



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 06:23 PM JST

PDB ID : 6JIU
EMDB ID : EMD-9836
Title : Structure of RyR2 (F/A/C/L-Ca²⁺/Ca²⁺+CaM dataset)
Authors : Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.
Deposited on : 2019-02-23
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

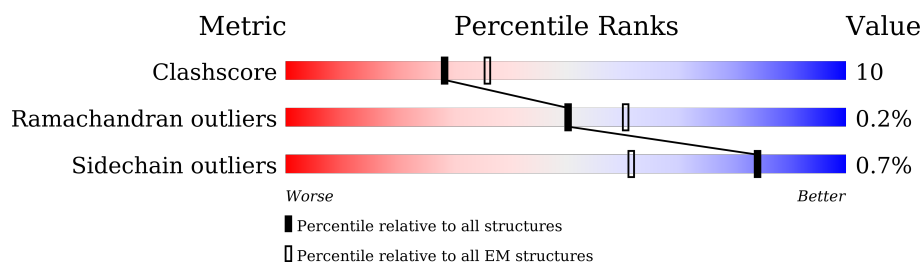
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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



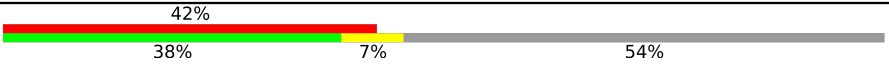



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	4968	 6% 54% 16% 30%
1	D	4968	 6% 54% 16% 30%
1	G	4968	 6% 54% 16% 30%
1	J	4968	 6% 54% 16% 30%
2	B	108	 79% 19% ..
2	E	108	 79% 19% ..
2	H	108	 80% 19% ..
2	K	108	 80% 19% ..

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Mol	Chain	Length	Quality of chain
3	C	149	
3	F	149	
3	I	149	
3	L	149	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 112212 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 RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3496	Total	C	N	O	S	0	0
			26661	16986	4571	4947	157		
1	D	3496	Total	C	N	O	S	0	0
			26661	16986	4571	4947	157		
1	G	3496	Total	C	N	O	S	0	0
			26661	16986	4571	4947	157		
1	J	3496	Total	C	N	O	S	0	0
			26661	16986	4571	4947	157		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	E	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	H	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	K	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	68	Total	C	N	O	S	0	0
			524	326	83	110	5		
3	F	68	Total	C	N	O	S	0	0
			524	326	83	110	5		
3	I	68	Total	C	N	O	S	0	0
			524	326	83	110	5		
3	L	68	Total	C	N	O	S	0	0
			524	326	83	110	5		

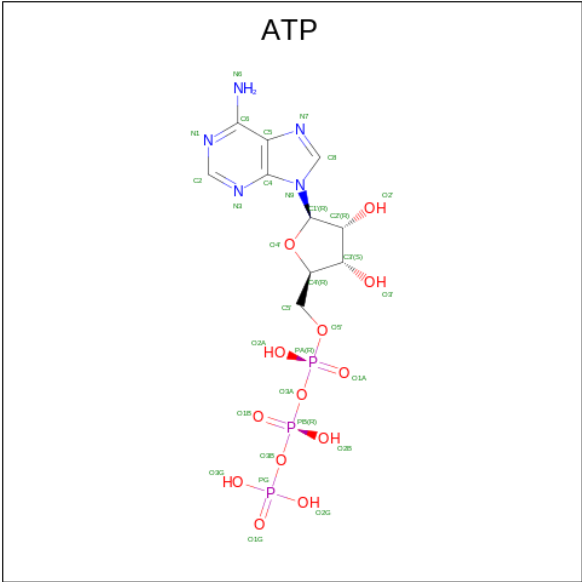
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Zn 1	0
4	D	1	Total 1	Zn 1	0
4	G	1	Total 1	Zn 1	0
4	J	1	Total 1	Zn 1	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

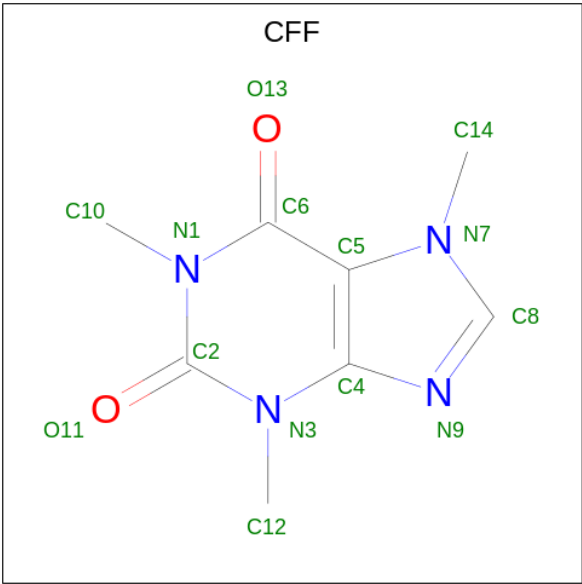
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total 1	Ca 1	0
5	C	2	Total 2	Ca 2	0
5	D	1	Total 1	Ca 1	0
5	F	2	Total 2	Ca 2	0
5	G	1	Total 1	Ca 1	0
5	I	2	Total 2	Ca 2	0
5	J	1	Total 1	Ca 1	0
5	L	2	Total 2	Ca 2	0

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 7 is CAFFEINE (three-letter code: CFF) (formula: C₈H₁₀N₄O₂).

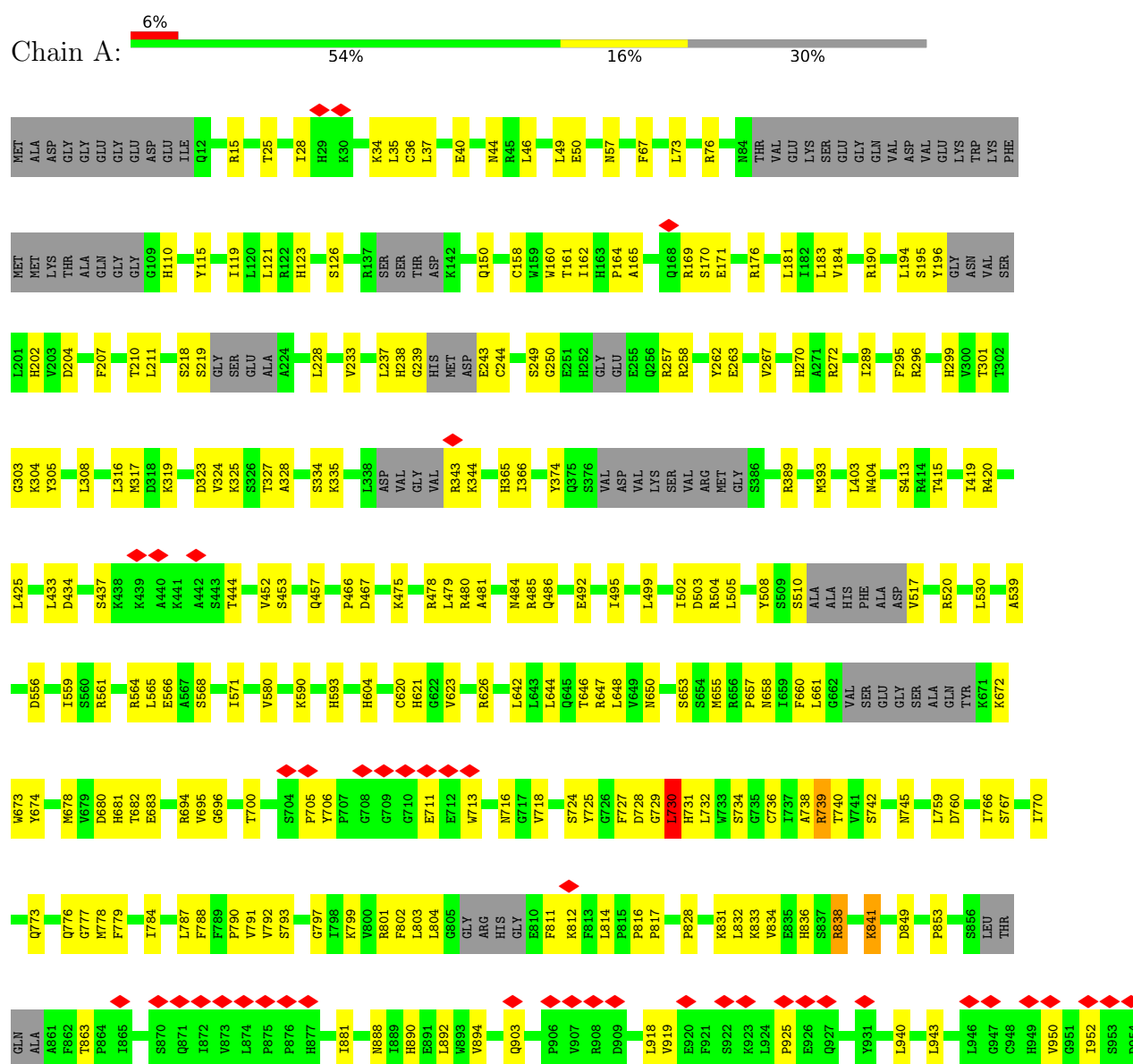


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total 14	C 8	N 4	O 2	0
7	D	1	Total 14	C 8	N 4	O 2	0
7	G	1	Total 14	C 8	N 4	O 2	0
7	J	1	Total 14	C 8	N 4	O 2	0

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: RyR2

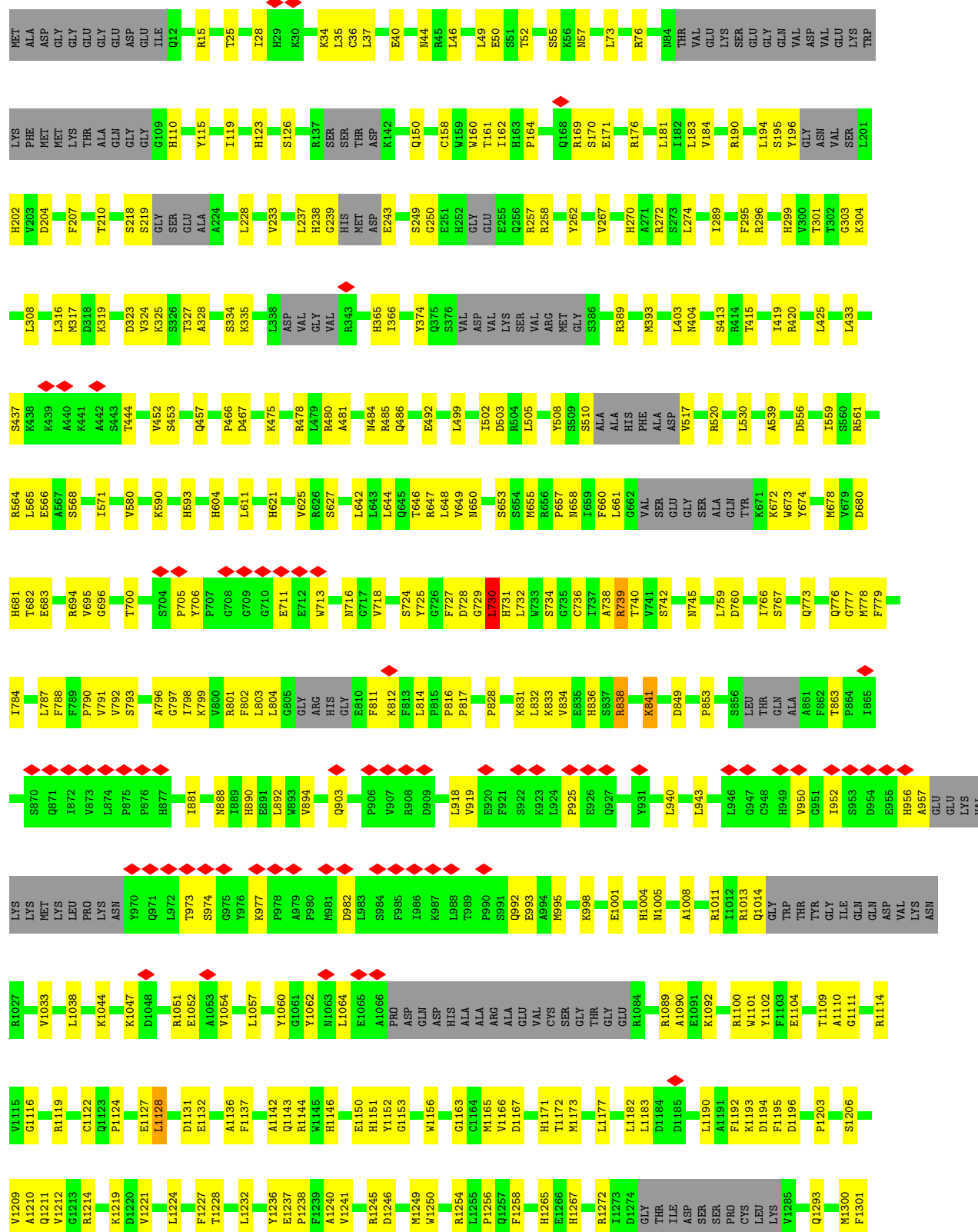




WORLDWIDE
PDB
PROTEIN DATA BANK



● Molecule 1: RyR2



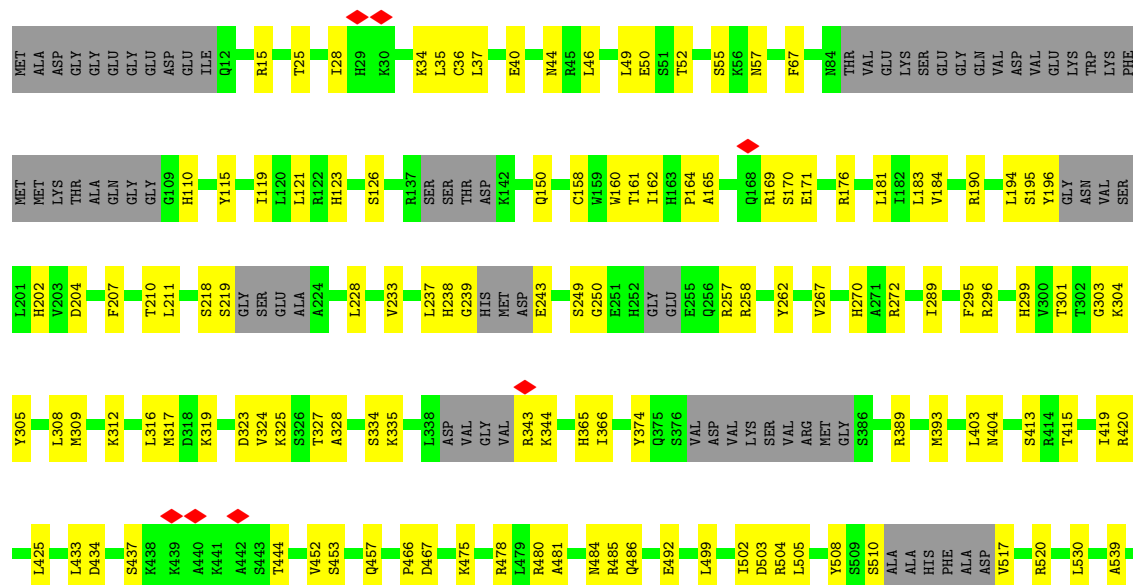
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PDB
PROTEIN DATA BANK





A2846	E2847	N2848	Y2849	H2850	N2851	I2852	W2853	A2854	K2855	K2856	K2857	K2858	L2859	E2860	L2861	E2862	S2863	K2864	G2865	G2866	G2867	N2868	H2869	P2870	L2871	L2872	V2873	P2874	Y2875	T2877	L2878	T2879	A2880	K2881	E2882	K2883	A2884	K2885	D2886	K2887	E2888	K2889	A2890	Q2891	D2892	L2893	L2894	K2895	F2896	L2897	Q2898	I2899	N2900	G2901	Y2902	A2903	V2904	S2905
W2786	G2787	W2788	R2789	I2790	E2791	R2792	T2793	R2794	E2795	G2796	D2797	SER	MET	ALA	LEU	TYR	ASN	ARG	THR	ARG	ARG	ILE	SER	GLN	THR	SER	GLN	VAL	VAL	ASP	A2818	A2819	H2820	G2821	V2822	S2823	P2824	R2825	A2826	T2827	D2828	W2829	S2830	N2831	V2832	T2833	L2834	S2835	R2836	D2837	L2838	H2839	K2840	W2841	A2842	E2843	N2844	W2845
A2726	E2727	H2728	S2729	D2730	D2731	K2732	W2733	S2734	M2735	D2736	K2737	L2738	A2739	N2740	G2741	W2742	I2743	Y2744	G2745	E2746	I2747	Y2748	S2749	D2750	S2751	S2752	K2753	V2754	Q2755	P2756	L2757	M2758	K2759	P2760	Y2761	K2762	L2763	L2764	S2765	E2766	K2767	E2768	K2769	E2770	I2771	Y2772	R2773	W2774	P2775	I2776	K2777	E2778	S2779	L2780	T2782	M2783	L2784	A2785
R2643	K2644	G2648	L2653	SER	GLN	LYS	LYS	LYS	Y2658	P2679	ASP	TYR	MET	GLU	SER	ASN	VAL	SER	MET	GLU	LYS	GLN	SER	SER	MET	ASP	SER	GLU	GLY	W2701	F2702	N2703	P2704	Q2705	P2706	V2707	D2708	T2709	S2710	N2711	I2712	T2713	L2714	P2715	E2716	K2717	L2718	E2719	Y2720	F2721	N2723	K2724	Y2725					
R2421	S2422	I2423	P2429	L2433	V2434	W2435	V2436	S2438	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP	GLY	VAL	VAL	GLU	PRO	ASP	MET	ALA	GLY	F2461	D2464	H2465	R2475	V2476	Y2477	GLY	ILE	GLU	V2481	Q2482	L2485	L2503	ASP	THR	ALA	ALA	LEU	SER	PHE	GLY	ALA	T2511	A2514	L2515								
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R2643	K2644	G2648	L2653	SER	GLN	LYS	LYS	LYS	Y2658	P2679	ASP	TYR	MET	GLU	SER	ASN	VAL	SER	MET	GLU	LYS	GLN	SER	SER	MET	ASP	SER	GLU	GLY	W2701	F2702	N2703	P2704	Q2705	P2706	V2707	D2708	T2709	S2710	N2711	I2712	T2713	L2714	P2715	E2716	K2717	L2718	E2719	Y2720	F2721	N2723	K2724	Y2725					
A2726	E2727	H2728	S2729	D2730	D2731	K2732	W2733	S2734	M2735	D2736	K2737	L2738	A2739	N2740	G2741	W2742	I2743	Y2744	G2745	E2746	I2747	Y2748	S2749	D2750	S2751	S2752	K2753	V2754	Q2755	P2756	L2757	M2758	K2759	P2760	Y2761	K2762	L2763	L2764	S2765	E2766	K2767	E2768	K2769	E2770	I2771	Y2772	R2773	W2774	P2775	I2776	K2777	E2778	S2779	L2780	T2782	M2783	L2784	A2785
W2786	G2787	W2788	R2789	I2790	E2791	R2792	T2793	R2794	E2795	G2796	D2797	SER	MET	ALA	LEU	TYR	ASN	ARG	THR	ARG	ARG	ILE	SER	GLN	THR	SER	GLN	VAL	VAL	ASP	A2818	A2819	H2820	G2821	V2822	S2823	P2824	R2825	A2826	T2827	D2828	W2829	S2830	N2831	V2832	T2833	L2834	S2835	R2836	D2837	L2838	H2839	K2840	W2841	A2842	E2843	N2844	W2845
A2846	E2847	N2848	Y2849	H2850	N2851	I2852	W2853	A2854	K2855	K2856	K2857	K2858	L2859	E2860	L2861	E2862	S2863	K2864	G2865	G2866	G2867	N2868	H2869	P2870	L2871	L2872	V2873	P2874	Y2875	T2877	L2878	T2879	A2880	K2881	E2882	K2883	A2884	K2885	D2886	K2887	E2888	K2889	A2890	Q2891	D2892	L2893	L2894	K2895	F2896	L2897	Q2898	I2899	N2900	G2901	Y2902	A2903	V2904	S2905
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Y1703	D1704	L1705	I1709	S1712	S1713	A1715	R1718	L1719	N1722	P1728	M1729	T1730	I1736	L1738	D1741	GLU	ASN	GLY	LYS	PRO	GLU	HIS	G1747	I1751	G1752	L1753	S1756	L1757	R1758	P1759	P1766	S1767	F1768	V1769	S1770	G1775	Y1776	Q1777	Y1778	D1785	E1690	N1691	K1790	M1794	V1799													
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L1904	L1905	C1908	Q1918	H1921	R1922	A1925	A1928	Q1938	Q1941	R1944	Y1945	N1953	MET	SER	ALA	LEU	THR	ALA	ARG	LYS	THR	LYS	PHE	ARG	SER	PRO	PRO	GLN	GLN	ILE	ASN	MET	LEU	LEU	ASN	PHE	LYS	ASP	L2081																			
L1989	K1990	D2013	ASP	GLY	SER	LEU	ASP	GLY	GLY	ASP	L2024	L2025	R2029	V2037	T2038	Y2039	LYS	LYS	LYS	GLN	ALA	GLU	VAL	GLU	SER	GLY	ASP	LYS	LYS	PHE	ARG	SER	PRO	GLN	GLU	GLN	ILE	ASN	MET	LEU	ASN	PHE	LYS	ASP	GLY													
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N2196	F2204	N2211	K2213	V2228	GLY	LEU	ALA	SER	PRO	ALA	MET	ARG	GLY	SER	ASP	GLN	CYS	GLN	PRO	MET	THR	L2283	L2275	SER	CYS	GLN	GLY	VAL	LYS	GLY	TYR	ASP	PRO	ILE	ILE	GLY	TRP	ASN	F2308	S2313	R2323	I2326	R2327	R2328	F2329	E2330	CYS											
PHE	GLY	PRO	ALA	LEU	ARG	GLY	GLY	GLY	ASN	G2343	I2354	ALA	GLU	ASP	PRO	GLY	PRO	SER	ARG	ASP	GLY	PRO	VAL	GLU	THR	SER	GLY	GLY	LYS	MET	PRO	ASP	THR	GLY	ASP	THR	ILE	HIS	MET	G2386	T2391	R2402	G2403	A2404	L2409	H2411	A2412	I2418										
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R2643	K2644	G2648	L2653	SER	GLN	LYS	LYS	LYS	Y2658	P2679	ASP	TYR	MET	GLU	SER	ASN	VAL	SER	MET	GLU	LYS	GLN	SER	SER	MET	ASP	SER	GLU	GLY	W2701	F2702	N2703	P2704	Q2705	P2706	V2707	D2708	T2709	S2710	N2711	I2712	T2713	L2714	P2715	E2716	K2717	L2718	E2719	Y2720	F2721	N2723	K2724	Y2725					
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W2786	G2787	W2788	R2789	I2790	E2791	R2792	T2793	R2794	E2795	G2796	D2797	SER	MET	ALA	LEU	TYR	ASN	ARG	THR	ARG	ARG	ILE	SER	GLN	THR	SER	GLN	VAL	VAL	ASP	A2818	A2819	H2820	G2821	V2822	S2823	P2824	R2825	A2826	T2827	D2828	W2829	S2830	N2831	V2832	T2833	L2834	S2835	R2836	D2837	L2838	H2839	K2840	W2841	A2842	E2843	N2844	W2845
A2846	E2847	N2848	Y2849	H2850	N2851	I2852	W2853	A2854	K2855	K2856	K2857	K2858	L2859	E2860	L2861	E2862	S2863	K2864	G2865	G2866	G2867	N2868	H2869	P2870	L2871	L2872	V2873	P2874	Y2875	T2877	L2878	T2879	A2880	K2881	E2882	K2883	A2884	K2885	D2886	K2887	E2888	K2889	A2890	Q2891	D2892	L2893	L2894	K2895	F2896	L2897	Q2898	I2899	N2900	G2901	Y2902	A2903	V2904	S2905

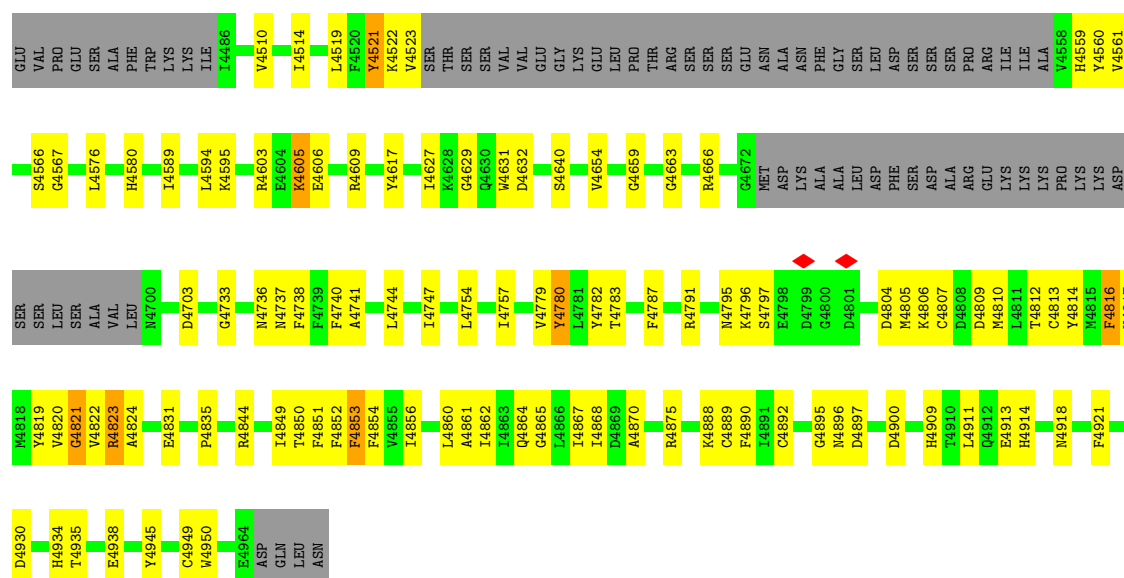




D566	M678	G777	I965	H956	I196	E1104	D1196	LEU	ARG	ASP	GLY	W1596	Y1703
I559	V679	M778	S870	A957	P1203	T1109	P1203	LYS	VAL	TYR	GLN	S1597	I1709
S560	D680	F779	Q871	GLU	Q1203	A1110	Q1203	V1285	ASP	LEU	ARG	R1598	M1599
R561	H681	I784	L872	LYS	S1206	G1111	S1206	Q1293	ASP	GLN	ASN	P1600	S1712
R564	T682	L787	V873	VAL	V1209	R1114	V1209	M1300	LYS	THR	N1502	K1605	Y1714
L565	E683	F788	L874	LYS	A1210	V1115	A1210	F1301	ALA	ALA	E1506	A1715	A1715
E566	R694	F789	L874	MET	Q1211	G1116	Q1211	Y1302	THR	THR	I1507	S1609	R1718
A567	V695	L789	L874	LYS	V1212	R1119	V1212	R1303	LYS	LYS	V1510	R1610	L1719
S568	G696	P875	P876	LEU	G1213	R1119	G1213	L1304	PRO	PRO	V1511	S1612	L1722
I571	T700	S793	H877	PRO	R1214	C1122	R1214	C1310	GLU	PHE	ASP	E1613	M1722
V580	S704	G797	I881	LYS	K1219	Q1123	K1219	ALA	ASN	ASN	ALA	R1614	M1728
K590	P705	I798	N888	ASN	K1220	P1124	K1220	GLU	VAL	VAL	ALA	W1617	M1729
H593	Y706	K799	H890	Y970	V1221	E1127	V1221	GLU	VAL	GLU	SER	T1730	T1730
H604	P707	V800	R801	L972	S1222	L1128	S1222	PHE	LYS	LYS	G1516	V1619	V1619
H621	G708	R801	F802	T973	T1223	D1131	T1223	LYS	THR	THR	F1520	Q1620	Q1620
V625	G709	F802	L804	S974	K1225	D1131	K1225	THR	ALA	ALA	T1521	C1621	C1621
R626	G710	L804	V893	G975	Y1226	F1136	Y1226	SER	GLN	GLN	A1522	L1622	L1622
S627	E711	G805	V894	Y976	F1227	A1136	F1227	ALA	GLU	GLU	W1444	W1444	W1444
I632	E712	ARG	Q903	K977	T1228	F1137	T1228	GLY	LYS	LYS	W1445	W1445	W1445
L644	W713	HIS	P906	P978	L1232	A1142	L1232	ILE	PRO	PRO	T1447	T1447	T1447
G645	N716	GLY	P906	A979	Y1060	Q1143	Y1060	PRO	ARG	ARG	S1448	S1448	S1448
T646	G717	GLY	V907	A979	G1061	R1144	G1061	GLY	LEU	LEU	F1450	F1450	F1450
R647	V718	E810	R908	P980	Y1062	E1150	Y1062	ALA	LYS	LYS	L1450	L1450	L1450
L648	P815	F811	D909	M981	Y1063	E1150	Y1063	SER	GLN	GLN	F1450	F1450	F1450
V649	P816	K812	P909	D982	M1063	H1151	M1063	LEU	ARG	ARG	E1451	E1451	E1451
M650	L814	F813	H915	L983	E1065	Y1152	E1065	PHE	PHE	PHE	L1459	L1459	L1459
S653	S724	P815	P816	S984	A1066	G1153	A1066	PRO	LEU	LEU	ASP	ASP	ASP
M655	Y725	P816	P817	F985	PRO	W1156	PRO	ASN	LEU	LEU	ARG	ARG	ARG
R656	G726	L814	P817	P986	ASP	G1163	ASP	ASP	THR	THR	VAL	VAL	VAL
P657	L730	L814	P817	K987	ASP	M1249	M1249	LEU	LYS	LYS	THR	THR	THR
M658	L731	L814	P817	T988	ASP	W1250	W1250	GLU	PRO	PRO	ASP	ASP	ASP
I659	L732	L814	P817	T989	ALA	M1165	M1165	ASP	THR	THR	ASP	ASP	ASP
F660	L733	L814	P817	P990	ALA	V1166	V1166	ASP	TYR	TYR	ASP	ASP	ASP
L661	L734	L814	P817	S991	ARG	D1167	D1167	ASP	ALA	ALA	ASP	ASP	ASP
G662	L735	L814	P817	Q992	ALA	H1171	R1254	PHE	THR	THR	ASP	ASP	ASP
VAL	L736	L814	P817	E993	GLU	T1172	L1255	VAL	ALA	ALA	ASP	ASP	ASP
SER	L737	L814	P817	A994	VAL	M1173	Q1257	GLU	ASP	ASP	ASP	ASP	ASP
GLY	L738	L814	P817	M995	CYS	M1174	F1258	THR	ASP	ASP	ASP	ASP	ASP
ALA	L739	L814	P817	Q927	GLY	F1175	H1265	LEU	ALA	ALA	ASP	ASP	ASP
GLN	L740	L814	P817	Y931	THR	L1177	H1267	VAL	ARG	ARG	ASP	ASP	ASP
TYR	L741	L814	P817	E338	GLY	L1182	R1272	LEU	LEU	LEU	THR	THR	THR
K671	L742	L814	P817	T939	GLU	L1183	I1273	MET	GLU	GLU	ASP	ASP	ASP
K672	L743	L814	P817	L940	ALA	D1184	D1274	LYS	VAL	VAL	ASP	ASP	ASP
ALA	L745	L814	P817	L943	ALA	D1185	GLY	THR	ALA	ALA	THR	THR	THR
ALA	L759	L814	P817	L943	ALA	L1190	ILE	GLY	ALA	ALA	ASP	ASP	ASP
GLN	D760	L814	P817	L943	ALA	A1191	THR	GLY	ASP	ASP	ASP	ASP	ASP
K671	I766	L814	P817	L946	ALA	K1193	ASP	LEU	THR	THR	ASP	ASP	ASP
K672	S767	L814	P817	G947	ALA	D1194	SER	VAL	ASP	ASP	ASP	ASP	ASP
W673	S767	L814	P817	C948	ALA	W1101	SER	VAL	ASP	ASP	ASP	ASP	ASP
Y674	Q773	L814	P817	H949	ALA	Y1102	CYS	PRO	PRO	PRO	PRO	PRO	PRO
	Q776	L814	P817	G951	ALA	F1195	GLY	ASP	TYR	TYR	TYR	TYR	TYR
		L814	P817	I952	ALA		GLY	ASP	TYR	TYR	TYR	TYR	TYR
		L814	P817	S953	ALA		GLY	ASP	TYR	TYR	TYR	TYR	TYR
		L814	P817	D954	ALA		GLY	ASP	TYR	TYR	TYR	TYR	TYR
		L814	P817	E955	ALA		GLY	ASP	TYR	TYR	TYR	TYR	TYR

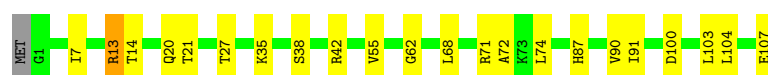
WORLDWIDE
PDB
PROTEIN DATA BANK





• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain B: 79% 19% ..



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 79% 19% ..



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 80% 19% ..



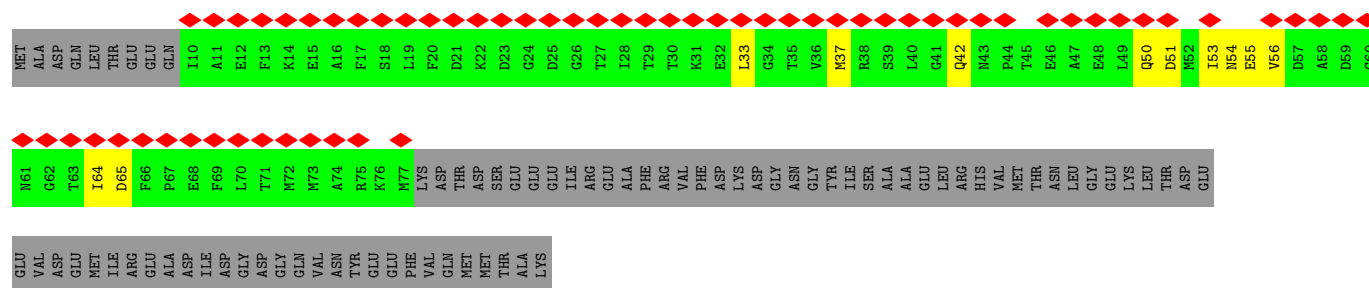
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain K: 80% 19% ..

