2807
V4049	V4049	M3437	LYS	M3437	D3330	R3225	T3131	Y3016	K2928	GLY	P2808
M4057	M4057	E3454	LYS	E3454	A3331	T3229	T3132	T3020	F2929	GLY	K2872
L4059	L4059	N3450	LYS	N3450	A3332	L3230	V3134	A3022	L2874	GLY	A2873
K4060	K4060	R3453	LYS	R3453	K3336	G3231	A3135	V3024	E2876	GLY	T2809
F4061	F4061	E3454	LYS	E3454	R3337	G3231	L3136	L3023	Q2877	GLY	K2810
K4069	K4069	N3457	LYS	N3457	L3338	E3238	L3140	V3024	A2879	GLY	E2811
F3887	F3887	R3465	LYS	R3465	A3339	P3241	F3144	L3025	G2893	GLY	L2813
L3888	L3888	N3466	LYS	N3466	V3340	D3242	Q3145	A2936	G2894	GLY	K2814
Q3889	Q3889	K3467	LYS	K3467	Q3343	T3243	H3146	V2935	N2884	GLY	E2815
L3890	L3890	S3468	LYS	S3468	P3344	P3244	I3147	G3026	E2820	GLY	L2817
L3891	L3891	F3469	LYS	F3469	I3345	V3245	Q3149	S3027	W2821	GLY	A2818
Q3900	Q3900	L3470	LYS	L3470	R3350	D3247	F3152	G3028	N2885	GLY	W2819
G4073	G4073	T3471	LYS	T3471	R3350	R3248	D3153	ASP	L2889	GLY	E2822
S4074	S4074	A3472	LYS	A3472	L3354	L3249	D3154	M3038	K2890	GLY	L2823
		M3573	LYS	M3573	F3356	M3250	G3153	E3035	E2892	GLY	E2824
		L3569	LYS	L3569	T3361	G3254	D3154	K3036	K2825	GLY	K2826
		E3670	LYS	E3670	G3254	G3254	G3153	E3037	E2892	GLY	E2827
		T3674	LYS	T3674	G3254	G3254	D3154	M3038	E2893	GLY	E2828
			LYS						E2894	GLY	E2830
			LYS						E2895	GLY	GLU
			LYS							GLY	GLU
			LYS							GLY	ARG
			LYS							GLY	THR
			LYS							GLY	GLU



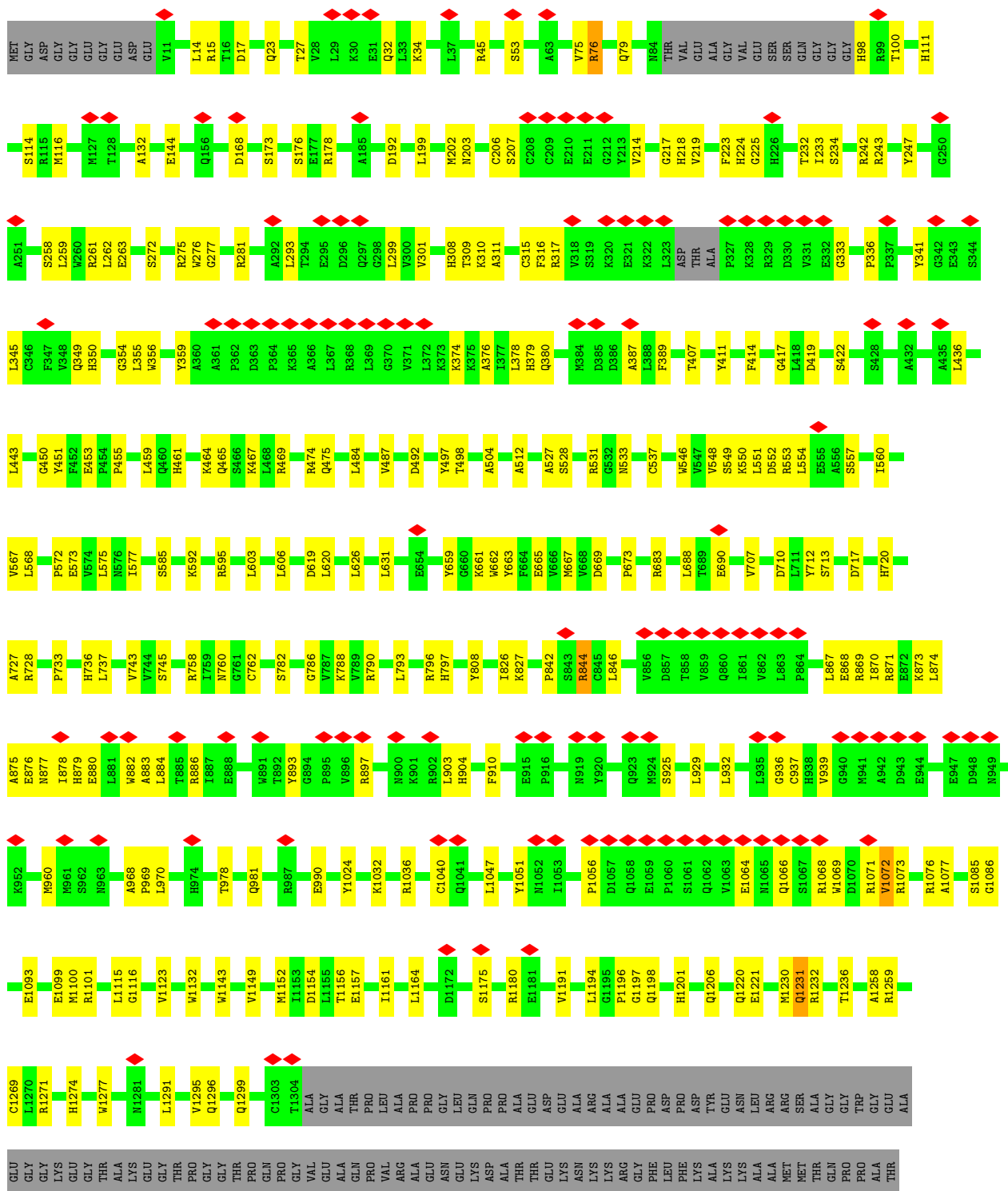
K3222	N3128	T3011	N2933	A2873	L2813	D2752	V2661	L2622	V2397	V2190	ARG	E1944
S3223	L3129	Y3016	Q2934	M2874	K2814	S2763	E2669	F2526	ARG	Q2193	ASP	Y1965
P3224	T3130	T3020	Y2935	A2875	A2815	F2754	R2676	R2531	ARG	R2199	THR	K1968
R3225	T3133	T3021	A2936	Q2877	T2817	I2765	K2677	R2531	ARG	V2207	VAL	L1969
I3229	V3134	A3022	T2937	L2878	A2818	N2756	K2678	R2531	ARG	M2211	LEU	A1983
L3230	A3135	K3023	T2938	A2879	W2819	K2757	F2679	Y2553	GLU	P2207	LEU	F1984
G3231	L3136	R3024	R2939	E2880	E2820	F2758	W2680	K2564	HIS	G2215	VAL	T1985
E3238	L3140	V3024	GLY	N2881	W2821	A2769	G2681	P2567	GLY	L2216	LYS	M1986
F3241	L3143	L3025	LEU	Y2882	T2822	E2760	I2682	H2574	GLU	G2217	LYS	S1987
D3242	F3144	G3026	ASP	Y2883	I2823	H2763	L2686	G2574	GLU	G2218	GLU	A1988
H3243	G3027	S3027	MET	N2884	E2824	E2764	A2687	R2574	GLU	E2219	LYS	A1989
I3244	H3145	G3028	GLU	T2885	K2825	K2765	H2688	L2583	GLU	T2220	PRO	E1990
P3244	H3146	G3029	L2946	W2886	A2826	W2766	K2689	V2586	GLU	M2228	GLU	R1994
V3245	I3147	E3035	D2947	G2887	E2827	A2767	K2690	L2595	GLU	N2246	LEU	S2000
L3246	A3148	K3036	T2948	R2888	E2828	F2768	Y2691	R2600	GLU	Q2247	ALA	P2001
D3247	Q3149	E3037	S2949	K2889	G2829	D2769	Y2696	D2431	GLU	R2248	ALA	P2002
L3249	F3152	K3038	R2954	K2890	E2830	K2770	A2707	D2443	GLU	L2288	GLU	Q2003
K3250	G3153	A3048	F2955	K2891	GLU	I2771	P2711	G2446	GLU	E2296	LEU	E2004
G3254	D3154	L3049	L2960	Q2892	GLU	Q2772	P2712	L2451	GLU	V2299	LEU	Q2005
R3262	I3157	V3050	L2963	E2893	THR	N2773	P2712	R2452	GLU	Q2097	LEU	T2006
E3265	L3158	H3051	L2963	L2894	THR	N2774	D2716	R2453	GLU	V2102	LEU	N2007
K3266	D3159	R3052	M2967	E2895	LYS	W2775	Q2776	R2454	GLU	Q2107	GLU	W2008
E3271	D3160	L3056	S2970	A2896	LYS	S2776	S2770	R2455	GLU	E2108	GLU	L2009
K3275	Q3161	F3057	Q2971	K2897	THR	Y2777	K2772	R2456	GLU	D2109	GLU	H2011
P3276	V3162	V3064	E2972	G2898	ARG	Q2778	E2723	R2459	GLU	Y2110	GLU	V2014
E3290	I3171	V3064	F2973	G2899	ILE	E2779	E2724	S2459	GLU	Q2112	GLU	D2017
A3291	S3174	L3075	I2974	G2900	SER	N2780	E2725	D2464	GLU	M2120	GLU	C2021
F3292	S3174	K3081	E2978	T2901	GLN	W2781	K2725	D2465	GLU	F2121	GLU	P2022
P3293	R3187	G3084	A2979	H2902	THR	D2782	LYS	D2469	GLU	S2122	GLU	L2023
P3294	P3188	P3085	S2982	L2903	ALA	E2783	ALA	T2469	GLU	L2123	GLU	T2027
A3295	G3191	P3085	S2983	L2904	GLN	E2784	THR	L2472	GLU	R2126	GLU	R2028
L3296	L3194	E3104	G2984	L2905	TYR	L2785	VAL	L2479	GLU	Q2127	GLU	L2046
P3297	A3195	K3106	G2985	V2906	ASP	K2786	ASP	K2481	GLU	P2146	GLU	GLY
A3298	R3196	V3107	V2986	V2908	PRO	T2787	ALA	D2482	GLU	R2163	GLU	GLU
G3299	M3201	M3105	V2987	D2909	ARG	H2788	GLY	A2484	GLU	I2167	GLU	GLU
A3300	P3202	R3111	K2988	T2910	GLY	E2789	N2734	F2484	GLU	M2170	GLU	PRO
P3301	A3204	L3112	S2989	L2911	LYS	M2790	F2735	R2650	GLU	E2175	GLU	GLU
P3302	G3208	G3113	K2988	T2912	THR	L2791	D2736	C2651	GLU	E2370	GLU	GLU
P3303	N3211	G3114	K2988	A2913	THR	K2792	P2737	Y2654	GLU	E2371	GLU	THR
C3304	N3214	V3115	K2990	E2915	THR	K2795	P2739	Y2655	GLU	G2372	GLU	SER
S3309	A3215	S3116	K2996	K2916	THR	T2796	E2741	C2656	GLU	G2373	GLU	LEU
N3318	C3216	ALA	F2997	A2917	GLN	F2797	T2742	G2660	GLU	L2377	GLU	SER
L3320	S3217	THR	F2998	D2918	GLN	S2798	N2744	E2513	GLU	P2395	GLU	ARG
R3321	G3218	GLN	F2998	R2920	GLN	E2799	V2745	N2514	GLU	G2396	GLU	LEU
I3322	T3221	VAL	L3001	E2921	THR	K2800	I2746		GLU			
N3325			N3007	K2922	THR	D2801	I2747		GLU			
N3326			Q3008	A2923	THR	K2802	P2748		GLU			
			Y3009	Q2924	THR	E2803	E2749		GLU			
			F3010	E2925	THR	I2804	K2750		GLU			
				L2926	THR	Y2805	L2761		GLU			
				L2927	THR	R2806			GLU			
				K2928	THR	W2807			GLU			
				F2929	THR	P2808			GLU			
				L2930	THR	I2809			GLU			
				Q2931	THR	K2810			GLU			
				M2932	THR	S2812			GLU			





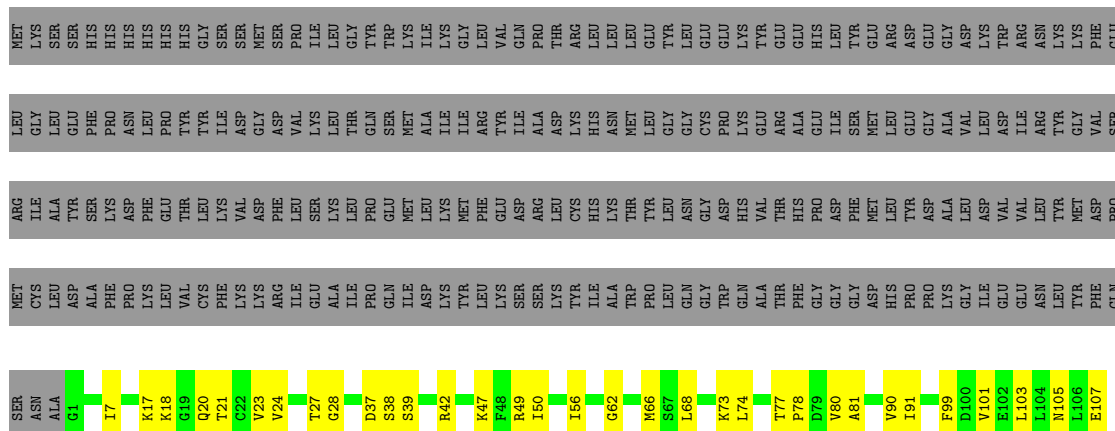












- [illegible]

SER	ASN	ALA	G1	I7	K17	K18	G19	Q20	T21	C22	V23	V24	T27	S38	S39	R42	K47	F48	R49	I50	I56	G62	M66	S67	L68	R71	A72	K73	L74	P78	A81	Y82	V90	I91	F99	D100	V101	E102	L103	L104	N105	L106	E107
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21706	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.200	Depositor
Minimum map value	-0.744	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.305	Depositor
Map size (Å)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.288, 1.288, 1.288	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADE, 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	A	0.30	0/35720	0.67	8/48374 (0.0%)
1	B	0.30	0/35720	0.67	8/48374 (0.0%)
1	C	0.30	0/35720	0.67	8/48374 (0.0%)
1	D	0.30	0/35720	0.67	6/48374 (0.0%)
2	E	0.26	0/834	0.64	0/1123
2	F	0.26	0/834	0.64	0/1123
2	G	0.26	0/834	0.64	0/1123
2	H	0.26	0/834	0.64	0/1123
All	All	0.30	0/146216	0.67	30/197988 (0.0%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	844	ARG	CA-CB-CG	7.34	128.78	114.10
1	D	844	ARG	CA-CB-CG	7.34	128.78	114.10
1	A	844	ARG	CA-CB-CG	7.33	128.77	114.10
1	B	844	ARG	CA-CB-CG	7.32	128.75	114.10
1	A	76	ARG	CG-CD-NE	6.59	126.51	112.00
1	B	76	ARG	CG-CD-NE	6.57	126.46	112.00
1	C	76	ARG	CG-CD-NE	6.57	126.46	112.00
1	D	76	ARG	CG-CD-NE	6.57	126.46	112.00
1	A	844	ARG	N-CA-CB	6.14	119.63	110.29
1	B	844	ARG	N-CA-CB	6.14	119.62	110.29
1	C	844	ARG	N-CA-CB	6.14	119.62	110.29
1	D	844	ARG	N-CA-CB	6.14	119.62	110.29
1	B	1072	VAL	N-CA-CB	-5.66	101.33	111.92
1	C	1072	VAL	N-CA-CB	-5.66	101.33	111.92
1	D	1072	VAL	N-CA-CB	-5.65	101.35	111.92
1	A	1072	VAL	N-CA-CB	-5.65	101.36	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3265	GLU	CA-C-N	-5.08	117.10	122.28
1	B	3265	GLU	C-N-CA	-5.08	117.10	122.28
1	C	3265	GLU	CA-C-N	-5.08	117.10	122.28
1	C	3265	GLU	C-N-CA	-5.08	117.10	122.28
1	A	4909	TYR	CA-C-N	5.06	131.20	121.54
1	A	4909	TYR	C-N-CA	5.06	131.20	121.54
1	A	3265	GLU	CA-C-N	-5.05	117.13	122.28
1	A	3265	GLU	C-N-CA	-5.05	117.13	122.28
1	B	4909	TYR	CA-C-N	5.05	131.18	121.54
1	B	4909	TYR	C-N-CA	5.05	131.18	121.54
1	D	4909	TYR	CA-C-N	5.03	131.15	121.54
1	D	4909	TYR	C-N-CA	5.03	131.15	121.54
1	C	4909	TYR	CA-C-N	5.02	131.13	121.54
1	C	4909	TYR	C-N-CA	5.02	131.13	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	34906	0	34529	508	0
1	B	34906	0	34529	520	0
1	C	34906	0	34529	524	0
1	D	34906	0	34529	523	0
2	E	818	0	824	20	0
2	F	818	0	824	20	0
2	G	818	0	824	19	0
2	H	818	0	824	20	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	10	0	4	1	0
4	B	10	0	4	1	0
4	C	10	0	4	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	10	0	4	1	0
All	All	142940	0	141428	2122	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 7.

