



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 09:20 AM UTC

PDB ID : 6JIU / pdb_00006jiu
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:

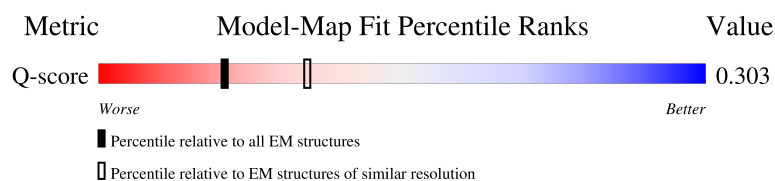
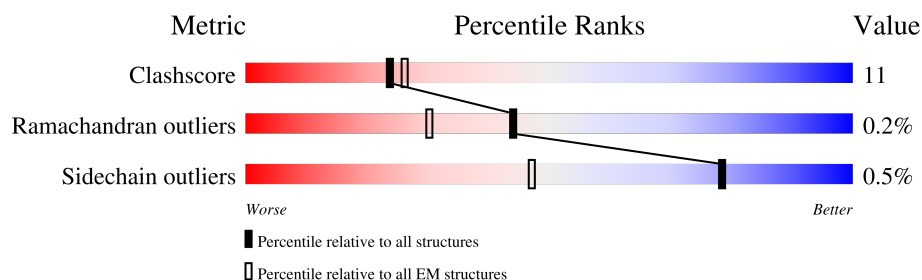
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	
1	D	4968	
1	G	4968	
1	J	4968	

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Mol	Chain	Length	Quality of chain
2	B	108	 77% 22%
2	E	108	 77% 22%
2	H	108	 78% 21%
2	K	108	 78% 21%
3	C	149	 42% 37% 9% 54%
3	F	149	 42% 38% 8% 54%
3	I	149	 42% 38% 8% 54%
3	L	149	 42% 38% 8% 54%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CFF	A	6003	-	X	-	-
7	CFF	D	6003	-	X	-	-
7	CFF	G	6003	-	X	-	-
7	CFF	J	6003	-	X	-	-

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 (CCD ID: 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 (CCD ID: CA) (formula: Ca).

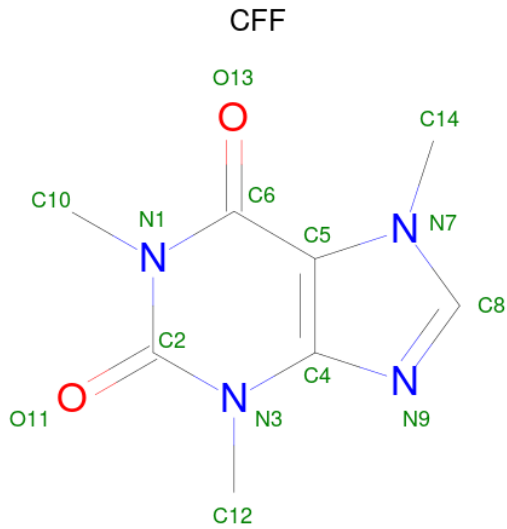
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total 1	Ca 1	0
5	C	2	Total 2	Ca 2	0
5	D	1	Total 1	Ca 1	0
5	F	2	Total 2	Ca 2	0
5	G	1	Total 1	Ca 1	0
5	I	2	Total 2	Ca 2	0
5	J	1	Total 1	Ca 1	0
5	L	2	Total 2	Ca 2	0

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 7 is CAFFEINE (CCD ID: CFF) (formula: $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$).

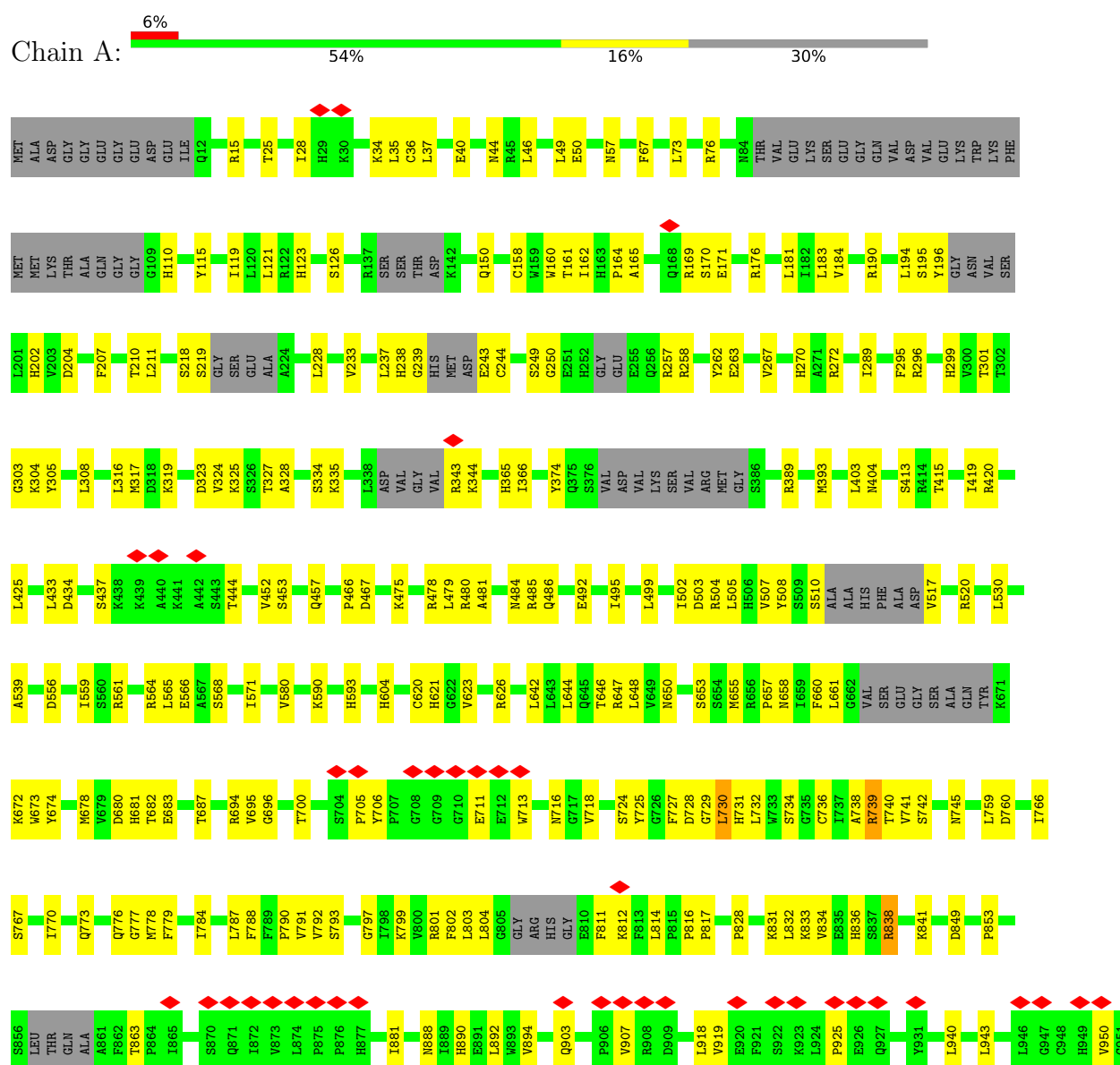


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total 14	C 8	N 4	O 2	0
7	D	1	Total 14	C 8	N 4	O 2	0
7	G	1	Total 14	C 8	N 4	O 2	0
7	J	1	Total 14	C 8	N 4	O 2	0

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.

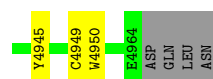
• Molecule 1: RyR2



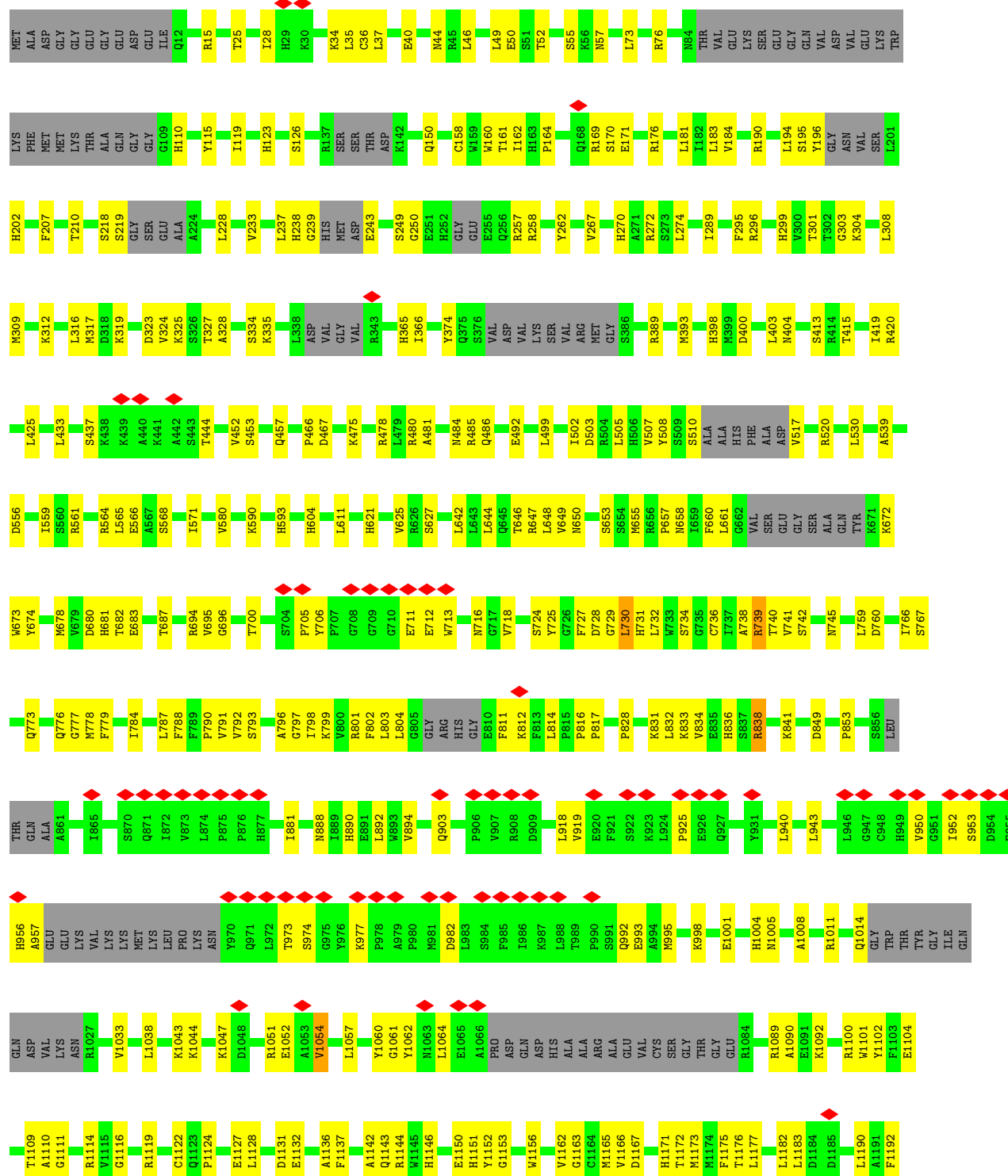






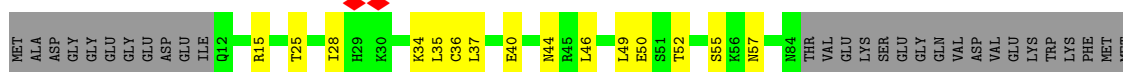


• Molecule 1: RyR2





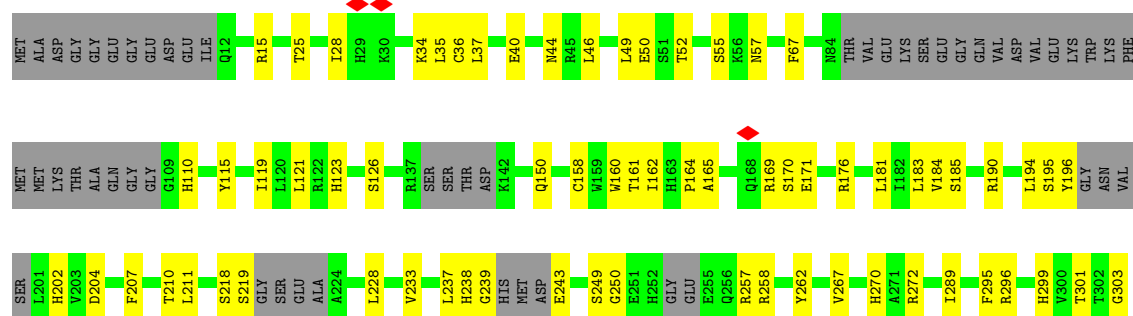






D2708	HIS	L2611	GLU	ILE	ASP	E2170	S2064	GLN	PRO	Y1778	E1690	V1488	VAL
D2709	ALA	K2605	V2481	MET	ILE	M2176	M2067	ASN	ALA	D1785	M1691	C1489	LEU
S2710	M2606	G2386	G2386	TRP	TRP	G2181	G2386	LEU	GLU	Q1588	V1588	GLY	ALA
D2711	P2607	L2485	L2485	ASN	ASN	G2181	W2070	LEU	GLU	K1790	Q1589	GLU	ASP
D2712	L2611	L2803	L2803	P2283	P2283	GLY	S2074	LEU	SER	M1794	L1595	SER	ARG
D2713	G2627	THR	THR	F2308	F2308	GLU	V2075	ASN	GLY	V1596	L1596	MET	ASP
D2714	ALA	A2404	ALA	S2313	S2313	SER	I2076	GLY	GLY	V1799	S1597	PRO	TYR
D2715	GLN	ALA	ALA	R2393	R2393	GLU	P2079	ASP	LYS	R1807	R1598	GLN	ASP
D2716	ASN	L2409	LEU	R2393	R2393	ILE	E2080	LYS	PRO	D1808	M1599	GLN	TYR
D2717	PHE	L2410	SER	L2410	L2410	THR	L2081	SER	LYS	P1809	P1600	GLY	LEU
D2718	GLY	A2411	ALA	I2326	I2326	PHE	L2081	GLU	GLU	K1605	K1605	ARG	MET
E2719	ALA	T2511	T2511	R2327	R2327	P2191	M2085	GLU	GLU	G1812	T1709	ASN	GLN
D2720	A2634	A2514	A2514	E2330	E2330	K2192	M2085	C1987	G1893	G1812	N1502	THR	SER
D2721	L2639	L2515	L2515	CYS	CYS	K2192	H2090	C1988	L1894	L1817	E1506	VAL	THR
D2722	R2643	M2518	M2518	PHE	PHE	M2193	L2089	P1990	K1904	L1817	E1506	VAL	THR
D2723	K2644	L2528	L2528	GLY	GLY	V2194	L2089	P1990	L1905	L1821	I1507	VAL	THR
D2724	G2648	L2528	L2528	ALA	ALA	A2195	L2089	P1990	L1905	L1821	I1507	VAL	THR
D2725	G2648	L2528	L2528	ALA	ALA	A2195	L2089	P1990	L1905	L1821	I1507	VAL	THR
D2726	L2653	THR	THR	ARG	ARG	N2211	D2116	GLY	Q1918	L1839	M1722	ALA	GLU
E2727	SER	L2433	ARG	GLY	GLY	G2212	N2119	LEU	H1921	L1839	M1722	ALA	GLU
D2728	GLN	V2434	CYS	GLU	GLU	K2213	N2119	ASP	R1922	I1842	P1728	ALA	GLU
S2729	LYS	G2435	ALA	GLY	GLY	A2122	A2122	GLY	A1925	I1846	M1729	ALA	GLU
D2730	LYS	L2535	PRO	GLY	GLY	V2228	Q2126	ASN	A1925	I1846	T1730	ALA	GLU
D2731	Y2658	L2437	LYS	ASN	ASN	GLY	Q2126	SER	A1925	I1846	T1730	ALA	GLU
D2732	P2679	S2438	A2543	G2343	G2343	LEU	V2133	ASP	A1928	S1849	I1736	SER	PRO
D2733	ASP	G2442	L2546	L2354	L2354	SER	ARG	T2024	Q1938	VAL	P1626	GLY	ALA
D2734	TYR	THR	THR	ALA	ALA	PRO	MET	T2025	Q1938	VAL	P1626	GLY	ALA
S2735	MET	GLU	GLU	GLU	GLU	ALA	GLY	R2029	Q1941	PHE	L1738	ASP	GLU
D2736	GLU	ILE	GLU	PRO	PRO	ARG	E2138	LYS	Q1941	GLY	P1739	GLY	GLU
D2737	SER	ALA	ALA	SER	SER	GLY	E2139	GLY	Y1945	ALA	E1634	GLY	GLU
D2738	ASN	LYS	LYS	ARG	ARG	SER	E2140	LEU	Y1948	GLY	ASN	GLY	GLU
D2739	VAL	ASP	ASP	ASP	ASP	GLY	K2141	LYS	M1949	PRO	LYS	GLY	GLU
D2740	SER	ASN	ASN	PRO	PRO	L2254	M2143	LYS	M1949	PRO	LYS	GLY	GLU
D2741	MET	VAL	VAL	SER	SER	L2254	M2143	LYS	M1953	GLU	HIS	GLY	GLU
D2742	LYS	GLU	GLU	THR	THR	L2258	L2147	GLN	SER	GLU	E1568	GLY	GLU
D2743	GLN	PRO	PRO	THR	THR	D2262	T2150	ALA	ALA	ASP	E1568	GLY	GLU
D2744	SER	ASP	ASP	GLY	GLY	L2263	T2150	LYS	ALA	THR	E1568	ILE	THR
D2745	SER	MET	MET	SER	SER	L2275	N2153	VAL	ALA	GLU	R1659	ASN	THR
D2746	MET	GLY	GLY	SER	SER	GLN	K2154	GLU	ALA	GLU	R1659	VAL	THR
E2745	ASP	ALA	ALA	LYS	LYS	SER	V2155	SER	ARG	GLU	Y1661	MET	THR
D2746	ASP	GLY	GLY	MET	MET	SER	F2156	THR	LYS	PRO	P1759	GLY	GLU
D2747	SER	ILE	ILE	PRO	PRO	THR	Y2157	ASP	THR	CYS	H1670	PRO	THR
D2748	GLY	D2464	GLY	GLN	GLN	GLN	Q2168	SER	LYS	ALA	P1766	LEU	GLU
D2749	GLN	H2465	GLN	THR	THR	MET	H2159	LYS	GLY	SER	L1676	SER	GLU
D2750	GLY	GLY	GLY	GLU	GLU	VAL	P2160	LYS	PHE	ASP	A1568	GLU	GLU
D2751	F2701	F2702	ARG	GLY	GLY	LYS	N2161	SER	SER	ASP	E1682	G1569	GLU
S2752	F2703	F2704	ARG	GLY	GLY	LYS	L2162	SER	SER	SER	S1770	L1570	GLU
D2753	Q2705	Q2706	M2601	ILE	THR	PRO	A2165	T2058	PRO	ARG	L1685	L1570	GLU
D2754	P2707	P2708	GLU	GLY	GLY	TYR	L2166	L2059	PRO	LEU	C1775	S1573	GLU
D2755	P2709	P2710	GLU	GLY	THR	PRO	L2166	Q2060	GLU	GLY	Q1777	V1579	GLU