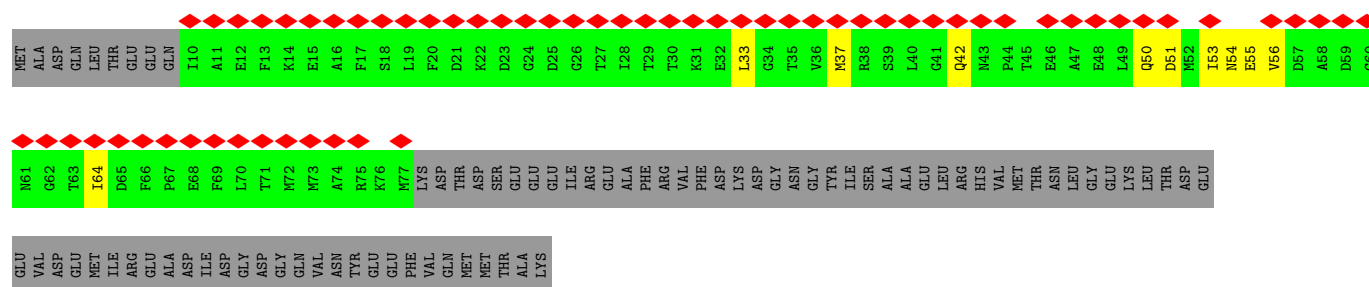
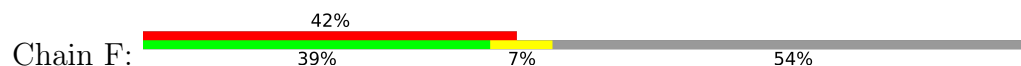


• Molecule 3: Calmodulin-1

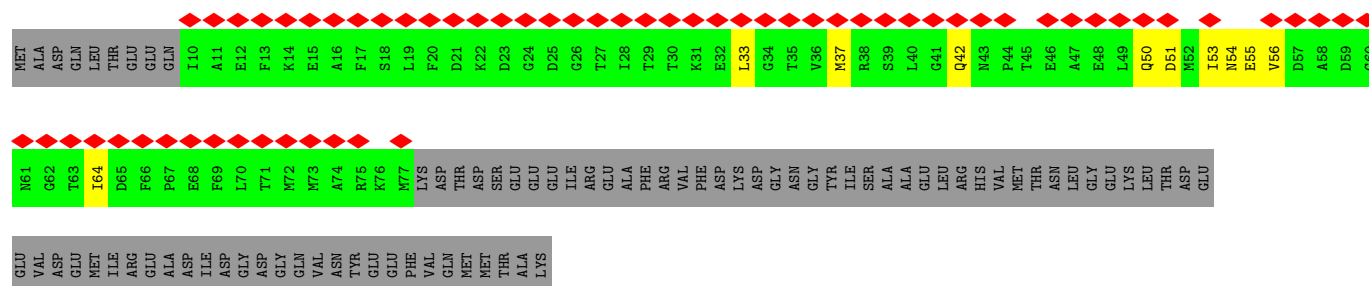
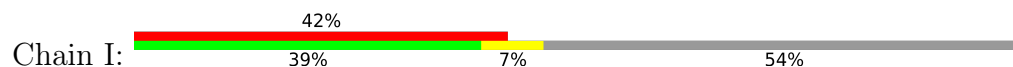
Chain C: 42% 38% 7% 54%



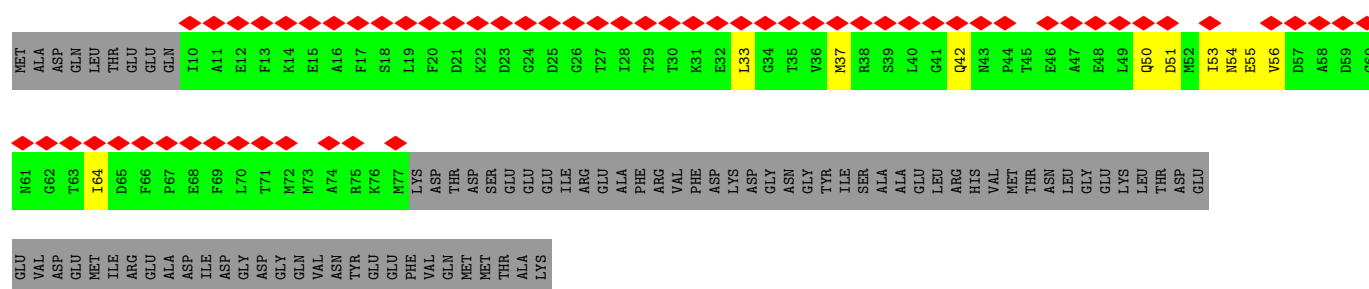
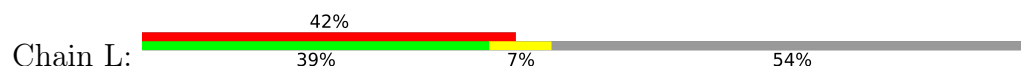
• Molecule 3: Calmodulin-1



• Molecule 3: Calmodulin-1



• Molecule 3: Calmodulin-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	77092	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.023	Depositor
Map size (\AA)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.338, 1.338, 1.338	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.35	2/27161 (0.0%)	0.55	7/36737 (0.0%)
1	D	0.34	0/27161	0.55	9/36737 (0.0%)
1	G	0.34	0/27161	0.55	5/36737 (0.0%)
1	J	0.34	0/27161	0.55	6/36737 (0.0%)
2	B	0.33	0/835	0.53	0/1123
2	E	0.33	0/835	0.53	0/1123
2	H	0.33	0/835	0.53	0/1123
2	K	0.33	0/835	0.53	0/1123
3	C	0.29	0/530	0.49	0/711
3	F	0.29	0/530	0.49	0/711
3	I	0.29	0/530	0.49	0/711
3	L	0.29	0/530	0.49	0/711
All	All	0.34	2/114104 (0.0%)	0.55	27/154284 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	23
1	D	0	23
1	G	0	23
1	J	0	23
All	All	0	92

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4521	TYR	N-CA	7.55	1.61	1.46
1	A	4522	LYS	CA-C	-6.22	1.36	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4823	ARG	N-CA-C	10.38	139.02	111.00
1	D	4823	ARG	CB-CA-C	-7.98	94.43	110.40
1	A	730	LEU	CA-CB-CG	6.89	131.16	115.30
1	D	730	LEU	CA-CB-CG	6.89	131.16	115.30
1	G	730	LEU	CA-CB-CG	6.89	131.16	115.30
1	J	730	LEU	CA-CB-CG	6.89	131.16	115.30
1	A	4522	LYS	N-CA-CB	-6.62	98.69	110.60
1	A	2326	ILE	CB-CA-C	5.51	122.62	111.60
1	G	2326	ILE	CB-CA-C	5.51	122.62	111.60
1	A	4821	GLY	N-CA-C	-5.44	99.49	113.10
1	G	2130	LEU	CA-CB-CG	5.42	127.77	115.30
1	A	3984	LEU	CA-CB-CG	5.42	127.75	115.30
1	D	3984	LEU	CA-CB-CG	5.42	127.75	115.30
1	G	3984	LEU	CA-CB-CG	5.42	127.75	115.30
1	J	3984	LEU	CA-CB-CG	5.42	127.75	115.30
1	D	2130	LEU	CA-CB-CG	5.41	127.74	115.30
1	A	2130	LEU	CA-CB-CG	5.40	127.73	115.30
1	J	2130	LEU	CA-CB-CG	5.40	127.73	115.30
1	J	4521	TYR	CB-CA-C	-5.36	99.68	110.40
1	D	4823	ARG	N-CA-CB	-5.18	101.28	110.60
1	J	4821	GLY	N-CA-C	-5.14	100.25	113.10
1	D	4822	VAL	CB-CA-C	5.08	121.06	111.40
1	A	1128	LEU	CA-CB-CG	5.04	126.90	115.30
1	D	1128	LEU	CA-CB-CG	5.04	126.90	115.30
1	G	1128	LEU	CA-CB-CG	5.04	126.90	115.30
1	J	1128	LEU	CA-CB-CG	5.04	126.90	115.30
1	D	2326	ILE	CB-CA-C	5.00	121.60	111.60

There are no chirality outliers.

All (92) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1127	GLU	Peptide
1	A	1447	THR	Peptide
1	A	1579	VAL	Peptide
1	A	1596	TRP	Peptide
1	A	1635	GLU	Peptide
1	A	1759	PRO	Peptide
1	A	1775	CYS	Peptide
1	A	1808	ASP	Peptide
1	A	1809	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	A	1847	GLU	Peptide
1	A	2037	VAL	Peptide
1	A	2429	PRO	Peptide
1	A	295	PHE	Peptide
1	A	3829	LYS	Peptide
1	A	4074	ASP	Peptide
1	A	4091	PRO	Peptide
1	A	728	ASP	Peptide
1	A	729	GLY	Peptide
1	A	739	ARG	Peptide
1	A	816	PRO	Peptide
1	A	817	PRO	Peptide
1	A	838	ARG	Peptide
1	A	841	LYS	Peptide
1	D	1127	GLU	Peptide
1	D	1447	THR	Peptide
1	D	1579	VAL	Peptide
1	D	1596	TRP	Peptide
1	D	1635	GLU	Peptide
1	D	1759	PRO	Peptide
1	D	1775	CYS	Peptide
1	D	1808	ASP	Peptide
1	D	1809	PRO	Peptide
1	D	1847	GLU	Peptide
1	D	2037	VAL	Peptide
1	D	2429	PRO	Peptide
1	D	295	PHE	Peptide
1	D	3829	LYS	Peptide
1	D	4074	ASP	Peptide
1	D	4091	PRO	Peptide
1	D	728	ASP	Peptide
1	D	729	GLY	Peptide
1	D	739	ARG	Peptide
1	D	816	PRO	Peptide
1	D	817	PRO	Peptide
1	D	838	ARG	Peptide
1	D	841	LYS	Peptide
1	G	1127	GLU	Peptide
1	G	1447	THR	Peptide
1	G	1579	VAL	Peptide
1	G	1596	TRP	Peptide
1	G	1635	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	G	1759	PRO	Peptide
1	G	1775	CYS	Peptide
1	G	1808	ASP	Peptide
1	G	1809	PRO	Peptide
1	G	1847	GLU	Peptide
1	G	2037	VAL	Peptide
1	G	2429	PRO	Peptide
1	G	295	PHE	Peptide
1	G	3829	LYS	Peptide
1	G	4074	ASP	Peptide
1	G	4091	PRO	Peptide
1	G	728	ASP	Peptide
1	G	729	GLY	Peptide
1	G	739	ARG	Peptide
1	G	816	PRO	Peptide
1	G	817	PRO	Peptide
1	G	838	ARG	Peptide
1	G	841	LYS	Peptide
1	J	1127	GLU	Peptide
1	J	1447	THR	Peptide
1	J	1579	VAL	Peptide
1	J	1596	TRP	Peptide
1	J	1635	GLU	Peptide
1	J	1759	PRO	Peptide
1	J	1775	CYS	Peptide
1	J	1808	ASP	Peptide
1	J	1809	PRO	Peptide
1	J	1847	GLU	Peptide
1	J	2037	VAL	Peptide
1	J	2429	PRO	Peptide
1	J	295	PHE	Peptide
1	J	3829	LYS	Peptide
1	J	4074	ASP	Peptide
1	J	4091	PRO	Peptide
1	J	728	ASP	Peptide
1	J	729	GLY	Peptide
1	J	739	ARG	Peptide
1	J	816	PRO	Peptide
1	J	817	PRO	Peptide
1	J	838	ARG	Peptide
1	J	841	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	26661	0	25136	600	0
1	D	26661	0	25136	589	0
1	G	26661	0	25136	605	0
1	J	26661	0	25136	598	0
2	B	819	0	824	15	0
2	E	819	0	824	15	0
2	H	819	0	824	14	0
2	K	819	0	824	14	0
3	C	524	0	504	8	0
3	F	524	0	504	7	0
3	I	524	0	504	7	0
3	L	524	0	504	7	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	A	1	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
5	F	2	0	0	0	0
5	G	1	0	0	0	0
5	I	2	0	0	0	0
5	J	1	0	0	0	0
5	L	2	0	0	0	0
6	A	31	0	12	0	0
6	D	31	0	12	0	0
6	G	31	0	12	0	0
6	J	31	0	12	0	0
7	A	14	0	10	1	0
7	D	14	0	10	1	0
7	G	14	0	10	1	0
7	J	14	0	10	1	0
All	All	112212	0	105944	2282	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 10.