All (2122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:844:ARG:HH12	1:C:1197:GLY:HA3	1.45	0.80
1:B:844:ARG:HH12	1:B:1197:GLY:HA3	1.45	0.80
1:A:844:ARG:HH12	1:A:1197:GLY:HA3	1.45	0.79
1:D:844:ARG:HH12	1:D:1197:GLY:HA3	1.45	0.79
1:B:34:LYS:H	1:B:53:SER:HB3	1.49	0.78
1:C:34:LYS:H	1:C:53:SER:HB3	1.49	0.78
1:D:34:LYS:H	1:D:53:SER:HB3	1.49	0.77
1:A:34:LYS:H	1:A:53:SER:HB3	1.49	0.76
1:C:3377:GLU:HA	1:C:3380:ARG:HG2	1.72	0.72
1:D:3377:GLU:HA	1:D:3380:ARG:HG2	1.72	0.72
1:A:2927:LEU:HG	1:A:2931:GLN:HE22	1.55	0.72
1:B:2423:MET:HE1	1:B:2494:PHE:HA	1.72	0.71
1:B:3377:GLU:HA	1:B:3380:ARG:HG2	1.72	0.71
1:D:2927:LEU:HG	1:D:2931:GLN:HE22	1.55	0.71
1:A:3377:GLU:HA	1:A:3380:ARG:HG2	1.72	0.71
1:C:2927:LEU:HG	1:C:2931:GLN:HE22	1.55	0.70
1:C:2423:MET:HE1	1:C:2494:PHE:HA	1.72	0.70
1:A:2423:MET:HE1	1:A:2494:PHE:HA	1.72	0.70
1:D:2423:MET:HE1	1:D:2494:PHE:HA	1.72	0.70
1:B:2927:LEU:HG	1:B:2931:GLN:HE22	1.55	0.70
1:B:4211:LYS:HB3	1:B:4215:ARG:HH21	1.57	0.70
1:A:4211:LYS:HB3	1:A:4215:ARG:HH21	1.57	0.69
1:A:4892:ARG:NH2	1:B:4899:ASP:OD1	2.25	0.69
1:D:4211:LYS:HB3	1:D:4215:ARG:HH21	1.57	0.69
1:A:2215:LEU:O	1:A:2219:GLU:HB2	1.93	0.69
1:C:3420:ARG:HH12	1:C:3519:PRO:HD2	1.57	0.69
1:D:2215:LEU:O	1:D:2219:GLU:HB2	1.93	0.69
1:C:4211:LYS:HB3	1:C:4215:ARG:HH21	1.57	0.68
1:B:3420:ARG:HH12	1:B:3519:PRO:HD2	1.57	0.68
1:A:168:ASP:HB3	1:A:199:LEU:HD11	1.76	0.68
1:A:533:ASN:O	1:A:537:CYS:HB2	1.94	0.68
1:A:3420:ARG:HH12	1:A:3519:PRO:HD2	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:ASN:O	1:C:537:CYS:HB2	1.94	0.67
1:D:3420:ARG:HH12	1:D:3519:PRO:HD2	1.57	0.67
1:B:168:ASP:HB3	1:B:199:LEU:HD11	1.76	0.67
1:D:533:ASN:O	1:D:537:CYS:HB2	1.94	0.67
1:B:533:ASN:O	1:B:537:CYS:HB2	1.94	0.67
1:C:2215:LEU:O	1:C:2219:GLU:HB2	1.93	0.67
1:D:168:ASP:HB3	1:D:199:LEU:HD11	1.76	0.67
1:C:168:ASP:HB3	1:C:199:LEU:HD11	1.76	0.67
1:D:728:ARG:NH2	1:D:1489:CYS:SG	2.69	0.66
1:B:842:PRO:HG3	1:B:1073:ARG:HE	1.60	0.66
2:G:90:VAL:HG12	2:G:91:ILE:HG13	1.78	0.66
1:C:842:PRO:HG3	1:C:1073:ARG:HE	1.61	0.66
1:C:1258:ALA:HB3	1:C:1271:ARG:HB3	1.77	0.66
1:A:842:PRO:HG3	1:A:1073:ARG:HE	1.61	0.66
1:B:2215:LEU:O	1:B:2219:GLU:HB2	1.93	0.66
1:A:1258:ALA:HB3	1:A:1271:ARG:HB3	1.77	0.66
1:B:1258:ALA:HB3	1:B:1271:ARG:HB3	1.77	0.66
1:D:842:PRO:HG3	1:D:1073:ARG:HE	1.61	0.66
1:D:3948:LYS:HD3	1:D:4009:GLN:HE21	1.61	0.66
1:B:728:ARG:NH2	1:B:1489:CYS:SG	2.69	0.66
1:C:728:ARG:NH2	1:C:1489:CYS:SG	2.69	0.65
1:A:728:ARG:NH2	1:A:1489:CYS:SG	2.69	0.65
1:B:2469:ILE:HB	1:B:2502:MET:HE1	1.78	0.65
1:D:981:GLN:HG2	1:D:1047:LEU:HD11	1.78	0.65
1:B:2248:ARG:HH22	1:B:3870:ASN:HB2	1.61	0.65
1:C:2469:ILE:HB	1:C:2502:MET:HE1	1.78	0.65
2:F:90:VAL:HG12	2:F:91:ILE:HG13	1.78	0.65
2:H:90:VAL:HG12	2:H:91:ILE:HG13	1.78	0.65
1:C:981:GLN:HG2	1:C:1047:LEU:HD11	1.78	0.65
1:C:2248:ARG:HH22	1:C:3870:ASN:HB2	1.61	0.65
1:A:475:GLN:NE2	1:A:528:SER:O	2.30	0.65
1:A:3842:LEU:HD23	1:A:3875:MET:HE3	1.78	0.65
1:B:233:ILE:HD12	1:B:242:ARG:HB3	1.78	0.65
1:C:3842:LEU:HD23	1:C:3875:MET:HE3	1.78	0.65
1:D:475:GLN:NE2	1:D:528:SER:O	2.30	0.65
1:A:3247:ASP:HA	1:A:3250:MET:HE2	1.79	0.65
1:B:4978:HIS:HA	1:B:4982:GLU:HG3	1.78	0.65
1:D:3247:ASP:HA	1:D:3250:MET:HE2	1.79	0.65
1:B:981:GLN:HG2	1:B:1047:LEU:HD11	1.78	0.65
1:C:4978:HIS:HA	1:C:4982:GLU:HG3	1.78	0.65
1:D:233:ILE:HD12	1:D:242:ARG:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:GLN:NE2	1:C:528:SER:O	2.30	0.65
1:D:2469:ILE:HB	1:D:2502:MET:HE1	1.78	0.65
1:B:173:SER:HB3	1:B:178:ARG:H	1.62	0.64
1:B:1093:GLU:HB3	1:B:1201:HIS:HB3	1.79	0.64
1:D:1258:ALA:HB3	1:D:1271:ARG:HB3	1.77	0.64
1:A:3948:LYS:HD3	1:A:4009:GLN:HE21	1.61	0.64
1:A:4978:HIS:HA	1:A:4982:GLU:HG3	1.78	0.64
1:C:233:ILE:HD12	1:C:242:ARG:HB3	1.78	0.64
1:D:1093:GLU:HB3	1:D:1201:HIS:HB3	1.79	0.64
1:A:2469:ILE:HB	1:A:2502:MET:HE1	1.78	0.64
1:B:3842:LEU:HD23	1:B:3875:MET:HE3	1.78	0.64
1:B:3948:LYS:HD3	1:B:4009:GLN:HE21	1.61	0.64
1:D:2248:ARG:HH22	1:D:3870:ASN:HB2	1.61	0.64
2:E:90:VAL:HG12	2:E:91:ILE:HG13	1.78	0.64
1:A:981:GLN:HG2	1:A:1047:LEU:HD11	1.79	0.64
1:D:4978:HIS:HA	1:D:4982:GLU:HG3	1.78	0.64
1:A:2248:ARG:HH22	1:A:3870:ASN:HB2	1.61	0.64
1:B:475:GLN:NE2	1:B:528:SER:O	2.30	0.64
1:B:3247:ASP:HA	1:B:3250:MET:HE2	1.79	0.64
1:C:173:SER:HB3	1:C:178:ARG:H	1.62	0.64
1:C:3247:ASP:HA	1:C:3250:MET:HE2	1.79	0.64
1:C:3948:LYS:HD3	1:C:4009:GLN:HE21	1.61	0.64
1:B:3927:GLN:HE21	1:B:3991:GLY:HA3	1.63	0.64
1:D:3842:LEU:HD23	1:D:3875:MET:HE3	1.78	0.64
1:A:1093:GLU:HB3	1:A:1201:HIS:HB3	1.79	0.64
1:C:1093:GLU:HB3	1:C:1201:HIS:HB3	1.79	0.64
1:A:233:ILE:HD12	1:A:242:ARG:HB3	1.78	0.63
1:D:745:SER:HB2	1:D:758:ARG:HB2	1.81	0.63
1:D:173:SER:HB3	1:D:178:ARG:H	1.62	0.63
1:A:173:SER:HB3	1:A:178:ARG:H	1.62	0.63
1:D:293:LEU:HD12	1:D:378:LEU:HD23	1.81	0.63
1:C:3927:GLN:HE21	1:C:3991:GLY:HA3	1.63	0.63
1:D:3927:GLN:HE21	1:D:3991:GLY:HA3	1.63	0.63
1:A:293:LEU:HD12	1:A:378:LEU:HD23	1.81	0.63
1:A:3927:GLN:HE21	1:A:3991:GLY:HA3	1.63	0.63
1:A:745:SER:HB2	1:A:758:ARG:HB2	1.81	0.62
1:B:745:SER:HB2	1:B:758:ARG:HB2	1.81	0.62
1:A:451:TYR:O	1:A:474:ARG:NH1	2.33	0.62
1:C:1100:MET:HE3	1:C:1198:GLN:HB3	1.81	0.62
1:D:897:ARG:HB2	1:D:903:LEU:HD11	1.82	0.62
1:B:293:LEU:HD12	1:B:378:LEU:HD23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:TYR:O	1:B:474:ARG:NH1	2.33	0.62
1:A:897:ARG:HB2	1:A:903:LEU:HD11	1.82	0.62
1:B:1100:MET:HE3	1:B:1198:GLN:HB3	1.81	0.62
1:D:451:TYR:O	1:D:474:ARG:NH1	2.33	0.62
1:D:667:MET:HB3	1:D:790:ARG:HB2	1.82	0.62
1:A:978:THR:OG1	1:A:981:GLN:OE1	2.18	0.62
1:B:234:SER:HB2	1:B:242:ARG:HA	1.82	0.62
1:C:234:SER:HB2	1:C:242:ARG:HA	1.82	0.62
1:C:745:SER:HB2	1:C:758:ARG:HB2	1.81	0.62
2:F:49:ARG:HH21	2:F:50:ILE:HG12	1.65	0.62
1:A:3050:VAL:HG11	1:A:3064:VAL:HG11	1.82	0.61
2:H:49:ARG:HH21	2:H:50:ILE:HG12	1.65	0.61
1:C:293:LEU:HD12	1:C:378:LEU:HD23	1.81	0.61
1:D:3050:VAL:HG11	1:D:3064:VAL:HG11	1.82	0.61
1:A:1024:TYR:O	1:A:1032:LYS:NZ	2.34	0.61
1:A:1100:MET:HE3	1:A:1198:GLN:HB3	1.81	0.61
1:B:978:THR:OG1	1:B:981:GLN:OE1	2.18	0.61
2:E:49:ARG:HH21	2:E:50:ILE:HG12	1.65	0.61
1:C:451:TYR:O	1:C:474:ARG:NH1	2.33	0.61
1:D:1100:MET:HE3	1:D:1198:GLN:HB3	1.81	0.61
1:A:234:SER:HB2	1:A:242:ARG:HA	1.82	0.61
1:B:2630:VAL:HG12	1:B:2682:ILE:HD11	1.83	0.61
1:C:978:THR:OG1	1:C:981:GLN:OE1	2.18	0.61
1:C:1024:TYR:O	1:C:1032:LYS:NZ	2.33	0.61
1:C:2630:VAL:HG12	1:C:2682:ILE:HD11	1.83	0.61
1:D:3420:ARG:HH22	1:D:3519:PRO:HB2	1.66	0.61
1:B:1575:LEU:HB3	1:B:1579:MET:HE1	1.83	0.61
1:C:3420:ARG:HH22	1:C:3519:PRO:HB2	1.66	0.61
1:A:3420:ARG:HH22	1:A:3519:PRO:HB2	1.66	0.61
1:B:897:ARG:HB2	1:B:903:LEU:HD11	1.82	0.61
1:B:4892:ARG:NH2	1:C:4899:ASP:OD1	2.34	0.61
1:C:3050:VAL:HG11	1:C:3064:VAL:HG11	1.82	0.61
1:D:234:SER:HB2	1:D:242:ARG:HA	1.82	0.61
2:G:49:ARG:HH21	2:G:50:ILE:HG12	1.65	0.61
1:A:2630:VAL:HG12	1:A:2682:ILE:HD11	1.83	0.60
1:B:1024:TYR:O	1:B:1032:LYS:NZ	2.34	0.60
1:A:1575:LEU:HB3	1:A:1579:MET:HE1	1.83	0.60
1:B:3050:VAL:HG11	1:B:3064:VAL:HG11	1.82	0.60
1:B:3420:ARG:HH22	1:B:3519:PRO:HB2	1.66	0.60
1:D:2630:VAL:HG12	1:D:2682:ILE:HD11	1.83	0.60
1:A:1569:GLN:HB2	1:A:1572:ILE:HD12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:667:MET:HB3	1:C:790:ARG:HB2	1.82	0.60
1:A:667:MET:HB3	1:A:790:ARG:HB2	1.82	0.60
1:A:4680:LYS:HE3	1:A:4686:LEU:HD22	1.83	0.60
1:B:317:ARG:NH1	1:B:349:GLN:OE1	2.34	0.60
1:B:4680:LYS:HE3	1:B:4686:LEU:HD22	1.83	0.60
1:D:1575:LEU:HB3	1:D:1579:MET:HE1	1.83	0.60
1:D:3106:MET:HE1	1:D:3129:LEU:HA	1.83	0.60
1:B:667:MET:HB3	1:B:790:ARG:HB2	1.82	0.60
1:C:897:ARG:HB2	1:C:903:LEU:HD11	1.82	0.60
1:C:1569:GLN:HB2	1:C:1572:ILE:HD12	1.84	0.60
1:C:4892:ARG:NH2	1:D:4899:ASP:OD1	2.34	0.60
1:D:978:THR:OG1	1:D:981:GLN:OE1	2.18	0.60
1:A:1653:LEU:O	1:A:1660:GLN:NE2	2.35	0.60
1:C:1575:LEU:HB3	1:C:1579:MET:HE1	1.83	0.60
1:C:3106:MET:HE1	1:C:3129:LEU:HA	1.83	0.60
1:D:1569:GLN:HB2	1:D:1572:ILE:HD12	1.84	0.60
1:C:317:ARG:NH1	1:C:349:GLN:OE1	2.34	0.60
1:D:3157:ILE:HG22	1:D:3162:GLN:HG2	1.83	0.60
1:B:1569:GLN:HB2	1:B:1572:ILE:HD12	1.84	0.60
1:D:317:ARG:NH1	1:D:349:GLN:OE1	2.34	0.60
1:B:3157:ILE:HG22	1:B:3162:GLN:HG2	1.83	0.59
1:D:1024:TYR:O	1:D:1032:LYS:NZ	2.33	0.59
1:A:317:ARG:NH1	1:A:349:GLN:OE1	2.34	0.59
1:D:359:TYR:HA	1:D:376:ALA:HA	1.85	0.59
1:C:3157:ILE:HG22	1:C:3162:GLN:HG2	1.83	0.59
1:A:359:TYR:HA	1:A:376:ALA:HA	1.85	0.59
1:A:1808:ARG:NH1	1:A:1853:ILE:O	2.36	0.59
1:C:359:TYR:HA	1:C:376:ALA:HA	1.85	0.59
1:C:1196:PRO:O	1:C:1198:GLN:NE2	2.36	0.59
1:C:1653:LEU:O	1:C:1660:GLN:NE2	2.34	0.59
1:D:4680:LYS:HE3	1:D:4686:LEU:HD22	1.83	0.59
1:B:3106:MET:HE1	1:B:3129:LEU:HA	1.83	0.59
1:A:3106:MET:HE1	1:A:3129:LEU:HA	1.83	0.59
1:D:2001:PRO:HG2	1:D:3864:THR:HB	1.85	0.59
1:B:359:TYR:HA	1:B:376:ALA:HA	1.85	0.59
1:D:683:ARG:HG2	1:D:717:ASP:HB3	1.85	0.59
1:A:2929:PHE:O	1:A:2933:ASN:ND2	2.36	0.58
1:A:3157:ILE:HG22	1:A:3162:GLN:HG2	1.83	0.58
1:B:2929:PHE:O	1:B:2933:ASN:ND2	2.36	0.58
1:C:1808:ARG:NH1	1:C:1853:ILE:O	2.36	0.58
1:C:4680:LYS:HE3	1:C:4686:LEU:HD22	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1969:LEU:HD12	1:C:2009:LEU:HD13	1.85	0.58
1:D:3053:ARG:HA	1:D:3056:LEU:HD13	1.86	0.58
1:B:3053:ARG:HA	1:B:3056:LEU:HD13	1.86	0.58
1:C:683:ARG:HG2	1:C:717:ASP:HB3	1.85	0.58
1:D:1561:VAL:HG12	1:D:1562:ILE:HG23	1.85	0.58
1:A:882:TRP:O	1:A:886:ARG:NH1	2.36	0.58
1:A:1196:PRO:O	1:A:1198:GLN:NE2	2.36	0.58
1:A:3007:ASN:O	1:A:3011:THR:OG1	2.21	0.58
1:C:1808:ARG:HD3	1:C:1853:ILE:HG22	1.85	0.58
1:C:3007:ASN:O	1:C:3011:THR:OG1	2.21	0.58
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	1.85	0.58
1:A:1969:LEU:HD12	1:A:2009:LEU:HD13	1.85	0.58
1:A:2001:PRO:HG2	1:A:3864:THR:HB	1.85	0.58
1:B:1808:ARG:HD3	1:B:1853:ILE:HG22	1.85	0.58
1:D:707:VAL:HG23	1:D:782:SER:HB3	1.85	0.58
1:D:1808:ARG:NH1	1:D:1853:ILE:O	2.36	0.58
1:A:683:ARG:HG2	1:A:717:ASP:HB3	1.85	0.58
1:A:3051:ARG:O	1:A:3053:ARG:NE	2.36	0.58
1:B:882:TRP:O	1:B:886:ARG:NH1	2.37	0.58
1:B:1561:VAL:HG12	1:B:1562:ILE:HG23	1.85	0.58
1:C:3053:ARG:HA	1:C:3056:LEU:HD13	1.86	0.58
1:D:3007:ASN:O	1:D:3011:THR:OG1	2.21	0.58
1:A:3053:ARG:HA	1:A:3056:LEU:HD13	1.86	0.58
1:B:707:VAL:HG23	1:B:782:SER:HB3	1.85	0.58
1:C:882:TRP:O	1:C:886:ARG:NH1	2.37	0.58
1:C:3309:SER:OG	1:C:3350:ARG:NH2	2.37	0.58
1:D:459:LEU:O	1:D:464:LYS:NZ	2.37	0.58
1:A:707:VAL:HG23	1:A:782:SER:HB3	1.85	0.58
1:B:1808:ARG:NH1	1:B:1853:ILE:O	2.36	0.58
1:D:882:TRP:O	1:D:886:ARG:NH1	2.37	0.58
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	1.85	0.58
1:B:1653:LEU:O	1:B:1660:GLN:NE2	2.34	0.57
1:B:3007:ASN:O	1:B:3011:THR:OG1	2.21	0.57
1:C:2747:ILE:HB	1:C:2814:LYS:HG2	1.86	0.57
1:C:3075:LEU:O	1:C:3146:HIS:NE2	2.33	0.57
1:D:1969:LEU:HD12	1:D:2009:LEU:HD13	1.85	0.57
1:D:2929:PHE:O	1:D:2933:ASN:ND2	2.36	0.57
1:A:1808:ARG:HD3	1:A:1853:ILE:HG22	1.85	0.57
1:A:2000:SER:O	1:A:2005:GLN:NE2	2.37	0.57
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	1.85	0.57
1:B:1969:LEU:HD12	1:B:2009:LEU:HD13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3309:SER:OG	1:B:3350:ARG:NH2	2.37	0.57
1:C:1561:VAL:HG12	1:C:1562:ILE:HG23	1.85	0.57
1:C:3051:ARG:O	1:C:3053:ARG:NE	2.36	0.57
1:A:659:TYR:O	1:A:662:TRP:NE1	2.37	0.57
1:B:2001:PRO:HG2	1:B:3864:THR:HB	1.85	0.57
1:C:277:GLY:HA2	1:C:315:CYS:HB3	1.87	0.57
1:C:659:TYR:O	1:C:662:TRP:NE1	2.37	0.57
1:D:1808:ARG:HD3	1:D:1853:ILE:HG22	1.85	0.57
1:A:4899:ASP:OD1	1:D:4892:ARG:NH2	2.38	0.57
1:B:277:GLY:HA2	1:B:315:CYS:HB3	1.87	0.57
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.85	0.57
1:B:683:ARG:HG2	1:B:717:ASP:HB3	1.85	0.57
1:D:3075:LEU:O	1:D:3146:HIS:NE2	2.33	0.57
1:A:1683:HIS:NE2	1:A:1798:LEU:O	2.36	0.57
1:B:2747:ILE:HB	1:B:2814:LYS:HG2	1.86	0.57
1:B:4864:ASN:ND2	1:B:4874:MET:SD	2.78	0.57
1:C:459:LEU:O	1:C:464:LYS:NZ	2.37	0.57
1:A:459:LEU:O	1:A:464:LYS:NZ	2.37	0.57
1:A:3850:GLN:NE2	1:A:3872:GLU:OE1	2.38	0.57
1:A:1561:VAL:HG12	1:A:1562:ILE:HG23	1.85	0.57
1:B:659:TYR:O	1:B:662:TRP:NE1	2.37	0.57
1:B:1196:PRO:O	1:B:1198:GLN:NE2	2.36	0.57
1:C:707:VAL:HG23	1:C:782:SER:HB3	1.85	0.57
1:D:659:TYR:O	1:D:662:TRP:NE1	2.37	0.57
1:A:3107:VAL:HG11	1:A:3171:SER:HB2	1.87	0.57
1:C:277:GLY:N	1:C:316:PHE:O	2.38	0.57
1:C:2446:GLY:HA2	1:C:2451:LEU:HD21	1.86	0.57
1:C:4864:ASN:ND2	1:C:4874:MET:SD	2.78	0.57
1:D:1870:VAL:HG11	1:D:2097:LEU:HD22	1.86	0.57
1:D:2595:LEU:O	1:D:2600:ARG:NH2	2.38	0.57
1:D:3051:ARG:O	1:D:3053:ARG:NE	2.36	0.57
1:A:277:GLY:N	1:A:316:PHE:O	2.38	0.57
1:A:886:ARG:HE	1:A:904:HIS:HB2	1.70	0.57
1:B:2000:SER:O	1:B:2005:GLN:NE2	2.37	0.57
1:D:1653:LEU:O	1:D:1660:GLN:NE2	2.35	0.57
1:D:2446:GLY:HA2	1:D:2451:LEU:HD21	1.86	0.57
1:D:3850:GLN:NE2	1:D:3872:GLU:OE1	2.38	0.57
1:C:2929:PHE:O	1:C:2933:ASN:ND2	2.36	0.56
1:C:3107:VAL:HG11	1:C:3171:SER:HB2	1.87	0.56
1:D:1299:GLN:NE2	1:D:1545:ASN:OD1	2.38	0.56
1:D:2747:ILE:HB	1:D:2814:LYS:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2747:ILE:HB	1:A:2814:LYS:HG2	1.86	0.56
1:B:886:ARG:HE	1:B:904:HIS:HB2	1.70	0.56
1:D:4864:ASN:ND2	1:D:4874:MET:SD	2.78	0.56
1:A:1870:VAL:HG11	1:A:2097:LEU:HD22	1.86	0.56
1:B:277:GLY:N	1:B:316:PHE:O	2.38	0.56
1:B:1870:VAL:HG11	1:B:2097:LEU:HD22	1.86	0.56
1:B:2110:TYR:O	1:B:2112:GLN:NE2	2.39	0.56
1:B:2891:LYS:HA	1:B:2894:LEU:HB3	1.87	0.56
1:B:3107:VAL:HG11	1:B:3171:SER:HB2	1.87	0.56
1:B:3850:GLN:NE2	1:B:3872:GLU:OE1	2.38	0.56
1:C:1277:TRP:HD1	1:C:1559:GLN:HG3	1.71	0.56
1:C:2001:PRO:HG2	1:C:3864:THR:HB	1.85	0.56
1:D:277:GLY:HA2	1:D:315:CYS:HB3	1.87	0.56
1:D:1196:PRO:O	1:D:1198:GLN:NE2	2.36	0.56
1:D:1277:TRP:HD1	1:D:1559:GLN:HG3	1.71	0.56
1:D:2110:TYR:O	1:D:2112:GLN:NE2	2.39	0.56
1:D:2656:CYS:HA	1:D:2711:PRO:HG3	1.87	0.56
1:D:2770:LYS:HD3	1:D:2787:THR:HB	1.88	0.56
1:D:2891:LYS:HA	1:D:2894:LEU:HB3	1.87	0.56
1:A:277:GLY:HA2	1:A:315:CYS:HB3	1.87	0.56
1:A:2595:LEU:O	1:A:2600:ARG:NH2	2.38	0.56
1:A:3628:ARG:NH1	1:A:3857:GLY:O	2.38	0.56
1:A:4864:ASN:ND2	1:A:4874:MET:SD	2.78	0.56
1:C:1299:GLN:NE2	1:C:1545:ASN:OD1	2.38	0.56
1:C:4581:LYS:NZ	1:C:4582:VAL:O	2.38	0.56
1:D:3628:ARG:NH1	1:D:3857:GLY:O	2.38	0.56
1:A:1299:GLN:NE2	1:A:1545:ASN:OD1	2.38	0.56
1:A:3309:SER:OG	1:A:3350:ARG:NH2	2.37	0.56
1:B:2446:GLY:HA2	1:B:2451:LEU:HD21	1.86	0.56
1:B:2595:LEU:O	1:B:2600:ARG:NH2	2.38	0.56
1:B:3322:ILE:O	1:B:3326:ASN:ND2	2.33	0.56
1:C:3628:ARG:NH1	1:C:3857:GLY:O	2.38	0.56
1:C:3850:GLN:NE2	1:C:3872:GLU:OE1	2.38	0.56
1:D:3107:VAL:HG11	1:D:3171:SER:HB2	1.87	0.56
1:B:2656:CYS:HA	1:B:2711:PRO:HG3	1.87	0.56
1:C:2595:LEU:O	1:C:2600:ARG:NH2	2.38	0.56
1:D:3322:ILE:O	1:D:3326:ASN:ND2	2.33	0.56
1:A:2110:TYR:O	1:A:2112:GLN:NE2	2.39	0.56
1:C:1870:VAL:HG11	1:C:2097:LEU:HD22	1.86	0.56
1:C:2656:CYS:HA	1:C:2711:PRO:HG3	1.87	0.56
1:D:277:GLY:N	1:D:316:PHE:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:ARG:NH2	1:A:631:LEU:O	2.39	0.56
1:B:1299:GLN:NE2	1:B:1545:ASN:OD1	2.38	0.56
1:C:223:PHE:HB2	1:C:389:PHE:HB2	1.88	0.56
1:D:2000:SER:O	1:D:2005:GLN:NE2	2.37	0.56
1:B:4030:LEU:HG	1:B:4040:ILE:HD11	1.88	0.56
1:C:2770:LYS:HD3	1:C:2787:THR:HB	1.87	0.56
1:D:886:ARG:HE	1:D:904:HIS:HB2	1.70	0.56
1:D:3420:ARG:NH1	1:D:3516:LYS:O	2.39	0.56
1:A:2927:LEU:O	1:A:2931:GLN:NE2	2.39	0.56
1:B:595:ARG:NH2	1:B:631:LEU:O	2.39	0.56
1:B:1277:TRP:HD1	1:B:1559:GLN:HG3	1.71	0.56
1:B:3420:ARG:NH1	1:B:3516:LYS:O	2.39	0.56
1:C:2110:TYR:O	1:C:2112:GLN:NE2	2.39	0.56
1:C:3769:ARG:O	1:C:3773:ARG:NH1	2.39	0.56
1:C:4030:LEU:HG	1:C:4040:ILE:HD11	1.88	0.56
1:D:4581:LYS:NZ	1:D:4582:VAL:O	2.38	0.56
1:D:4983:HIS:O	4:D:5102:ADE:N6	2.39	0.56
1:A:1277:TRP:HD1	1:A:1559:GLN:HG3	1.71	0.55
1:A:2770:LYS:HD3	1:A:2787:THR:HB	1.87	0.55
1:A:3420:ARG:NH1	1:A:3516:LYS:O	2.39	0.55
1:B:2971:GLN:HA	1:B:2974:ILE:HG12	1.88	0.55
1:B:3051:ARG:O	1:B:3053:ARG:NE	2.36	0.55
1:B:3693:LYS:NZ	1:B:3695:PRO:O	2.39	0.55
1:C:886:ARG:HE	1:C:904:HIS:HB2	1.70	0.55
1:C:1206:GLN:NE2	1:C:1230:MET:O	2.39	0.55
1:D:1101:ARG:NH1	1:D:1115:LEU:O	2.39	0.55
1:D:3900:GLN:NE2	1:D:3967:GLU:O	2.40	0.55
1:A:2656:CYS:HA	1:A:2711:PRO:HG3	1.87	0.55
1:A:2971:GLN:HA	1:A:2974:ILE:HG12	1.89	0.55
1:B:1206:GLN:NE2	1:B:1230:MET:O	2.39	0.55
1:C:1792:ALA:O	1:C:2176:ASN:ND2	2.38	0.55
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	2.24	0.55
1:A:2891:LYS:HA	1:A:2894:LEU:HB3	1.87	0.55
1:C:595:ARG:NH2	1:C:631:LEU:O	2.39	0.55
1:C:2927:LEU:O	1:C:2931:GLN:NE2	2.39	0.55
1:D:595:ARG:NH2	1:D:631:LEU:O	2.39	0.55
1:A:1156:THR:OG1	1:A:1157:GLU:OE1	2.24	0.55
1:A:2021:CYS:O	1:A:2028:ARG:NH2	2.40	0.55
1:A:3693:LYS:NZ	1:A:3695:PRO:O	2.39	0.55
1:D:2021:CYS:O	1:D:2028:ARG:NH2	2.40	0.55
1:D:2927:LEU:O	1:D:2931:GLN:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3309:SER:OG	1:D:3350:ARG:NH2	2.37	0.55
1:D:3693:LYS:NZ	1:D:3695:PRO:O	2.39	0.55
1:A:1101:ARG:NH1	1:A:1115:LEU:O	2.39	0.55
1:B:3628:ARG:NH1	1:B:3857:GLY:O	2.38	0.55
1:C:1156:THR:OG1	1:C:1157:GLU:OE1	2.24	0.55
1:C:2021:CYS:O	1:C:2028:ARG:NH2	2.40	0.55
1:D:417:GLY:HA3	1:D:436:LEU:HD21	1.88	0.55
1:A:144:GLU:OE1	1:D:2452:ARG:NH1	2.40	0.55
1:A:2626:LEU:HD22	1:A:2640:PRO:HB3	1.89	0.55
1:A:3900:GLN:NE2	1:A:3967:GLU:O	2.40	0.55
1:B:2021:CYS:O	1:B:2028:ARG:NH2	2.40	0.55
1:B:2770:LYS:HD3	1:B:2787:THR:HB	1.87	0.55
1:C:3693:LYS:NZ	1:C:3695:PRO:O	2.39	0.55
1:D:223:PHE:HB2	1:D:389:PHE:HB2	1.88	0.55
1:D:2875:ALA:HB2	1:D:2927:LEU:HD22	1.89	0.55
1:A:3132:THR:HG23	1:A:3136:LEU:HD23	1.88	0.55
1:B:1792:ALA:O	1:B:2176:ASN:ND2	2.38	0.55
1:B:2927:LEU:O	1:B:2931:GLN:NE2	2.39	0.55
1:C:1101:ARG:NH1	1:C:1115:LEU:O	2.39	0.55
1:C:2000:SER:O	1:C:2005:GLN:NE2	2.37	0.55
1:C:2891:LYS:HA	1:C:2894:LEU:HB3	1.87	0.55
1:C:4983:HIS:O	4:C:5102:ADE:N6	2.39	0.55
1:D:1792:ALA:O	1:D:2176:ASN:ND2	2.38	0.55
1:A:223:PHE:HB2	1:A:389:PHE:HB2	1.88	0.55
1:A:1206:GLN:NE2	1:A:1230:MET:O	2.39	0.55
1:A:2446:GLY:HA2	1:A:2451:LEU:HD21	1.86	0.55
1:A:4983:HIS:O	4:A:5102:ADE:N6	2.39	0.55
1:B:459:LEU:O	1:B:464:LYS:NZ	2.37	0.55
1:B:2626:LEU:HD22	1:B:2640:PRO:HB3	1.89	0.55
1:D:2626:LEU:HD22	1:D:2640:PRO:HB3	1.89	0.55
1:D:3769:ARG:O	1:D:3773:ARG:NH1	2.39	0.55
1:B:1152:MET:HB2	1:B:1161:ILE:HB	1.89	0.55
1:B:3132:THR:HG23	1:B:3136:LEU:HD23	1.88	0.55
1:C:2452:ARG:NH1	1:D:144:GLU:OE1	2.40	0.55
1:A:3769:ARG:O	1:A:3773:ARG:NH1	2.39	0.55
1:A:867:LEU:HD13	1:A:929:LEU:HB3	1.89	0.54
1:A:4030:LEU:HG	1:A:4040:ILE:HD11	1.88	0.54
1:B:3769:ARG:O	1:B:3773:ARG:NH1	2.39	0.54
1:C:867:LEU:HD13	1:C:929:LEU:HB3	1.89	0.54
1:C:3420:ARG:NH1	1:C:3516:LYS:O	2.39	0.54
1:D:2177:LEU:O	1:D:2181:SER:OG	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3825:GLU:OE1	1:A:3828:PHE:N	2.36	0.54
1:B:223:PHE:HB2	1:B:389:PHE:HB2	1.88	0.54
1:B:417:GLY:HA3	1:B:436:LEU:HD21	1.88	0.54
1:B:4581:LYS:NZ	1:B:4582:VAL:O	2.38	0.54
1:C:417:GLY:HA3	1:C:436:LEU:HD21	1.88	0.54
1:C:3900:GLN:NE2	1:C:3967:GLU:O	2.40	0.54
1:D:2971:GLN:HA	1:D:2974:ILE:HG12	1.89	0.54
1:D:2978:GLU:OE2	1:D:3053:ARG:NH1	2.39	0.54
2:F:74:LEU:HB2	2:F:99:PHE:HB2	1.90	0.54
1:A:1152:MET:HB2	1:A:1161:ILE:HB	1.89	0.54
1:B:1101:ARG:NH1	1:B:1115:LEU:O	2.39	0.54
1:C:2626:LEU:HD22	1:C:2640:PRO:HB3	1.89	0.54
1:C:3132:THR:HG23	1:C:3136:LEU:HD23	1.88	0.54
1:A:417:GLY:HA3	1:A:436:LEU:HD21	1.88	0.54
1:C:1448:VAL:HG22	1:C:1554:VAL:HG23	1.90	0.54
1:D:497:TYR:O	1:D:553:ARG:NH2	2.37	0.54
1:D:867:LEU:HD13	1:D:929:LEU:HB3	1.89	0.54
1:D:1733:GLU:OE2	1:D:2163:ARG:NH2	2.41	0.54
1:D:4030:LEU:HG	1:D:4040:ILE:HD11	1.88	0.54
1:B:3208:PRO:HA	1:B:3211:ASN:HB2	1.89	0.54
1:C:3053:ARG:HG3	1:C:3056:LEU:HD22	1.90	0.54
1:C:3208:PRO:HA	1:C:3211:ASN:HB2	1.89	0.54
2:H:74:LEU:HB2	2:H:99:PHE:HB2	1.90	0.54
1:C:2971:GLN:HA	1:C:2974:ILE:HG12	1.89	0.54
1:A:2875:ALA:HB2	1:A:2927:LEU:HD22	1.89	0.54
1:B:355:LEU:HD22	1:B:380:GLN:HA	1.90	0.54
1:B:2452:ARG:NH1	1:C:144:GLU:OE1	2.40	0.54
1:B:3434:LEU:HD22	1:B:3517:MET:HE2	1.90	0.54
1:D:2992:GLU:OE2	1:D:2996:LYS:NZ	2.41	0.54
1:D:3208:PRO:HA	1:D:3211:ASN:HB2	1.89	0.54
1:A:4704:LEU:O	1:A:4774:LYS:NZ	2.36	0.54
1:C:1152:MET:HB2	1:C:1161:ILE:HB	1.89	0.54
1:B:1733:GLU:OE2	1:B:2163:ARG:NH2	2.41	0.54
1:D:2650:ARG:NH1	1:D:2651:CYS:SG	2.81	0.54
1:D:3053:ARG:HG3	1:D:3056:LEU:HD22	1.90	0.54
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	1.90	0.54
1:B:2650:ARG:NH1	1:B:2651:CYS:SG	2.81	0.54
1:C:3434:LEU:HD22	1:C:3517:MET:HE2	1.90	0.54
1:D:2507:ASP:OD2	1:D:2564:LYS:NZ	2.41	0.54
1:D:3434:LEU:HD22	1:D:3517:MET:HE2	1.90	0.54
1:A:3329:ILE:O	1:A:3403:ARG:NH2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:LEU:HD11	1:B:585:SER:HB3	1.90	0.53
1:B:3900:GLN:NE2	1:B:3967:GLU:O	2.40	0.53
1:C:2480:GLY:O	1:C:2484:ALA:N	2.42	0.53
1:C:2875:ALA:HB2	1:C:2927:LEU:HD22	1.89	0.53
1:C:3111:ARG:HH12	1:C:3174:SER:HB2	1.74	0.53
1:D:551:LEU:HD11	1:D:585:SER:HB3	1.90	0.53
1:D:1206:GLN:NE2	1:D:1230:MET:O	2.39	0.53
1:D:3132:THR:HG23	1:D:3136:LEU:HD23	1.88	0.53
2:G:74:LEU:HB2	2:G:99:PHE:HB2	1.90	0.53
1:A:1733:GLU:OE2	1:A:2163:ARG:NH2	2.41	0.53
1:A:2480:GLY:O	1:A:2484:ALA:N	2.41	0.53
1:B:707:VAL:HG13	1:B:713:SER:HB2	1.90	0.53
1:B:2875:ALA:HB2	1:B:2927:LEU:HD22	1.89	0.53
1:C:2170:MET:HE3	1:C:2228:MET:HE3	1.89	0.53
1:C:2507:ASP:OD2	1:C:2564:LYS:NZ	2.41	0.53
1:C:2919:ASP:HA	1:C:2922:LYS:HD2	1.89	0.53
1:C:2978:GLU:OE2	1:C:3053:ARG:NH1	2.39	0.53
1:D:2919:ASP:HA	1:D:2922:LYS:HD2	1.89	0.53
1:A:2207:VAL:HG12	1:A:2211:MET:HE1	1.89	0.53
1:A:4581:LYS:NZ	1:A:4582:VAL:O	2.38	0.53
1:B:867:LEU:HD13	1:B:929:LEU:HB3	1.89	0.53
1:B:1259:ARG:NH2	1:B:1591:CYS:SG	2.82	0.53
1:B:2919:ASP:HA	1:B:2922:LYS:HD2	1.89	0.53
1:D:1259:ARG:NH2	1:D:1591:CYS:SG	2.82	0.53
1:A:355:LEU:HD22	1:A:380:GLN:HA	1.90	0.53
1:A:455:PRO:HB3	1:A:467:LYS:HD2	1.91	0.53
1:A:2507:ASP:OD2	1:A:2564:LYS:NZ	2.41	0.53
1:A:2650:ARG:NH1	1:A:2651:CYS:SG	2.81	0.53
1:A:3053:ARG:HG3	1:A:3056:LEU:HD22	1.90	0.53
1:A:3322:ILE:O	1:A:3326:ASN:ND2	2.33	0.53
1:C:2003:GLN:O	1:C:2007:ASN:ND2	2.42	0.53
1:C:2650:ARG:NH1	1:C:2651:CYS:SG	2.81	0.53
1:D:455:PRO:HB3	1:D:467:LYS:HD2	1.91	0.53
1:D:707:VAL:HG13	1:D:713:SER:HB2	1.90	0.53
1:D:1683:HIS:NE2	1:D:1798:LEU:O	2.36	0.53
1:A:2003:GLN:O	1:A:2007:ASN:ND2	2.41	0.53
1:A:2967:MET:SD	1:A:2970:SER:OG	2.67	0.53
1:A:3075:LEU:O	1:A:3146:HIS:NE2	2.33	0.53
1:B:2003:GLN:O	1:B:2007:ASN:ND2	2.42	0.53
1:B:2170:MET:HE3	1:B:2228:MET:HE3	1.89	0.53
1:B:2654:TYR:HB2	1:B:2661:TRP:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3329:ILE:O	1:B:3403:ARG:NH2	2.40	0.53
1:B:3827:GLY:HA2	1:B:3830:GLN:HB2	1.91	0.53
1:C:2654:TYR:HB2	1:C:2661:TRP:HB2	1.91	0.53
1:C:2967:MET:SD	1:C:2970:SER:OG	2.67	0.53
1:D:206:CYS:SG	1:D:207:SER:N	2.82	0.53
1:D:1152:MET:HB2	1:D:1161:ILE:HB	1.89	0.53
1:D:2003:GLN:O	1:D:2007:ASN:ND2	2.42	0.53
1:D:3366:ARG:NH1	1:D:3437:MET:SD	2.82	0.53
2:F:38:SER:O	2:F:42:ARG:NH2	2.42	0.53
1:A:1259:ARG:NH2	1:A:1591:CYS:SG	2.82	0.53
1:A:3434:LEU:HD22	1:A:3517:MET:HE2	1.90	0.53
1:B:1448:VAL:HG22	1:B:1554:VAL:HG23	1.90	0.53
1:C:2207:VAL:HG12	1:C:2211:MET:HE1	1.89	0.53
1:D:1461:ASP:OD2	1:D:1468:LYS:NZ	2.40	0.53
1:A:2170:MET:HE3	1:A:2228:MET:HE3	1.89	0.53
1:B:2023:LEU:O	1:B:2028:ARG:NE	2.41	0.53
1:B:3366:ARG:NH1	1:B:3437:MET:SD	2.82	0.53
1:C:356:TRP:O	1:C:379:HIS:N	2.42	0.53
2:E:38:SER:O	2:E:42:ARG:NH2	2.42	0.53
2:G:38:SER:O	2:G:42:ARG:NH2	2.42	0.53
1:A:707:VAL:HG13	1:A:713:SER:HB2	1.90	0.53
1:A:3208:PRO:HA	1:A:3211:ASN:HB2	1.89	0.53
1:A:3875:MET:HB3	1:A:3878:ASP:HB3	1.91	0.53
1:B:2480:GLY:O	1:B:2484:ALA:N	2.41	0.53
1:B:3053:ARG:HG3	1:B:3056:LEU:HD22	1.90	0.53
1:B:4983:HIS:O	4:B:5102:ADE:N6	2.39	0.53
1:C:355:LEU:HD22	1:C:380:GLN:HA	1.90	0.53
1:C:1259:ARG:NH2	1:C:1591:CYS:SG	2.82	0.53
1:D:3825:GLU:OE1	1:D:3828:PHE:N	2.36	0.53
1:A:3827:GLY:HA2	1:A:3830:GLN:HB2	1.91	0.53
1:B:455:PRO:HB3	1:B:467:LYS:HD2	1.91	0.53
1:B:3111:ARG:HH12	1:B:3174:SER:HB2	1.74	0.53
1:B:3145:GLN:OE1	1:B:3196:ARG:NE	2.42	0.53
1:B:3875:MET:HB3	1:B:3878:ASP:HB3	1.91	0.53
1:C:497:TYR:O	1:C:553:ARG:NH2	2.37	0.53
1:C:4958:CYS:SG	1:C:4978:HIS:CD2	3.02	0.53
1:D:2170:MET:HE3	1:D:2228:MET:HE3	1.89	0.53
1:B:206:CYS:SG	1:B:207:SER:N	2.82	0.53
1:B:3825:GLU:OE1	1:B:3828:PHE:N	2.36	0.53
1:C:455:PRO:HB3	1:C:467:LYS:HD2	1.91	0.53
1:C:707:VAL:HG13	1:C:713:SER:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	1.90	0.53
1:D:2480:GLY:O	1:D:2484:ALA:N	2.42	0.53
1:D:3111:ARG:HH12	1:D:3174:SER:HB2	1.73	0.53
1:A:497:TYR:O	1:A:553:ARG:NH2	2.37	0.52
1:A:2919:ASP:HA	1:A:2922:LYS:HD2	1.89	0.52
1:B:2927:LEU:HD12	1:B:2930:LEU:HD12	1.92	0.52
1:C:1291:LEU:HD12	1:C:1550:PRO:HG2	1.92	0.52
1:C:3875:MET:HB3	1:C:3878:ASP:HB3	1.91	0.52
1:A:2927:LEU:HD12	1:A:2930:LEU:HD12	1.91	0.52
1:A:3111:ARG:HH12	1:A:3174:SER:HB2	1.74	0.52
1:B:497:TYR:O	1:B:553:ARG:NH2	2.37	0.52
1:B:2507:ASP:OD2	1:B:2564:LYS:NZ	2.41	0.52
1:B:2967:MET:SD	1:B:2970:SER:OG	2.67	0.52
1:C:688:LEU:HD23	1:C:690:GLU:H	1.75	0.52
1:C:1454:THR:OG1	1:C:1456:ASP:OD1	2.24	0.52
1:C:1461:ASP:OD2	1:C:1468:LYS:NZ	2.40	0.52
1:D:2654:TYR:HB2	1:D:2661:TRP:HB2	1.91	0.52
1:D:4958:CYS:SG	1:D:4978:HIS:CD2	3.02	0.52
2:E:74:LEU:HB2	2:E:99:PHE:HB2	1.90	0.52
1:A:2707:ALA:HB1	1:A:3009:TYR:HD1	1.75	0.52
1:A:3366:ARG:NH1	1:A:3437:MET:SD	2.82	0.52
1:A:3579:LEU:HD12	1:A:3582:ARG:HE	1.75	0.52
1:B:1291:LEU:HD12	1:B:1550:PRO:HG2	1.92	0.52
1:B:3415:TYR:O	1:B:3419:ASN:ND2	2.37	0.52
1:B:4138:ASP:O	1:B:4142:ASN:ND2	2.41	0.52
1:C:1733:GLU:OE2	1:C:2163:ARG:NH2	2.41	0.52
1:C:3415:TYR:O	1:C:3419:ASN:ND2	2.37	0.52
1:D:2207:VAL:HG12	1:D:2211:MET:HE1	1.90	0.52
1:D:2967:MET:SD	1:D:2970:SER:OG	2.67	0.52
1:D:3875:MET:HB3	1:D:3878:ASP:HB3	1.91	0.52
1:A:551:LEU:HD11	1:A:585:SER:HB3	1.90	0.52
1:A:4138:ASP:O	1:A:4142:ASN:ND2	2.41	0.52
1:B:2707:ALA:HB1	1:B:3009:TYR:HD1	1.75	0.52
1:B:4958:CYS:SG	1:B:4978:HIS:CD2	3.02	0.52
1:C:551:LEU:HD11	1:C:585:SER:HB3	1.90	0.52
1:C:2707:ALA:HB1	1:C:3009:TYR:HD1	1.75	0.52
1:C:2927:LEU:HD12	1:C:2930:LEU:HD12	1.92	0.52
1:A:4958:CYS:SG	1:A:4978:HIS:CD2	3.02	0.52
1:B:2207:VAL:HG12	1:B:2211:MET:HE1	1.90	0.52
1:B:3579:LEU:HD12	1:B:3582:ARG:HE	1.75	0.52
1:B:3603:LEU:HD13	1:B:3606:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3603:LEU:HD13	1:C:3606:LEU:HD13	1.92	0.52
1:D:355:LEU:HD22	1:D:380:GLN:HA	1.90	0.52
1:D:1291:LEU:HD12	1:D:1550:PRO:HG2	1.91	0.52
1:D:2927:LEU:HD12	1:D:2930:LEU:HD12	1.91	0.52
1:A:3145:GLN:OE1	1:A:3196:ARG:NE	2.42	0.52
1:B:1683:HIS:NE2	1:B:1798:LEU:O	2.36	0.52
1:C:1683:HIS:NE2	1:C:1798:LEU:O	2.36	0.52
1:C:3145:GLN:OE1	1:C:3196:ARG:NE	2.42	0.52
1:C:3366:ARG:NH1	1:C:3437:MET:SD	2.82	0.52
2:H:38:SER:O	2:H:42:ARG:NH2	2.42	0.52
1:A:688:LEU:HD23	1:A:690:GLU:H	1.75	0.52
1:A:1291:LEU:HD12	1:A:1550:PRO:HG2	1.92	0.52
1:B:4057:MET:HA	1:B:4060:LYS:HB3	1.91	0.52
1:C:206:CYS:SG	1:C:207:SER:N	2.82	0.52
1:D:2707:ALA:HB1	1:D:3009:TYR:HD1	1.75	0.52
1:D:3145:GLN:OE1	1:D:3196:ARG:NE	2.42	0.52
1:D:3579:LEU:HD12	1:D:3582:ARG:HE	1.75	0.52
1:D:3827:GLY:HA2	1:D:3830:GLN:HB2	1.91	0.52
1:A:2452:ARG:NH1	1:B:144:GLU:OE1	2.42	0.52
1:A:2801:ASP:HA	1:A:2804:ILE:HG12	1.92	0.52
1:A:2902:HIS:HB3	1:A:2905:LEU:HG	1.92	0.52
1:B:2777:TYR:HB3	1:B:2791:LEU:HD23	1.92	0.52
1:B:2902:HIS:HB3	1:B:2905:LEU:HG	1.92	0.52
1:C:2902:HIS:HB3	1:C:2905:LEU:HG	1.92	0.52
1:D:356:TRP:O	1:D:379:HIS:N	2.42	0.52
1:D:688:LEU:HD23	1:D:690:GLU:H	1.75	0.52
1:D:2902:HIS:HB3	1:D:2905:LEU:HG	1.92	0.52
1:A:595:ARG:NH1	1:A:1643:GLU:OE2	2.43	0.52
1:A:3641:LEU:HA	1:A:3644:LEU:HD23	1.92	0.52
1:B:356:TRP:O	1:B:379:HIS:N	2.42	0.52
1:B:1156:THR:OG1	1:B:1157:GLU:OE1	2.24	0.52
1:C:2777:TYR:HB3	1:C:2791:LEU:HD23	1.92	0.52
1:C:3825:GLU:OE1	1:C:3828:PHE:N	2.36	0.52
1:D:595:ARG:NH1	1:D:1643:GLU:OE2	2.43	0.52
1:A:15:ARG:HA	1:A:100:THR:HA	1.91	0.52
1:A:2654:TYR:HB2	1:A:2661:TRP:HB2	1.91	0.52
1:C:355:LEU:HB2	1:C:378:LEU:HG	1.92	0.52
1:D:355:LEU:HB2	1:D:378:LEU:HG	1.92	0.52
1:D:554:LEU:HD11	1:D:1593:PRO:HD3	1.93	0.52
1:D:3603:LEU:HD13	1:D:3606:LEU:HD13	1.92	0.52
1:A:355:LEU:HB2	1:A:378:LEU:HG	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:LEU:HD11	1:A:1593:PRO:HD3	1.92	0.51
1:A:932:LEU:HB3	1:A:937:CYS:HB3	1.91	0.51
1:A:2296:GLU:HA	1:A:2299:VAL:HG12	1.93	0.51
1:A:4097:MET:HE2	1:A:4108:ILE:HG23	1.92	0.51
1:B:595:ARG:NH1	1:B:1643:GLU:OE2	2.43	0.51
1:B:3751:VAL:HG13	1:B:3756:LYS:HD3	1.93	0.51
1:C:15:ARG:HA	1:C:100:THR:HA	1.92	0.51
1:A:1438:ARG:HA	1:A:1514:LEU:O	2.10	0.51
1:A:3751:VAL:HG13	1:A:3756:LYS:HD3	1.92	0.51
1:B:355:LEU:HB2	1:B:378:LEU:HG	1.92	0.51
1:B:688:LEU:HD23	1:B:690:GLU:H	1.75	0.51
1:B:4097:MET:HE2	1:B:4108:ILE:HG23	1.92	0.51
1:C:2960:LEU:HD23	1:C:2963:LEU:HD12	1.93	0.51
1:D:1438:ARG:HA	1:D:1514:LEU:O	2.10	0.51
2:H:21:THR:HG22	2:H:49:ARG:HD2	1.93	0.51
1:A:1154:ASP:OD1	1:A:1156:THR:OG1	2.29	0.51
1:A:3421:ALA:O	1:A:3425:THR:OG1	2.27	0.51
1:B:554:LEU:HD11	1:B:1593:PRO:HD3	1.93	0.51
1:B:932:LEU:HB3	1:B:937:CYS:HB3	1.91	0.51
1:C:3827:GLY:HA2	1:C:3830:GLN:HB2	1.91	0.51
1:D:247:TYR:HB2	1:D:374:LYS:HB2	1.92	0.51
1:D:2296:GLU:HA	1:D:2299:VAL:HG12	1.93	0.51
1:D:2960:LEU:HD23	1:D:2963:LEU:HD12	1.93	0.51
2:F:21:THR:HG22	2:F:49:ARG:HD2	1.93	0.51
1:A:206:CYS:SG	1:A:207:SER:N	2.82	0.51
1:B:2954:ARG:NH1	1:B:3016:TYR:OH	2.44	0.51
1:C:2023:LEU:O	1:C:2028:ARG:NE	2.41	0.51
1:C:3751:VAL:HG13	1:C:3756:LYS:HD3	1.92	0.51
1:D:932:LEU:HB3	1:D:937:CYS:HB3	1.91	0.51
1:D:2801:ASP:HA	1:D:2804:ILE:HG12	1.92	0.51
1:D:3204:ALA:HB3	1:D:3214:ASN:HD21	1.74	0.51
1:A:1792:ALA:O	1:A:2176:ASN:ND2	2.38	0.51
1:B:1454:THR:OG1	1:B:1456:ASP:OD1	2.24	0.51
1:B:1461:ASP:OD2	1:B:1468:LYS:NZ	2.40	0.51
1:B:2992:GLU:OE2	1:B:2996:LYS:NZ	2.41	0.51
1:C:247:TYR:HB2	1:C:374:LYS:HB2	1.92	0.51
1:D:1154:ASP:OD1	1:D:1156:THR:OG1	2.29	0.51
1:D:1156:THR:OG1	1:D:1157:GLU:OE1	2.24	0.51
1:D:2954:ARG:NH1	1:D:3016:TYR:OH	2.44	0.51
1:A:3603:LEU:HD13	1:A:3606:LEU:HD13	1.92	0.51
1:B:247:TYR:HB2	1:B:374:LYS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2801:ASP:HA	1:B:2804:ILE:HG12	1.92	0.51
1:C:554:LEU:HD11	1:C:1593:PRO:HD3	1.93	0.51
1:C:3421:ALA:O	1:C:3425:THR:OG1	2.28	0.51
1:C:3579:LEU:HD12	1:C:3582:ARG:HE	1.75	0.51
1:D:4057:MET:HA	1:D:4060:LYS:HB3	1.91	0.51
2:E:21:THR:HG22	2:E:49:ARG:HD2	1.93	0.51
2:G:21:THR:HG22	2:G:49:ARG:HD2	1.93	0.51
1:A:4219:PHE:HE1	1:A:4946:GLN:HB3	1.76	0.51
1:B:1438:ARG:HA	1:B:1514:LEU:O	2.10	0.51
1:B:3204:ALA:HB3	1:B:3214:ASN:HD21	1.74	0.51
1:C:595:ARG:NH1	1:C:1643:GLU:OE2	2.43	0.51
1:C:844:ARG:NH1	1:C:1197:GLY:HA3	2.21	0.51
1:C:932:LEU:HB3	1:C:937:CYS:HB3	1.91	0.51
1:C:1438:ARG:HA	1:C:1514:LEU:O	2.10	0.51
1:D:15:ARG:HA	1:D:100:THR:HA	1.92	0.51
1:D:3329:ILE:O	1:D:3403:ARG:NH2	2.40	0.51
1:A:2954:ARG:NH1	1:A:3016:TYR:OH	2.44	0.51
1:A:4057:MET:HA	1:A:4060:LYS:HB3	1.91	0.51
1:B:788:LYS:HA	1:B:1628:VAL:O	2.11	0.51
1:B:1154:ASP:OD1	1:B:1156:THR:OG1	2.29	0.51
1:A:356:TRP:O	1:A:379:HIS:N	2.42	0.51
1:A:403:MET:O	1:A:407:THR:OG1	2.19	0.51
1:A:450:GLY:HA2	1:A:453:GLU:HG2	1.93	0.51
1:A:546:TRP:O	1:A:549:SER:OG	2.28	0.51
1:A:2777:TYR:HB3	1:A:2791:LEU:HD23	1.92	0.51
1:A:2913:ALA:HA	1:A:2916:LYS:HB3	1.93	0.51
1:A:3204:ALA:HB3	1:A:3214:ASN:HD21	1.74	0.51
1:B:2978:GLU:OE2	1:B:3053:ARG:NH1	2.39	0.51
1:B:3075:LEU:O	1:B:3146:HIS:NE2	2.33	0.51
1:C:1154:ASP:OD1	1:C:1156:THR:OG1	2.29	0.51
1:D:2777:TYR:HB3	1:D:2791:LEU:HD23	1.92	0.51
1:D:3037:GLU:HG2	1:D:3085:PRO:HD2	1.93	0.51
1:D:3366:ARG:HA	1:D:3441:ILE:HD11	1.93	0.51
1:A:247:TYR:HB2	1:A:374:LYS:HB2	1.92	0.51
1:B:15:ARG:HA	1:B:100:THR:HA	1.92	0.51
1:C:2296:GLU:HA	1:C:2299:VAL:HG12	1.92	0.51
1:C:2992:GLU:OE2	1:C:2996:LYS:NZ	2.41	0.51
1:C:3329:ILE:O	1:C:3403:ARG:NH2	2.40	0.51
1:D:450:GLY:HA2	1:D:453:GLU:HG2	1.93	0.51
2:E:27:THR:HA	2:E:38:SER:HA	1.93	0.51
1:A:2960:LEU:HD23	1:A:2963:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2296:GLU:HA	1:B:2299:VAL:HG12	1.93	0.50
1:B:3245:VAL:O	1:B:3249:LEU:HB2	2.12	0.50
1:C:2954:ARG:NH1	1:C:3016:TYR:OH	2.44	0.50
1:C:3204:ALA:HB3	1:C:3214:ASN:HD21	1.74	0.50
1:D:2464:ASP:OD1	1:D:2464:ASP:N	2.44	0.50
1:D:3751:VAL:HG13	1:D:3756:LYS:HD3	1.92	0.50
1:D:4219:PHE:HE1	1:D:4946:GLN:HB3	1.76	0.50
2:G:27:THR:HA	2:G:38:SER:HA	1.93	0.50
1:A:2023:LEU:O	1:A:2028:ARG:NE	2.41	0.50
1:A:3037:GLU:HG2	1:A:3085:PRO:HD2	1.93	0.50
1:A:4563:ARG:NH2	1:A:4815:ASP:OD1	2.45	0.50
1:B:2960:LEU:HD23	1:B:2963:LEU:HD12	1.93	0.50
1:B:3641:LEU:HA	1:B:3644:LEU:HD23	1.92	0.50
1:C:546:TRP:O	1:C:549:SER:OG	2.28	0.50
1:C:2801:ASP:HA	1:C:2804:ILE:HG12	1.92	0.50
1:C:2913:ALA:HA	1:C:2916:LYS:HB3	1.93	0.50
1:D:1944:GLU:HB3	1:D:2123:LEU:HD21	1.93	0.50
1:C:3322:ILE:O	1:C:3326:ASN:ND2	2.33	0.50
1:C:4069:LYS:HD3	1:C:4133:GLN:HG3	1.94	0.50
1:C:4853:VAL:O	1:C:4857:ASN:ND2	2.44	0.50
1:D:3641:LEU:HA	1:D:3644:LEU:HD23	1.92	0.50