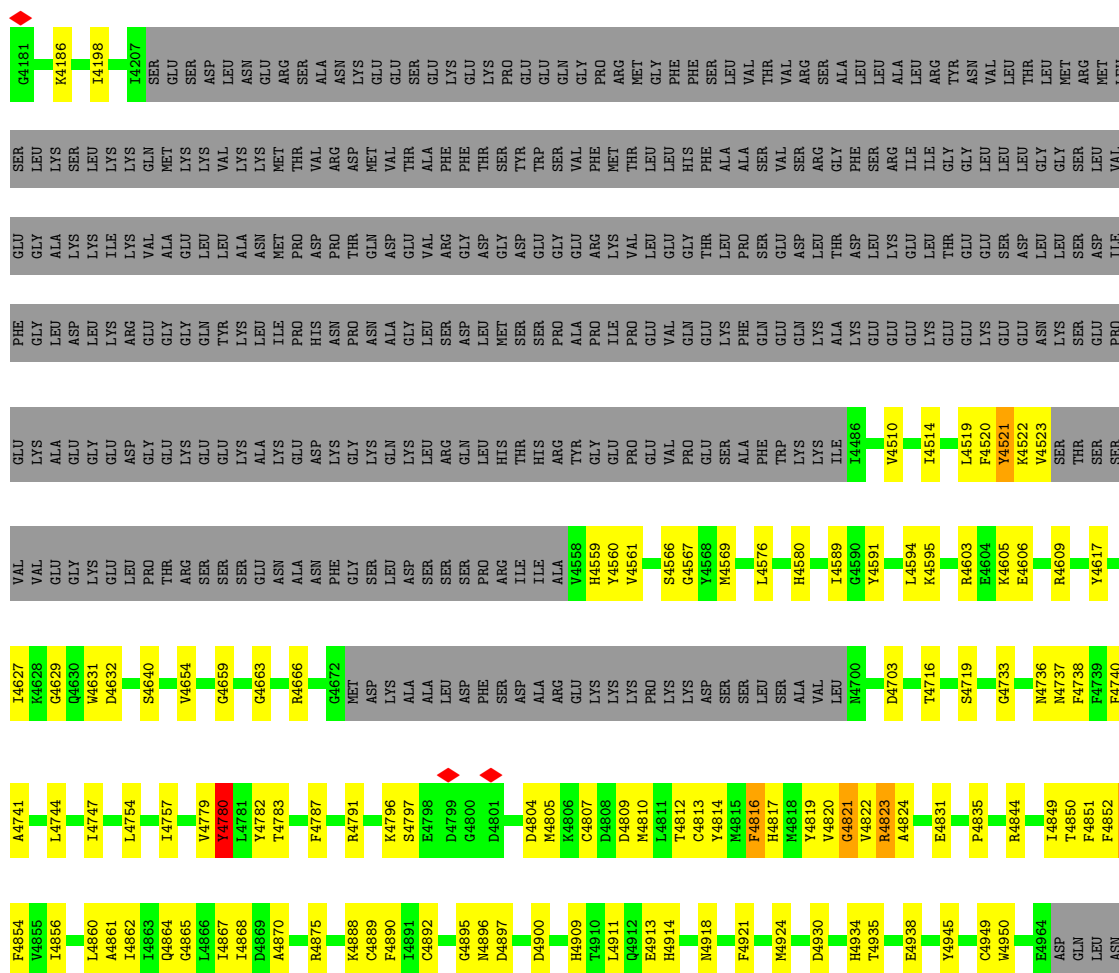








Y4046	I3925	A3737	GLY	LYS	VAL	TRP	GLU	LYS	CYS	VAL	S3137	CYS	LEU	E2882	◆
R4047	Q3926	M3740	ALA	SER	SER	LEU	VAL	LYS	CYS	CYS	L3138	L3034	GLU	K2883	◆
D4048	Q3934	F4049	VAL	THR	THR	GLY	ARG	LYS	THR	PRO	+	K3055	PHE	A2884	◆
H4050	S3935	S3748	PRO	CYS	GLN	GLY	ILE	LYS	ALA	ASN	+	SER	GLY	K2885	◆
K4051	L3936	+	GLU	ARG	ILE	ASN	ARG	LYS	ASN	PRO	+	ALA	GLY	D2886	◆
A4052	A3937	K3777	GLU	ARG	ARG	PRO	GLY	ALA	SER	SER	+	LEU	SER	D2887	◆
H4053	H3938	Y3781	ASP	ARG	ARG	GLU	GLY	VAL	GLU	GLU	+	ALA	ARG	E2888	◆
E4054	S3939	+	GLY	THR	TYR	GLY	ASN	VAL	HIS	LEU	+	SER	SER	K2889	◆
S4055	R3940	K3785	THR	SER	LYS	GLY	HIS	ASP	VAL	LEU	+	ALA	LYS	A2890	◆
H4056	+	K3786	LYS	SER	LEU	GLY	LEU	SER	THR	GLU	+	SER	GLY	D2891	◆
H4058	D3943	D3787	VAL	VAL	VAL	GLY	GLN	PHE	ARG	GLU	+	ILE	GLY	D2892	◆
Y4059	V3946	+	R3661	GLU	ASP	GLY	GLY	ARG	THR	GLU	+	D3068	HIS	T2893	◆
T4060	T3940	F3790	V3662	HIS	ARG	THR	GLY	ASP	GLY	GLU	+	+	PHE	D2894	◆
Q4061	L3949	+	D3663	PRO	TYR	VAL	LEU	ASP	ILE	VAL	+	T3072	PRO	L2895	◆
S4062	H3950	S3800	L3665	GLN	THR	ALA	GLY	LEU	ILE	ASP	+	+	GLY	K2896	◆
E4063	+	C3801	H3666	SER	THR	VAL	ASP	LYS	LEU	LEU	+	G3079	GLN	K2895	◆
+	M3955	L3804	L3667	GLY	ALA	THR	PRO	SER	LYS	ALA	+	T3082	GLY	F2896	◆
C4070	Q3956	+	L3668	LYS	ALA	ILE	ALA	GLU	ILE	GLU	+	HIS	ILE	L2897	◆
A4071	M3957	+	I3669	LYS	THR	ILE	SER	VAL	ILE	SER	+	THR	LYS	Q2898	◆
E4072	K3958	F3809	+	ALA	ARG	TRP	GLY	ARG	TYR	GLY	+	ARG	PHE	T2899	◆
T4073	L3959	E3810	R3674	VAL	ILE	TRP	TRP	GLY	ASN	ASN	+	ASN	ALA	A2900	◆
D4074	S3960	R3811	+	TRP	GLN	VAL	GLN	ASP	LYS	ARG	+	PRO	VAL	G2901	◆
+	+	Q3812	L3677	HIS	ALA	ALA	MET	LYS	GLY	THR	+	LYS	VAL	T2902	◆
T4078	M3973	+	+	LYS	ALA	ALA	ALA	SER	GLY	THR	+	GLY	VAL	A2903	◆
L4079	Q3976	G3819	K3682	L3591	LEU	LEU	LEU	HIS	GLY	PRO	+	VAL	LEU	V2904	◆
D4080	K3977	MET	L3683	L3592	TYR	TYR	TYR	ASN	ALA	ASP	+	THR	LEU	K2905	◆
Y4081	+	VAL	+	S3593	LYS	LYS	ARG	PHE	GLY	GLY	+	THR	ILE	R2906	◆
+	+	THR	Y3689	+	ASP	ASP	ARG	LEU	GLY	ILE	+	ILE	GLN	G2907	◆
+	+	GLY	Y3692	K3594	LEU	LEU	LEU	ARG	LEU	ALA	+	TYR	THR	PHE	◆
D4094	+	GLU	+	Q3595	PRO	PRO	ILE	GLY	GLN	VAL	+	T3098	PHE	LYS	◆
F4097	L3987	G3825	I3695	R3596	ARG	ARG	GLY	ASN	GLY	VAL	+	T3099	THR	LEU	◆
+	+	+	C3700	+	THR	GLY	THR	GLY	ASN	PHE	+	V3100	THR	ASP	◆
M4110	+	D3834	ASP	R3605	ASP	ILE	ASP	VAL	ALA	VAL	+	+	THR	LYS	◆
+	N3993	+	GLU	Y3610	THR	THR	ASP	THR	THR	PRO	+	+	LEU	ASN	◆
D4113	+	L3844	GLU	N3611	SER	SER	THR	GLN	PHE	LEU	+	+	GLU	HIS	◆
R4115	I3996	+	GLU	+	ASP	ASP	ASP	ASN	ALA	LEU	+	+	LEU	ARG	◆
L4116	S4007	L3879	ASP	L3612	PRO	PRO	GLY	GLY	GLY	SER	+	P3104	LEU	ASP	◆
Q4117	+	L3880	ASP	+	GLY	GLY	ASP	ILE	ASP	GLN	+	M3105	THR	THR	◆
T4118	M4010	R3881	GLY	R3616	LYS	LYS	GLN	ASN	LEU	PRO	+	L3106	PRO	PRO	◆
F4119	+	V3882	GLY	+	THR	THR	GLY	ASN	TYR	ILE	+	G3114	SER	ILE	◆
+	L4015	S3885	GLU	F3621	VAL	VAL	LEU	MET	ALA	ASN	+	+	GLU	GLY	◆
L4122	D4031	D3888	GLU	L3622	GLU	GLU	ILE	SER	PHE	LYS	+	Q3115	ARG	LYS	◆
A4123	T4032	+	GLU	Q3623	ARG	ARG	ARG	PHE	TYR	TRP	+	H3116	THR	ARG	◆
F4130	F4033	F3889	VAL	G3624	VAL	VAL	VAL	LEU	PRO	LYS	+	Q3117	SER	PHE	◆
+	K4034	Y3890	LYS	E3626	LEU	LEU	LEU	ILE	LEU	GLN	+	F3118	LEU	ALA	◆
L4134	E4035	W3891	S3714	K3627	ASP	ASP	LYS	THR	ILE	GLY	+	GLY	SER	TYR	◆
+	Y4036	+	+	+	ILE	ASN	ASN	ASP	ARG	PRO	+	ASP	GLU	GLY	◆
M4140	D4039	D3900	K3724	E3633	THR	THR	ARG	THR	THR	GLY	+	ILE	LEU	PHE	◆
+	+	A3910	R3731	E3634	VAL	VAL	VAL	SER	VAL	ASN	+	+	+	LEU	◆
R4148	+	+	L3732	H3635	LEU	LEU	LEU	LYS	ASP	PRO	+	+	+	GLN	◆
+	G4042	N3919	H3733	E3638	PHE	PHE	LYS	MET	TYR	GLY	+	L3124	ARG	ILE	◆
S4154	V4043	+	+	+	HIS	HIS	ASP	SER	ASN	ARG	+	+	ALA	LEU	◆
E4155	I4044	T3922	D3734	E3643	LEU	LEU	THR	LYS	ARG	ALA	+	S3130	SER	ILE	◆
+	S4045	+	G3736	L3645	GLN	GLY	GLU	ALA	LEU	VAL	+	C3131	ILE	VAL	◆
+	+	+	+	+	+	+	ASP	ALA	ALA	MET	+	Y3132	ASN	VAL	◆
+	+	+	+	+	+	+	+	+	+	+	+	R3133	THR	ASP	◆
+	+	+	+	+	+	+	+	+	+	+	+	I3134	GLY	GLU	◆
+	+	+	+	+	+	+	+	+	+	+	+	+	+	HIS	◆
+	+	+	+	+	+	+	+	+	+	+	+	+	+	GLN	◆
+	+	+	+	+	+	+	+	+	+	+	+	+	+	TYR	◆
+	+	+	+	+	+	+	+	+	+	+	+	+	+	ILE	◆



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

Chain B: 77% 22%

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

Chain E: 77% 22%

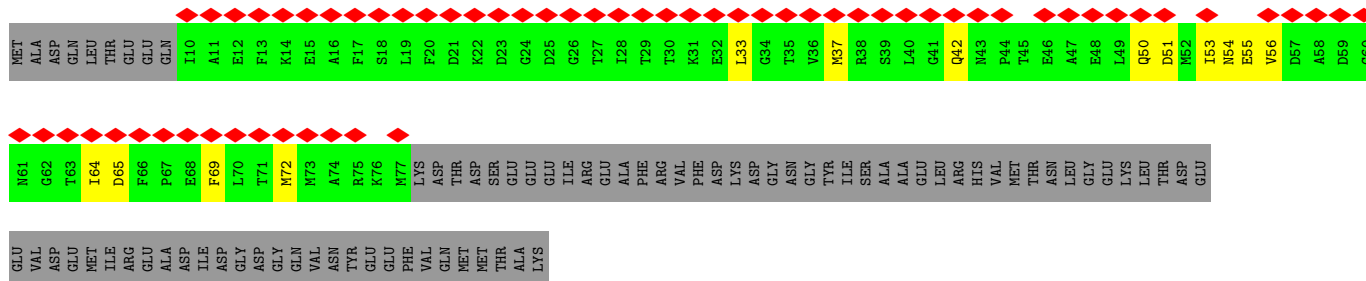
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 78% 21%