All (2282) 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:A:4852:PHE:CZ	1:D:4823:ARG:HA	1.59	1.37
1:G:4861:ALA:CB	1:J:4864:GLN:HE21	1.53	1.22
1:D:4861:ALA:CB	1:G:4864:GLN:HE21	1.52	1.22
1:A:4861:ALA:CB	1:D:4864:GLN:HE21	1.52	1.21
1:A:4782:TYR:CD2	1:A:4851:PHE:CD1	2.30	1.20
1:A:4864:GLN:HE21	1:J:4861:ALA:CB	1.54	1.20
1:A:4861:ALA:HB1	1:D:4864:GLN:HE21	1.08	1.17
1:A:4782:TYR:HD2	1:A:4851:PHE:CE1	1.60	1.17
1:G:4782:TYR:HD2	1:G:4851:PHE:CE1	1.63	1.17
1:G:4782:TYR:CD2	1:G:4851:PHE:CD1	2.32	1.17
1:D:4782:TYR:CD2	1:D:4851:PHE:CD1	2.33	1.16
1:D:4782:TYR:HD2	1:D:4851:PHE:CE1	1.64	1.15
1:D:4861:ALA:HB1	1:G:4864:GLN:HE21	1.08	1.14
1:J:4782:TYR:CD2	1:J:4851:PHE:CD1	2.35	1.14
1:A:4822:VAL:HG12	1:J:4852:PHE:HE2	1.05	1.14
1:D:4787:PHE:HE2	1:G:4521:TYR:CE2	1.67	1.13
1:A:4521:TYR:CE2	1:J:4787:PHE:HE2	1.64	1.13
1:A:4861:ALA:HB1	1:D:4868:ILE:HD11	1.28	1.13
1:A:4787:PHE:HE2	1:D:4521:TYR:CE2	1.67	1.12
1:G:4787:PHE:HE2	1:J:4521:TYR:CE2	1.66	1.12
1:J:4782:TYR:HD2	1:J:4851:PHE:CE1	1.67	1.12
1:G:4852:PHE:HE2	1:J:4822:VAL:HG12	1.07	1.11
1:A:4868:ILE:HD11	1:J:4861:ALA:HB1	1.26	1.11
1:D:4852:PHE:HE2	1:G:4822:VAL:HG12	0.96	1.11
1:D:4852:PHE:CE2	1:G:4822:VAL:HG12	1.86	1.09
1:G:4861:ALA:HB1	1:J:4868:ILE:HD11	1.28	1.09
1:A:4864:GLN:HE21	1:J:4861:ALA:HB1	1.11	1.07
1:D:4861:ALA:HB1	1:G:4868:ILE:HD11	1.28	1.07
1:G:4861:ALA:HB1	1:J:4864:GLN:HE21	1.09	1.06
1:A:4852:PHE:CZ	1:D:4823:ARG:CA	2.37	1.06
1:A:4782:TYR:HD2	1:A:4851:PHE:CD1	1.71	1.03
1:G:4782:TYR:HD2	1:G:4851:PHE:CD1	1.74	1.03
1:J:4782:TYR:HD2	1:J:4851:PHE:CD1	1.75	1.03
1:G:4861:ALA:CB	1:J:4864:GLN:NE2	2.23	1.02
1:A:4822:VAL:HG12	1:J:4852:PHE:CE2	1.93	1.02
1:G:4852:PHE:CE2	1:J:4822:VAL:HG12	1.95	1.01
1:A:4861:ALA:CB	1:D:4864:GLN:NE2	2.22	1.01
1:D:4861:ALA:CB	1:G:4864:GLN:NE2	2.22	1.00
1:G:4782:TYR:CD2	1:G:4851:PHE:CE1	2.49	1.00
1:A:4782:TYR:CD2	1:A:4851:PHE:CE1	2.46	0.99
1:A:4852:PHE:CE1	1:D:4823:ARG:CA	2.45	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4864:GLN:NE2	1:J:4861:ALA:CB	2.25	0.99
1:D:4782:TYR:CD2	1:D:4851:PHE:CE1	2.51	0.99
1:D:4782:TYR:HD2	1:D:4851:PHE:CD1	1.74	0.99
1:A:4521:TYR:CE2	1:J:4787:PHE:CE2	2.51	0.99
1:G:4787:PHE:CE2	1:J:4521:TYR:CE2	2.53	0.96
1:D:4787:PHE:CE2	1:G:4521:TYR:CE2	2.53	0.96
1:J:4782:TYR:CD2	1:J:4851:PHE:CE1	2.54	0.96
1:A:4787:PHE:CE2	1:D:4521:TYR:CE2	2.53	0.95
1:D:4782:TYR:CD2	1:D:4851:PHE:HD1	1.81	0.95
1:A:4861:ALA:HB2	1:D:4864:GLN:NE2	1.82	0.94
1:G:4861:ALA:HB2	1:J:4864:GLN:NE2	1.82	0.94
1:J:4782:TYR:CD2	1:J:4851:PHE:HD1	1.82	0.94
1:A:4852:PHE:CE1	1:D:4823:ARG:HA	2.01	0.94
1:A:4523:VAL:HB	1:J:4791:ARG:HH22	1.32	0.94
1:A:4779:VAL:HG12	1:A:4851:PHE:HZ	1.33	0.94
1:D:4861:ALA:HB2	1:G:4864:GLN:NE2	1.82	0.93
1:A:4852:PHE:CE1	1:D:4823:ARG:O	2.22	0.93
1:A:4849:ILE:HD11	1:D:4819:TYR:CD1	2.04	0.93
1:D:4787:PHE:HE2	1:G:4521:TYR:HE2	1.12	0.93
1:G:4782:TYR:CD2	1:G:4851:PHE:HD1	1.81	0.93
1:A:4787:PHE:HE2	1:D:4521:TYR:HE2	1.12	0.92
1:A:4864:GLN:NE2	1:J:4861:ALA:HB2	1.83	0.92
1:D:4791:ARG:HH22	1:G:4523:VAL:HB	1.32	0.91
1:G:4791:ARG:HH21	1:J:4523:VAL:HG11	1.35	0.91
1:A:4791:ARG:HH22	1:D:4523:VAL:HB	1.33	0.91
1:A:207:PHE:CB	1:D:2326:ILE:HB	2.01	0.90
1:A:4521:TYR:HE2	1:J:4787:PHE:HE2	1.10	0.90
1:D:4791:ARG:HH21	1:G:4523:VAL:HG11	1.36	0.90
1:G:4791:ARG:HH22	1:J:4523:VAL:HB	1.31	0.90
1:A:2326:ILE:HB	1:J:207:PHE:CB	2.02	0.90
1:G:4779:VAL:HG12	1:G:4851:PHE:HZ	1.37	0.90
1:A:4782:TYR:CD2	1:A:4851:PHE:HD1	1.79	0.89
1:D:207:PHE:CB	1:G:2326:ILE:HB	2.02	0.89
1:G:4787:PHE:HE2	1:J:4521:TYR:HE2	1.12	0.88
1:A:4523:VAL:HG11	1:J:4791:ARG:HH21	1.37	0.88
1:G:207:PHE:CB	1:J:2326:ILE:HB	2.02	0.88
1:A:4779:VAL:HG12	1:A:4851:PHE:CZ	2.09	0.88
1:A:4791:ARG:HH21	1:D:4523:VAL:HG11	1.37	0.88
1:D:4779:VAL:HG12	1:D:4851:PHE:HZ	1.38	0.88
1:D:4845:ILE:HG23	1:G:4819:TYR:CD1	2.08	0.88
1:D:4861:ALA:CB	1:G:4868:ILE:HD11	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4868:ILE:HD11	1:J:4861:ALA:CB	2.03	0.87
1:J:4779:VAL:HG12	1:J:4851:PHE:HZ	1.39	0.87
1:A:4861:ALA:CB	1:D:4868:ILE:HD11	2.04	0.87
1:G:4861:ALA:CB	1:J:4868:ILE:HD11	2.04	0.86
1:A:4852:PHE:HE1	1:D:4823:ARG:O	1.58	0.85
1:G:4779:VAL:HG12	1:G:4851:PHE:CZ	2.12	0.85
1:G:4813:CYS:O	1:G:4817:HIS:HB2	1.77	0.84
1:J:4779:VAL:HG12	1:J:4851:PHE:CZ	2.13	0.84
1:D:4779:VAL:HG12	1:D:4851:PHE:CZ	2.12	0.84
1:D:4852:PHE:HE2	1:G:4822:VAL:CG1	1.88	0.83
1:A:4810:MET:CB	1:D:4521:TYR:O	2.26	0.83
1:G:4791:ARG:NH2	1:J:4523:VAL:HG11	1.93	0.83
1:D:4791:ARG:NH2	1:G:4523:VAL:HG11	1.94	0.83
1:A:4791:ARG:NH2	1:D:4523:VAL:HG11	1.94	0.81
1:A:4852:PHE:CZ	1:D:4822:VAL:O	2.34	0.80
1:A:4515:ASN:HB3	1:J:4780:TYR:OH	1.80	0.80
1:G:4777:VAL:O	1:G:4780:TYR:HD2	1.63	0.80
1:A:4523:VAL:HG11	1:J:4791:ARG:NH2	1.96	0.80
1:G:4736:ASN:OD1	1:G:4738:PHE:HD2	1.66	0.79
1:D:4736:ASN:OD1	1:D:4738:PHE:HD2	1.66	0.79
1:A:4822:VAL:CG1	1:J:4852:PHE:HE2	1.91	0.79
1:G:4791:ARG:HH22	1:J:4523:VAL:CB	1.94	0.79
1:D:4791:ARG:HH22	1:G:4523:VAL:CB	1.96	0.79
1:J:4736:ASN:OD1	1:J:4738:PHE:HD2	1.66	0.78
1:J:4822:VAL:C	1:J:4824:ALA:H	1.87	0.78
1:A:4813:CYS:O	1:A:4817:HIS:HB2	1.84	0.78
1:A:4736:ASN:OD1	1:A:4738:PHE:HD2	1.66	0.78
1:A:4849:ILE:HD11	1:D:4819:TYR:HA	1.66	0.78
1:A:4849:ILE:HD11	1:D:4819:TYR:HD1	1.47	0.77
1:A:4791:ARG:HH22	1:D:4523:VAL:CB	1.96	0.77
1:A:4864:GLN:HG2	1:A:4868:ILE:CD1	2.15	0.77
1:G:4864:GLN:HG2	1:G:4868:ILE:CD1	2.15	0.77
1:A:190:ARG:NH1	1:D:2423:ILE:HG23	1.99	0.77
1:A:4868:ILE:CD1	1:J:4861:ALA:HB1	2.12	0.77
1:D:4864:GLN:HG2	1:D:4868:ILE:CD1	2.15	0.77
1:A:2423:ILE:HG23	1:J:190:ARG:NH1	2.00	0.77
1:A:4861:ALA:HB1	1:D:4868:ILE:CD1	2.13	0.77
1:A:4523:VAL:CB	1:J:4791:ARG:HH22	1.96	0.76
1:A:4521:TYR:HE2	1:J:4787:PHE:CE2	1.98	0.76
1:J:4864:GLN:HG2	1:J:4868:ILE:CD1	2.15	0.76
1:D:190:ARG:NH1	1:G:2423:ILE:HG23	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:190:ARG:NH1	1:J:2423:ILE:HG23	2.01	0.76
1:G:4852:PHE:HE2	1:J:4822:VAL:CG1	1.92	0.76
1:G:4861:ALA:HB1	1:J:4864:GLN:NE2	1.93	0.75
1:A:4522:LYS:CB	1:J:4809:ASP:HA	2.16	0.75
1:A:4521:TYR:O	1:J:4810:MET:CB	2.34	0.75
1:D:4861:ALA:HB1	1:G:4868:ILE:CD1	2.13	0.75
1:J:4559:HIS:ND1	1:J:4738:PHE:CZ	2.55	0.75
1:D:4559:HIS:ND1	1:D:4738:PHE:CZ	2.55	0.74
1:G:4559:HIS:ND1	1:G:4738:PHE:CZ	2.55	0.74
1:A:4559:HIS:ND1	1:A:4738:PHE:CZ	2.55	0.74
1:D:4852:PHE:CE2	1:G:4823:ARG:HA	2.22	0.74
1:G:4791:ARG:NH2	1:J:4523:VAL:CG1	2.50	0.74
1:A:4822:VAL:C	1:A:4824:ALA:H	1.87	0.74
1:A:4864:GLN:NE2	1:J:4861:ALA:HB1	1.95	0.74
1:G:4809:ASP:HA	1:J:4522:LYS:CB	2.17	0.74
1:A:4809:ASP:HA	1:D:4522:LYS:CB	2.18	0.74
1:D:4852:PHE:CD2	1:G:4823:ARG:HA	2.23	0.73
1:G:4787:PHE:CE2	1:J:4521:TYR:HE2	2.00	0.73
1:A:4861:ALA:HB1	1:D:4864:GLN:NE2	1.92	0.73
1:D:4809:ASP:HA	1:G:4522:LYS:CB	2.18	0.73
1:D:4791:ARG:NH2	1:G:4523:VAL:CG1	2.51	0.73
1:G:4861:ALA:HB1	1:J:4868:ILE:CD1	2.14	0.73
2:B:21:THR:H	2:B:107:GLU:HB2	1.54	0.73
2:E:21:THR:H	2:E:107:GLU:HB2	1.54	0.72
2:K:21:THR:H	2:K:107:GLU:HB2	1.54	0.72
1:G:4791:ARG:NH2	1:J:4523:VAL:HB	2.04	0.72
2:H:21:THR:H	2:H:107:GLU:HB2	1.54	0.72
1:J:4864:GLN:HG2	1:J:4868:ILE:HD12	1.72	0.71
1:A:4791:ARG:NH2	1:D:4523:VAL:CG1	2.52	0.71
1:G:4864:GLN:HG2	1:G:4868:ILE:HD12	1.72	0.71
1:A:4523:VAL:CB	1:J:4791:ARG:NH2	2.54	0.71
1:A:4787:PHE:CE2	1:D:4521:TYR:HE2	2.00	0.71
1:D:4791:ARG:NH2	1:G:4523:VAL:HB	2.06	0.71
1:D:4861:ALA:HB1	1:G:4864:GLN:NE2	1.93	0.71
1:D:4845:ILE:HG23	1:G:4819:TYR:CE1	2.25	0.71
1:A:4822:VAL:O	1:A:4824:ALA:N	2.22	0.71
1:G:4791:ARG:NH2	1:J:4523:VAL:CB	2.53	0.71
1:J:4822:VAL:O	1:J:4824:ALA:N	2.22	0.71
1:A:4523:VAL:CG1	1:J:4791:ARG:NH2	2.52	0.71
1:J:4813:CYS:O	1:J:4817:HIS:HB2	1.90	0.71
1:A:4864:GLN:HG2	1:A:4868:ILE:HD12	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4864:GLN:HG2	1:D:4868:ILE:HD12	1.72	0.70
1:D:4814:TYR:O	1:D:4818:MET:N	2.24	0.70
1:D:4791:ARG:NH2	1:G:4523:VAL:CB	2.54	0.70
1:A:4849:ILE:CD1	1:D:4819:TYR:CD1	2.75	0.69
1:A:4791:ARG:NH2	1:D:4523:VAL:CB	2.55	0.69
1:A:4791:ARG:NH2	1:D:4523:VAL:HB	2.07	0.69
1:G:4807:CYS:SG	1:G:4816:PHE:CE2	2.85	0.68
1:G:4822:VAL:C	1:G:4824:ALA:H	1.96	0.68
1:A:4862:ILE:HG22	1:D:4868:ILE:HG12	1.76	0.68
1:G:4807:CYS:SG	1:G:4816:PHE:CD2	2.82	0.68
1:A:4523:VAL:HB	1:J:4791:ARG:NH2	2.05	0.68
1:A:4852:PHE:CE1	1:D:4823:ARG:C	2.66	0.68
1:D:4862:ILE:HG22	1:G:4868:ILE:HG12	1.76	0.68
1:A:4807:CYS:SG	1:A:4816:PHE:CD2	2.85	0.67
1:D:2025:THR:O	1:D:2029:ARG:NH1	2.27	0.67
1:A:2025:THR:O	1:A:2029:ARG:NH1	2.27	0.67
1:D:4787:PHE:CE2	1:G:4521:TYR:HE2	2.00	0.67
1:G:2025:THR:O	1:G:2029:ARG:NH1	2.27	0.67
1:G:4862:ILE:HG22	1:J:4868:ILE:HG12	1.77	0.66
1:J:1111:GLY:HA3	1:J:1211:GLN:HE21	1.60	0.66
1:G:1111:GLY:HA3	1:G:1211:GLN:HE21	1.60	0.66
1:J:2025:THR:O	1:J:2029:ARG:NH1	2.27	0.66
1:D:4810:MET:CB	1:G:4521:TYR:O	2.42	0.66
1:A:4829:GLY:HA3	1:D:4819:TYR:OH	1.94	0.66
1:J:4888:LYS:HA	1:J:4895:GLY:HA2	1.78	0.66
1:A:4888:LYS:HA	1:A:4895:GLY:HA2	1.78	0.65
1:D:4820:VAL:CG1	1:D:4831:GLU:OE2	2.44	0.65
1:A:4852:PHE:HZ	1:D:4822:VAL:O	1.80	0.65
1:J:233:VAL:HG21	1:J:413:SER:HB3	1.78	0.65
1:A:4797:SER:HB3	1:A:4805:MET:H	1.62	0.65
1:A:4849:ILE:CD1	1:D:4819:TYR:HD1	2.10	0.65
1:A:4819:TYR:CD1	1:J:4849:ILE:HD11	2.32	0.65
1:D:233:VAL:HG21	1:D:413:SER:HB3	1.78	0.65
1:A:4868:ILE:HG12	1:J:4862:ILE:HG22	1.78	0.65
1:A:1111:GLY:HA3	1:A:1211:GLN:HE21	1.60	0.65
1:D:1111:GLY:HA3	1:D:1211:GLN:HE21	1.60	0.65
1:D:4797:SER:HB3	1:D:4805:MET:H	1.62	0.65
1:G:4888:LYS:HA	1:G:4895:GLY:HA2	1.78	0.65
1:G:1173:MET:HB3	1:G:1192:PHE:HB2	1.79	0.64
1:G:4820:VAL:CG1	1:G:4831:GLU:HG3	2.27	0.64
1:D:1173:MET:HB3	1:D:1192:PHE:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:VAL:HG21	1:A:413:SER:HB3	1.78	0.64
1:D:4888:LYS:HA	1:D:4895:GLY:HA2	1.78	0.64
1:D:3993:ASN:HD22	1:D:4110:MET:HG3	1.62	0.64
1:A:3993:ASN:HD22	1:A:4110:MET:HG3	1.62	0.64
1:J:3993:ASN:HD22	1:J:4110:MET:HG3	1.62	0.64
1:A:681:HIS:HB2	1:A:799:LYS:HG2	1.80	0.64
1:A:2076:ILE:H	1:A:3667:GLN:HE22	1.45	0.64
1:J:4797:SER:HB3	1:J:4805:MET:H	1.62	0.64
1:D:1482:ARG:HH11	1:D:1531:TYR:HA	1.63	0.63
1:G:4797:SER:HB3	1:G:4805:MET:H	1.62	0.63
1:J:681:HIS:HB2	1:J:799:LYS:HG2	1.80	0.63
1:G:233:VAL:HG21	1:G:413:SER:HB3	1.78	0.63
1:J:1482:ARG:HH11	1:J:1531:TYR:HA	1.63	0.63
1:G:1645:THR:HG22	1:G:1695:PRO:HG3	1.81	0.63
1:G:3993:ASN:HD22	1:G:4110:MET:HG3	1.62	0.63
1:J:1241:VAL:HB	1:J:1807:ARG:HH22	1.64	0.63
1:A:1645:THR:HG22	1:A:1695:PRO:HG3	1.81	0.63
1:D:681:HIS:HB2	1:D:799:LYS:HG2	1.80	0.63
1:A:1241:VAL:HB	1:A:1807:ARG:HH22	1.63	0.63
2:E:87:HIS:H	2:E:91:ILE:HB	1.63	0.63
1:A:1482:ARG:HH11	1:A:1531:TYR:HA	1.63	0.63
1:G:681:HIS:HB2	1:G:799:LYS:HG2	1.80	0.63
1:J:1645:THR:HG22	1:J:1695:PRO:HG3	1.81	0.63
1:J:4736:ASN:OD1	1:J:4738:PHE:CD2	2.51	0.63
1:A:1173:MET:HB3	1:A:1192:PHE:HB2	1.79	0.63
1:D:2076:ILE:H	1:D:3667:GLN:HE22	1.45	0.63
1:J:2076:ILE:H	1:J:3667:GLN:HE22	1.45	0.63
1:J:4521:TYR:O	1:J:4521:TYR:CD2	2.51	0.63
1:A:4812:THR:O	1:A:4816:PHE:HB3	1.99	0.63
1:D:1645:THR:HG22	1:D:1695:PRO:HG3	1.81	0.63
1:D:4889:CYS:SG	1:D:4890:PHE:N	2.72	0.63
1:G:1482:ARG:HH11	1:G:1531:TYR:HA	1.63	0.63
1:G:4889:CYS:SG	1:G:4890:PHE:N	2.72	0.63
1:A:2323:ARG:O	1:A:2326:ILE:HG13	1.99	0.62
2:B:87:HIS:H	2:B:91:ILE:HB	1.63	0.62
1:G:2076:ILE:H	1:G:3667:GLN:HE22	1.45	0.62
1:G:2876:ASP:OD1	1:G:2876:ASP:N	2.31	0.62
1:G:1241:VAL:HB	1:G:1807:ARG:HH22	1.63	0.62
1:A:4736:ASN:OD1	1:A:4738:PHE:CD2	2.51	0.62
1:G:2323:ARG:O	1:G:2326:ILE:HG13	1.99	0.62
1:J:4889:CYS:SG	1:J:4890:PHE:N	2.72	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1442:TRP:HD1	1:A:1488:VAL:HG13	1.65	0.62
1:D:1241:VAL:HB	1:D:1807:ARG:HH22	1.63	0.62
1:J:1173:MET:HB3	1:J:1192:PHE:HB2	1.79	0.62
1:A:4807:CYS:SG	1:A:4816:PHE:CE2	2.89	0.62
1:D:802:PHE:HB2	1:D:1617:TRP:HB2	1.81	0.62
2:H:87:HIS:H	2:H:91:ILE:HB	1.63	0.62
1:G:802:PHE:HB2	1:G:1617:TRP:HB2	1.81	0.62
1:G:1442:TRP:HD1	1:G:1488:VAL:HG13	1.65	0.62
1:J:1442:TRP:HD1	1:J:1488:VAL:HG13	1.65	0.62
1:J:2323:ARG:O	1:J:2326:ILE:HG13	1.99	0.62
1:J:694:ARG:HB2	1:J:793:SER:HB2	1.82	0.62
1:G:694:ARG:HB2	1:G:793:SER:HB2	1.82	0.62
1:G:4820:VAL:O	1:G:4824:ALA:HB2	1.99	0.62
1:A:4889:CYS:SG	1:A:4890:PHE:N	2.72	0.61
1:A:802:PHE:HB2	1:A:1617:TRP:HB2	1.81	0.61
1:D:694:ARG:HB2	1:D:793:SER:HB2	1.82	0.61
1:G:1303:ARG:HH21	1:G:1595:LEU:HD13	1.64	0.61
2:K:87:HIS:H	2:K:91:ILE:HB	1.63	0.61
2:K:13:ARG:NH2	2:K:14:THR:OG1	2.34	0.61
1:D:4054:GLU:HG3	1:D:4061:GLN:HE21	1.66	0.61
1:A:4850:THR:O	1:A:4854:PHE:HB3	2.00	0.61
1:J:4812:THR:O	1:J:4816:PHE:HB3	2.00	0.61
1:A:694:ARG:HB2	1:A:793:SER:HB2	1.82	0.61
1:A:4849:ILE:HD11	1:D:4819:TYR:CA	2.31	0.61
1:D:2323:ARG:O	1:D:2326:ILE:HG13	1.99	0.61
1:D:1044:LYS:HA	1:D:1047:LYS:HB2	1.83	0.61
1:J:802:PHE:HB2	1:J:1617:TRP:HB2	1.81	0.61
1:A:1303:ARG:HH21	1:A:1595:LEU:HD13	1.64	0.61
1:D:1303:ARG:HH21	1:D:1595:LEU:HD13	1.64	0.61
1:D:1442:TRP:HD1	1:D:1488:VAL:HG13	1.65	0.61
1:D:1507:ILE:HB	1:D:1521:THR:HB	1.83	0.61
1:G:1044:LYS:HA	1:G:1047:LYS:HB2	1.83	0.61
2:H:13:ARG:NH2	2:H:14:THR:OG1	2.34	0.61
1:J:4056:HIS:O	1:J:4057:LYS:HG2	2.01	0.60
1:A:1507:ILE:HB	1:A:1521:THR:HB	1.82	0.60
1:A:4054:GLU:HG3	1:A:4061:GLN:HE21	1.66	0.60
1:D:4056:HIS:O	1:D:4057:LYS:HG2	2.01	0.60
1:A:797:GLY:HA2	1:A:1622:LEU:HA	1.84	0.60
1:A:4849:ILE:CD1	1:D:4819:TYR:HA	2.31	0.60
2:B:13:ARG:NH2	2:B:14:THR:OG1	2.34	0.60
1:J:1044:LYS:HA	1:J:1047:LYS:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4070:CYS:SG	1:D:4071:ALA:N	2.75	0.60
1:G:1507:ILE:HB	1:G:1521:THR:HB	1.82	0.60
1:J:797:GLY:HA2	1:J:1622:LEU:HA	1.84	0.60
1:J:1303:ARG:HH21	1:J:1595:LEU:HD13	1.64	0.60
1:D:415:THR:HG21	1:D:485:ARG:HG2	1.84	0.60
1:G:4054:GLU:HG3	1:G:4061:GLN:HE21	1.66	0.60
1:G:2204:PHE:O	1:G:2211:ASN:ND2	2.35	0.60
1:J:415:THR:HG21	1:J:485:ARG:HG2	1.84	0.60
1:A:4056:HIS:O	1:A:4057:LYS:HG2	2.01	0.60
1:J:4070:CYS:SG	1:J:4071:ALA:N	2.75	0.60
1:D:1089:ARG:NH1	1:D:1122:CYS:SG	2.75	0.60
1:J:4850:THR:O	1:J:4854:PHE:HB3	2.02	0.60
1:D:4007:SER:HG	1:D:4010:ASN:HD21	1.48	0.59
1:G:4812:THR:O	1:G:4816:PHE:HB3	2.02	0.59
1:G:4850:THR:O	1:G:4854:PHE:HB3	2.02	0.59
1:A:508:TYR:O	1:A:564:ARG:NH1	2.36	0.59
1:A:1044:LYS:HA	1:A:1047:LYS:HB2	1.83	0.59
1:A:3891:TRP:HE1	1:A:3950:HIS:HE1	1.50	0.59
1:J:2204:PHE:O	1:J:2211:ASN:ND2	2.35	0.59
1:D:508:TYR:O	1:D:564:ARG:NH1	2.35	0.59
2:E:13:ARG:NH2	2:E:14:THR:OG1	2.34	0.59
1:A:415:THR:HG21	1:A:485:ARG:HG2	1.84	0.59
1:G:1089:ARG:NH1	1:G:1122:CYS:SG	2.75	0.59
1:G:4736:ASN:OD1	1:G:4738:PHE:CD2	2.51	0.59
1:J:4054:GLU:HG3	1:J:4061:GLN:HE21	1.66	0.59
1:A:731:HIS:ND1	1:A:739:ARG:O	2.36	0.59
1:A:2528:LEU:HD11	1:A:2568:ASP:HA	1.85	0.59
1:D:731:HIS:ND1	1:D:739:ARG:O	2.36	0.59
1:D:4736:ASN:OD1	1:D:4738:PHE:CD2	2.51	0.59
1:G:731:HIS:ND1	1:G:739:ARG:O	2.36	0.59
1:G:3891:TRP:HE1	1:G:3950:HIS:HE1	1.50	0.59
1:J:2528:LEU:HD11	1:J:2568:ASP:HA	1.85	0.59
1:J:3891:TRP:HE1	1:J:3950:HIS:HE1	1.50	0.59
1:J:4822:VAL:C	1:J:4824:ALA:N	2.55	0.59
1:A:4777:VAL:O	1:A:4780:TYR:HD2	1.84	0.59
1:D:797:GLY:HA2	1:D:1622:LEU:HA	1.84	0.59
1:D:2204:PHE:O	1:D:2211:ASN:ND2	2.35	0.59
1:G:486:GLN:NE2	1:G:539:ALA:O	2.36	0.59
1:J:486:GLN:NE2	1:J:539:ALA:O	2.36	0.59
1:J:508:TYR:O	1:J:564:ARG:NH1	2.36	0.59
1:A:4515:ASN:CB	1:J:4780:TYR:OH	2.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:508:TYR:O	1:G:564:ARG:NH1	2.36	0.59
1:A:4070:CYS:SG	1:A:4071:ALA:N	2.75	0.59
1:G:4056:HIS:O	1:G:4057:LYS:HG2	2.01	0.59
1:A:888:ASN:ND2	1:A:957:ALA:O	2.33	0.59
1:D:207:PHE:CB	1:G:2326:ILE:CB	2.80	0.59
1:J:1507:ILE:HB	1:J:1521:THR:HB	1.82	0.59
1:D:4594:LEU:HB3	1:D:4595:LYS:HZ2	1.68	0.59
1:J:1089:ARG:NH1	1:J:1122:CYS:SG	2.75	0.59
1:A:2204:PHE:O	1:A:2211:ASN:ND2	2.35	0.58
1:A:4782:TYR:CE2	1:A:4851:PHE:CD1	2.87	0.58
1:D:486:GLN:NE2	1:D:539:ALA:O	2.36	0.58
1:G:415:THR:HG21	1:G:485:ARG:HG2	1.84	0.58
2:K:7:ILE:H	2:K:72:ALA:HA	1.68	0.58
1:A:2326:ILE:CB	1:J:207:PHE:CB	2.80	0.58
2:B:7:ILE:H	2:B:72:ALA:HA	1.68	0.58
1:D:3891:TRP:HE1	1:D:3950:HIS:HE1	1.50	0.58
1:G:797:GLY:HA2	1:G:1622:LEU:HA	1.84	0.58
1:G:4822:VAL:O	1:G:4824:ALA:N	2.36	0.58
1:A:3888:ASP:HA	1:A:3891:TRP:HB2	1.85	0.58
1:A:4783:THR:HG21	1:A:4814:TYR:HB2	1.85	0.58
1:J:4783:THR:HG21	1:J:4814:TYR:HB2	1.85	0.58
1:A:1089:ARG:NH1	1:A:1122:CYS:SG	2.75	0.58
1:D:4850:THR:O	1:D:4854:PHE:HB3	2.02	0.58
1:G:2528:LEU:HD11	1:G:2568:ASP:HA	1.85	0.58
1:J:731:HIS:ND1	1:J:739:ARG:O	2.36	0.58
1:A:486:GLN:NE2	1:A:539:ALA:O	2.36	0.58
1:G:4070:CYS:SG	1:G:4071:ALA:N	2.75	0.58
1:G:4663:GLY:H	1:G:4666:ARG:HD2	1.69	0.58
1:A:4819:TYR:HD1	1:J:4849:ILE:HD11	1.67	0.58
1:D:2528:LEU:HD11	1:D:2568:ASP:HA	1.85	0.58
1:A:258:ARG:NH1	1:A:317:MET:SD	2.77	0.58
1:D:3888:ASP:HA	1:D:3891:TRP:HB2	1.85	0.58
1:G:4864:GLN:HG2	1:G:4868:ILE:HD11	1.84	0.58
1:J:3939:SER:OG	1:J:3940:ARG:N	2.37	0.58
2:B:62:GLY:HA3	2:B:74:LEU:HD11	1.86	0.58
1:G:4782:TYR:CE2	1:G:4851:PHE:CD1	2.90	0.58
1:D:258:ARG:NH1	1:D:317:MET:SD	2.77	0.58
1:J:258:ARG:NH1	1:J:317:MET:SD	2.77	0.58
1:J:4594:LEU:HB3	1:J:4595:LYS:HZ2	1.68	0.58
1:J:4663:GLY:H	1:J:4666:ARG:HD2	1.69	0.58
1:J:4864:GLN:HG2	1:J:4868:ILE:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4782:TYR:CE2	1:D:4851:PHE:CD1	2.91	0.58
1:G:4852:PHE:CD2	1:J:4823:ARG:HA	2.39	0.58
1:J:4186:LYS:NZ	1:J:4890:PHE:O	2.37	0.58
1:J:267:VAL:HA	1:J:270:HIS:HB2	1.87	0.57
1:A:2262:ASP:OD1	1:A:2262:ASP:N	2.37	0.57
1:A:4864:GLN:HG2	1:A:4868:ILE:HD11	1.84	0.57
1:G:267:VAL:HA	1:G:270:HIS:HB2	1.86	0.57
1:G:700:THR:O	1:G:838:ARG:NH1	2.37	0.57
1:G:4186:LYS:NZ	1:G:4890:PHE:O	2.37	0.57
1:G:4782:TYR:CD2	1:G:4851:PHE:HE1	2.16	0.57
2:H:7:ILE:H	2:H:72:ALA:HA	1.68	0.57
1:J:195:SER:HB2	1:J:202:HIS:HB2	1.87	0.57
1:A:767:SER:HA	1:A:777:GLY:HA3	1.86	0.57
1:D:767:SER:HA	1:D:777:GLY:HA3	1.86	0.57
1:A:195:SER:HB2	1:A:202:HIS:HB2	1.87	0.57
1:A:4186:LYS:NZ	1:A:4890:PHE:O	2.37	0.57
1:D:3939:SER:OG	1:D:3940:ARG:N	2.37	0.57
2:E:62:GLY:HA3	2:E:74:LEU:HD11	1.86	0.57
1:D:1256:PRO:O	1:D:1451:HIS:ND1	2.36	0.57
1:D:4663:GLY:H	1:D:4666:ARG:HD2	1.69	0.57
2:E:7:ILE:H	2:E:72:ALA:HA	1.68	0.57
1:G:3888:ASP:HA	1:G:3891:TRP:HB2	1.85	0.57
1:J:3888:ASP:HA	1:J:3891:TRP:HB2	1.85	0.57
1:A:2876:ASP:OD1	1:A:2876:ASP:N	2.31	0.57
1:G:767:SER:HA	1:G:777:GLY:HA3	1.86	0.57
2:K:62:GLY:HA3	2:K:74:LEU:HD11	1.86	0.57
1:A:700:THR:O	1:A:838:ARG:NH1	2.37	0.57
1:D:4864:GLN:HG2	1:D:4868:ILE:HD11	1.84	0.57
1:G:2262:ASP:OD1	1:G:2262:ASP:N	2.37	0.57
1:G:3682:LYS:NZ	1:G:3683:LEU:O	2.38	0.57
1:J:767:SER:HA	1:J:777:GLY:HA3	1.86	0.57
1:A:1256:PRO:O	1:A:1451:HIS:ND1	2.36	0.57
1:D:3682:LYS:NZ	1:D:3683:LEU:O	2.38	0.57
1:G:258:ARG:NH1	1:G:317:MET:SD	2.77	0.57
1:J:1655:TYR:OH	1:J:1659:ARG:NH2	2.38	0.57
1:A:4782:TYR:CD2	1:A:4851:PHE:HE1	2.14	0.57
1:G:1655:TYR:OH	1:G:1659:ARG:NH2	2.38	0.57
1:G:2308:PHE:HA	1:G:2313:SER:HA	1.87	0.57
1:J:4782:TYR:CE2	1:J:4851:PHE:CD1	2.92	0.57
3:L:56:VAL:HG11	3:L:64:ILE:HG23	1.86	0.57
1:A:2308:PHE:HA	1:A:2313:SER:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4663:GLY:H	1:A:4666:ARG:HD2	1.69	0.56
1:D:195:SER:HB2	1:D:202:HIS:HB2	1.87	0.56
1:D:4783:THR:HG21	1:D:4814:TYR:HB2	1.85	0.56
1:G:195:SER:HB2	1:G:202:HIS:HB2	1.87	0.56
1:D:2192:LYS:O	1:D:2196:ASN:ND2	2.38	0.56
1:G:3939:SER:OG	1:G:3940:ARG:N	2.37	0.56
1:G:4796:LYS:NZ	1:G:4805:MET:O	2.38	0.56
1:A:267:VAL:HA	1:A:270:HIS:HB2	1.87	0.56
1:A:1676:LEU:HD23	1:A:1709:ILE:HD11	1.88	0.56
1:A:4566:SER:OG	1:A:4567:GLY:N	2.39	0.56
1:A:4796:LYS:NZ	1:A:4805:MET:O	2.38	0.56
1:D:267:VAL:HA	1:D:270:HIS:HB2	1.87	0.56
1:D:700:THR:O	1:D:838:ARG:NH1	2.37	0.56
3:F:56:VAL:HG11	3:F:64:ILE:HG23	1.86	0.56
1:G:207:PHE:CB	1:J:2326:ILE:CB	2.81	0.56
3:I:56:VAL:HG11	3:I:64:ILE:HG23	1.86	0.56
1:J:700:THR:O	1:J:838:ARG:NH1	2.37	0.56
1:J:1676:LEU:HD23	1:J:1709:ILE:HD11	1.88	0.56
1:J:4521:TYR:O	1:J:4521:TYR:CG	2.54	0.56
3:C:56:VAL:HG11	3:C:64:ILE:HG23	1.86	0.56
1:G:169:ARG:HH12	1:G:176:ARG:HB2	1.71	0.56
1:G:4783:THR:HG21	1:G:4814:TYR:HB2	1.85	0.56
1:A:2192:LYS:O	1:A:2196:ASN:ND2	2.38	0.56
2:H:62:GLY:HA3	2:H:74:LEU:HD11	1.86	0.56
1:D:1655:TYR:OH	1:D:1659:ARG:NH2	2.38	0.56
1:G:1445:TRP:O	1:G:1486:TYR:N	2.39	0.56
1:G:4566:SER:OG	1:G:4567:GLY:N	2.39	0.56
1:J:2192:LYS:O	1:J:2196:ASN:ND2	2.38	0.56
1:D:706:TYR:OH	1:D:1254:ARG:N	2.38	0.56
1:G:888:ASN:ND2	1:G:957:ALA:O	2.33	0.56
1:J:1445:TRP:O	1:J:1486:TYR:N	2.39	0.56
1:J:4007:SER:HG	1:J:4010:ASN:HD21	1.52	0.56
1:J:4796:LYS:NZ	1:J:4805:MET:O	2.38	0.56
1:A:1445:TRP:O	1:A:1486:TYR:N	2.39	0.56
1:D:1676:LEU:HD23	1:D:1709:ILE:HD11	1.87	0.56
1:J:2308:PHE:HA	1:J:2313:SER:HA	1.87	0.56
1:J:2262:ASP:OD1	1:J:2262:ASP:N	2.37	0.56
1:A:503:ASP:OD1	1:A:561:ARG:NH2	2.39	0.56
1:A:1272:ARG:NH1	1:A:1587:HIS:O	2.39	0.56
1:A:1655:TYR:OH	1:A:1659:ARG:NH2	2.38	0.56
1:A:3682:LYS:NZ	1:A:3683:LEU:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:ARG:HH12	1:D:176:ARG:HB2	1.71	0.56
1:D:903:GLN:NE2	1:D:974:SER:OG	2.39	0.56
1:D:2262:ASP:OD1	1:D:2262:ASP:N	2.37	0.56
1:J:4566:SER:OG	1:J:4567:GLY:N	2.39	0.56
1:A:207:PHE:CB	1:D:2326:ILE:CB	2.80	0.55
1:A:903:GLN:NE2	1:A:974:SER:OG	2.39	0.55
1:A:1728:PRO:HB2	1:A:1730:THR:HG23	1.88	0.55
1:D:2308:PHE:HA	1:D:2313:SER:HA	1.87	0.55
1:G:503:ASP:OD1	1:G:561:ARG:NH2	2.39	0.55
1:G:903:GLN:NE2	1:G:974:SER:OG	2.39	0.55
1:G:2192:LYS:O	1:G:2196:ASN:ND2	2.38	0.55
1:J:706:TYR:OH	1:J:1254:ARG:N	2.38	0.55
1:D:565:LEU:HD22	1:D:604:HIS:HE1	1.72	0.55
1:D:1445:TRP:O	1:D:1486:TYR:N	2.39	0.55
1:D:3800:SER:OG	1:D:3801:CYS:N	2.39	0.55
1:D:4777:VAL:O	1:D:4780:TYR:HD2	1.90	0.55
1:J:169:ARG:HH12	1:J:176:ARG:HB2	1.71	0.55
1:G:565:LEU:HD22	1:G:604:HIS:HE1	1.72	0.55
1:G:718:VAL:HA	1:G:736:CYS:H	1.71	0.55
1:G:1676:LEU:HD23	1:G:1709:ILE:HD11	1.87	0.55
1:J:1256:PRO:O	1:J:1451:HIS:ND1	2.36	0.55
1:J:2730:HIS:NE2	1:J:2759:LYS:O	2.40	0.55
1:J:4782:TYR:CD2	1:J:4851:PHE:HE1	2.21	0.55
1:A:169:ARG:HH12	1:A:176:ARG:HB2	1.71	0.55
1:A:718:VAL:HA	1:A:736:CYS:H	1.71	0.55
1:D:1272:ARG:NH1	1:D:1587:HIS:O	2.39	0.55
1:J:1728:PRO:HB2	1:J:1730:THR:HG23	1.88	0.55
1:D:4782:TYR:CD2	1:D:4851:PHE:HE1	2.18	0.55
1:J:503:ASP:OD1	1:J:561:ARG:NH2	2.39	0.55
1:A:499:LEU:HD12	1:A:502:ILE:HD12	1.89	0.55
1:A:674:TYR:HE2	1:A:814:LEU:HB2	1.72	0.55
1:G:804:LEU:HD13	1:G:832:LEU:HD11	1.88	0.55
1:J:1440:ASN:N	1:J:1490:ALA:O	2.40	0.55
1:J:1846:ILE:HG12	1:J:1894:LEU:HD23	1.89	0.55
1:J:4918:ASN:HA	1:J:4921:PHE:HD2	1.72	0.55
1:A:1011:ARG:HA	1:A:1014:GLN:HB3	1.89	0.55
1:A:3809:PHE:O	1:A:3812:GLN:NE2	2.37	0.55
1:D:503:ASP:OD1	1:D:561:ARG:NH2	2.39	0.55
1:A:2213:LYS:HG2	1:A:2254:LEU:HD11	1.89	0.55
1:D:674:TYR:HE2	1:D:814:LEU:HB2	1.72	0.55
2:E:20:GLN:HB3	2:E:107:GLU:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4594:LEU:HB3	1:G:4595:LYS:HZ2	1.70	0.55
1:J:565:LEU:HD22	1:J:604:HIS:HE1	1.72	0.55
1:J:1209:VAL:N	1:J:1211:GLN:OE1	2.40	0.55
1:J:3682:LYS:NZ	1:J:3683:LEU:O	2.38	0.55
1:A:1440:ASN:N	1:A:1490:ALA:O	2.40	0.55
1:A:1613:GLU:HB3	1:A:1618:LEU:H	1.72	0.55
1:A:3683:LEU:HD22	1:A:3748:SER:HB3	1.88	0.55
1:A:4835:PRO:HG3	1:A:4844:ARG:HE	1.72	0.55
1:D:499:LEU:HD12	1:D:502:ILE:HD12	1.89	0.55
1:D:734:SER:O	1:D:739:ARG:NH1	2.40	0.55
1:D:1219:LYS:H	1:D:1240:ALA:HB2	1.72	0.55
1:D:4845:ILE:CG2	1:G:4819:TYR:CD1	2.88	0.55
1:G:1756:SER:OG	1:G:1757:LEU:N	2.40	0.55
1:J:1011:ARG:HA	1:J:1014:GLN:HB3	1.89	0.55
1:A:565:LEU:HD22	1:A:604:HIS:HE1	1.72	0.55
1:A:940:LEU:HA	1:A:943:LEU:HB2	1.90	0.55
1:A:2730:HIS:NE2	1:A:2759:LYS:O	2.40	0.55
1:D:1440:ASN:N	1:D:1490:ALA:O	2.40	0.55
1:D:2876:ASP:OD1	1:D:2876:ASP:N	2.31	0.55
1:D:4835:PRO:HG3	1:D:4844:ARG:HE	1.72	0.55
1:G:1846:ILE:HG12	1:G:1894:LEU:HD23	1.89	0.55
1:G:3683:LEU:HD22	1:G:3748:SER:HB3	1.88	0.55
1:G:4777:VAL:O	1:G:4780:TYR:CD2	2.53	0.55
1:J:903:GLN:NE2	1:J:974:SER:OG	2.39	0.55
1:J:1736:ILE:HG23	1:J:1753:LEU:HD12	1.89	0.55
3:L:37:MET:HG3	3:L:42:GLN:HB3	1.89	0.55
1:A:1738:LEU:HD22	1:A:1925:ALA:HA	1.89	0.54
1:D:1756:SER:OG	1:D:1757:LEU:N	2.40	0.54
1:D:4566:SER:OG	1:D:4567:GLY:N	2.39	0.54
1:G:1440:ASN:N	1:G:1490:ALA:O	2.40	0.54
1:G:4835:PRO:HG3	1:G:4844:ARG:HE	1.72	0.54
1:J:718:VAL:HA	1:J:736:CYS:H	1.71	0.54
1:A:734:SER:O	1:A:739:ARG:NH1	2.40	0.54
1:A:1209:VAL:N	1:A:1211:GLN:OE1	2.40	0.54
1:A:2790:ILE:HG12	1:A:2904:VAL:HG13	1.90	0.54
1:A:4823:ARG:HA	1:J:4852:PHE:CD2	2.42	0.54
1:D:1846:ILE:HG12	1:D:1894:LEU:HD23	1.89	0.54
1:D:2213:LYS:HG2	1:D:2254:LEU:HD11	1.89	0.54
1:D:3683:LEU:HD22	1:D:3748:SER:HB3	1.88	0.54
1:D:4186:LYS:NZ	1:D:4890:PHE:O	2.37	0.54
1:G:674:TYR:HE2	1:G:814:LEU:HB2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1613:GLU:HB3	1:G:1618:LEU:H	1.72	0.54
1:G:2730:HIS:NE2	1:G:2759:LYS:O	2.40	0.54
2:H:20:GLN:HB3	2:H:107:GLU:H	1.72	0.54
1:J:1613:GLU:HB3	1:J:1618:LEU:H	1.72	0.54
1:J:2790:ILE:HG12	1:J:2904:VAL:HG13	1.90	0.54
1:J:4835:PRO:HG3	1:J:4844:ARG:HE	1.72	0.54
1:A:1846:ILE:HG12	1:A:1894:LEU:HD23	1.89	0.54
1:A:4605:LYS:NZ	1:A:4606:GLU:OE1	2.41	0.54
1:A:4918:ASN:HA	1:A:4921:PHE:HD2	1.72	0.54
1:D:718:VAL:HA	1:D:736:CYS:H	1.71	0.54
1:G:517:VAL:HG23	1:G:520:ARG:HE	1.73	0.54
1:G:680:ASP:HB2	1:G:799:LYS:HG3	1.90	0.54
1:G:706:TYR:OH	1:G:1254:ARG:N	2.38	0.54
1:G:1272:ARG:NH1	1:G:1587:HIS:O	2.39	0.54
1:G:4852:PHE:CE2	1:J:4823:ARG:HA	2.42	0.54
1:J:804:LEU:HD13	1:J:832:LEU:HD11	1.88	0.54
1:J:1272:ARG:NH1	1:J:1587:HIS:O	2.39	0.54
1:A:1736:ILE:HG23	1:A:1753:LEU:HD12	1.89	0.54
1:A:3781:TYR:HE1	1:A:3785:LYS:HD2	1.73	0.54
3:C:37:MET:HG3	3:C:42:GLN:HB3	1.89	0.54
1:D:1670:HIS:ND1	1:D:1778:TYR:O	2.41	0.54
1:G:940:LEU:HA	1:G:943:LEU:HB2	1.90	0.54
1:G:1219:LYS:H	1:G:1240:ALA:HB2	1.72	0.54
1:G:1728:PRO:HB2	1:G:1730:THR:HG23	1.88	0.54
1:J:517:VAL:HG23	1:J:520:ARG:HE	1.73	0.54
1:J:2213:LYS:HG2	1:J:2254:LEU:HD11	1.89	0.54
1:J:3781:TYR:HE1	1:J:3785:LYS:HD2	1.73	0.54
1:A:680:ASP:HB2	1:A:799:LYS:HG3	1.90	0.54
1:A:1756:SER:OG	1:A:1757:LEU:N	2.40	0.54
1:G:734:SER:O	1:G:739:ARG:NH1	2.40	0.54
1:G:1736:ILE:HG23	1:G:1753:LEU:HD12	1.89	0.54
1:G:2213:LYS:HG2	1:G:2254:LEU:HD11	1.89	0.54
1:G:3781:TYR:HE1	1:G:3785:LYS:HD2	1.73	0.54
1:J:4807:CYS:SG	1:J:4816:PHE:CE2	2.98	0.54
1:D:2730:HIS:NE2	1:D:2759:LYS:O	2.40	0.54
1:D:2790:ILE:HG12	1:D:2904:VAL:HG13	1.89	0.54
1:G:499:LEU:HD12	1:G:502:ILE:HD12	1.89	0.54
1:G:1011:ARG:HA	1:G:1014:GLN:HB3	1.89	0.54
1:J:499:LEU:HD12	1:J:502:ILE:HD12	1.88	0.54
1:A:4617:TYR:OH	1:A:4629:GLY:O	2.24	0.54
1:D:804:LEU:HD13	1:D:832:LEU:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3781:TYR:HE1	1:D:3785:LYS:HD2	1.73	0.54
1:J:1738:LEU:HD22	1:J:1925:ALA:HA	1.89	0.54
1:A:2553:VAL:O	1:A:2605:LYS:N	2.41	0.54
1:A:3939:SER:OG	1:A:3940:ARG:N	2.37	0.54
1:A:4044:ILE:HG13	1:A:4045:SER:H	1.73	0.54
2:B:20:GLN:HB3	2:B:107:GLU:H	1.72	0.54
1:D:1728:PRO:HB2	1:D:1730:THR:HG23	1.88	0.54
1:G:1209:VAL:N	1:G:1211:GLN:OE1	2.40	0.54
1:J:3800:SER:OG	1:J:3801:CYS:N	2.39	0.54
1:A:1219:LYS:H	1:A:1240:ALA:HB2	1.72	0.54
1:A:1670:HIS:ND1	1:A:1778:TYR:O	2.41	0.54
1:D:680:ASP:HB2	1:D:799:LYS:HG3	1.90	0.54
1:D:1738:LEU:HD22	1:D:1925:ALA:HA	1.89	0.54
1:D:3984:LEU:HA	1:D:3987:LEU:HD12	1.90	0.54
1:G:2402:ARG:O	1:G:2475:ARG:NH2	2.41	0.54
1:G:2790:ILE:HG12	1:G:2904:VAL:HG13	1.90	0.54
1:J:734:SER:O	1:J:739:ARG:NH1	2.40	0.54
1:A:4594:LEU:HB3	1:A:4595:LYS:HZ2	1.73	0.54
1:D:4780:TYR:OH	1:G:4515:ASN:HB3	2.07	0.54
1:G:2553:VAL:O	1:G:2605:LYS:N	2.41	0.54
1:J:3809:PHE:O	1:J:3812:GLN:NE2	2.37	0.54
1:D:4044:ILE:HG13	1:D:4045:SER:H	1.73	0.53
1:G:2434:VAL:O	1:G:2438:SER:OG	2.26	0.53
1:G:3809:PHE:O	1:G:3812:GLN:NE2	2.37	0.53
1:J:1756:SER:OG	1:J:1757:LEU:N	2.40	0.53
1:J:3683:LEU:HD22	1:J:3748:SER:HB3	1.88	0.53
1:J:4044:ILE:HG13	1:J:4045:SER:H	1.73	0.53
1:A:580:VAL:O	1:A:621:HIS:NE2	2.42	0.53
1:A:660:PHE:HB3	1:A:787:LEU:HD22	1.90	0.53
1:A:804:LEU:HD13	1:A:832:LEU:HD11	1.88	0.53
1:D:580:VAL:O	1:D:621:HIS:NE2	2.42	0.53
1:D:1011:ARG:HA	1:D:1014:GLN:HB3	1.89	0.53
1:D:1209:VAL:N	1:D:1211:GLN:OE1	2.40	0.53
1:G:4918:ASN:HA	1:G:4921:PHE:HD2	1.72	0.53
3:I:37:MET:HG3	3:I:42:GLN:HB3	1.89	0.53
1:A:4521:TYR:CD2	1:J:4787:PHE:CE2	2.95	0.53
1:D:2553:VAL:O	1:D:2605:LYS:N	2.41	0.53
1:G:1670:HIS:ND1	1:G:1778:TYR:O	2.41	0.53
1:G:4617:TYR:OH	1:G:4629:GLY:O	2.24	0.53
1:G:4822:VAL:C	1:G:4824:ALA:N	2.60	0.53
1:J:940:LEU:HA	1:J:943:LEU:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1670:HIS:ND1	1:J:1778:TYR:O	2.41	0.53
1:J:3984:LEU:HA	1:J:3987:LEU:HD12	1.90	0.53
1:J:4052:ALA:O	1:J:4056:HIS:ND1	2.39	0.53
2:K:20:GLN:HB3	2:K:107:GLU:H	1.72	0.53
1:A:2402:ARG:O	1:A:2475:ARG:NH2	2.41	0.53
1:D:3809:PHE:O	1:D:3812:GLN:NE2	2.37	0.53
1:D:4031:ASP:HA	1:D:4034:LYS:HB3	1.91	0.53
1:D:4605:LYS:NZ	1:D:4606:GLU:OE1	2.41	0.53
1:G:4605:LYS:NZ	1:G:4606:GLU:OE1	2.41	0.53
1:J:674:TYR:HE2	1:J:814:LEU:HB2	1.72	0.53
1:J:2116:ASP:OD2	1:J:2155:VAL:N	2.42	0.53
1:D:239:GLY:O	1:D:243:GLU:N	2.42	0.53
1:G:1738:LEU:HD22	1:G:1925:ALA:HA	1.89	0.53
1:G:4804:ASP:N	1:G:4804:ASP:OD1	2.42	0.53
1:A:1589:GLN:NE2	1:A:1634:GLU:OE1	2.42	0.53
1:A:2116:ASP:OD2	1:A:2155:VAL:N	2.42	0.53
1:D:833:LYS:HA	1:D:1614:ARG:HH22	1.74	0.53
1:D:1613:GLU:HB3	1:D:1618:LEU:H	1.72	0.53
1:D:4918:ASN:HA	1:D:4921:PHE:HD2	1.72	0.53
1:G:2644:LYS:O	1:G:2648:GLY:N	2.41	0.53
1:G:3984:LEU:HA	1:G:3987:LEU:HD12	1.90	0.53
1:J:239:GLY:O	1:J:243:GLU:N	2.42	0.53
1:J:657:PRO:HD2	1:J:790:PRO:HG2	1.90	0.53
1:J:680:ASP:HB2	1:J:799:LYS:HG3	1.90	0.53
1:J:888:ASN:ND2	1:J:957:ALA:O	2.33	0.53
1:J:1219:LYS:H	1:J:1240:ALA:HB2	1.72	0.53
1:A:650:ASN:HA	1:A:1626:GLN:HA	1.91	0.53
1:D:517:VAL:HG23	1:D:520:ARG:HE	1.73	0.53
1:D:657:PRO:HD2	1:D:790:PRO:HG2	1.90	0.53
1:D:1736:ILE:HG23	1:D:1753:LEU:HD12	1.89	0.53
1:G:1589:GLN:NE2	1:G:1634:GLU:OE1	2.42	0.53
1:G:4031:ASP:HA	1:G:4034:LYS:HB3	1.91	0.53
1:J:580:VAL:O	1:J:621:HIS:NE2	2.42	0.53
1:J:650:ASN:HA	1:J:1626:GLN:HA	1.91	0.53
1:J:833:LYS:HA	1:J:1614:ARG:HH22	1.74	0.53
1:J:2553:VAL:O	1:J:2605:LYS:N	2.41	0.53
1:A:239:GLY:O	1:A:243:GLU:N	2.42	0.53
1:A:833:LYS:HA	1:A:1614:ARG:HH22	1.74	0.53
1:A:2434:VAL:O	1:A:2438:SER:OG	2.26	0.53
1:A:4823:ARG:HA	1:J:4852:PHE:CE2	2.44	0.53
1:G:1256:PRO:O	1:G:1451:HIS:ND1	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2402:ARG:O	1:J:2475:ARG:NH2	2.41	0.53
1:J:4617:TYR:OH	1:J:4629:GLY:O	2.24	0.53
1:A:517:VAL:HG23	1:A:520:ARG:HE	1.73	0.53
1:A:657:PRO:HD2	1:A:790:PRO:HG2	1.90	0.53
1:A:1143:GLN:HA	1:A:1151:HIS:HA	1.91	0.53
1:D:1589:GLN:NE2	1:D:1634:GLU:OE1	2.42	0.53
1:D:2402:ARG:O	1:D:2475:ARG:NH2	2.41	0.53
1:G:170:SER:OG	1:G:171:GLU:N	2.42	0.53
1:G:890:HIS:NE2	1:G:919:VAL:O	2.42	0.53
1:G:4810:MET:CB	1:J:4519:LEU:O	2.57	0.53
1:J:1143:GLN:HA	1:J:1151:HIS:HA	1.91	0.53
1:J:4605:LYS:NZ	1:J:4606:GLU:OE1	2.41	0.53
1:G:580:VAL:O	1:G:621:HIS:NE2	2.42	0.53
1:G:650:ASN:HA	1:G:1626:GLN:HA	1.91	0.53
1:G:1172:THR:HG22	1:G:1193:LYS:HG3	1.91	0.53
1:G:4813:CYS:O	1:G:4817:HIS:N	2.38	0.53
1:J:776:GLN:HG2	1:J:1472:GLU:HA	1.91	0.53
1:A:776:GLN:HG2	1:A:1472:GLU:HA	1.91	0.52
1:D:660:PHE:HB3	1:D:787:LEU:HD22	1.90	0.52
1:D:776:GLN:HG2	1:D:1472:GLU:HA	1.91	0.52
1:D:940:LEU:HA	1:D:943:LEU:HB2	1.89	0.52
1:D:4796:LYS:NZ	1:D:4805:MET:O	2.38	0.52
3:F:37:MET:HG3	3:F:42:GLN:HB3	1.89	0.52
1:G:833:LYS:HA	1:G:1614:ARG:HH22	1.74	0.52
1:J:660:PHE:HB3	1:J:787:LEU:HD22	1.90	0.52
1:J:1589:GLN:NE2	1:J:1634:GLU:OE1	2.42	0.52
1:A:890:HIS:NE2	1:A:919:VAL:O	2.42	0.52
1:A:3984:LEU:HA	1:A:3987:LEU:HD12	1.90	0.52
1:D:453:SER:O	1:D:457:GLN:NE2	2.42	0.52
1:J:1172:THR:HG22	1:J:1193:LYS:HG3	1.91	0.52
1:J:2883:LYS:O	1:J:2887:ARG:N	2.42	0.52
1:A:1114:ARG:HB3	1:A:1128:LEU:HD22	1.92	0.52
1:D:678:MET:HB3	1:D:801:ARG:HB2	1.91	0.52
1:D:888:ASN:ND2	1:D:957:ALA:O	2.33	0.52
1:G:239:GLY:O	1:G:243:GLU:N	2.42	0.52
1:G:4044:ILE:HG13	1:G:4045:SER:H	1.73	0.52
1:G:4787:PHE:CE2	1:J:4521:TYR:CD2	2.97	0.52
1:J:28:ILE:HG12	1:J:196:TYR:HE1	1.74	0.52
1:J:1114:ARG:HB3	1:J:1128:LEU:HD22	1.92	0.52
1:A:4052:ALA:O	1:A:4056:HIS:ND1	2.39	0.52
1:A:4780:TYR:OH	1:D:4741:ALA:HB1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4782:TYR:CE2	1:A:4851:PHE:HD1	2.25	0.52
1:A:4852:PHE:CD1	1:D:4823:ARG:CB	2.93	0.52
1:D:237:LEU:HB3	1:D:404:ASN:HB3	1.91	0.52
1:D:650:ASN:HA	1:D:1626:GLN:HA	1.91	0.52
1:D:1171:HIS:O	1:D:1194:ASP:N	2.41	0.52
1:D:1172:THR:HG22	1:D:1193:LYS:HG3	1.91	0.52
1:D:4052:ALA:O	1:D:4056:HIS:ND1	2.39	0.52
1:D:4617:TYR:OH	1:D:4629:GLY:O	2.24	0.52
1:J:1171:HIS:O	1:J:1194:ASP:N	2.41	0.52
1:A:678:MET:HB3	1:A:801:ARG:HB2	1.91	0.52
1:A:1004:HIS:O	1:A:1008:ALA:N	2.39	0.52
1:A:4031:ASP:HA	1:A:4034:LYS:HB3	1.91	0.52
1:D:1143:GLN:HA	1:D:1151:HIS:HA	1.91	0.52
1:D:2434:VAL:O	1:D:2438:SER:OG	2.26	0.52
1:J:170:SER:OG	1:J:171:GLU:N	2.42	0.52
1:J:2193:MET:HA	1:J:2196:ASN:HD22	1.75	0.52
1:J:2846:ALA:HA	1:J:2849:TYR:HB2	1.92	0.52
1:A:453:SER:O	1:A:457:GLN:NE2	2.42	0.52
1:A:4519:LEU:O	1:J:4810:MET:CB	2.58	0.52
1:G:28:ILE:HG12	1:G:196:TYR:HE1	1.74	0.52
1:G:453:SER:O	1:G:457:GLN:NE2	2.42	0.52
1:G:657:PRO:HD2	1:G:790:PRO:HG2	1.90	0.52
1:G:660:PHE:HB3	1:G:787:LEU:HD22	1.90	0.52
1:G:4119:PHE:HA	1:G:4122:LEU:HD12	1.92	0.52
1:J:890:HIS:NE2	1:J:919:VAL:O	2.42	0.52
1:J:1004:HIS:O	1:J:1008:ALA:N	2.39	0.52
1:J:1699:ARG:NH2	1:J:1703:TYR:OH	2.43	0.52
1:J:4119:PHE:HA	1:J:4122:LEU:HD12	1.92	0.52
1:A:1172:THR:HG22	1:A:1193:LYS:HG3	1.91	0.52
1:A:1699:ARG:NH2	1:A:1703:TYR:OH	2.43	0.52
1:A:2193:MET:HA	1:A:2196:ASN:HD22	1.75	0.52
1:A:2883:LYS:O	1:A:2887:ARG:N	2.42	0.52
1:D:28:ILE:HG12	1:D:196:TYR:HE1	1.74	0.52
1:D:170:SER:OG	1:D:171:GLU:N	2.42	0.52
1:G:2158:GLN:O	1:G:3616:ARG:NH1	2.43	0.52
1:J:237:LEU:HB3	1:J:404:ASN:HB3	1.91	0.52
1:D:2846:ALA:HA	1:D:2849:TYR:HB2	1.92	0.52
1:G:218:SER:OG	1:G:219:SER:N	2.43	0.52
1:J:453:SER:O	1:J:457:GLN:NE2	2.42	0.52
1:J:4015:LEU:HD13	1:J:4123:ALA:HB2	1.92	0.52
1:J:4070:CYS:HB2	1:J:4073:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ILE:HG12	1:A:196:TYR:HE1	1.74	0.52
1:A:207:PHE:O	1:D:2327:ARG:HA	2.09	0.52
1:A:1736:ILE:HB	1:A:1738:LEU:HD23	1.92	0.52
1:A:2158:GLN:O	1:A:3616:ARG:NH1	2.43	0.52
1:A:4070:CYS:HB2	1:A:4073:THR:HG23	1.92	0.52
1:D:4787:PHE:CE2	1:G:4521:TYR:CD2	2.97	0.52
1:D:4949:CYS:SG	1:D:4950:TRP:N	2.83	0.52
1:G:237:LEU:HB3	1:G:404:ASN:HB3	1.91	0.52
1:G:678:MET:HB3	1:G:801:ARG:HB2	1.91	0.52
1:G:776:GLN:HG2	1:G:1472:GLU:HA	1.91	0.52
1:G:4070:CYS:HB2	1:G:4073:THR:HG23	1.92	0.52
1:J:218:SER:OG	1:J:219:SER:N	2.43	0.52
1:J:678:MET:HB3	1:J:801:ARG:HB2	1.91	0.52
1:J:2107:TYR:CG	1:J:2162:LEU:HD21	2.45	0.52
1:J:2158:GLN:O	1:J:3616:ARG:NH1	2.43	0.52
1:J:4804:ASP:N	1:J:4804:ASP:OD1	2.42	0.52
1:A:2076:ILE:HG21	1:A:2081:LEU:HD22	1.92	0.52
1:A:4059:TYR:HB3	1:A:4063:GLU:HB2	1.92	0.52
1:D:4070:CYS:HB2	1:D:4073:THR:HG23	1.92	0.52
1:G:1114:ARG:HB3	1:G:1128:LEU:HD22	1.92	0.52
1:G:1699:ARG:NH2	1:G:1703:TYR:OH	2.43	0.52
1:G:2116:ASP:OD2	1:G:2155:VAL:N	2.42	0.52
1:G:4059:TYR:HB3	1:G:4063:GLU:HB2	1.92	0.52