1:D:4097:MET:HE2	1:D:4108:ILE:HG23	1.92	0.50
2:H:78:PRO:HA	2:H:81:ALA:HB3	1.93	0.50
1:A:2992:GLU:OE2	1:A:2996:LYS:NZ	2.41	0.50
1:A:3245:VAL:O	1:A:3249:LEU:HB2	2.11	0.50
1:A:3771:HIS:NE2	1:A:3811:GLU:OE2	2.45	0.50
1:B:2913:ALA:HA	1:B:2916:LYS:HB3	1.93	0.50
1:C:450:GLY:HA2	1:C:453:GLU:HG2	1.93	0.50
1:C:2177:LEU:O	1:C:2181:SER:OG	2.25	0.50
1:C:4057:MET:HA	1:C:4060:LYS:HB3	1.91	0.50
1:D:4069:LYS:HD3	1:D:4133:GLN:HG3	1.94	0.50
1:A:788:LYS:HA	1:A:1628:VAL:O	2.11	0.50
1:B:450:GLY:HA2	1:B:453:GLU:HG2	1.93	0.50
1:B:3052:HIS:NE2	1:B:3128:ASN:OD1	2.45	0.50
1:C:3366:ARG:HA	1:C:3441:ILE:HD11	1.93	0.50
1:D:939:VAL:HB	1:D:1051:TYR:HB3	1.94	0.50
2:F:78:PRO:HA	2:F:81:ALA:HB3	1.93	0.50
2:H:27:THR:HA	2:H:38:SER:HA	1.93	0.50
1:A:939:VAL:HB	1:A:1051:TYR:HB3	1.94	0.50
1:B:3037:GLU:HG2	1:B:3085:PRO:HD2	1.93	0.50
1:B:3104:GLU:HA	1:B:3107:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4097:MET:HE2	1:C:4108:ILE:HG23	1.92	0.50
1:D:3771:HIS:NE2	1:D:3811:GLU:OE2	2.45	0.50
1:B:272:SER:OG	1:B:333:GLY:O	2.29	0.50
1:B:870:ILE:HG13	1:B:874:LEU:HD23	1.94	0.50
1:B:4563:ARG:NH2	1:B:4815:ASP:OD1	2.45	0.50
1:D:3048:ALA:O	1:D:3053:ARG:NH2	2.45	0.50
1:A:3688:GLU:HG3	1:A:3690:VAL:HG12	1.94	0.50
1:A:4069:LYS:HD3	1:A:4133:GLN:HG3	1.93	0.50
1:A:4938:ASP:OD1	1:D:4944:ARG:NH2	2.45	0.50
1:B:1944:GLU:HB3	1:B:2123:LEU:HD21	1.93	0.50
1:B:3048:ALA:O	1:B:3053:ARG:NH2	2.45	0.50
1:D:2913:ALA:HA	1:D:2916:LYS:HB3	1.93	0.50
2:F:27:THR:HA	2:F:38:SER:HA	1.93	0.50
1:A:1864:LYS:NZ	1:A:1871:PHE:O	2.45	0.50
1:A:2464:ASP:OD1	1:A:2464:ASP:N	2.44	0.50
1:A:4853:VAL:O	1:A:4857:ASN:ND2	2.44	0.50
1:B:1724:CYS:SG	1:B:1728:ARG:NH1	2.83	0.50
1:B:4725:LEU:HA	1:B:4737:ILE:HG21	1.94	0.50
1:C:842:PRO:O	1:C:1197:GLY:N	2.45	0.50
1:C:1640:HIS:HA	1:C:1647:CYS:HA	1.94	0.50
1:C:1782:PHE:O	2:G:82:TYR:OH	2.29	0.50
1:C:3354:LEU:HA	1:C:3358:PHE:HB2	1.93	0.50
1:C:4563:ARG:NH2	1:C:4815:ASP:OD1	2.45	0.50
1:A:349:GLN:NE2	1:A:354:GLY:O	2.45	0.49
1:A:842:PRO:O	1:A:1197:GLY:N	2.45	0.49
1:B:1640:HIS:HA	1:B:1647:CYS:HA	1.94	0.49
1:C:3052:HIS:NE2	1:C:3128:ASN:OD1	2.45	0.49
1:C:3641:LEU:HA	1:C:3644:LEU:HD23	1.92	0.49
2:G:78:PRO:HA	2:G:81:ALA:HB3	1.93	0.49
1:A:1944:GLU:HB3	1:A:2123:LEU:HD21	1.93	0.49
1:A:3188:PRO:O	1:A:3191:GLY:N	2.45	0.49
1:B:939:VAL:HB	1:B:1051:TYR:HB3	1.94	0.49
1:C:272:SER:OG	1:C:333:GLY:O	2.29	0.49
1:C:3771:HIS:NE2	1:C:3811:GLU:OE2	2.45	0.49
1:D:868:GLU:HA	1:D:871:ARG:HB2	1.95	0.49
1:D:3104:GLU:HA	1:D:3107:VAL:HG22	1.94	0.49
1:D:3524:MET:O	1:D:3595:ARG:NH1	2.45	0.49
1:D:4138:ASP:O	1:D:4142:ASN:ND2	2.41	0.49
1:A:868:GLU:HA	1:A:871:ARG:HB2	1.95	0.49
1:A:3965:LEU:HA	1:A:3968:TYR:HD2	1.78	0.49
1:B:3188:PRO:O	1:B:3191:GLY:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3771:HIS:NE2	1:B:3811:GLU:OE2	2.45	0.49
1:C:1944:GLU:HB3	1:C:2123:LEU:HD21	1.93	0.49
1:C:3037:GLU:HG2	1:C:3085:PRO:HD2	1.93	0.49
1:C:4138:ASP:O	1:C:4142:ASN:ND2	2.41	0.49
1:D:3245:VAL:O	1:D:3249:LEU:HB2	2.11	0.49
1:A:3159:ASP:OD1	1:A:3159:ASP:N	2.46	0.49
1:B:3524:MET:O	1:B:3595:ARG:NH1	2.45	0.49
1:B:4069:LYS:HD3	1:B:4133:GLN:HG3	1.94	0.49
1:C:3048:ALA:O	1:C:3053:ARG:NH2	2.45	0.49
1:D:272:SER:OG	1:D:333:GLY:O	2.29	0.49
1:D:1640:HIS:HA	1:D:1647:CYS:HA	1.94	0.49
1:A:870:ILE:HG13	1:A:874:LEU:HD23	1.94	0.49
1:A:1640:HIS:HA	1:A:1647:CYS:HA	1.94	0.49
1:A:3524:MET:O	1:A:3595:ARG:NH1	2.45	0.49
1:C:788:LYS:HA	1:C:1628:VAL:O	2.11	0.49
1:C:3187:ARG:HD3	1:C:3271:GLU:HG3	1.94	0.49
1:C:3188:PRO:O	1:C:3191:GLY:N	2.45	0.49
1:D:743:VAL:HB	1:D:760:ASN:HA	1.95	0.49
1:D:4563:ARG:NH2	1:D:4815:ASP:OD1	2.45	0.49
1:A:1699:GLU:OE2	1:A:1813:ARG:NH2	2.38	0.49
1:A:1724:CYS:SG	1:A:1728:ARG:NH1	2.83	0.49
1:A:3048:ALA:O	1:A:3053:ARG:NH2	2.45	0.49
1:A:3052:HIS:NE2	1:A:3128:ASN:OD1	2.45	0.49
1:B:842:PRO:O	1:B:1197:GLY:N	2.45	0.49
1:B:3354:LEU:HA	1:B:3358:PHE:HB2	1.93	0.49
1:B:3366:ARG:HA	1:B:3441:ILE:HD11	1.93	0.49
1:B:3965:LEU:HA	1:B:3968:TYR:HD2	1.78	0.49
1:B:4179:GLY:O	1:B:4194:TYR:HA	2.12	0.49
1:C:939:VAL:HB	1:C:1051:TYR:HB3	1.94	0.49
1:C:4090:LYS:HG2	1:C:4123:ILE:HD11	1.95	0.49
1:D:1232:ARG:NH2	1:D:1828:ASP:O	2.36	0.49
1:D:1724:CYS:SG	1:D:1728:ARG:NH1	2.83	0.49
1:D:3188:PRO:O	1:D:3191:GLY:N	2.45	0.49
1:D:3354:LEU:HA	1:D:3358:PHE:HB2	1.93	0.49
1:B:1864:LYS:NZ	1:B:1871:PHE:O	2.45	0.49
1:B:3688:GLU:HG3	1:B:3690:VAL:HG12	1.94	0.49
1:B:4219:PHE:HE1	1:B:4946:GLN:HB3	1.76	0.49
1:B:4848:VAL:HG11	1:B:4887:MET:HG3	1.95	0.49
1:C:877:ASN:HA	1:C:970:LEU:H	1.78	0.49
1:C:2464:ASP:N	1:C:2464:ASP:OD1	2.44	0.49
1:C:3524:MET:O	1:C:3595:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4848:VAL:HG11	1:D:4887:MET:HG3	1.95	0.49
1:C:710:ASP:OD1	1:C:710:ASP:N	2.45	0.49
1:C:1642:PRO:O	1:C:1645:ASN:ND2	2.46	0.49
1:C:3245:VAL:O	1:C:3249:LEU:HB2	2.11	0.49
1:C:3886:ARG:NH1	1:C:3889:GLN:OE1	2.46	0.49
1:D:3688:GLU:HG3	1:D:3690:VAL:HG12	1.94	0.49
1:D:4090:LYS:HG2	1:D:4123:ILE:HD11	1.95	0.49
1:D:4179:GLY:O	1:D:4194:TYR:HA	2.12	0.49
2:G:68:LEU:HA	2:G:103:LEU:HD22	1.95	0.49
1:A:27:THR:OG1	1:A:32:GLN:OE1	2.28	0.49
1:A:2102:VAL:HG13	1:A:2120:MET:HG2	1.95	0.49
1:A:2640:PRO:HA	1:A:2643:LEU:HB3	1.95	0.49
1:A:3104:GLU:HA	1:A:3107:VAL:HG22	1.94	0.49
1:A:4001:MET:HE1	1:A:4061:PHE:HB2	1.94	0.49
1:B:796:ARG:O	1:B:1619:ARG:NH2	2.45	0.49
1:B:4001:MET:HE1	1:B:4061:PHE:HB2	1.94	0.49
1:C:743:VAL:HB	1:C:760:ASN:HA	1.95	0.49
1:C:1724:CYS:SG	1:C:1728:ARG:NH1	2.83	0.49
1:C:3414:ARG:HE	1:C:3472:ALA:HB3	1.78	0.49
1:C:3965:LEU:HA	1:C:3968:TYR:HD2	1.78	0.49
1:C:4179:GLY:O	1:C:4194:TYR:HA	2.12	0.49
1:D:1454:THR:OG1	1:D:1456:ASP:OD1	2.24	0.49
1:D:2640:PRO:HA	1:D:2643:LEU:HB3	1.95	0.49
1:D:3052:HIS:NE2	1:D:3128:ASN:OD1	2.45	0.49
1:D:3414:ARG:HE	1:D:3472:ALA:HB3	1.78	0.49
1:D:4152:GLU:OE2	1:D:4192:ARG:NH1	2.46	0.49
1:D:4725:LEU:HA	1:D:4737:ILE:HG21	1.94	0.49
2:F:68:LEU:HA	2:F:103:LEU:HD22	1.95	0.49
1:A:877:ASN:HA	1:A:970:LEU:H	1.78	0.49
1:A:2862:LEU:O	1:A:2928:LYS:NZ	2.41	0.49
1:A:4848:VAL:HG11	1:A:4887:MET:HG3	1.95	0.49
1:C:4725:LEU:HA	1:C:4737:ILE:HG21	1.94	0.49
1:C:4848:VAL:HG11	1:C:4887:MET:HG3	1.95	0.49
1:D:796:ARG:O	1:D:1619:ARG:NH2	2.45	0.49
1:D:3187:ARG:HD3	1:D:3271:GLU:HG3	1.94	0.49
1:D:4001:MET:HE1	1:D:4061:PHE:HB2	1.94	0.49
2:E:78:PRO:HA	2:E:81:ALA:HB3	1.93	0.49
2:H:68:LEU:HA	2:H:103:LEU:HD22	1.95	0.49
1:A:1965:TYR:OH	1:A:2027:ILE:O	2.31	0.48
1:A:4090:LYS:HG2	1:A:4123:ILE:HD11	1.95	0.48
1:A:4548:ARG:HE	1:A:4548:ARG:HB3	1.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1642:PRO:O	1:B:1645:ASN:ND2	2.46	0.48
1:B:3187:ARG:HD3	1:B:3271:GLU:HG3	1.94	0.48
1:C:1072:VAL:HG23	1:C:1194:LEU:C	2.38	0.48
1:C:4214:LYS:HB3	1:C:4214:LYS:HE2	1.61	0.48
1:D:875:ALA:O	1:D:879:HIS:ND1	2.46	0.48
1:D:877:ASN:HA	1:D:970:LEU:H	1.78	0.48
1:D:1965:TYR:OH	1:D:2027:ILE:O	2.31	0.48
1:D:2023:LEU:O	1:D:2028:ARG:NE	2.41	0.48
1:D:3415:TYR:O	1:D:3419:ASN:ND2	2.37	0.48
1:D:3965:LEU:HA	1:D:3968:TYR:HD2	1.78	0.48
1:A:4725:LEU:HA	1:A:4737:ILE:HG21	1.94	0.48
1:B:3566:SER:HB3	1:B:3569:LEU:HG	1.95	0.48
1:B:4704:LEU:O	1:B:4774:LYS:NZ	2.36	0.48
1:C:4152:GLU:OE2	1:C:4192:ARG:NH1	2.46	0.48
1:C:4219:PHE:HE1	1:C:4946:GLN:HB3	1.76	0.48
1:D:842:PRO:O	1:D:1197:GLY:N	2.45	0.48
1:D:870:ILE:HG13	1:D:874:LEU:HD23	1.94	0.48
1:D:2431:ASP:HB2	1:D:2501:SER:HB3	1.96	0.48
2:G:24:VAL:HG12	2:G:103:LEU:HA	1.95	0.48
1:B:1072:VAL:HG23	1:B:1194:LEU:C	2.38	0.48
1:B:1525:GLY:O	1:B:1541:GLN:HA	2.13	0.48
1:C:796:ARG:O	1:C:1619:ARG:NH2	2.45	0.48
1:C:2431:ASP:HB2	1:C:2501:SER:HB3	1.95	0.48
1:C:4888:TYR:HD2	1:C:4889:VAL:HG22	1.78	0.48
1:D:349:GLN:NE2	1:D:354:GLY:O	2.44	0.48
1:D:788:LYS:HA	1:D:1628:VAL:O	2.11	0.48
1:D:2102:VAL:HG13	1:D:2120:MET:HG2	1.95	0.48
1:D:3524:MET:HA	1:D:3582:ARG:HH22	1.78	0.48
2:F:24:VAL:HG12	2:F:103:LEU:HA	1.95	0.48
1:A:111:HIS:ND1	1:A:114:SER:OG	2.35	0.48
1:A:3354:LEU:HA	1:A:3358:PHE:HB2	1.93	0.48
1:A:4918:ILE:HD11	1:D:4888:TYR:HA	1.94	0.48
1:B:877:ASN:HA	1:B:970:LEU:H	1.78	0.48
1:B:884:LEU:HB2	1:B:969:PRO:HD3	1.95	0.48
1:B:1863:LEU:HD13	1:B:1866:ILE:HD11	1.95	0.48
1:B:2640:PRO:HA	1:B:2643:LEU:HB3	1.95	0.48
1:B:4152:GLU:OE2	1:B:4192:ARG:NH1	2.46	0.48
1:C:4001:MET:HE1	1:C:4061:PHE:HB2	1.94	0.48
1:D:1699:GLU:OE2	1:D:1813:ARG:NH2	2.38	0.48
1:A:1175:SER:OG	1:A:1180:ARG:NH2	2.47	0.48
1:A:4152:GLU:OE2	1:A:4192:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4179:GLY:O	1:A:4194:TYR:HA	2.12	0.48
1:B:868:GLU:HA	1:B:871:ARG:HB2	1.94	0.48
1:B:2514:ASN:OD1	1:B:2514:ASN:N	2.45	0.48
1:B:2627:VAL:HG22	1:B:2678:LEU:HG	1.95	0.48
1:B:3414:ARG:HE	1:B:3472:ALA:HB3	1.78	0.48
1:B:3524:MET:HA	1:B:3582:ARG:HH22	1.78	0.48
1:C:868:GLU:HA	1:C:871:ARG:HB2	1.94	0.48
1:C:1525:GLY:O	1:C:1541:GLN:HA	2.13	0.48
1:C:1863:LEU:HD13	1:C:1866:ILE:HD11	1.95	0.48
1:C:2640:PRO:HA	1:C:2643:LEU:HB3	1.95	0.48
1:C:3104:GLU:HA	1:C:3107:VAL:HG22	1.94	0.48
1:D:1072:VAL:HG23	1:D:1194:LEU:C	2.38	0.48
1:D:1525:GLY:O	1:D:1541:GLN:HA	2.13	0.48
1:A:345:LEU:HB3	1:A:387:ALA:HB1	1.96	0.48
1:A:2616:PRO:HA	1:A:2619:LEU:HB2	1.96	0.48
1:A:3171:SER:O	1:A:3174:SER:OG	2.28	0.48
1:B:111:HIS:ND1	1:B:114:SER:OG	2.35	0.48
1:B:2107:GLN:O	1:B:3683:GLN:NE2	2.47	0.48
1:B:4853:VAL:O	1:B:4857:ASN:ND2	2.44	0.48
1:C:1965:TYR:OH	1:C:2027:ILE:O	2.31	0.48
1:C:2742:THR:HG22	1:C:2815:ALA:HB2	1.96	0.48
1:C:3566:SER:HB3	1:C:3569:LEU:HG	1.95	0.48
1:D:2616:PRO:HA	1:D:2619:LEU:HB2	1.96	0.48
1:D:4888:TYR:HD2	1:D:4889:VAL:HG22	1.78	0.48
2:H:24:VAL:HG12	2:H:103:LEU:HA	1.95	0.48
1:A:743:VAL:HB	1:A:760:ASN:HA	1.95	0.48
1:A:796:ARG:O	1:A:1619:ARG:NH2	2.45	0.48
1:A:1216:ILE:HG12	1:D:3424:LEU:HD11	1.96	0.48
1:A:3414:ARG:HE	1:A:3472:ALA:HB3	1.78	0.48
1:B:875:ALA:O	1:B:879:HIS:ND1	2.46	0.48
1:B:2102:VAL:HG13	1:B:2120:MET:HG2	1.95	0.48
1:B:4090:LYS:HG2	1:B:4123:ILE:HD11	1.95	0.48
1:C:870:ILE:HG13	1:C:874:LEU:HD23	1.94	0.48
1:C:1296:GLN:HA	1:C:1546:THR:O	2.14	0.48
1:C:3688:GLU:HG3	1:C:3690:VAL:HG12	1.94	0.48
1:C:4892:ARG:HD3	1:D:4918:ILE:HD13	1.96	0.48
1:D:345:LEU:HB3	1:D:387:ALA:HB1	1.96	0.48
1:D:546:TRP:O	1:D:549:SER:OG	2.28	0.48
1:D:1295:VAL:O	1:D:1547:LYS:HA	2.14	0.48
2:F:99:PHE:HB3	2:F:101:VAL:HG23	1.96	0.48
1:A:1072:VAL:HG23	1:A:1194:LEU:C	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1525:GLY:O	1:A:1541:GLN:HA	2.13	0.48
1:A:3886:ARG:NH1	1:A:3889:GLN:OE1	2.46	0.48
1:B:349:GLN:NE2	1:B:354:GLY:O	2.44	0.48
1:B:710:ASP:OD1	1:B:710:ASP:N	2.45	0.48
1:B:1076:ARG:HB3	1:B:1191:VAL:HG23	1.96	0.48
1:B:1175:SER:OG	1:B:1180:ARG:NH2	2.47	0.48
1:B:1296:GLN:HA	1:B:1546:THR:O	2.14	0.48
1:B:2522:LEU:HD12	1:B:2526:PHE:HB2	1.95	0.48
1:B:4157:ASP:OD1	1:B:4159:ARG:NH1	2.47	0.48
1:C:345:LEU:HB3	1:C:387:ALA:HB1	1.96	0.48
1:C:875:ALA:O	1:C:879:HIS:ND1	2.46	0.48
1:C:2107:GLN:O	1:C:3683:GLN:NE2	2.47	0.48
1:D:844:ARG:NH1	1:D:1197:GLY:HA3	2.21	0.48
1:D:1698:LEU:O	1:D:1712:TYR:OH	2.28	0.48
1:D:1863:LEU:HD13	1:D:1866:ILE:HD11	1.95	0.48
1:D:2742:THR:HG22	1:D:2815:ALA:HB2	1.96	0.48
1:A:875:ALA:O	1:A:879:HIS:ND1	2.46	0.48
1:A:1076:ARG:HB3	1:A:1191:VAL:HG23	1.96	0.48
1:A:1295:VAL:O	1:A:1547:LYS:HA	2.14	0.48
1:A:2017:ASP:OD1	1:A:2017:ASP:N	2.47	0.48
1:A:2978:GLU:OE2	1:A:3053:ARG:NH1	2.39	0.48
1:A:3366:ARG:HA	1:A:3441:ILE:HD11	1.93	0.48
1:B:2616:PRO:HA	1:B:2619:LEU:HB2	1.96	0.48
1:B:4892:ARG:HD3	1:C:4918:ILE:HD13	1.96	0.48
1:C:2102:VAL:HG13	1:C:2120:MET:HG2	1.95	0.48
1:C:2522:LEU:HD12	1:C:2526:PHE:HB2	1.95	0.48
1:C:3524:MET:HA	1:C:3582:ARG:HH22	1.79	0.48
1:A:710:ASP:N	1:A:710:ASP:OD1	2.45	0.48
1:A:884:LEU:HB2	1:A:969:PRO:HD3	1.95	0.48
1:A:1642:PRO:O	1:A:1645:ASN:ND2	2.46	0.48
1:A:2469:ILE:HA	1:A:2472:LEU:HG	1.96	0.48
1:A:2522:LEU:HD12	1:A:2526:PHE:HB2	1.95	0.48
1:A:4627:MET:H	1:A:4627:MET:HG3	1.42	0.48
1:B:3130:THR:HA	1:B:3133:THR:HG22	1.96	0.48
1:C:2736:ASP:HA	1:C:2891:LYS:HE2	1.96	0.48
1:D:2522:LEU:HD12	1:D:2526:PHE:HB2	1.95	0.48
1:A:3187:ARG:HD3	1:A:3271:GLU:HG3	1.95	0.47
1:B:3927:GLN:HA	1:B:3992:PHE:HE1	1.79	0.47
1:B:4888:TYR:HD2	1:B:4889:VAL:HG22	1.78	0.47
1:C:884:LEU:HB2	1:C:969:PRO:HD3	1.95	0.47
1:C:4704:LEU:O	1:C:4774:LYS:NZ	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4722:ARG:H	1:C:4722:ARG:HG2	1.45	0.47
1:D:1864:LYS:NZ	1:D:1871:PHE:O	2.45	0.47
1:D:3421:ALA:O	1:D:3425:THR:OG1	2.28	0.47
2:E:68:LEU:HA	2:E:103:LEU:HD22	1.95	0.47
1:A:1296:GLN:HA	1:A:1546:THR:O	2.14	0.47
1:A:2177:LEU:O	1:A:2181:SER:OG	2.25	0.47
1:A:2736:ASP:HA	1:A:2891:LYS:HE2	1.96	0.47
1:B:1295:VAL:O	1:B:1547:LYS:HA	2.14	0.47
1:B:1782:PHE:O	2:F:82:TYR:OH	2.30	0.47
1:B:2309:SER:OG	1:B:2321:ILE:O	2.26	0.47
1:B:2742:THR:HG22	1:B:2815:ALA:HB2	1.96	0.47
1:B:4241:THR:HB	1:B:4989:MET:HE1	1.96	0.47
1:C:2616:PRO:HA	1:C:2619:LEU:HB2	1.96	0.47
1:D:1175:SER:OG	1:D:1180:ARG:NH2	2.47	0.47
1:D:1642:PRO:O	1:D:1645:ASN:ND2	2.46	0.47
1:D:2469:ILE:HA	1:D:2472:LEU:HG	1.96	0.47
2:G:99:PHE:HB3	2:G:101:VAL:HG23	1.96	0.47
1:A:3519:PRO:HB3	1:B:1220:GLN:HB2	1.96	0.47
1:A:3566:SER:HB3	1:A:3569:LEU:HG	1.95	0.47
1:A:4157:ASP:OD1	1:A:4159:ARG:NH1	2.47	0.47
1:B:345:LEU:HB3	1:B:387:ALA:HB1	1.96	0.47
1:B:2736:ASP:HA	1:B:2891:LYS:HE2	1.96	0.47
1:C:1776:HIS:HB3	1:C:1798:LEU:HD13	1.97	0.47
1:C:3130:THR:HA	1:C:3133:THR:HG22	1.96	0.47
1:D:1296:GLN:HA	1:D:1546:THR:O	2.14	0.47
1:D:2736:ASP:HA	1:D:2891:LYS:HE2	1.96	0.47
1:D:3195:ALA:HB2	1:D:3275:PRO:HB3	1.97	0.47
1:D:4627:MET:H	1:D:4627:MET:HG3	1.42	0.47
2:E:24:VAL:HG12	2:E:103:LEU:HA	1.95	0.47
1:B:1232:ARG:NH2	1:B:1828:ASP:O	2.36	0.47
1:C:3596:VAL:O	1:C:3600:SER:OG	2.27	0.47
1:C:4138:ASP:OD1	1:C:4139:ILE:N	2.48	0.47
1:D:884:LEU:HB2	1:D:969:PRO:HD3	1.95	0.47
1:A:4888:TYR:HD2	1:A:4889:VAL:HG22	1.78	0.47
1:B:743:VAL:HB	1:B:760:ASN:HA	1.95	0.47
1:B:1776:HIS:HB3	1:B:1798:LEU:HD13	1.97	0.47
1:C:592:LYS:HB3	1:C:1592:PRO:HB3	1.97	0.47
1:C:1175:SER:OG	1:C:1180:ARG:NH2	2.47	0.47
1:C:1698:LEU:O	1:C:1712:TYR:OH	2.28	0.47
1:C:2309:SER:OG	1:C:2321:ILE:O	2.26	0.47
1:D:2107:GLN:O	1:D:3683:GLN:NE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3842:LEU:HB2	1:D:3929:SER:HB2	1.97	0.47
1:A:1863:LEU:HD13	1:A:1866:ILE:HD11	1.95	0.47
1:A:3524:MET:HA	1:A:3582:ARG:HH22	1.79	0.47
1:B:688:LEU:HD22	1:B:712:TYR:HD1	1.80	0.47
1:B:733:PRO:HG2	1:B:762:CYS:HB3	1.97	0.47
1:B:2689:LYS:O	1:B:2993:GLN:NE2	2.47	0.47
1:B:4138:ASP:OD1	1:B:4139:ILE:N	2.48	0.47
1:C:3195:ALA:HB2	1:C:3275:PRO:HB3	1.97	0.47
1:C:4157:ASP:OD1	1:C:4159:ARG:NH1	2.47	0.47
1:D:688:LEU:HD22	1:D:712:TYR:HD1	1.80	0.47
1:D:3130:THR:HA	1:D:3133:THR:HG22	1.96	0.47
2:E:99:PHE:HB3	2:E:101:VAL:HG23	1.96	0.47
1:A:592:LYS:HB3	1:A:1592:PRO:HB3	1.97	0.47
1:A:688:LEU:HD22	1:A:712:TYR:HD1	1.80	0.47
1:A:733:PRO:HG2	1:A:762:CYS:HB3	1.97	0.47
1:B:567:VAL:HG13	1:B:568:LEU:HD12	1.97	0.47
1:B:592:LYS:HB3	1:B:1592:PRO:HB3	1.97	0.47
1:B:2431:ASP:HB2	1:B:2501:SER:HB3	1.95	0.47
1:B:2464:ASP:OD1	1:B:2464:ASP:N	2.44	0.47
1:B:5030:LYS:HB2	1:B:5030:LYS:HE2	1.59	0.47
1:C:1699:GLU:OE2	1:C:1813:ARG:NH2	2.38	0.47
1:C:2689:LYS:O	1:C:2993:GLN:NE2	2.47	0.47
1:D:27:THR:OG1	1:D:32:GLN:OE1	2.28	0.47
1:D:592:LYS:HB3	1:D:1592:PRO:HB3	1.97	0.47
1:D:884:LEU:HD13	1:D:968:ALA:H	1.80	0.47
1:D:3886:ARG:NH1	1:D:3889:GLN:OE1	2.46	0.47
1:D:3927:GLN:HA	1:D:3992:PHE:HE1	1.79	0.47
1:D:4157:ASP:OD1	1:D:4159:ARG:NH1	2.47	0.47
1:A:1776:HIS:HB3	1:A:1798:LEU:HD13	1.97	0.47
1:A:2742:THR:HG22	1:A:2815:ALA:HB2	1.96	0.47
1:A:2817:ILE:HG13	1:A:2822:THR:HA	1.96	0.47
1:A:3130:THR:HA	1:A:3133:THR:HG22	1.96	0.47
1:A:4823:LEU:HD23	1:A:4823:LEU:HA	1.80	0.47
1:C:673:PRO:HB3	2:G:71:ARG:HH22	1.80	0.47
1:C:884:LEU:HD13	1:C:968:ALA:H	1.80	0.47
1:C:1077:ALA:HA	1:C:1236:THR:HG22	1.96	0.47
1:C:2627:VAL:HG22	1:C:2678:LEU:HG	1.95	0.47
1:D:567:VAL:HG13	1:D:568:LEU:HD12	1.97	0.47
1:D:4138:ASP:OD1	1:D:4139:ILE:N	2.48	0.47
1:D:4241:THR:HB	1:D:4989:MET:HE1	1.96	0.47
1:A:272:SER:OG	1:A:333:GLY:O	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2107:GLN:O	1:A:3683:GLN:NE2	2.47	0.47
1:A:2431:ASP:HB2	1:A:2501:SER:HB3	1.96	0.47
1:A:3081:MET:HE2	1:A:3081:MET:HB3	1.83	0.47
1:B:844:ARG:NH1	1:B:1197:GLY:HA3	2.21	0.47
1:B:3886:ARG:NH1	1:B:3889:GLN:OE1	2.46	0.47
1:B:4772:ASP:HB3	1:B:4775:TYR:HB3	1.97	0.47
1:C:349:GLN:NE2	1:C:354:GLY:O	2.44	0.47
1:C:1076:ARG:HB3	1:C:1191:VAL:HG23	1.96	0.47
1:C:4241:THR:HB	1:C:4989:MET:HE1	1.96	0.47
1:C:4548:ARG:HE	1:C:4548:ARG:HB3	1.43	0.47
1:D:673:PRO:HB3	2:H:71:ARG:HH22	1.80	0.47
1:D:733:PRO:HG2	1:D:762:CYS:HB3	1.97	0.47
1:D:1077:ALA:HA	1:D:1236:THR:HG22	1.96	0.47
1:D:2627:VAL:HG22	1:D:2678:LEU:HG	1.95	0.47
2:H:99:PHE:HB3	2:H:101:VAL:HG23	1.96	0.47
1:A:572:PRO:HA	1:A:575:LEU:HD13	1.97	0.47
1:A:1232:ARG:NH2	1:A:1828:ASP:O	2.36	0.47
1:A:2627:VAL:HG22	1:A:2678:LEU:HG	1.96	0.47
1:A:4902:GLU:O	1:A:4913:ARG:NH2	2.32	0.47
1:C:1232:ARG:NH2	1:C:1828:ASP:O	2.36	0.47
1:C:1295:VAL:O	1:C:1547:LYS:HA	2.14	0.47
1:C:4190:ILE:H	1:C:4190:ILE:HG12	1.43	0.47
1:D:2689:LYS:O	1:D:2993:GLN:NE2	2.47	0.47
2:G:23:VAL:HG22	2:G:47:LYS:HB3	1.97	0.47
1:A:114:SER:HB2	1:A:116:MET:HE2	1.98	0.46
1:A:567:VAL:HG13	1:A:568:LEU:HD12	1.97	0.46
1:A:603:LEU:HA	1:A:606:LEU:HD12	1.98	0.46
1:A:2689:LYS:O	1:A:2993:GLN:NE2	2.47	0.46
1:B:1077:ALA:HA	1:B:1236:THR:HG22	1.96	0.46
1:B:2469:ILE:HA	1:B:2472:LEU:HG	1.96	0.46
1:B:2817:ILE:HG13	1:B:2822:THR:HA	1.96	0.46
1:C:567:VAL:HG13	1:C:568:LEU:HD12	1.97	0.46
1:C:688:LEU:HD22	1:C:712:TYR:HD1	1.80	0.46
1:C:2469:ILE:HA	1:C:2472:LEU:HG	1.96	0.46
1:C:3337:ARG:HA	1:C:3340:VAL:HG12	1.97	0.46
1:C:4772:ASP:HB3	1:C:4775:TYR:HB3	1.97	0.46
1:D:1076:ARG:HB3	1:D:1191:VAL:HG23	1.96	0.46
1:D:4677:LEU:HD12	1:D:4677:LEU:HA	1.83	0.46
1:D:4853:VAL:O	1:D:4857:ASN:ND2	2.44	0.46
1:A:3195:ALA:HB2	1:A:3275:PRO:HB3	1.97	0.46
1:A:3927:GLN:HA	1:A:3992:PHE:HE1	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4168:GLU:O	1:A:4171:LEU:N	2.48	0.46
1:A:4241:THR:HB	1:A:4989:MET:HE1	1.96	0.46
1:A:4576:ILE:HD13	1:A:4639:MET:HB3	1.97	0.46
1:B:2625:ARG:NE	1:B:2629:ASP:OD2	2.47	0.46
1:B:3343:GLN:NE2	1:B:3469:PHE:O	2.47	0.46
1:C:2817:ILE:HG13	1:C:2822:THR:HA	1.96	0.46
1:D:3335:MET:HE3	1:D:3335:MET:HB3	1.80	0.46
1:D:3566:SER:HB3	1:D:3569:LEU:HG	1.95	0.46
2:E:62:GLY:O	2:E:66:MET:HG3	2.16	0.46
2:G:62:GLY:O	2:G:66:MET:HG3	2.16	0.46
1:A:1461:ASP:OD2	1:A:1468:LYS:NZ	2.40	0.46
1:A:3805:LEU:HB3	1:A:3890:LEU:HB3	1.98	0.46
1:A:4138:ASP:OD1	1:A:4139:ILE:N	2.48	0.46
1:A:4772:ASP:HB3	1:A:4775:TYR:HB3	1.97	0.46
1:B:1036:ARG:O	1:B:1040:CYS:HB2	2.15	0.46
1:B:2815:ALA:HB1	1:B:2881:ASN:HD21	1.80	0.46
1:B:3454:GLU:HA	1:B:3457:ASN:HB2	1.98	0.46
1:B:4151:SER:HA	1:B:4160:LEU:HD21	1.97	0.46
1:C:3157:ILE:HG23	1:C:3161:VAL:HG12	1.98	0.46
1:C:3842:LEU:HB2	1:C:3929:SER:HB2	1.97	0.46
1:D:3343:GLN:NE2	1:D:3469:PHE:O	2.47	0.46
1:D:4958:CYS:HB3	1:D:4961:CYS:SG	2.56	0.46
2:F:62:GLY:O	2:F:66:MET:HG3	2.16	0.46
1:B:884:LEU:HD13	1:B:968:ALA:H	1.80	0.46
1:B:1851:MET:HB3	1:B:1853:ILE:HG12	1.98	0.46
1:B:2017:ASP:N	1:B:2017:ASP:OD1	2.47	0.46
1:B:3335:MET:HE3	1:B:3335:MET:HB3	1.80	0.46
1:B:4214:LYS:HB3	1:B:4214:LYS:HE2	1.61	0.46
1:C:1036:ARG:O	1:C:1040:CYS:HB2	2.15	0.46
1:C:4861:LYS:H	1:C:4861:LYS:HG3	1.46	0.46
1:D:710:ASP:N	1:D:710:ASP:OD1	2.45	0.46
1:D:2815:ALA:HB1	1:D:2881:ASN:HD21	1.80	0.46
1:D:4151:SER:HA	1:D:4160:LEU:HD21	1.97	0.46
2:H:62:GLY:O	2:H:66:MET:HG3	2.16	0.46
1:A:5030:LYS:HB2	1:A:5030:LYS:HE2	1.59	0.46
1:B:1698:LEU:O	1:B:1712:TYR:OH	2.28	0.46
1:B:3157:ILE:HG23	1:B:3161:VAL:HG12	1.97	0.46
1:B:4576:ILE:HD13	1:B:4639:MET:HB3	1.97	0.46
1:C:3454:GLU:HA	1:C:3457:ASN:HB2	1.98	0.46
1:D:3596:VAL:O	1:D:3600:SER:OG	2.27	0.46
1:D:4772:ASP:HB3	1:D:4775:TYR:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:23:VAL:HG22	2:E:47:LYS:HB3	1.97	0.46
2:F:23:VAL:HG22	2:F:47:LYS:HB3	1.97	0.46
1:A:419:ASP:HA	1:A:422:SER:HB3	1.98	0.46
1:A:573:GLU:O	1:A:577:ILE:HG12	2.16	0.46
1:A:826:ILE:HG22	1:A:827:LYS:HD2	1.98	0.46
1:A:884:LEU:HD13	1:A:968:ALA:H	1.80	0.46
1:A:2815:ALA:HB1	1:A:2881:ASN:HD21	1.80	0.46
1:B:3195:ALA:HB2	1:B:3275:PRO:HB3	1.97	0.46
1:B:3713:LYS:NZ	1:B:3715:LYS:O	2.42	0.46
1:B:3932:ASP:HA	1:B:3935:TRP:HB2	1.98	0.46
1:C:826:ILE:HG22	1:C:827:LYS:HD2	1.98	0.46
1:C:1099:GLU:OE2	1:C:1101:ARG:NE	2.46	0.46
1:C:3927:GLN:HA	1:C:3992:PHE:HE1	1.79	0.46
1:C:4958:CYS:HB3	1:C:4961:CYS:SG	2.55	0.46
1:D:3157:ILE:HG23	1:D:3161:VAL:HG12	1.98	0.46
1:D:3337:ARG:HA	1:D:3340:VAL:HG12	1.97	0.46
1:D:4190:ILE:N	1:D:5031:GLN:HE22	2.14	0.46
1:D:4214:LYS:HE2	1:D:4214:LYS:HB3	1.61	0.46
1:D:5030:LYS:HE2	1:D:5030:LYS:HB2	1.59	0.46
1:A:1077:ALA:HA	1:A:1236:THR:HG22	1.96	0.46
1:A:4958:CYS:HB3	1:A:4961:CYS:SG	2.55	0.46
1:B:114:SER:HB2	1:B:116:MET:HE2	1.98	0.46
1:B:403:MET:O	1:B:407:THR:OG1	2.19	0.46
1:B:3842:LEU:HB2	1:B:3929:SER:HB2	1.97	0.46
1:C:733:PRO:HG2	1:C:762:CYS:HB3	1.97	0.46
1:C:1851:MET:HB3	1:C:1853:ILE:HG12	1.98	0.46
1:C:1864:LYS:NZ	1:C:1871:PHE:O	2.45	0.46
1:D:1036:ARG:O	1:D:1040:CYS:HB2	2.15	0.46
1:A:844:ARG:NH1	1:A:1197:GLY:HA3	2.21	0.46
1:B:603:LEU:HA	1:B:606:LEU:HD12	1.98	0.46
1:B:4580:TYR:HE2	1:B:4630:TYR:HB3	1.81	0.46
1:B:4958:CYS:HB3	1:B:4961:CYS:SG	2.55	0.46
1:C:224:HIS:CD2	1:C:225:GLY:H	2.34	0.46
1:D:573:GLU:O	1:D:577:ILE:HG12	2.16	0.46
1:D:826:ILE:HG22	1:D:827:LYS:HD2	1.98	0.46
1:D:1782:PHE:O	2:H:82:TYR:OH	2.29	0.46
1:D:2973:PHE:HB2	1:D:2991:HIS:CD2	2.51	0.46
1:D:3254:GLY:HA2	1:D:3318:ASN:ND2	2.31	0.46
1:D:4867:GLU:H	1:D:4867:GLU:HG2	1.35	0.46
1:A:3254:GLY:HA2	1:A:3318:ASN:ND2	2.31	0.46
1:B:572:PRO:HA	1:B:575:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2456:ILE:O	1:B:2459:SER:OG	2.26	0.46
1:C:572:PRO:HA	1:C:575:LEU:HD13	1.97	0.46
1:C:2616:PRO:HG3	1:C:2647:HIS:HE1	1.81	0.46
1:C:2625:ARG:NE	1:C:2629:ASP:OD2	2.47	0.46
1:C:2973:PHE:HB2	1:C:2991:HIS:CD2	2.51	0.46
1:C:4151:SER:HA	1:C:4160:LEU:HD21	1.97	0.46
1:D:414:PHE:HA	1:D:436:LEU:HD22	1.98	0.46
1:D:419:ASP:HA	1:D:422:SER:HB3	1.98	0.46
1:D:572:PRO:HA	1:D:575:LEU:HD13	1.97	0.46
1:D:1776:HIS:HB3	1:D:1798:LEU:HD13	1.97	0.46
1:D:1851:MET:HB3	1:D:1853:ILE:HG12	1.98	0.46
1:D:2286:LEU:HD12	1:D:2286:LEU:HA	1.82	0.46
1:D:3454:GLU:HA	1:D:3457:ASN:HB2	1.97	0.46
1:A:224:HIS:CD2	1:A:225:GLY:H	2.34	0.46
1:A:2443:ILE:HD12	1:A:2454:ARG:HE	1.81	0.46
1:A:3454:GLU:HA	1:A:3457:ASN:HB2	1.98	0.46
1:A:4183:ILE:HG12	1:A:4193:ILE:HD11	1.98	0.46
1:A:4190:ILE:N	1:A:5031:GLN:HE22	2.14	0.46
1:A:4677:LEU:HD12	1:A:4677:LEU:HA	1.82	0.46
1:B:27:THR:OG1	1:B:32:GLN:OE1	2.28	0.46
1:B:3805:LEU:HB3	1:B:3890:LEU:HB3	1.98	0.46
1:C:2443:ILE:HD12	1:C:2454:ARG:HE	1.81	0.46
1:D:2817:ILE:HG13	1:D:2822:THR:HA	1.96	0.46
1:D:3674:ILE:HD13	1:D:3770:LEU:HD21	1.98	0.46
1:D:4902:GLU:O	1:D:4913:ARG:NH2	2.32	0.46
1:A:1851:MET:HB3	1:A:1853:ILE:HG12	1.98	0.45
1:A:4627:MET:HE2	1:A:4627:MET:HB2	1.75	0.45
1:B:3392:LEU:HA	1:B:3395:ARG:HD2	1.98	0.45
1:C:2815:ALA:HB1	1:C:2881:ASN:HD21	1.80	0.45
1:C:3890:LEU:HD23	1:C:3890:LEU:HA	1.85	0.45
1:D:4183:ILE:HG12	1:D:4193:ILE:HD11	1.98	0.45
1:A:2175:GLU:HG3	1:A:2228:MET:HB3	1.98	0.45
1:A:3729:MET:HG3	1:A:3800:LEU:HD13	1.99	0.45
1:A:3842:LEU:HB2	1:A:3929:SER:HB2	1.97	0.45
1:A:3932:ASP:HA	1:A:3935:TRP:HB2	1.98	0.45
1:B:224:HIS:CD2	1:B:225:GLY:H	2.34	0.45
1:B:2973:PHE:HB2	1:B:2991:HIS:CD2	2.51	0.45
1:B:3337:ARG:HA	1:B:3340:VAL:HG12	1.97	0.45
1:B:3995:VAL:O	1:B:3999:MET:HB2	2.16	0.45
1:C:4190:ILE:N	1:C:5031:GLN:HE22	2.14	0.45
1:D:114:SER:HB2	1:D:116:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:603:LEU:HA	1:D:606:LEU:HD12	1.97	0.45
2:H:23:VAL:HG22	2:H:47:LYS:HB3	1.97	0.45
1:A:1036:ARG:O	1:A:1040:CYS:HB2	2.15	0.45
1:A:2817:ILE:HD12	1:A:2823:ILE:HG22	1.99	0.45
1:A:3157:ILE:HG23	1:A:3161:VAL:HG12	1.98	0.45
1:A:4580:TYR:HE2	1:A:4630:TYR:HB3	1.81	0.45
1:B:826:ILE:HG22	1:B:827:LYS:HD2	1.98	0.45
1:B:2686:LEU:HB3	1:B:2997:PHE:HE1	1.82	0.45
1:C:3254:GLY:HA2	1:C:3318:ASN:ND2	2.31	0.45
1:C:4183:ILE:HG12	1:C:4193:ILE:HD11	1.98	0.45
1:D:217:GLY:N	1:D:262:LEU:O	2.45	0.45
1:D:224:HIS:CD2	1:D:225:GLY:H	2.34	0.45
1:D:4576:ILE:HD13	1:D:4639:MET:HB3	1.97	0.45
1:A:548:VAL:HA	1:A:551:LEU:HD23	1.99	0.45
1:A:893:TYR:HB3	1:A:960:MET:HE2	1.99	0.45
1:B:2121:PHE:O	1:B:3725:TYR:OH	2.28	0.45
1:B:4190:ILE:N	1:B:5031:GLN:HE22	2.14	0.45
1:C:3713:LYS:NZ	1:C:3715:LYS:O	2.42	0.45
1:C:3785:ALA:HA	1:C:3787:LYS:HE3	1.99	0.45
1:D:407:THR:HG22	1:D:411:TYR:CE2	2.52	0.45
1:D:3729:MET:HG3	1:D:3800:LEU:HD13	1.98	0.45
1:D:3805:LEU:HB3	1:D:3890:LEU:HB3	1.98	0.45
1:D:4704:LEU:O	1:D:4774:LYS:NZ	2.36	0.45
1:A:484:LEU:HA	1:A:487:VAL:HG22	1.99	0.45
1:A:1220:GLN:HB2	1:D:3519:PRO:HB3	1.99	0.45
1:A:2616:PRO:HG3	1:A:2647:HIS:HE1	1.81	0.45
1:A:2973:PHE:HB2	1:A:2991:HIS:CD2	2.51	0.45
1:A:4861:LYS:H	1:A:4861:LYS:HG3	1.46	0.45
1:B:1866:ILE:HA	1:B:1926:LEU:HD23	1.98	0.45
1:B:2443:ILE:HD12	1:B:2454:ARG:HE	1.81	0.45
1:B:3519:PRO:HB3	1:C:1220:GLN:HB2	1.99	0.45
1:B:4059:LEU:HD12	1:B:4170:ILE:HG21	1.99	0.45
1:C:484:LEU:HA	1:C:487:VAL:HG22	1.99	0.45
1:C:4580:TYR:HE2	1:C:4630:TYR:HB3	1.81	0.45
1:D:484:LEU:HA	1:D:487:VAL:HG22	1.99	0.45
1:D:2686:LEU:HB3	1:D:2997:PHE:HE1	1.82	0.45
1:D:3959:LYS:NZ	1:D:4018:ASP:OD1	2.45	0.45
1:D:4168:GLU:O	1:D:4171:LEU:N	2.48	0.45
1:D:4821:LYS:HE3	1:D:4821:LYS:HB3	1.76	0.45
1:A:1738:LEU:HB2	1:A:2146:PRO:HD3	1.99	0.45
1:A:3634:ALA:O	1:A:3638:MET:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3674:ILE:HD13	1:A:3770:LEU:HD21	1.98	0.45
1:B:3785:ALA:HA	1:B:3787:LYS:HE3	1.99	0.45
1:B:4168:GLU:O	1:B:4171:LEU:N	2.48	0.45
1:B:4183:ILE:HG12	1:B:4193:ILE:HD11	1.98	0.45
1:C:414:PHE:HA	1:C:436:LEU:HD22	1.98	0.45
1:D:893:TYR:HB3	1:D:960:MET:HE2	1.99	0.45
1:D:1676:LEU:HD22	1:D:2167:ILE:HD12	1.99	0.45
1:D:2175:GLU:HG3	1:D:2228:MET:HB3	1.99	0.45
1:A:76:ARG:O	1:A:79:GLN:N	2.49	0.45
1:A:243:ARG:HA	1:A:301:VAL:HG22	1.99	0.45
1:A:4151:SER:HA	1:A:4160:LEU:HD21	1.97	0.45
1:B:419:ASP:HA	1:B:422:SER:HB3	1.98	0.45
1:B:484:LEU:HA	1:B:487:VAL:HG22	1.99	0.45
1:B:863:LEU:HA	1:B:864:PRO:HD3	1.85	0.45
1:B:893:TYR:HB3	1:B:960:MET:HE2	1.99	0.45
1:B:1965:TYR:OH	1:B:2027:ILE:O	2.31	0.45
1:B:3194:LEU:HD13	1:B:3276:MET:HE3	1.99	0.45
1:B:3634:ALA:O	1:B:3638:MET:HB3	2.16	0.45
1:B:3729:MET:HG3	1:B:3800:LEU:HD13	1.99	0.45
1:B:4989:MET:HE3	1:B:4989:MET:HB2	1.72	0.45
1:C:243:ARG:HA	1:C:301:VAL:HG22	1.99	0.45
1:C:419:ASP:HA	1:C:422:SER:HB3	1.98	0.45
1:C:1676:LEU:HD22	1:C:2167:ILE:HD12	1.99	0.45
1:C:2175:GLU:HG3	1:C:2228:MET:HB3	1.98	0.45
1:C:3779:VAL:HG13	1:C:3797:THR:HG22	1.99	0.45
1:C:3805:LEU:HB3	1:C:3890:LEU:HB3	1.98	0.45
1:D:3416:VAL:HG13	1:D:3423:TRP:HZ3	1.82	0.45
1:D:3932:ASP:HA	1:D:3935:TRP:HB2	1.98	0.45
1:D:4059:LEU:HD12	1:D:4170:ILE:HG21	1.99	0.45
1:A:1698:LEU:O	1:A:1712:TYR:OH	2.28	0.45
1:A:2677:LYS:HE2	1:A:2677:LYS:HB3	1.77	0.45
1:A:3337:ARG:HA	1:A:3340:VAL:HG12	1.97	0.45
1:B:407:THR:HG22	1:B:411:TYR:CE2	2.52	0.45
1:B:548:VAL:HA	1:B:551:LEU:HD23	1.99	0.45
1:B:573:GLU:O	1:B:577:ILE:HG12	2.16	0.45
1:C:647:ASN:OD1	1:C:647:ASN:N	2.50	0.45
1:C:2686:LEU:HB3	1:C:2997:PHE:HE1	1.82	0.45
1:C:3519:PRO:HB3	1:D:1220:GLN:HB2	1.99	0.45
1:C:3634:ALA:O	1:C:3638:MET:HB3	2.16	0.45
2:F:105:ASN:ND2	2:F:107:GLU:O	2.50	0.45
1:A:1866:ILE:HA	1:A:1926:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3194:LEU:HD13	1:A:3276:MET:HE3	1.99	0.45
1:A:3392:LEU:HA	1:A:3395:ARG:HD2	1.98	0.45
1:B:1676:LEU:HD22	1:B:2167:ILE:HD12	1.99	0.45
1:B:2616:PRO:HG3	1:B:2647:HIS:HE1	1.81	0.45
1:B:3254:GLY:HA2	1:B:3318:ASN:ND2	2.31	0.45
1:B:3524:MET:HG2	1:B:3595:ARG:HD2	1.99	0.45
1:C:114:SER:HB2	1:C:116:MET:HE2	1.98	0.45
1:C:893:TYR:HB3	1:C:960:MET:HE2	1.99	0.45
1:C:3932:ASP:HA	1:C:3935:TRP:HB2	1.98	0.45
1:C:3995:VAL:O	1:C:3999:MET:HB2	2.16	0.45
1:B:243:ARG:HA	1:B:301:VAL:HG22	1.99	0.45
1:B:673:PRO:HB3	2:F:71:ARG:HH22	1.80	0.45
1:B:2817:ILE:HD12	1:B:2823:ILE:HG22	1.99	0.45
1:C:1866:ILE:HA	1:C:1926:LEU:HD23	1.98	0.45
1:C:3809:ASN:HB3	1:C:3812:VAL:HB	1.99	0.45
1:D:76:ARG:O	1:D:79:GLN:N	2.49	0.45
1:D:243:ARG:HA	1:D:301:VAL:HG22	1.99	0.45
1:D:299:LEU:HD13	1:D:378:LEU:HD22	1.98	0.45
1:D:1738:LEU:HB2	1:D:2146:PRO:HD3	1.99	0.45
1:D:1866:ILE:HA	1:D:1926:LEU:HD23	1.98	0.45
1:D:2443:ILE:HD12	1:D:2454:ARG:HE	1.81	0.45
1:D:2616:PRO:HG3	1:D:2647:HIS:HE1	1.81	0.45
1:D:4580:TYR:HE2	1:D:4630:TYR:HB3	1.81	0.45
1:D:4911:LEU:HD22	1:D:4911:LEU:HA	1.87	0.45
1:A:299:LEU:HD13	1:A:378:LEU:HD22	1.98	0.44
1:A:414:PHE:HA	1:A:436:LEU:HD22	1.98	0.44
1:A:1676:LEU:HD22	1:A:2167:ILE:HD12	1.99	0.44
1:A:3995:VAL:O	1:A:3999:MET:HB2	2.16	0.44
1:B:4722:ARG:H	1:B:4722:ARG:HG2	1.45	0.44
1:B:4861:LYS:H	1:B:4861:LYS:HG3	1.46	0.44
1:C:603:LEU:HA	1:C:606:LEU:HD12	1.98	0.44
1:C:661:LYS:HB3	1:C:808:TYR:HA	1.99	0.44
1:C:4049:VAL:HG21	1:C:4159:ARG:HE	1.82	0.44
1:C:4576:ILE:HD13	1:C:4639:MET:HB3	1.97	0.44
1:D:548:VAL:HA	1:D:551:LEU:HD23	1.99	0.44
1:D:2190:VAL:HA	1:D:2193:GLN:HB2	2.00	0.44
1:D:3301:PRO:HA	1:D:3302:PRO:HD3	1.88	0.44
1:D:3785:ALA:HA	1:D:3787:LYS:HE3	1.99	0.44
1:D:4861:LYS:H	1:D:4861:LYS:HG3	1.46	0.44
1:A:407:THR:HG22	1:A:411:TYR:CE2	2.52	0.44
1:A:793:LEU:HB2	1:A:797:HIS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1149:VAL:HG12	1:A:1164:LEU:HA	1.99	0.44
1:A:1839:VAL:HG23	1:A:1935:VAL:HG22	1.99	0.44
1:A:4059:LEU:HD12	1:A:4170:ILE:HG21	1.99	0.44
1:B:661:LYS:HB3	1:B:808:TYR:HA	1.99	0.44
1:C:2017:ASP:N	1:C:2017:ASP:OD1	2.47	0.44
1:C:2190:VAL:HA	1:C:2193:GLN:HB2	1.99	0.44
1:C:2586:VAL:HG13	1:C:2607:LEU:HD21	2.00	0.44
1:C:3392:LEU:HA	1:C:3395:ARG:HD2	1.98	0.44
1:C:3524:MET:HG2	1:C:3595:ARG:HD2	1.99	0.44
1:C:4732:PHE:HD2	1:C:4737:ILE:HG12	1.82	0.44
1:D:2017:ASP:OD1	1:D:2017:ASP:N	2.47	0.44
1:D:2712:PRO:HA	1:D:2955:PHE:HD2	1.83	0.44
1:D:3634:ALA:O	1:D:3638:MET:HB3	2.16	0.44
1:D:3995:VAL:O	1:D:3999:MET:HB2	2.16	0.44
1:D:4548:ARG:HE	1:D:4548:ARG:HB3	1.43	0.44
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.33	0.44
1:D:4584:ASP:HA	1:D:4628:VAL:HG12	2.00	0.44
2:E:105:ASN:ND2	2:E:107:GLU:O	2.50	0.44
1:A:1442:GLY:HA2	1:A:1509:ILE:HG23	2.00	0.44
1:A:3107:VAL:O	1:A:3111:ARG:HB2	2.18	0.44
1:A:3596:VAL:O	1:A:3600:SER:OG	2.27	0.44
1:A:3785:ALA:HA	1:A:3787:LYS:HE3	1.99	0.44
1:B:2199:ARG:NE	1:B:2246:ASN:OD1	2.50	0.44
1:B:2604:GLU:HB3	1:B:2608:MET:HE1	2.00	0.44
1:B:3674:ILE:HD13	1:B:3770:LEU:HD21	1.98	0.44
1:C:34:LYS:HD3	1:C:34:LYS:HA	1.82	0.44
1:C:461:HIS:O	1:C:465:GLN:HG2	2.18	0.44
1:C:573:GLU:O	1:C:577:ILE:HG12	2.16	0.44
1:C:1149:VAL:HG12	1:C:1164:LEU:HA	1.99	0.44
1:C:2817:ILE:HD12	1:C:2823:ILE:HG22	1.99	0.44
1:C:3674:ILE:HD13	1:C:3770:LEU:HD21	1.98	0.44
1:D:1926:LEU:HA	1:D:1929:MET:HE2	2.00	0.44
1:D:2325:PRO:O	1:D:2329:GLU:HB2	2.18	0.44
1:D:3579:LEU:HB2	1:D:3582:ARG:HG2	1.99	0.44
1:D:4865:LYS:HD2	1:D:4865:LYS:HA	1.63	0.44
1:A:45:ARG:HG2	1:A:443:LEU:HD21	2.00	0.44
1:A:2686:LEU:HB3	1:A:2997:PHE:HE1	1.82	0.44
1:A:3779:VAL:HG13	1:A:3797:THR:HG22	1.99	0.44
1:A:4732:PHE:HD2	1:A:4737:ILE:HG12	1.83	0.44
1:B:465:GLN:O	1:B:469:ARG:HG2	2.18	0.44
1:B:1738:LEU:HB2	1:B:2146:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3416:VAL:HG13	1:B:3423:TRP:HZ3	1.82	0.44
1:B:4190:ILE:H	1:B:4190:ILE:HG12	1.43	0.44
1:C:2286:LEU:HD12	1:C:2286:LEU:HA	1.82	0.44
1:C:2736:ASP:OD1	1:C:2736:ASP:N	2.50	0.44
1:C:4888:TYR:HA	1:D:4918:ILE:HD11	1.99	0.44
1:D:3670:GLU:HG3	1:D:3728:ILE:HG23	2.00	0.44
1:D:4049:VAL:HG21	1:D:4159:ARG:HE	1.82	0.44
1:A:2586:VAL:HG13	1:A:2607:LEU:HD21	2.00	0.44
1:B:76:ARG:O	1:B:79:GLN:N	2.49	0.44
1:B:1442:GLY:HA2	1:B:1509:ILE:HG23	2.00	0.44
1:B:1926:LEU:HA	1:B:1929:MET:HE2	2.00	0.44
1:B:2780:ASN:ND2	1:B:2782:ASP:OD2	2.51	0.44
1:B:3020:THR:HG23	1:B:3023:LYS:H	1.83	0.44
1:B:4000:MET:HE2	1:B:4058:ILE:HD13	2.00	0.44
1:C:76:ARG:O	1:C:79:GLN:N	2.49	0.44
1:C:3670:GLU:HG3	1:C:3728:ILE:HG23	2.00	0.44
1:C:4059:LEU:HD12	1:C:4170:ILE:HG21	1.99	0.44
1:C:4989:MET:HE3	1:C:4989:MET:HB2	1.72	0.44
1:D:465:GLN:O	1:D:469:ARG:HG2	2.18	0.44
1:D:3779:VAL:HG13	1:D:3797:THR:HG22	1.99	0.44
2:E:17:LYS:HG2	2:E:20:GLN:HE22	1.83	0.44
2:H:105:ASN:ND2	2:H:107:GLU:O	2.50	0.44
1:B:2175:GLU:HG3	1:B:2228:MET:HB3	1.98	0.44
1:B:3107:VAL:O	1:B:3111:ARG:HB2	2.18	0.44
1:B:3779:VAL:HG13	1:B:3797:THR:HG22	1.99	0.44
1:C:407:THR:HG22	1:C:411:TYR:CE2	2.52	0.44
1:C:1839:VAL:HG23	1:C:1935:VAL:HG22	1.99	0.44
1:C:1926:LEU:HA	1:C:1929:MET:HE2	2.00	0.44
1:C:3051:ARG:HA	1:C:3131:TYR:CZ	2.53	0.44
1:C:3729:MET:HG3	1:C:3800:LEU:HD13	1.98	0.44
1:D:461:HIS:O	1:D:465:GLN:HG2	2.18	0.44
1:D:786:GLY:HA2	1:D:1631:GLN:HA	1.99	0.44
1:D:2199:ARG:NE	1:D:2246:ASN:OD1	2.50	0.44
1:D:3140:LEU:HA	1:D:3143:LEU:HD12	2.00	0.44
1:A:661:LYS:HB3	1:A:808:TYR:HA	2.00	0.44
1:A:873:LYS:HG2	1:A:970:LEU:HD13	1.99	0.44