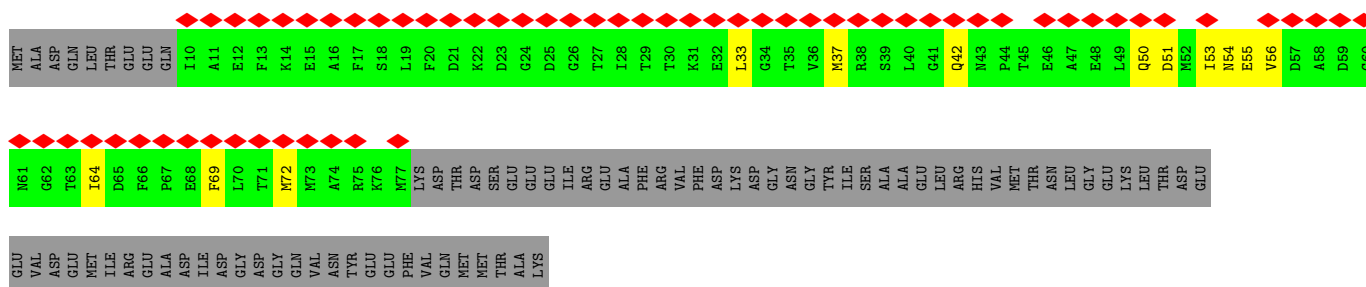
● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain K:  78% 21%

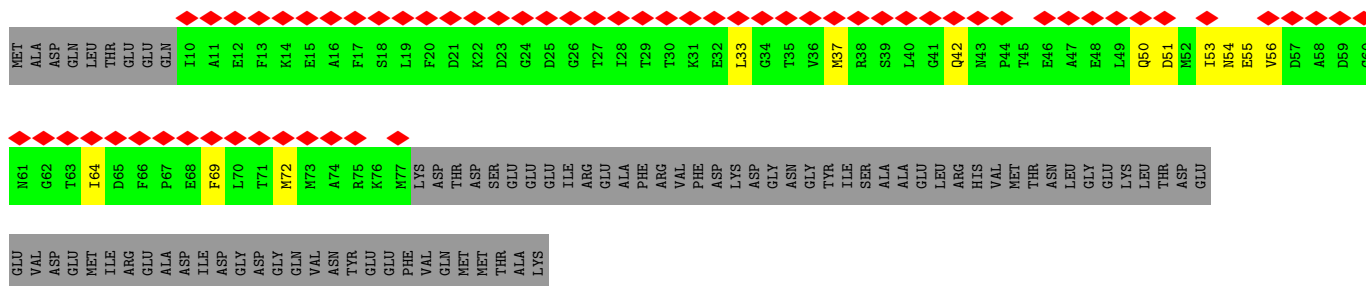
● Molecule 3: Calmodulin-1

Chain C:  42% 37% 9% 54%

● Molecule 3: Calmodulin-1

Chain F:  42% 38% 8% 54%

● Molecule 3: Calmodulin-1

Chain I:  42% 38% 8% 54%

● Molecule 3: Calmodulin-1

Chain L:  42% 38% 8% 54%

GLU	VAL	ASP	GLU	MET	ILE	ARG	GLU	ALA	ASP	ILE	ASP	GLY	ASP	GLN	VAL	VAL	GLN	MET	MET	THR	ALA	LYS																																				
N61	G62	T63	I64	D65	F66	P67	E68	F69	L70	T71	M72	M73	A74	R75	K76	M77	LYS	ASP	THR	ASP	SER	GLU	GLU	ILE	ARG	GLU	ALA	PHE	ARG	VAL	PHE	ASP	LYS	ASP	GLY	ASN	GLY	TYR	SER	ILE	ALA	GLU	LEU	ARG	HIS	VAL	MET	THR	ASN	LEU	GLY	GLU	LYS	LEU	THR	ASP	GLU	
ALA	ASP	GLN	LEU	THR	GLU	GLU	GLN	I10	A11	E12	F13	K14	E15	A16	F17	S18	L19	F20	D21	K22	D23	G24	D25	G26	T27	I28	T29	T30	K31	E32	L33	G34	T35	V36	M37	R38	S39	L40	G41	Q42	M43	P44	T45	E46	A47	E48	L49	Q50	D51	M52	I53	N54	E55	V56	D57	A58	D59	C60

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 (Å)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: ATP, ZN, CA, CFF

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	0.31	3/27161 (0.0%)	0.59	9/36737 (0.0%)
1	D	0.29	0/27161	0.60	12/36737 (0.0%)
1	G	0.29	0/27161	0.59	7/36737 (0.0%)
1	J	0.29	0/27161	0.59	10/36737 (0.0%)
2	B	0.25	0/835	0.54	0/1123
2	E	0.26	0/835	0.54	0/1123
2	H	0.25	0/835	0.54	0/1123
2	K	0.25	0/835	0.54	0/1123
3	C	0.18	0/530	0.53	0/711
3	F	0.18	0/530	0.53	0/711
3	I	0.18	0/530	0.53	0/711
3	L	0.18	0/530	0.53	0/711
All	All	0.29	3/114104 (0.0%)	0.59	38/154284 (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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4522	LYS	CA-C	-13.08	1.36	1.52
1	A	4521	TYR	N-CA	12.78	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4522	LYS	N-CA	5.60	1.53	1.45

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4823	ARG	N-CA-C	19.57	139.02	113.97
1	J	2326	ILE	N-CA-C	-8.74	103.32	111.45
1	D	4823	ARG	CB-CA-C	-8.71	94.43	109.07
1	J	2326	ILE	CB-CA-C	7.26	121.44	111.92
1	A	4522	LYS	N-CA-CB	-6.97	98.69	111.37
1	A	2326	ILE	CB-CA-C	6.91	122.62	111.29
1	G	2326	ILE	CB-CA-C	6.91	122.62	111.29
1	J	4521	TYR	CB-CA-C	-6.87	99.68	110.74
1	D	4823	ARG	N-CA-CB	-6.75	101.28	110.67
1	D	4822	VAL	CB-CA-C	6.58	121.06	112.24
1	D	2326	ILE	CB-CA-C	6.29	121.60	111.29
1	G	4780	TYR	N-CA-C	-5.84	104.82	111.07
1	A	4780	TYR	N-CA-C	-5.81	104.85	111.07
1	D	4780	TYR	N-CA-C	-5.81	104.85	111.07
1	J	4780	TYR	N-CA-C	-5.79	104.88	111.07
1	A	4821	GLY	N-CA-C	-5.78	99.49	113.18
1	D	2327	ARG	N-CA-C	5.78	119.14	111.75
1	D	4824	ALA	N-CA-C	-5.69	104.47	111.75
1	J	4521	TYR	N-CA-C	5.65	117.91	108.02
1	G	4521	TYR	CB-CA-C	-5.53	101.84	110.74
1	A	1739	PHE	N-CA-C	5.51	115.22	108.11
1	D	1739	PHE	N-CA-C	5.51	115.22	108.11
1	G	1739	PHE	N-CA-C	5.51	115.22	108.11
1	J	1739	PHE	N-CA-C	5.51	115.22	108.11
1	A	4522	LYS	N-CA-C	5.48	118.16	109.50
1	J	4821	GLY	N-CA-C	-5.45	100.25	113.18
1	G	507	VAL	N-CA-C	-5.20	107.75	112.12
1	A	507	VAL	N-CA-C	-5.16	107.79	112.12
1	D	507	VAL	N-CA-C	-5.16	107.79	112.12
1	J	507	VAL	N-CA-C	-5.16	107.79	112.12
1	A	2156	PHE	N-CA-C	-5.12	106.37	113.18
1	D	2156	PHE	N-CA-C	-5.12	106.37	113.18
1	G	2156	PHE	N-CA-C	-5.12	106.37	113.18
1	J	2156	PHE	N-CA-C	-5.12	106.37	113.18
1	D	687	THR	N-CA-C	-5.08	99.97	110.80
1	A	687	THR	N-CA-C	-5.07	100.01	110.80
1	G	687	THR	N-CA-C	-5.07	100.01	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	687	THR	N-CA-C	-5.06	100.02	110.80

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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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	624	0
1	D	26661	0	25136	615	0
1	G	26661	0	25136	624	0
1	J	26661	0	25136	622	0
2	B	819	0	824	16	0
2	E	819	0	824	16	0
2	H	819	0	824	15	0
2	K	819	0	824	15	0
3	C	524	0	504	9	0
3	F	524	0	504	8	0
3	I	524	0	504	8	0
3	L	524	0	504	8	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0
7	D	14	0	10	2	0
7	G	14	0	10	2	0
7	J	14	0	10	2	0
All	All	112212	0	105944	2381	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 11.