1:J:4807:CYS:SG	1:J:4816:PHE:CD2	2.91	0.52
1:D:1114:ARG:HB3	1:D:1128:LEU:HD22	1.92	0.51
1:D:2193:MET:HA	1:D:2196:ASN:HD22	1.75	0.51
1:D:4804:ASP:OD1	1:D:4804:ASP:N	2.42	0.51
1:G:228:LEU:HB3	1:G:289:ILE:HD12	1.92	0.51
1:G:2881:LYS:HA	1:G:2884:ALA:HB3	1.92	0.51
1:G:4015:LEU:HD13	1:G:4123:ALA:HB2	1.92	0.51
1:J:803:LEU:HD13	1:J:812:LYS:H	1.75	0.51
1:J:2881:LYS:HA	1:J:2884:ALA:HB3	1.92	0.51
1:A:2327:ARG:HA	1:J:207:PHE:O	2.11	0.51
1:A:4852:PHE:CE2	1:D:4822:VAL:O	2.63	0.51
1:D:700:THR:HG23	1:D:838:ARG:HD3	1.92	0.51
1:D:1250:TRP:HB3	1:D:1600:PRO:HB2	1.92	0.51
1:D:2158:GLN:O	1:D:3616:ARG:NH1	2.43	0.51
1:D:4119:PHE:HA	1:D:4122:LEU:HD12	1.92	0.51
1:J:228:LEU:HB3	1:J:289:ILE:HD12	1.92	0.51
1:J:1241:VAL:H	1:J:1807:ARG:HH12	1.57	0.51
1:J:4031:ASP:HA	1:J:4034:LYS:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1241:VAL:H	1:A:1807:ARG:HH12	1.57	0.51
1:A:2832:VAL:O	1:A:2895:LYS:NZ	2.43	0.51
1:D:480:ARG:O	1:D:484:ASN:ND2	2.42	0.51
1:D:803:LEU:HD13	1:D:812:LYS:H	1.75	0.51
1:D:4810:MET:CB	1:G:4519:LEU:O	2.59	0.51
1:G:4864:GLN:CG	1:G:4868:ILE:HD11	2.40	0.51
1:J:2558:LYS:O	1:J:2562:LEU:N	2.43	0.51
1:J:4521:TYR:HB2	1:J:4561:VAL:HG22	1.91	0.51
1:A:849:ASP:OD2	1:A:1214:ARG:NH2	2.44	0.51
1:A:3800:SER:OG	1:A:3801:CYS:N	2.39	0.51
1:D:672:LYS:HA	1:D:760:ASP:HA	1.93	0.51
1:D:1699:ARG:NH2	1:D:1703:TYR:OH	2.43	0.51
1:G:328:ALA:O	1:G:365:HIS:ND1	2.42	0.51
1:G:644:LEU:HB3	1:G:1630:LEU:HD12	1.93	0.51
1:G:672:LYS:HA	1:G:760:ASP:HA	1.93	0.51
1:G:1137:PHE:HA	1:G:1144:ARG:HA	1.93	0.51
1:G:1250:TRP:HB3	1:G:1600:PRO:HB2	1.92	0.51
1:G:1719:LEU:HA	1:G:1722:ASN:HD22	1.76	0.51
1:G:1736:ILE:HB	1:G:1738:LEU:HD23	1.92	0.51
1:J:849:ASP:OD2	1:J:1214:ARG:NH2	2.44	0.51
1:A:4804:ASP:OD1	1:A:4804:ASP:N	2.42	0.51
1:A:4949:CYS:SG	1:A:4950:TRP:N	2.83	0.51
1:D:849:ASP:OD2	1:D:1214:ARG:NH2	2.44	0.51
1:D:1690:GLU:OE2	1:D:1790:LYS:NZ	2.36	0.51
1:D:2732:LYS:HD3	1:D:2829:MET:HB2	1.92	0.51
1:D:2881:LYS:HA	1:D:2884:ALA:HB3	1.92	0.51
1:G:1143:GLN:HA	1:G:1151:HIS:HA	1.91	0.51
1:G:2732:LYS:HD3	1:G:2829:MET:HB2	1.92	0.51
1:J:249:SER:OG	1:J:250:GLY:N	2.44	0.51
1:A:218:SER:OG	1:A:219:SER:N	2.43	0.51
1:A:644:LEU:HB3	1:A:1630:LEU:HD12	1.93	0.51
1:A:672:LYS:HA	1:A:760:ASP:HA	1.93	0.51
1:A:2107:TYR:CG	1:A:2162:LEU:HD21	2.45	0.51
1:D:249:SER:OG	1:D:250:GLY:N	2.44	0.51
1:G:849:ASP:OD2	1:G:1214:ARG:NH2	2.44	0.51
1:G:1090:ALA:HA	1:G:1249:MET:HG2	1.93	0.51
1:G:2119:ASN:N	1:G:2119:ASN:OD1	2.44	0.51
1:G:3692:TYR:HA	1:G:3695:ILE:HD12	1.93	0.51
1:J:559:ILE:HD13	1:J:593:HIS:HB3	1.93	0.51
1:J:3934:GLN:OE1	1:J:3938:HIS:NE2	2.44	0.51
1:A:559:ILE:HD13	1:A:593:HIS:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4007:SER:HG	1:A:4010:ASN:HD21	1.52	0.51
1:A:4852:PHE:CE1	1:D:4823:ARG:CB	2.94	0.51
1:D:2832:VAL:O	1:D:2895:LYS:NZ	2.43	0.51
1:G:559:ILE:HD13	1:G:593:HIS:HB3	1.93	0.51
1:G:803:LEU:HD13	1:G:812:LYS:H	1.75	0.51
1:G:3922:THR:O	1:G:3926:GLN:N	2.44	0.51
1:J:4059:TYR:HB3	1:J:4063:GLU:HB2	1.92	0.51
1:A:249:SER:OG	1:A:250:GLY:N	2.44	0.51
1:A:700:THR:HG23	1:A:838:ARG:HD3	1.92	0.51
1:A:1228:THR:HA	1:A:1232:LEU:HD12	1.93	0.51
1:A:4864:GLN:CG	1:A:4868:ILE:HD11	2.40	0.51
1:D:218:SER:OG	1:D:219:SER:N	2.43	0.51
1:D:228:LEU:HB3	1:D:289:ILE:HD12	1.92	0.51
1:D:1090:ALA:HA	1:D:1249:MET:HG2	1.93	0.51
1:D:2107:TYR:CG	1:D:2162:LEU:HD21	2.45	0.51
1:D:3692:TYR:HA	1:D:3695:ILE:HD12	1.93	0.51
1:D:3922:THR:O	1:D:3926:GLN:N	2.44	0.51
1:D:3934:GLN:OE1	1:D:3938:HIS:NE2	2.44	0.51
1:G:480:ARG:O	1:G:484:ASN:ND2	2.42	0.51
1:G:1144:ARG:NH2	1:G:1150:GLU:OE1	2.43	0.51
1:G:1241:VAL:H	1:G:1807:ARG:HH12	1.57	0.51
1:G:2193:MET:HA	1:G:2196:ASN:HD22	1.75	0.51
1:G:2846:ALA:HA	1:G:2849:TYR:HB2	1.92	0.51
1:G:4094:ASP:OD1	1:G:4094:ASP:N	2.44	0.51
1:J:4949:CYS:SG	1:J:4950:TRP:N	2.83	0.51
1:D:559:ILE:HD13	1:D:593:HIS:HB3	1.93	0.51
1:D:1137:PHE:HA	1:D:1144:ARG:HA	1.93	0.51
1:G:467:ASP:O	1:G:475:LYS:NZ	2.40	0.51
1:G:2107:TYR:CG	1:G:2162:LEU:HD21	2.45	0.51
1:G:4521:TYR:HB2	1:G:4561:VAL:HG22	1.91	0.51
1:J:1137:PHE:HA	1:J:1144:ARG:HA	1.93	0.51
1:J:1736:ILE:HB	1:J:1738:LEU:HD23	1.92	0.51
1:J:2076:ILE:HG21	1:J:2081:LEU:HD22	1.92	0.51
1:A:40:GLU:HB3	1:A:44:ASN:HB3	1.93	0.51
1:A:4119:PHE:HA	1:A:4122:LEU:HD12	1.92	0.51
1:D:40:GLU:HB3	1:D:44:ASN:HB3	1.93	0.51
1:D:890:HIS:NE2	1:D:919:VAL:O	2.42	0.51
1:D:1228:THR:HA	1:D:1232:LEU:HD12	1.93	0.51
1:D:1736:ILE:HB	1:D:1738:LEU:HD23	1.92	0.51
1:D:2258:LEU:O	1:D:3811:ARG:NH2	2.44	0.51
1:D:2644:LYS:O	1:D:2648:GLY:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:480:ARG:O	1:J:484:ASN:ND2	2.42	0.51
1:J:4754:LEU:H	1:J:4757:ILE:HD12	1.76	0.51
1:A:170:SER:OG	1:A:171:GLU:N	2.42	0.50
1:A:237:LEU:HB3	1:A:404:ASN:HB3	1.91	0.50
1:A:2258:LEU:O	1:A:3811:ARG:NH2	2.44	0.50
1:A:2846:ALA:HA	1:A:2849:TYR:HB2	1.92	0.50
1:A:4015:LEU:HD13	1:A:4123:ALA:HB2	1.92	0.50
1:A:4754:LEU:H	1:A:4757:ILE:HD12	1.76	0.50
1:D:1004:HIS:O	1:D:1008:ALA:N	2.39	0.50
1:D:1699:ARG:HH22	1:D:1821:LEU:HD21	1.76	0.50
1:D:4864:GLN:CG	1:D:4868:ILE:HD11	2.40	0.50
1:G:2076:ILE:HG21	1:G:2081:LEU:HD22	1.92	0.50
1:G:2558:LYS:O	1:G:2562:LEU:N	2.43	0.50
1:J:1092:LYS:H	1:J:1250:TRP:HZ3	1.58	0.50
1:J:3925:ILE:HD11	1:J:3936:LEU:HD13	1.93	0.50
1:A:1090:ALA:HA	1:A:1249:MET:HG2	1.93	0.50
1:A:1699:ARG:HH22	1:A:1821:LEU:HD21	1.76	0.50
1:A:2881:LYS:HA	1:A:2884:ALA:HB3	1.92	0.50
1:G:1228:THR:HA	1:G:1232:LEU:HD12	1.93	0.50
1:G:2258:LEU:O	1:G:3811:ARG:NH2	2.44	0.50
1:G:4052:ALA:O	1:G:4056:HIS:ND1	2.39	0.50
1:G:4949:CYS:SG	1:G:4950:TRP:N	2.83	0.50
1:J:700:THR:HG23	1:J:838:ARG:HD3	1.92	0.50
1:A:228:LEU:HB3	1:A:289:ILE:HD12	1.92	0.50
1:A:480:ARG:O	1:A:484:ASN:ND2	2.42	0.50
1:A:803:LEU:HD13	1:A:812:LYS:H	1.75	0.50
1:A:2138:GLU:O	1:A:2141:LYS:NZ	2.34	0.50
1:A:2732:LYS:HD3	1:A:2829:MET:HB2	1.92	0.50
1:A:3922:THR:O	1:A:3926:GLN:N	2.44	0.50
1:D:1670:HIS:HE1	1:D:1713:SER:HB2	1.77	0.50
1:D:1719:LEU:HA	1:D:1722:ASN:HD22	1.76	0.50
1:D:4015:LEU:HD13	1:D:4123:ALA:HB2	1.92	0.50
1:D:4059:TYR:HB3	1:D:4063:GLU:HB2	1.92	0.50
1:G:2832:VAL:O	1:G:2895:LYS:NZ	2.43	0.50
1:G:3934:GLN:OE1	1:G:3938:HIS:NE2	2.44	0.50
1:J:2832:VAL:O	1:J:2895:LYS:NZ	2.43	0.50
1:A:1119:ARG:NH2	1:A:1196:ASP:O	2.45	0.50
1:A:2159:HIS:HB3	1:A:2162:LEU:HD23	1.93	0.50
2:B:71:ARG:NH2	2:B:100:ASP:OD2	2.44	0.50
1:D:2119:ASN:N	1:D:2119:ASN:OD1	2.44	0.50
1:D:4945:TYR:OH	7:D:6003:CFF:H81	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4945:TYR:OH	7:G:6003:CFF:H81	2.11	0.50
1:J:644:LEU:HB3	1:J:1630:LEU:HD12	1.93	0.50
1:J:711:GLU:OE1	1:J:1448:SER:OG	2.25	0.50
1:J:1228:THR:HA	1:J:1232:LEU:HD12	1.93	0.50
1:J:1766:PRO:HG2	2:K:42:ARG:HH21	1.77	0.50
1:J:2119:ASN:N	1:J:2119:ASN:OD1	2.44	0.50
1:A:1092:LYS:H	1:A:1250:TRP:HZ3	1.58	0.50
1:A:1250:TRP:HB3	1:A:1600:PRO:HB2	1.92	0.50
1:A:3934:GLN:OE1	1:A:3938:HIS:NE2	2.44	0.50
1:A:4787:PHE:CE2	1:D:4521:TYR:CD2	2.98	0.50
2:H:71:ARG:NH2	2:H:100:ASP:OD2	2.44	0.50
1:J:1719:LEU:HA	1:J:1722:ASN:HD22	1.76	0.50
1:J:2732:LYS:HD3	1:J:2829:MET:HB2	1.92	0.50
2:K:71:ARG:NH2	2:K:100:ASP:OD2	2.44	0.50
1:A:706:TYR:OH	1:A:1254:ARG:N	2.38	0.50
1:A:1144:ARG:NH2	1:A:1150:GLU:OE1	2.43	0.50
1:A:3925:ILE:HD11	1:A:3936:LEU:HD13	1.93	0.50
1:D:644:LEU:HB3	1:D:1630:LEU:HD12	1.93	0.50
1:D:731:HIS:HE1	1:D:738:ALA:HB1	1.77	0.50
1:D:1092:LYS:H	1:D:1250:TRP:HZ3	1.58	0.50
1:D:2159:HIS:HB3	1:D:2162:LEU:HD23	1.93	0.50
1:D:4521:TYR:HB2	1:D:4561:VAL:HG22	1.91	0.50
1:G:1109:THR:OG1	1:G:1212:VAL:N	2.45	0.50
1:G:2728:HIS:O	1:G:2732:LYS:N	2.45	0.50
1:J:672:LYS:HA	1:J:760:ASP:HA	1.93	0.50
1:D:658:ASN:ND2	1:D:831:LYS:O	2.45	0.50
1:G:1004:HIS:O	1:G:1008:ALA:N	2.39	0.50
1:G:1301:PHE:HD2	1:G:1595:LEU:HD23	1.77	0.50
1:G:1670:HIS:HE1	1:G:1713:SER:HB2	1.77	0.50
1:G:4754:LEU:H	1:G:4757:ILE:HD12	1.76	0.50
1:J:1250:TRP:HB3	1:J:1600:PRO:HB2	1.92	0.50
1:A:658:ASN:ND2	1:A:831:LYS:O	2.45	0.50
1:A:1425:THR:N	1:A:1510:VAL:O	2.45	0.50
1:A:1766:PRO:HG2	2:B:42:ARG:HH21	1.76	0.50
1:A:2558:LYS:O	1:A:2562:LEU:N	2.43	0.50
1:A:4852:PHE:HZ	1:D:4823:ARG:HA	1.58	0.50
1:D:207:PHE:O	1:G:2327:ARG:HA	2.12	0.50
1:D:3925:ILE:HD11	1:D:3936:LEU:HD13	1.93	0.50
1:G:40:GLU:HB3	1:G:44:ASN:HB3	1.93	0.50
1:G:249:SER:OG	1:G:250:GLY:N	2.44	0.50
1:G:700:THR:HG23	1:G:838:ARG:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1092:LYS:H	1:G:1250:TRP:HZ3	1.58	0.50
1:G:1766:PRO:HG2	2:H:42:ARG:HH21	1.76	0.50
1:J:655:MET:HG2	1:J:836:HIS:HA	1.94	0.50
1:J:1918:GLN:HE21	1:J:1922:ARG:HH21	1.60	0.50
1:J:2433:LEU:HA	1:J:2436:VAL:HB	1.94	0.50
1:A:467:ASP:O	1:A:475:LYS:NZ	2.40	0.50
1:A:742:SER:OG	1:A:1472:GLU:OE2	2.28	0.50
1:A:2433:LEU:HA	1:A:2436:VAL:HB	1.94	0.50
1:A:3692:TYR:HA	1:A:3695:ILE:HD12	1.93	0.50
1:A:4810:MET:CB	1:D:4519:LEU:O	2.60	0.50
1:D:655:MET:HG2	1:D:836:HIS:HA	1.94	0.50
1:D:1301:PHE:HD2	1:D:1595:LEU:HD23	1.77	0.50
1:D:2076:ILE:HG21	1:D:2081:LEU:HD22	1.92	0.50
1:D:2116:ASP:OD2	1:D:2155:VAL:N	2.42	0.50
1:D:2558:LYS:O	1:D:2562:LEU:N	2.43	0.50
1:D:4754:LEU:H	1:D:4757:ILE:HD12	1.76	0.50
1:G:658:ASN:ND2	1:G:831:LYS:O	2.45	0.50
1:J:1090:ALA:HA	1:J:1249:MET:HG2	1.93	0.50
1:J:3922:THR:O	1:J:3926:GLN:N	2.44	0.50
1:A:655:MET:HG2	1:A:836:HIS:HA	1.94	0.49
1:A:1137:PHE:HA	1:A:1144:ARG:HA	1.93	0.49
1:A:2728:HIS:O	1:A:2732:LYS:N	2.45	0.49
1:D:1144:ARG:NH2	1:D:1150:GLU:OE1	2.43	0.49
1:D:1425:THR:N	1:D:1510:VAL:O	2.45	0.49
2:E:71:ARG:NH2	2:E:100:ASP:OD2	2.44	0.49
1:G:219:SER:O	1:G:219:SER:OG	2.29	0.49
1:G:4853:PHE:CD1	1:G:4853:PHE:C	2.85	0.49
1:J:1144:ARG:NH2	1:J:1150:GLU:OE1	2.43	0.49
1:J:3692:TYR:HA	1:J:3695:ILE:HD12	1.93	0.49
1:A:1670:HIS:HE1	1:A:1713:SER:HB2	1.77	0.49
1:D:2418:ILE:HG23	1:D:2421:ARG:HD3	1.94	0.49
1:G:1918:GLN:HE21	1:G:1922:ARG:HH21	1.60	0.49
1:J:1109:THR:OG1	1:J:1212:VAL:N	2.45	0.49
1:J:1301:PHE:HD2	1:J:1595:LEU:HD23	1.77	0.49
1:J:2159:HIS:HB3	1:J:2162:LEU:HD23	1.93	0.49
1:A:57:ASN:HA	1:A:323:ASP:HA	1.95	0.49
1:A:219:SER:O	1:A:219:SER:OG	2.29	0.49
1:D:328:ALA:O	1:D:365:HIS:ND1	2.42	0.49
1:D:1241:VAL:H	1:D:1807:ARG:HH12	1.57	0.49
3:F:51:ASP:O	3:F:55:GLU:N	2.45	0.49
1:G:655:MET:HG2	1:G:836:HIS:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:40:GLU:HB3	1:J:44:ASN:HB3	1.93	0.49
1:J:467:ASP:O	1:J:475:LYS:NZ	2.40	0.49
1:J:3986:MET:HG2	1:J:3996:ILE:HD11	1.95	0.49
1:J:4864:GLN:CG	1:J:4868:ILE:HD11	2.40	0.49
1:A:4853:PHE:CD1	1:A:4853:PHE:C	2.85	0.49
1:D:2138:GLU:O	1:D:2141:LYS:NZ	2.34	0.49
1:D:2883:LYS:O	1:D:2887:ARG:N	2.42	0.49
1:J:1699:ARG:HH22	1:J:1821:LEU:HD21	1.76	0.49
1:J:4945:TYR:OH	7:J:6003:CFF:H81	2.11	0.49
1:D:2855:LYS:HA	1:D:2858:LYS:HB2	1.95	0.49
1:G:207:PHE:O	1:J:2327:ARG:HA	2.12	0.49
1:G:711:GLU:OE1	1:G:1448:SER:OG	2.25	0.49
1:G:731:HIS:HE1	1:G:738:ALA:HB1	1.77	0.49
1:G:1171:HIS:O	1:G:1194:ASP:N	2.41	0.49
1:G:1425:THR:N	1:G:1510:VAL:O	2.45	0.49
1:J:328:ALA:O	1:J:365:HIS:ND1	2.42	0.49
1:J:658:ASN:ND2	1:J:831:LYS:O	2.45	0.49
1:J:2855:LYS:HA	1:J:2858:LYS:HB2	1.95	0.49
1:A:1719:LEU:HA	1:A:1722:ASN:HD22	1.76	0.49
1:D:1119:ARG:NH2	1:D:1196:ASP:O	2.45	0.49
1:D:1766:PRO:HG2	2:E:42:ARG:HH21	1.77	0.49
1:G:742:SER:OG	1:G:1472:GLU:OE2	2.28	0.49
1:G:1699:ARG:HH22	1:G:1821:LEU:HD21	1.76	0.49
1:J:696:GLY:HA3	1:J:724:SER:HA	1.94	0.49
1:J:2258:LEU:O	1:J:3811:ARG:NH2	2.45	0.49
1:D:57:ASN:HA	1:D:323:ASP:HA	1.95	0.49
1:G:1119:ARG:NH2	1:G:1196:ASP:O	2.45	0.49
1:A:568:SER:HA	1:A:571:ILE:HD12	1.95	0.49
1:A:2119:ASN:OD1	1:A:2119:ASN:N	2.44	0.49
1:A:3986:MET:HG2	1:A:3996:ILE:HD11	1.95	0.49
1:A:4819:TYR:CD1	1:A:4819:TYR:C	2.85	0.49
1:A:4945:TYR:OH	7:A:6003:CFF:H81	2.11	0.49
1:D:568:SER:HA	1:D:571:ILE:HD12	1.95	0.49
1:D:2433:LEU:HA	1:D:2436:VAL:HB	1.94	0.49
1:G:2433:LEU:HA	1:G:2436:VAL:HB	1.94	0.49
1:J:1506:GLU:HA	1:J:1522:ALA:HA	1.95	0.49
1:A:4852:PHE:C	1:A:4852:PHE:CD2	2.85	0.49
1:D:2897:LEU:HD13	1:D:2904:VAL:HG21	1.95	0.49
1:G:2159:HIS:HB3	1:G:2162:LEU:HD23	1.93	0.49
1:G:2418:ILE:HG23	1:G:2421:ARG:HD3	1.94	0.49
1:G:2855:LYS:HA	1:G:2858:LYS:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3925:ILE:HD11	1:G:3936:LEU:HD13	1.93	0.49
1:G:4819:TYR:C	1:G:4819:TYR:CD2	2.85	0.49
3:I:51:ASP:O	3:I:55:GLU:N	2.45	0.49
1:J:57:ASN:HA	1:J:323:ASP:HA	1.95	0.49
1:J:1425:THR:N	1:J:1510:VAL:O	2.45	0.49
1:J:1670:HIS:HE1	1:J:1713:SER:HB2	1.77	0.49
3:L:51:ASP:O	3:L:55:GLU:N	2.45	0.49
1:J:731:HIS:HE1	1:J:738:ALA:HB1	1.77	0.49
1:J:1570:LEU:O	1:J:1573:SER:OG	2.31	0.49
1:A:731:HIS:HE1	1:A:738:ALA:HB1	1.77	0.48
1:A:1301:PHE:HD2	1:A:1595:LEU:HD23	1.77	0.48
1:A:2855:LYS:HA	1:A:2858:LYS:HB2	1.95	0.48
1:A:4640:SER:OG	1:A:4703:ASP:OD2	2.31	0.48
1:D:1918:GLN:HE21	1:D:1922:ARG:HH21	1.60	0.48
1:D:2258:LEU:HD21	1:D:2263:LEU:HD21	1.95	0.48
1:G:696:GLY:HA3	1:G:724:SER:HA	1.94	0.48
1:G:1630:LEU:HD22	1:G:1641:ILE:HD13	1.95	0.48
1:G:4820:VAL:HG11	1:G:4831:GLU:HG3	1.94	0.48
1:J:1449:ASP:N	1:J:1449:ASP:OD1	2.46	0.48
1:J:4640:SER:OG	1:J:4703:ASP:OD2	2.31	0.48
1:A:1918:GLN:HE21	1:A:1922:ARG:HH21	1.60	0.48
1:A:2897:LEU:HD13	1:A:2904:VAL:HG21	1.95	0.48
1:A:4521:TYR:HB2	1:A:4561:VAL:HG22	1.94	0.48
1:D:1506:GLU:HA	1:D:1522:ALA:HA	1.95	0.48
1:J:1119:ARG:NH2	1:J:1196:ASP:O	2.45	0.48
1:A:1445:TRP:HE3	1:A:1539:LEU:HB3	1.78	0.48
1:A:2258:LEU:HD21	1:A:2263:LEU:HD21	1.95	0.48
1:A:2418:ILE:HG23	1:A:2421:ARG:HD3	1.94	0.48
1:J:3900:ASP:OD1	1:J:3900:ASP:N	2.39	0.48
1:D:711:GLU:OE1	1:D:1448:SER:OG	2.25	0.48
1:D:1221:VAL:HA	1:D:1224:LEU:HG	1.96	0.48
1:G:3986:MET:HG2	1:G:3996:ILE:HD11	1.95	0.48
1:G:4849:ILE:HD11	1:J:4819:TYR:CD1	2.48	0.48
1:J:2897:LEU:HD13	1:J:2904:VAL:HG21	1.95	0.48
1:D:696:GLY:HA3	1:D:724:SER:HA	1.94	0.48
1:D:1109:THR:OG1	1:D:1212:VAL:N	2.45	0.48
1:D:1570:LEU:O	1:D:1573:SER:OG	2.31	0.48
1:D:3986:MET:HG2	1:D:3996:ILE:HD11	1.95	0.48
1:D:4794:TYR:OH	1:D:4817:HIS:CE1	2.66	0.48
1:G:1445:TRP:HE3	1:G:1539:LEU:HB3	1.78	0.48
1:G:2897:LEU:HD13	1:G:2904:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4810:MET:CB	1:J:4521:TYR:O	2.61	0.48
1:J:2841:MET:O	1:J:2845:MET:N	2.40	0.48
1:A:2122:ALA:O	1:A:2126:GLN:N	2.47	0.48
1:A:2639:LEU:O	1:A:2643:ARG:N	2.44	0.48
1:D:766:ILE:HB	1:D:779:PHE:HB2	1.96	0.48
1:G:568:SER:HA	1:G:571:ILE:HD12	1.95	0.48
1:G:1221:VAL:HA	1:G:1224:LEU:HG	1.96	0.48
1:G:4816:PHE:C	1:G:4816:PHE:CD1	2.86	0.48
1:J:556:ASP:N	1:J:556:ASP:OD1	2.46	0.48
1:J:727:PHE:H	1:J:730:LEU:HD12	1.78	0.48
1:J:2434:VAL:O	1:J:2438:SER:OG	2.26	0.48
1:A:1449:ASP:N	1:A:1449:ASP:OD1	2.46	0.48
1:D:1445:TRP:HE3	1:D:1539:LEU:HB3	1.78	0.48
1:D:1630:LEU:HD22	1:D:1641:ILE:HD13	1.95	0.48
1:G:556:ASP:N	1:G:556:ASP:OD1	2.46	0.48
1:G:4820:VAL:HG12	1:G:4831:GLU:HG3	1.95	0.48
1:A:308:LEU:HD22	1:A:393:MET:HG3	1.96	0.48
1:A:556:ASP:N	1:A:556:ASP:OD1	2.46	0.48
1:A:1661:TYR:HB3	1:A:1676:LEU:HD21	1.96	0.48
1:A:4515:ASN:HB3	1:J:4780:TYR:CZ	2.49	0.48
1:A:4816:PHE:CD1	1:A:4816:PHE:C	2.87	0.48
1:D:15:ARG:HD3	1:D:110:HIS:HB3	1.96	0.48
1:D:2729:SER:HA	1:D:2732:LYS:HB3	1.96	0.48
1:D:4819:TYR:CD1	1:D:4819:TYR:C	2.85	0.48
1:G:57:ASN:HA	1:G:323:ASP:HA	1.95	0.48
1:G:1570:LEU:O	1:G:1573:SER:OG	2.31	0.48
1:G:2176:MET:HE1	1:G:2194:VAL:HG13	1.95	0.48
1:G:4514:ILE:HD11	1:G:4576:LEU:HB3	1.96	0.48
1:J:2122:ALA:O	1:J:2126:GLN:N	2.47	0.48
1:A:766:ILE:HB	1:A:779:PHE:HB2	1.96	0.48
1:A:1245:ARG:HE	1:A:1692:LYS:HB3	1.79	0.48
1:A:2147:LEU:HA	1:A:2150:ILE:HD12	1.95	0.48
1:A:3919:ASN:O	1:A:3922:THR:OG1	2.31	0.48
1:A:4114:THR:HA	1:A:4117:GLN:HB2	1.96	0.48
1:D:1245:ARG:HE	1:D:1692:LYS:HB3	1.79	0.48
1:D:2728:HIS:O	1:D:2732:LYS:N	2.45	0.48
1:D:4033:PHE:HA	1:D:4036:TYR:HB2	1.96	0.48
1:D:4817:HIS:NE2	1:D:4828:ILE:HG12	2.28	0.48
1:G:2258:LEU:HD21	1:G:2263:LEU:HD21	1.95	0.48
1:J:1221:VAL:HA	1:J:1224:LEU:HG	1.96	0.48
1:J:1938:GLN:HA	1:J:3610:TYR:HE2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2418:ILE:HG23	1:J:2421:ARG:HD3	1.94	0.48
1:A:50:GLU:OE2	1:A:319:LYS:NZ	2.46	0.48
1:A:2644:LYS:O	1:A:2648:GLY:N	2.41	0.48
3:C:51:ASP:O	3:C:55:GLU:N	2.45	0.48
1:D:4514:ILE:HD11	1:D:4576:LEU:HB3	1.96	0.48
1:G:766:ILE:HB	1:G:779:PHE:HB2	1.96	0.48
1:G:2639:LEU:O	1:G:2643:ARG:N	2.44	0.48
1:G:4819:TYR:HD2	1:G:4820:VAL:HG23	1.79	0.48
1:J:1001:GLU:O	1:J:1005:ASN:ND2	2.47	0.48
1:J:2728:HIS:O	1:J:2732:LYS:N	2.45	0.48
1:A:1001:GLU:O	1:A:1005:ASN:ND2	2.47	0.47
1:A:4056:HIS:C	1:A:4057:LYS:HG2	2.35	0.47
1:D:556:ASP:N	1:D:556:ASP:OD1	2.46	0.47
1:D:2122:ALA:O	1:D:2126:GLN:N	2.47	0.47
1:G:727:PHE:H	1:G:730:LEU:HD12	1.78	0.47
1:G:2884:ALA:HA	1:G:2887:ARG:HB3	1.97	0.47
1:G:3623:GLN:O	1:G:3627:LYS:NZ	2.47	0.47
1:J:766:ILE:HB	1:J:779:PHE:HB2	1.96	0.47
1:J:1630:LEU:HD22	1:J:1641:ILE:HD13	1.95	0.47
1:J:3623:GLN:O	1:J:3627:LYS:NZ	2.47	0.47
1:A:1109:THR:OG1	1:A:1212:VAL:N	2.45	0.47
1:A:1221:VAL:HA	1:A:1224:LEU:HG	1.96	0.47
1:A:1304:LEU:HB2	1:A:1541:PRO:HG2	1.96	0.47
1:D:1661:TYR:HB3	1:D:1676:LEU:HD21	1.96	0.47
1:G:1938:GLN:HA	1:G:3610:TYR:HE2	1.79	0.47
1:G:2729:SER:HA	1:G:2732:LYS:HB3	1.95	0.47
1:G:3973:MET:HA	1:G:3976:GLN:HB3	1.96	0.47
1:J:682:THR:OG1	1:J:683:GLU:N	2.47	0.47
1:J:1245:ARG:HE	1:J:1692:LYS:HB3	1.79	0.47
1:J:3919:ASN:O	1:J:3922:THR:OG1	2.31	0.47
1:A:1506:GLU:HA	1:A:1522:ALA:HA	1.95	0.47
1:A:4033:PHE:HA	1:A:4036:TYR:HB2	1.96	0.47
1:D:1001:GLU:O	1:D:1005:ASN:ND2	2.47	0.47
1:D:3973:MET:HA	1:D:3976:GLN:HB3	1.96	0.47
1:G:15:ARG:HD3	1:G:110:HIS:HB3	1.96	0.47
1:G:4033:PHE:HA	1:G:4036:TYR:HB2	1.96	0.47
1:G:4780:TYR:OH	1:J:4741:ALA:HB1	2.14	0.47
1:J:308:LEU:HD22	1:J:393:MET:HG3	1.96	0.47
1:J:568:SER:HA	1:J:571:ILE:HD12	1.95	0.47
1:J:1304:LEU:HB2	1:J:1541:PRO:HG2	1.96	0.47
1:J:1661:TYR:HB3	1:J:1676:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2070:TRP:O	1:J:2074:SER:OG	2.32	0.47
1:J:4033:PHE:HA	1:J:4036:TYR:HB2	1.96	0.47
1:A:328:ALA:O	1:A:365:HIS:ND1	2.42	0.47
1:A:1570:LEU:O	1:A:1573:SER:OG	2.31	0.47
1:A:4039:ASP:OD2	1:A:4039:ASP:N	2.41	0.47
1:D:1768:PHE:HE1	2:E:90:VAL:HG21	1.80	0.47
1:D:1938:GLN:HA	1:D:3610:TYR:HE2	1.79	0.47
1:G:1104:GLU:HA	1:G:1163:GLY:HA2	1.96	0.47
1:G:1506:GLU:HA	1:G:1522:ALA:HA	1.95	0.47
1:G:1768:PHE:HE1	2:H:90:VAL:HG21	1.80	0.47
1:G:4780:TYR:OH	1:J:4744:LEU:HD23	2.14	0.47
1:J:1445:TRP:HE3	1:J:1539:LEU:HB3	1.78	0.47
1:J:2514:ALA:O	1:J:2518:ASN:ND2	2.48	0.47
1:J:4853:PHE:CD1	1:J:4853:PHE:C	2.85	0.47
1:A:123:HIS:CD2	1:A:126:SER:H	2.33	0.47
1:A:696:GLY:HA3	1:A:724:SER:HA	1.94	0.47
1:A:2176:MET:HE1	1:A:2194:VAL:HG13	1.95	0.47
1:D:123:HIS:CD2	1:D:126:SER:H	2.33	0.47
1:D:3919:ASN:O	1:D:3922:THR:OG1	2.31	0.47
1:G:1001:GLU:O	1:G:1005:ASN:ND2	2.47	0.47
1:G:2147:LEU:HA	1:G:2150:ILE:HD12	1.95	0.47
1:G:3663:ASP:OD2	1:G:3735:ARG:NH2	2.47	0.47
1:J:123:HIS:CD2	1:J:126:SER:H	2.33	0.47
1:A:658:ASN:HB2	1:A:833:LYS:H	1.80	0.47
1:A:3623:GLN:O	1:A:3627:LYS:NZ	2.47	0.47
1:D:299:HIS:N	1:D:304:LYS:O	2.43	0.47
1:D:1104:GLU:HA	1:D:1163:GLY:HA2	1.97	0.47
1:D:2176:MET:HE1	1:D:2194:VAL:HG13	1.96	0.47
1:D:2884:ALA:HA	1:D:2887:ARG:HB3	1.97	0.47
1:D:4591:TYR:HH	1:D:4719:SER:HG	1.60	0.47
1:G:2883:LYS:O	1:G:2887:ARG:N	2.42	0.47
1:J:3890:TYR:HE1	1:J:3958:LYS:HD2	1.79	0.47
1:A:1171:HIS:O	1:A:1194:ASP:N	2.41	0.47
1:A:1630:LEU:HD22	1:A:1641:ILE:HD13	1.95	0.47
1:A:1768:PHE:HE1	2:B:90:VAL:HG21	1.80	0.47
1:A:3663:ASP:OD2	1:A:3735:ARG:NH2	2.47	0.47
1:A:3890:TYR:HE1	1:A:3958:LYS:HD2	1.79	0.47
1:D:50:GLU:OE2	1:D:319:LYS:NZ	2.46	0.47
1:D:467:ASP:O	1:D:475:LYS:NZ	2.40	0.47
1:D:505:LEU:HD23	1:D:530:LEU:HD13	1.96	0.47
1:D:682:THR:OG1	1:D:683:GLU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:727:PHE:H	1:D:730:LEU:HD12	1.78	0.47
1:D:742:SER:OG	1:D:1472:GLU:OE2	2.28	0.47
1:D:1799:VAL:HG22	1:D:1894:LEU:HD13	1.97	0.47
1:D:2147:LEU:HA	1:D:2150:ILE:HD12	1.95	0.47
1:D:3623:GLN:O	1:D:3627:LYS:NZ	2.47	0.47
1:D:3645:LEU:HB3	1:D:3665:LEU:HB2	1.97	0.47
1:D:3663:ASP:OD2	1:D:3735:ARG:NH2	2.47	0.47
1:D:4056:HIS:O	1:D:4057:LYS:CG	2.63	0.47
1:G:123:HIS:CD2	1:G:126:SER:H	2.33	0.47
1:G:658:ASN:HB2	1:G:833:LYS:H	1.80	0.47
1:G:1449:ASP:OD1	1:G:1449:ASP:N	2.46	0.47
1:G:2138:GLU:O	1:G:2141:LYS:NZ	2.34	0.47
1:G:2404:ALA:HB3	1:G:2475:ARG:HE	1.79	0.47
1:G:2514:ALA:O	1:G:2518:ASN:ND2	2.48	0.47
1:G:3800:SER:OG	1:G:3801:CYS:N	2.39	0.47
1:G:3919:ASN:O	1:G:3922:THR:OG1	2.31	0.47
1:J:15:ARG:HD3	1:J:110:HIS:HB3	1.96	0.47
1:J:510:SER:O	1:J:520:ARG:NH2	2.48	0.47
1:J:1104:GLU:HA	1:J:1163:GLY:HA2	1.97	0.47
1:J:1768:PHE:HE1	2:K:90:VAL:HG21	1.80	0.47
1:J:2258:LEU:HD21	1:J:2263:LEU:HD21	1.95	0.47
1:J:3663:ASP:OD2	1:J:3735:ARG:NH2	2.47	0.47
1:J:4056:HIS:C	1:J:4057:LYS:HG2	2.35	0.47
1:A:15:ARG:HD3	1:A:110:HIS:HB3	1.96	0.47
1:A:4822:VAL:C	1:A:4824:ALA:N	2.56	0.47
1:D:308:LEU:HD22	1:D:393:MET:HG3	1.96	0.47
1:D:2070:TRP:O	1:D:2074:SER:OG	2.32	0.47
1:D:3890:TYR:HE1	1:D:3958:LYS:HD2	1.79	0.47
1:D:4114:THR:HA	1:D:4117:GLN:HB2	1.96	0.47
1:G:505:LEU:HD23	1:G:530:LEU:HD13	1.96	0.47
1:G:682:THR:OG1	1:G:683:GLU:N	2.47	0.47
1:G:2122:ALA:O	1:G:2126:GLN:N	2.47	0.47
1:G:4591:TYR:OH	1:G:4719:SER:OG	2.31	0.47
1:J:303:GLY:HA2	1:J:420:ARG:HH11	1.80	0.47
1:J:1131:ASP:OD1	1:J:1131:ASP:N	2.48	0.47
1:J:2176:MET:HE1	1:J:2194:VAL:HG13	1.96	0.47
1:J:2729:SER:HA	1:J:2732:LYS:HB3	1.95	0.47
1:J:4039:ASP:OD2	1:J:4039:ASP:N	2.41	0.47
1:A:303:GLY:HA2	1:A:420:ARG:HH11	1.80	0.47
1:A:510:SER:O	1:A:520:ARG:NH2	2.48	0.47
1:A:1171:HIS:ND1	1:A:1195:PHE:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1770:SER:O	1:A:1770:SER:OG	2.32	0.47
1:A:1938:GLN:HA	1:A:3610:TYR:HE2	1.79	0.47
1:A:4849:ILE:HD11	1:D:4819:TYR:CG	2.48	0.47
1:D:4039:ASP:OD2	1:D:4039:ASP:N	2.41	0.47
1:G:1171:HIS:ND1	1:G:1195:PHE:O	2.48	0.47
1:J:1769:VAL:HB	2:K:55:VAL:HA	1.97	0.47
1:J:1799:VAL:HG22	1:J:1894:LEU:HD13	1.97	0.47
1:J:2884:ALA:HA	1:J:2887:ARG:HB3	1.97	0.47
1:J:4514:ILE:HD11	1:J:4576:LEU:HB3	1.96	0.47
1:A:2070:TRP:O	1:A:2074:SER:OG	2.32	0.47
1:A:2514:ALA:O	1:A:2518:ASN:ND2	2.48	0.47
1:A:2515:LEU:HA	1:A:2518:ASN:HD22	1.80	0.47
1:A:4514:ILE:HD11	1:A:4576:LEU:HB3	1.96	0.47
1:D:510:SER:O	1:D:520:ARG:NH2	2.48	0.47
1:D:1171:HIS:ND1	1:D:1195:PHE:O	2.48	0.47
1:D:4627:ILE:O	1:D:4631:TRP:N	2.48	0.47
1:G:50:GLU:OE2	1:G:319:LYS:NZ	2.46	0.47
1:G:1444:GLY:HA2	1:G:1487:MET:HB2	1.97	0.47
1:G:1718:ARG:O	1:G:1722:ASN:ND2	2.48	0.47
1:G:4114:THR:HA	1:G:4117:GLN:HB2	1.96	0.47
1:A:711:GLU:OE1	1:A:1448:SER:OG	2.25	0.46
1:D:194:LEU:HB3	1:D:210:THR:HG21	1.98	0.46
1:D:425:LEU:HD21	1:D:452:VAL:HG13	1.98	0.46
1:D:1444:GLY:HA2	1:D:1487:MET:HB2	1.97	0.46
1:D:1718:ARG:O	1:D:1722:ASN:ND2	2.48	0.46
1:D:2116:ASP:OD1	1:D:2153:ASN:ND2	2.47	0.46
1:G:194:LEU:HB3	1:G:210:THR:HG21	1.97	0.46
1:G:308:LEU:HD22	1:G:393:MET:HG3	1.96	0.46
1:G:503:ASP:HA	1:G:561:ARG:HH22	1.80	0.46
1:G:3645:LEU:HB3	1:G:3665:LEU:HB2	1.97	0.46
1:J:503:ASP:HA	1:J:561:ARG:HH22	1.80	0.46
1:J:2515:LEU:HA	1:J:2518:ASN:HD22	1.80	0.46
1:J:4056:HIS:O	1:J:4057:LYS:CG	2.63	0.46
1:J:4094:ASP:OD1	1:J:4094:ASP:N	2.44	0.46
1:J:4114:THR:HA	1:J:4117:GLN:HB2	1.96	0.46
1:J:4816:PHE:C	1:J:4816:PHE:CD1	2.87	0.46
1:J:4831:GLU:N	1:J:4831:GLU:OE1	2.49	0.46
1:A:727:PHE:H	1:A:730:LEU:HD12	1.78	0.46
1:A:1104:GLU:HA	1:A:1163:GLY:HA2	1.96	0.46
1:A:1775:CYS:SG	1:A:1776:TYR:N	2.88	0.46
1:A:4094:ASP:OD1	1:A:4094:ASP:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:658:ASN:HB2	1:D:833:LYS:H	1.80	0.46
1:D:863:THR:O	1:D:863:THR:OG1	2.33	0.46
1:D:1775:CYS:SG	1:D:1776:TYR:N	2.88	0.46
1:G:590:LYS:H	1:G:593:HIS:CD2	2.34	0.46
1:G:1661:TYR:HB3	1:G:1676:LEU:HD21	1.96	0.46
1:G:3665:LEU:HD23	1:G:3735:ARG:HH11	1.80	0.46
1:G:3890:TYR:HE1	1:G:3958:LYS:HD2	1.79	0.46
1:J:219:SER:O	1:J:219:SER:OG	2.29	0.46
1:J:1227:PHE:HE2	1:J:1238:PRO:HG3	1.81	0.46
1:A:784:ILE:HG23	1:A:788:PHE:HE2	1.80	0.46
1:A:1718:ARG:O	1:A:1722:ASN:ND2	2.48	0.46
1:A:2841:MET:O	1:A:2845:MET:N	2.40	0.46
1:A:2884:ALA:HA	1:A:2887:ARG:HB3	1.97	0.46
1:A:3665:LEU:HD23	1:A:3735:ARG:HH11	1.80	0.46
1:A:4831:GLU:OE1	1:A:4831:GLU:N	2.49	0.46
1:D:303:GLY:HA2	1:D:420:ARG:HH11	1.80	0.46
1:D:503:ASP:HA	1:D:561:ARG:HH22	1.80	0.46
1:D:2514:ALA:O	1:D:2518:ASN:ND2	2.48	0.46
1:G:510:SER:O	1:G:520:ARG:NH2	2.48	0.46
1:G:1245:ARG:HE	1:G:1692:LYS:HB3	1.79	0.46
1:G:4627:ILE:O	1:G:4631:TRP:N	2.48	0.46
1:J:1171:HIS:ND1	1:J:1195:PHE:O	2.48	0.46
1:J:1718:ARG:O	1:J:1722:ASN:ND2	2.48	0.46
1:J:2147:LEU:HA	1:J:2150:ILE:HD12	1.95	0.46
2:K:27:THR:HA	2:K:38:SER:HA	1.98	0.46
1:A:425:LEU:HD21	1:A:452:VAL:HG13	1.98	0.46
1:A:1227:PHE:HE2	1:A:1238:PRO:HG3	1.81	0.46
1:A:1444:GLY:HA2	1:A:1487:MET:HB2	1.97	0.46
1:A:2391:THR:HG22	1:A:2465:HIS:HE1	1.81	0.46
1:A:3973:MET:HA	1:A:3976:GLN:HB3	1.96	0.46
2:B:27:THR:HA	2:B:38:SER:HA	1.98	0.46
1:D:784:ILE:HG23	1:D:788:PHE:HE2	1.80	0.46
1:D:3804:LEU:HD13	1:D:3910:ALA:HB2	1.98	0.46
1:D:4780:TYR:OH	1:G:4741:ALA:HB1	2.15	0.46
1:G:207:PHE:CB	1:J:2326:ILE:C	2.84	0.46
1:G:1131:ASP:OD1	1:G:1131:ASP:N	2.48	0.46
1:G:1227:PHE:HE2	1:G:1238:PRO:HG3	1.81	0.46
1:G:2543:ALA:HA	1:G:2877:THR:HB	1.97	0.46
1:J:194:LEU:HB3	1:J:210:THR:HG21	1.97	0.46
1:J:334:SER:OG	1:J:335:LYS:N	2.49	0.46
1:J:1444:GLY:HA2	1:J:1487:MET:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2404:ALA:HB3	1:J:2475:ARG:HE	1.79	0.46
1:J:3645:LEU:HB3	1:J:3665:LEU:HB2	1.97	0.46
1:A:194:LEU:HB3	1:A:210:THR:HG21	1.97	0.46
1:A:682:THR:OG1	1:A:683:GLU:N	2.47	0.46
1:A:2404:ALA:HB3	1:A:2475:ARG:HE	1.79	0.46
1:D:334:SER:OG	1:D:335:LYS:N	2.49	0.46
1:D:1131:ASP:OD1	1:D:1131:ASP:N	2.48	0.46
1:D:1227:PHE:HE2	1:D:1238:PRO:HG3	1.81	0.46
1:D:2543:ALA:HA	1:D:2877:THR:HB	1.97	0.46
1:D:2841:MET:O	1:D:2845:MET:N	2.40	0.46
1:D:4056:HIS:C	1:D:4057:LYS:HG2	2.35	0.46
1:D:4094:ASP:OD1	1:D:4094:ASP:N	2.44	0.46
1:G:44:ASN:HD21	1:G:46:LEU:HB2	1.81	0.46
1:G:425:LEU:HD21	1:G:452:VAL:HG13	1.98	0.46
1:G:1611:ILE:N	1:G:1620:GLN:O	2.38	0.46
1:G:4056:HIS:C	1:G:4057:LYS:HG2	2.35	0.46
1:G:4737:ASN:OD1	1:G:4737:ASN:N	2.39	0.46
1:J:2391:THR:HG22	1:J:2465:HIS:HE1	1.81	0.46
1:J:4861:ALA:O	1:J:4865:GLY:N	2.47	0.46
1:A:1265:HIS:CD2	1:A:1267:HIS:H	2.34	0.46
1:A:3804:LEU:HD13	1:A:3910:ALA:HB2	1.98	0.46
1:A:4856:ILE:HA	1:A:4860:LEU:HD23	1.97	0.46
1:D:590:LYS:H	1:D:593:HIS:CD2	2.34	0.46
1:D:1304:LEU:HB2	1:D:1541:PRO:HG2	1.96	0.46
1:G:4056:HIS:O	1:G:4057:LYS:CG	2.63	0.46
2:H:27:THR:HA	2:H:38:SER:HA	1.98	0.46
1:A:2729:SER:HA	1:A:2732:LYS:HB3	1.96	0.46
1:A:4056:HIS:O	1:A:4057:LYS:CG	2.63	0.46
1:A:4813:CYS:O	1:A:4817:HIS:N	2.42	0.46
1:D:44:ASN:HD21	1:D:46:LEU:HB2	1.81	0.46
1:G:190:ARG:HH12	1:J:2423:ILE:HG23	1.81	0.46
1:G:4787:PHE:HZ	1:J:4522:LYS:HA	1.81	0.46
1:J:2562:LEU:O	1:J:2566:GLN:N	2.46	0.46
1:J:2848:ASN:O	1:J:2852:ILE:N	2.49	0.46
1:J:3804:LEU:HD13	1:J:3910:ALA:HB2	1.98	0.46
1:A:503:ASP:HA	1:A:561:ARG:HH22	1.80	0.46
1:A:564:ARG:HG3	1:A:566:GLU:HG3	1.98	0.46
1:A:1769:VAL:HB	2:B:55:VAL:HA	1.97	0.46
1:A:1799:VAL:HG22	1:A:1894:LEU:HD13	1.97	0.46
1:A:4603:ARG:NE	1:A:4632:ASP:OD2	2.49	0.46
1:G:881:ILE:HD11	1:G:952:ILE:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1799:VAL:HG22	1:G:1894:LEU:HD13	1.97	0.46
1:J:658:ASN:HB2	1:J:833:LYS:H	1.80	0.46
1:J:2644:LYS:O	1:J:2648:GLY:N	2.41	0.46
1:J:4603:ARG:NE	1:J:4632:ASP:OD2	2.49	0.46
1:A:169:ARG:HH22	1:A:176:ARG:HD2	1.81	0.46
1:D:881:ILE:HD11	1:D:952:ILE:HG23	1.98	0.46
1:D:1153:GLY:N	1:D:1183:LEU:O	2.49	0.46
1:D:1690:GLU:O	1:D:1692:LYS:NZ	2.45	0.46
1:D:1769:VAL:HB	2:E:55:VAL:HA	1.98	0.46
1:D:2391:THR:HG22	1:D:2465:HIS:HE1	1.81	0.46
1:D:2404:ALA:HB3	1:D:2475:ARG:HE	1.79	0.46
1:G:649:VAL:O	1:G:1627:PHE:N	2.46	0.46
1:G:4782:TYR:CE2	1:G:4851:PHE:HD1	2.27	0.46
1:J:160:TRP:HB3	1:J:183:LEU:HD11	1.98	0.46
1:J:3973:MET:HA	1:J:3976:GLN:HB3	1.96	0.46
1:A:44:ASN:HD21	1:A:46:LEU:HB2	1.81	0.46
1:A:160:TRP:HB3	1:A:183:LEU:HD11	1.98	0.46
1:A:505:LEU:HD23	1:A:530:LEU:HD13	1.96	0.46
1:A:590:LYS:H	1:A:593:HIS:CD2	2.34	0.46
1:A:3943:ASP:N	1:A:3943:ASP:OD1	2.49	0.46
1:A:4045:SER:HB3	1:A:4048:ASP:HB2	1.98	0.46
1:D:160:TRP:HB3	1:D:183:LEU:HD11	1.98	0.46
1:D:1265:HIS:CD2	1:D:1267:HIS:H	2.34	0.46
1:D:1609:SER:OG	1:D:1621:CYS:SG	2.72	0.46
1:D:4603:ARG:NE	1:D:4632:ASP:OD2	2.49	0.46
2:E:27:THR:HA	2:E:38:SER:HA	1.98	0.46
1:G:160:TRP:HB3	1:G:183:LEU:HD11	1.98	0.46
1:G:303:GLY:HA2	1:G:420:ARG:HH11	1.80	0.46
1:G:4733:GLY:HA3	1:G:4740:PHE:HD1	1.81	0.46
1:J:590:LYS:H	1:J:593:HIS:CD2	2.34	0.46
1:J:1265:HIS:CD2	1:J:1267:HIS:H	2.34	0.46
1:J:2543:ALA:HA	1:J:2877:THR:HB	1.97	0.46
1:A:3787:ASP:OD1	1:A:3790:PHE:N	2.49	0.45
1:D:36:CYS:SG	1:D:37:LEU:N	2.89	0.45
1:D:564:ARG:HG3	1:D:566:GLU:HG3	1.98	0.45
1:D:2515:LEU:HA	1:D:2518:ASN:HD22	1.80	0.45
1:G:25:THR:HG22	1:G:34:LYS:HG2	1.99	0.45
1:G:36:CYS:SG	1:G:37:LEU:N	2.89	0.45
1:G:150:GLN:NE2	1:G:158:CYS:SG	2.89	0.45
1:G:1153:GLY:N	1:G:1183:LEU:O	2.49	0.45
1:G:3804:LEU:HD13	1:G:3910:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:25:THR:HG22	1:J:34:LYS:HG2	1.99	0.45
1:J:44:ASN:HD21	1:J:46:LEU:HB2	1.81	0.45
1:J:505:LEU:HD23	1:J:530:LEU:HD13	1.96	0.45
1:J:784:ILE:HG23	1:J:788:PHE:HE2	1.80	0.45
1:A:3645:LEU:HB3	1:A:3665:LEU:HB2	1.97	0.45
1:A:4849:ILE:HD11	1:D:4819:TYR:CB	2.46	0.45
1:D:649:VAL:O	1:D:1627:PHE:N	2.46	0.45
1:G:161:THR:HG23	1:G:184:VAL:HB	1.98	0.45
1:G:169:ARG:HH22	1:G:176:ARG:HD2	1.81	0.45
1:G:784:ILE:HG23	1:G:788:PHE:HE2	1.80	0.45
1:G:1304:LEU:HB2	1:G:1541:PRO:HG2	1.96	0.45
1:G:1769:VAL:HB	2:H:55:VAL:HA	1.97	0.45
1:G:4831:GLU:N	1:G:4831:GLU:OE1	2.49	0.45
1:J:3665:LEU:HD23	1:J:3735:ARG:HH11	1.80	0.45
1:J:4856:ILE:HA	1:J:4860:LEU:HD23	1.97	0.45
1:A:36:CYS:SG	1:A:37:LEU:N	2.89	0.45
1:A:161:THR:HG23	1:A:184:VAL:HB	1.98	0.45
1:D:162:ILE:HG23	1:D:181:LEU:HD13	1.99	0.45
1:D:1449:ASP:OD1	1:D:1449:ASP:N	2.46	0.45
1:D:3665:LEU:HD23	1:D:3735:ARG:HH11	1.80	0.45
1:D:4911:LEU:HD23	1:D:4911:LEU:HA	1.81	0.45
1:G:1690:GLU:O	1:G:1692:LYS:NZ	2.45	0.45
1:J:36:CYS:SG	1:J:37:LEU:N	2.89	0.45
1:J:881:ILE:HD11	1:J:952:ILE:HG23	1.98	0.45
1:A:2409:LEU:HA	1:A:2412:ALA:HB3	1.98	0.45
1:A:3900:ASP:OD1	1:A:3900:ASP:N	2.39	0.45
1:D:4856:ILE:HA	1:D:4860:LEU:HD23	1.97	0.45
1:G:309:MET:SD	1:G:312:LYS:NZ	2.75	0.45
1:G:1751:ILE:HG13	1:G:1921:HIS:HB2	1.98	0.45
1:G:2409:LEU:HA	1:G:2412:ALA:HB3	1.98	0.45
1:G:2515:LEU:HA	1:G:2518:ASN:HD22	1.80	0.45
1:J:150:GLN:NE2	1:J:158:CYS:SG	2.89	0.45
1:J:425:LEU:HD21	1:J:452:VAL:HG13	1.98	0.45
1:J:3844:LEU:HD23	1:J:3844:LEU:HA	1.78	0.45
1:J:4045:SER:HB3	1:J:4048:ASP:HB2	1.98	0.45
1:A:207:PHE:CB	1:D:2326:ILE:C	2.85	0.45
1:A:1938:GLN:NE2	1:A:3611:ASN:O	2.50	0.45
1:A:2326:ILE:C	1:J:207:PHE:CB	2.85	0.45
1:A:4930:ASP:O	1:A:4934:HIS:NE2	2.50	0.45
1:D:25:THR:HG22	1:D:34:LYS:HG2	1.99	0.45
1:D:169:ARG:HH22	1:D:176:ARG:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2562:LEU:O	1:G:2566:GLN:N	2.46	0.45
1:J:1751:ILE:HG13	1:J:1921:HIS:HB2	1.98	0.45
1:A:2543:ALA:HA	1:A:2877:THR:HB	1.97	0.45
1:D:1116:GLY:HA3	1:D:1136:ALA:HA	1.99	0.45
1:D:3730:ALA:HA	1:D:3733:HIS:CE1	2.52	0.45
1:D:3880:LEU:HD11	1:D:3940:ARG:HD2	1.99	0.45
1:D:3946:VAL:HA	1:D:3949:LEU:HD12	1.99	0.45
1:D:4831:GLU:OE1	1:D:4831:GLU:N	2.49	0.45
1:G:695:VAL:HG22	1:G:792:VAL:HG23	1.99	0.45
1:G:1116:GLY:HA3	1:G:1136:ALA:HA	1.99	0.45
1:G:3730:ALA:HA	1:G:3733:HIS:CE1	2.52	0.45
1:G:4856:ILE:HA	1:G:4860:LEU:HD23	1.97	0.45
1:J:1116:GLY:HA3	1:J:1136:ALA:HA	1.99	0.45
1:A:334:SER:OG	1:A:335:LYS:N	2.49	0.45
1:A:1116:GLY:HA3	1:A:1136:ALA:HA	1.99	0.45
1:A:1152:TYR:OH	1:A:1175:PHE:O	2.35	0.45
1:D:161:THR:HG23	1:D:184:VAL:HB	1.98	0.45
1:G:974:SER:OG	1:G:974:SER:O	2.35	0.45
1:G:3714:SER:OG	1:G:3717:GLU:OE2	2.31	0.45
1:G:4045:SER:HB3	1:G:4048:ASP:HB2	1.98	0.45
1:G:4820:VAL:O	1:G:4824:ALA:CB	2.65	0.45
1:J:52:THR:O	1:J:55:SER:OG	2.33	0.45
1:J:1611:ILE:N	1:J:1620:GLN:O	2.38	0.45
1:J:1775:CYS:SG	1:J:1776:TYR:N	2.88	0.45
1:A:162:ILE:HG23	1:A:181:LEU:HD13	1.99	0.45
1:D:119:ILE:HD13	1:D:162:ILE:HD11	1.99	0.45
1:D:150:GLN:NE2	1:D:158:CYS:SG	2.89	0.45
1:G:334:SER:OG	1:G:335:LYS:N	2.49	0.45
1:G:564:ARG:HG3	1:G:566:GLU:HG3	1.98	0.45
1:G:1265:HIS:CD2	1:G:1267:HIS:H	2.34	0.45
1:G:1293:GLN:NE2	1:G:1548:THR:O	2.43	0.45
1:J:50:GLU:OE2	1:J:319:LYS:NZ	2.46	0.45
1:J:162:ILE:HG23	1:J:181:LEU:HD13	1.99	0.45
1:J:305:TYR:N	1:J:317:MET:O	2.41	0.45
1:J:3730:ALA:HA	1:J:3733:HIS:CE1	2.52	0.45
1:J:4733:GLY:HA3	1:J:4740:PHE:HD1	1.81	0.45
1:A:25:THR:HG22	1:A:34:LYS:HG2	1.99	0.45
1:A:881:ILE:HD11	1:A:952:ILE:HG23	1.98	0.45
1:D:3787:ASP:OD1	1:D:3790:PHE:N	2.49	0.45
1:D:4733:GLY:HA3	1:D:4740:PHE:HD1	1.81	0.45
1:D:4854:PHE:CD1	1:D:4854:PHE:O	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:119:ILE:HD13	1:G:162:ILE:HD11	1.99	0.45
1:G:992:GLN:HA	1:G:1064:LEU:HD12	1.99	0.45
1:G:1682:GLU:HG2	1:G:1685:LEU:HD12	1.99	0.45
1:G:1775:CYS:SG	1:G:1776:TYR:N	2.88	0.45
1:G:1904:LYS:O	1:G:1908:CYS:N	2.49	0.45
1:G:2391:THR:HG22	1:G:2465:HIS:HE1	1.81	0.45
1:J:4930:ASP:O	1:J:4934:HIS:NE2	2.50	0.45
1:A:150:GLN:NE2	1:A:158:CYS:SG	2.89	0.45
1:A:716:ASN:HD21	1:A:791:VAL:HG23	1.82	0.45
1:A:4819:TYR:CD1	1:A:4819:TYR:O	2.70	0.45
1:D:706:TYR:HH	1:D:1254:ARG:H	1.64	0.45
1:D:2409:LEU:HA	1:D:2412:ALA:HB3	1.98	0.45
1:D:4130:PHE:O	1:D:4134:LEU:N	2.50	0.45
1:G:162:ILE:HG23	1:G:181:LEU:HD13	1.99	0.45
1:G:272:ARG:HA	1:G:301:THR:HG21	1.98	0.45
1:G:778:MET:HE3	1:G:1480:ILE:HD11	1.99	0.45
1:G:3787:ASP:OD1	1:G:3790:PHE:N	2.49	0.45
1:G:3946:VAL:HA	1:G:3949:LEU:HD12	1.99	0.45
1:G:4852:PHE:CD1	1:G:4852:PHE:O	2.70	0.45
1:J:4510:VAL:HG23	1:J:4576:LEU:HD12	1.99	0.45
1:J:4819:TYR:CD1	1:J:4819:TYR:O	2.70	0.45
1:A:4854:PHE:O	1:A:4854:PHE:CD1	2.70	0.44
1:D:716:ASN:HD21	1:D:791:VAL:HG23	1.82	0.44
1:D:778:MET:HE3	1:D:1480:ILE:HD11	1.99	0.44
1:D:1611:ILE:N	1:D:1620:GLN:O	2.38	0.44
1:D:1682:GLU:HG2	1:D:1685:LEU:HD12	1.99	0.44
1:D:2607:PRO:O	1:D:2611:LEU:N	2.51	0.44
1:D:4045:SER:HB3	1:D:4048:ASP:HB2	1.98	0.44
1:G:308:LEU:HD23	1:G:365:HIS:CD2	2.52	0.44
1:G:4603:ARG:NE	1:G:4632:ASP:OD2	2.49	0.44
1:G:4815:MET:O	1:G:4819:TYR:HB3	2.17	0.44
1:J:2162:LEU:O	1:J:2166:LEU:N	2.45	0.44
1:J:2876:ASP:OD1	1:J:2876:ASP:N	2.31	0.44
1:A:119:ILE:HD13	1:A:162:ILE:HD11	1.99	0.44
1:A:308:LEU:HD23	1:A:365:HIS:CD2	2.52	0.44
1:A:1738:LEU:HD21	1:A:1928:ALA:HB3	1.99	0.44
1:A:2790:ILE:HG23	1:A:2904:VAL:HG22	2.00	0.44
1:A:4782:TYR:CB	1:A:4851:PHE:HE1	2.30	0.44
1:A:4816:PHE:CD1	1:A:4816:PHE:O	2.70	0.44
1:A:4861:ALA:HB2	1:D:4864:GLN:CD	2.37	0.44
1:D:695:VAL:HG22	1:D:792:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2327:ARG:H	1:D:2327:ARG:HG3	1.49	0.44
1:D:4852:PHE:O	1:D:4852:PHE:CG	2.70	0.44
1:D:4896:ASN:O	1:D:4900:ASP:N	2.50	0.44
1:G:1938:GLN:NE2	1:G:3611:ASN:O	2.50	0.44
1:G:2070:TRP:O	1:G:2074:SER:OG	2.32	0.44
1:G:4640:SER:OG	1:G:4703:ASP:OD2	2.31	0.44
1:J:169:ARG:HH22	1:J:176:ARG:HD2	1.81	0.44
1:J:1153:GLY:N	1:J:1183:LEU:O	2.49	0.44
1:J:1790:LYS:O	1:J:1794:MET:N	2.48	0.44
1:J:4854:PHE:CD1	1:J:4854:PHE:O	2.70	0.44
1:A:1682:GLU:HG2	1:A:1685:LEU:HD12	1.99	0.44
3:C:50:GLN:HA	3:C:53:ILE:HG22	2.00	0.44