1:A:1926:LEU:HA	1:A:1929:MET:HE2	2.00	0.44
1:A:2625:ARG:NE	1:A:2629:ASP:OD2	2.47	0.44
1:A:2676:ARG:HE	1:A:2680:TRP:HE1	1.66	0.44
1:A:4000:MET:HE2	1:A:4058:ILE:HD13	2.00	0.44
1:B:1099:GLU:OE2	1:B:1101:ARG:NE	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2586:VAL:HG13	1:B:2607:LEU:HD21	2.00	0.44
1:B:3809:ASN:HB3	1:B:3812:VAL:HB	1.99	0.44
1:B:4865:LYS:HD2	1:B:4865:LYS:HA	1.63	0.44
1:C:548:VAL:HA	1:C:551:LEU:HD23	1.99	0.44
1:C:876:GLU:HG2	1:C:910:PHE:CE2	2.53	0.44
1:C:2780:ASN:ND2	1:C:2782:ASP:OD2	2.51	0.44
1:C:3107:VAL:O	1:C:3111:ARG:HB2	2.18	0.44
1:C:3140:LEU:HA	1:C:3143:LEU:HD12	2.00	0.44
1:C:4168:GLU:O	1:C:4171:LEU:N	2.48	0.44
1:C:4902:GLU:O	1:C:4913:ARG:NH2	2.32	0.44
1:D:1099:GLU:OE2	1:D:1101:ARG:NE	2.46	0.44
1:D:2586:VAL:HG13	1:D:2607:LEU:HD21	2.00	0.44
1:D:2817:ILE:HD12	1:D:2823:ILE:HG22	1.99	0.44
1:D:3020:THR:HG23	1:D:3023:LYS:H	1.83	0.44
1:D:3107:VAL:O	1:D:3111:ARG:HB2	2.18	0.44
1:D:3332:ALA:O	1:D:3336:LYS:NZ	2.51	0.44
1:D:3752:SER:OG	1:D:3755:GLU:OE1	2.25	0.44
2:G:105:ASN:ND2	2:G:107:GLU:O	2.50	0.44
1:A:281:ARG:NH2	1:A:309:THR:OG1	2.51	0.44
1:A:626:LEU:HB3	1:A:1688:HIS:CE1	2.53	0.44
1:A:3020:THR:HG23	1:A:3023:LYS:H	1.83	0.44
1:A:3332:ALA:O	1:A:3336:LYS:NZ	2.51	0.44
1:A:3779:VAL:O	1:A:3783:ILE:HG12	2.18	0.44
1:B:414:PHE:HA	1:B:436:LEU:HD22	1.98	0.44
1:B:626:LEU:HB3	1:B:1688:HIS:CE1	2.53	0.44
1:B:786:GLY:HA2	1:B:1631:GLN:HA	1.99	0.44
1:C:45:ARG:HG2	1:C:443:LEU:HD21	2.00	0.44
1:C:299:LEU:HD13	1:C:378:LEU:HD22	1.98	0.44
1:C:2098:VAL:HG13	1:C:2127:GLN:HG3	2.00	0.44
1:C:2325:PRO:O	1:C:2329:GLU:HB2	2.18	0.44
1:C:3020:THR:HG23	1:C:3023:LYS:H	1.83	0.44
1:C:4584:ASP:HA	1:C:4628:VAL:HG12	2.00	0.44
1:C:4796:MET:HE3	1:C:4796:MET:HB2	1.74	0.44
1:D:45:ARG:HG2	1:D:443:LEU:HD21	2.00	0.44
1:D:876:GLU:HG2	1:D:910:PHE:CE2	2.53	0.44
1:D:2621:HIS:HA	1:D:2624:ARG:HG2	2.00	0.44
2:F:17:LYS:HG2	2:F:20:GLN:HE22	1.83	0.44
1:A:2712:PRO:HA	1:A:2955:PHE:HD2	1.83	0.44
1:A:3524:MET:HG2	1:A:3595:ARG:HD2	1.99	0.44
1:A:4918:ILE:HD13	1:D:4892:ARG:HD3	2.00	0.44
1:B:876:GLU:HG2	1:B:910:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1686:CYS:HB2	1:B:1782:PHE:HZ	1.83	0.44
1:B:2676:ARG:HE	1:B:2680:TRP:HE1	1.66	0.44
1:B:3081:MET:HE2	1:B:3081:MET:HB3	1.83	0.44
1:C:2737:PRO:HG2	1:C:2888:ARG:HB2	1.99	0.44
1:C:3332:ALA:O	1:C:3336:LYS:NZ	2.51	0.44
1:C:5030:LYS:HE2	1:C:5030:LYS:HB2	1.59	0.44
1:D:626:LEU:HB3	1:D:1688:HIS:CE1	2.53	0.44
1:D:1686:CYS:HB2	1:D:1782:PHE:HZ	1.83	0.44
1:D:1839:VAL:HG23	1:D:1935:VAL:HG22	1.99	0.44
1:D:2098:VAL:HG13	1:D:2127:GLN:HG3	2.00	0.44
1:D:3985:LEU:HD11	1:D:4026:MET:HE1	2.00	0.44
2:E:7:ILE:HD11	2:E:73:LYS:HB2	2.00	0.44
2:H:17:LYS:HG2	2:H:20:GLN:HE22	1.83	0.44
1:A:876:GLU:HG2	1:A:910:PHE:CE2	2.53	0.43
1:A:2621:HIS:HA	1:A:2624:ARG:HG2	2.00	0.43
1:A:2737:PRO:HG2	1:A:2888:ARG:HB2	1.99	0.43
1:A:3354:LEU:N	1:A:3415:TYR:OH	2.51	0.43
1:A:4570:ALA:O	1:A:4574:ASN:ND2	2.33	0.43
1:B:17:ASP:N	1:B:69:LEU:O	2.44	0.43
1:B:663:TYR:OH	1:B:665:GLU:OE2	2.35	0.43
1:B:3354:LEU:N	1:B:3415:TYR:OH	2.51	0.43
1:B:4049:VAL:HG21	1:B:4159:ARG:HE	1.83	0.43
1:C:403:MET:O	1:C:407:THR:OG1	2.19	0.43
1:C:793:LEU:HB2	1:C:797:HIS:HB2	1.99	0.43
1:C:2199:ARG:NE	1:C:2246:ASN:OD1	2.50	0.43
1:C:2712:PRO:HA	1:C:2955:PHE:HD2	1.83	0.43
1:C:3035:GLU:HA	1:C:3038:MET:HE2	2.00	0.43
1:C:3147:ILE:HA	1:C:3152:PHE:HB2	2.01	0.43
1:C:3194:LEU:HD13	1:C:3276:MET:HE3	1.99	0.43
1:C:3985:LEU:HD11	1:C:4026:MET:HE1	2.00	0.43
1:D:661:LYS:HB3	1:D:808:TYR:HA	1.99	0.43
1:D:1149:VAL:HG12	1:D:1164:LEU:HA	1.99	0.43
1:D:2625:ARG:NE	1:D:2629:ASP:OD2	2.47	0.43
1:D:3081:MET:HE2	1:D:3081:MET:HB3	1.83	0.43
1:D:3194:LEU:HD13	1:D:3276:MET:HE3	1.99	0.43
1:D:3809:ASN:HB3	1:D:3812:VAL:HB	1.99	0.43
1:D:4796:MET:HB2	1:D:4796:MET:HE3	1.73	0.43
2:H:7:ILE:HD11	2:H:73:LYS:HB2	2.00	0.43
1:A:293:LEU:H	1:A:311:ALA:HB1	1.84	0.43
1:A:2325:PRO:O	1:A:2329:GLU:HB2	2.18	0.43
1:A:3579:LEU:HB2	1:A:3582:ARG:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2621:HIS:HA	1:B:2624:ARG:HG2	2.00	0.43
1:B:3596:VAL:O	1:B:3600:SER:OG	2.27	0.43
1:C:465:GLN:O	1:C:469:ARG:HG2	2.18	0.43
1:C:1738:LEU:HB2	1:C:2146:PRO:HD3	1.99	0.43
1:C:3416:VAL:HG13	1:C:3423:TRP:HZ3	1.82	0.43
1:D:2676:ARG:HE	1:D:2680:TRP:HE1	1.66	0.43
1:D:2716:ASP:OD1	1:D:2716:ASP:N	2.51	0.43
1:D:2780:ASN:ND2	1:D:2782:ASP:OD2	2.51	0.43
1:D:4204:GLN:HB3	1:D:4245:MET:HE2	2.00	0.43
1:A:786:GLY:HA2	1:A:1631:GLN:HA	1.99	0.43
1:A:2567:PRO:HG3	1:A:2613:TYR:CZ	2.53	0.43
1:A:2604:GLU:HB3	1:A:2608:MET:HE1	1.99	0.43
1:A:2765:LYS:HD3	1:A:2765:LYS:HA	1.85	0.43
1:A:2998:PHE:HA	1:A:3002:LEU:HD13	2.00	0.43
1:A:3140:LEU:HA	1:A:3143:LEU:HD12	2.00	0.43
1:A:3416:VAL:HG13	1:A:3423:TRP:HZ3	1.82	0.43
1:B:299:LEU:HD13	1:B:378:LEU:HD22	1.98	0.43
1:B:2736:ASP:OD1	1:B:2736:ASP:N	2.50	0.43
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.33	0.43
1:C:1100:MET:HB2	1:C:1143:TRP:CZ2	2.53	0.43
1:C:1686:CYS:HB2	1:C:1782:PHE:HZ	1.83	0.43
1:C:2621:HIS:HA	1:C:2624:ARG:HG2	2.00	0.43
1:C:2998:PHE:HA	1:C:3002:LEU:HD13	2.00	0.43
1:C:3579:LEU:HB2	1:C:3582:ARG:HG2	1.99	0.43
1:C:4000:MET:HE2	1:C:4058:ILE:HD13	2.00	0.43
1:D:281:ARG:NH2	1:D:309:THR:OG1	2.51	0.43
1:D:720:HIS:CG	1:D:727:ALA:HB1	2.54	0.43
1:D:873:LYS:HG2	1:D:970:LEU:HD13	1.99	0.43
1:D:1100:MET:HB2	1:D:1143:TRP:CZ2	2.53	0.43
1:D:2309:SER:OG	1:D:2321:ILE:O	2.26	0.43
1:D:2604:GLU:HB3	1:D:2608:MET:HE1	2.00	0.43
1:D:2737:PRO:HG2	1:D:2888:ARG:HB2	1.99	0.43
1:D:3392:LEU:HA	1:D:3395:ARG:HD2	1.98	0.43
1:A:465:GLN:O	1:A:469:ARG:HG2	2.18	0.43
1:A:647:ASN:OD1	1:A:647:ASN:N	2.50	0.43
1:A:1686:CYS:HB2	1:A:1782:PHE:HZ	1.83	0.43
1:A:2286:LEU:HD12	1:A:2286:LEU:HA	1.82	0.43
1:B:2190:VAL:HA	1:B:2193:GLN:HB2	2.00	0.43
1:B:2739:PRO:HG3	1:B:2888:ARG:HG2	2.00	0.43
1:B:3035:GLU:HA	1:B:3038:MET:HE2	2.00	0.43
1:B:3201:MET:HG3	1:B:3203:VAL:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4888:TYR:HA	1:C:4918:ILE:HD11	1.99	0.43
1:C:863:LEU:HA	1:C:864:PRO:HD3	1.85	0.43
1:C:936:GLY:HA3	1:C:1056:PRO:HB3	2.00	0.43
1:C:1115:LEU:HB3	1:C:1123:VAL:HG11	2.01	0.43
1:C:2677:LYS:HB3	1:C:2677:LYS:HE2	1.77	0.43
1:C:2739:PRO:HG3	1:C:2888:ARG:HG2	2.00	0.43
1:D:552:ASP:OD1	1:D:552:ASP:N	2.50	0.43
1:D:1442:GLY:HA2	1:D:1509:ILE:HG23	2.00	0.43
1:D:2677:LYS:HE2	1:D:2677:LYS:HB3	1.77	0.43
1:D:3147:ILE:HA	1:D:3152:PHE:HB2	2.01	0.43
1:D:3262:ARG:O	1:D:3266:MET:HG2	2.18	0.43
2:G:7:ILE:HD11	2:G:73:LYS:HB2	2.00	0.43
1:A:3415:TYR:O	1:A:3419:ASN:ND2	2.37	0.43
1:A:3890:LEU:HD23	1:A:3890:LEU:HA	1.85	0.43
1:A:3945:GLU:OE1	1:A:3949:ARG:NH1	2.52	0.43
1:A:4204:GLN:HB3	1:A:4245:MET:HE2	2.00	0.43
1:A:4584:ASP:HA	1:A:4628:VAL:HG12	2.00	0.43
1:B:873:LYS:HG2	1:B:970:LEU:HD13	1.99	0.43
1:B:936:GLY:HA3	1:B:1056:PRO:HB3	2.00	0.43
1:B:1100:MET:HB2	1:B:1143:TRP:CZ2	2.53	0.43
1:B:2677:LYS:HB3	1:B:2677:LYS:HE2	1.77	0.43
1:B:2712:PRO:HA	1:B:2955:PHE:HD2	1.83	0.43
1:B:3959:LYS:NZ	1:B:4018:ASP:OD1	2.45	0.43
1:B:4902:GLU:O	1:B:4913:ARG:NH2	2.32	0.43
1:C:17:ASP:HB2	1:C:98:HIS:HE1	1.84	0.43
1:C:111:HIS:ND1	1:C:114:SER:OG	2.35	0.43
1:C:504:ALA:HB2	1:C:512:ALA:HB2	2.00	0.43
1:C:626:LEU:HB3	1:C:1688:HIS:CE1	2.53	0.43
1:C:786:GLY:HA2	1:C:1631:GLN:HA	1.99	0.43
1:C:1435:TYR:HB3	1:C:1575:LEU:HD21	2.00	0.43
1:C:2567:PRO:HG3	1:C:2613:TYR:CZ	2.53	0.43
1:C:2676:ARG:HE	1:C:2680:TRP:HE1	1.66	0.43
1:C:3779:VAL:O	1:C:3783:ILE:HG12	2.18	0.43
1:C:3945:GLU:OE1	1:C:3949:ARG:NH1	2.52	0.43
1:D:17:ASP:HB2	1:D:98:HIS:HE1	1.84	0.43
1:D:2567:PRO:HG3	1:D:2613:TYR:CZ	2.53	0.43
1:D:3573:MET:HA	1:D:3576:TYR:HB3	2.00	0.43
1:D:3945:GLU:OE1	1:D:3949:ARG:NH1	2.52	0.43
1:D:4888:TYR:CD2	1:D:4889:VAL:HG22	2.54	0.43
2:G:56:ILE:HG12	2:G:81:ALA:HA	2.01	0.43
2:H:56:ILE:HG12	2:H:81:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1100:MET:HB2	1:A:1143:TRP:CZ2	2.53	0.43
1:A:2190:VAL:HA	1:A:2193:GLN:HB2	2.00	0.43
1:A:2716:ASP:OD1	1:A:2716:ASP:N	2.52	0.43
1:A:3262:ARG:O	1:A:3266:MET:HG2	2.18	0.43
1:A:4171:LEU:O	1:A:4175:ARG:HB2	2.19	0.43
1:B:504:ALA:HB2	1:B:512:ALA:HB2	2.00	0.43
1:B:793:LEU:HB2	1:B:797:HIS:HB2	1.99	0.43
1:B:1149:VAL:HG12	1:B:1164:LEU:HA	1.99	0.43
1:B:3579:LEU:HB2	1:B:3582:ARG:HG2	1.99	0.43
1:C:878:ILE:HD11	1:C:925:SER:HB2	2.01	0.43
1:C:3343:GLN:NE2	1:C:3469:PHE:O	2.47	0.43
1:C:3354:LEU:N	1:C:3415:TYR:OH	2.51	0.43
1:C:4204:GLN:HB3	1:C:4245:MET:HE2	2.00	0.43
1:D:878:ILE:HD11	1:D:925:SER:HB2	2.01	0.43
1:D:2617:SER:OG	1:D:2618:MET:SD	2.72	0.43
1:D:3944:GLU:OE1	1:D:3946:GLN:N	2.47	0.43
2:F:56:ILE:HG12	2:F:81:ALA:HA	2.00	0.43
1:A:878:ILE:HD11	1:A:925:SER:HB2	2.01	0.43
1:A:2739:PRO:HG3	1:A:2888:ARG:HG2	2.00	0.43
1:A:3147:ILE:HA	1:A:3152:PHE:HB2	2.01	0.43
1:A:3809:ASN:HB3	1:A:3812:VAL:HB	1.99	0.43
1:A:4968:PHE:O	1:A:4974:GLY:HA3	2.19	0.43
1:B:3140:LEU:HA	1:B:3143:LEU:HD12	2.00	0.43
1:B:3262:ARG:O	1:B:3266:MET:HG2	2.18	0.43
1:B:3670:GLU:HG3	1:B:3728:ILE:HG23	2.00	0.43
1:B:3945:GLU:OE1	1:B:3949:ARG:NH1	2.52	0.43
1:C:3201:MET:HG3	1:C:3203:VAL:H	1.83	0.43
1:C:3262:ARG:O	1:C:3266:MET:HG2	2.18	0.43
1:C:4888:TYR:CD2	1:C:4889:VAL:HG22	2.54	0.43
1:D:936:GLY:HA3	1:D:1056:PRO:HB3	2.00	0.43
1:D:1115:LEU:HB3	1:D:1123:VAL:HG11	2.01	0.43
1:D:2006:ILE:HG23	1:D:3641:LEU:HD11	2.01	0.43
1:D:3201:MET:HG3	1:D:3203:VAL:H	1.83	0.43
1:D:4732:PHE:HD2	1:D:4737:ILE:HG12	1.83	0.43
1:A:2006:ILE:HG23	1:A:3641:LEU:HD11	2.01	0.43
1:B:45:ARG:HG2	1:B:443:LEU:HD21	2.00	0.43
1:B:461:HIS:O	1:B:465:GLN:HG2	2.18	0.43
1:B:720:HIS:CG	1:B:727:ALA:HB1	2.54	0.43
1:B:2098:VAL:HG13	1:B:2127:GLN:HG3	2.00	0.43
1:B:2325:PRO:O	1:B:2329:GLU:HB2	2.18	0.43
1:B:4732:PHE:HD2	1:B:4737:ILE:HG12	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4823:LEU:HD23	1:B:4823:LEU:HA	1.80	0.43
1:C:27:THR:OG1	1:C:32:GLN:OE1	2.28	0.43
1:C:2339:VAL:HG12	1:C:2349:ASN:HB3	2.01	0.43
1:C:3249:LEU:HD12	1:C:3249:LEU:HA	1.86	0.43
1:C:3450:ASN:HA	1:C:3453:ARG:HG2	2.01	0.43
1:D:3524:MET:HG2	1:D:3595:ARG:HD2	1.99	0.43
1:D:3779:VAL:O	1:D:3783:ILE:HG12	2.18	0.43
1:D:4171:LEU:O	1:D:4175:ARG:HB2	2.19	0.43
1:A:461:HIS:O	1:A:465:GLN:HG2	2.18	0.43
1:A:720:HIS:CG	1:A:727:ALA:HB1	2.54	0.43
1:A:2309:SER:OG	1:A:2321:ILE:O	2.26	0.43
1:A:3573:MET:HA	1:A:3576:TYR:HB3	2.00	0.43
1:A:4049:VAL:HG21	1:A:4159:ARG:HE	1.82	0.43
1:B:217:GLY:N	1:B:262:LEU:O	2.45	0.43
1:B:2567:PRO:HG3	1:B:2613:TYR:CZ	2.53	0.43
1:B:3147:ILE:HA	1:B:3152:PHE:HB2	2.01	0.43
1:B:3779:VAL:O	1:B:3783:ILE:HG12	2.18	0.43
1:B:3944:GLU:OE1	1:B:3946:GLN:N	2.47	0.43
1:C:293:LEU:H	1:C:311:ALA:HB1	1.83	0.43
1:C:873:LYS:HG2	1:C:970:LEU:HD13	1.99	0.43
1:C:1442:GLY:HA2	1:C:1509:ILE:HG23	2.00	0.43
1:C:2006:ILE:HG23	1:C:3641:LEU:HD11	2.01	0.43
1:C:4646:LEU:HD23	1:C:4646:LEU:HA	1.89	0.43
1:C:4968:PHE:O	1:C:4974:GLY:HA3	2.19	0.43
1:D:293:LEU:H	1:D:311:ALA:HB1	1.84	0.43
1:D:4000:MET:HE2	1:D:4058:ILE:HD13	2.00	0.43
1:D:4968:PHE:O	1:D:4974:GLY:HA3	2.19	0.43
1:A:2780:ASN:ND2	1:A:2782:ASP:OD2	2.51	0.43
1:A:3343:GLN:NE2	1:A:3469:PHE:O	2.47	0.43
1:A:3670:GLU:HG3	1:A:3728:ILE:HG23	2.00	0.43
1:B:261:ARG:HH11	1:B:263:GLU:HG2	1.84	0.43
1:B:293:LEU:H	1:B:311:ALA:HB1	1.83	0.43
1:B:878:ILE:HD11	1:B:925:SER:HB2	2.01	0.43
1:B:1839:VAL:HG23	1:B:1935:VAL:HG22	1.99	0.43
1:B:2862:LEU:O	1:B:2928:LYS:NZ	2.41	0.43
1:B:3320:LEU:HD21	1:B:3361:THR:HG21	2.01	0.43
1:B:3332:ALA:O	1:B:3336:LYS:NZ	2.51	0.43
1:B:4968:PHE:O	1:B:4974:GLY:HA3	2.19	0.43
1:C:720:HIS:CG	1:C:727:ALA:HB1	2.54	0.43
1:C:3238:GLU:HA	1:C:3241:PRO:HG3	2.01	0.43
1:D:2288:LEU:O	1:D:3849:ARG:NH1	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2339:VAL:HG12	1:D:2349:ASN:HB3	2.01	0.43
1:D:4864:ASN:HD21	1:D:4872:PRO:HB2	1.84	0.43
1:A:3051:ARG:HA	1:A:3131:TYR:CZ	2.53	0.42
1:A:3245:VAL:H	1:A:3248:ARG:HE	1.67	0.42
1:A:4821:LYS:HE3	1:A:4821:LYS:HB3	1.76	0.42
1:A:4944:ARG:NH2	1:B:4938:ASP:OD1	2.50	0.42
1:B:736:HIS:ND1	1:B:737:LEU:O	2.38	0.42
1:B:1435:TYR:HB3	1:B:1575:LEU:HD21	2.00	0.42
1:B:2006:ILE:HG23	1:B:3641:LEU:HD11	2.01	0.42
1:B:2737:PRO:HG2	1:B:2888:ARG:HB2	1.99	0.42
1:B:3051:ARG:HA	1:B:3131:TYR:CZ	2.53	0.42
1:C:2716:ASP:OD1	1:C:2716:ASP:N	2.51	0.42
1:D:218:HIS:O	1:D:261:ARG:HA	2.19	0.42
1:D:504:ALA:HB2	1:D:512:ALA:HB2	2.00	0.42
1:D:1435:TYR:HB3	1:D:1575:LEU:HD21	2.00	0.42
1:D:2736:ASP:OD1	1:D:2736:ASP:N	2.50	0.42
1:D:3535:LEU:O	1:D:3538:THR:OG1	2.29	0.42
2:H:18:LYS:HA	2:H:50:ILE:HD11	2.01	0.42
1:A:261:ARG:HH11	1:A:263:GLU:HG2	1.85	0.42
1:A:504:ALA:HB2	1:A:512:ALA:HB2	2.00	0.42
1:A:1064:GLU:O	1:A:1071:ARG:NH2	2.53	0.42
1:A:2604:GLU:HG2	1:A:2639:MET:HG3	2.01	0.42
1:B:1115:LEU:HB3	1:B:1123:VAL:HG11	2.01	0.42
1:B:2998:PHE:HA	1:B:3002:LEU:HD13	2.00	0.42
1:B:3450:ASN:HA	1:B:3453:ARG:HG2	2.01	0.42
1:B:4584:ASP:HA	1:B:4628:VAL:HG12	2.00	0.42
1:C:261:ARG:HH11	1:C:263:GLU:HG2	1.84	0.42
1:C:2604:GLU:HB3	1:C:2608:MET:HE1	2.00	0.42
1:D:793:LEU:HB2	1:D:797:HIS:HB2	1.99	0.42
1:D:2111:VAL:HG21	1:D:2120:MET:HE1	2.01	0.42
1:D:2998:PHE:HA	1:D:3002:LEU:HD13	2.00	0.42
1:D:3051:ARG:HA	1:D:3131:TYR:CZ	2.53	0.42
2:G:17:LYS:HG2	2:G:20:GLN:HE22	1.83	0.42
1:A:217:GLY:N	1:A:262:LEU:O	2.45	0.42
1:A:1115:LEU:HB3	1:A:1123:VAL:HG11	2.01	0.42
1:A:1435:TYR:HB3	1:A:1575:LEU:HD21	2.00	0.42
1:A:3201:MET:HG3	1:A:3203:VAL:H	1.84	0.42
1:A:3424:LEU:HD11	1:B:1216:ILE:HG12	2.00	0.42
1:B:17:ASP:HB2	1:B:98:HIS:HE1	1.84	0.42
1:B:281:ARG:NH2	1:B:309:THR:OG1	2.51	0.42
1:B:4112:LEU:O	1:B:4115:SER:OG	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4627:MET:HE2	1:B:4627:MET:HB2	1.75	0.42
1:C:4171:LEU:O	1:C:4175:ARG:HB2	2.19	0.42
1:D:34:LYS:HD3	1:D:34:LYS:HA	1.82	0.42
1:D:736:HIS:ND1	1:D:737:LEU:O	2.38	0.42
1:D:3354:LEU:N	1:D:3415:TYR:OH	2.51	0.42
1:A:2288:LEU:O	1:A:3849:ARG:NH1	2.42	0.42
1:A:2871:LEU:HG	1:A:2927:LEU:HD21	2.02	0.42
1:A:3035:GLU:HA	1:A:3038:MET:HE2	2.00	0.42
1:A:4869:GLU:H	1:A:4869:GLU:HG2	1.69	0.42
1:B:546:TRP:O	1:B:549:SER:OG	2.28	0.42
1:B:1066:GLN:NE2	1:B:1461:ASP:OD1	2.53	0.42
1:B:2607:LEU:HD23	1:B:2607:LEU:HA	1.91	0.42
1:B:2765:LYS:HA	1:B:2765:LYS:HD3	1.85	0.42
1:B:3354:LEU:HD11	1:B:3434:LEU:HD12	2.00	0.42
1:B:3573:MET:HA	1:B:3576:TYR:HB3	2.00	0.42
1:B:4171:LEU:O	1:B:4175:ARG:HB2	2.19	0.42
1:B:4867:GLU:H	1:B:4867:GLU:HG2	1.34	0.42
1:B:4888:TYR:CD2	1:B:4889:VAL:HG22	2.54	0.42
1:D:3238:GLU:HA	1:D:3241:PRO:HG3	2.01	0.42
1:D:3320:LEU:HD21	1:D:3361:THR:HG21	2.01	0.42
1:D:3354:LEU:HD11	1:D:3434:LEU:HD12	2.00	0.42
1:D:4874:MET:HE3	1:D:4874:MET:HB3	1.88	0.42
1:A:936:GLY:HA3	1:A:1056:PRO:HB3	2.01	0.42
1:A:2098:VAL:HG13	1:A:2127:GLN:HG3	2.00	0.42
1:A:2736:ASP:OD1	1:A:2736:ASP:N	2.50	0.42
1:B:1064:GLU:O	1:B:1071:ARG:NH2	2.53	0.42
1:B:2122:SER:O	1:B:2126:ARG:HG3	2.20	0.42
1:B:2604:GLU:HG2	1:B:2639:MET:HG3	2.00	0.42
1:B:2716:ASP:OD1	1:B:2716:ASP:N	2.51	0.42
1:B:3821:LYS:O	1:B:3824:LYS:NZ	2.47	0.42
1:C:1277:TRP:CD1	1:C:1559:GLN:HG3	2.52	0.42
1:C:3244:PRO:HB2	1:C:3249:LEU:HD13	2.02	0.42
1:C:4675:LYS:O	1:C:4679:ARG:HG2	2.20	0.42
1:C:4944:ARG:NH2	1:D:4938:ASP:OD1	2.52	0.42
1:D:275:ARG:HE	1:D:336:PRO:HD2	1.85	0.42
1:D:3788:GLY:HA2	1:D:3835:LEU:HG	2.02	0.42
1:D:4675:LYS:O	1:D:4679:ARG:HG2	2.20	0.42
2:F:7:ILE:HD11	2:F:73:LYS:HB2	2.00	0.42
1:A:3244:PRO:HB2	1:A:3249:LEU:HD13	2.02	0.42
1:A:4850:LEU:HD23	1:A:4850:LEU:HA	1.86	0.42
1:B:34:LYS:HD3	1:B:34:LYS:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3985:LEU:HD11	1:B:4026:MET:HE1	2.00	0.42
1:C:1000:ARG:HA	1:C:1000:ARG:HD3	1.82	0.42
1:C:2604:GLU:HG2	1:C:2639:MET:HG3	2.00	0.42
1:C:2871:LEU:HG	1:C:2927:LEU:HD21	2.02	0.42
1:C:3573:MET:HA	1:C:3576:TYR:HB3	2.00	0.42
1:D:2871:LEU:HG	1:D:2927:LEU:HD21	2.02	0.42
1:A:17:ASP:HB2	1:A:98:HIS:HE1	1.84	0.42
1:A:3320:LEU:HD21	1:A:3361:THR:HG21	2.01	0.42
1:A:3985:LEU:HD11	1:A:4026:MET:HE1	2.00	0.42
1:A:4675:LYS:O	1:A:4679:ARG:HG2	2.20	0.42
1:A:4867:GLU:H	1:A:4867:GLU:HG2	1.34	0.42
1:B:1277:TRP:CD1	1:B:1559:GLN:HG3	2.52	0.42
1:B:2288:LEU:O	1:B:3849:ARG:NH1	2.42	0.42
1:B:3768:SER:HA	1:B:3771:HIS:CD2	2.55	0.42
1:C:218:HIS:O	1:C:261:ARG:HA	2.19	0.42
1:C:552:ASP:N	1:C:552:ASP:OD1	2.50	0.42
1:C:3535:LEU:O	1:C:3538:THR:OG1	2.29	0.42
1:D:261:ARG:HH11	1:D:263:GLU:HG2	1.84	0.42
1:D:492:ASP:OD1	1:D:546:TRP:NE1	2.49	0.42
1:D:1066:GLN:NE2	1:D:1461:ASP:OD1	2.53	0.42
1:D:3244:PRO:HB2	1:D:3249:LEU:HD13	2.02	0.42
2:E:56:ILE:HG12	2:E:81:ALA:HA	2.01	0.42
1:A:2121:PHE:O	1:A:3725:TYR:OH	2.28	0.42
1:A:3301:PRO:HA	1:A:3302:PRO:HD3	1.88	0.42
1:B:1968:LYS:HB3	1:B:1968:LYS:HE2	1.90	0.42
1:B:2871:LEU:HG	1:B:2927:LEU:HD21	2.02	0.42
1:B:3244:PRO:HA	1:B:3248:ARG:HH21	1.84	0.42
1:B:3245:VAL:H	1:B:3248:ARG:HE	1.67	0.42
1:C:1066:GLN:NE2	1:C:1461:ASP:OD1	2.53	0.42
1:C:2122:SER:O	1:C:2126:ARG:HG3	2.20	0.42
1:C:2862:LEU:O	1:C:2928:LYS:NZ	2.41	0.42
1:C:3768:SER:HA	1:C:3771:HIS:CD2	2.55	0.42
1:C:4864:ASN:HD21	1:C:4872:PRO:HB2	1.84	0.42
1:D:2514:ASN:OD1	1:D:2514:ASN:N	2.45	0.42
1:D:2604:GLU:HG2	1:D:2639:MET:HG3	2.00	0.42
1:D:3245:VAL:H	1:D:3248:ARG:HE	1.67	0.42
2:G:18:LYS:HA	2:G:50:ILE:HD11	2.01	0.42
1:A:1066:GLN:NE2	1:A:1461:ASP:OD1	2.52	0.42
1:A:1269:CYS:HA	1:A:1564:PHE:O	2.20	0.42
1:A:2111:VAL:HG21	1:A:2120:MET:HE1	2.01	0.42
1:A:3823:LYS:HA	1:A:3823:LYS:HD3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2111:VAL:HG21	1:B:2120:MET:HE1	2.01	0.42
1:B:3238:GLU:HA	1:B:3241:PRO:HG3	2.01	0.42
1:B:4850:LEU:HD23	1:B:4850:LEU:HA	1.86	0.42
1:C:3354:LEU:HD11	1:C:3434:LEU:HD12	2.00	0.42
1:C:4813:LEU:HD23	1:C:4813:LEU:HA	1.95	0.42
1:D:132:ALA:HB1	1:D:192:ASP:HB3	2.01	0.42
1:D:308:HIS:HD2	1:D:310:LYS:HB2	1.85	0.42
1:D:2500:ALA:HB2	1:D:2553:TYR:HD1	1.85	0.42
1:D:3244:PRO:HA	1:D:3248:ARG:HH21	1.84	0.42
1:D:3768:SER:HA	1:D:3771:HIS:CD2	2.55	0.42
1:A:2339:VAL:HG12	1:A:2349:ASN:HB3	2.01	0.42
1:A:2583:LEU:HA	1:A:2586:VAL:HG12	2.02	0.42
1:B:546:TRP:CE2	1:B:550:LYS:HE2	2.55	0.42
1:B:557:SER:HA	1:B:560:ILE:HG22	2.01	0.42
1:B:2339:VAL:HG12	1:B:2349:ASN:HB3	2.01	0.42
1:B:4204:GLN:HB3	1:B:4245:MET:HE2	2.00	0.42
1:B:4864:ASN:HD21	1:B:4872:PRO:HB2	1.84	0.42
1:C:14:LEU:HD13	1:C:202:MET:HE2	2.02	0.42
1:C:217:GLY:N	1:C:262:LEU:O	2.45	0.42
1:C:276:TRP:HD1	1:C:316:PHE:HB3	1.85	0.42
1:C:2111:VAL:HG21	1:C:2120:MET:HE1	2.01	0.42
1:C:2765:LYS:HD3	1:C:2765:LYS:HA	1.85	0.42
1:C:3320:LEU:HD21	1:C:3361:THR:HG21	2.01	0.42
1:D:1064:GLU:O	1:D:1071:ARG:NH2	2.53	0.42
1:D:4581:LYS:HB3	1:D:4581:LYS:HE3	1.78	0.42
1:D:4661:TYR:OH	1:D:4786:ASP:OD2	2.34	0.42
2:E:18:LYS:HA	2:E:50:ILE:HD11	2.01	0.42
1:A:863:LEU:HA	1:A:864:PRO:HD3	1.85	0.41
1:A:3249:LEU:HD12	1:A:3249:LEU:HA	1.86	0.41
1:A:3788:GLY:HA2	1:A:3835:LEU:HG	2.02	0.41
1:A:4743:MET:H	1:A:4743:MET:HG3	1.63	0.41
1:B:276:TRP:HD1	1:B:316:PHE:HB3	1.85	0.41
1:B:2583:LEU:HA	1:B:2586:VAL:HG12	2.02	0.41
1:C:546:TRP:CE2	1:C:550:LYS:HE2	2.55	0.41
1:D:2318:TYR:CZ	1:D:2395:PRO:HD3	2.55	0.41
1:D:2739:PRO:HG3	1:D:2888:ARG:HG2	2.00	0.41
1:D:3035:GLU:HA	1:D:3038:MET:HE2	2.00	0.41
1:A:308:HIS:HD2	1:A:310:LYS:HB2	1.85	0.41
1:A:1968:LYS:HB3	1:A:1968:LYS:HE2	1.90	0.41
1:A:2691:TYR:HA	1:A:2696:TYR:HE2	1.85	0.41
1:A:3354:LEU:HD11	1:A:3434:LEU:HD12	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3450:ASN:HA	1:A:3453:ARG:HG2	2.01	0.41
1:A:3768:SER:HA	1:A:3771:HIS:CD2	2.55	0.41
1:A:4569:LEU:HD12	1:A:4569:LEU:HA	1.95	0.41
1:A:4888:TYR:CD2	1:A:4889:VAL:HG22	2.54	0.41
1:B:308:HIS:HD2	1:B:310:LYS:HB2	1.85	0.41
1:B:1269:CYS:HA	1:B:1564:PHE:O	2.20	0.41
1:B:2682:ILE:O	1:B:2686:LEU:HB2	2.21	0.41
1:B:3244:PRO:HB2	1:B:3249:LEU:HD13	2.02	0.41
1:C:132:ALA:HB1	1:C:192:ASP:HB3	2.02	0.41
1:C:2481:LYS:HE2	1:C:2481:LYS:HB2	1.92	0.41
1:C:2617:SER:OG	1:C:2618:MET:SD	2.72	0.41
1:C:3718:GLU:OE2	1:C:3719:ASP:N	2.54	0.41
1:D:276:TRP:HD1	1:D:316:PHE:HB3	1.85	0.41
1:D:880:GLU:HB3	1:D:883:ALA:HB3	2.02	0.41
1:D:2682:ILE:O	1:D:2686:LEU:HB2	2.21	0.41
1:A:552:ASP:OD1	1:A:552:ASP:N	2.50	0.41
1:A:3238:GLU:HA	1:A:3241:PRO:HG3	2.01	0.41
1:A:3718:GLU:OE2	1:A:3719:ASP:N	2.54	0.41
1:A:3780:LEU:HD23	1:A:3780:LEU:HA	1.88	0.41
1:A:4864:ASN:HD21	1:A:4872:PRO:HB2	1.84	0.41
1:B:219:VAL:HG12	1:B:259:LEU:HD12	2.02	0.41
1:B:880:GLU:HB3	1:B:883:ALA:HB3	2.02	0.41
1:B:1699:GLU:OE2	1:B:1813:ARG:NH2	2.38	0.41
1:C:2318:TYR:CZ	1:C:2395:PRO:HD3	2.55	0.41
1:C:2691:TYR:HA	1:C:2696:TYR:HE2	1.85	0.41
1:C:3780:LEU:HD23	1:C:3780:LEU:HA	1.88	0.41
1:D:546:TRP:CE2	1:D:550:LYS:HE2	2.55	0.41
1:D:669:ASP:HB2	1:D:788:LYS:O	2.20	0.41
1:D:1269:CYS:HA	1:D:1564:PHE:O	2.20	0.41
1:D:2377:LEU:N	1:D:2465:ASP:OD2	2.54	0.41
1:D:3159:ASP:OD1	1:D:3159:ASP:N	2.46	0.41
1:A:546:TRP:CE2	1:A:550:LYS:HE2	2.55	0.41
1:A:3944:GLU:OE1	1:A:3946:GLN:N	2.47	0.41
1:A:4188:ARG:HA	1:A:4188:ARG:HD2	1.78	0.41
1:A:4795:TYR:CZ	1:A:4812:HIS:HB3	2.55	0.41
1:A:4914:VAL:HG12	1:D:4888:TYR:CD1	2.56	0.41
1:B:1088:TRP:HB2	1:B:1153:ILE:HG22	2.03	0.41
1:C:2500:ALA:HB2	1:C:2553:TYR:HD1	1.85	0.41
1:C:2696:TYR:HD1	1:C:3001:ILE:HD11	1.86	0.41
1:C:4188:ARG:HD2	1:C:4188:ARG:HA	1.78	0.41
1:D:1231[B]:GLN:H	1:D:1231[B]:GLN:HG3	1.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2696:TYR:HD1	1:D:3001:ILE:HD11	1.86	0.41
1:D:3718:GLU:OE2	1:D:3719:ASP:N	2.54	0.41
1:A:132:ALA:HB1	1:A:192:ASP:HB3	2.02	0.41
1:A:176:SER:O	1:A:178:ARG:NH1	2.54	0.41
1:A:218:HIS:O	1:A:261:ARG:HA	2.19	0.41
1:A:1277:TRP:CD1	1:A:1559:GLN:HG3	2.52	0.41
1:A:2500:ALA:HB2	1:A:2553:TYR:HD1	1.85	0.41
1:A:2682:ILE:O	1:A:2686:LEU:HB2	2.21	0.41
1:A:4930:ALA:HB2	1:D:4933:GLN:HE21	1.86	0.41
1:B:464:LYS:HE2	1:B:464:LYS:HB2	1.89	0.41
1:B:990:GLU:HG3	1:B:1024:TYR:HB3	2.03	0.41
1:B:1231[B]:GLN:H	1:B:1231[B]:GLN:HG3	1.51	0.41
1:B:1694:LEU:HD12	1:B:1715:LEU:HB2	2.02	0.41
1:B:2377:LEU:N	1:B:2465:ASP:OD2	2.54	0.41
1:B:2500:ALA:HB2	1:B:2553:TYR:HD1	1.85	0.41
1:B:2696:TYR:HD1	1:B:3001:ILE:HD11	1.86	0.41
1:B:4795:TYR:CZ	1:B:4812:HIS:HB3	2.56	0.41
1:B:4827:LEU:HD23	1:B:4827:LEU:HA	1.87	0.41
1:C:176:SER:O	1:C:178:ARG:NH1	2.54	0.41
1:C:275:ARG:HE	1:C:336:PRO:HD2	1.85	0.41
1:C:669:ASP:HB2	1:C:788:LYS:O	2.20	0.41
1:C:990:GLU:HG3	1:C:1024:TYR:HB3	2.03	0.41
1:C:2377:LEU:N	1:C:2465:ASP:OD2	2.54	0.41
1:C:3162:GLN:OE1	1:C:3166:TYR:OH	2.30	0.41
1:C:4865:LYS:HD2	1:C:4865:LYS:HA	1.63	0.41
1:D:219:VAL:HG12	1:D:259:LEU:HD12	2.02	0.41
1:D:869:ARG:CZ	1:D:870:ILE:HB	2.51	0.41
1:D:2122:SER:O	1:D:2126:ARG:HG3	2.20	0.41
1:D:2583:LEU:HA	1:D:2586:VAL:HG12	2.02	0.41
1:D:3862:ASP:OD1	1:D:3862:ASP:N	2.45	0.41
1:A:275:ARG:HE	1:A:336:PRO:HD2	1.85	0.41
1:A:557:SER:HA	1:A:560:ILE:HG22	2.01	0.41
1:A:669:ASP:HB2	1:A:788:LYS:O	2.20	0.41
1:A:990:GLU:HG3	1:A:1024:TYR:HB3	2.03	0.41
1:A:1694:LEU:HD12	1:A:1715:LEU:HB2	2.02	0.41
1:A:2122:SER:O	1:A:2126:ARG:HG3	2.20	0.41
1:A:2696:TYR:HD1	1:A:3001:ILE:HD11	1.86	0.41
1:A:2927:LEU:HD12	1:A:2927:LEU:HA	1.92	0.41
1:A:3244:PRO:HA	1:A:3248:ARG:HH21	1.84	0.41
1:A:4581:LYS:HE3	1:A:4581:LYS:HB3	1.77	0.41
1:B:67:PHE:HB3	1:B:109:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:VAL:O	1:B:79:GLN:HG2	2.21	0.41
1:B:3890:LEU:HD23	1:B:3890:LEU:HA	1.85	0.41
1:B:4675:LYS:O	1:B:4679:ARG:HG2	2.20	0.41
1:C:3245:VAL:H	1:C:3248:ARG:HE	1.67	0.41
1:C:3788:GLY:HA2	1:C:3835:LEU:HG	2.02	0.41
1:C:4112:LEU:O	1:C:4115:SER:OG	2.37	0.41
1:D:3890:LEU:HD23	1:D:3890:LEU:HA	1.85	0.41
1:D:4066:LEU:HD23	1:D:4133:GLN:HE22	1.86	0.41
1:A:14:LEU:HD13	1:A:202:MET:HE2	2.02	0.41
1:A:67:PHE:HB3	1:A:109:LEU:HD11	2.03	0.41
1:A:2199:ARG:NE	1:A:2246:ASN:OD1	2.50	0.41
1:B:487:VAL:O	1:B:491:ILE:HD12	2.21	0.41
1:B:2792:ARG:HB2	1:B:2797:PHE:HD1	1.86	0.41
1:B:3159:ASP:OD1	1:B:3159:ASP:N	2.46	0.41
1:C:475:GLN:OE1	1:C:533:ASN:ND2	2.53	0.41
1:C:557:SER:HA	1:C:560:ILE:HG22	2.01	0.41
1:C:736:HIS:ND1	1:C:737:LEU:O	2.38	0.41
1:C:1064:GLU:O	1:C:1071:ARG:NH2	2.53	0.41
1:C:3244:PRO:HA	1:C:3248:ARG:HH21	1.84	0.41
1:C:3888:LEU:HD23	1:C:3891:LEU:HD21	2.03	0.41
1:C:4020:GLN:HA	1:C:4023:MET:HB3	2.02	0.41
1:C:4911:LEU:HD22	1:C:4911:LEU:HA	1.87	0.41
1:D:557:SER:HA	1:D:560:ILE:HG22	2.01	0.41
1:D:3888:LEU:HD23	1:D:3891:LEU:HD21	2.03	0.41
1:D:4850:LEU:HD23	1:D:4850:LEU:HA	1.86	0.41
1:A:1088:TRP:HB2	1:A:1153:ILE:HG22	2.03	0.41
1:A:1221:GLU:OE1	1:A:1221:GLU:N	2.54	0.41
1:B:176:SER:O	1:B:178:ARG:NH1	2.54	0.41
1:B:869:ARG:CZ	1:B:870:ILE:HB	2.51	0.41
1:B:2318:TYR:CZ	1:B:2395:PRO:HD3	2.55	0.41
1:C:281:ARG:NH2	1:C:309:THR:OG1	2.51	0.41
1:C:1068:ARG:O	1:C:1071:ARG:HG2	2.21	0.41
1:C:2001:PRO:O	1:C:2005:GLN:HG3	2.21	0.41
1:C:2583:LEU:HA	1:C:2586:VAL:HG12	2.02	0.41
1:C:2682:ILE:O	1:C:2686:LEU:HB2	2.21	0.41
1:C:3842:LEU:HD12	1:C:3930:ILE:HA	2.03	0.41
1:C:4795:TYR:CZ	1:C:4812:HIS:HB3	2.55	0.41
1:C:4869:GLU:H	1:C:4869:GLU:HG2	1.69	0.41
1:C:4878:ASP:HB3	1:C:4881:THR:OG1	2.21	0.41
1:D:23:GLN:OE1	1:D:203:ASN:ND2	2.54	0.41
1:D:1277:TRP:CD1	1:D:1559:GLN:HG3	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4878:ASP:HB3	1:D:4881:THR:OG1	2.21	0.41
2:F:18:LYS:HA	2:F:50:ILE:HD11	2.01	0.41
1:A:75:VAL:O	1:A:79:GLN:HG2	2.21	0.41
1:A:498:THR:HA	1:A:553:ARG:HH12	1.86	0.41
1:A:619:ASP:OD1	1:A:620:LEU:N	2.54	0.41
1:A:1099:GLU:OE2	1:A:1101:ARG:NE	2.46	0.41
1:A:2318:TYR:CZ	1:A:2395:PRO:HD3	2.55	0.41
1:A:2494:PHE:HE2	1:A:2499:LYS:HE3	1.86	0.41
1:A:3989:VAL:HG13	1:A:4023:MET:HE2	2.03	0.41
1:B:23:GLN:OE1	1:B:203:ASN:ND2	2.54	0.41
1:B:218:HIS:O	1:B:261:ARG:HA	2.19	0.41
1:B:436:LEU:HD23	1:B:436:LEU:HA	1.87	0.41
1:B:1068:ARG:O	1:B:1071:ARG:HG2	2.21	0.41
1:B:1085:SER:OG	1:B:1086:GLY:N	2.54	0.41
1:B:1274:HIS:HB3	1:B:1277:TRP:HB2	2.03	0.41
1:B:2691:TYR:HA	1:B:2696:TYR:HE2	1.85	0.41
1:B:3788:GLY:HA2	1:B:3835:LEU:HG	2.02	0.41
1:C:487:VAL:O	1:C:491:ILE:HD12	2.21	0.41
1:C:663:TYR:OH	1:C:665:GLU:OE2	2.35	0.41
1:C:815:VAL:O	1:C:1007:TYR:OH	2.37	0.41
1:C:880:GLU:HB3	1:C:883:ALA:HB3	2.02	0.41
1:C:1434:TYR:HD1	1:C:1519:LEU:HG	1.86	0.41
1:C:2927:LEU:HD12	1:C:2927:LEU:HA	1.91	0.41
1:C:4627:MET:H	1:C:4627:MET:HG3	1.42	0.41
1:D:1500:PHE:HB3	1:D:1531:ALA:HB1	2.03	0.41
1:D:2456:ILE:O	1:D:2459:SER:OG	2.26	0.41
1:D:2691:TYR:HA	1:D:2696:TYR:HE2	1.85	0.41
1:D:2862:LEU:O	1:D:2928:LYS:NZ	2.41	0.41
1:D:3420:ARG:HE	1:D:3420:ARG:HB3	1.50	0.41
1:D:3713:LYS:NZ	1:D:3715:LYS:O	2.42	0.41
1:D:4646:LEU:HD23	1:D:4646:LEU:HA	1.89	0.41
1:A:23:GLN:OE1	1:A:203:ASN:ND2	2.54	0.41
1:A:492:ASP:OD1	1:A:546:TRP:NE1	2.49	0.41
1:A:1068:ARG:O	1:A:1071:ARG:HG2	2.21	0.41
1:A:2181:SER:O	1:A:2185:ILE:HG12	2.21	0.41
1:A:3420:ARG:HE	1:A:3420:ARG:HB3	1.50	0.41
1:B:14:LEU:HD13	1:B:202:MET:HE2	2.02	0.41
1:B:498:THR:HA	1:B:553:ARG:HH12	1.86	0.41
1:B:1434:TYR:HD1	1:B:1519:LEU:HG	1.86	0.41
1:B:4085:ARG:O	1:B:4085:ARG:NH1	2.50	0.41
1:B:4582:VAL:HG11	1:C:4860:ARG:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4627:MET:H	1:B:4627:MET:HG3	1.42	0.41
1:B:4874:MET:HE3	1:B:4874:MET:HB3	1.88	0.41
1:C:436:LEU:HD23	1:C:436:LEU:HA	1.87	0.41
1:C:464:LYS:HB2	1:C:464:LYS:HE2	1.90	0.41
1:C:527:ALA:O	1:C:531:ARG:HB2	2.21	0.41
1:C:1500:PHE:HB3	1:C:1531:ALA:HB1	2.03	0.41
1:C:2792:ARG:HB2	1:C:2797:PHE:HD1	1.86	0.41
1:C:4801:LEU:HD23	1:C:4801:LEU:HA	1.93	0.41
1:C:4823:LEU:HD23	1:C:4823:LEU:HA	1.80	0.41
1:D:498:THR:HA	1:D:553:ARG:HH12	1.86	0.41
1:D:990:GLU:HG3	1:D:1024:TYR:HB3	2.03	0.41
1:D:1274:HIS:HB3	1:D:1277:TRP:HB2	2.03	0.41
1:D:2607:LEU:HD23	1:D:2607:LEU:HA	1.91	0.41
1:A:219:VAL:HG12	1:A:259:LEU:HD12	2.02	0.40
1:A:665:GLU:HG2	1:A:745:SER:HA	2.04	0.40
1:A:880:GLU:HB3	1:A:883:ALA:HB3	2.02	0.40
1:A:2377:LEU:N	1:A:2465:ASP:OD2	2.54	0.40
1:A:2792:ARG:HB2	1:A:2797:PHE:HD1	1.86	0.40
1:A:3888:LEU:HD23	1:A:3891:LEU:HD21	2.03	0.40
1:B:132:ALA:HB1	1:B:192:ASP:HB3	2.02	0.40
1:B:1849:LEU:HD23	1:B:1849:LEU:HA	1.91	0.40
1:B:1990:GLU:OE2	1:B:1994:ARG:NH1	2.48	0.40
1:B:2181:SER:O	1:B:2185:ILE:HG12	2.21	0.40
1:B:3718:GLU:OE2	1:B:3719:ASP:N	2.54	0.40
1:B:3842:LEU:HD12	1:B:3930:ILE:HA	2.03	0.40
1:B:4020:GLN:HA	1:B:4023:MET:HB3	2.02	0.40
1:B:4743:MET:H	1:B:4743:MET:HG3	1.63	0.40
1:C:23:GLN:OE1	1:C:203:ASN:ND2	2.54	0.40
1:C:219:VAL:HG12	1:C:259:LEU:HD12	2.02	0.40
1:C:639:ASN:ND2	1:C:676:THR:OG1	2.55	0.40
1:C:4661:TYR:OH	1:C:4786:ASP:OD2	2.34	0.40
1:D:14:LEU:HD13	1:D:202:MET:HE2	2.02	0.40
1:D:111:HIS:ND1	1:D:114:SER:OG	2.35	0.40
1:D:214:VAL:HG22	1:D:341:TYR:CZ	2.57	0.40
1:D:663:TYR:OH	1:D:665:GLU:OE2	2.35	0.40
1:D:4112:LEU:O	1:D:4115:SER:OG	2.38	0.40
1:D:4869:GLU:H	1:D:4869:GLU:HG2	1.69	0.40
2:E:28:GLY:N	2:E:37:ASP:O	2.54	0.40
1:A:1254:HIS:HB3	1:A:1274:HIS:CE1	2.57	0.40
1:A:1274:HIS:HB3	1:A:1277:TRP:HB2	2.03	0.40
1:A:2001:PRO:O	1:A:2005:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4020:GLN:HA	1:A:4023:MET:HB3	2.02	0.40
1:B:275:ARG:HE	1:B:336:PRO:HD2	1.85	0.40
1:B:492:ASP:OD1	1:B:546:TRP:NE1	2.49	0.40
1:B:790:ARG:HA	1:B:1626:TRP:O	2.21	0.40
1:B:2007:ASN:O	1:B:2011:HIS:HB2	2.21	0.40
1:B:2109:ASP:OD1	1:B:2109:ASP:N	2.55	0.40
1:B:2927:LEU:HD12	1:B:2927:LEU:HA	1.92	0.40
1:B:3989:VAL:HG13	1:B:4023:MET:HE2	2.03	0.40
1:B:4059:LEU:HD13	1:B:4059:LEU:HA	1.88	0.40
1:C:492:ASP:OD1	1:C:546:TRP:NE1	2.49	0.40
1:C:869:ARG:CZ	1:C:870:ILE:HB	2.51	0.40
1:C:1088:TRP:HB2	1:C:1153:ILE:HG22	2.03	0.40
1:C:1221:GLU:N	1:C:1221:GLU:OE1	2.54	0.40
1:C:1694:LEU:HD12	1:C:1715:LEU:HB2	2.02	0.40
1:C:2268[A]:GLN:H	1:C:2268[A]:GLN:HG3	1.68	0.40
1:C:2456:ILE:O	1:C:2459:SER:OG	2.26	0.40
1:D:232:THR:HG22	1:D:258:SER:HB3	2.03	0.40
1:D:527:ALA:O	1:D:531:ARG:HB2	2.21	0.40
1:D:1068:ARG:O	1:D:1071:ARG:HG2	2.21	0.40
1:D:1085:SER:OG	1:D:1086:GLY:N	2.54	0.40
1:D:2001:PRO:O	1:D:2005:GLN:HG3	2.21	0.40
1:D:2109:ASP:OD1	1:D:2109:ASP:N	2.55	0.40
1:D:2554:LEU:HB3	1:D:2559:LEU:HD13	2.04	0.40
1:D:2610:LEU:O	1:D:2614:ILE:HG12	2.22	0.40
1:D:3582:ARG:HD3	1:D:3582:ARG:HA	1.77	0.40
1:D:3989:VAL:HG13	1:D:4023:MET:HE2	2.03	0.40
1:D:4020:GLN:HA	1:D:4023:MET:HB3	2.02	0.40
2:E:38:SER:OG	2:E:39:SER:N	2.54	0.40
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.89	0.40
1:A:2007:ASN:O	1:A:2011:HIS:HB2	2.21	0.40
1:A:2159:LEU:HD11	1:A:2163:ARG:HE	1.87	0.40
1:A:4808:PHE:HD1	1:A:4808:PHE:HA	1.80	0.40
1:A:4874:MET:HE3	1:A:4874:MET:HB3	1.88	0.40
1:B:214:VAL:HG22	1:B:341:TYR:CZ	2.57	0.40
1:B:619:ASP:OD1	1:B:620:LEU:N	2.54	0.40
1:B:1221:GLU:OE1	1:B:1221:GLU:N	2.54	0.40
1:B:1254:HIS:HB3	1:B:1274:HIS:CE1	2.57	0.40
1:B:2494:PHE:HE2	1:B:2499:LYS:HE3	1.86	0.40
1:B:4677:LEU:HD12	1:B:4677:LEU:HA	1.83	0.40
1:C:75:VAL:O	1:C:79:GLN:HG2	2.21	0.40
1:C:619:ASP:OD1	1:C:620:LEU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1254:HIS:HB3	1:C:1274:HIS:CE1	2.57	0.40
1:C:2109:ASP:OD1	1:C:2109:ASP:N	2.55	0.40
1:C:2181:SER:O	1:C:2185:ILE:HG12	2.21	0.40
1:C:2268[B]:GLN:H	1:C:2268[B]:GLN:HG3	1.68	0.40
1:C:3963:ASN:O	1:C:3966:THR:OG1	2.34	0.40
1:C:4066:LEU:HD23	1:C:4133:GLN:HE22	1.86	0.40
1:D:350:HIS:O	1:D:354:GLY:N	2.54	0.40
1:D:2792:ARG:HB2	1:D:2797:PHE:HD1	1.86	0.40
1:D:3450:ASN:HA	1:D:3453:ARG:HG2	2.01	0.40
2:H:38:SER:OG	2:H:39:SER:N	2.54	0.40
1:B:665:GLU:HG2	1:B:745:SER:HA	2.04	0.40
1:B:4066:LEU:HD23	1:B:4133:GLN:HE22	1.86	0.40
1:C:214:VAL:HG22	1:C:341:TYR:CZ	2.57	0.40
1:C:1274:HIS:HB3	1:C:1277:TRP:HB2	2.03	0.40
1:C:2610:LEU:O	1:C:2614:ILE:HG12	2.22	0.40
1:D:75:VAL:O	1:D:79:GLN:HG2	2.21	0.40
1:D:475:GLN:OE1	1:D:533:ASN:ND2	2.53	0.40
1:D:1221:GLU:OE1	1:D:1221:GLU:N	2.54	0.40
1:D:1694:LEU:HD12	1:D:1715:LEU:HB2	2.02	0.40
1:D:2161:GLN:O	1:D:2164:SER:OG	2.39	0.40
1:D:4722:ARG:H	1:D:4722:ARG:HG2	1.45	0.40
2:F:77:THR:HG22	2:F:80:VAL:HG22	2.03	0.40
1:A:639:ASN:ND2	1:A:676:THR:OG1	2.54	0.40
1:A:736:HIS:ND1	1:A:737:LEU:O	2.38	0.40
1:B:2001:PRO:O	1:B:2005:GLN:HG3	2.21	0.40
1:B:2355:ARG:HA	1:B:2358:ILE:HG12	2.04	0.40
1:B:3888:LEU:HD23	1:B:3891:LEU:HD21	2.03	0.40
1:C:308:HIS:HD2	1:C:310:LYS:HB2	1.85	0.40
1:C:498:THR:HA	1:C:553:ARG:HH12	1.86	0.40
1:C:1650:ILE:HA	1:C:1653:LEU:HD23	2.03	0.40
1:C:2007:ASN:O	1:C:2011:HIS:HB2	2.21	0.40
1:C:2554:LEU:HB3	1:C:2559:LEU:HD13	2.04	0.40
1:C:3081:MET:HB3	1:C:3081:MET:HE2	1.83	0.40
1:C:3296:LEU:HG	1:C:3297:PRO:HD3	2.04	0.40
1:D:176:SER:O	1:D:178:ARG:NH1	2.54	0.40
1:D:619:ASP:OD1	1:D:620:LEU:N	2.54	0.40
1:D:665:GLU:HG2	1:D:745:SER:HA	2.04	0.40
1:D:790:ARG:HA	1:D:1626:TRP:O	2.21	0.40
1:D:3842:LEU:HD12	1:D:3930:ILE:HA	2.03	0.40
2:E:77:THR:HG22	2:E:80:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4353/5037 (86%)	4129 (95%)	217 (5%)	7 (0%)	43	75
1	B	4353/5037 (86%)	4128 (95%)	218 (5%)	7 (0%)	43	75
1	C	4353/5037 (86%)	4131 (95%)	215 (5%)	7 (0%)	43	75
1	D	4353/5037 (86%)	4129 (95%)	217 (5%)	7 (0%)	43	75
2	E	105/350 (30%)	95 (90%)	10 (10%)	0	100	100
2	F	105/350 (30%)	96 (91%)	9 (9%)	0	100	100
2	G	105/350 (30%)	95 (90%)	10 (10%)	0	100	100
2	H	105/350 (30%)	95 (90%)	10 (10%)	0	100	100
All	All	17832/21548 (83%)	16898 (95%)	906 (5%)	28 (0%)	44	75