All (2381) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:J:4822:VAL:C	1:J:4824:ALA:H	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:4822:VAL:C	1:A:4824:ALA:H	1.87	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4822:VAL:C	1:G:4824:ALA:H	1.96	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
1:A:4852:PHE:CE1	1:D:4823:ARG:C	2.66	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1482:ARG:HH11	1:A:1531:TYR:HA	1.63	0.63
1:A:4822:VAL:C	1:A:4824:ALA:N	2.56	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4822:VAL:C	1:J:4824:ALA:N	2.55	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
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:A:2176:MET:HE1	1:A:2194:VAL:HG13	1.84	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:D:2176:MET:HE1	1:D:2194:VAL:HG13	1.84	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3891:TRP:HE1	1:A:3950:HIS:HE1	1.50	0.59
1:D:2138:GLU:O	1:D:2141:LYS:NZ	2.34	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: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:G:2176:MET:HE1	1:G:2194:VAL:HG13	1.84	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:J:2176:MET:HE1	1:J:2194:VAL:HG13	1.84	0.59
1:A:2138:GLU:O	1:A:2141:LYS:NZ	2.34	0.59
1:A:4515:ASN:CB	1:J:4780:TYR:OH	2.48	0.59
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:2138:GLU:O	1:G:2141:LYS:NZ	2.34	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:J:4594:LEU:HB3	1:J:4595:LYS:HZ2	1.67	0.58
1:A:486:GLN:NE2	1:A:539:ALA:O	2.36	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
1:J:4070:CYS:SG	1:J:4071:ALA:N	2.75	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: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
1:D:4782:TYR:CE2	1:D:4851:PHE:CD1	2.91	0.58
1:G:4070:CYS:SG	1:G:4071:ALA:N	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:D:4594:LEU:HB3	1:D:4595:LYS:HZ2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:4594:LEU:HB3	1:G:4595:LYS:HZ2	1.69	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:J:4007:SER:HG	1:J:4010:ASN:HD21	1.51	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:2138:GLU:O	1:J:2141:LYS:NZ	2.34	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:D:1948:VAL:HG13	1:D:1949:MET:HE2	1.89	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:1948:VAL:HG13	1:A:1949:MET:HE2	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:J:309:MET:SD	1:J:312:LYS:NZ	2.75	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
1:G:1948:VAL:HG13	1:G:1949:MET:HE2	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:4853:PHE:CD1	1:G:4853:PHE:C	2.85	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
1:A:3804:LEU:O	1:A:3885:SER:OG	2.26	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: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:A:4853:PHE:CD1	1:A:4853:PHE:C	2.85	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:J:1948:VAL:HG13	1:J:1949:MET:HE2	1.89	0.54
1:J:2434:VAL:O	1:J:2438:SER:OG	2.26	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:467:ASP:O	1:J:475:LYS:NZ	2.40	0.54
1:J:1690:GLU:OE2	1:J:1790:LYS:NZ	2.36	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:A:4819:TYR:CD1	1:A:4819:TYR:C	2.85	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:A:4852:PHE:C	1:A:4852:PHE:CD2	2.85	0.53
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:G:4819:TYR:C	1:G:4819:TYR:CD2	2.85	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:J:940:LEU:HA	1:J:943:LEU:HB2	1.89	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:4816:PHE:C	1:G:4816:PHE:CD1	2.86	0.53
1:J:2402:ARG:O	1:J:2475:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:4816:PHE:CD1	1:A:4816:PHE:C	2.87	0.53
1:D:467:ASP:O	1:D:475:LYS:NZ	2.40	0.53
1:D:4819:TYR:CD1	1:D:4819:TYR:C	2.85	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:G:4822:VAL:C	1:G:4824:ALA:N	2.60	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
2:B:63:ALA:HA	2:B:66:MET:HE2	1.92	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:A:1756:SER:OG	1:A:1757:LEU:N	2.40	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:3804:LEU:O	1:G:3885:SER:OG	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:E:63:ALA:HA	2:E:66:MET:HE2	1.92	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:J:3804:LEU:O	1:J:3885:SER:OG	2.26	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:J:4853:PHE:CD1	1:J:4853:PHE:C	2.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:ILE:HG12	1:D:196:TYR:HE1	1.74	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
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:4056:HIS:C	1:J:4057:LYS:HG2	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:J:4816:PHE:CD1	1:J:4816:PHE:C	2.87	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2107:TYR:CG	1:A:2162:LEU:HD21	2.45	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:2783:MET:HE3	1:J:2845:MET:HE2	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
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:309:MET:SD	1:D:312:LYS:NZ	2.75	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:207:PHE:CB	1:J:2326:ILE:C	2.84	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:4056:HIS:C	1:G:4057:LYS:HG2	2.35	0.51
1:G:4094:ASP:OD1	1:G:4094:ASP:N	2.44	0.51
2:H:63:ALA:HA	2:H:66:MET:HE2	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4056:HIS:C	1:A:4057:LYS:HG2	2.35	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:170:SER:OG	1:D:171:GLU:N	2.42	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
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:4056:HIS:C	1:D:4057:LYS:HG2	2.35	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:G:2783:MET:HE3	1:G:2845:MET:HE2	1.93	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
2:K:63:ALA:HA	2:K:66:MET:HE2	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:G:4796:LYS:NZ	1:G:4805:MET:O	2.38	0.50
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: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:207:PHE:CB	1:D:2326:ILE:C	2.85	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:2783:MET:HE3	1:A:2845:MET:HE2	1.93	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:742:SER:OG	1:J:1472:GLU:OE2	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2326:ILE:C	1:J:207:PHE:CB	2.85	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:1688:ALA:HA	1:D:1694:MET:HE1	1.94	0.49
2:E:71:ARG:NH2	2:E:100:ASP:OD2	2.44	0.49
1:J:1144:ARG:NH2	1:J:1150:GLU:OE1	2.43	0.49
1:J:1688:ALA:HA	1:J:1694:MET:HE1	1.94	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:D:3804:LEU:O	1:D:3885:SER:OG	2.26	0.49
1:G:1688:ALA:HA	1:G:1694:MET:HE1	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: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
1:D:2783:MET:HE3	1:D:2845:MET:HE2	1.93	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
1:J:40:GLU:HB3	1:J:44:ASN:HB3	1.93	0.49
1:J:2140:GLU:HB2	1:J:2143:MET:HE2	1.94	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: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:1688:ALA:HA	1:A:1694:MET:HE1	1.94	0.49
1:A:1719:LEU:HA	1:A:1722:ASN:HD22	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4861:ALA:HB2	1:D:4864:GLN:CD	2.37	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: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: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
1:G:3925:ILE:HD11	1:G:3936:LEU:HD13	1.93	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:207:PHE:CB	1:G:2326:ILE:C	2.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:4591:TYR:OH	1:A:4719:SER:OG	2.31	0.48
1:A:4945:TYR:HH	7:A:6003:CFF:H81	1.77	0.48
1:D:742:SER:OG	1:D:1472:GLU:OE2	2.28	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:G:2140:GLU:HB2	1:G:2143:MET:HE2	1.94	0.48
1:J:3900:ASP:OD1	1:J:3900:ASP:N	2.39	0.48
1:J:4819:TYR:CD1	1:J:4819:TYR:C	2.90	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
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: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:3800:SER:OG	1:J:3801:CYS:N	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:4514:ILE:HD11	1:G:4576:LEU:HB3	1.96	0.48
1:J:1730:THR:O	1:J:1733:THR:OG1	2.29	0.48
1:J:2060:GLN:O	1:J:2064:SER:OG	2.32	0.48
1:J:2122:ALA:O	1:J:2126:GLN:N	2.47	0.48
1:A:218:SER:OG	1:A:219:SER:N	2.43	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
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:2140:GLU:HB2	1:D:2143:MET:HE2	1.94	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:2140:GLU:HB2	1:A:2143:MET:HE2	1.94	0.47
1:D:556:ASP:N	1:D:556:ASP:OD1	2.46	0.47
1:D:2060:GLN:O	1:D:2064:SER:OG	2.32	0.47
1:D:2122:ALA:O	1:D:2126:GLN:N	2.47	0.47
1:D:4861:ALA:HB2	1:G:4864:GLN:CD	2.38	0.47
1:G:727:PHE:H	1:G:730:LEU:HD12	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2070:TRP:O	1:G:2074:SER:OG	2.32	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
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:711:GLU:OE1	1:D:1448:SER:OG	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:4945:TYR:HH	7:G:6003:CFF:H81	1.78	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:2737:LYS:HZ3	1:A:2755:GLN:HE22	1.62	0.47
1:A:3623:GLN:O	1:A:3627:LYS:NZ	2.47	0.47
1:A:4864:GLN:CD	1:J:4861:ALA:HB2	2.39	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:2884:ALA:HA	1:D:2887:ARG:HB3	1.97	0.47
1:G:2883:LYS:O	1:G:2887:ARG:N	2.42	0.47
1:G:3919:ASN:O	1:G:3922:THR:OG1	2.31	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:2060:GLN:O	1:A:2064:SER:OG	2.32	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: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
1:D:706:TYR:HH	1:D:1254:ARG:H	1.62	0.47
1:D:727:PHE:H	1:D:730:LEU:HD12	1.78	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:1599:MET:HE3	1:G:1599:MET:HB2	1.80	0.47
1:G:2404:ALA:HB3	1:G:2475:ARG:HE	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:706:TYR:HH	1:J:1254:ARG:H	1.62	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:A:15:ARG:HD3	1:A:110:HIS:HB3	1.96	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:D:4591:TYR:OH	1:D:4719:SER:OG	2.31	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:D:658:ASN:HB2	1:D:833:LYS:H	1.80	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1245:ARG:HE	1:G:1692:LYS:HB3	1.79	0.46
1:G:2060:GLN:O	1:G:2064:SER:OG	2.32	0.46
1:G:2737:LYS:HZ3	1:G:2755:GLN:HE22	1.64	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:249:SER:OG	1:D:250:GLY:N	2.44	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: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:741:VAL:HB	1:J:778:MET:HE2	1.97	0.46
1:J:1444:GLY:HA2	1:J:1487:MET:HB2	1.97	0.46
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
3:C:69:PHE:HA	3:C:72:MET:HE2	1.98	0.46
1:D:334:SER:OG	1:D:335:LYS:N	2.49	0.46
1:D:741:VAL:HB	1:D:778:MET:HE2	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4737:ASN:OD1	1:G:4737:ASN:N	2.39	0.46
1:J:712:GLU:OE2	1:J:1638:SER:OG	2.33	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:1038:LEU:HD11	1:J:1043:LYS:HZ2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3973:MET:HA	1:J:3976:GLN:HB3	1.96	0.46
1:J:4591:TYR:OH	1:J:4719:SER:OG	2.31	0.46
3:L:69:PHE:HA	3:L:72:MET:HE2	1.98	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:1694:MET:HE3	1:D:1694:MET:HB2	1.71	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:741:VAL:HB	1:A:778:MET:HE2	1.97	0.45
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
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:3689:TYR:HE1	1:A:3740:MET:HE1	1.81	0.45
1:A:3740:MET:HE2	1:A:3740:MET:HB2	1.87	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:D:4945:TYR:HH	7:D:6003:CFF:H81	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1152:TYR:OH	1:J:1175:PHE:O	2.35	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:A:1694:MET:HE3	1:A:1694:MET:HB2	1.71	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:J:3689:TYR:HE1	1:J:3740:MET:HE1	1.81	0.45
1:A:706:TYR:HH	1:A:1254:ARG:H	1.62	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:1938:GLN:NE2	1:A:3611:ASN:O	2.50	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
1:D:1152:TYR:OH	1:D:1175:PHE:O	2.35	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:I:69:PHE:HA	3:I:72:MET:HE2	1.98	0.45
1:J:1116:GLY:HA3	1:J:1136:ALA:HA	1.99	0.45
1:A:556:ASP:N	1:A:556:ASP:OD1	2.46	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: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:J:2737:LYS:HZ3	1:J:2755:GLN:HE22	1.65	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: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:G:4861:ALA:HB2	1:J:4864:GLN:CD	2.38	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:3740:MET:HE2	1:J:3740:MET:HB2	1.87	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4140:MET:HB3	1:A:4140:MET:HE2	1.87	0.45
1:A:4819:TYR:CD1	1:A:4819:TYR:O	2.70	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: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: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:D:4140:MET:HE2	1:D:4140:MET:HB3	1.87	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:334:SER:OG	1:A:335:LYS:N	2.49	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:D:695:VAL:HG22	1:D:792:VAL:HG23	1.99	0.44
1:D:2327:ARG:H	1:D:2327:ARG:HG3	1.49	0.44
1:D:2782:THR:HG23	1:D:2845:MET:HE1	1.99	0.44
1:D:4852:PHE:O	1:D:4852:PHE:CG	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4896:ASN:O	1:D:4900:ASP:N	2.50	0.44
1:G:741:VAL:HB	1:G:778:MET:HE2	1.97	0.44
1:G:1938:GLN:NE2	1:G:3611:ASN:O	2.50	0.44
1:G:3689:TYR:HE1	1:G:3740:MET:HE1	1.81	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:1900:PRO:O	1:D:1904:LYS:NZ	2.40	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:3957:MET:O	1:G:3960:SER:OG	2.34	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:4796:LYS:NZ	1:J:4805:MET:O	2.38	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:2070:TRP:O	1:A:2074:SER:OG	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:334:SER:OG	1:G:335:LYS:N	2.49	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:2782:THR:HG23	1:J:2845:MET:HE1	1.99	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: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
3:F:69:PHE:HA	3:F:72:MET:HE2	1.98	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:2782:THR:HG23	1:G:2845:MET:HE1	1.99	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:335:LYS:NZ	1:J:398:HIS:O	2.50	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: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:3689:TYR:HE1	1:D:3740:MET:HE1	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:335:LYS:NZ	1:D:398:HIS:O	2.50	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:D:4520:PHE:HD2	1:D:4569:MET:HE1	1.83	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:3957:MET:O	1:J:3960:SER:OG	2.34	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:4520:PHE:HD2	1:A:4569:MET:HE1	1.83	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
1:D:3740:MET:HE2	1:D:3740:MET:HB2	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:3981:VAL:O	1:A:3985:SER:OG	2.36	0.43
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: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: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: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:A:190:ARG:HH12	1:D:2423:ILE:HG23	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1730:THR:O	1:D:1733:THR:OG1	2.29	0.43
1:D:4817:HIS:NE2	1:D:4828:ILE:CD1	2.81	0.43
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:1599:MET:HE3	1:J:1599:MET:HB2	1.80	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: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: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:J:3981:VAL:O	1:J:3985:SER:OG	2.36	0.43
1:J:4520:PHE:HD2	1:J:4569:MET:HE1	1.83	0.43
1:A:2782:THR:HG23	1:A:2845:MET:HE1	1.99	0.43
1:A:2897:LEU:HD23	1:A:2897:LEU:HA	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:4198:ILE:HG12	1:D:4924:MET:HE3	2.01	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
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:G:4140:MET:HE2	1:G:4140:MET:HB3	1.87	0.43
1:J:1712:SER:HA	1:J:1715:ALA:HB3	1.99	0.43
1:J:3724:LYS:HA	1:J:3724:LYS:HD3	1.81	0.43
1:J:4198:ILE:HG12	1:J:4924:MET:HE3	2.01	0.43
1:J:4945:TYR:HH	7:J:6003:CFF:H81	1.82	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:1628:MET:HE3	1:A:1641:ILE:HG13	2.01	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:3981:VAL:O	1:D:3985:SER:OG	2.36	0.43
1:D:4651:LYS:NZ	1:D:4672:GLY:O	2.40	0.43
1:G:335:LYS:NZ	1:G:398:HIS:O	2.50	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:4520:PHE:HD2	1:G:4569:MET:HE1	1.83	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: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
1:A:4198:ILE:HG12	1:A:4924:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:973:THR:HG21	1:D:977:LYS:HA	2.01	0.43
1:D:1162:VAL:O	1:D:1176:THR:OG1	2.35	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
2:B:104:LEU:HD23	2:B:104:LEU:HA	1.90	0.43
1:D:374:TYR:OH	1:D:400:ASP:OD2	2.34	0.43
1:D:745:ASN:ND2	1:D:773:GLN:OE1	2.49	0.43
1:D:1038:LEU:HD11	1:D:1043:LYS:HZ2	1.84	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: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:3740:MET:HE2	1:G:3740:MET:HB2	1.87	0.43
1:G:4198:ILE:HG12	1:G:4924:MET:HE3	2.01	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: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:1124:PRO:O	1:A:1598:ARG:NE	2.51	0.42
1:A:3879:LEU:HA	1:A:3882:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:4852:PHE:O	1:A:4852:PHE:CG	2.70	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:1628:MET:HE3	1:G:1641:ILE:HG13	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:974:SER:OG	1:A:974:SER:O	2.35	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
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:3981:VAL:O	1:G:3985:SER:OG	2.36	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:J:4852:PHE:O	1:J:4852:PHE:CG	2.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4140:MET:HE2	1:J:4140:MET:HB3	1.87	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
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:711:GLU:OE1	1:J:1448:SER:OG	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:185:SER:HG	1:J:190:ARG:H	1.62	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
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: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
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:1628:MET:HE3	1:D:1641:ILE:HG13	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2067:MET:HE3	1:J:2085:MET:HE3	2.02	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
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: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:2067:MET:HE3	1:A:2085:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1162:VAL:O	1:G:1176:THR:OG1	2.35	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
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:1628:MET:HE3	1:J:1641:ILE:HG13	2.01	0.41
1:J:2090:HIS:HD2	1:J:3695:ILE:HD11	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:D:3957:MET:O	1:D:3960:SER:OG	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1945:TYR:OH	1:A:1993:ILE:O	2.35	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:2067:MET:HE3	1:D:2085:MET:HE3	2.02	0.41
1:D:2154:LYS:O	1:D:2154:LYS:NZ	2.53	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
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:1730:THR:O	1:A:1733:THR:OG1	2.29	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:725:TYR:HA	1:D:732:LEU:HA	2.01	0.41
1:D:3945:VAL:HB	1:D:4003:MET:HE1	2.03	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:3911:ILE:HD13	1:A:3911:ILE:HA	1.93	0.41
1:A:3957:MET:O	1:A:3960:SER:OG	2.34	0.41
1:A:4875:ARG:HD2	1:A:4875:ARG:O	2.20	0.41
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:D:3998:LYS:HG3	1:D:4110:MET:HE1	2.03	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:2085:MET:HE2	1:A:2085:MET:HB3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2154:LYS:HA	1:A:2154:LYS:HD2	1.93	0.41
1:A:4515:ASN:CG	1:J:4780:TYR:OH	2.64	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:712:GLU:OE2	1:G:1638:SER:OG	2.33	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
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: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:712:GLU:OE2	1:D:1638:SER:OG	2.33	0.41
1:D:892:LEU:HD13	1:D:1052:GLU:HB3	2.02	0.41
1:D:953:SER:OG	1:D:1061:GLY:O	2.38	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:2067:MET:HE3	1:G:2085:MET:HE3	2.02	0.41
1:G:2085:MET:HE2	1:G:2085:MET:HB3	1.84	0.41
1:G:2170:GLU:H	1:G:2170:GLU:HG2	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1162:VAL:O	1:A:1176:THR:OG1	2.35	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:1038:LEU:HD11	1:G:1043:LYS:HZ2	1.85	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:3998:LYS:HG3	1:G:4110:MET:HE1	2.03	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:J:4737:ASN:OD1	1:J:4737:ASN:N	2.39	0.41
1:A:123:HIS:HD2	1:A:126:SER:H	1.69	0.40
1:A:219:SER:O	1:A:219:SER:OG	2.29	0.40
1:A:505:LEU:HD12	1:A:505:LEU:HA	1.88	0.40
1:A:770:ILE:HD13	1:A:770:ILE:HA	1.96	0.40
1:A:953:SER:OG	1:A:1061:GLY:O	2.38	0.40
1:A:1165:MET:HB3	1:A:1236:TYR:CZ	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3955:MET:HE3	1:G:3958:LYS:HG3	2.03	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:3955:MET:HE3	1:J:3958:LYS:HG3	2.03	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: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:A:3998:LYS:HG3	1:A:4110:MET:HE1	2.03	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:1945:TYR:OH	1:D:1993:ILE:O	2.35	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:1764:SER:OG	1:J:1779:SER:O	2.32	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:219:SER:O	1:J:219:SER:OG	2.29	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: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:4852:PHE:CZ	1:D:4822:VAL:C	2.98	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:D:653:SER:O	1:D:653:SER:OG	2.37	0.40
1:D:3955:MET:HE3	1:D:3958:LYS:HG3	2.03	0.40
1:G:123:HIS:HD2	1:G:126:SER:H	1.69	0.40
1:G:219:SER:O	1:G:219:SER:OG	2.29	0.40
1:G:434:ASP:OD1	1:G:504:ARG:NE	2.52	0.40
1:G:847:THR:OG1	1:G:1215:MET:O	2.33	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3945:VAL:HB	1:A:4003:MET:HE1	2.03	0.40
1:A:3955:MET:HE3	1:A:3958:LYS:HG3	2.03	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: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%)	43 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	3374/4968 (68%)	3012 (89%)	355 (10%)	7 (0%)	43	77
1	G	3374/4968 (68%)	3012 (89%)	354 (10%)	8 (0%)	43	77
1	J	3374/4968 (68%)	3010 (89%)	355 (10%)	9 (0%)	36	71
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%)	44	77

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%)	2656 (99%)	16 (1%)	78	80
1	D	2671/4355 (61%)	2656 (99%)	15 (1%)	78	80
1	G	2671/4355 (61%)	2655 (99%)	16 (1%)	78	80
1	J	2671/4355 (61%)	2657 (100%)	14 (0%)	81	81
2	B	88/89 (99%)	88 (100%)	0	100	100
2	E	88/89 (99%)	88 (100%)	0	100	100
2	H	88/89 (99%)	88 (100%)	0	100	100
2	K	88/89 (99%)	88 (100%)	0	100	100
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%)	11204 (100%)	61 (0%)	78	81

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	324	VAL
1	A	444	THR
1	A	907	VAL
1	A	925	PRO
1	A	950	VAL
1	A	1054	VAL
1	A	2076	ILE
1	A	2099	LEU
1	A	2793	THR
1	A	2876	ASP
1	A	3996	ILE
1	A	4716	THR
1	A	4780	TYR
1	A	4816	PHE
1	A	4852	PHE
1	A	4853	PHE
1	D	324	VAL
1	D	444	THR
1	D	925	PRO
1	D	950	VAL
1	D	1054	VAL
1	D	2076	ILE
1	D	2099	LEU
1	D	2793	THR
1	D	2876	ASP
1	D	3996	ILE
1	D	4716	THR
1	D	4780	TYR
1	D	4817	HIS
1	D	4853	PHE
1	D	4875	ARG
1	G	324	VAL
1	G	444	THR
1	G	907	VAL
1	G	925	PRO
1	G	950	VAL
1	G	2076	ILE
1	G	2099	LEU
1	G	2793	THR
1	G	2876	ASP
1	G	3996	ILE
1	G	4716	THR
1	G	4780	TYR

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Mol	Chain	Res	Type
1	G	4816	PHE
1	G	4818	MET
1	G	4853	PHE
1	G	4875	ARG
1	J	324	VAL
1	J	444	THR
1	J	907	VAL
1	J	925	PRO
1	J	950	VAL
1	J	2076	ILE
1	J	2099	LEU
1	J	2793	THR
1	J	2876	ASP
1	J	3996	ILE
1	J	4716	THR
1	J	4780	TYR
1	J	4816	PHE
1	J	4853	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (214) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	44	ASN
1	A	163	HIS
1	A	476	GLN
1	A	544	ASN
1	A	593	HIS
1	A	604	HIS
1	A	607	ASN
1	A	635	ASN
1	A	783	ASN
1	A	903	GLN
1	A	1005	ASN
1	A	1157	GLN
1	A	1265	HIS
1	A	1440	ASN
1	A	1589	GLN
1	A	1631	HIS
1	A	1636	ASN
1	A	1722	ASN
1	A	1793	GLN