1:D:272:ARG:HA	1:D:301:THR:HG21	1.98	0.44
1:D:308:LEU:HD23	1:D:365:HIS:CD2	2.52	0.44
1:D:1712:SER:HA	1:D:1715:ALA:HB3	1.99	0.44
1:G:4930:ASP:O	1:G:4934:HIS:NE2	2.50	0.44
1:J:119:ILE:HD13	1:J:162:ILE:HD11	1.99	0.44
1:J:564:ARG:HG3	1:J:566:GLU:HG3	1.98	0.44
1:J:649:VAL:O	1:J:1627:PHE:N	2.46	0.44
1:J:992:GLN:HA	1:J:1064:LEU:HD12	1.99	0.44
1:J:3943:ASP:OD1	1:J:3943:ASP:N	2.49	0.44
1:A:272:ARG:HA	1:A:301:THR:HG21	1.98	0.44
1:A:1057:LEU:O	1:A:1062:TYR:N	2.47	0.44
1:A:1293:GLN:NE2	1:A:1548:THR:O	2.43	0.44
1:D:1751:ILE:HG13	1:D:1921:HIS:HB2	1.98	0.44
1:D:4782:TYR:CE2	1:D:4851:PHE:HD1	2.27	0.44
1:D:4787:PHE:HZ	1:G:4522:LYS:HA	1.82	0.44
1:D:4930:ASP:O	1:D:4934:HIS:NE2	2.50	0.44
1:G:4861:ALA:O	1:G:4865:GLY:N	2.47	0.44
2:H:35:LYS:HE2	2:H:35:LYS:HB3	1.81	0.44
1:J:1057:LEU:O	1:J:1062:TYR:N	2.47	0.44
1:J:1682:GLU:HG2	1:J:1685:LEU:HD12	1.99	0.44
1:J:2327:ARG:H	1:J:2327:ARG:HG3	1.53	0.44
1:J:2790:ILE:HG23	1:J:2904:VAL:HG22	2.00	0.44
1:J:4852:PHE:O	1:J:4852:PHE:CD1	2.70	0.44
1:A:1153:GLY:N	1:A:1183:LEU:O	2.49	0.44
1:A:1690:GLU:OE2	1:A:1790:LYS:NZ	2.36	0.44
1:A:4733:GLY:HA3	1:A:4740:PHE:HD1	1.81	0.44
2:B:35:LYS:HE2	2:B:35:LYS:HB3	1.81	0.44
1:D:1922:ARG:HH22	1:D:2039:TYR:HD1	1.66	0.44
1:D:3844:LEU:HD23	1:D:3844:LEU:HA	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4510:VAL:HG23	1:D:4576:LEU:HD12	1.99	0.44
1:D:4852:PHE:O	1:D:4852:PHE:CD1	2.70	0.44
1:G:1922:ARG:HH22	1:G:2039:TYR:HD1	1.66	0.44
1:G:4130:PHE:O	1:G:4134:LEU:N	2.50	0.44
1:G:4854:PHE:CD1	1:G:4854:PHE:O	2.70	0.44
1:J:716:ASN:HD21	1:J:791:VAL:HG23	1.82	0.44
1:J:1190:LEU:HB2	1:J:1193:LYS:HE2	2.00	0.44
1:J:1938:GLN:NE2	1:J:3611:ASN:O	2.50	0.44
1:J:4605:LYS:HE3	1:J:4605:LYS:HB3	1.74	0.44
1:J:4627:ILE:O	1:J:4631:TRP:N	2.48	0.44
1:J:4852:PHE:O	1:J:4852:PHE:CG	2.70	0.44
1:A:328:ALA:HB1	1:A:366:ILE:HD12	2.00	0.44
1:A:1098:ALA:O	1:A:1101:TRP:NE1	2.31	0.44
1:D:190:ARG:HH12	1:G:2423:ILE:HG23	1.80	0.44
1:D:1938:GLN:NE2	1:D:3611:ASN:O	2.50	0.44
1:G:299:HIS:N	1:G:304:LYS:O	2.43	0.44
1:G:1101:TRP:HA	1:G:1237:GLU:HB2	1.99	0.44
1:G:1102:TYR:N	1:G:1237:GLU:O	2.51	0.44
1:G:1246:ASP:HB2	1:G:1605:LYS:HE2	2.00	0.44
1:G:3880:LEU:HD11	1:G:3940:ARG:HD2	1.99	0.44
1:J:308:LEU:HD23	1:J:365:HIS:CD2	2.52	0.44
1:J:505:LEU:HD12	1:J:505:LEU:HA	1.88	0.44
1:J:1246:ASP:HB2	1:J:1605:LYS:HE2	2.00	0.44
1:J:2409:LEU:HA	1:J:2412:ALA:HB3	1.98	0.44
1:J:4605:LYS:HD2	1:J:4609:ARG:HD3	2.00	0.44
1:J:4816:PHE:CD1	1:J:4816:PHE:O	2.70	0.44
1:A:894:VAL:HG22	1:A:918:LEU:HA	2.00	0.44
1:A:1751:ILE:HG13	1:A:1921:HIS:HB2	1.98	0.44
1:A:1790:LYS:O	1:A:1794:MET:N	2.48	0.44
1:A:2848:ASN:O	1:A:2852:ILE:N	2.49	0.44
1:A:3946:VAL:HA	1:A:3949:LEU:HD12	1.99	0.44
1:A:4852:PHE:O	1:A:4852:PHE:CG	2.70	0.44
1:A:4896:ASN:O	1:A:4900:ASP:N	2.50	0.44
1:D:705:PRO:HG3	1:D:838:ARG:HB2	2.00	0.44
1:D:1246:ASP:HB2	1:D:1605:LYS:HE2	2.00	0.44
1:D:4640:SER:OG	1:D:4703:ASP:OD2	2.31	0.44
1:G:1098:ALA:O	1:G:1101:TRP:NE1	2.31	0.44
1:G:3943:ASP:OD1	1:G:3943:ASP:N	2.49	0.44
1:J:343:ARG:HB3	1:J:344:LYS:H	1.72	0.44
1:J:695:VAL:HG22	1:J:792:VAL:HG23	1.99	0.44
1:J:742:SER:OG	1:J:1472:GLU:OE2	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2061:GLN:O	1:J:2064:SER:OG	2.36	0.44
1:J:4782:TYR:CE2	1:J:4851:PHE:HD1	2.28	0.44
1:J:4853:PHE:CD1	1:J:4853:PHE:O	2.71	0.44
1:A:1131:ASP:N	1:A:1131:ASP:OD1	2.48	0.44
1:A:1190:LEU:HB2	1:A:1193:LYS:HE2	2.00	0.44
1:A:2607:PRO:O	1:A:2611:LEU:N	2.51	0.44
1:A:4787:PHE:HZ	1:D:4522:LYS:HA	1.83	0.44
1:D:207:PHE:CB	1:G:2326:ILE:C	2.86	0.44
1:D:982:ASP:OD2	1:D:982:ASP:N	2.41	0.44
1:D:1738:LEU:HD21	1:D:1928:ALA:HB3	1.99	0.44
1:J:894:VAL:HG22	1:J:918:LEU:HA	2.00	0.44
1:J:1089:ARG:HH21	1:J:1600:PRO:HG3	1.83	0.44
1:J:3787:ASP:OD1	1:J:3790:PHE:N	2.49	0.44
1:J:4796:LYS:HE2	1:J:4805:MET:HB3	2.00	0.44
1:J:4875:ARG:O	1:J:4875:ARG:HD2	2.18	0.44
1:J:4896:ASN:O	1:J:4900:ASP:N	2.50	0.44
3:L:50:GLN:HA	3:L:53:ILE:HG22	2.00	0.44
3:L:50:GLN:O	3:L:54:ASN:HB2	2.18	0.44
1:A:705:PRO:HG3	1:A:838:ARG:HB2	2.00	0.44
1:A:1102:TYR:N	1:A:1237:GLU:O	2.51	0.44
1:A:4510:VAL:HG23	1:A:4576:LEU:HD12	1.99	0.44
1:A:4595:LYS:HA	1:A:4595:LYS:HD3	1.77	0.44
1:D:1057:LEU:O	1:D:1062:TYR:N	2.47	0.44
1:D:1102:TYR:N	1:D:1237:GLU:O	2.51	0.44
1:D:1839:LEU:HA	1:D:1842:ILE:HG22	2.00	0.44
3:F:50:GLN:NE2	3:F:54:ASN:OD1	2.51	0.44
1:G:328:ALA:HB1	1:G:366:ILE:HD12	2.00	0.44
1:G:1210:ALA:N	1:G:1211:GLN:OE1	2.51	0.44
1:G:1258:PHE:HA	1:G:1595:LEU:HA	1.99	0.44
1:G:1839:LEU:HA	1:G:1842:ILE:HG22	2.00	0.44
1:G:4816:PHE:CD1	1:G:4816:PHE:O	2.70	0.44
1:G:4853:PHE:CD1	1:G:4853:PHE:O	2.71	0.44
1:J:121:LEU:HD23	1:J:121:LEU:HA	1.82	0.44
1:J:706:TYR:HH	1:J:1254:ARG:H	1.64	0.44
1:J:1258:PHE:HA	1:J:1595:LEU:HA	1.99	0.44
1:J:1738:LEU:HD21	1:J:1928:ALA:HB3	1.99	0.44
1:J:1839:LEU:HA	1:J:1842:ILE:HG22	2.00	0.44
1:J:3880:LEU:HD11	1:J:3940:ARG:HD2	1.99	0.44
1:J:4819:TYR:CD1	1:J:4819:TYR:C	2.90	0.44
1:A:1246:ASP:HB2	1:A:1605:LYS:HE2	2.00	0.43
1:A:3730:ALA:HA	1:A:3733:HIS:CE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:505:LEU:HD12	1:D:505:LEU:HA	1.88	0.43
1:D:1210:ALA:N	1:D:1211:GLN:OE1	2.51	0.43
1:D:4034:LYS:HZ2	1:D:4081:TYR:HE2	1.64	0.43
1:D:4861:ALA:O	1:D:4865:GLY:N	2.47	0.43
1:D:4909:HIS:HA	1:D:4913:GLU:HG2	2.00	0.43
2:E:35:LYS:HE2	2:E:35:LYS:HB3	1.81	0.43
1:G:4852:PHE:O	1:G:4852:PHE:CG	2.70	0.43
1:G:4896:ASN:O	1:G:4900:ASP:N	2.50	0.43
1:J:272:ARG:HA	1:J:301:THR:HG21	1.98	0.43
1:J:299:HIS:N	1:J:304:LYS:O	2.43	0.43
1:J:309:MET:SD	1:J:312:LYS:NZ	2.75	0.43
1:J:1102:TYR:N	1:J:1237:GLU:O	2.51	0.43
1:J:1124:PRO:O	1:J:1598:ARG:NE	2.51	0.43
1:J:3946:VAL:HA	1:J:3949:LEU:HD12	1.99	0.43
1:J:4094:ASP:HA	1:J:4097:PHE:HB3	2.00	0.43
1:J:4148:ARG:NH1	1:J:4913:GLU:OE1	2.40	0.43
1:J:4819:TYR:CD1	1:J:4823:ARG:CB	3.01	0.43
1:A:244:CYS:N	1:A:263:GLU:O	2.48	0.43
1:A:1089:ARG:HH21	1:A:1600:PRO:HG3	1.83	0.43
1:A:1101:TRP:HA	1:A:1237:GLU:HB2	1.99	0.43
1:A:1125:ASP:OD1	1:A:1597:SER:OG	2.29	0.43
1:A:1839:LEU:HA	1:A:1842:ILE:HG22	2.00	0.43
3:C:50:GLN:NE2	3:C:54:ASN:OD1	2.51	0.43
1:D:803:LEU:HB3	1:D:811:PHE:HA	2.00	0.43
1:D:992:GLN:HA	1:D:1064:LEU:HD12	1.99	0.43
1:D:1101:TRP:HA	1:D:1237:GLU:HB2	1.99	0.43
1:D:1790:LYS:O	1:D:1794:MET:N	2.48	0.43
1:D:2061:GLN:O	1:D:2064:SER:OG	2.36	0.43
1:D:4747:ILE:HD12	1:D:4747:ILE:HA	1.92	0.43
1:D:4892:CYS:SG	1:D:4914:HIS:NE2	2.92	0.43
1:G:2607:PRO:O	1:G:2611:LEU:N	2.51	0.43
1:G:4595:LYS:HA	1:G:4595:LYS:HD3	1.77	0.43
3:I:50:GLN:HA	3:I:53:ILE:HG22	2.00	0.43
1:J:161:THR:HG23	1:J:184:VAL:HB	1.98	0.43
1:J:626:ARG:NH2	1:J:1668:GLY:O	2.36	0.43
1:J:3677:LEU:HD23	1:J:3677:LEU:HA	1.88	0.43
1:J:3804:LEU:O	1:J:3885:SER:OG	2.26	0.43
1:A:190:ARG:HH12	1:D:2423:ILE:HG23	1.78	0.43
1:A:695:VAL:HG22	1:A:792:VAL:HG23	1.99	0.43
3:C:50:GLN:O	3:C:54:ASN:HB2	2.18	0.43
1:D:4817:HIS:NE2	1:D:4828:ILE:CD1	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:68:LEU:HA	2:E:103:LEU:HD23	2.00	0.43
3:F:50:GLN:HA	3:F:53:ILE:HG22	2.00	0.43
1:G:647:ARG:NH1	1:G:648:LEU:O	2.51	0.43
1:G:803:LEU:HB3	1:G:811:PHE:HA	2.00	0.43
1:G:1190:LEU:HB2	1:G:1193:LYS:HE2	2.00	0.43
1:G:1738:LEU:HD21	1:G:1928:ALA:HB3	1.99	0.43
1:G:4892:CYS:SG	1:G:4914:HIS:NE2	2.92	0.43
1:J:974:SER:OG	1:J:974:SER:O	2.35	0.43
1:J:1101:TRP:HA	1:J:1237:GLU:HB2	1.99	0.43
1:J:1609:SER:OG	1:J:1621:CYS:SG	2.72	0.43
1:J:3973:MET:O	1:J:3977:LYS:N	2.44	0.43
1:A:2562:LEU:O	1:A:2566:GLN:N	2.46	0.43
1:A:4605:LYS:HD2	1:A:4609:ARG:HD3	2.00	0.43
1:A:4627:ILE:O	1:A:4631:TRP:N	2.48	0.43
1:A:4852:PHE:CD2	1:A:4852:PHE:O	2.70	0.43
1:D:374:TYR:HB2	1:D:389:ARG:HB3	2.00	0.43
1:D:1124:PRO:O	1:D:1598:ARG:NE	2.52	0.43
1:G:1712:SER:HA	1:G:1715:ALA:HB3	1.99	0.43
1:G:2061:GLN:O	1:G:2064:SER:OG	2.36	0.43
1:G:2855:LYS:HA	1:G:2855:LYS:HD2	1.88	0.43
1:A:481:ALA:O	1:A:485:ARG:NE	2.51	0.43
1:A:495:ILE:O	1:A:499:LEU:N	2.51	0.43
1:A:1712:SER:HA	1:A:1715:ALA:HB3	1.99	0.43
1:A:2643:ARG:O	1:A:2647:TRP:N	2.47	0.43
1:A:4515:ASN:HB3	1:J:4780:TYR:HH	1.80	0.43
1:A:4892:CYS:SG	1:A:4914:HIS:NE2	2.92	0.43
1:D:35:LEU:HB3	1:D:49:LEU:HB3	2.01	0.43
1:D:4042:GLY:O	1:D:4081:TYR:N	2.48	0.43
1:D:4796:LYS:HE2	1:D:4805:MET:HB3	2.00	0.43
1:G:374:TYR:HB2	1:G:389:ARG:HB3	2.00	0.43
1:G:1090:ALA:HB3	1:G:1203:PRO:HD2	2.01	0.43
1:G:2845:MET:HB3	1:G:2845:MET:HE2	1.88	0.43
1:G:4589:ILE:HD13	1:G:4589:ILE:HA	1.89	0.43
1:J:2161:ASN:O	1:J:2165:ALA:N	2.48	0.43
1:A:2897:LEU:HD23	1:A:2897:LEU:HA	1.92	0.43
1:A:3880:LEU:HD11	1:A:3940:ARG:HD2	1.99	0.43
1:A:4094:ASP:HA	1:A:4097:PHE:HB3	2.00	0.43
1:A:4850:THR:O	1:A:4854:PHE:CB	2.66	0.43
1:D:2790:ILE:HG23	1:D:2904:VAL:HG22	2.00	0.43
1:G:705:PRO:HG3	1:G:838:ARG:HB2	2.00	0.43
1:G:1124:PRO:O	1:G:1598:ARG:NE	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3879:LEU:HA	1:G:3882:VAL:HB	2.01	0.43
1:G:4047:ARG:HA	1:G:4050:HIS:HB3	2.00	0.43
1:J:1712:SER:HA	1:J:1715:ALA:HB3	1.99	0.43
1:J:2138:GLU:O	1:J:2141:LYS:NZ	2.34	0.43
1:J:3724:LYS:HA	1:J:3724:LYS:HD3	1.81	0.43
1:A:803:LEU:HB3	1:A:811:PHE:HA	2.00	0.43
1:A:1210:ALA:N	1:A:1211:GLN:OE1	2.51	0.43
1:A:1258:PHE:HA	1:A:1595:LEU:HA	1.99	0.43
1:A:1611:ILE:N	1:A:1620:GLN:O	2.38	0.43
1:A:2116:ASP:OD1	1:A:2153:ASN:ND2	2.47	0.43
1:A:4605:LYS:HE3	1:A:4605:LYS:HB3	1.74	0.43
1:D:328:ALA:HB1	1:D:366:ILE:HD12	2.00	0.43
1:D:1089:ARG:HH21	1:D:1600:PRO:HG3	1.83	0.43
1:D:4651:LYS:NZ	1:D:4672:GLY:O	2.40	0.43
1:G:657:PRO:HB3	1:G:834:VAL:HG12	2.01	0.43
1:G:716:ASN:HD21	1:G:791:VAL:HG23	1.82	0.43
1:G:725:TYR:HA	1:G:732:LEU:HA	2.01	0.43
1:G:894:VAL:HG22	1:G:918:LEU:HA	2.00	0.43
1:G:2154:LYS:HA	1:G:2154:LYS:HD2	1.93	0.43
1:G:3804:LEU:O	1:G:3885:SER:OG	2.26	0.43
1:G:4605:LYS:HD2	1:G:4609:ARG:HD3	2.00	0.43
1:G:4909:HIS:HA	1:G:4913:GLU:HG2	2.00	0.43
1:J:657:PRO:HB3	1:J:834:VAL:HG12	2.01	0.43
1:J:778:MET:HE3	1:J:1480:ILE:HD11	2.00	0.43
1:J:1210:ALA:N	1:J:1211:GLN:OE1	2.51	0.43
1:J:4909:HIS:HA	1:J:4913:GLU:HG2	2.00	0.43
1:A:1905:LEU:HB2	1:A:2081:LEU:HD12	2.01	0.43
2:B:68:LEU:HA	2:B:103:LEU:HD23	2.00	0.43
1:D:250:GLY:HA2	1:D:257:ARG:HE	1.84	0.43
1:D:973:THR:HG21	1:D:977:LYS:HA	2.01	0.43
1:D:1258:PHE:HA	1:D:1595:LEU:HA	1.99	0.43
1:D:4817:HIS:CD2	1:D:4828:ILE:CD1	3.02	0.43
1:G:1089:ARG:HH21	1:G:1600:PRO:HG3	1.83	0.43
1:G:2790:ILE:HG23	1:G:2904:VAL:HG22	2.00	0.43
1:G:4796:LYS:HE2	1:G:4805:MET:HB3	2.00	0.43
1:J:1905:LEU:HB2	1:J:2081:LEU:HD12	2.01	0.43
1:J:1922:ARG:HH22	1:J:2039:TYR:HD1	1.66	0.43
2:K:68:LEU:HA	2:K:103:LEU:HD23	2.00	0.43
1:A:992:GLN:HA	1:A:1064:LEU:HD12	1.99	0.43
1:A:1609:SER:OG	1:A:1621:CYS:SG	2.72	0.43
1:A:4853:PHE:CD1	1:A:4853:PHE:O	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:LEU:HD23	2:B:104:LEU:HA	1.90	0.43
1:D:745:ASN:ND2	1:D:773:GLN:OE1	2.49	0.43
1:D:1190:LEU:HB2	1:D:1193:LYS:HE2	2.00	0.43
1:D:2537:ALA:O	1:D:2541:HIS:N	2.50	0.43
1:D:3879:LEU:HA	1:D:3882:VAL:HB	2.01	0.43
1:D:3943:ASP:OD1	1:D:3943:ASP:N	2.49	0.43
1:D:4861:ALA:HB2	1:G:4864:GLN:CD	2.38	0.43
1:G:305:TYR:N	1:G:317:MET:O	2.41	0.43
1:G:325:LYS:O	1:G:365:HIS:NE2	2.52	0.43
1:G:4654:VAL:O	1:G:4659:GLY:N	2.52	0.43
1:J:2116:ASP:OD1	1:J:2153:ASN:ND2	2.47	0.43
1:J:2639:LEU:O	1:J:2643:ARG:N	2.44	0.43
1:J:4892:CYS:SG	1:J:4914:HIS:NE2	2.92	0.43
1:A:1256:PRO:HD2	1:A:1451:HIS:HB3	2.01	0.43
1:D:2717:LYS:H	1:D:2717:LYS:HG2	1.60	0.43
1:D:3756:VAL:O	1:D:3759:THR:OG1	2.34	0.43
1:G:1110:ALA:HA	1:G:1156:TRP:CZ2	2.54	0.43
1:G:2116:ASP:OD1	1:G:2153:ASN:ND2	2.47	0.43
1:G:4094:ASP:HA	1:G:4097:PHE:HB3	2.00	0.43
1:J:705:PRO:HG3	1:J:838:ARG:HB2	2.00	0.43
1:J:1166:VAL:HG13	1:J:1173:MET:HG3	2.01	0.43
1:J:3879:LEU:HA	1:J:3882:VAL:HB	2.01	0.43
1:A:262:TYR:HB2	1:A:389:ARG:HB2	2.01	0.42
1:A:745:ASN:ND2	1:A:773:GLN:OE1	2.49	0.42
1:A:778:MET:HE3	1:A:1480:ILE:HD11	2.00	0.42
1:A:1124:PRO:O	1:A:1598:ARG:NE	2.51	0.42
1:A:1945:TYR:OH	1:A:1993:ILE:O	2.35	0.42
1:A:3879:LEU:HA	1:A:3882:VAL:HB	2.01	0.42
1:A:4130:PHE:O	1:A:4134:LEU:N	2.50	0.42
3:C:65:ASP:OD1	3:C:65:ASP:N	2.50	0.42
1:D:894:VAL:HG22	1:D:918:LEU:HA	2.00	0.42
1:D:974:SER:OG	1:D:974:SER:O	2.35	0.42
1:D:3669:ILE:HD13	1:D:3737:ALA:HB2	2.01	0.42
1:D:4047:ARG:HA	1:D:4050:HIS:HB3	2.00	0.42
1:G:35:LEU:HB3	1:G:49:LEU:HB3	2.01	0.42
1:G:673:TRP:HB2	1:G:759:LEU:HB3	2.01	0.42
1:J:296:ARG:HG2	1:J:327:THR:HG23	2.01	0.42
1:J:745:ASN:ND2	1:J:773:GLN:OE1	2.49	0.42
1:J:2607:PRO:O	1:J:2611:LEU:N	2.51	0.42
1:J:4559:HIS:ND1	1:J:4738:PHE:CE2	2.87	0.42
1:A:673:TRP:HB2	1:A:759:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1922:ARG:HH22	1:A:2039:TYR:HD1	1.66	0.42
1:A:4045:SER:HA	1:A:4078:THR:HA	2.02	0.42
1:D:425:LEU:HD11	1:D:452:VAL:HA	2.01	0.42
1:D:1177:LEU:HB3	1:D:1182:LEU:HD21	2.02	0.42
1:D:1905:LEU:HB2	1:D:2081:LEU:HD12	2.01	0.42
1:D:2222:LEU:HD12	1:D:2222:LEU:HA	1.89	0.42
1:D:3643:GLU:OE2	1:D:3731:ARG:NH2	2.53	0.42
1:D:4045:SER:HA	1:D:4078:THR:HA	2.02	0.42
1:D:4148:ARG:NH1	1:D:4913:GLU:OE1	2.40	0.42
1:D:4605:LYS:HD2	1:D:4609:ARG:HD3	2.00	0.42
3:F:50:GLN:O	3:F:54:ASN:HB2	2.18	0.42
1:G:52:THR:O	1:G:55:SER:OG	2.33	0.42
1:G:4510:VAL:HG23	1:G:4576:LEU:HD12	1.99	0.42
1:J:328:ALA:HB1	1:J:366:ILE:HD12	2.00	0.42
1:J:433:LEU:O	1:J:437:SER:N	2.53	0.42
1:J:731:HIS:CG	1:J:740:THR:HA	2.54	0.42
1:J:1177:LEU:HB3	1:J:1182:LEU:HD21	2.02	0.42
1:A:325:LYS:O	1:A:365:HIS:NE2	2.52	0.42
1:A:374:TYR:HB2	1:A:389:ARG:HB3	2.00	0.42
1:A:725:TYR:HA	1:A:732:LEU:HA	2.01	0.42
1:A:1090:ALA:HB3	1:A:1203:PRO:HD2	2.01	0.42
1:A:1114:ARG:HB2	1:A:1206:SER:HB3	2.01	0.42
1:A:4909:HIS:HA	1:A:4913:GLU:HG2	2.00	0.42
1:D:2154:LYS:HA	1:D:2154:LYS:HD2	1.93	0.42
1:D:2161:ASN:O	1:D:2165:ALA:N	2.48	0.42
1:D:2162:LEU:O	1:D:2166:LEU:N	2.45	0.42
1:D:4654:VAL:O	1:D:4659:GLY:N	2.52	0.42
1:G:851:LEU:HD12	1:G:851:LEU:HA	1.91	0.42
1:G:1054:VAL:HA	1:G:1057:LEU:HB2	2.01	0.42
1:G:1905:LEU:HB2	1:G:2081:LEU:HD12	2.01	0.42
1:G:3016:VAL:O	1:G:3020:ILE:N	2.47	0.42
3:I:50:GLN:NE2	3:I:54:ASN:OD1	2.51	0.42
1:J:647:ARG:NH1	1:J:648:LEU:O	2.51	0.42
1:J:4576:LEU:O	1:J:4580:HIS:N	2.47	0.42
1:A:2061:GLN:O	1:A:2064:SER:OG	2.36	0.42
1:A:3643:GLU:OE2	1:A:3731:ARG:NH2	2.53	0.42
1:D:52:THR:O	1:D:55:SER:OG	2.33	0.42
1:D:296:ARG:HG2	1:D:327:THR:HG23	2.01	0.42
1:D:1033:VAL:HG23	1:D:1038:LEU:HD23	2.02	0.42
1:D:1166:VAL:HG13	1:D:1173:MET:HG3	2.01	0.42
1:D:4605:LYS:HB3	1:D:4605:LYS:HE3	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:34:LYS:O	1:G:52:THR:N	2.46	0.42
1:G:1166:VAL:HG13	1:G:1173:MET:HG3	2.01	0.42
1:G:3893:TYR:HA	1:G:3896:LYS:HZ3	1.85	0.42
1:G:4839:GLU:H	1:G:4839:GLU:HG3	1.69	0.42
3:I:50:GLN:O	3:I:54:ASN:HB2	2.18	0.42
1:J:1033:VAL:HG23	1:J:1038:LEU:HD23	2.02	0.42
1:J:1256:PRO:HD2	1:J:1451:HIS:HB3	2.01	0.42
1:J:2421:ARG:O	1:J:2425:ARG:NE	2.50	0.42
1:J:2643:ARG:O	1:J:2647:TRP:N	2.47	0.42
1:J:3643:GLU:OE2	1:J:3731:ARG:NH2	2.53	0.42
1:J:4047:ARG:HA	1:J:4050:HIS:HB3	2.00	0.42
1:A:250:GLY:HA2	1:A:257:ARG:HE	1.84	0.42
1:A:433:LEU:O	1:A:437:SER:N	2.53	0.42
1:A:653:SER:O	1:A:653:SER:OG	2.37	0.42
1:A:973:THR:HG21	1:A:977:LYS:HA	2.01	0.42
1:A:2161:ASN:O	1:A:2165:ALA:N	2.48	0.42
1:A:3621:PHE:O	1:A:3625:TYR:N	2.53	0.42
1:A:3844:LEU:HD23	1:A:3844:LEU:HA	1.78	0.42
1:A:4780:TYR:HH	1:D:4741:ALA:HB1	1.84	0.42
1:A:4935:THR:H	1:A:4938:GLU:HB2	1.85	0.42
1:D:262:TYR:HB2	1:D:389:ARG:HB2	2.01	0.42
1:D:325:LYS:O	1:D:365:HIS:NE2	2.52	0.42
1:D:481:ALA:O	1:D:485:ARG:NE	2.51	0.42
1:D:1054:VAL:HA	1:D:1057:LEU:HB2	2.01	0.42
1:D:1110:ALA:HA	1:D:1156:TRP:CZ2	2.54	0.42
1:D:2639:LEU:O	1:D:2643:ARG:N	2.44	0.42
1:G:479:LEU:HD12	1:G:479:LEU:HA	1.90	0.42
1:G:1431:ARG:HE	1:G:1431:ARG:HB2	1.56	0.42
1:G:4045:SER:HA	1:G:4078:THR:HA	2.02	0.42
1:J:325:LYS:O	1:J:365:HIS:NE2	2.52	0.42
1:J:4589:ILE:HD13	1:J:4589:ILE:HA	1.89	0.42
1:A:590:LYS:HE2	1:A:590:LYS:HB2	1.86	0.42
1:A:731:HIS:CG	1:A:740:THR:HA	2.54	0.42
1:A:1177:LEU:HB3	1:A:1182:LEU:HD21	2.02	0.42
1:A:3777:LYS:HE2	1:A:3777:LYS:HB2	1.89	0.42
1:D:1114:ARG:HB2	1:D:1206:SER:HB3	2.01	0.42
1:D:3638:GLU:N	1:D:3638:GLU:OE1	2.53	0.42
1:D:4094:ASP:HA	1:D:4097:PHE:HB3	2.00	0.42
1:D:4559:HIS:ND1	1:D:4738:PHE:CE2	2.87	0.42
1:G:250:GLY:HA2	1:G:257:ARG:HE	1.84	0.42
1:G:973:THR:HG21	1:G:977:LYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2841:MET:O	1:G:2845:MET:N	2.40	0.42
1:G:4022:LEU:HD12	1:G:4022:LEU:HA	1.86	0.42
1:G:4521:TYR:O	1:G:4521:TYR:CD2	2.72	0.42
1:J:374:TYR:HB2	1:J:389:ARG:HB3	2.00	0.42
1:J:1293:GLN:NE2	1:J:1548:THR:O	2.43	0.42
1:J:1921:HIS:O	1:J:1925:ALA:N	2.52	0.42
1:J:4113:ASP:OD2	1:J:4115:ARG:NH2	2.53	0.42
1:J:4935:THR:H	1:J:4938:GLU:HB2	1.85	0.42
1:A:419:ILE:HD13	1:A:492:GLU:HG3	2.02	0.42
1:A:1033:VAL:HG23	1:A:1038:LEU:HD23	2.02	0.42
1:A:1110:ALA:HA	1:A:1156:TRP:CZ2	2.54	0.42
1:A:4654:VAL:O	1:A:4659:GLY:N	2.52	0.42
1:A:4861:ALA:O	1:A:4865:GLY:N	2.47	0.42
1:D:433:LEU:O	1:D:437:SER:N	2.53	0.42
1:D:992:GLN:HB3	1:D:1054:VAL:HG11	2.02	0.42
1:D:1293:GLN:NE2	1:D:1548:THR:O	2.43	0.42
1:G:425:LEU:HD11	1:G:452:VAL:HA	2.01	0.42
1:G:433:LEU:O	1:G:437:SER:N	2.53	0.42
1:G:1790:LYS:O	1:G:1794:MET:N	2.48	0.42
1:G:4039:ASP:OD2	1:G:4039:ASP:N	2.41	0.42
1:G:4559:HIS:ND1	1:G:4738:PHE:CE2	2.87	0.42
1:G:4605:LYS:HB3	1:G:4605:LYS:HE3	1.74	0.42
2:H:68:LEU:HA	2:H:103:LEU:HD23	2.00	0.42
1:J:466:PRO:HB3	1:J:478:ARG:HG2	2.02	0.42
1:J:673:TRP:HB2	1:J:759:LEU:HB3	2.01	0.42
1:J:803:LEU:HB3	1:J:811:PHE:HA	2.00	0.42
1:J:973:THR:HG21	1:J:977:LYS:HA	2.01	0.42
1:J:4654:VAL:O	1:J:4659:GLY:N	2.52	0.42
1:J:4737:ASN:OD1	1:J:4737:ASN:N	2.39	0.42
3:L:50:GLN:NE2	3:L:54:ASN:OD1	2.51	0.42
1:A:1166:VAL:HG13	1:A:1173:MET:HG3	2.01	0.42
1:A:1265:HIS:HD2	1:A:1267:HIS:H	1.67	0.42
1:A:1785:ASP:N	1:A:1785:ASP:OD1	2.53	0.42
1:A:3669:ILE:HD13	1:A:3737:ALA:HB2	2.02	0.42
1:A:4047:ARG:HA	1:A:4050:HIS:HB3	2.00	0.42
1:A:4796:LYS:HE2	1:A:4805:MET:HB3	2.00	0.42
1:D:73:LEU:HD23	1:D:73:LEU:HA	1.90	0.42
1:D:995:MET:HA	1:D:998:LYS:HD2	2.02	0.42
1:D:3786:LYS:HB3	1:D:3786:LYS:HE2	1.84	0.42
1:G:892:LEU:HD13	1:G:1052:GLU:HB3	2.02	0.42
1:G:1177:LEU:HB3	1:G:1182:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1770:SER:O	1:G:1770:SER:OG	2.32	0.42
1:G:2482:GLN:HA	1:G:2485:LEU:HD13	2.02	0.42
1:G:4576:LEU:O	1:G:4580:HIS:N	2.47	0.42
1:J:35:LEU:HB3	1:J:49:LEU:HB3	2.01	0.42
1:J:892:LEU:HD13	1:J:1052:GLU:HB3	2.01	0.42
1:J:3068:ASP:O	1:J:3072:THR:N	2.47	0.42
1:J:4130:PHE:O	1:J:4134:LEU:N	2.50	0.42
1:A:35:LEU:HB3	1:A:49:LEU:HB3	2.01	0.42
1:A:425:LEU:HD11	1:A:452:VAL:HA	2.01	0.42
1:A:992:GLN:HB3	1:A:1054:VAL:HG11	2.02	0.42
1:D:258:ARG:NH1	1:D:316:LEU:O	2.53	0.42
1:D:731:HIS:CG	1:D:740:THR:HA	2.54	0.42
1:D:993:GLU:HG2	1:D:1051:ARG:HG2	2.02	0.42
1:D:1440:ASN:N	1:D:1440:ASN:OD1	2.53	0.42
1:D:1785:ASP:OD1	1:D:1785:ASP:N	2.53	0.42
1:D:1921:HIS:O	1:D:1925:ALA:N	2.52	0.42
1:D:2079:PRO:HB3	1:D:3674:ARG:HH21	1.85	0.42
1:D:2848:ASN:O	1:D:2852:ILE:N	2.49	0.42
1:D:3016:VAL:O	1:D:3020:ILE:N	2.47	0.42
1:D:4935:THR:H	1:D:4938:GLU:HB2	1.85	0.42
1:G:262:TYR:HB2	1:G:389:ARG:HB2	2.01	0.42
1:G:481:ALA:O	1:G:485:ARG:NE	2.51	0.42
1:G:745:ASN:ND2	1:G:773:GLN:OE1	2.49	0.42
1:J:713:TRP:CH2	1:J:1629:SER:HB2	2.55	0.42
1:J:725:TYR:HA	1:J:732:LEU:HA	2.01	0.42
1:J:992:GLN:HB3	1:J:1054:VAL:HG21	2.02	0.42
1:J:1090:ALA:HB3	1:J:1203:PRO:HD2	2.01	0.42
1:J:1431:ARG:HE	1:J:1431:ARG:HB2	1.56	0.42
1:J:2482:GLN:HA	1:J:2485:LEU:HD13	2.02	0.42
1:J:2769:LYS:HB3	1:J:2769:LYS:HE2	1.91	0.42
1:J:4045:SER:HA	1:J:4078:THR:HA	2.02	0.42
1:A:657:PRO:HB3	1:A:834:VAL:HG12	2.01	0.42
1:A:713:TRP:HZ3	1:A:1627:PHE:HB2	1.85	0.42
1:A:4113:ASP:OD2	1:A:4115:ARG:NH2	2.53	0.42
2:B:87:HIS:HB3	2:B:90:VAL:HB	2.02	0.42
1:D:1734:LYS:HB2	1:D:1734:LYS:HE3	1.78	0.42
1:D:3724:LYS:HD3	1:D:3724:LYS:HA	1.81	0.42
1:D:4113:ASP:OD2	1:D:4115:ARG:NH2	2.53	0.42
1:G:296:ARG:HG2	1:G:327:THR:HG23	2.01	0.42
1:G:938:GLU:OE1	1:G:1002:ASN:ND2	2.45	0.42
1:G:993:GLU:HG2	1:G:1051:ARG:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1599:MET:HE3	1:G:1599:MET:HB2	1.97	0.42
1:G:2079:PRO:HB3	1:G:3674:ARG:HH21	1.85	0.42
1:G:3669:ILE:HD13	1:G:3737:ALA:HB2	2.02	0.42
1:G:3973:MET:O	1:G:3977:LYS:N	2.44	0.42
1:J:211:LEU:HD23	1:J:211:LEU:HA	1.88	0.42
1:J:590:LYS:HE2	1:J:590:LYS:HB2	1.86	0.42
1:J:713:TRP:HZ3	1:J:1627:PHE:HB2	1.85	0.42
1:J:995:MET:HA	1:J:998:LYS:HD2	2.02	0.42
1:J:1114:ARG:HB2	1:J:1206:SER:HB3	2.01	0.42
1:J:1265:HIS:HD2	1:J:1267:HIS:H	1.67	0.42
1:J:1709:ILE:HD13	1:J:1709:ILE:HA	1.90	0.42
1:J:1734:LYS:HE3	1:J:1734:LYS:HB2	1.78	0.42
1:J:1785:ASP:N	1:J:1785:ASP:OD1	2.53	0.42
1:J:3621:PHE:O	1:J:3625:TYR:N	2.53	0.42
1:A:238:HIS:HA	1:A:403:LEU:HD22	2.02	0.41
1:A:2090:HIS:HD2	1:A:3695:ILE:HD11	1.85	0.41
1:A:2162:LEU:O	1:A:2166:LEU:N	2.45	0.41
1:A:3891:TRP:HE1	1:A:3950:HIS:CE1	2.35	0.41
1:A:4867:ILE:HD12	1:A:4870:ALA:HB3	2.02	0.41
1:D:673:TRP:HB2	1:D:759:LEU:HB3	2.01	0.41
1:D:1090:ALA:HB3	1:D:1203:PRO:HD2	2.01	0.41
1:D:1256:PRO:HD2	1:D:1451:HIS:HB3	2.01	0.41
1:D:2546:ILE:O	1:D:2550:LEU:N	2.53	0.41
1:D:4072:GLU:HB2	1:D:4079:LEU:HA	2.01	0.41
1:G:713:TRP:CH2	1:G:1629:SER:HB2	2.55	0.41
1:G:4782:TYR:CB	1:G:4851:PHE:HE1	2.33	0.41
1:J:115:TYR:HB3	1:J:164:PRO:HD3	2.02	0.41
1:J:1110:ALA:HA	1:J:1156:TRP:CZ2	2.54	0.41
1:J:4747:ILE:HD12	1:J:4747:ILE:HA	1.92	0.41
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.90	0.41
1:A:299:HIS:N	1:A:304:LYS:O	2.43	0.41
1:A:647:ARG:NH1	1:A:648:LEU:O	2.51	0.41
1:A:1054:VAL:HA	1:A:1057:LEU:HB2	2.01	0.41
1:D:647:ARG:NH1	1:D:648:LEU:O	2.51	0.41
1:D:713:TRP:HZ3	1:D:1627:PHE:HB2	1.85	0.41
1:D:1809:PRO:HB3	1:D:1817:LEU:HD13	2.02	0.41
1:D:2482:GLN:HA	1:D:2485:LEU:HD13	2.02	0.41
1:D:4521:TYR:HE1	1:D:4560:TYR:H	1.68	0.41
2:E:87:HIS:HB3	2:E:90:VAL:HB	2.02	0.41
1:G:211:LEU:HD23	1:G:211:LEU:HA	1.88	0.41
1:G:466:PRO:HB3	1:G:478:ARG:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:992:GLN:HB3	1:G:1054:VAL:HG21	2.02	0.41
1:J:250:GLY:HA2	1:J:257:ARG:HE	1.84	0.41
1:J:1054:VAL:HA	1:J:1057:LEU:HB2	2.01	0.41
1:J:2090:HIS:HD2	1:J:3695:ILE:HD11	1.85	0.41
1:J:4795:ASN:HB2	1:J:4806:LYS:HZ3	1.85	0.41
1:J:4850:THR:O	1:J:4854:PHE:CB	2.67	0.41
1:J:4911:LEU:HD23	1:J:4911:LEU:HA	1.81	0.41
3:L:33:LEU:O	3:L:37:MET:HB2	2.21	0.41
1:A:466:PRO:HB3	1:A:478:ARG:HG2	2.02	0.41
1:A:2482:GLN:HA	1:A:2485:LEU:HD13	2.02	0.41
1:A:4559:HIS:ND1	1:A:4738:PHE:CE2	2.87	0.41
1:D:657:PRO:HB3	1:D:834:VAL:HG12	2.01	0.41
1:D:2562:LEU:O	1:D:2566:GLN:N	2.46	0.41
1:G:258:ARG:NH1	1:G:316:LEU:O	2.53	0.41
1:G:419:ILE:HD13	1:G:492:GLU:HG3	2.02	0.41
1:G:1033:VAL:HG23	1:G:1038:LEU:HD23	2.02	0.41
1:G:1256:PRO:HD2	1:G:1451:HIS:HB3	2.01	0.41
1:G:3643:GLU:OE2	1:G:3731:ARG:NH2	2.53	0.41
1:G:4521:TYR:HE1	1:G:4560:TYR:H	1.68	0.41
1:J:238:HIS:HA	1:J:403:LEU:HD22	2.02	0.41
1:J:258:ARG:NH1	1:J:316:LEU:O	2.53	0.41
1:J:419:ILE:HD13	1:J:492:GLU:HG3	2.02	0.41
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.88	0.41
1:A:1809:PRO:HB3	1:A:1817:LEU:HD13	2.02	0.41
1:A:1921:HIS:O	1:A:1925:ALA:N	2.52	0.41
1:A:4072:GLU:HB2	1:A:4079:LEU:HA	2.01	0.41
1:A:4897:ASP:OD1	1:A:4897:ASP:N	2.53	0.41
1:D:713:TRP:CH2	1:D:1629:SER:HB2	2.55	0.41
1:D:3804:LEU:O	1:D:3885:SER:OG	2.26	0.41
1:G:238:HIS:HA	1:G:403:LEU:HD22	2.02	0.41
1:G:713:TRP:HZ3	1:G:1627:PHE:HB2	1.85	0.41
1:G:3621:PHE:O	1:G:3625:TYR:N	2.53	0.41
1:G:4911:LEU:HA	1:G:4911:LEU:HD23	1.81	0.41
1:G:4935:THR:H	1:G:4938:GLU:HB2	1.85	0.41
1:J:1828:LEU:HD12	1:J:1828:LEU:HA	1.90	0.41
1:J:2546:ILE:O	1:J:2550:LEU:N	2.53	0.41
1:J:3638:GLU:OE1	1:J:3638:GLU:N	2.53	0.41
1:J:4867:ILE:HD12	1:J:4870:ALA:HB3	2.02	0.41
1:A:296:ARG:HG2	1:A:327:THR:HG23	2.01	0.41
1:A:343:ARG:HB3	1:A:344:LYS:H	1.72	0.41
1:A:434:ASP:OD1	1:A:504:ARG:NE	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:LEU:HA	1:A:502:ILE:HD12	2.03	0.41
1:A:1181:ILE:H	1:A:1181:ILE:HG13	1.72	0.41
1:A:4521:TYR:HE1	1:A:4560:TYR:H	1.68	0.41
3:C:33:LEU:O	3:C:37:MET:HB2	2.20	0.41
1:D:115:TYR:HB3	1:D:164:PRO:HD3	2.02	0.41
1:D:661:LEU:O	1:D:788:PHE:N	2.54	0.41
1:G:1785:ASP:OD1	1:G:1785:ASP:N	2.53	0.41
1:G:3638:GLU:OE1	1:G:3638:GLU:N	2.53	0.41
1:G:3777:LYS:HE2	1:G:3777:LYS:HB2	1.89	0.41
1:J:499:LEU:HA	1:J:502:ILE:HD12	2.03	0.41
1:J:1842:ILE:HD12	1:J:1842:ILE:HA	1.90	0.41
1:J:2138:GLU:HB3	1:J:2141:LYS:HZ2	1.85	0.41
2:K:87:HIS:HB3	2:K:90:VAL:HB	2.02	0.41
1:A:76:ARG:CB	1:D:3891:TRP:HE3	2.32	0.41
1:A:892:LEU:HD13	1:A:1052:GLU:HB3	2.02	0.41
1:A:2079:PRO:HB3	1:A:3674:ARG:HH21	1.85	0.41
1:A:2326:ILE:CA	1:J:207:PHE:CB	2.98	0.41
1:D:123:HIS:HD2	1:D:126:SER:H	1.69	0.41
1:D:419:ILE:HD13	1:D:492:GLU:HG3	2.02	0.41
1:D:725:TYR:HA	1:D:732:LEU:HA	2.01	0.41
1:D:4780:TYR:HH	1:G:4741:ALA:HB1	1.85	0.41
3:F:33:LEU:O	3:F:37:MET:HB2	2.20	0.41
1:G:770:ILE:HD13	1:G:770:ILE:HA	1.96	0.41
1:G:1152:TYR:OH	1:G:1175:PHE:O	2.35	0.41
1:G:2464:ASP:OD1	1:G:2464:ASP:N	2.41	0.41
1:G:2546:ILE:O	1:G:2550:LEU:N	2.53	0.41
1:G:3633:GLU:HA	1:G:3635:HIS:HD2	1.86	0.41
1:J:204:ASP:OD1	1:J:204:ASP:N	2.54	0.41
1:J:262:TYR:HB2	1:J:389:ARG:HB2	2.01	0.41
1:J:434:ASP:OD1	1:J:504:ARG:NE	2.52	0.41
1:J:3891:TRP:HE1	1:J:3950:HIS:CE1	2.35	0.41
1:J:4521:TYR:HE1	1:J:4560:TYR:H	1.68	0.41
1:A:642:LEU:HD12	1:A:642:LEU:HA	1.91	0.41
1:A:1989:CYS:SG	1:A:3605:ARG:NH2	2.94	0.41
1:A:2154:LYS:O	1:A:2154:LYS:NZ	2.53	0.41
1:A:2327:ARG:H	1:A:2327:ARG:HG3	1.49	0.41
1:A:2423:ILE:HG23	1:J:190:ARG:HH12	1.79	0.41
1:A:2849:TYR:HB3	1:A:2886:ASP:HB3	2.03	0.41
1:A:3893:TYR:HA	1:A:3896:LYS:HZ3	1.86	0.41
1:A:3911:ILE:HD13	1:A:3911:ILE:HA	1.93	0.41
1:A:4875:ARG:HD2	1:A:4875:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:LEU:HD23	1:D:274:LEU:HA	1.96	0.41
1:D:3621:PHE:O	1:D:3625:TYR:N	2.53	0.41
1:G:731:HIS:CG	1:G:740:THR:HA	2.54	0.41
1:G:995:MET:HA	1:G:998:LYS:HD2	2.02	0.41
1:G:1114:ARG:HB2	1:G:1206:SER:HB3	2.01	0.41
1:G:1440:ASN:N	1:G:1440:ASN:OD1	2.53	0.41
1:G:1475:LYS:HE2	1:G:1475:LYS:HB2	1.90	0.41
1:G:1989:CYS:SG	1:G:3605:ARG:NH2	2.94	0.41
1:G:2849:TYR:HB3	1:G:2886:ASP:HB3	2.03	0.41
1:G:3677:LEU:HA	1:G:3677:LEU:HD23	1.88	0.41
1:G:4072:GLU:HB2	1:G:4079:LEU:HA	2.01	0.41
1:J:653:SER:O	1:J:653:SER:OG	2.37	0.41
1:J:1760:ARG:HA	1:J:1760:ARG:HD3	1.89	0.41
1:J:4072:GLU:HB2	1:J:4079:LEU:HA	2.01	0.41
1:A:165:ALA:HB3	1:A:211:LEU:HD21	2.02	0.41
1:A:995:MET:HA	1:A:998:LYS:HD2	2.02	0.41
1:A:1440:ASN:N	1:A:1440:ASN:OD1	2.53	0.41
1:A:2154:LYS:HA	1:A:2154:LYS:HD2	1.93	0.41
1:D:466:PRO:HB3	1:D:478:ARG:HG2	2.02	0.41
1:D:4705:LYS:HE3	1:D:4705:LYS:HB3	1.92	0.41
1:D:4867:ILE:HD12	1:D:4870:ALA:HB3	2.02	0.41
1:G:115:TYR:HB3	1:G:164:PRO:HD3	2.02	0.41
1:G:499:LEU:HA	1:G:502:ILE:HD12	2.03	0.41
1:G:625:VAL:HG22	1:G:627:SER:H	1.86	0.41
1:G:653:SER:O	1:G:653:SER:OG	2.37	0.41
1:G:1100:ARG:HG2	1:G:1167:ASP:HA	2.03	0.41
1:G:3783:LYS:HD3	1:G:3783:LYS:HA	1.91	0.41
3:I:33:LEU:O	3:I:37:MET:HB2	2.21	0.41
1:J:425:LEU:HD11	1:J:452:VAL:HA	2.01	0.41
1:J:661:LEU:O	1:J:788:PHE:N	2.54	0.41
1:J:1142:ALA:O	1:J:1152:TYR:N	2.48	0.41
1:J:1809:PRO:HB3	1:J:1817:LEU:HD13	2.02	0.41
1:J:1989:CYS:SG	1:J:3605:ARG:NH2	2.94	0.41
1:J:3016:VAL:O	1:J:3020:ILE:N	2.47	0.41
1:J:3669:ILE:HD13	1:J:3737:ALA:HB2	2.02	0.41
1:J:3777:LYS:HE2	1:J:3777:LYS:HB2	1.89	0.41
2:K:104:LEU:HD23	2:K:104:LEU:HA	1.90	0.41
1:A:207:PHE:CB	1:D:2326:ILE:CA	2.99	0.41
1:A:258:ARG:NH1	1:A:316:LEU:O	2.53	0.41
1:A:620:CYS:N	1:A:623:VAL:O	2.43	0.41
1:A:626:ARG:NH2	1:A:1668:GLY:O	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:THR:HA	1:A:1630:LEU:HA	2.03	0.41
1:A:863:THR:O	1:A:863:THR:OG1	2.33	0.41
1:A:1709:ILE:HD13	1:A:1709:ILE:HA	1.90	0.41
1:A:2138:GLU:HB3	1:A:2141:LYS:HZ2	1.86	0.41
1:A:3638:GLU:OE1	1:A:3638:GLU:N	2.53	0.41
1:D:238:HIS:HA	1:D:403:LEU:HD22	2.02	0.41
1:D:892:LEU:HD13	1:D:1052:GLU:HB3	2.02	0.41
1:D:1989:CYS:SG	1:D:3605:ARG:NH2	2.94	0.41
1:D:2241:LEU:HD12	1:D:2241:LEU:HA	1.91	0.41
1:D:2849:TYR:HB3	1:D:2886:ASP:HB3	2.03	0.41
1:D:3998:LYS:HB2	1:D:3998:LYS:HE3	1.84	0.41
1:G:2170:GLU:H	1:G:2170:GLU:HG2	1.75	0.41
1:G:3834:ASP:N	1:G:3834:ASP:OD1	2.54	0.41
1:G:4113:ASP:OD2	1:G:4115:ARG:NH2	2.53	0.41
1:G:4154:SER:OG	1:G:4155:GLU:N	2.54	0.41
1:J:481:ALA:O	1:J:485:ARG:NE	2.51	0.41
1:J:632:ILE:HD13	1:J:632:ILE:HA	1.93	0.41
1:J:956:HIS:HA	1:J:1060:TYR:HB3	2.03	0.41
1:J:1100:ARG:HG2	1:J:1167:ASP:HA	2.03	0.41
1:J:1165:MET:HB3	1:J:1236:TYR:CZ	2.56	0.41
1:J:2093:TYR:HD1	1:J:2093:TYR:HA	1.77	0.41
1:J:4888:LYS:HB2	1:J:4888:LYS:HE3	1.84	0.41
1:A:204:ASP:OD1	1:A:204:ASP:N	2.54	0.41
1:A:1792:ILE:O	1:A:1796:THR:OG1	2.31	0.41
1:D:625:VAL:HG22	1:D:627:SER:H	1.86	0.41
1:D:642:LEU:HD12	1:D:642:LEU:HA	1.91	0.41
1:D:646:THR:HA	1:D:1630:LEU:HA	2.03	0.41
1:D:1822:ILE:O	1:D:1826:TYR:N	2.54	0.41
1:D:2090:HIS:HD2	1:D:3695:ILE:HD11	1.85	0.41
1:D:2855:LYS:HA	1:D:2855:LYS:HD2	1.88	0.41
1:D:4782:TYR:CB	1:D:4851:PHE:HE1	2.34	0.41
1:D:4897:ASP:OD1	1:D:4897:ASP:N	2.53	0.41
1:G:956:HIS:HA	1:G:1060:TYR:HB3	2.03	0.41
1:G:1809:PRO:HB3	1:G:1817:LEU:HD13	2.02	0.41
1:G:2090:HIS:HD2	1:G:3695:ILE:HD11	1.85	0.41
1:G:2717:LYS:H	1:G:2717:LYS:HG2	1.60	0.41
1:G:4867:ILE:HD12	1:G:4870:ALA:HB3	2.02	0.41
1:J:1440:ASN:N	1:J:1440:ASN:OD1	2.53	0.41
1:J:2079:PRO:HB3	1:J:3674:ARG:HH21	1.85	0.41
1:A:123:HIS:HD2	1:A:126:SER:H	1.69	0.40
1:A:505:LEU:HD12	1:A:505:LEU:HA	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:ILE:HD13	1:A:770:ILE:HA	1.96	0.40
1:A:1165:MET:HB3	1:A:1236:TYR:CZ	2.56	0.40
1:A:4034:LYS:HZ2	1:A:4081:TYR:HE2	1.70	0.40
1:D:653:SER:O	1:D:653:SER:OG	2.37	0.40
1:G:121:LEU:HD23	1:G:121:LEU:HA	1.82	0.40
1:G:661:LEU:O	1:G:788:PHE:N	2.54	0.40
1:G:1705:LEU:HD12	1:G:1705:LEU:HA	1.95	0.40
1:G:1822:ILE:O	1:G:1826:TYR:N	2.54	0.40
1:G:1921:HIS:O	1:G:1925:ALA:N	2.52	0.40
2:H:87:HIS:HB3	2:H:90:VAL:HB	2.02	0.40
1:J:34:LYS:O	1:J:52:THR:N	2.46	0.40
1:J:1152:TYR:CZ	1:J:1182:LEU:HB2	2.56	0.40
1:J:1548:THR:OG1	1:J:1549:SER:N	2.55	0.40
1:J:4154:SER:OG	1:J:4155:GLU:N	2.54	0.40
1:J:4820:VAL:O	1:J:4831:GLU:OE2	2.39	0.40
1:A:46:LEU:HD23	1:A:46:LEU:HA	1.95	0.40
1:A:661:LEU:O	1:A:788:PHE:N	2.54	0.40
1:A:706:TYR:HH	1:A:1254:ARG:H	1.64	0.40
1:A:713:TRP:CH2	1:A:1629:SER:HB2	2.55	0.40
1:A:956:HIS:HA	1:A:1060:TYR:HB3	2.03	0.40
1:A:2546:ILE:O	1:A:2550:LEU:N	2.53	0.40
1:D:204:ASP:N	1:D:204:ASP:OD1	2.54	0.40
1:D:499:LEU:HA	1:D:502:ILE:HD12	2.03	0.40
1:D:611:LEU:HD12	1:D:611:LEU:HA	1.93	0.40
1:D:956:HIS:HA	1:D:1060:TYR:HB3	2.03	0.40
1:D:1132:GLU:HA	1:D:1146:HIS:CD2	2.56	0.40
1:D:3633:GLU:HA	1:D:3635:HIS:HD2	1.86	0.40
1:D:3645:LEU:HD23	1:D:3645:LEU:HA	1.84	0.40
1:D:4038:PRO:HG3	1:D:4044:ILE:HG22	2.04	0.40
2:E:50:ILE:H	2:E:50:ILE:HG13	1.74	0.40
1:G:1153:GLY:HA3	1:G:1182:LEU:HB3	2.03	0.40
1:G:1165:MET:HB3	1:G:1236:TYR:CZ	2.56	0.40
1:G:1265:HIS:CD2	1:G:1268:ILE:HG13	2.57	0.40
1:G:2162:LEU:O	1:G:2166:LEU:N	2.45	0.40
1:G:2725:TYR:HD1	1:G:2728:HIS:HB3	1.86	0.40
1:G:3724:LYS:HA	1:G:3724:LYS:HD3	1.81	0.40
1:G:4888:LYS:HE3	1:G:4888:LYS:HB2	1.84	0.40
1:J:67:PHE:HB3	1:J:121:LEU:HD22	2.04	0.40
1:J:625:VAL:HG22	1:J:627:SER:H	1.86	0.40
1:J:3633:GLU:HA	1:J:3635:HIS:HD2	1.86	0.40
1:A:1211:GLN:OE1	1:A:1211:GLN:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2430:LEU:HD11	1:A:2473:LEU:HD11	2.04	0.40
1:D:1142:ALA:O	1:D:1152:TYR:N	2.48	0.40
1:D:1152:TYR:CZ	1:D:1182:LEU:HB2	2.56	0.40
1:D:1165:MET:HB3	1:D:1236:TYR:CZ	2.56	0.40
1:D:1945:TYR:OH	1:D:1993:ILE:O	2.35	0.40
1:D:3834:ASP:OD1	1:D:3834:ASP:N	2.54	0.40
1:G:1117:TRP:CE2	1:G:1166:VAL:HG21	2.57	0.40
1:G:1211:GLN:OE1	1:G:1211:GLN:N	2.55	0.40
1:G:1690:GLU:OE2	1:G:1790:LYS:NZ	2.36	0.40
1:G:1809:PRO:O	1:G:1812:GLY:N	2.55	0.40
1:G:1941:GLN:O	1:G:1945:TYR:N	2.37	0.40
1:G:4897:ASP:N	1:G:4897:ASP:OD1	2.53	0.40
1:J:993:GLU:HG2	1:J:1051:ARG:HG2	2.02	0.40
1:J:1941:GLN:O	1:J:1945:TYR:N	2.37	0.40
1:J:2430:LEU:HD11	1:J:2473:LEU:HD11	2.04	0.40
1:J:2845:MET:HE2	1:J:2845:MET:HB3	1.89	0.40
1:J:4042:GLY:O	1:J:4081:TYR:N	2.48	0.40
1:A:305:TYR:N	1:A:317:MET:O	2.41	0.40
1:A:993:GLU:HG2	1:A:1051:ARG:HG2	2.02	0.40
1:A:2296:GLY:HA2	1:A:2299:TYR:HD2	1.87	0.40
1:A:2722:ILE:HG21	1:A:2773:ARG:HH11	1.87	0.40
1:A:4148:ARG:NH1	1:A:4913:GLU:OE1	2.40	0.40
1:A:4888:LYS:HE3	1:A:4888:LYS:HB2	1.84	0.40
1:D:76:ARG:CB	1:G:3891:TRP:HE3	2.34	0.40
1:G:123:HIS:HD2	1:G:126:SER:H	1.69	0.40
1:G:434:ASP:OD1	1:G:504:ARG:NE	2.52	0.40
1:G:706:TYR:HH	1:G:1254:ARG:H	1.63	0.40
1:G:915:HIS:CE1	1:G:917:CYS:HB2	2.57	0.40
1:G:1152:TYR:CZ	1:G:1182:LEU:HB2	2.56	0.40
1:G:1548:THR:OG1	1:G:1549:SER:N	2.55	0.40
1:G:2161:ASN:O	1:G:2165:ALA:N	2.48	0.40
1:G:2327:ARG:H	1:G:2327:ARG:HG3	1.49	0.40
1:J:165:ALA:HB3	1:J:211:LEU:HD21	2.02	0.40
1:J:646:THR:HA	1:J:1630:LEU:HA	2.03	0.40
1:J:915:HIS:CE1	1:J:917:CYS:HB2	2.57	0.40
1:J:938:GLU:OE1	1:J:1002:ASN:ND2	2.45	0.40
1:J:1152:TYR:OH	1:J:1175:PHE:O	2.35	0.40
1:J:1153:GLY:HA3	1:J:1182:LEU:HB3	2.03	0.40
1:J:2849:TYR:HB3	1:J:2886:ASP:HB3	2.03	0.40
1:J:4897:ASP:N	1:J:4897:ASP:OD1	2.53	0.40
1:A:67:PHE:HB3	1:A:121:LEU:HD22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TYR:HB3	1:A:164:PRO:HD3	2.02	0.40
1:A:479:LEU:HD12	1:A:479:LEU:HA	1.90	0.40
1:A:1152:TYR:CZ	1:A:1182:LEU:HB2	2.56	0.40
1:A:2725:TYR:HD1	1:A:2728:HIS:HB3	1.86	0.40
1:A:4042:GLY:O	1:A:4081:TYR:N	2.48	0.40
1:D:34:LYS:O	1:D:52:THR:N	2.46	0.40
1:D:35:LEU:HD13	1:D:49:LEU:HD13	2.03	0.40
1:D:796:ALA:HB3	1:D:798:ILE:HG13	2.04	0.40
1:D:1100:ARG:HG2	1:D:1167:ASP:HA	2.03	0.40
1:G:165:ALA:HB3	1:G:211:LEU:HD21	2.02	0.40
1:G:748:LEU:HB3	1:G:750:ARG:HG3	2.03	0.40
1:G:870:SER:HA	1:G:941:LYS:HD3	2.03	0.40
1:G:1609:SER:OG	1:G:1621:CYS:SG	2.72	0.40
1:G:1767:SER:OG	1:G:1768:PHE:N	2.55	0.40
1:G:2410:ILE:H	1:G:2410:ILE:HG13	1.69	0.40
1:G:2897:LEU:HD23	1:G:2897:LEU:HA	1.92	0.40
1:G:3891:TRP:HE1	1:G:3950:HIS:CE1	2.35	0.40
1:G:3911:ILE:HD13	1:G:3911:ILE:HA	1.93	0.40
1:G:4628:LYS:H	1:G:4628:LYS:HG2	1.70	0.40
1:G:4861:ALA:HB2	1:J:4864:GLN:CD	2.38	0.40
1:J:35:LEU:HD13	1:J:49:LEU:HD13	2.03	0.40
1:J:1223:THR:HA	1:J:1225:LYS:HE3	2.04	0.40
1:J:1520:PHE:HD2	1:J:1530:TYR:HA	1.86	0.40
1:J:2154:LYS:O	1:J:2154:LYS:NZ	2.53	0.40
1:J:2296:GLY:HA2	1:J:2299:TYR:HD2	1.87	0.40
1:J:2537:ALA:O	1:J:2541:HIS:N	2.50	0.40
1:J:3834:ASP:OD1	1:J:3834:ASP:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3374/4968 (68%)	3009 (89%)	357 (11%)	8 (0%)	47	80
1	D	3374/4968 (68%)	3012 (89%)	355 (10%)	7 (0%)	47	80
1	G	3374/4968 (68%)	3012 (89%)	354 (10%)	8 (0%)	47	80
1	J	3374/4968 (68%)	3010 (89%)	355 (10%)	9 (0%)	41	76
2	B	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
2	E	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
2	H	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
2	K	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
3	C	66/149 (44%)	64 (97%)	2 (3%)	0	100	100
3	F	66/149 (44%)	64 (97%)	2 (3%)	0	100	100
3	I	66/149 (44%)	63 (96%)	3 (4%)	0	100	100
3	L	66/149 (44%)	64 (97%)	2 (3%)	0	100	100
All	All	14180/20900 (68%)	12694 (90%)	1454 (10%)	32 (0%)	50	80