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1069	TRP
1	A	3615	SER
1	A	4910	GLU
1	B	1069	TRP
1	B	3615	SER
1	B	4910	GLU
1	C	1069	TRP
1	C	3615	SER
1	C	4910	GLU
1	D	1069	TRP
1	D	3615	SER
1	D	4910	GLU
1	A	3692	GLU
1	A	3693	LYS
1	A	4691	GLN
1	A	4694	ASP
1	B	3692	GLU

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Mol	Chain	Res	Type
1	B	3693	LYS
1	B	4691	GLN
1	B	4694	ASP
1	C	3692	GLU
1	C	3693	LYS
1	C	4691	GLN
1	C	4694	ASP
1	D	3692	GLU
1	D	3693	LYS
1	D	4691	GLN
1	D	4694	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3805/4276 (89%)	3667 (96%)	138 (4%)	31	53
1	B	3805/4276 (89%)	3666 (96%)	139 (4%)	30	52
1	C	3805/4276 (89%)	3667 (96%)	138 (4%)	31	53
1	D	3805/4276 (89%)	3666 (96%)	139 (4%)	30	52
2	E	88/304 (29%)	88 (100%)	0	100	100
2	F	88/304 (29%)	88 (100%)	0	100	100
2	G	88/304 (29%)	88 (100%)	0	100	100
2	H	88/304 (29%)	88 (100%)	0	100	100
All	All	15572/18320 (85%)	15018 (96%)	554 (4%)	32	53