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Mol	Chain	Res	Type
1	A	1836	ASN
1	A	1918	GLN
1	A	2090	HIS
1	A	2196	ASN
1	A	2518	ASN
1	A	2711	ASN
1	A	2755	GLN
1	A	2820	HIS
1	A	2898	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	3916	GLN
1	A	3950	HIS
1	A	3990	ASN
1	A	3993	ASN
1	A	4058	HIS
1	A	4061	GLN
1	A	4499	ASN
1	A	4515	ASN
1	A	4637	ASN
1	A	4644	ASN
1	A	4864	GLN
1	A	4880	GLN
1	A	4937	GLN
2	B	31	GLN
2	B	87	HIS
2	B	94	ASN
1	D	44	ASN
1	D	123	HIS
1	D	163	HIS
1	D	476	GLN
1	D	544	ASN
1	D	593	HIS
1	D	604	HIS
1	D	607	ASN
1	D	635	ASN
1	D	745	ASN
1	D	783	ASN

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Mol	Chain	Res	Type
1	D	903	GLN
1	D	1005	ASN
1	D	1157	GLN
1	D	1265	HIS
1	D	1440	ASN
1	D	1589	GLN
1	D	1631	HIS
1	D	1636	ASN
1	D	1722	ASN
1	D	1793	GLN
1	D	1836	ASN
1	D	1918	GLN
1	D	2090	HIS
1	D	2196	ASN
1	D	2252	ASN
1	D	2487	HIS
1	D	2518	ASN
1	D	2711	ASN
1	D	2755	GLN
1	D	2820	HIS
1	D	2898	GLN
1	D	2900	ASN
1	D	3595	GLN
1	D	3635	HIS
1	D	3667	GLN
1	D	3813	ASN
1	D	3852	ASN
1	D	3902	GLN
1	D	3916	GLN
1	D	3950	HIS
1	D	3990	ASN
1	D	3993	ASN
1	D	4058	HIS
1	D	4061	GLN
1	D	4499	ASN
1	D	4515	ASN
1	D	4637	ASN
1	D	4644	ASN
1	D	4817	HIS
1	D	4864	GLN
1	D	4880	GLN
1	D	4937	GLN

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Mol	Chain	Res	Type
2	E	31	GLN
2	E	87	HIS
1	G	44	ASN
1	G	123	HIS
1	G	163	HIS
1	G	476	GLN
1	G	544	ASN
1	G	593	HIS
1	G	604	HIS
1	G	607	ASN
1	G	635	ASN
1	G	783	ASN
1	G	842	GLN
1	G	903	GLN
1	G	1005	ASN
1	G	1157	GLN
1	G	1265	HIS
1	G	1440	ASN
1	G	1589	GLN
1	G	1631	HIS
1	G	1636	ASN
1	G	1722	ASN
1	G	1793	GLN
1	G	1836	ASN
1	G	1918	GLN
1	G	2090	HIS
1	G	2196	ASN
1	G	2252	ASN
1	G	2487	HIS
1	G	2518	ASN
1	G	2711	ASN
1	G	2755	GLN
1	G	2820	HIS
1	G	2898	GLN
1	G	2900	ASN
1	G	3635	HIS
1	G	3667	GLN
1	G	3813	ASN
1	G	3852	ASN
1	G	3902	GLN
1	G	3916	GLN
1	G	3950	HIS

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Mol	Chain	Res	Type
1	G	3990	ASN
1	G	3993	ASN
1	G	4058	HIS
1	G	4061	GLN
1	G	4499	ASN
1	G	4515	ASN
1	G	4637	ASN
1	G	4864	GLN
1	G	4880	GLN
1	G	4937	GLN
2	H	31	GLN
2	H	87	HIS
2	H	94	ASN
1	J	12	GLN
1	J	44	ASN
1	J	123	HIS
1	J	163	HIS
1	J	476	GLN
1	J	544	ASN
1	J	593	HIS
1	J	604	HIS
1	J	607	ASN
1	J	635	ASN
1	J	783	ASN
1	J	903	GLN
1	J	1005	ASN
1	J	1157	GLN
1	J	1265	HIS
1	J	1440	ASN
1	J	1589	GLN
1	J	1631	HIS
1	J	1636	ASN
1	J	1722	ASN
1	J	1793	GLN
1	J	1836	ASN
1	J	1918	GLN
1	J	2090	HIS
1	J	2196	ASN
1	J	2252	ASN
1	J	2317	ASN
1	J	2487	HIS
1	J	2518	ASN

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Mol	Chain	Res	Type
1	J	2711	ASN
1	J	2755	GLN
1	J	2820	HIS
1	J	2898	GLN
1	J	2900	ASN
1	J	3635	HIS
1	J	3667	GLN
1	J	3813	ASN
1	J	3852	ASN
1	J	3902	GLN
1	J	3906	ASN
1	J	3916	GLN
1	J	3950	HIS
1	J	3990	ASN
1	J	3993	ASN
1	J	4058	HIS
1	J	4061	GLN
1	J	4499	ASN
1	J	4515	ASN
1	J	4637	ASN
1	J	4864	GLN
1	J	4880	GLN
1	J	4937	GLN
2	K	31	GLN
2	K	87	HIS
2	K	94	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
6	ATP	D	6002	-	32,33,33	1.32	4 (12%)	48,52,52	1.85	10 (20%)
6	ATP	G	6002	-	32,33,33	1.32	4 (12%)	48,52,52	1.85	10 (20%)
7	CFF	A	6003	-	15,15,15	2.01	7 (46%)	23,23,23	2.75	9 (39%)
6	ATP	J	6002	-	32,33,33	1.32	4 (12%)	48,52,52	1.85	10 (20%)
7	CFF	G	6003	-	15,15,15	2.02	8 (53%)	23,23,23	2.75	9 (39%)
7	CFF	J	6003	-	15,15,15	2.01	7 (46%)	23,23,23	2.75	9 (39%)
6	ATP	A	6002	-	32,33,33	1.32	4 (12%)	48,52,52	1.85	10 (20%)
7	CFF	D	6003	-	15,15,15	2.01	8 (53%)	23,23,23	2.75	9 (39%)

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
6	ATP	D	6002	-	-	9/22/38/38	0/3/3/3
6	ATP	G	6002	-	-	9/22/38/38	0/3/3/3
7	CFF	A	6003	-	-	-	0/2/2/2
6	ATP	J	6002	-	-	9/22/38/38	0/3/3/3
7	CFF	G	6003	-	-	-	0/2/2/2
7	CFF	J	6003	-	-	-	0/2/2/2
6	ATP	A	6002	-	-	9/22/38/38	0/3/3/3
7	CFF	D	6003	-	-	-	0/2/2/2

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	6002	ATP	C5-C4	4.41	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	6002	ATP	C5-C4	4.41	1.47	1.39
6	D	6002	ATP	C5-C4	4.41	1.47	1.39
6	G	6002	ATP	C5-C4	4.41	1.47	1.39
7	A	6003	CFF	C6-N1	-4.00	1.32	1.40
7	D	6003	CFF	C6-N1	-4.00	1.32	1.40
7	G	6003	CFF	C6-N1	-4.00	1.32	1.40
7	J	6003	CFF	C6-N1	-4.00	1.32	1.40
7	A	6003	CFF	C4-N3	-2.81	1.33	1.38
7	D	6003	CFF	C4-N3	-2.81	1.33	1.38
7	G	6003	CFF	C4-N3	-2.81	1.33	1.38
7	J	6003	CFF	C4-N3	-2.81	1.33	1.38
6	A	6002	ATP	C5-N7	-2.62	1.34	1.39
6	D	6002	ATP	C5-N7	-2.62	1.34	1.39
6	G	6002	ATP	C5-N7	-2.62	1.34	1.39
6	J	6002	ATP	C5-N7	-2.62	1.34	1.39
7	A	6003	CFF	C5-N7	-2.49	1.34	1.38
7	D	6003	CFF	C5-N7	-2.49	1.34	1.38
7	G	6003	CFF	C5-N7	-2.49	1.34	1.38
7	J	6003	CFF	C5-N7	-2.49	1.34	1.38
6	A	6002	ATP	C5-C6	2.36	1.47	1.41
6	D	6002	ATP	C5-C6	2.36	1.47	1.41
6	G	6002	ATP	C5-C6	2.36	1.47	1.41
6	J	6002	ATP	C5-C6	2.36	1.47	1.41
7	A	6003	CFF	C5-C6	-2.27	1.37	1.43
7	D	6003	CFF	C5-C6	-2.27	1.37	1.43
7	G	6003	CFF	C5-C6	-2.27	1.37	1.43
7	J	6003	CFF	C5-C6	-2.27	1.37	1.43
7	A	6003	CFF	C2-N3	-2.21	1.34	1.39
7	D	6003	CFF	C2-N3	-2.21	1.34	1.39
7	G	6003	CFF	C2-N3	-2.21	1.34	1.39
7	J	6003	CFF	C2-N3	-2.21	1.34	1.39
7	A	6003	CFF	O13-C6	-2.21	1.18	1.23
7	D	6003	CFF	O13-C6	-2.21	1.18	1.23
7	G	6003	CFF	O13-C6	-2.21	1.18	1.23
7	J	6003	CFF	O13-C6	-2.21	1.18	1.23
7	A	6003	CFF	O11-C2	-2.14	1.18	1.22
7	D	6003	CFF	O11-C2	-2.14	1.18	1.22
7	G	6003	CFF	O11-C2	-2.14	1.18	1.22
7	J	6003	CFF	O11-C2	-2.14	1.18	1.22
6	A	6002	ATP	C8-N7	2.08	1.35	1.31
6	D	6002	ATP	C8-N7	2.08	1.35	1.31
6	G	6002	ATP	C8-N7	2.08	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	6002	ATP	C8-N7	2.05	1.35	1.31
7	G	6003	CFF	C2-N1	-2.03	1.35	1.39
7	D	6003	CFF	C2-N1	-2.01	1.35	1.39

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	6003	CFF	C14-N7-C8	-7.58	112.09	126.28
7	D	6003	CFF	C14-N7-C8	-7.58	112.09	126.28
7	G	6003	CFF	C14-N7-C8	-7.58	112.09	126.28
7	J	6003	CFF	C14-N7-C8	-7.58	112.09	126.28
6	A	6002	ATP	C5-C4-N3	-6.17	118.23	126.72
6	D	6002	ATP	C5-C4-N3	-6.17	118.23	126.72
6	G	6002	ATP	C5-C4-N3	-6.17	118.23	126.72
6	J	6002	ATP	C5-C4-N3	-6.14	118.27	126.72
7	A	6003	CFF	C14-N7-C5	5.34	140.49	127.77
7	D	6003	CFF	C14-N7-C5	5.34	140.49	127.77
7	G	6003	CFF	C14-N7-C5	5.34	140.49	127.77
7	J	6003	CFF	C14-N7-C5	5.34	140.49	127.77
6	A	6002	ATP	N3-C4-N9	5.18	135.98	127.17
6	D	6002	ATP	N3-C4-N9	5.18	135.98	127.17
6	G	6002	ATP	N3-C4-N9	5.18	135.98	127.17
6	J	6002	ATP	N3-C4-N9	5.18	135.98	127.17
7	A	6003	CFF	C5-C6-N1	4.32	119.97	112.06
7	D	6003	CFF	C5-C6-N1	4.32	119.97	112.06
7	G	6003	CFF	C5-C6-N1	4.32	119.97	112.06
7	J	6003	CFF	C5-C6-N1	4.32	119.97	112.06
6	A	6002	ATP	C2-N3-C4	3.70	120.86	111.83
6	D	6002	ATP	C2-N3-C4	3.70	120.86	111.83
6	G	6002	ATP	C2-N3-C4	3.70	120.86	111.83
6	J	6002	ATP	C2-N3-C4	3.70	120.86	111.83
7	D	6003	CFF	C6-N1-C2	-3.35	120.22	125.66
7	A	6003	CFF	C6-N1-C2	-3.33	120.25	125.66
7	J	6003	CFF	C6-N1-C2	-3.33	120.25	125.66
7	G	6003	CFF	C6-N1-C2	-3.31	120.28	125.66
6	J	6002	ATP	N3-C2-N1	-3.14	123.82	128.58
6	A	6002	ATP	N3-C2-N1	-3.12	123.87	128.58
6	D	6002	ATP	N3-C2-N1	-3.12	123.87	128.58
6	G	6002	ATP	N3-C2-N1	-3.12	123.87	128.58
7	A	6003	CFF	N3-C4-N9	3.07	131.09	126.27
7	D	6003	CFF	N3-C4-N9	3.07	131.09	126.27
7	G	6003	CFF	N3-C4-N9	3.07	131.09	126.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	6003	CFF	N3-C4-N9	3.07	131.09	126.27
7	A	6003	CFF	O13-C6-C5	-2.97	120.29	126.38
7	D	6003	CFF	O13-C6-C5	-2.97	120.29	126.38
7	G	6003	CFF	O13-C6-C5	-2.97	120.29	126.38
7	J	6003	CFF	O13-C6-C5	-2.97	120.29	126.38
6	A	6002	ATP	C4-C5-N7	-2.94	107.22	110.58
6	D	6002	ATP	C4-C5-N7	-2.94	107.22	110.58
6	G	6002	ATP	C4-C5-N7	-2.94	107.22	110.58
6	J	6002	ATP	C4-C5-N7	-2.91	107.25	110.58
6	D	6002	ATP	C2'-C1'-N9	-2.79	106.38	113.30
7	G	6003	CFF	C6-C5-C4	-2.79	119.41	122.92
6	A	6002	ATP	C2'-C1'-N9	-2.78	106.40	113.30
6	G	6002	ATP	C2'-C1'-N9	-2.78	106.40	113.30
6	J	6002	ATP	C2'-C1'-N9	-2.78	106.40	113.30
7	A	6003	CFF	C6-C5-C4	-2.76	119.44	122.92
7	J	6003	CFF	C6-C5-C4	-2.76	119.44	122.92
7	D	6003	CFF	C6-C5-C4	-2.74	119.47	122.92
6	A	6002	ATP	C4-N9-C8	2.72	108.60	105.74
6	D	6002	ATP	C4-N9-C8	2.72	108.60	105.74
6	G	6002	ATP	C4-N9-C8	2.72	108.60	105.74
6	J	6002	ATP	C4-N9-C8	2.72	108.60	105.74
7	G	6003	CFF	N7-C8-N9	-2.68	108.62	113.48
7	A	6003	CFF	N7-C8-N9	-2.66	108.66	113.48
7	J	6003	CFF	N7-C8-N9	-2.66	108.66	113.48
7	D	6003	CFF	N7-C8-N9	-2.65	108.68	113.48
6	D	6002	ATP	O4'-C1'-N9	2.51	112.90	108.09
6	A	6002	ATP	O4'-C1'-N9	2.50	112.89	108.09
6	G	6002	ATP	O4'-C1'-N9	2.50	112.89	108.09
6	J	6002	ATP	O4'-C1'-N9	2.50	112.89	108.09
6	A	6002	ATP	C5-N7-C8	2.30	107.06	103.45
6	D	6002	ATP	C5-N7-C8	2.30	107.06	103.45
6	G	6002	ATP	C5-N7-C8	2.30	107.06	103.45
6	J	6002	ATP	C5-N7-C8	2.28	107.03	103.45
6	A	6002	ATP	C3'-C2'-C1'	2.27	105.75	101.46
6	D	6002	ATP	C3'-C2'-C1'	2.27	105.75	101.46
6	G	6002	ATP	C3'-C2'-C1'	2.27	105.75	101.46
6	J	6002	ATP	C3'-C2'-C1'	2.27	105.75	101.46
7	D	6003	CFF	N3-C2-N1	2.08	119.73	117.14
7	A	6003	CFF	N3-C2-N1	2.05	119.70	117.14
7	J	6003	CFF	N3-C2-N1	2.05	119.70	117.14
7	G	6003	CFF	N3-C2-N1	2.03	119.68	117.14

There are no chirality outliers.