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4823	ARG
1	J	4823	ARG
1	G	4823	ARG
1	A	730	LEU
1	A	853	PRO
1	D	730	LEU
1	D	853	PRO
1	G	730	LEU
1	G	853	PRO
1	J	730	LEU
1	J	853	PRO
1	A	1580	PRO
1	A	1990	PRO
1	D	1580	PRO
1	D	1990	PRO
1	G	1580	PRO
1	G	1990	PRO
1	J	1580	PRO
1	J	1990	PRO
1	A	1535	PRO
1	D	1535	PRO
1	G	1535	PRO

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Mol	Chain	Res	Type
1	J	1535	PRO
1	A	1848	PRO
1	D	1848	PRO
1	G	1848	PRO
1	J	1848	PRO
1	J	4821	GLY
1	A	828	PRO
1	D	828	PRO
1	G	828	PRO
1	J	828	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2672/4355 (61%)	2653 (99%)	19 (1%)	84	90
1	D	2671/4355 (61%)	2650 (99%)	21 (1%)	81	89
1	G	2671/4355 (61%)	2651 (99%)	20 (1%)	84	90
1	J	2671/4355 (61%)	2653 (99%)	18 (1%)	84	90
2	B	88/89 (99%)	87 (99%)	1 (1%)	73	84
2	E	88/89 (99%)	87 (99%)	1 (1%)	73	84
2	H	88/89 (99%)	87 (99%)	1 (1%)	73	84
2	K	88/89 (99%)	87 (99%)	1 (1%)	73	84
3	C	57/127 (45%)	57 (100%)	0	100	100
3	F	57/127 (45%)	57 (100%)	0	100	100
3	I	57/127 (45%)	57 (100%)	0	100	100
3	L	57/127 (45%)	57 (100%)	0	100	100
All	All	11265/18284 (62%)	11183 (99%)	82 (1%)	84	90