All (554) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	846	LEU
1	A	1231[A]	GLN
1	A	1231[B]	GLN
1	A	1743[A]	ARG

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Mol	Chain	Res	Type
1	A	1743[B]	ARG
1	A	2369[A]	ARG
1	A	2369[B]	ARG
1	A	4181	ILE
1	A	4182	GLU
1	A	4183	ILE
1	A	4184	MET
1	A	4190	ILE
1	A	4198	SER
1	A	4199	GLU
1	A	4200	THR
1	A	4202	ARG
1	A	4204	GLN
1	A	4207	MET
1	A	4209	GLN
1	A	4211	LYS
1	A	4213	SER
1	A	4214	LYS
1	A	4222	VAL
1	A	4224	GLU
1	A	4230	LYS
1	A	4231	MET
1	A	4236	SER
1	A	4544	LEU
1	A	4545	GLU
1	A	4548	ARG
1	A	4550	LYS
1	A	4552	LEU
1	A	4555	LEU
1	A	4561	THR
1	A	4564	PHE
1	A	4567	LEU
1	A	4569	LEU
1	A	4576	ILE
1	A	4577	LEU
1	A	4578	LEU
1	A	4580	TYR
1	A	4581	LYS
1	A	4582	VAL
1	A	4583	SER
1	A	4584	ASP
1	A	4585	SER

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Mol	Chain	Res	Type
1	A	4627	MET
1	A	4628	VAL
1	A	4632	LEU
1	A	4634	GLU
1	A	4648	LEU
1	A	4651	THR
1	A	4658	ILE
1	A	4662	ASN
1	A	4676	GLU
1	A	4686	LEU
1	A	4697	VAL
1	A	4698	LYS
1	A	4700	GLN
1	A	4720	VAL
1	A	4722	ARG
1	A	4723	LYS
1	A	4730	ASP
1	A	4731	ILE
1	A	4734	ARG
1	A	4736	ARG
1	A	4743	MET
1	A	4745	LEU
1	A	4748	LEU
1	A	4772	ASP
1	A	4773	VAL
1	A	4779	LYS
1	A	4785	THR
1	A	4788	SER
1	A	4792	LEU
1	A	4796	MET
1	A	4797	VAL
1	A	4800	LEU
1	A	4813	LEU
1	A	4814	LEU
1	A	4821	LYS
1	A	4822	THR
1	A	4823	LEU
1	A	4843	LEU
1	A	4844	LEU
1	A	4852	THR
1	A	4853	VAL
1	A	4861	LYS

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Mol	Chain	Res	Type
1	A	4863	TYR
1	A	4865	LYS
1	A	4867	GLU
1	A	4870	ASP
1	A	4871	GLU
1	A	4873	ASP
1	A	4874	MET
1	A	4880	MET
1	A	4881	THR
1	A	4882	CYS
1	A	4884	LEU
1	A	4886	HIS
1	A	4887	MET
1	A	4889	VAL
1	A	4891	VAL
1	A	4902	GLU
1	A	4908	GLU
1	A	4911	LEU
1	A	4914	VAL
1	A	4917	ASP
1	A	4918	ILE
1	A	4924	VAL
1	A	4926	VAL
1	A	4932	ILE
1	A	4933	GLN
1	A	4936	ILE
1	A	4942	GLU
1	A	4945	ASP
1	A	4949	GLN
1	A	4950	VAL
1	A	4951	LYS
1	A	4952	GLU
1	A	4960	ILE
1	A	4965	SER
1	A	4966	ASP
1	A	4967	TYR
1	A	4970	THR
1	A	4971	THR
1	A	4973	HIS
1	A	4980	LEU
1	A	4982	GLU
1	A	4985	LEU

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Mol	Chain	Res	Type
1	A	4989	MET
1	A	4998	LYS
1	A	5002	GLU
1	A	5012	LYS
1	A	5029	ARG
1	A	5030	LYS
1	A	5034	ASP
1	A	5036	LEU
1	B	846	LEU
1	B	1231[A]	GLN
1	B	1231[B]	GLN
1	B	1743[A]	ARG
1	B	1743[B]	ARG
1	B	2369[A]	ARG
1	B	2369[B]	ARG
1	B	4181	ILE
1	B	4182	GLU
1	B	4183	ILE
1	B	4184	MET
1	B	4190	ILE
1	B	4198	SER
1	B	4199	GLU
1	B	4200	THR
1	B	4202	ARG
1	B	4204	GLN
1	B	4207	MET
1	B	4209	GLN
1	B	4211	LYS
1	B	4213	SER
1	B	4214	LYS
1	B	4222	VAL
1	B	4224	GLU
1	B	4230	LYS
1	B	4231	MET
1	B	4236	SER
1	B	4544	LEU
1	B	4545	GLU
1	B	4548	ARG
1	B	4550	LYS
1	B	4552	LEU
1	B	4555	LEU
1	B	4561	THR

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Mol	Chain	Res	Type
1	B	4564	PHE
1	B	4567	LEU
1	B	4569	LEU
1	B	4576	ILE
1	B	4577	LEU
1	B	4578	LEU
1	B	4580	TYR
1	B	4581	LYS
1	B	4582	VAL
1	B	4583	SER
1	B	4584	ASP
1	B	4585	SER
1	B	4627	MET
1	B	4628	VAL
1	B	4632	LEU
1	B	4634	GLU
1	B	4648	LEU
1	B	4651	THR
1	B	4658	ILE
1	B	4662	ASN
1	B	4676	GLU
1	B	4686	LEU
1	B	4697	VAL
1	B	4698	LYS
1	B	4700	GLN
1	B	4720	VAL
1	B	4722	ARG
1	B	4723	LYS
1	B	4730	ASP
1	B	4731	ILE
1	B	4734	ARG
1	B	4736	ARG
1	B	4743	MET
1	B	4745	LEU
1	B	4748	LEU
1	B	4772	ASP
1	B	4773	VAL
1	B	4779	LYS
1	B	4785	THR
1	B	4788	SER
1	B	4792	LEU
1	B	4796	MET

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Mol	Chain	Res	Type
1	B	4797	VAL
1	B	4800	LEU
1	B	4808	PHE
1	B	4813	LEU
1	B	4814	LEU
1	B	4821	LYS
1	B	4822	THR
1	B	4823	LEU
1	B	4843	LEU
1	B	4844	LEU
1	B	4852	THR
1	B	4853	VAL
1	B	4861	LYS
1	B	4863	TYR
1	B	4865	LYS
1	B	4867	GLU
1	B	4870	ASP
1	B	4871	GLU
1	B	4873	ASP
1	B	4874	MET
1	B	4880	MET
1	B	4881	THR
1	B	4882	CYS
1	B	4884	LEU
1	B	4886	HIS
1	B	4887	MET
1	B	4889	VAL
1	B	4891	VAL
1	B	4902	GLU
1	B	4908	GLU
1	B	4911	LEU
1	B	4914	VAL
1	B	4917	ASP
1	B	4918	ILE
1	B	4924	VAL
1	B	4926	VAL
1	B	4932	ILE
1	B	4933	GLN
1	B	4936	ILE
1	B	4942	GLU
1	B	4945	ASP
1	B	4949	GLN

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Mol	Chain	Res	Type
1	B	4950	VAL
1	B	4951	LYS
1	B	4952	GLU
1	B	4960	ILE
1	B	4965	SER
1	B	4966	ASP
1	B	4967	TYR
1	B	4970	THR
1	B	4971	THR
1	B	4973	HIS
1	B	4980	LEU
1	B	4982	GLU
1	B	4985	LEU
1	B	4989	MET
1	B	4998	LYS
1	B	5002	GLU
1	B	5012	LYS
1	B	5029	ARG
1	B	5030	LYS
1	B	5034	ASP
1	B	5036	LEU
1	C	846	LEU
1	C	1231[A]	GLN
1	C	1231[B]	GLN
1	C	1743[A]	ARG
1	C	1743[B]	ARG
1	C	2369[A]	ARG
1	C	2369[B]	ARG
1	C	4181	ILE
1	C	4182	GLU
1	C	4183	ILE
1	C	4184	MET
1	C	4190	ILE
1	C	4198	SER
1	C	4199	GLU
1	C	4200	THR
1	C	4202	ARG
1	C	4204	GLN
1	C	4207	MET
1	C	4209	GLN
1	C	4211	LYS
1	C	4213	SER