All (36) torsion outliers are listed below:

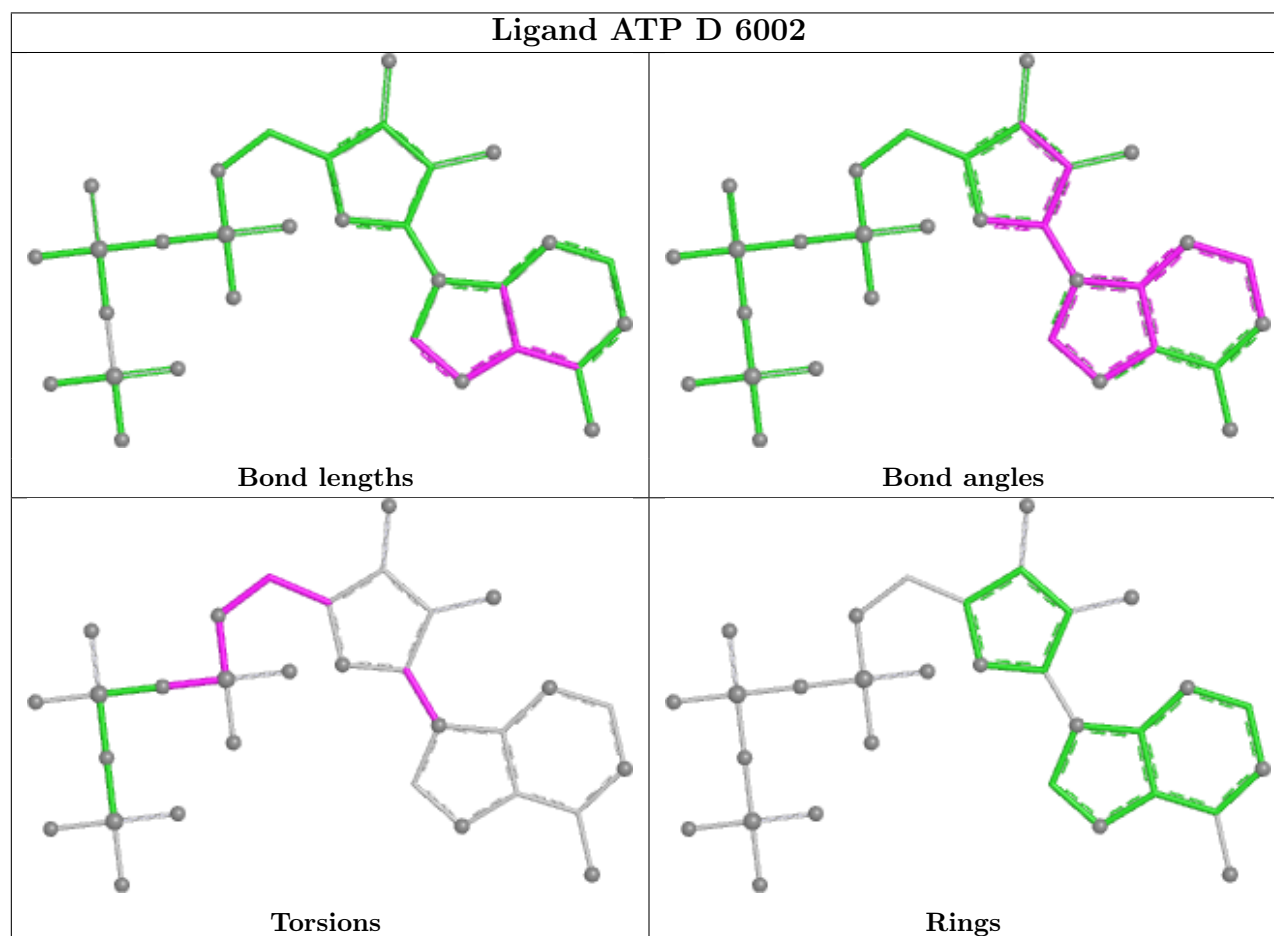
Mol	Chain	Res	Type	Atoms
6	A	6002	ATP	C5'-O5'-PA-O2A
6	A	6002	ATP	C5'-O5'-PA-O3A
6	A	6002	ATP	O4'-C1'-N9-C8
6	A	6002	ATP	O4'-C1'-N9-C4
6	D	6002	ATP	C5'-O5'-PA-O2A
6	D	6002	ATP	C5'-O5'-PA-O3A
6	D	6002	ATP	O4'-C1'-N9-C8
6	D	6002	ATP	O4'-C1'-N9-C4
6	G	6002	ATP	C5'-O5'-PA-O2A
6	G	6002	ATP	C5'-O5'-PA-O3A
6	G	6002	ATP	O4'-C1'-N9-C8
6	G	6002	ATP	O4'-C1'-N9-C4
6	J	6002	ATP	C5'-O5'-PA-O2A
6	J	6002	ATP	C5'-O5'-PA-O3A
6	J	6002	ATP	O4'-C1'-N9-C8
6	J	6002	ATP	O4'-C1'-N9-C4
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'
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

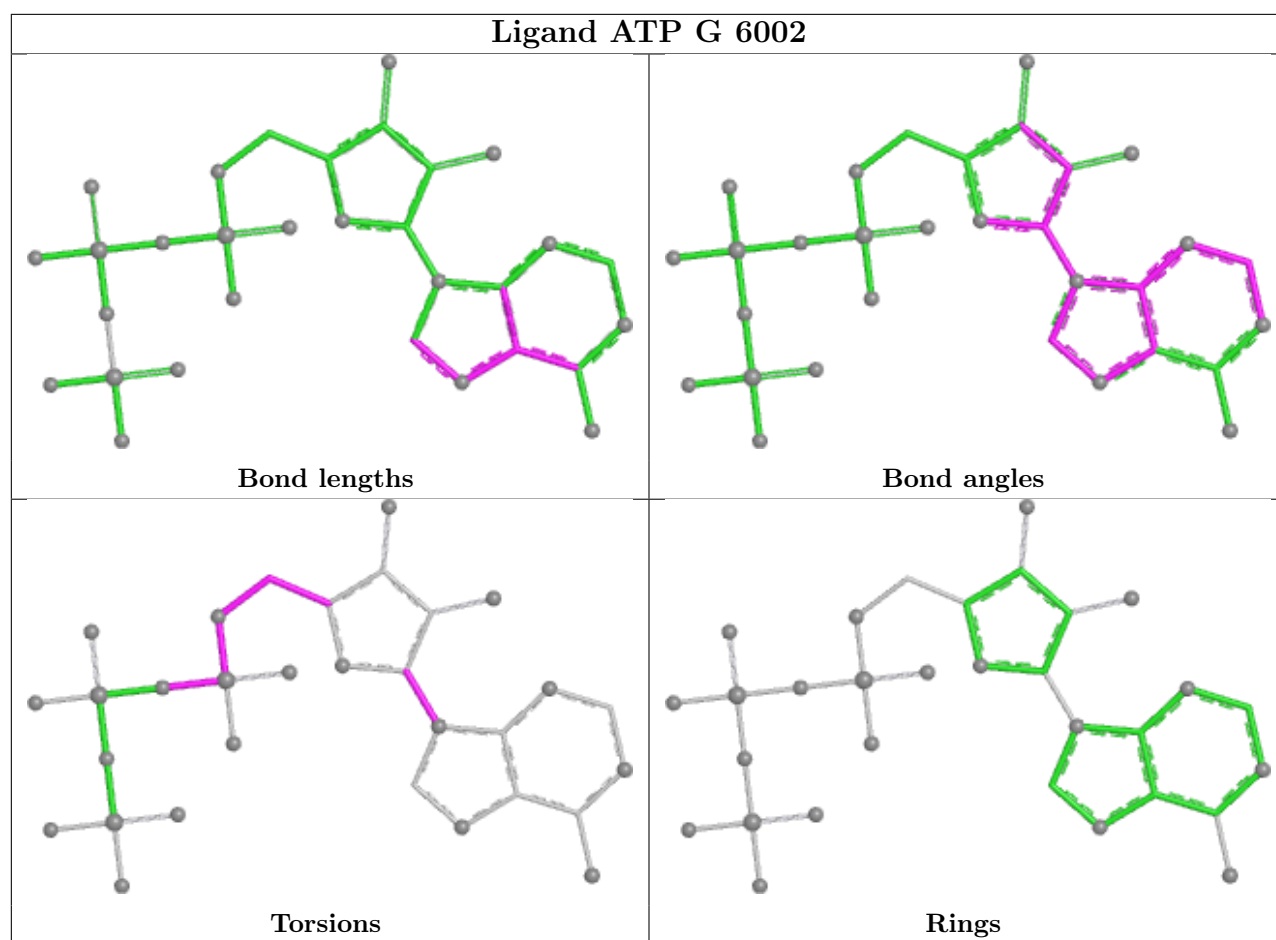
There are no ring outliers.

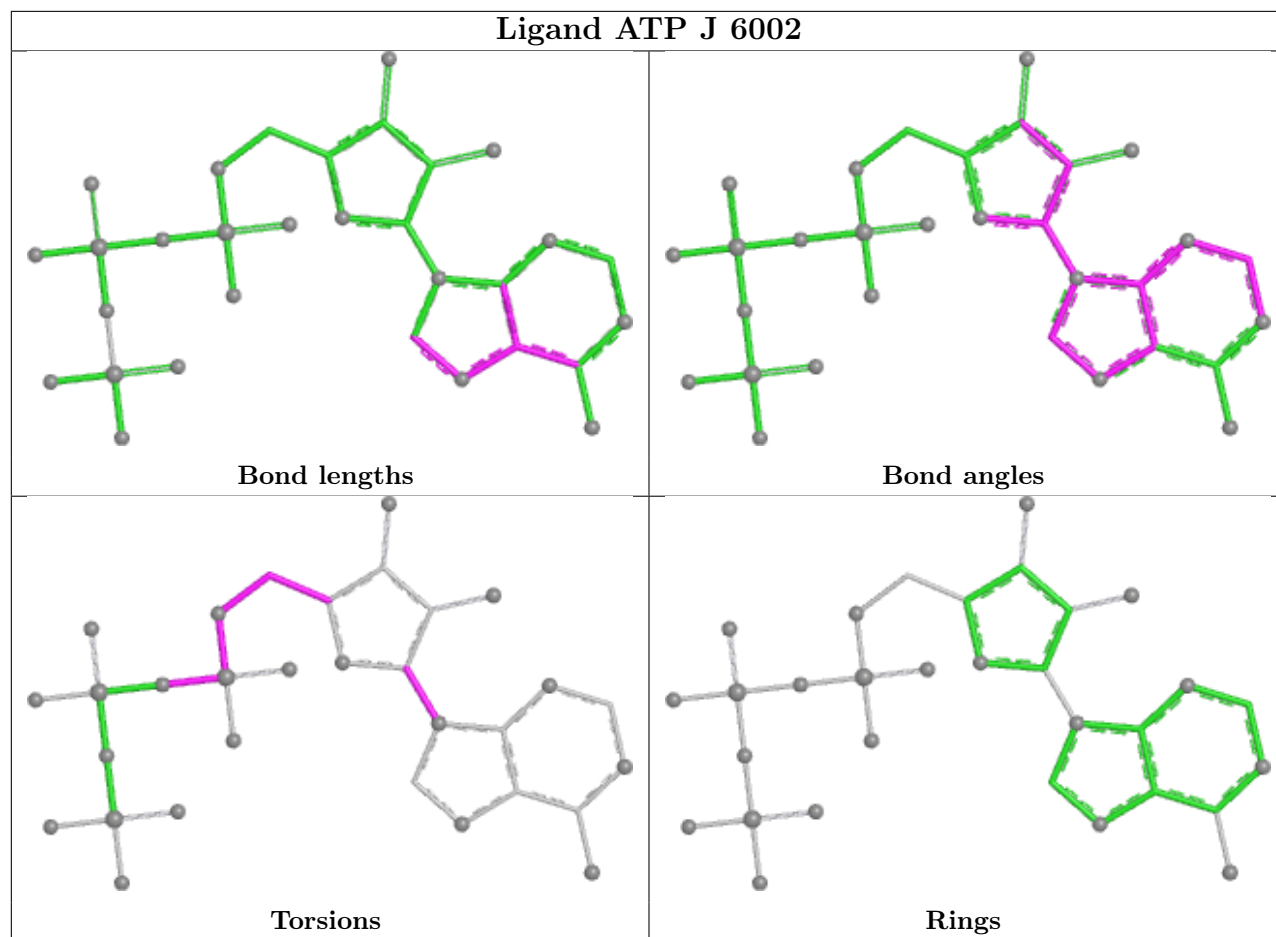
4 monomers are involved in 8 short contacts:

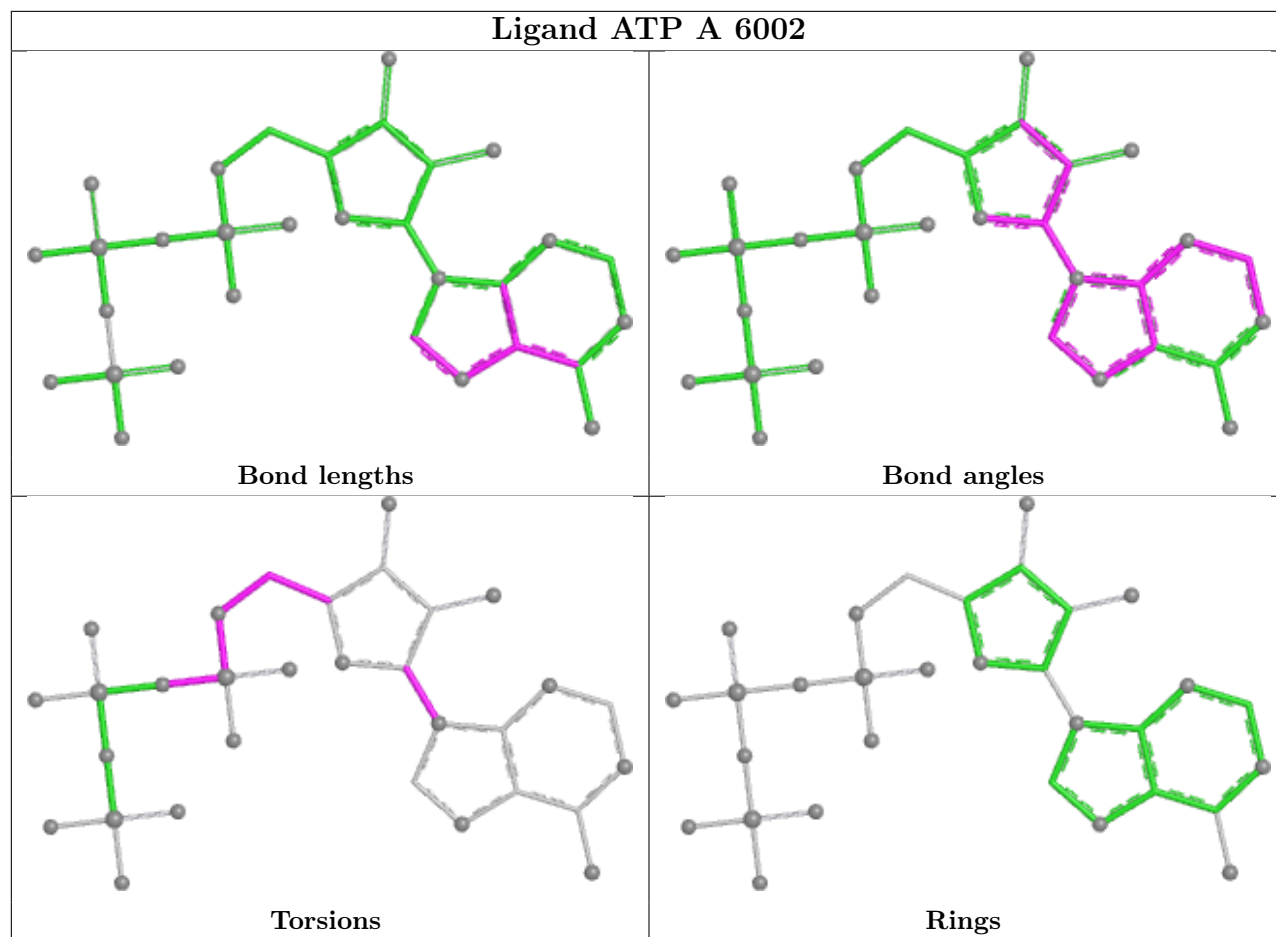
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	6003	CFF	2	0
7	G	6003	CFF	2	0
7	J	6003	CFF	2	0
7	D	6003	CFF	2	0

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.

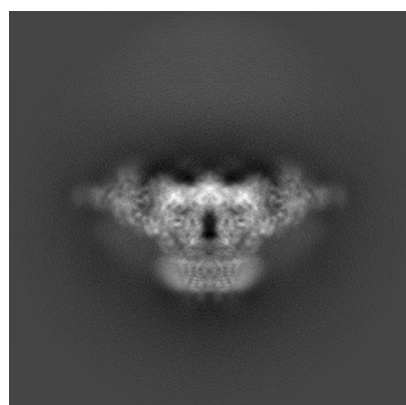
6 Map visualisation [i](#)

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.