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	324	VAL
1	A	444	THR
1	A	841	LYS
1	A	925	PRO
1	A	950	VAL
1	A	1013	ARG
1	A	1300	MET
1	A	1637	ARG
1	A	1683	PRO
1	A	1944	ARG
1	A	2328	ARG
1	A	2793	THR
1	A	2836	ARG
1	A	2876	ASP
1	A	4605	LYS
1	A	4780	TYR
1	A	4816	PHE
1	A	4852	PHE
1	A	4853	PHE
2	B	13	ARG
1	D	324	VAL
1	D	444	THR
1	D	841	LYS
1	D	925	PRO
1	D	950	VAL
1	D	1013	ARG
1	D	1300	MET
1	D	1637	ARG
1	D	1683	PRO
1	D	1944	ARG
1	D	2328	ARG
1	D	2793	THR
1	D	2836	ARG
1	D	2876	ASP
1	D	4605	LYS
1	D	4780	TYR
1	D	4817	HIS
1	D	4818	MET
1	D	4819	TYR
1	D	4853	PHE
1	D	4875	ARG
2	E	13	ARG
1	G	324	VAL

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Mol	Chain	Res	Type
1	G	444	THR
1	G	841	LYS
1	G	925	PRO
1	G	950	VAL
1	G	1013	ARG
1	G	1300	MET
1	G	1637	ARG
1	G	1683	PRO
1	G	1944	ARG
1	G	2328	ARG
1	G	2793	THR
1	G	2836	ARG
1	G	2876	ASP
1	G	4605	LYS
1	G	4780	TYR
1	G	4816	PHE
1	G	4818	MET
1	G	4853	PHE
1	G	4875	ARG
2	H	13	ARG
1	J	324	VAL
1	J	444	THR
1	J	841	LYS
1	J	925	PRO
1	J	950	VAL
1	J	1013	ARG
1	J	1300	MET
1	J	1637	ARG
1	J	1683	PRO
1	J	1944	ARG
1	J	2328	ARG
1	J	2793	THR
1	J	2836	ARG
1	J	2876	ASP
1	J	4605	LYS
1	J	4780	TYR
1	J	4816	PHE
1	J	4853	PHE
2	K	13	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (162) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	32	GLN
1	A	44	ASN
1	A	57	ASN
1	A	123	HIS
1	A	544	ASN
1	A	587	ASN
1	A	593	HIS
1	A	604	HIS
1	A	635	ASN
1	A	716	ASN
1	A	903	GLN
1	A	1005	ASN
1	A	1157	GLN
1	A	1265	HIS
1	A	1294	ASN
1	A	1589	GLN
1	A	1656	HIS
1	A	1684	GLN
1	A	1722	ASN
1	A	2090	HIS
1	A	2196	ASN
1	A	2211	ASN
1	A	2518	ASN
1	A	2755	GLN
1	A	2900	ASN
1	A	3635	HIS
1	A	3667	GLN
1	A	3813	ASN
1	A	3852	ASN
1	A	3902	GLN
1	A	3950	HIS
1	A	3961	GLN
1	A	3990	ASN
1	A	3993	ASN
1	A	4061	GLN
1	A	4089	HIS
1	A	4515	ASN
1	A	4864	GLN
1	A	4937	GLN
2	B	31	GLN
1	D	23	GLN
1	D	32	GLN

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Mol	Chain	Res	Type
1	D	44	ASN
1	D	57	ASN
1	D	123	HIS
1	D	544	ASN
1	D	587	ASN
1	D	593	HIS
1	D	604	HIS
1	D	635	ASN
1	D	716	ASN
1	D	903	GLN
1	D	1005	ASN
1	D	1157	GLN
1	D	1265	HIS
1	D	1294	ASN
1	D	1589	GLN
1	D	1656	HIS
1	D	1722	ASN
1	D	1836	ASN
1	D	2090	HIS
1	D	2196	ASN
1	D	2211	ASN
1	D	2518	ASN
1	D	2755	GLN
1	D	2900	ASN
1	D	3635	HIS
1	D	3667	GLN
1	D	3852	ASN
1	D	3902	GLN
1	D	3950	HIS
1	D	3961	GLN
1	D	3990	ASN
1	D	3993	ASN
1	D	4061	GLN
1	D	4089	HIS
1	D	4515	ASN
1	D	4817	HIS
1	D	4864	GLN
1	D	4937	GLN
2	E	31	GLN
1	G	23	GLN
1	G	32	GLN
1	G	44	ASN

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Mol	Chain	Res	Type
1	G	57	ASN
1	G	123	HIS
1	G	544	ASN
1	G	587	ASN
1	G	593	HIS
1	G	604	HIS
1	G	635	ASN
1	G	716	ASN
1	G	903	GLN
1	G	1005	ASN
1	G	1157	GLN
1	G	1265	HIS
1	G	1294	ASN
1	G	1589	GLN
1	G	1656	HIS
1	G	1722	ASN
1	G	1836	ASN
1	G	2090	HIS
1	G	2196	ASN
1	G	2211	ASN
1	G	2518	ASN
1	G	2755	GLN
1	G	2900	ASN
1	G	3635	HIS
1	G	3667	GLN
1	G	3852	ASN
1	G	3902	GLN
1	G	3950	HIS
1	G	3961	GLN
1	G	3990	ASN
1	G	3993	ASN
1	G	4061	GLN
1	G	4089	HIS
1	G	4515	ASN
1	G	4864	GLN
1	G	4937	GLN
2	H	31	GLN
1	J	23	GLN
1	J	32	GLN
1	J	44	ASN
1	J	57	ASN
1	J	123	HIS

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Mol	Chain	Res	Type
1	J	544	ASN
1	J	587	ASN
1	J	593	HIS
1	J	604	HIS
1	J	635	ASN
1	J	716	ASN
1	J	903	GLN
1	J	1005	ASN
1	J	1157	GLN
1	J	1265	HIS
1	J	1294	ASN
1	J	1589	GLN
1	J	1656	HIS
1	J	1722	ASN
1	J	1836	ASN
1	J	2090	HIS
1	J	2196	ASN
1	J	2211	ASN
1	J	2518	ASN
1	J	2755	GLN
1	J	2900	ASN
1	J	3635	HIS
1	J	3667	GLN
1	J	3852	ASN
1	J	3902	GLN
1	J	3950	HIS
1	J	3961	GLN
1	J	3990	ASN
1	J	3993	ASN
1	J	4061	GLN
1	J	4089	HIS
1	J	4515	ASN
1	J	4864	GLN
1	J	4937	GLN
2	K	31	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
7	CFF	G	6003	-	8,15,15	2.61	4 (50%)	8,23,23	1.31	1 (12%)
7	CFF	A	6003	-	8,15,15	2.60	4 (50%)	8,23,23	1.30	1 (12%)
6	ATP	A	6002	-	26,33,33	0.90	1 (3%)	31,52,52	1.46	5 (16%)
6	ATP	D	6002	-	26,33,33	0.90	1 (3%)	31,52,52	1.46	5 (16%)
7	CFF	D	6003	-	8,15,15	2.60	4 (50%)	8,23,23	1.30	1 (12%)
6	ATP	G	6002	-	26,33,33	0.90	1 (3%)	31,52,52	1.46	5 (16%)
6	ATP	J	6002	-	26,33,33	0.90	1 (3%)	31,52,52	1.46	5 (16%)
7	CFF	J	6003	-	8,15,15	2.60	4 (50%)	8,23,23	1.30	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CFF	G	6003	-	-	-	0/2/2/2
7	CFF	A	6003	-	-	-	0/2/2/2
6	ATP	A	6002	-	-	7/18/38/38	0/3/3/3
6	ATP	D	6002	-	-	7/18/38/38	0/3/3/3
7	CFF	D	6003	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	G	6002	-	-	7/18/38/38	0/3/3/3
6	ATP	J	6002	-	-	7/18/38/38	0/3/3/3
7	CFF	J	6003	-	-	-	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	6003	CFF	C5-C4	-4.65	1.33	1.39
7	D	6003	CFF	C5-C4	-4.63	1.33	1.39
7	A	6003	CFF	C5-C4	-4.61	1.33	1.39
7	J	6003	CFF	C5-C4	-4.61	1.33	1.39
7	A	6003	CFF	C6-N1	-4.27	1.32	1.38
7	D	6003	CFF	C6-N1	-4.27	1.32	1.38
7	G	6003	CFF	C6-N1	-4.27	1.32	1.38
7	J	6003	CFF	C6-N1	-4.27	1.32	1.38
7	A	6003	CFF	O13-C6	-2.41	1.18	1.24
7	D	6003	CFF	O13-C6	-2.41	1.18	1.24
7	G	6003	CFF	O13-C6	-2.41	1.18	1.24
7	J	6003	CFF	O13-C6	-2.41	1.18	1.24
7	A	6003	CFF	C5-C6	-2.39	1.37	1.41
7	D	6003	CFF	C5-C6	-2.39	1.37	1.41
7	G	6003	CFF	C5-C6	-2.39	1.37	1.41
7	J	6003	CFF	C5-C6	-2.39	1.37	1.41
6	J	6002	ATP	C5-C4	2.28	1.47	1.40
6	A	6002	ATP	C5-C4	2.28	1.47	1.40
6	D	6002	ATP	C5-C4	2.28	1.47	1.40
6	G	6002	ATP	C5-C4	2.28	1.47	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	6002	ATP	C3'-C2'-C1'	3.17	105.75	100.98
6	D	6002	ATP	C3'-C2'-C1'	3.17	105.75	100.98
6	G	6002	ATP	C3'-C2'-C1'	3.17	105.75	100.98
6	J	6002	ATP	C3'-C2'-C1'	3.17	105.75	100.98
6	A	6002	ATP	PB-O3B-PG	-3.15	122.02	132.83
6	D	6002	ATP	PB-O3B-PG	-3.15	122.02	132.83
6	G	6002	ATP	PB-O3B-PG	-3.15	122.02	132.83
6	J	6002	ATP	PB-O3B-PG	-3.15	122.02	132.83
6	J	6002	ATP	N3-C2-N1	-3.11	123.82	128.68
6	A	6002	ATP	N3-C2-N1	-3.08	123.87	128.68
6	D	6002	ATP	N3-C2-N1	-3.08	123.87	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	6002	ATP	N3-C2-N1	-3.08	123.87	128.68
6	A	6002	ATP	PA-O3A-PB	-3.03	122.42	132.83
6	D	6002	ATP	PA-O3A-PB	-3.03	122.42	132.83
6	G	6002	ATP	PA-O3A-PB	-3.03	122.42	132.83
6	J	6002	ATP	PA-O3A-PB	-3.03	122.42	132.83
7	A	6003	CFF	C14-N7-C8	-2.77	112.09	125.43
7	D	6003	CFF	C14-N7-C8	-2.77	112.09	125.43
7	G	6003	CFF	C14-N7-C8	-2.77	112.09	125.43
7	J	6003	CFF	C14-N7-C8	-2.77	112.09	125.43
6	A	6002	ATP	C4-C5-N7	-2.09	107.22	109.40
6	D	6002	ATP	C4-C5-N7	-2.09	107.22	109.40
6	G	6002	ATP	C4-C5-N7	-2.09	107.22	109.40
6	J	6002	ATP	C4-C5-N7	-2.06	107.25	109.40

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	6002	ATP	C5'-O5'-PA-O2A
6	A	6002	ATP	C5'-O5'-PA-O3A
6	D	6002	ATP	C5'-O5'-PA-O2A
6	D	6002	ATP	C5'-O5'-PA-O3A
6	G	6002	ATP	C5'-O5'-PA-O2A
6	G	6002	ATP	C5'-O5'-PA-O3A
6	J	6002	ATP	C5'-O5'-PA-O2A
6	J	6002	ATP	C5'-O5'-PA-O3A
6	A	6002	ATP	C3'-C4'-C5'-O5'
6	D	6002	ATP	C3'-C4'-C5'-O5'
6	G	6002	ATP	C3'-C4'-C5'-O5'
6	J	6002	ATP	C3'-C4'-C5'-O5'
6	A	6002	ATP	PB-O3A-PA-O5'
6	D	6002	ATP	PB-O3A-PA-O5'
6	G	6002	ATP	PB-O3A-PA-O5'
6	J	6002	ATP	PB-O3A-PA-O5'
6	A	6002	ATP	C4'-C5'-O5'-PA
6	D	6002	ATP	C4'-C5'-O5'-PA
6	G	6002	ATP	C4'-C5'-O5'-PA
6	J	6002	ATP	C4'-C5'-O5'-PA
6	A	6002	ATP	O4'-C4'-C5'-O5'
6	D	6002	ATP	O4'-C4'-C5'-O5'
6	G	6002	ATP	O4'-C4'-C5'-O5'
6	J	6002	ATP	O4'-C4'-C5'-O5'

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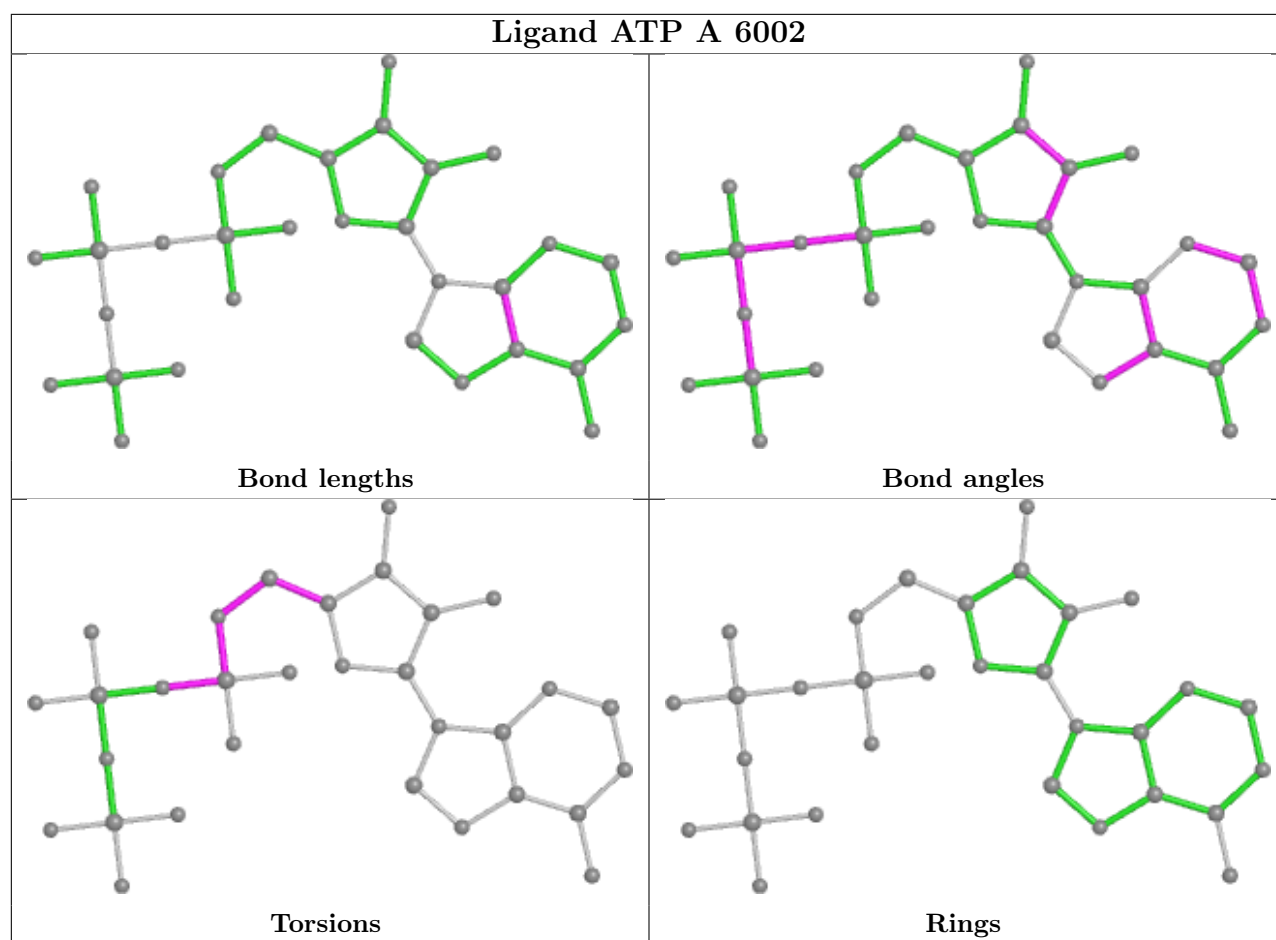
Mol	Chain	Res	Type	Atoms
6	A	6002	ATP	PB-O3A-PA-O2A
6	D	6002	ATP	PB-O3A-PA-O2A
6	G	6002	ATP	PB-O3A-PA-O2A
6	J	6002	ATP	PB-O3A-PA-O2A

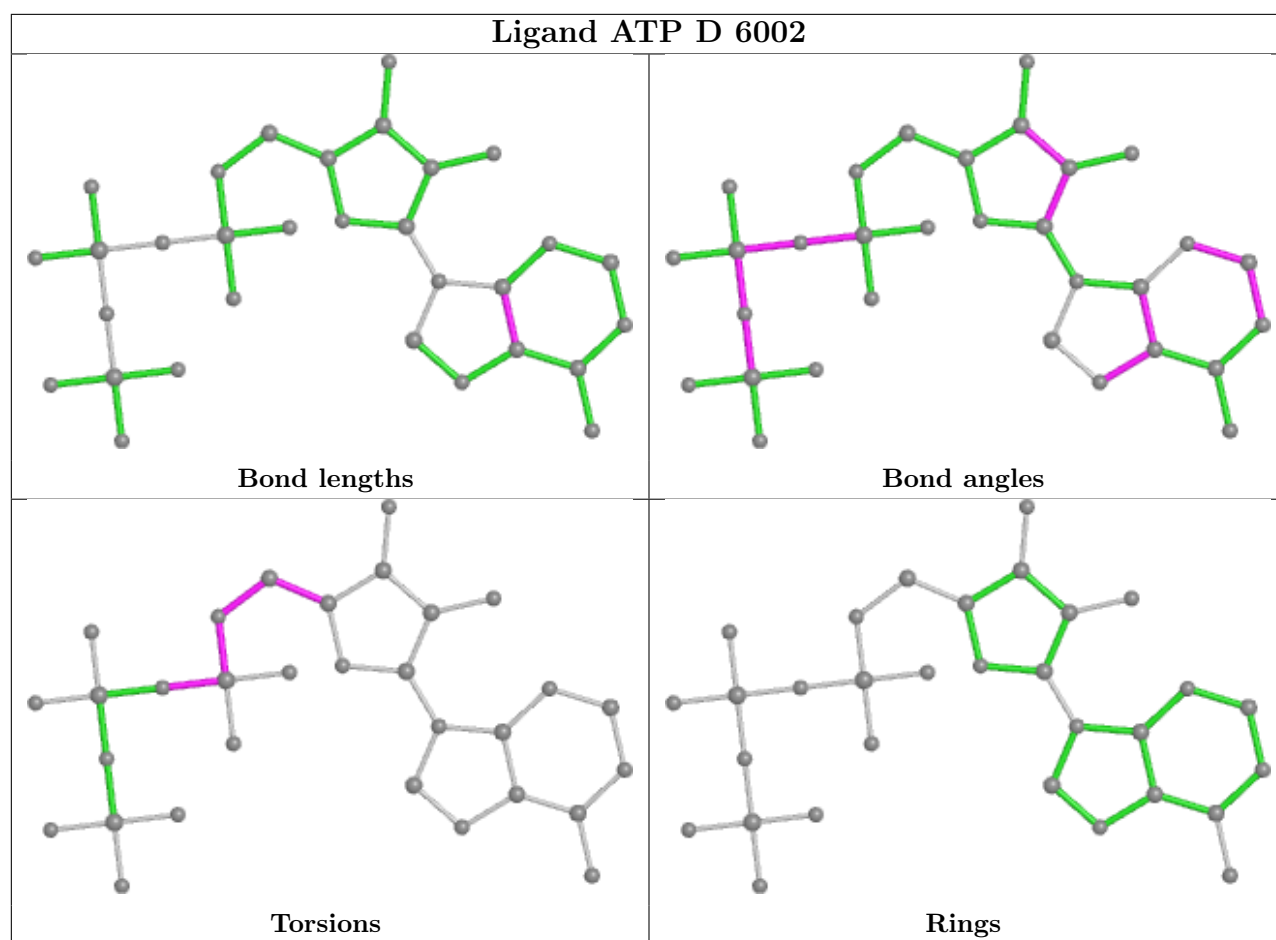
There are no ring outliers.