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Mol	Chain	Res	Type
1	C	4214	LYS
1	C	4222	VAL
1	C	4224	GLU
1	C	4230	LYS
1	C	4231	MET
1	C	4236	SER
1	C	4544	LEU
1	C	4545	GLU
1	C	4548	ARG
1	C	4550	LYS
1	C	4552	LEU
1	C	4555	LEU
1	C	4561	THR
1	C	4564	PHE
1	C	4567	LEU
1	C	4569	LEU
1	C	4576	ILE
1	C	4577	LEU
1	C	4578	LEU
1	C	4580	TYR
1	C	4581	LYS
1	C	4582	VAL
1	C	4583	SER
1	C	4584	ASP
1	C	4585	SER
1	C	4627	MET
1	C	4628	VAL
1	C	4632	LEU
1	C	4634	GLU
1	C	4648	LEU
1	C	4651	THR
1	C	4658	ILE
1	C	4662	ASN
1	C	4676	GLU
1	C	4686	LEU
1	C	4697	VAL
1	C	4698	LYS
1	C	4700	GLN
1	C	4720	VAL
1	C	4722	ARG
1	C	4723	LYS
1	C	4730	ASP

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Mol	Chain	Res	Type
1	C	4731	ILE
1	C	4734	ARG
1	C	4736	ARG
1	C	4743	MET
1	C	4745	LEU
1	C	4748	LEU
1	C	4772	ASP
1	C	4773	VAL
1	C	4779	LYS
1	C	4785	THR
1	C	4788	SER
1	C	4792	LEU
1	C	4796	MET
1	C	4797	VAL
1	C	4800	LEU
1	C	4813	LEU
1	C	4814	LEU
1	C	4821	LYS
1	C	4822	THR
1	C	4823	LEU
1	C	4843	LEU
1	C	4844	LEU
1	C	4852	THR
1	C	4853	VAL
1	C	4861	LYS
1	C	4863	TYR
1	C	4865	LYS
1	C	4867	GLU
1	C	4870	ASP
1	C	4871	GLU
1	C	4873	ASP
1	C	4874	MET
1	C	4880	MET
1	C	4881	THR
1	C	4882	CYS
1	C	4884	LEU
1	C	4886	HIS
1	C	4887	MET
1	C	4889	VAL
1	C	4891	VAL
1	C	4902	GLU
1	C	4908	GLU

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Mol	Chain	Res	Type
1	C	4911	LEU
1	C	4914	VAL
1	C	4917	ASP
1	C	4918	ILE
1	C	4924	VAL
1	C	4926	VAL
1	C	4932	ILE
1	C	4933	GLN
1	C	4936	ILE
1	C	4942	GLU
1	C	4945	ASP
1	C	4949	GLN
1	C	4950	VAL
1	C	4951	LYS
1	C	4952	GLU
1	C	4960	ILE
1	C	4965	SER
1	C	4966	ASP
1	C	4967	TYR
1	C	4970	THR
1	C	4971	THR
1	C	4973	HIS
1	C	4980	LEU
1	C	4982	GLU
1	C	4985	LEU
1	C	4989	MET
1	C	4998	LYS
1	C	5002	GLU
1	C	5012	LYS
1	C	5029	ARG
1	C	5030	LYS
1	C	5034	ASP
1	C	5036	LEU
1	D	846	LEU
1	D	1231[A]	GLN
1	D	1231[B]	GLN
1	D	1743[A]	ARG
1	D	1743[B]	ARG
1	D	2369[A]	ARG
1	D	2369[B]	ARG
1	D	4181	ILE
1	D	4182	GLU

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Mol	Chain	Res	Type
1	D	4183	ILE
1	D	4184	MET
1	D	4190	ILE
1	D	4198	SER
1	D	4199	GLU
1	D	4200	THR
1	D	4202	ARG
1	D	4204	GLN
1	D	4207	MET
1	D	4209	GLN
1	D	4211	LYS
1	D	4213	SER
1	D	4214	LYS
1	D	4222	VAL
1	D	4224	GLU
1	D	4230	LYS
1	D	4231	MET
1	D	4236	SER
1	D	4544	LEU
1	D	4545	GLU
1	D	4548	ARG
1	D	4550	LYS
1	D	4552	LEU
1	D	4555	LEU
1	D	4561	THR
1	D	4564	PHE
1	D	4567	LEU
1	D	4569	LEU
1	D	4576	ILE
1	D	4577	LEU
1	D	4578	LEU
1	D	4580	TYR
1	D	4581	LYS
1	D	4582	VAL
1	D	4583	SER
1	D	4584	ASP
1	D	4585	SER
1	D	4627	MET
1	D	4628	VAL
1	D	4632	LEU
1	D	4634	GLU
1	D	4648	LEU

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Mol	Chain	Res	Type
1	D	4651	THR
1	D	4658	ILE
1	D	4662	ASN
1	D	4676	GLU
1	D	4686	LEU
1	D	4697	VAL
1	D	4698	LYS
1	D	4700	GLN
1	D	4720	VAL
1	D	4722	ARG
1	D	4723	LYS
1	D	4730	ASP
1	D	4731	ILE
1	D	4734	ARG
1	D	4736	ARG
1	D	4743	MET
1	D	4745	LEU
1	D	4748	LEU
1	D	4772	ASP
1	D	4773	VAL
1	D	4779	LYS
1	D	4785	THR
1	D	4788	SER
1	D	4792	LEU
1	D	4796	MET
1	D	4797	VAL
1	D	4800	LEU
1	D	4808	PHE
1	D	4813	LEU
1	D	4814	LEU
1	D	4821	LYS
1	D	4822	THR
1	D	4823	LEU
1	D	4843	LEU
1	D	4844	LEU
1	D	4852	THR
1	D	4853	VAL
1	D	4861	LYS
1	D	4863	TYR
1	D	4865	LYS
1	D	4867	GLU
1	D	4870	ASP

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Mol	Chain	Res	Type
1	D	4871	GLU
1	D	4873	ASP
1	D	4874	MET
1	D	4880	MET
1	D	4881	THR
1	D	4882	CYS
1	D	4884	LEU
1	D	4886	HIS
1	D	4887	MET
1	D	4889	VAL
1	D	4891	VAL
1	D	4902	GLU
1	D	4908	GLU
1	D	4911	LEU
1	D	4914	VAL
1	D	4917	ASP
1	D	4918	ILE
1	D	4924	VAL
1	D	4926	VAL
1	D	4932	ILE
1	D	4933	GLN
1	D	4936	ILE
1	D	4942	GLU
1	D	4945	ASP
1	D	4949	GLN
1	D	4950	VAL
1	D	4951	LYS
1	D	4952	GLU
1	D	4960	ILE
1	D	4965	SER
1	D	4966	ASP
1	D	4967	TYR
1	D	4970	THR
1	D	4971	THR
1	D	4973	HIS
1	D	4980	LEU
1	D	4982	GLU
1	D	4985	LEU
1	D	4989	MET
1	D	4998	LYS
1	D	5002	GLU
1	D	5012	LYS

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Mol	Chain	Res	Type
1	D	5029	ARG
1	D	5030	LYS
1	D	5034	ASP
1	D	5036	LEU

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

Mol	Chain	Res	Type
1	A	12	GLN
1	A	98	HIS
1	A	201	ASN
1	A	203	ASN
1	A	241	GLN
1	A	284	HIS
1	A	489	ASN
1	A	533	ASN
1	A	596	ASN
1	A	838	HIS
1	A	877	ASN
1	A	1066	GLN
1	A	1158	ASN
1	A	1229	ASN
1	A	1299	GLN
1	A	1300	HIS
1	A	1463	ASN
1	A	1545	ASN
1	A	1611	HIS
1	A	1614	GLN
1	A	1631	GLN
1	A	1756	ASN
1	A	1938	GLN
1	A	2247	GLN
1	A	2881	ASN
1	A	2931	GLN
1	A	2976	HIS
1	A	2991	HIS
1	A	3214	ASN
1	A	3318	ASN
1	A	3325	ASN
1	A	3430	ASN
1	A	3457	ASN
1	A	3466	ASN

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Mol	Chain	Res	Type
1	A	3766	GLN
1	A	3927	GLN
1	A	4078	GLN
1	A	4547	GLN
1	A	4728	HIS
1	A	4812	HIS
1	A	4864	ASN
1	A	4886	HIS
1	A	4949	GLN
1	A	5031	GLN
1	B	12	GLN
1	B	98	HIS
1	B	201	ASN
1	B	203	ASN
1	B	241	GLN
1	B	284	HIS
1	B	461	HIS
1	B	465	GLN
1	B	489	ASN
1	B	533	ASN
1	B	596	ASN
1	B	838	HIS
1	B	877	ASN
1	B	1058	GLN
1	B	1066	GLN
1	B	1158	ASN
1	B	1229	ASN
1	B	1299	GLN
1	B	1300	HIS
1	B	1463	ASN
1	B	1545	ASN
1	B	1611	HIS
1	B	1614	GLN
1	B	1631	GLN
1	B	1756	ASN
1	B	1938	GLN
1	B	2247	GLN
1	B	2881	ASN
1	B	2924	GLN
1	B	2931	GLN
1	B	2991	HIS
1	B	3214	ASN

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Mol	Chain	Res	Type
1	B	3318	ASN
1	B	3325	ASN
1	B	3457	ASN
1	B	3466	ASN
1	B	3667	HIS
1	B	3766	GLN
1	B	3927	GLN
1	B	4078	GLN
1	B	4547	GLN
1	B	4728	HIS
1	B	4812	HIS
1	B	4864	ASN
1	B	4886	HIS
1	B	4933	GLN
1	B	4949	GLN
1	B	5031	GLN
1	C	12	GLN
1	C	98	HIS
1	C	201	ASN
1	C	203	ASN
1	C	241	GLN
1	C	284	HIS
1	C	461	HIS
1	C	465	GLN
1	C	489	ASN
1	C	596	ASN
1	C	838	HIS
1	C	877	ASN
1	C	1158	ASN
1	C	1229	ASN
1	C	1299	GLN
1	C	1300	HIS
1	C	1541	GLN
1	C	1545	ASN
1	C	1611	HIS
1	C	1614	GLN
1	C	1631	GLN
1	C	1756	ASN
1	C	1938	GLN
1	C	2247	GLN
1	C	2881	ASN
1	C	2924	GLN

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Mol	Chain	Res	Type
1	C	2931	GLN
1	C	2991	HIS
1	C	3214	ASN
1	C	3318	ASN
1	C	3325	ASN
1	C	3457	ASN
1	C	3466	ASN
1	C	3667	HIS
1	C	3766	GLN
1	C	3927	GLN
1	C	4078	GLN
1	C	4547	GLN
1	C	4728	HIS
1	C	4812	HIS
1	C	4864	ASN
1	C	4886	HIS
1	C	4933	GLN
1	C	4949	GLN
1	C	4973	HIS
1	C	5031	GLN
1	D	12	GLN
1	D	98	HIS
1	D	201	ASN
1	D	203	ASN
1	D	241	GLN
1	D	284	HIS
1	D	489	ASN
1	D	596	ASN
1	D	838	HIS
1	D	877	ASN
1	D	1066	GLN
1	D	1158	ASN
1	D	1229	ASN
1	D	1299	GLN
1	D	1300	HIS
1	D	1463	ASN
1	D	1545	ASN
1	D	1611	HIS
1	D	1631	GLN
1	D	1756	ASN
1	D	1938	GLN
1	D	2247	GLN

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Mol	Chain	Res	Type
1	D	2881	ASN
1	D	2931	GLN
1	D	2991	HIS
1	D	3214	ASN
1	D	3318	ASN
1	D	3325	ASN
1	D	3457	ASN
1	D	3466	ASN
1	D	3667	HIS
1	D	3766	GLN
1	D	3927	GLN
1	D	4078	GLN
1	D	4133	GLN
1	D	4547	GLN
1	D	4728	HIS
1	D	4812	HIS
1	D	4864	ASN
1	D	4886	HIS
1	D	4933	GLN
1	D	4949	GLN
1	D	4973	HIS
1	D	5031	GLN
2	E	43	ASN
2	E	65	GLN
2	F	43	ASN
2	F	65	GLN
2	G	43	ASN
2	G	65	GLN
2	H	43	ASN
2	H	65	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	ADE	A	5102	-	11,11,11	0.39	0	15,15,15	0.41	0
4	ADE	B	5102	-	11,11,11	0.39	0	15,15,15	0.41	0
4	ADE	C	5102	-	11,11,11	0.39	0	15,15,15	0.41	0
4	ADE	D	5102	-	11,11,11	0.39	0	15,15,15	0.41	0

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	ADE	A	5102	-	-	-	0/2/2/2
4	ADE	B	5102	-	-	-	0/2/2/2
4	ADE	C	5102	-	-	-	0/2/2/2
4	ADE	D	5102	-	-	-	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

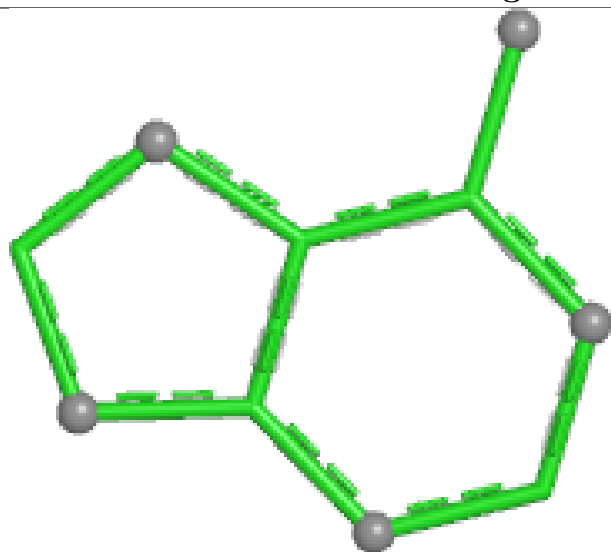
There are no ring outliers.

4 monomers are involved in 4 short contacts:

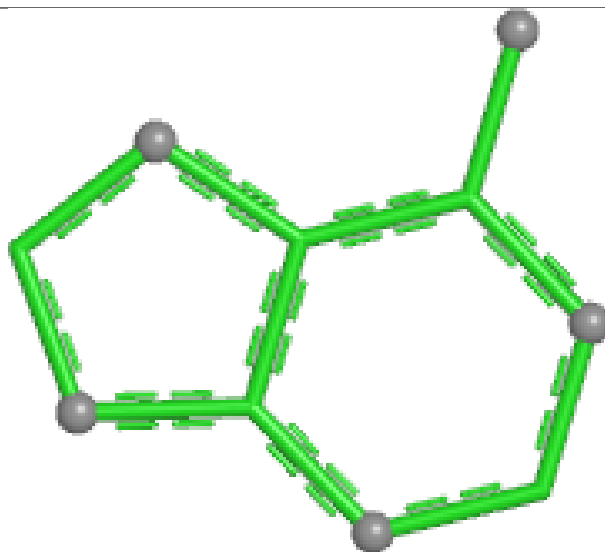
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5102	ADE	1	0
4	B	5102	ADE	1	0
4	C	5102	ADE	1	0
4	D	5102	ADE	1	0

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

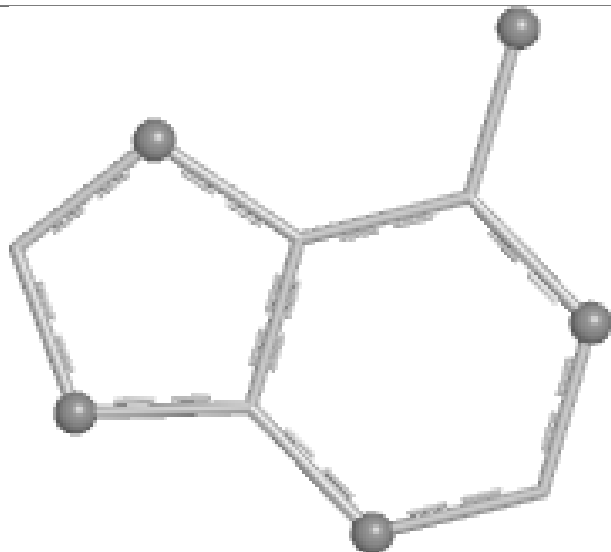
Ligand ADE A 5102



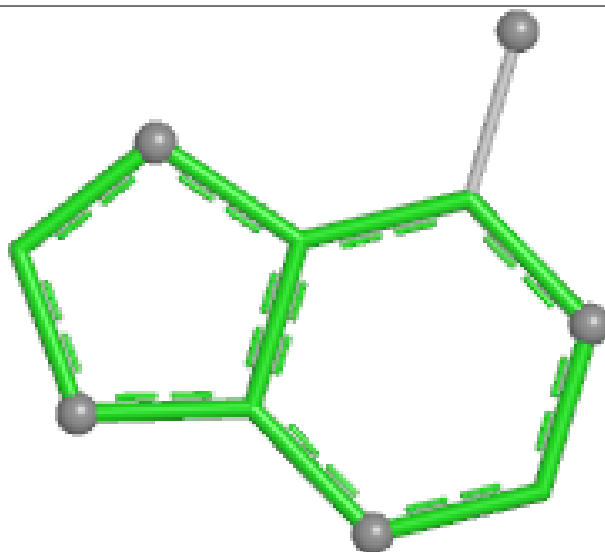
Bond lengths



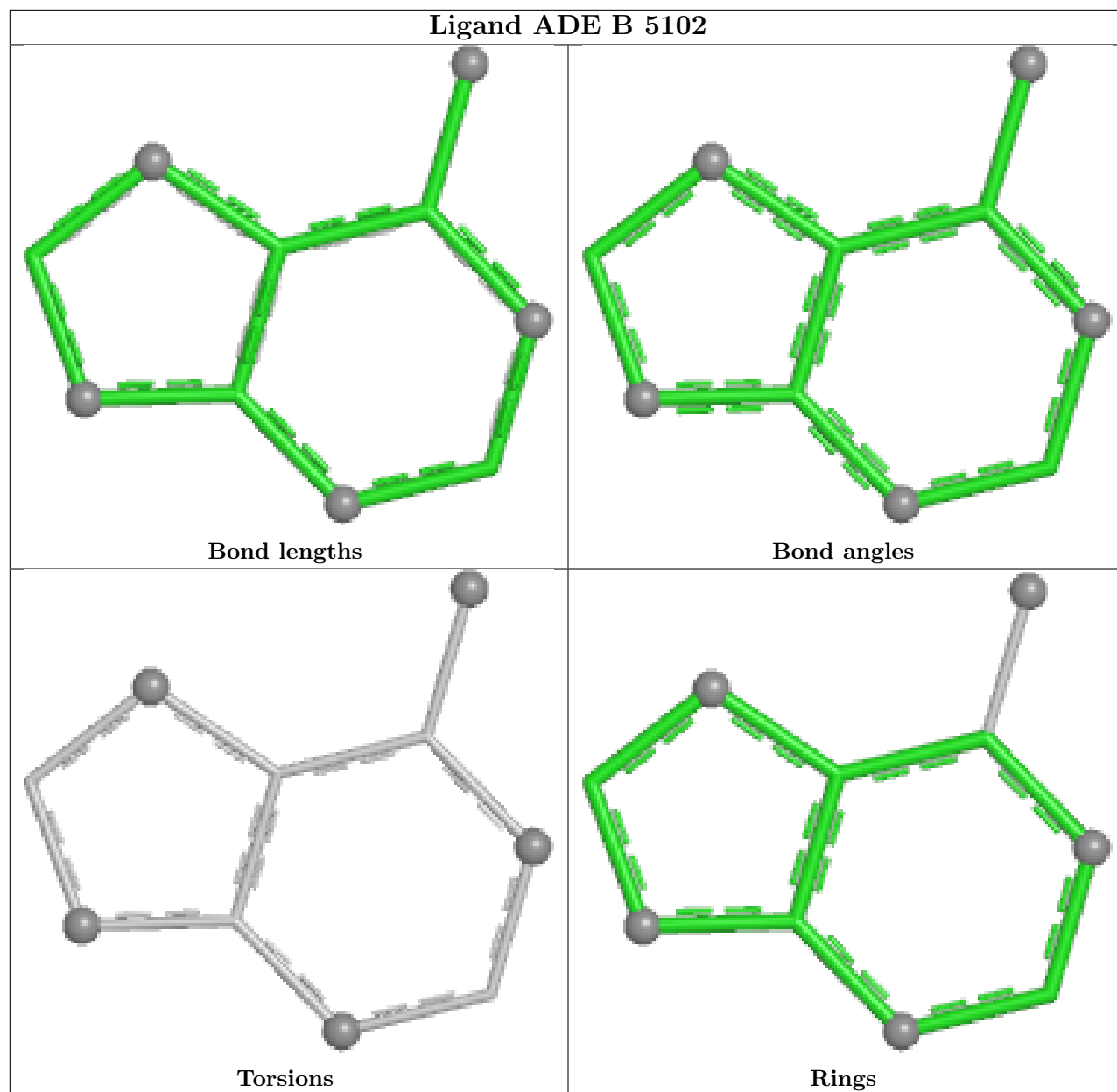
Bond angles

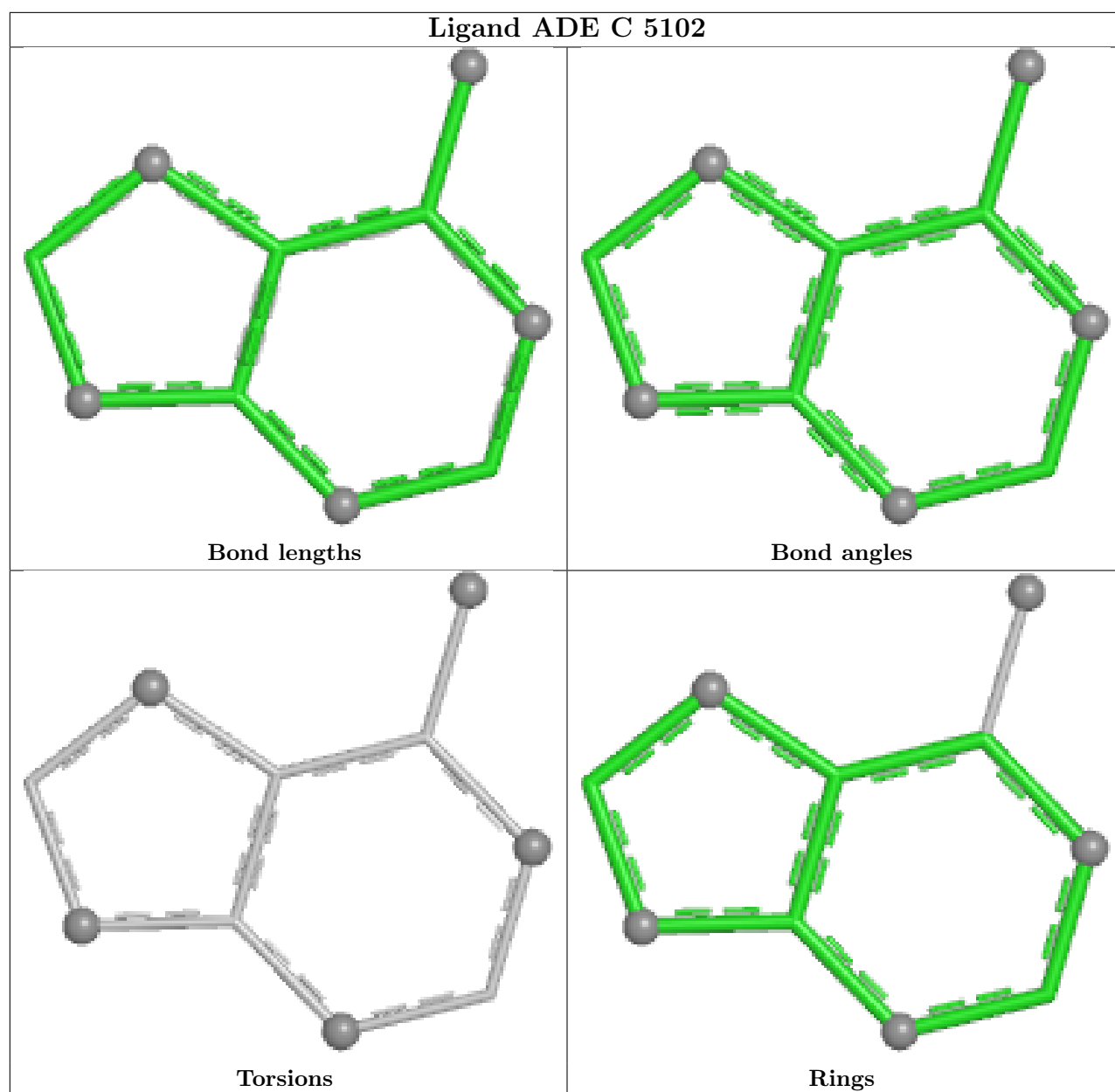


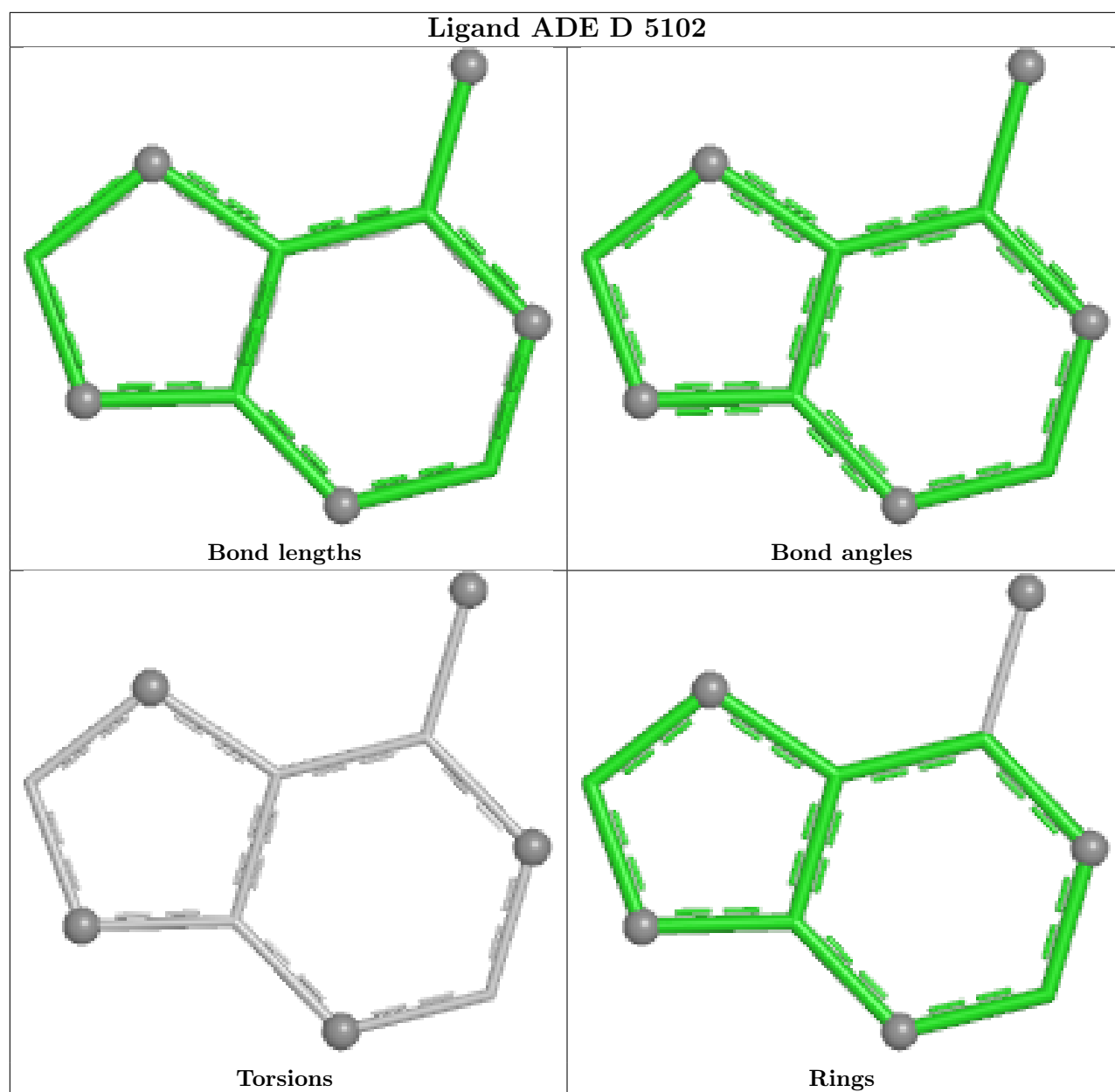
Torsions



Rings







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.

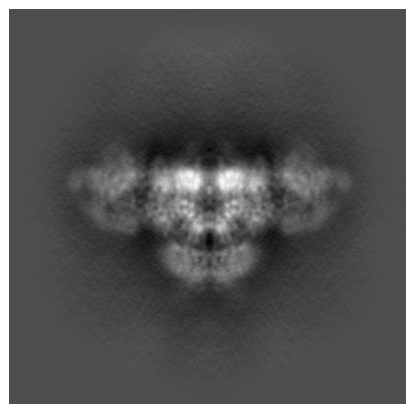
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40427. These allow visual inspection of the internal detail of the map and identification of artifacts.

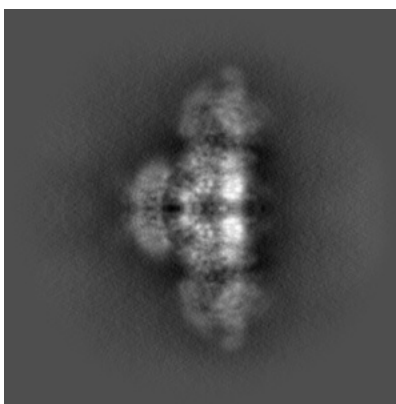
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

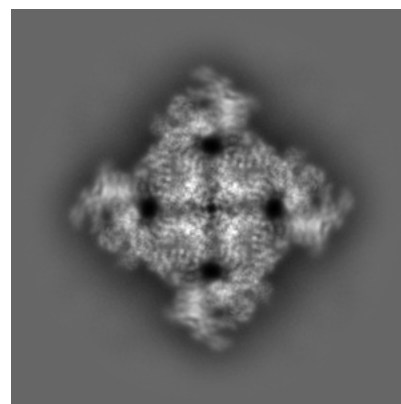
6.1.1 Primary map



X

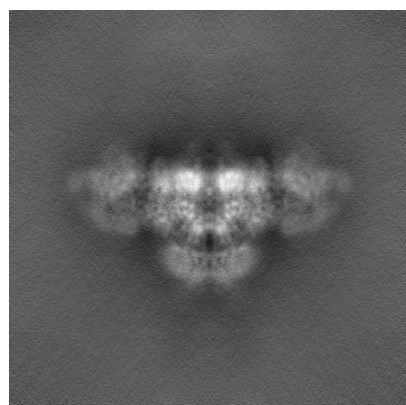


Y

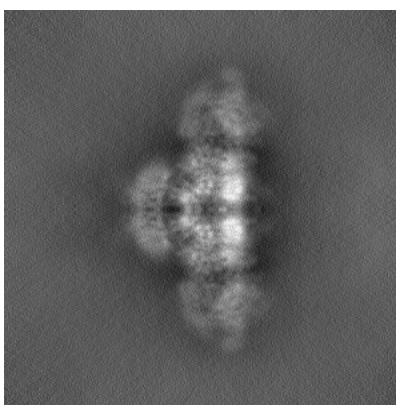


Z

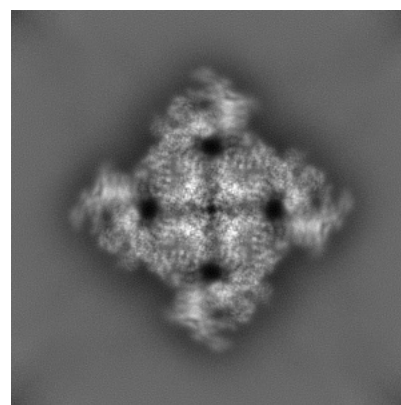
6.1.2 Raw map



X



Y

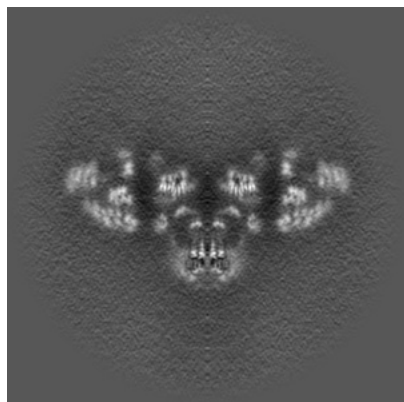


Z

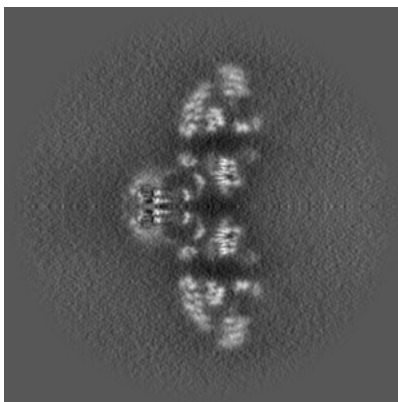
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

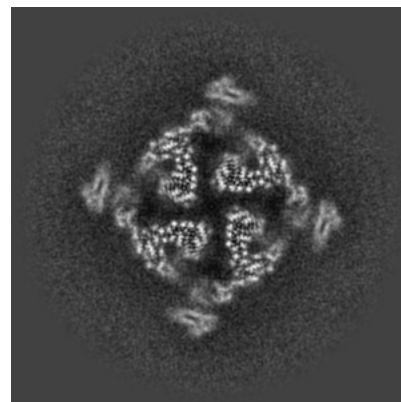
6.2.1 Primary map



X Index: 200

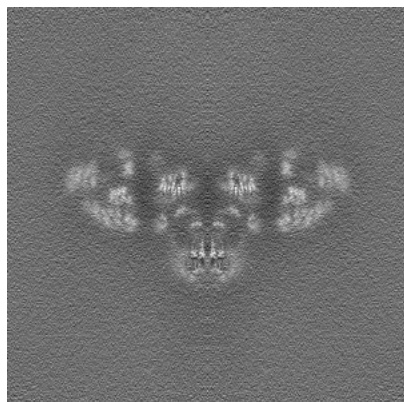


Y Index: 200

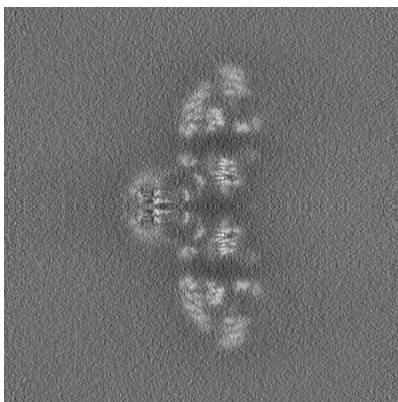


Z Index: 200

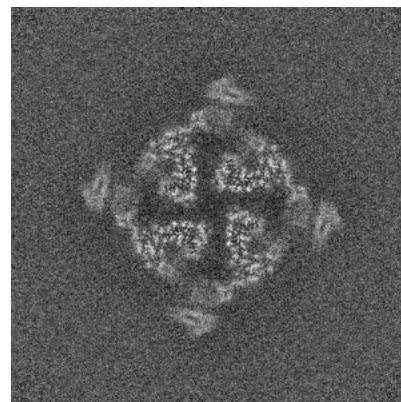
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

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

6.3 Largest variance slices [i](#)

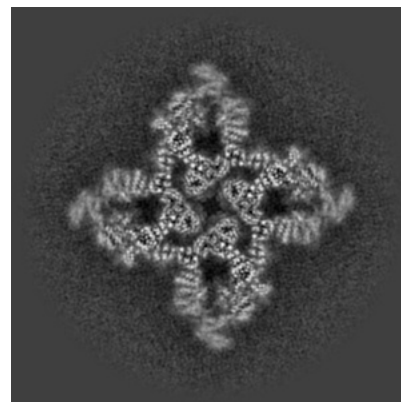
6.3.1 Primary map



X Index: 182

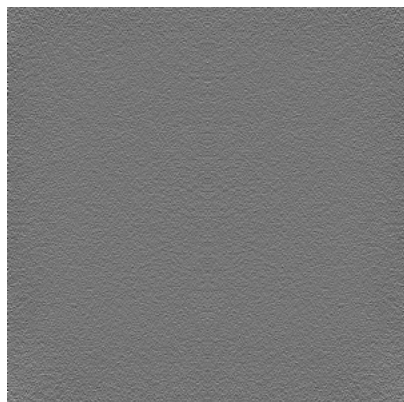


Y Index: 182

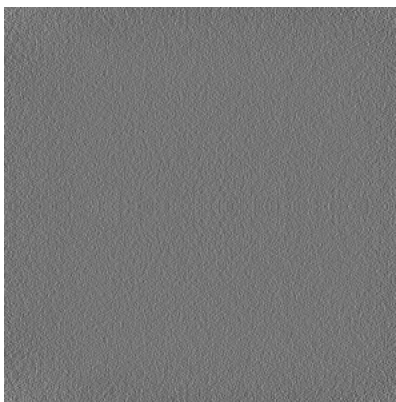


Z Index: 225

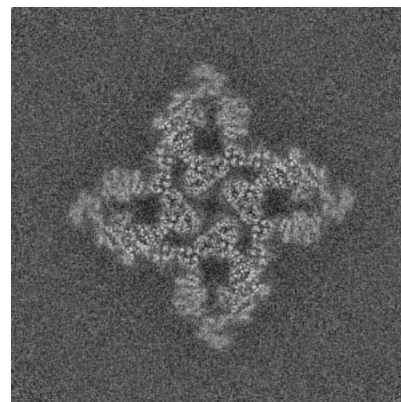
6.3.2 Raw map



X Index: 0



Y Index: 0

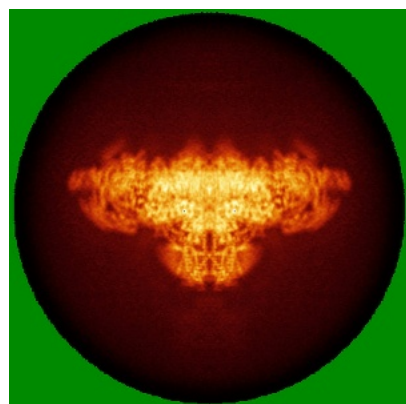


Z Index: 224

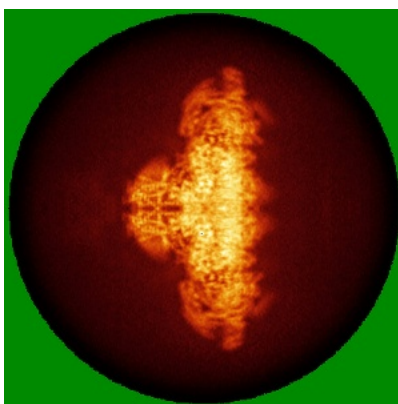
The images above show the largest variance slices of the map in three orthogonal directions.