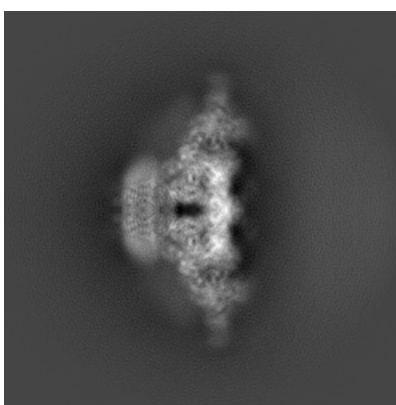
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

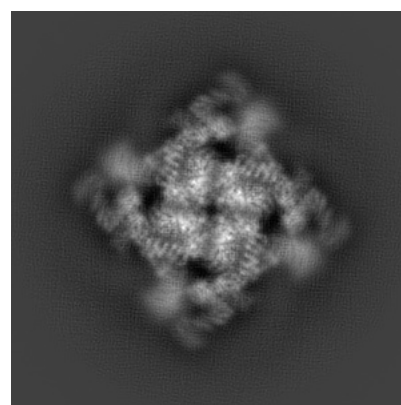
6.1.1 Primary map



X



Y

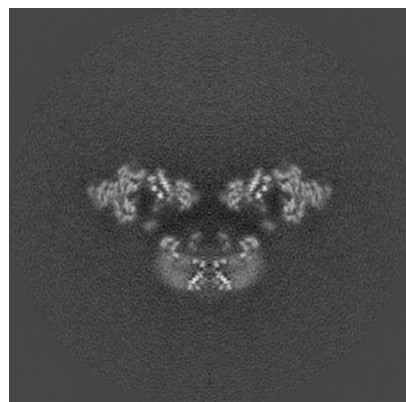


Z

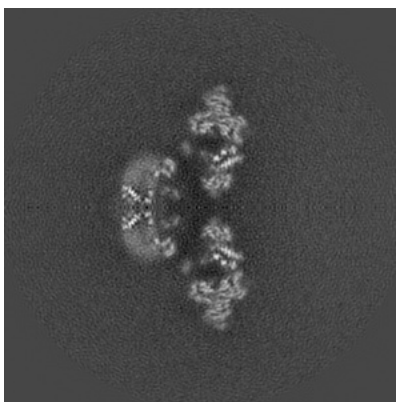
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

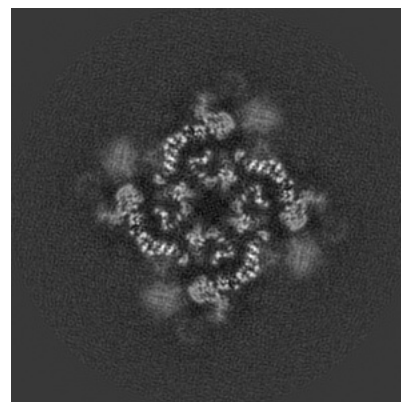
6.2.1 Primary map



X Index: 200



Y Index: 200

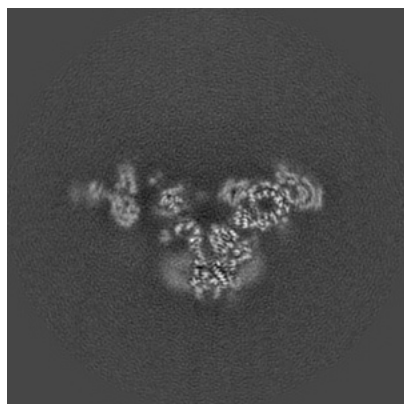


Z Index: 200

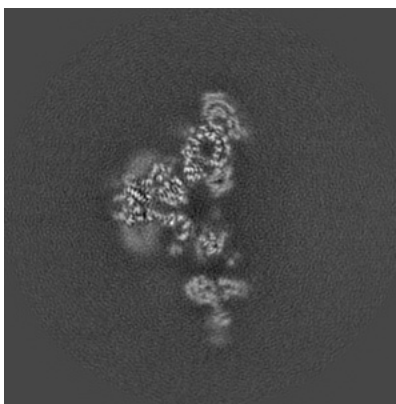
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

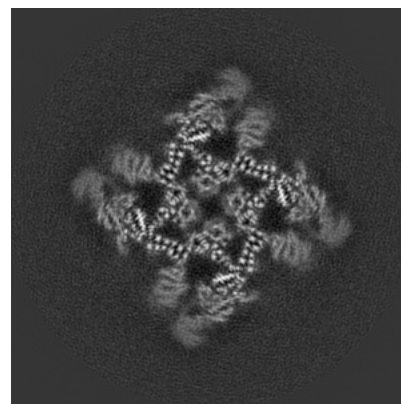
6.3.1 Primary map



X Index: 190



Y Index: 210

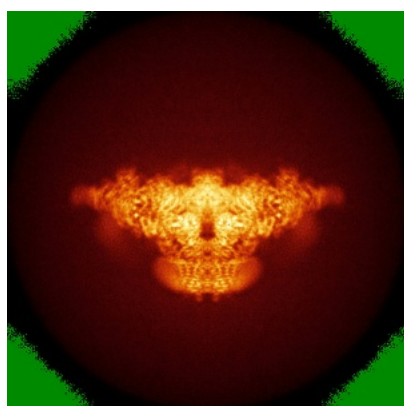


Z Index: 209

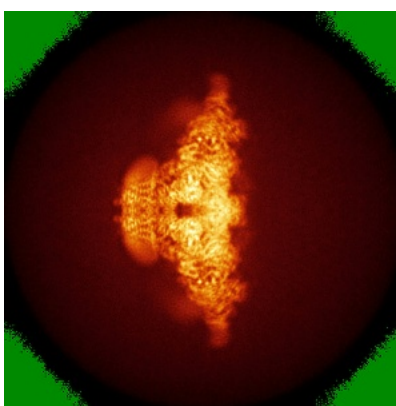
The images above show the largest variance slices of the map in three orthogonal directions.

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

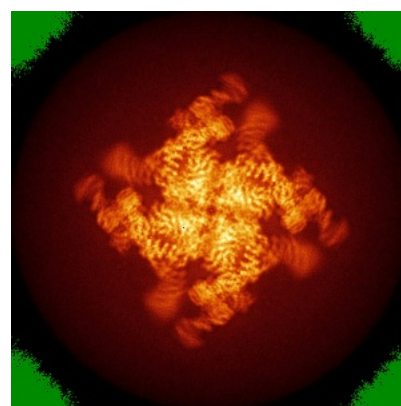
6.4.1 Primary map



X



Y

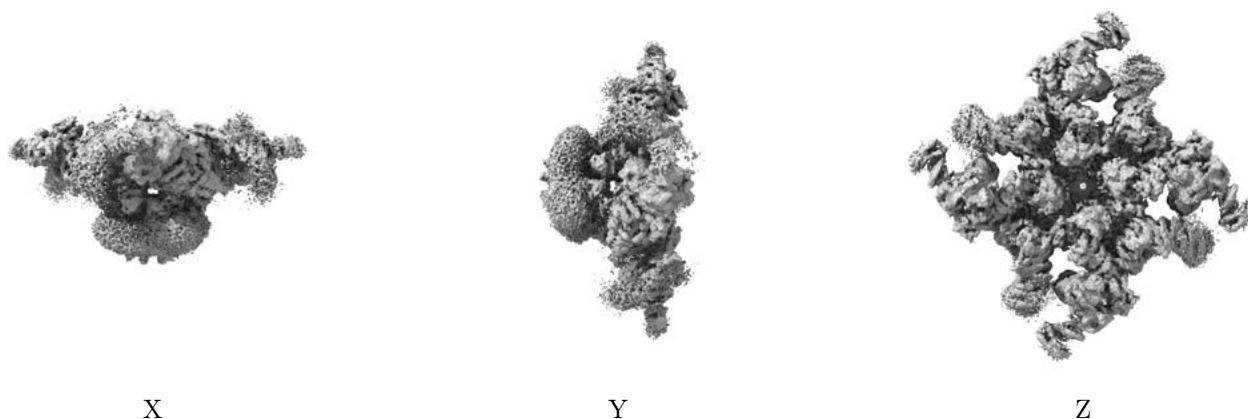


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

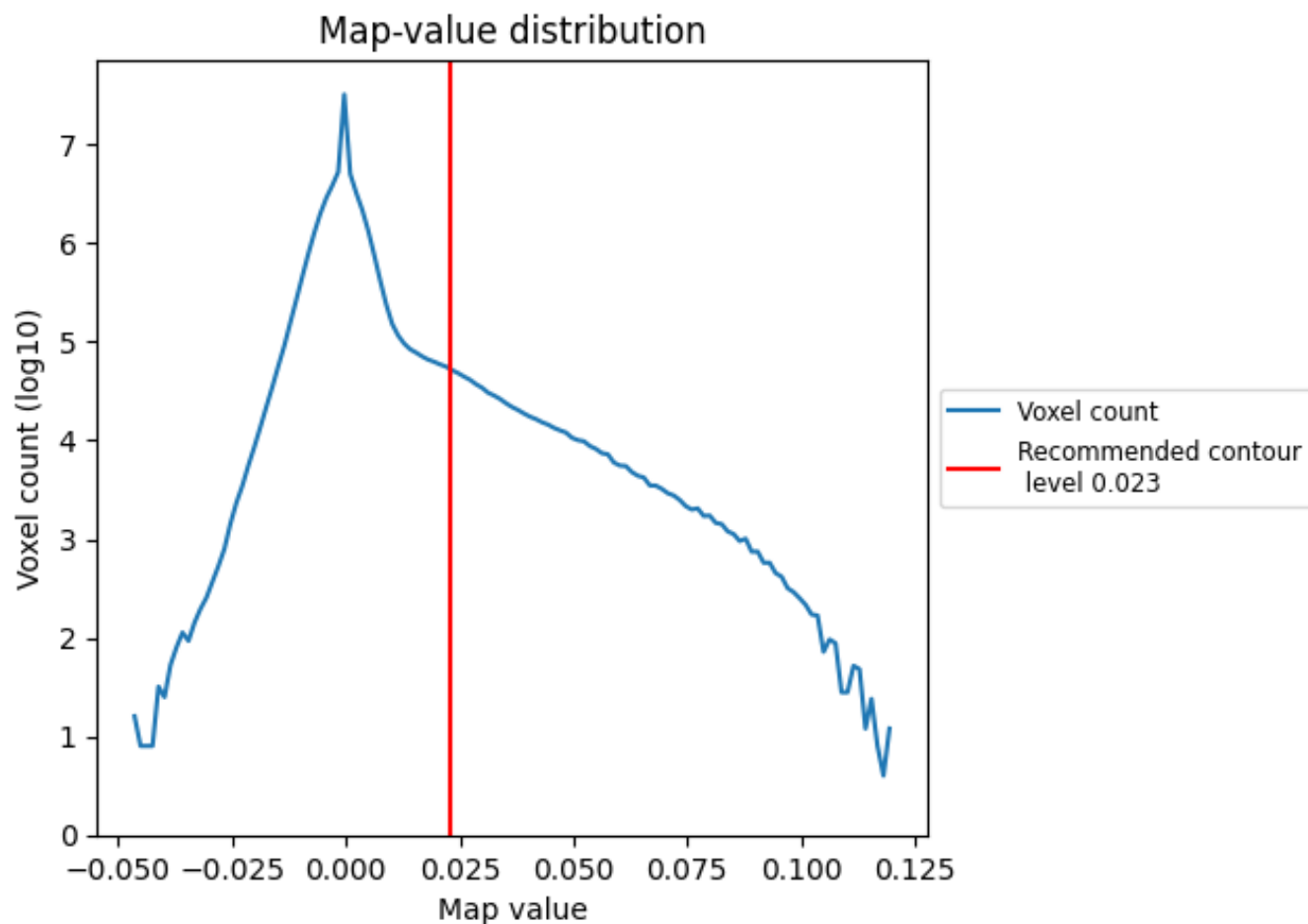
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

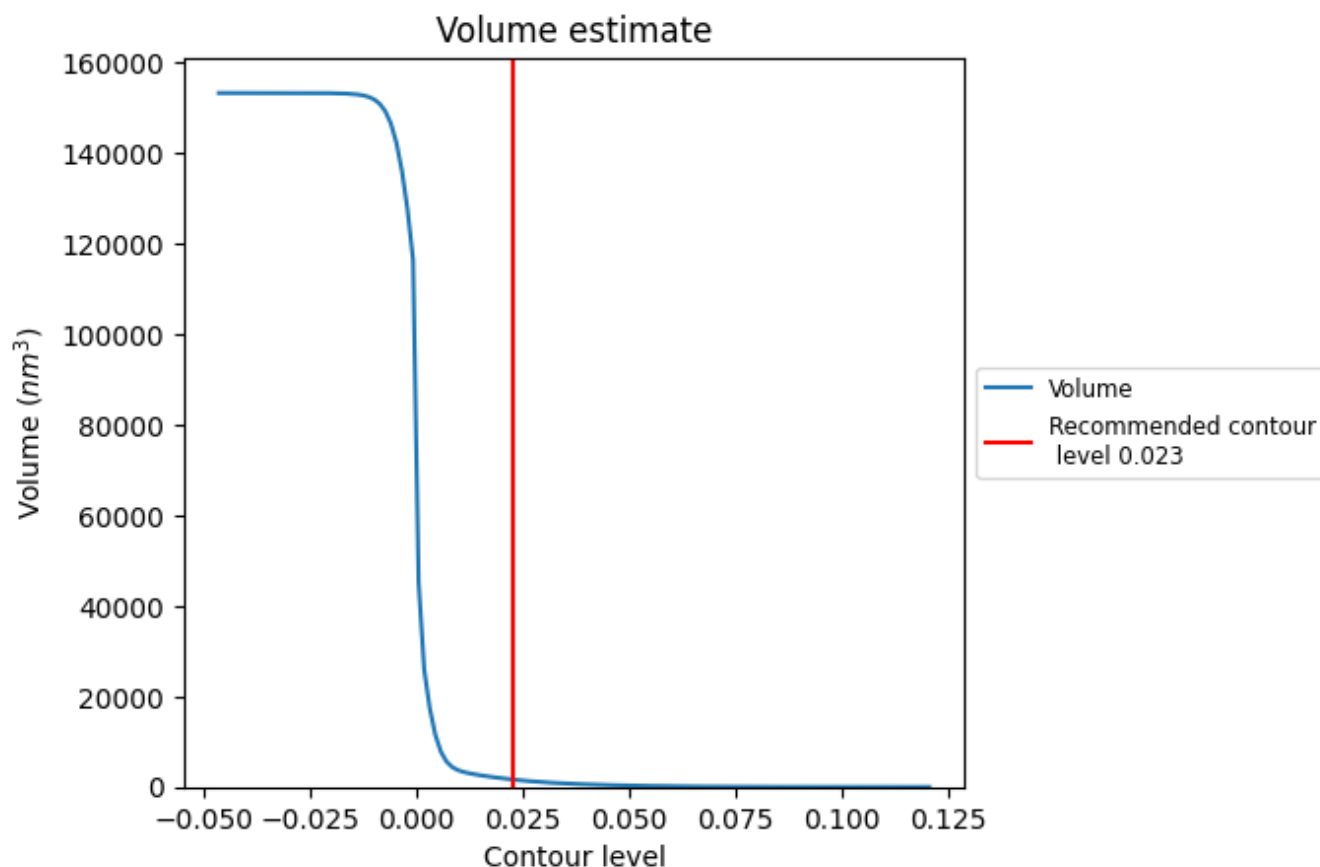
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