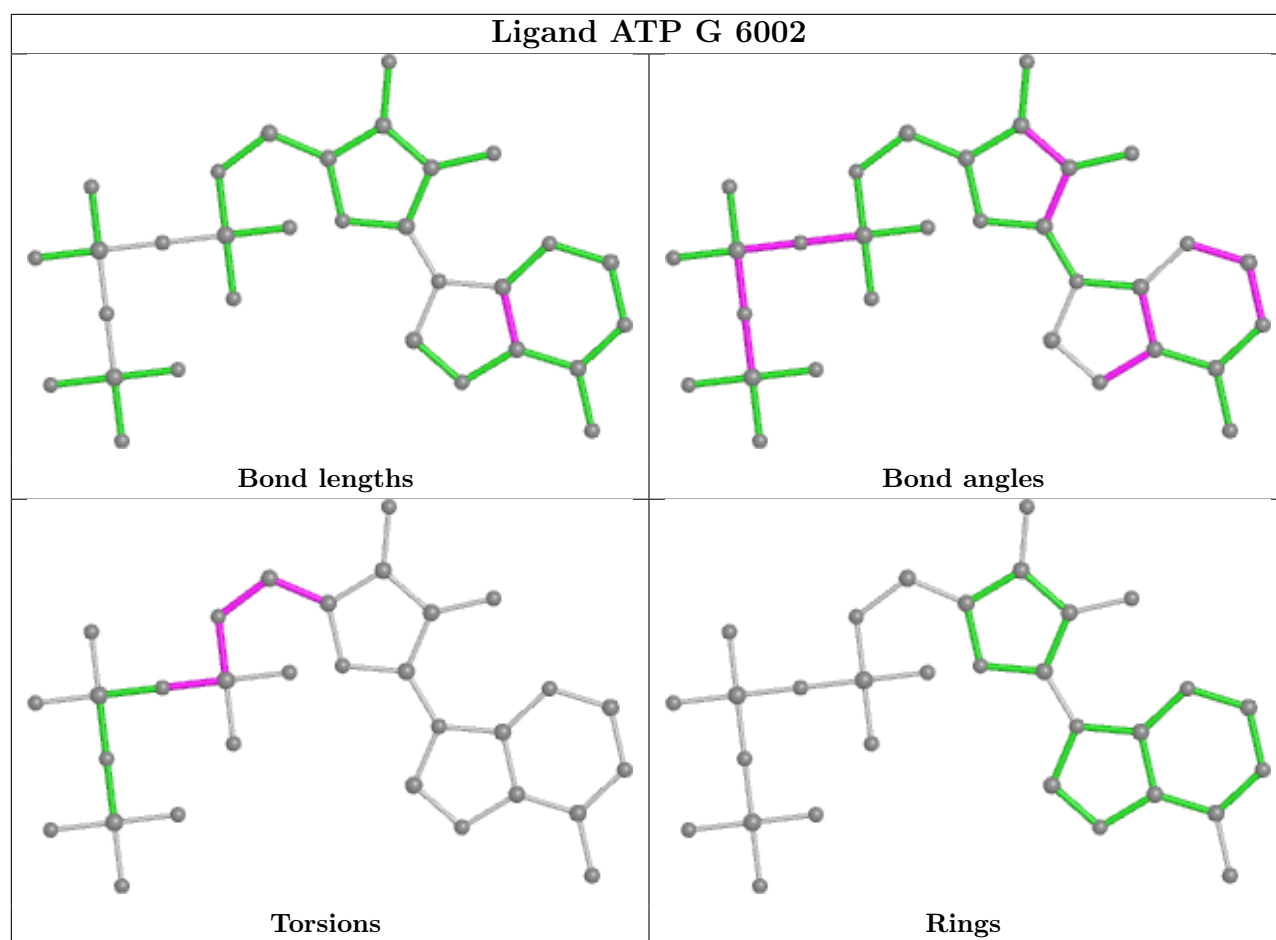
4 monomers are involved in 4 short contacts:

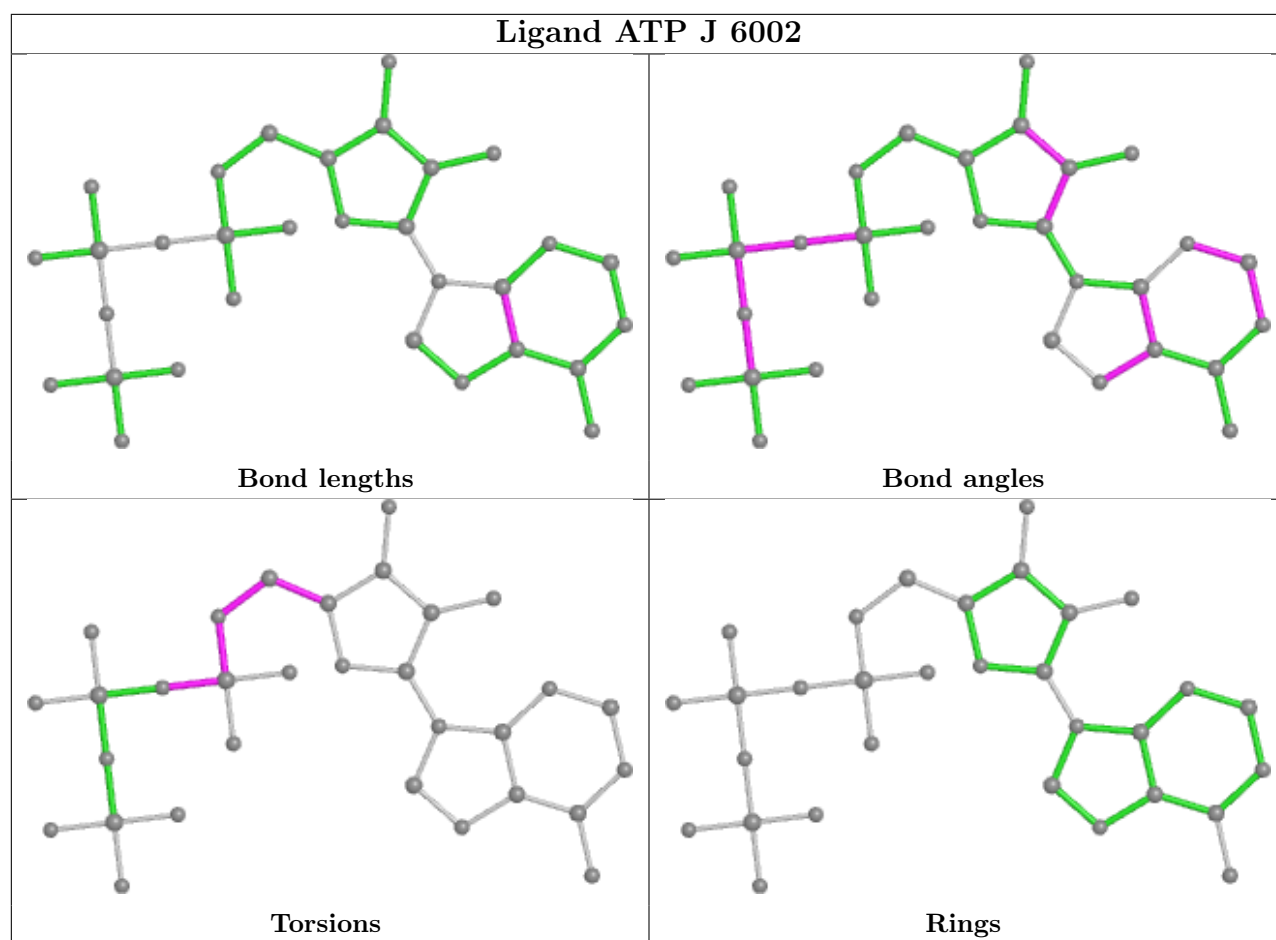
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	6003	CFF	1	0
7	A	6003	CFF	1	0
7	D	6003	CFF	1	0
7	J	6003	CFF	1	0

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.









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.

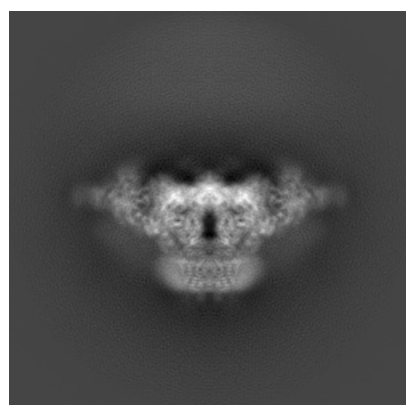
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9836. These allow visual inspection of the internal detail of the map and identification of artifacts.

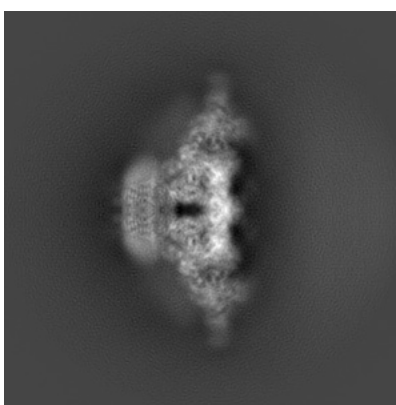
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

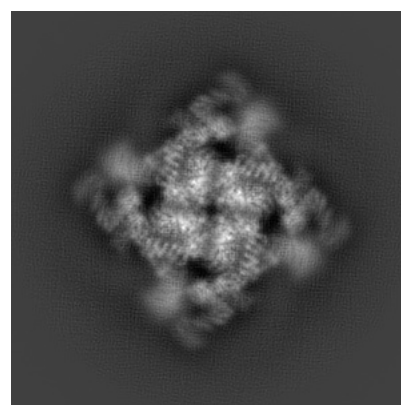
6.1.1 Primary map



X



Y

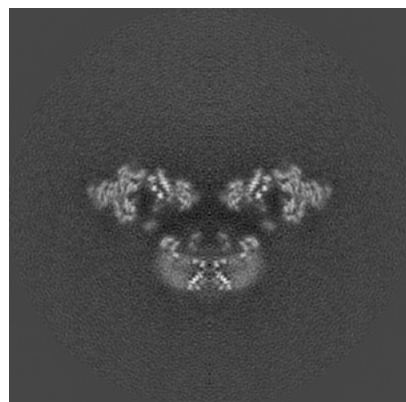


Z

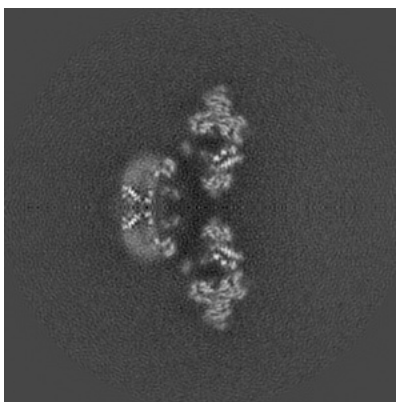
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

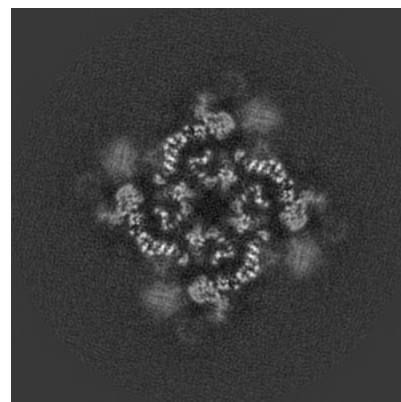
6.2.1 Primary map



X Index: 200



Y Index: 200

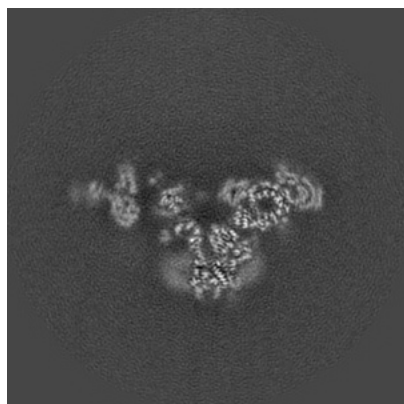


Z Index: 200

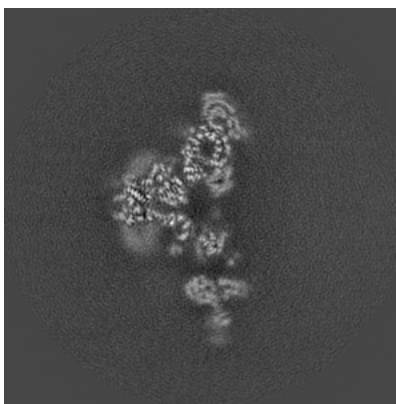
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

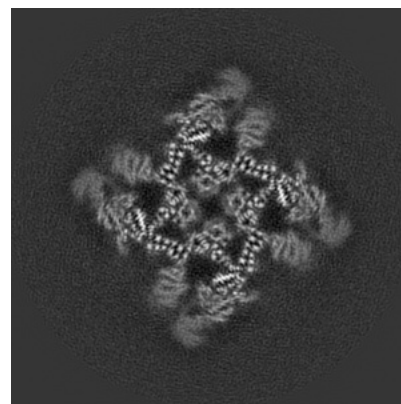
6.3.1 Primary map



X Index: 190



Y Index: 210

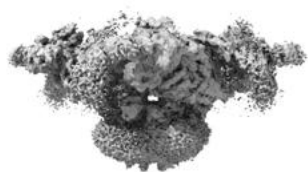


Z Index: 209

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

6.4 Orthogonal surface views [i](#)

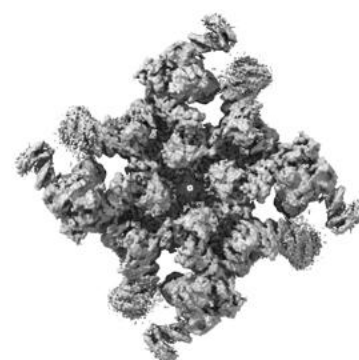
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

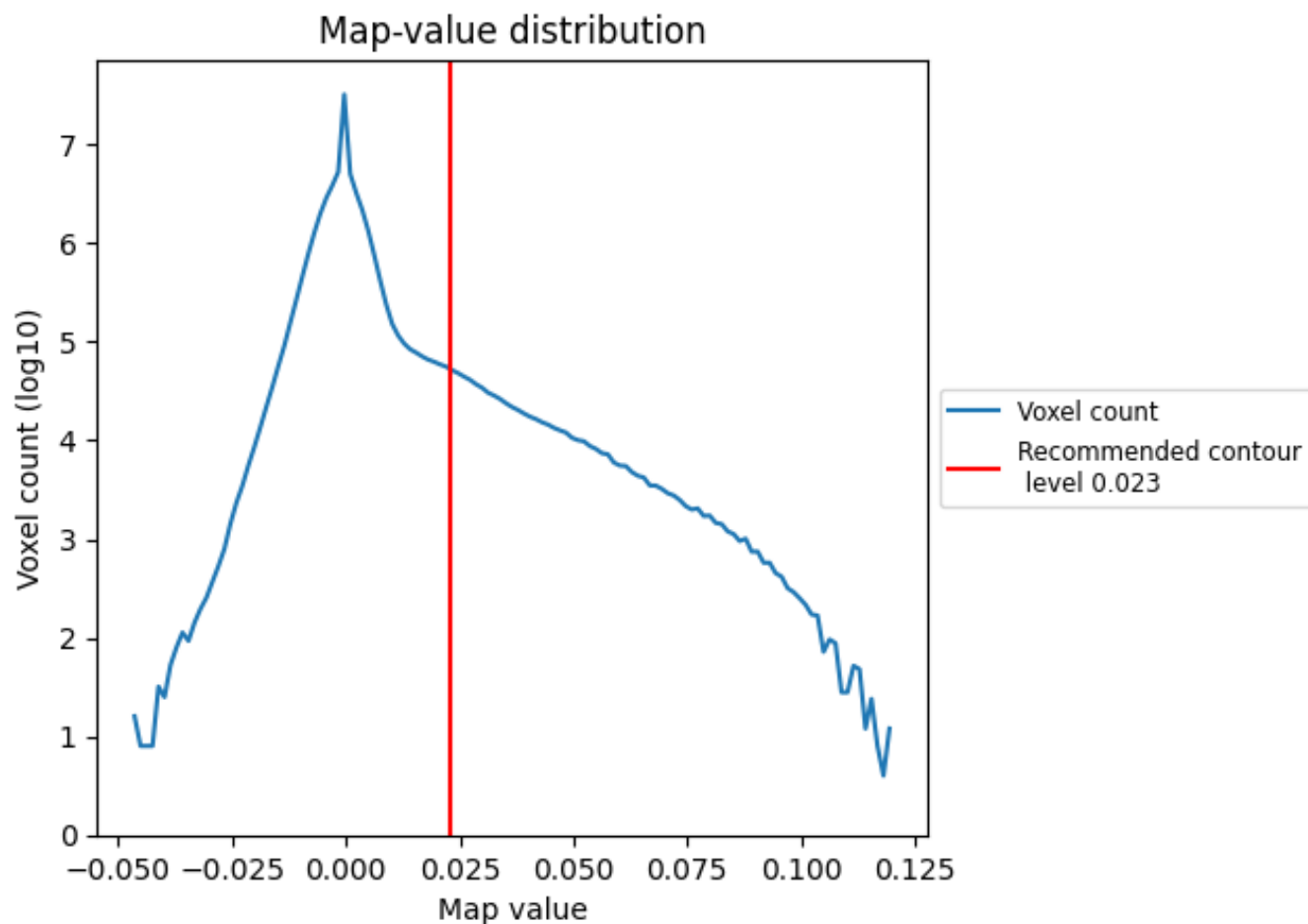
6.5 Mask visualisation

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

7 Map analysis [i](#)

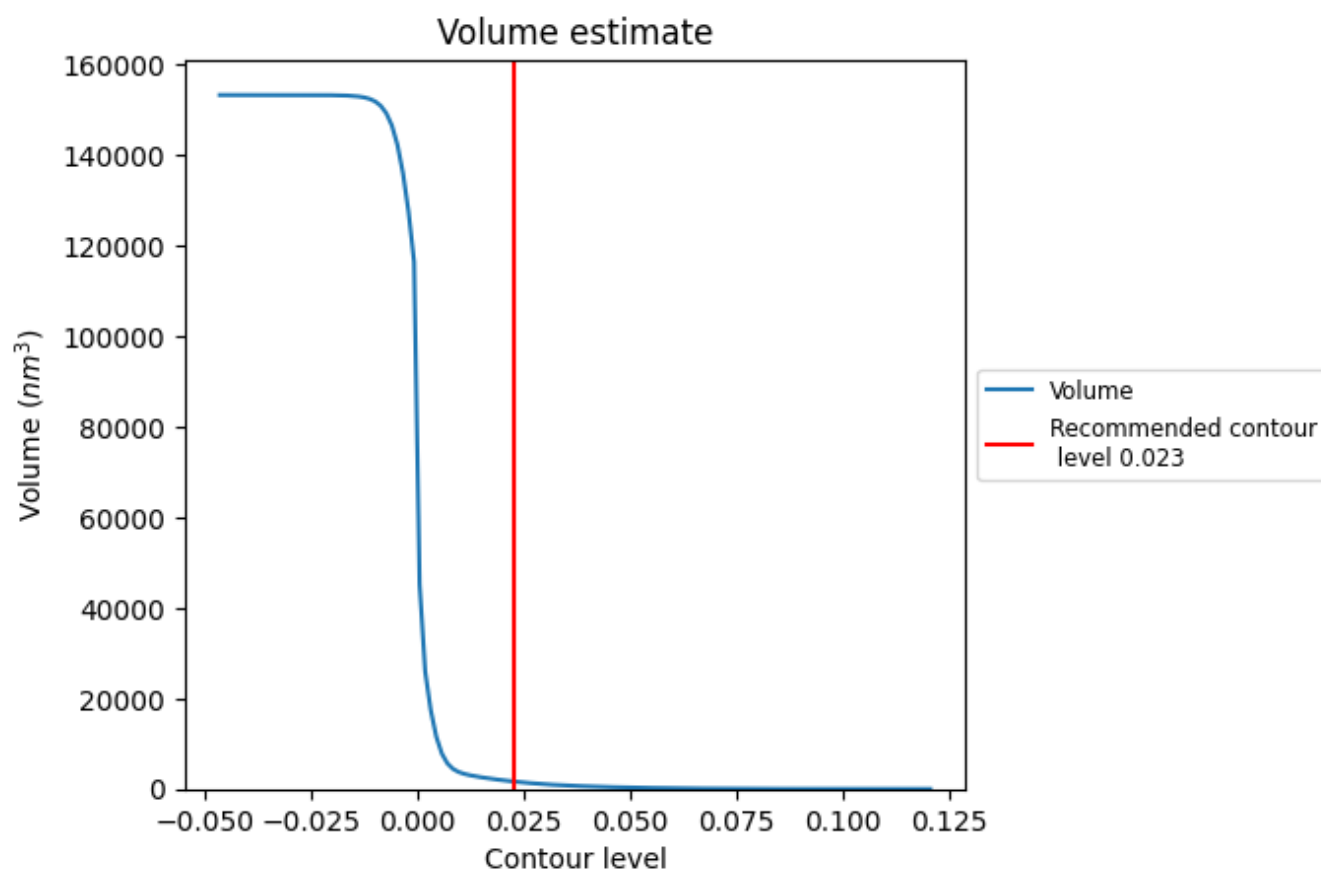
This section contains the results of statistical analysis of the map.

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.

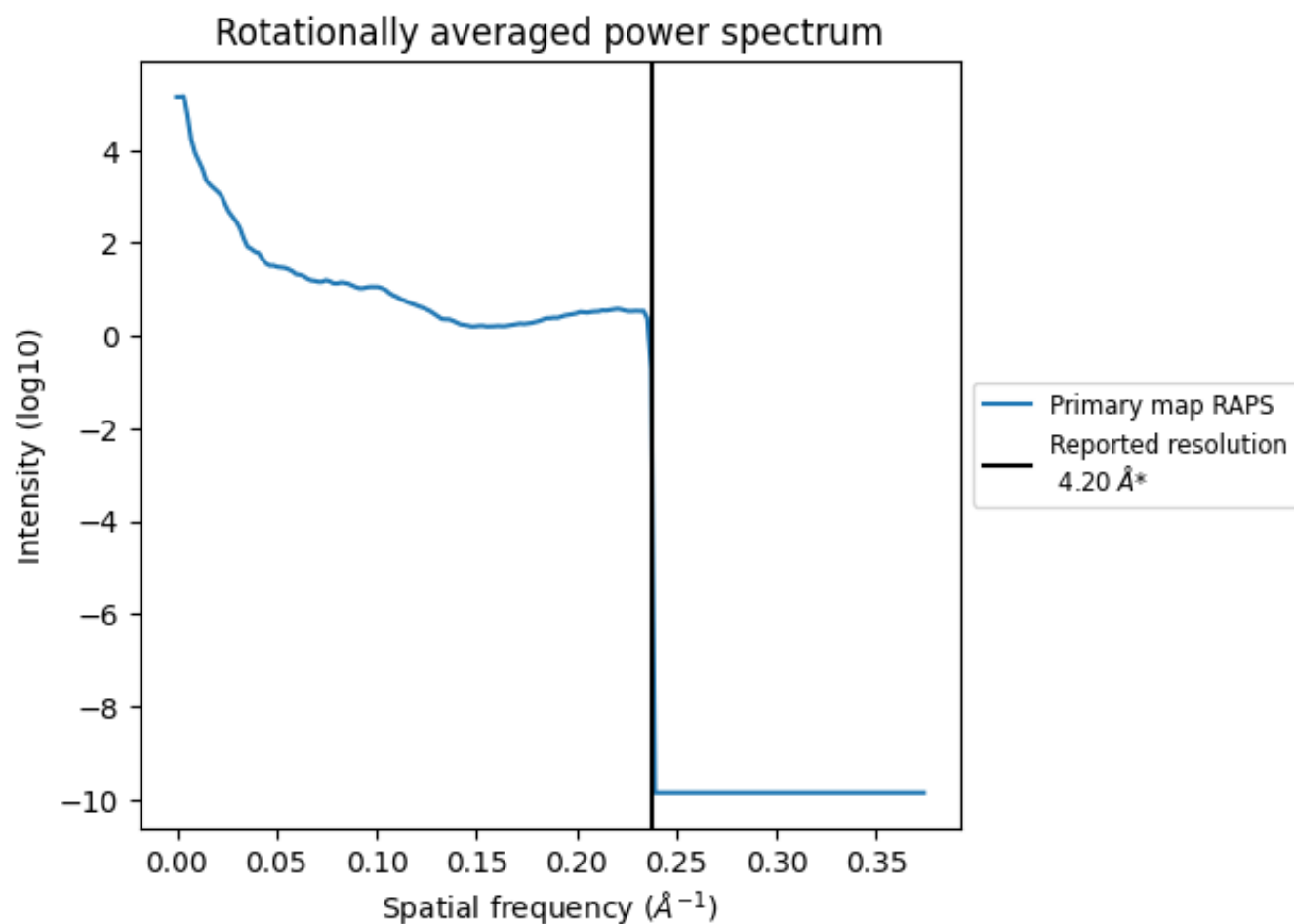
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1619 nm³; this corresponds to an approximate mass of 1462 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 ⓘ

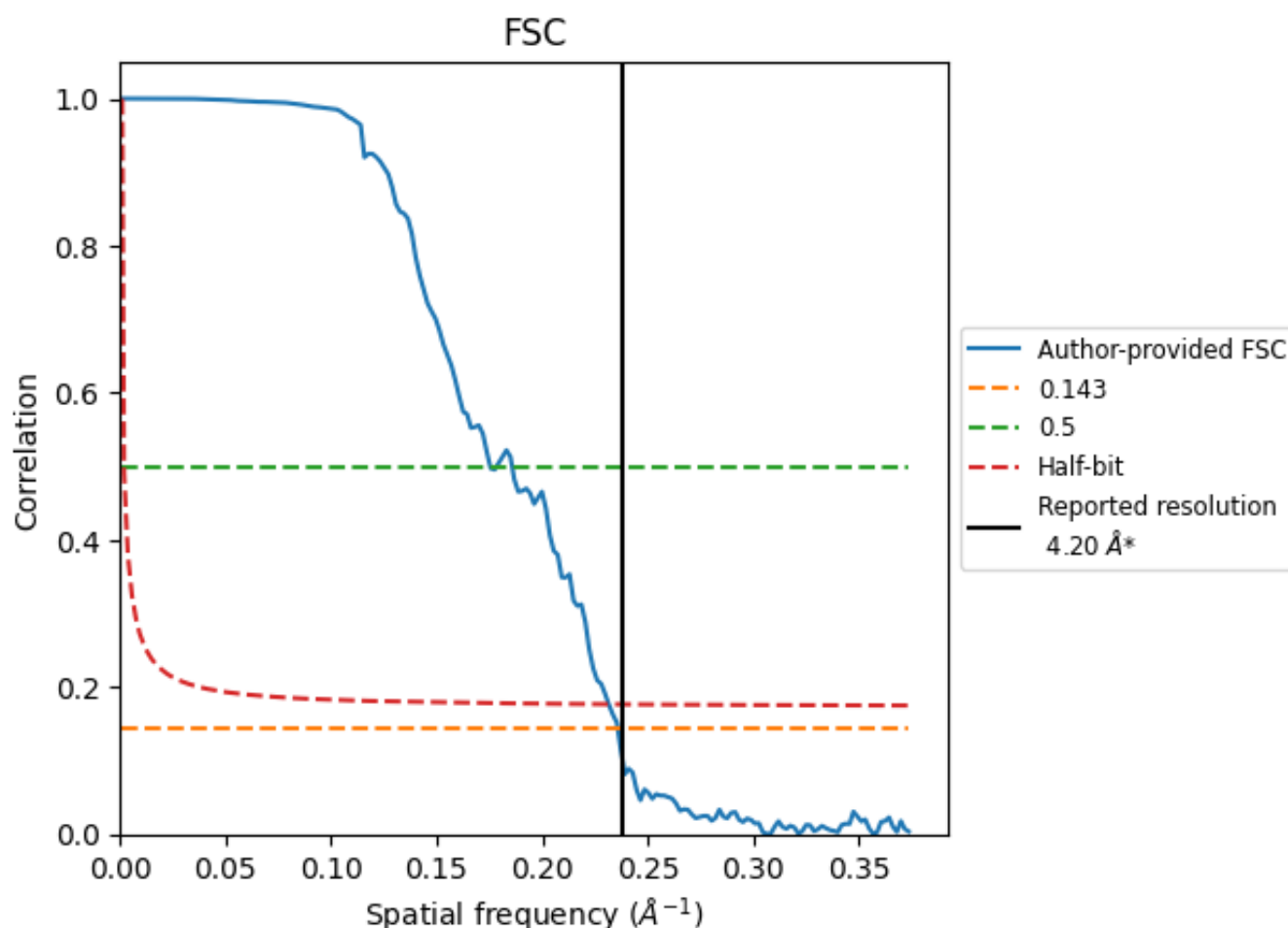


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 \AA^{-1}

8.2 Resolution estimates [i](#)

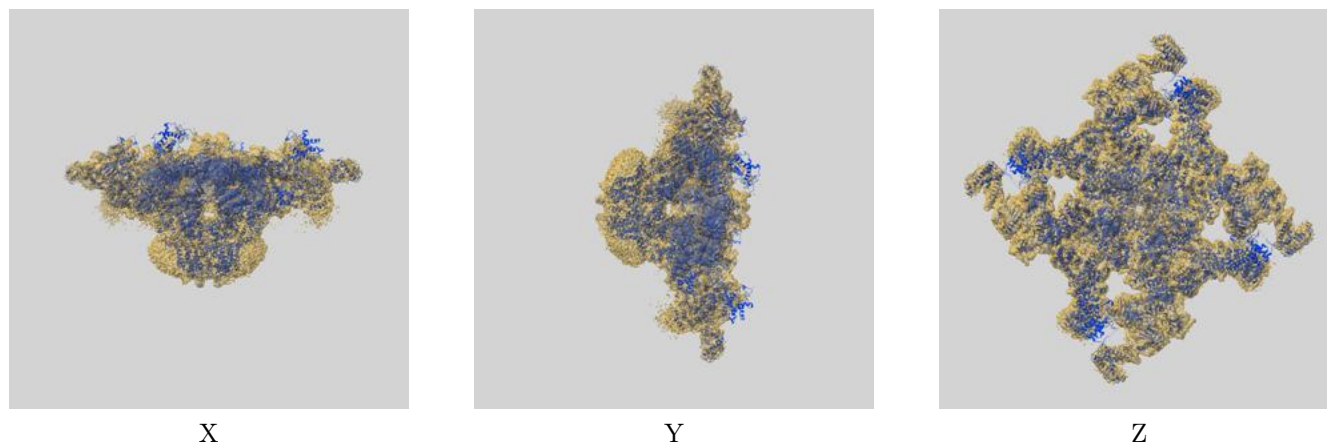
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.24	5.70	4.32
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

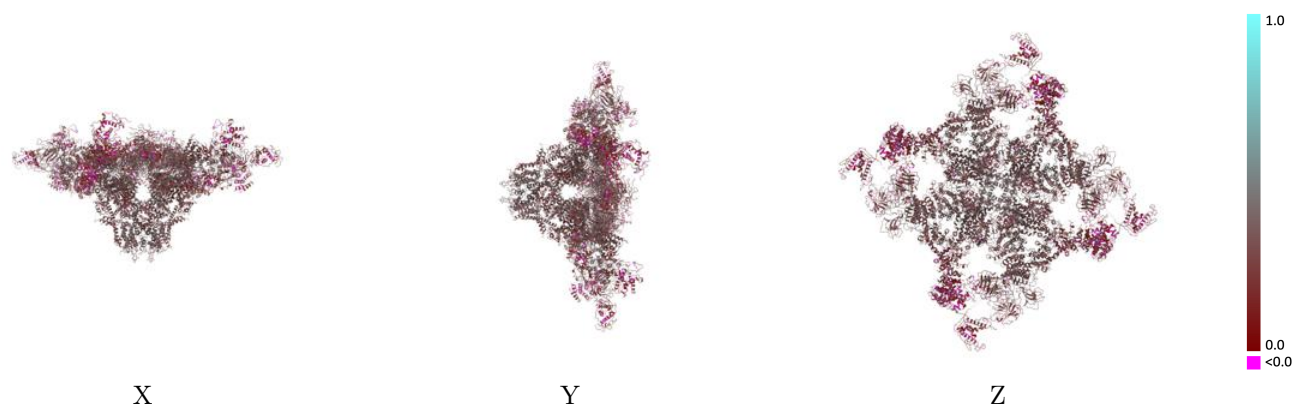
This section contains information regarding the fit between EMDB map EMD-9836 and PDB model 6JIU. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



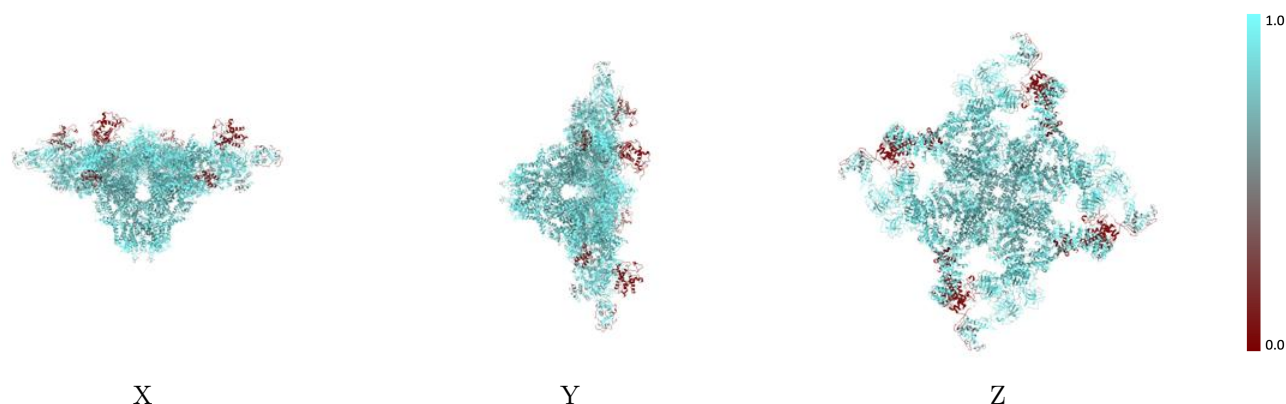
The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



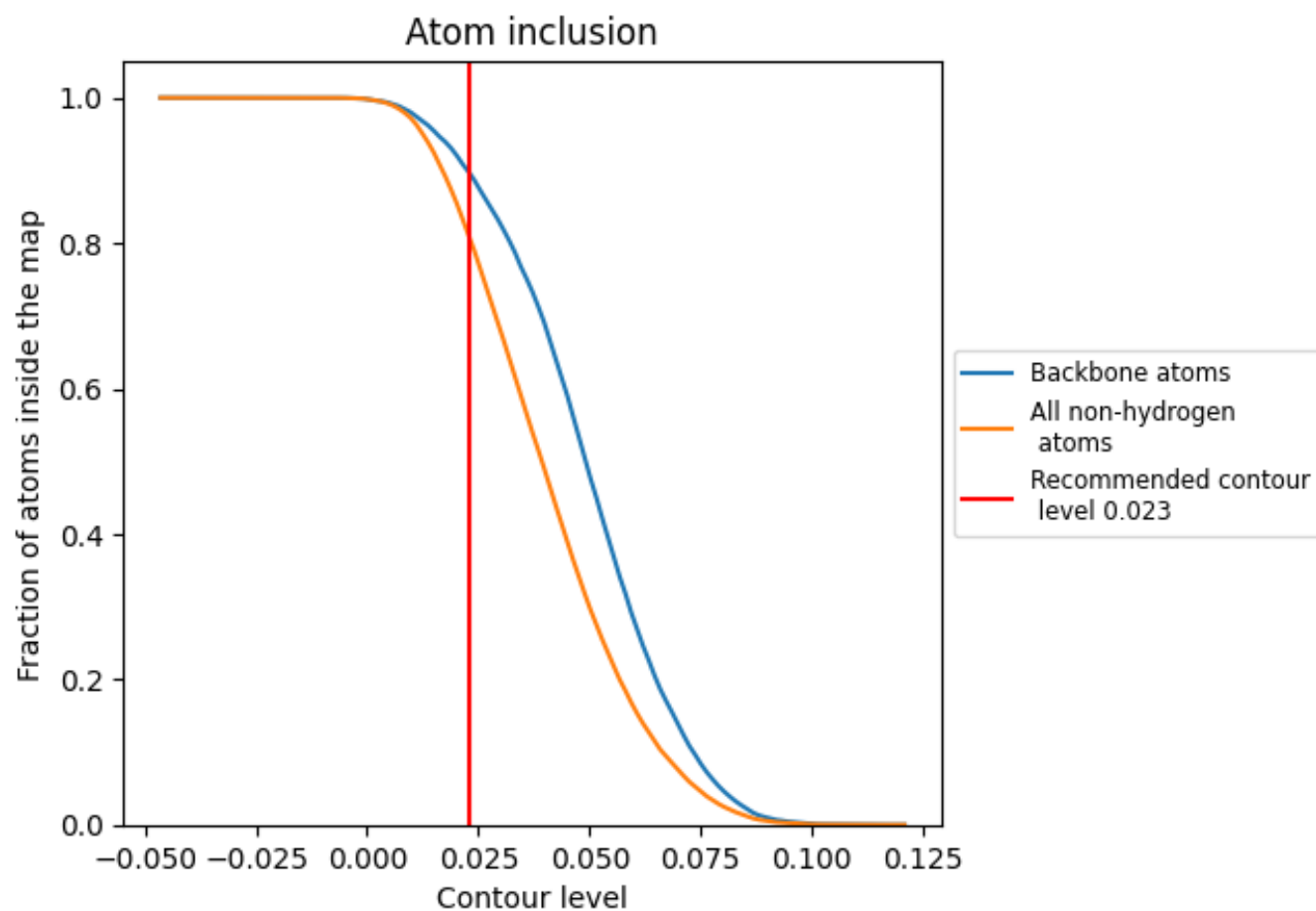
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.023).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 81% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8083	<div></div> 0.3030
A	<div></div> 0.8202	<div></div> 0.3050
B	<div></div> 0.8711	<div></div> 0.3450
C	<div></div> 0.1111	<div></div> 0.1780
D	<div></div> 0.8200	<div></div> 0.3050
E	<div></div> 0.8699	<div></div> 0.3430
F	<div></div> 0.1111	<div></div> 0.1750
G	<div></div> 0.8204	<div></div> 0.3040
H	<div></div> 0.8724	<div></div> 0.3420
I	<div></div> 0.1111	<div></div> 0.1790
J	<div></div> 0.8205	<div></div> 0.3040
K	<div></div> 0.8724	<div></div> 0.3420
L	<div></div> 0.1111	<div></div> 0.1800

1.0

0.0

<0.0