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

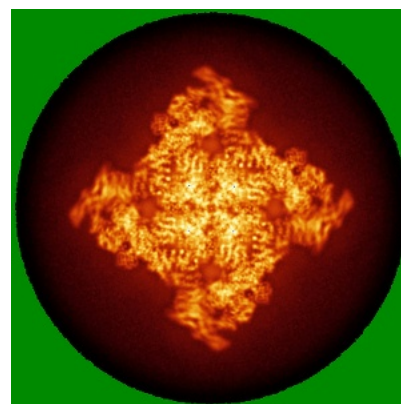
6.4.1 Primary map



X

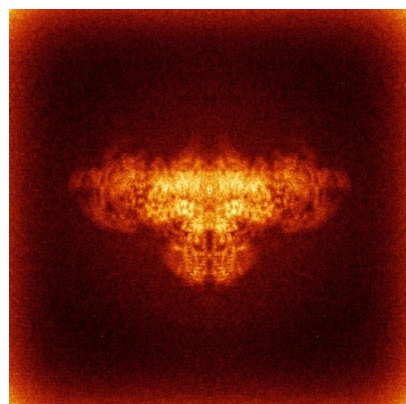


Y

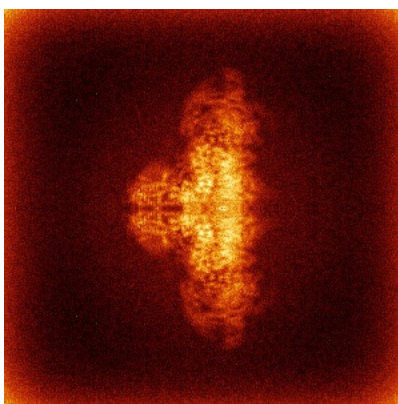


Z

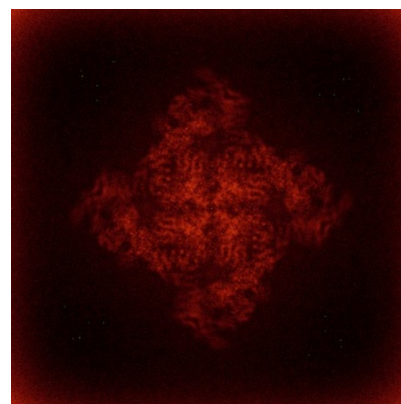
6.4.2 Raw map



X



Y

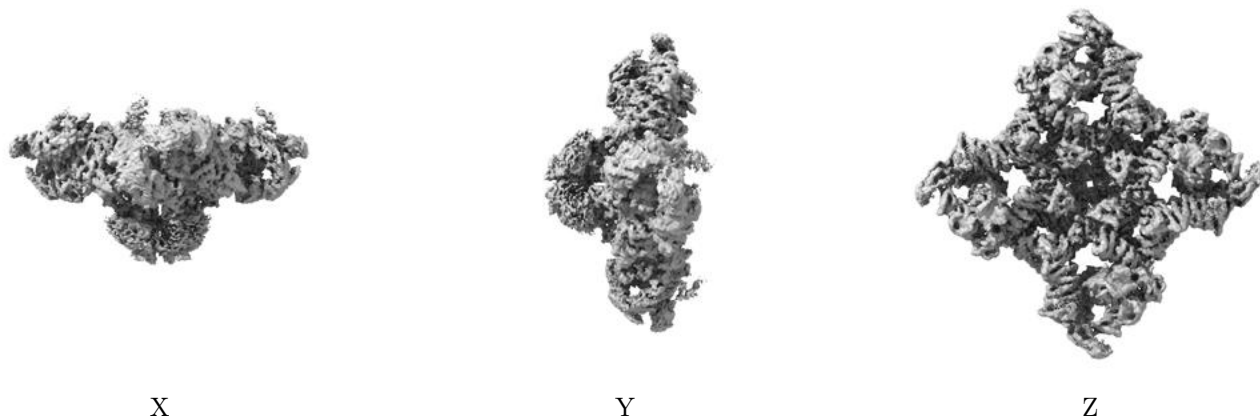


Z

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

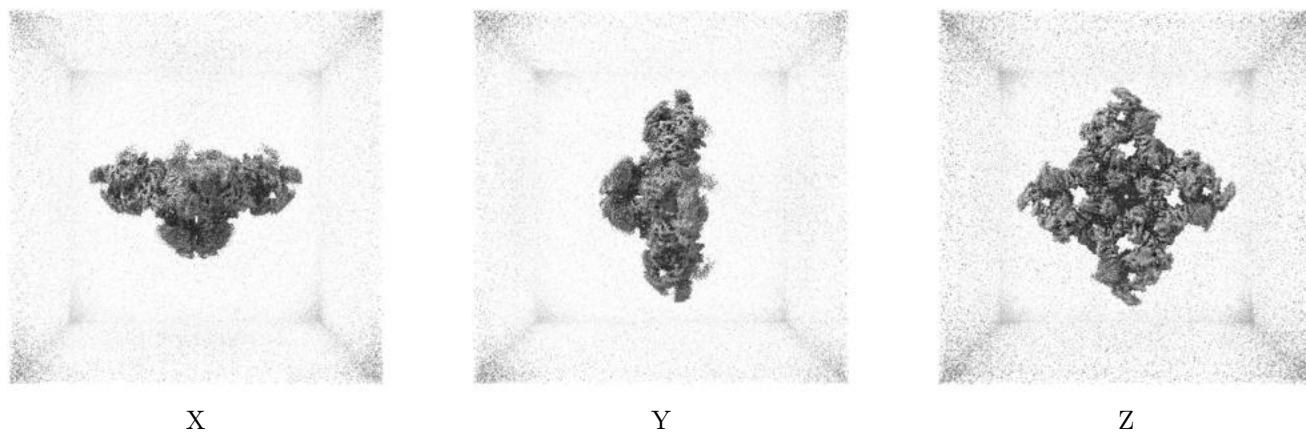
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.305. 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.

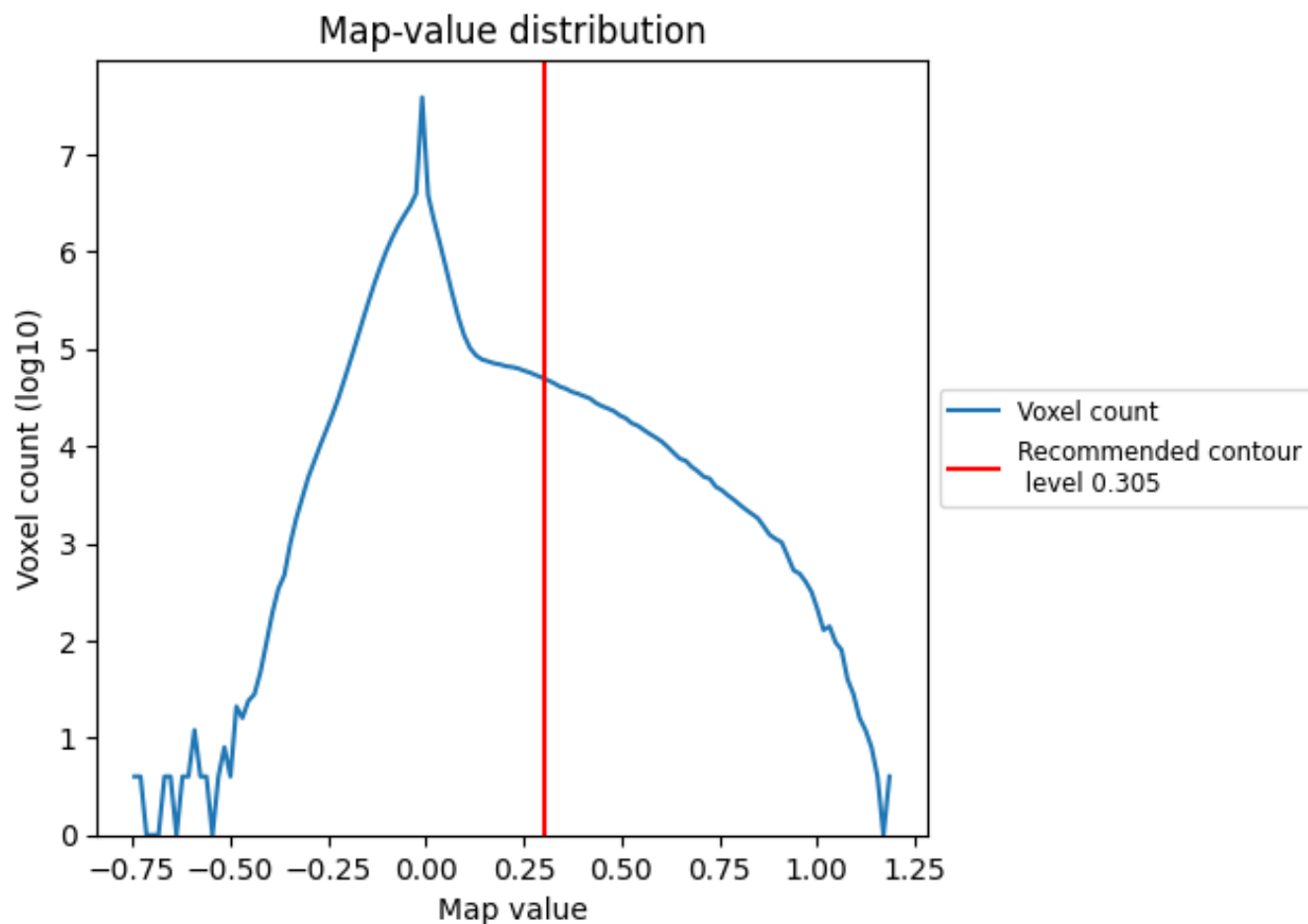
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

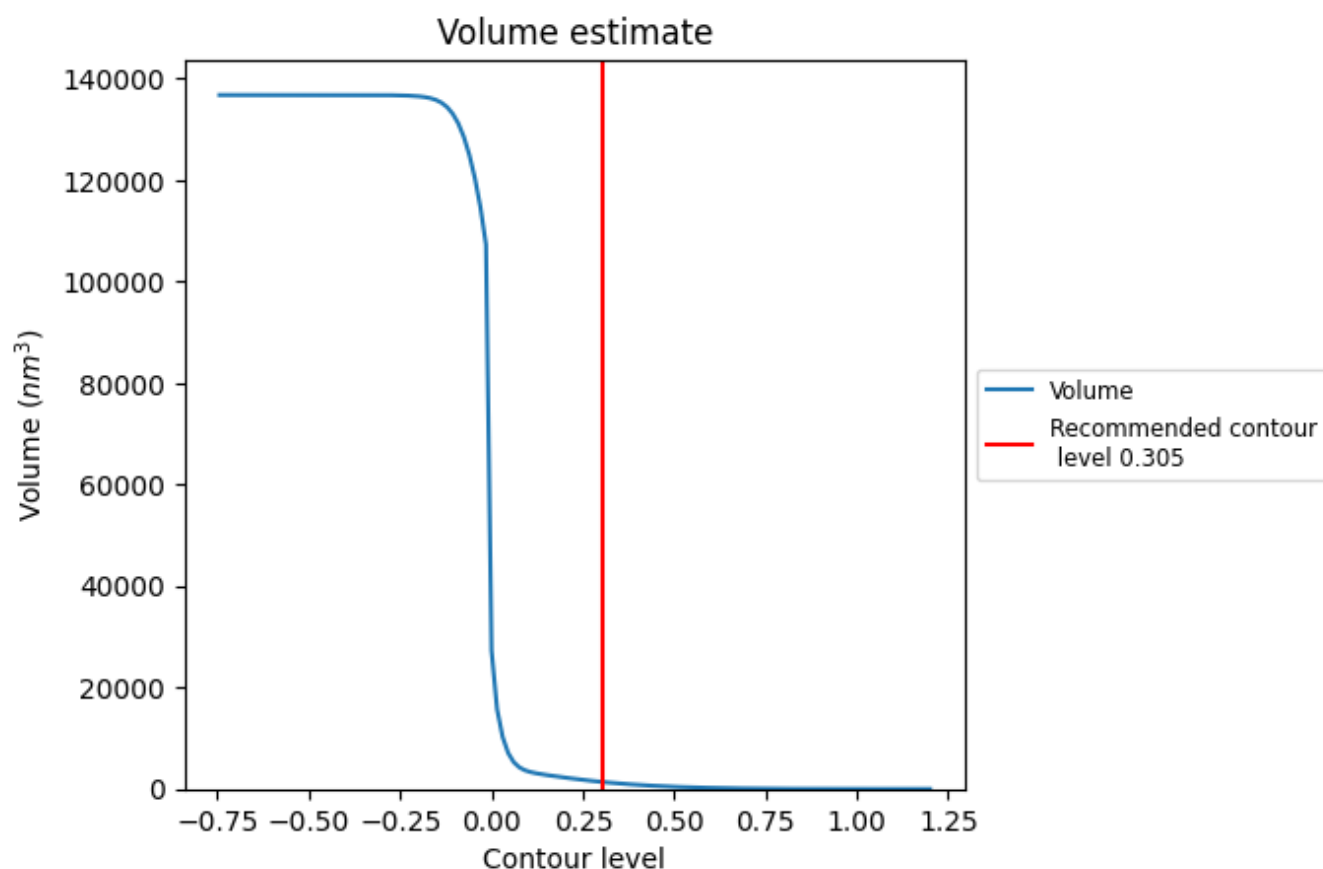
This section contains the results of statistical analysis of the map.

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.

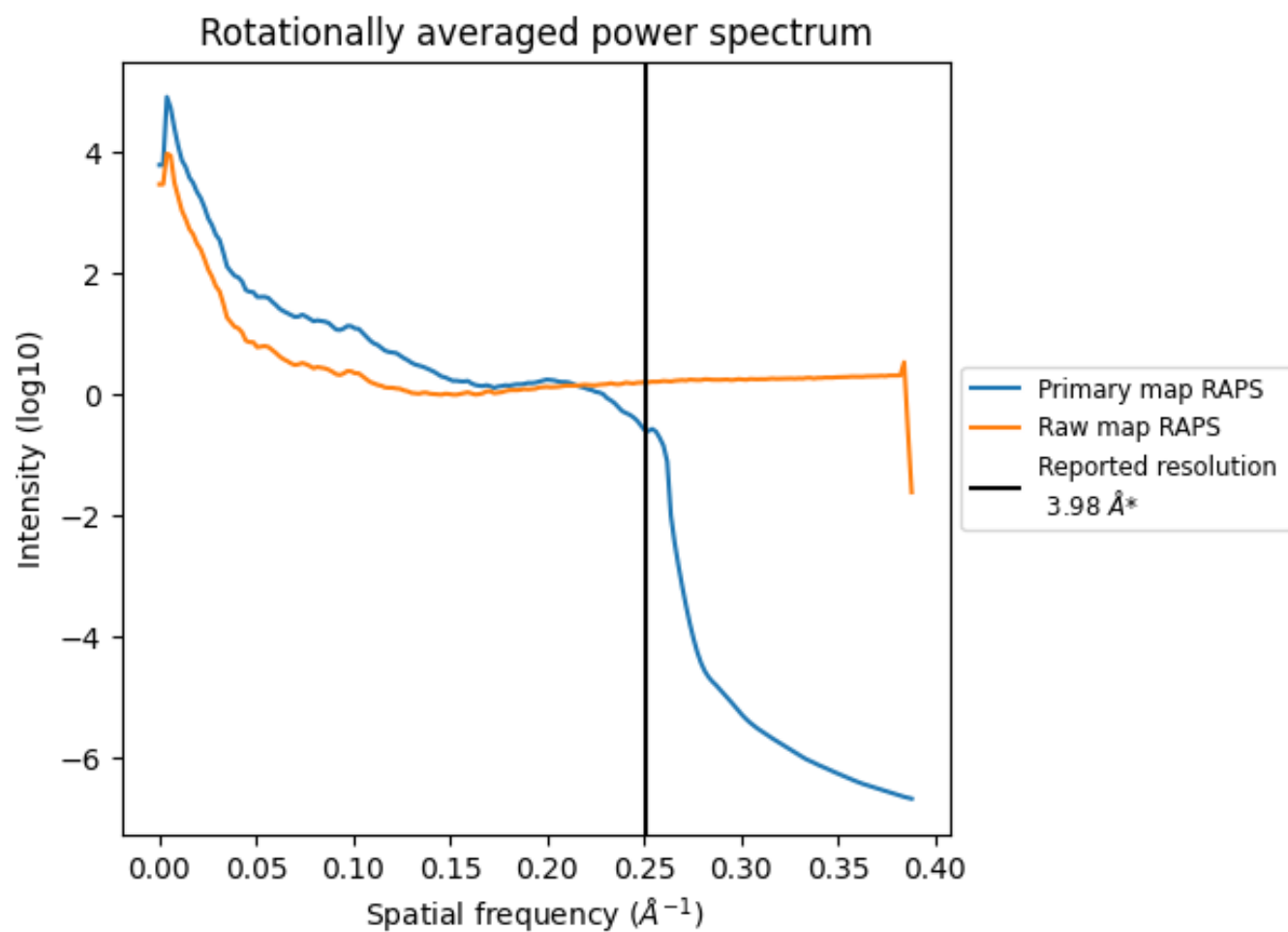
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1365 nm^3 ; this corresponds to an approximate mass of 1233 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 ⓘ

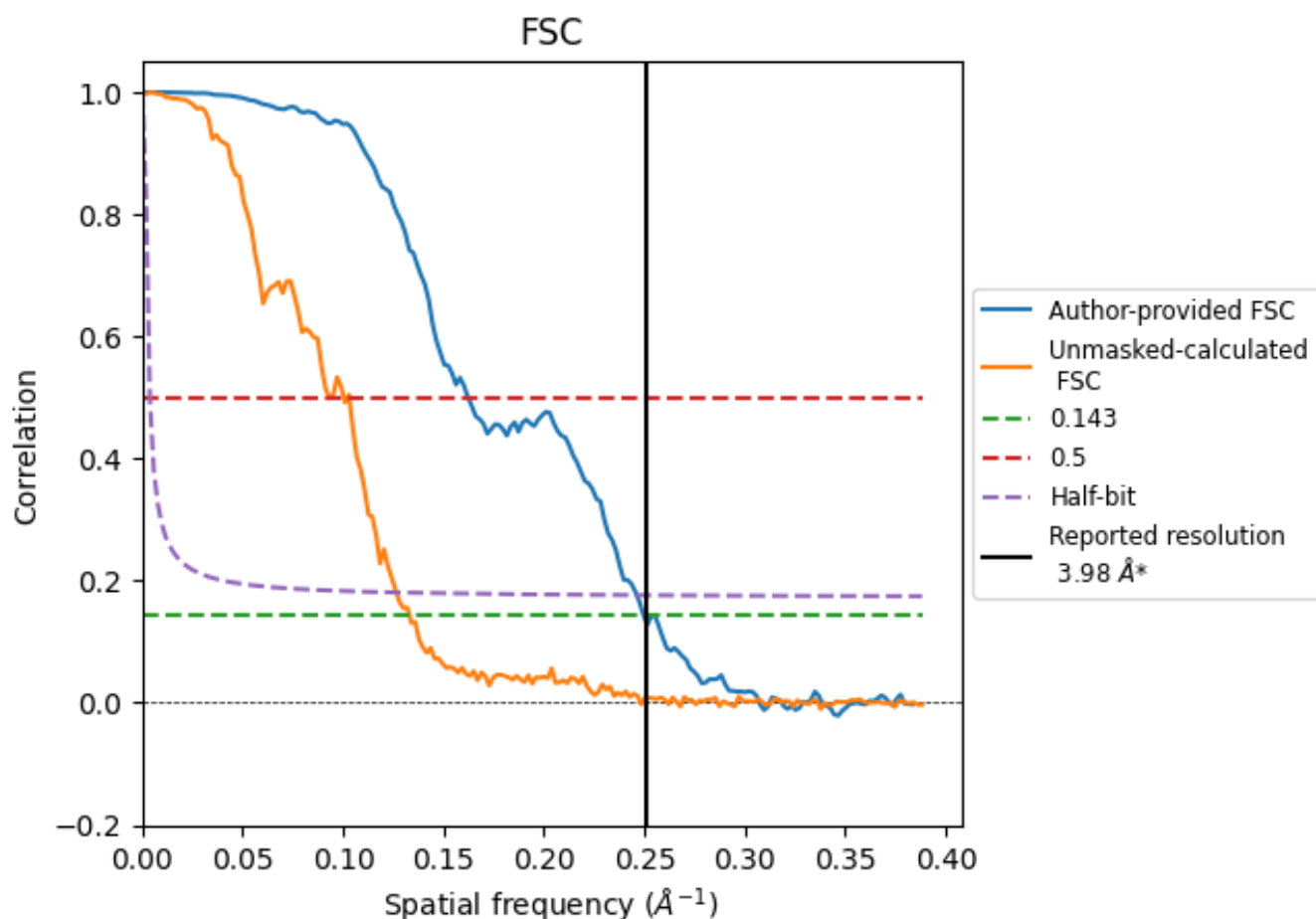


*Reported resolution corresponds to spatial frequency of 0.251 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.251 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

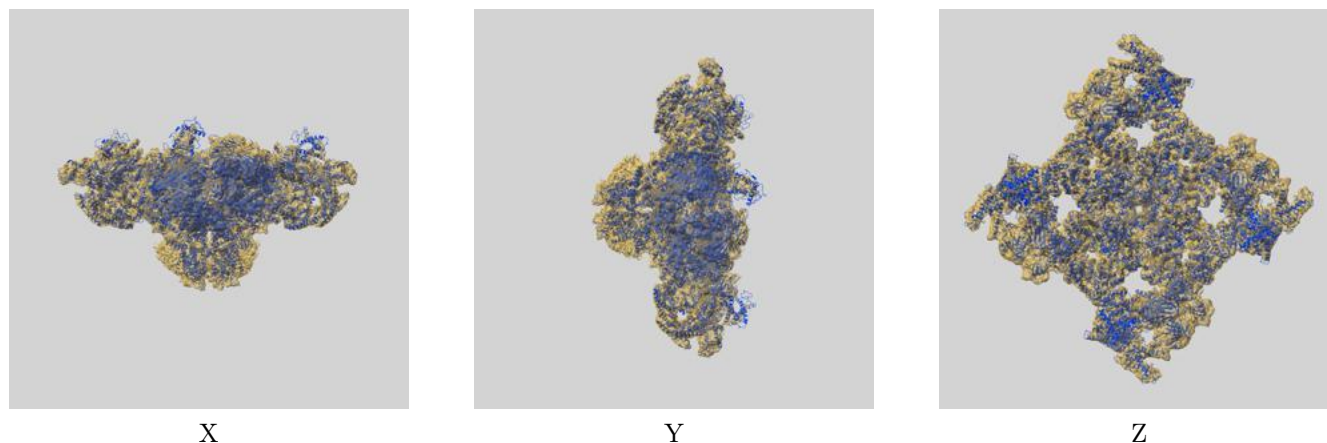
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.98	-	-
Author-provided FSC curve	4.01	6.17	4.06
Unmasked-calculated*	7.52	10.75	7.91

*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 7.52 differs from the reported value 3.98 by more than 10 %

9 Map-model fit [i](#)

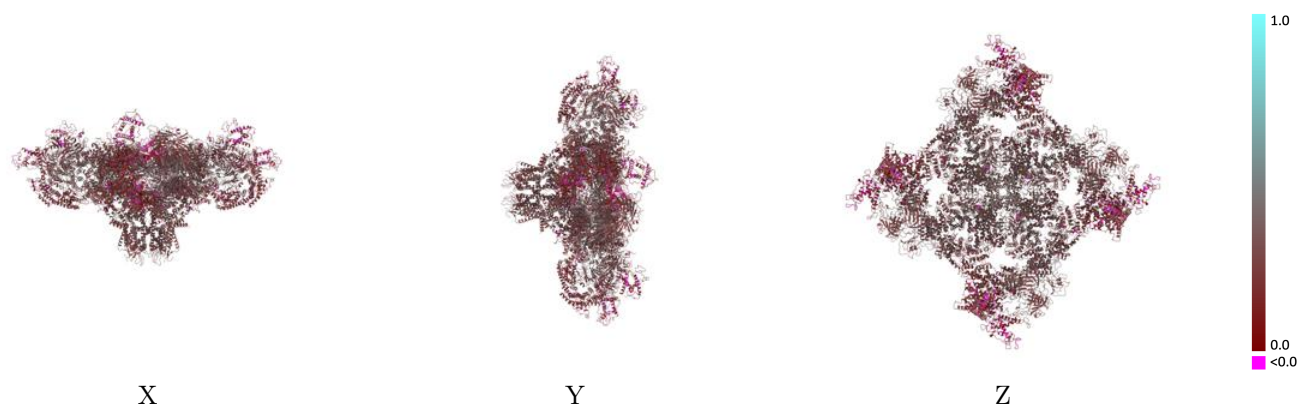
This section contains information regarding the fit between EMDB map EMD-40427 and PDB model 8SES. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



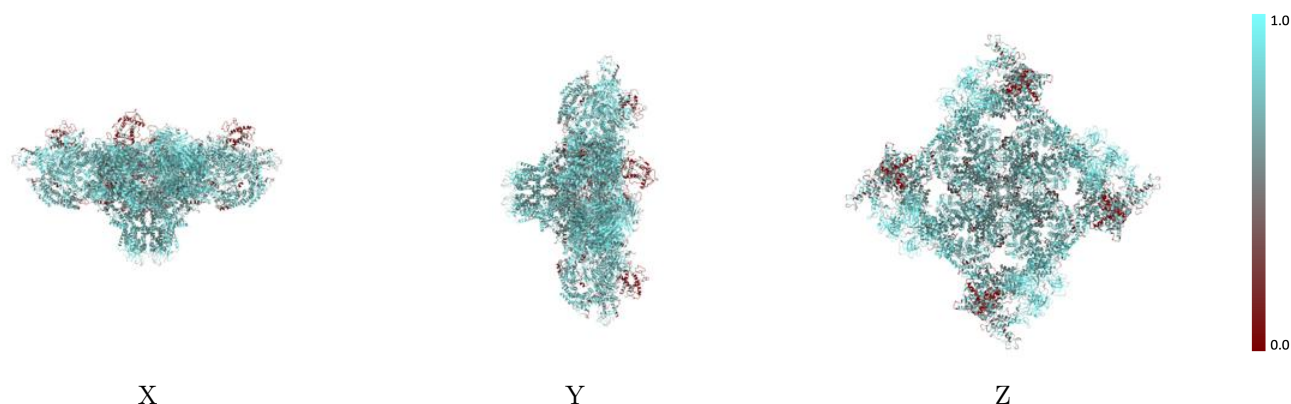
The images above show the 3D surface view of the map at the recommended contour level 0.305 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



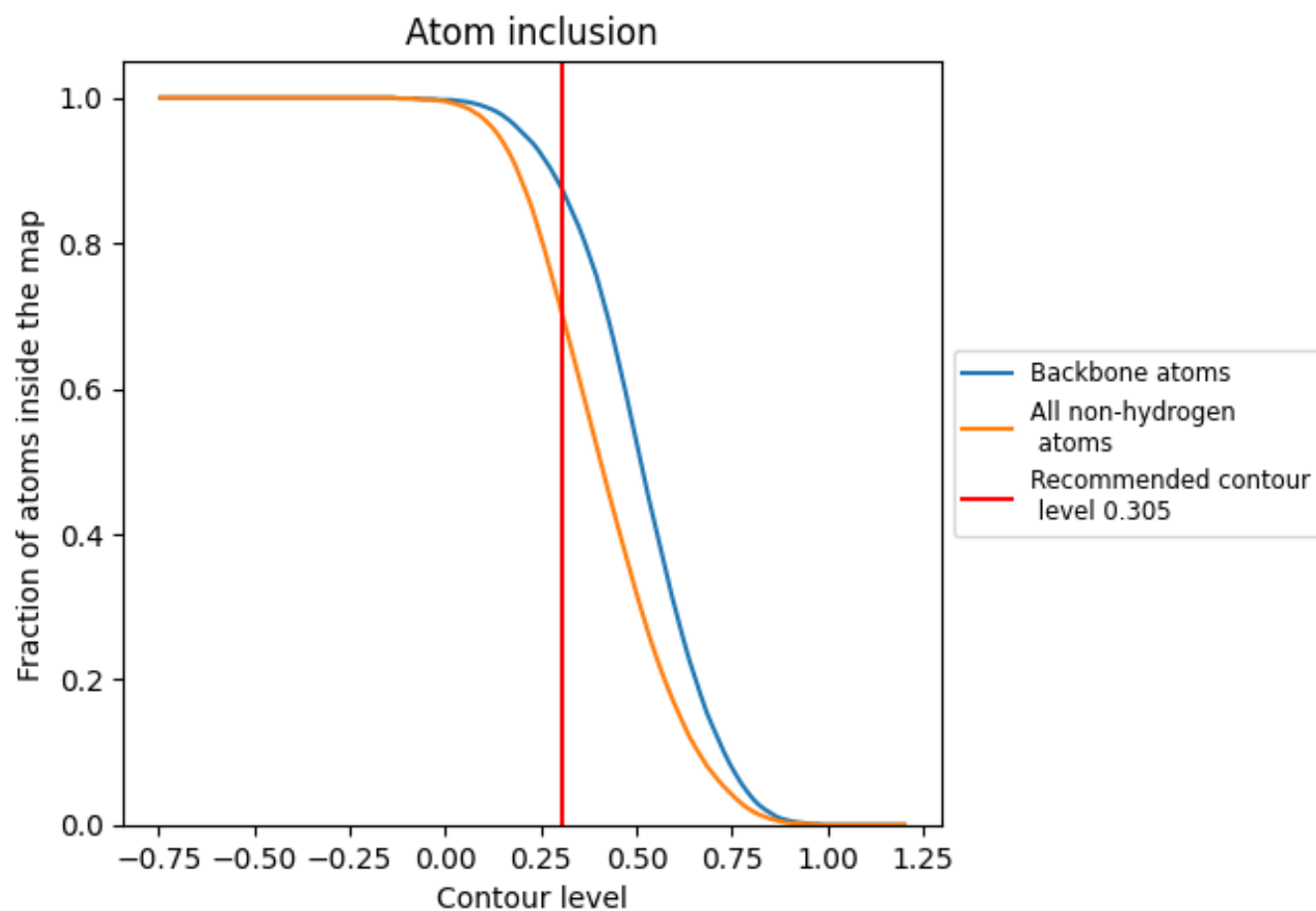
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.305).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 70% 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 (0.305) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7040	0.2840
A	0.7000	0.2820
B	0.7010	0.2820
C	0.7010	0.2820
D	0.7010	0.2830
E	0.8610	0.3440
F	0.8610	0.3430
G	0.8610	0.3420
H	0.8610	0.3450

1.0

0.0

<0.0