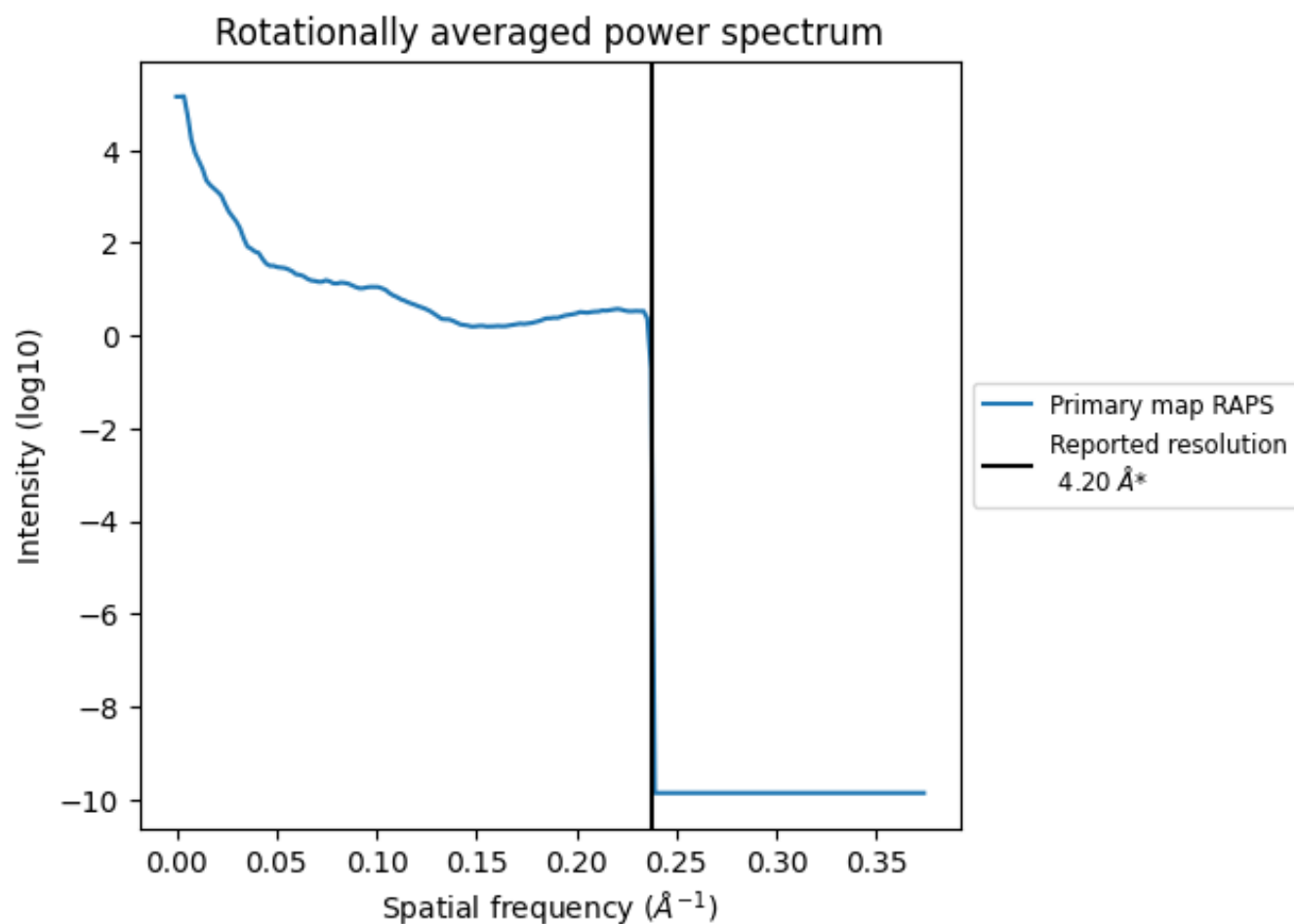
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

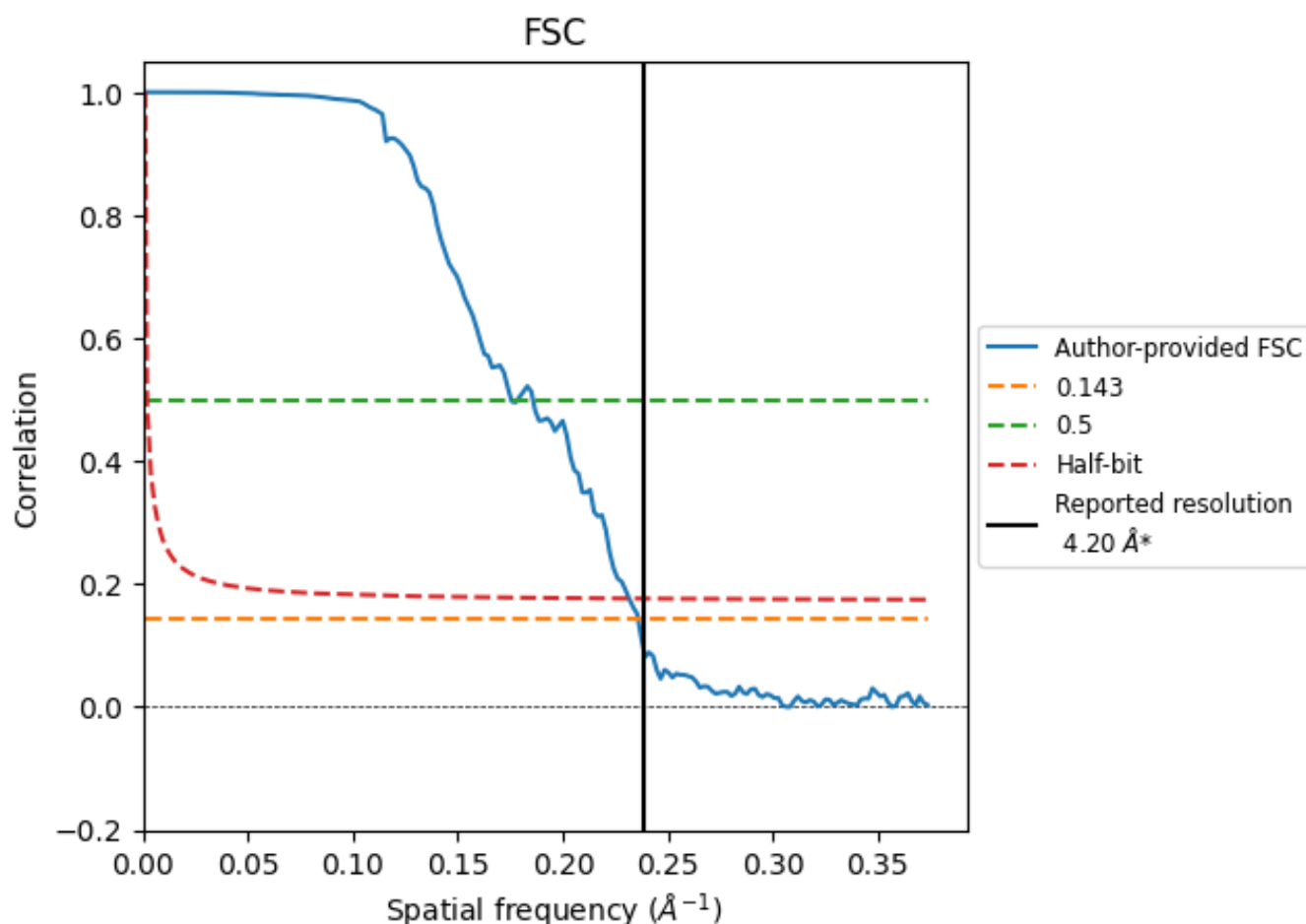


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

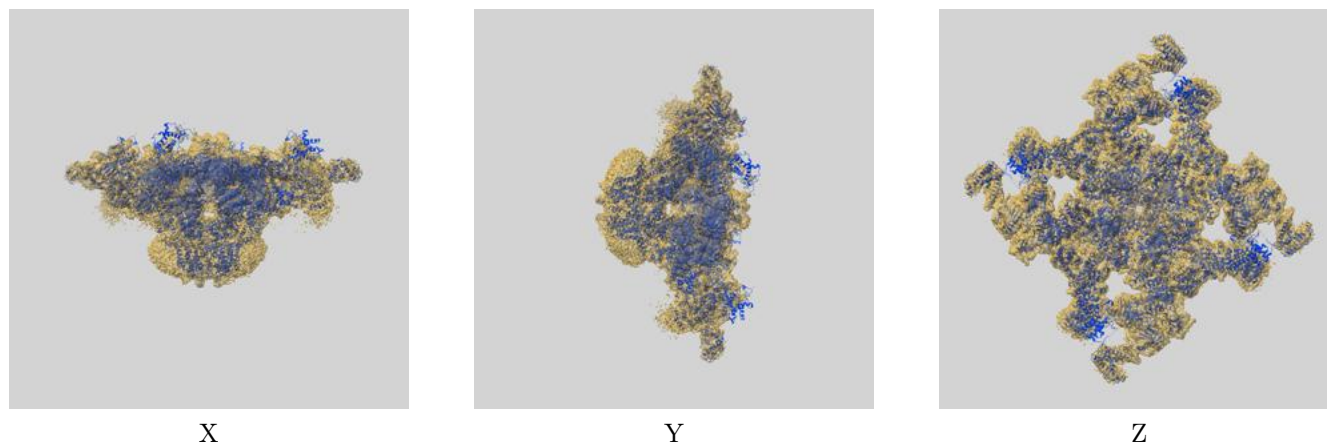
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.24	5.70	4.32
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

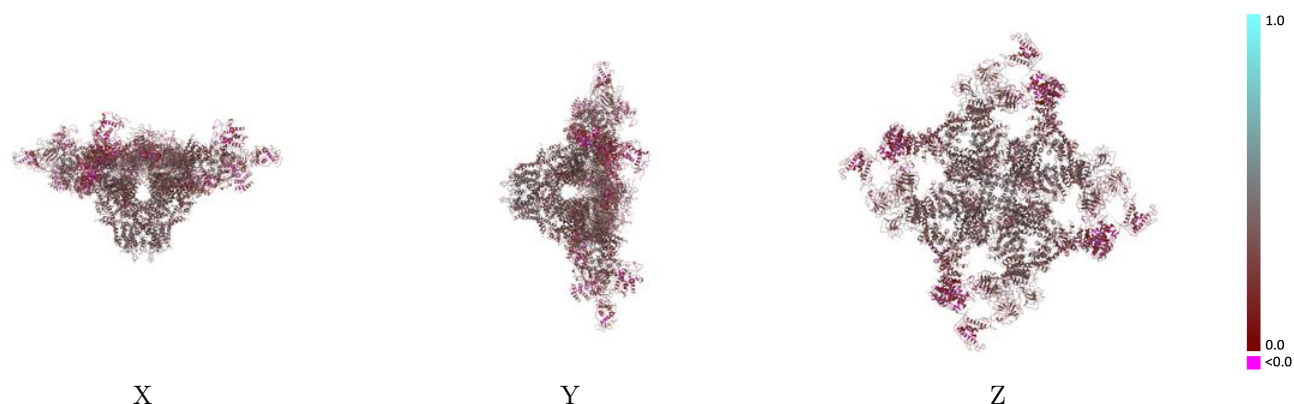
This section contains information regarding the fit between EMDB map EMD-9836 and PDB model 6JIU. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



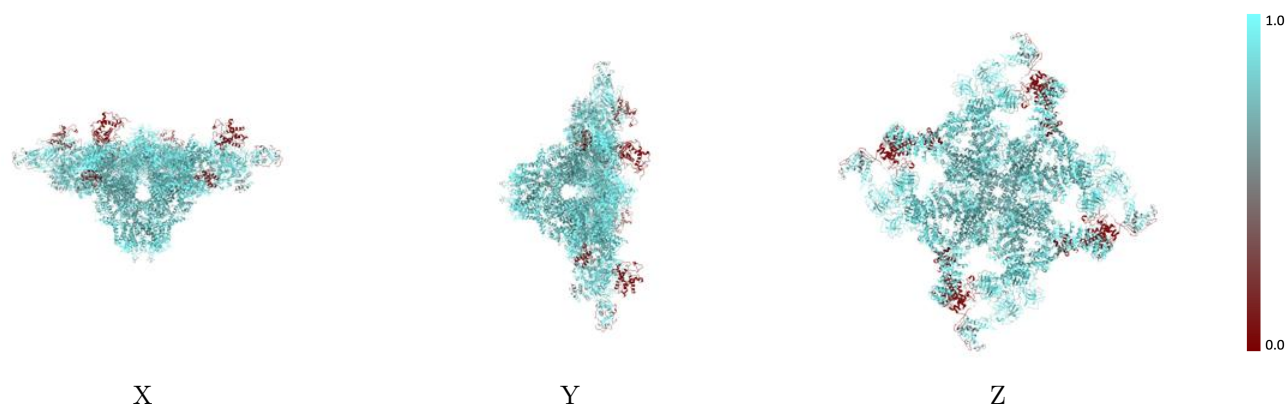
The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



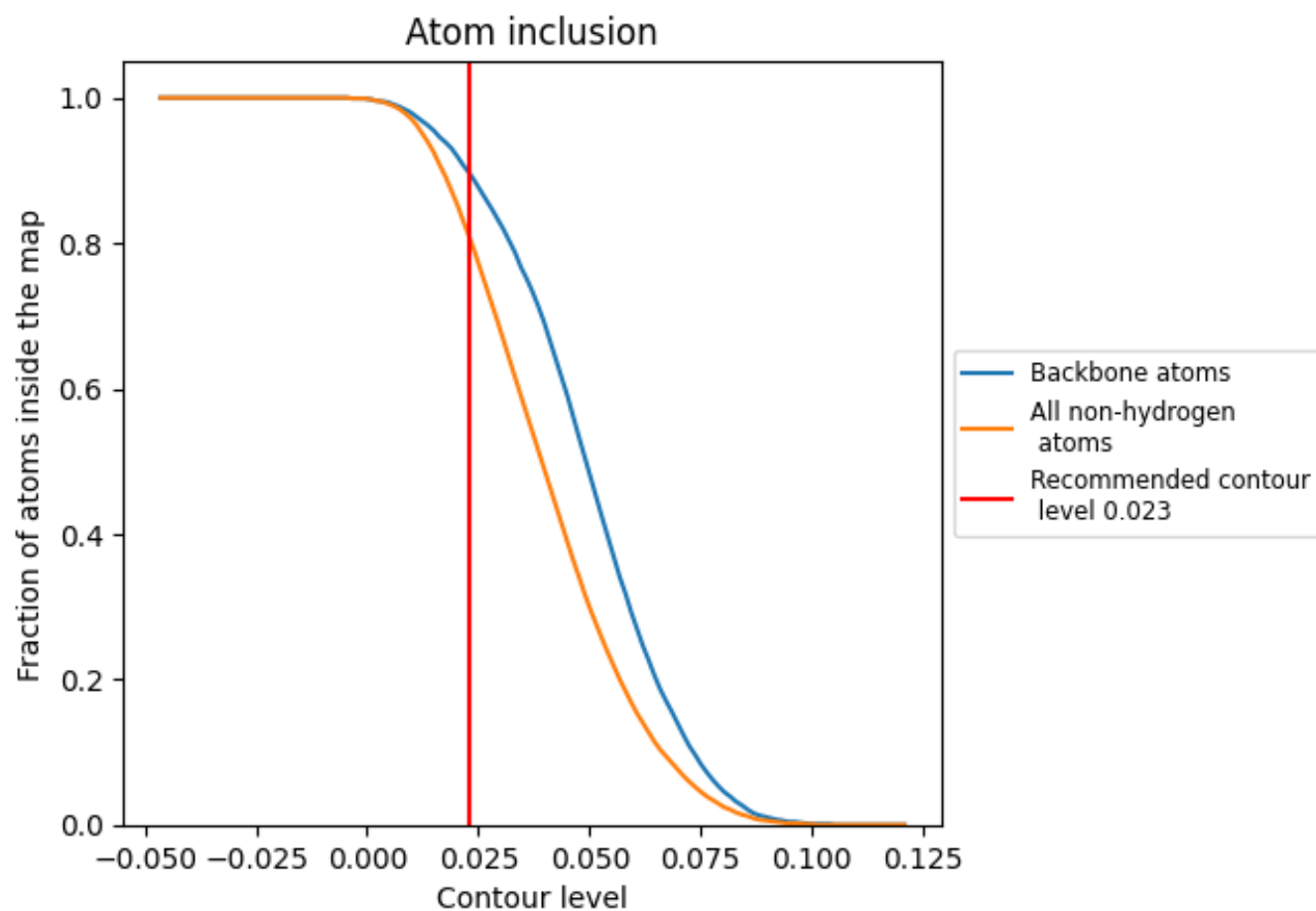
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.8080	0.3030
A	0.8200	0.3050
B	0.8710	0.3450
C	0.1110	0.1780
D	0.8200	0.3050
E	0.8700	0.3430
F	0.1110	0.1750
G	0.8200	0.3040
H	0.8720	0.3420
I	0.1110	0.1790
J	0.8210	0.3040
K	0.8720	0.3420
L	0.1110	0.1800

