



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:33 PM UTC

PDB ID : 6JRR / pdb_00006jrr
EMDB ID : EMD-9879
Title : Structure of RyR2 (*F/A/C/L-Ca²⁺ dataset)
Authors : Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.
Deposited on : 2019-04-05
Resolution : 3.90 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

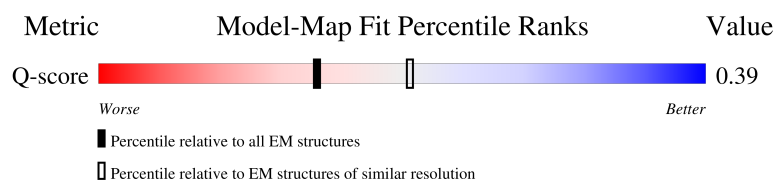
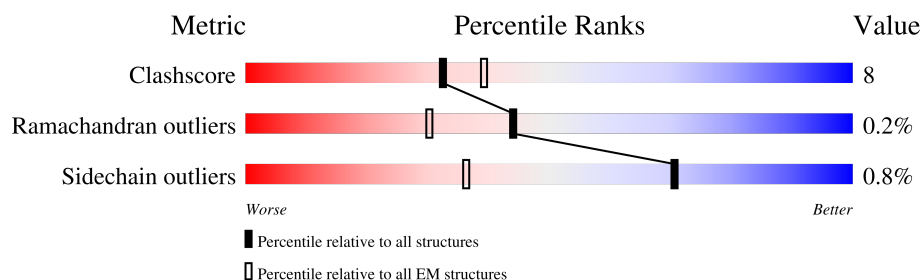
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	8855 (3.40 - 4.40)

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	9% 57% 13% 30%
1	C	4968	9% 57% 13% 30%
1	E	4968	9% 57% 13% 30%
1	G	4968	9% 57% 12% 30%

Continued on next page...

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 109132 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	3460	Total	C	N	O	S	0	0
			26417	16833	4528	4900	156		
1	C	3460	Total	C	N	O	S	0	0
			26417	16833	4528	4900	156		
1	E	3460	Total	C	N	O	S	0	0
			26417	16833	4528	4900	156		
1	G	3460	Total	C	N	O	S	0	0
			26417	16833	4528	4900	156		

- 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	D	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	F	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		

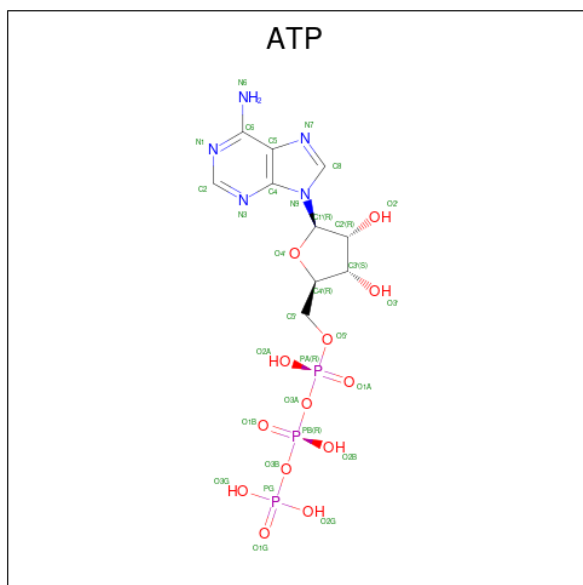
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

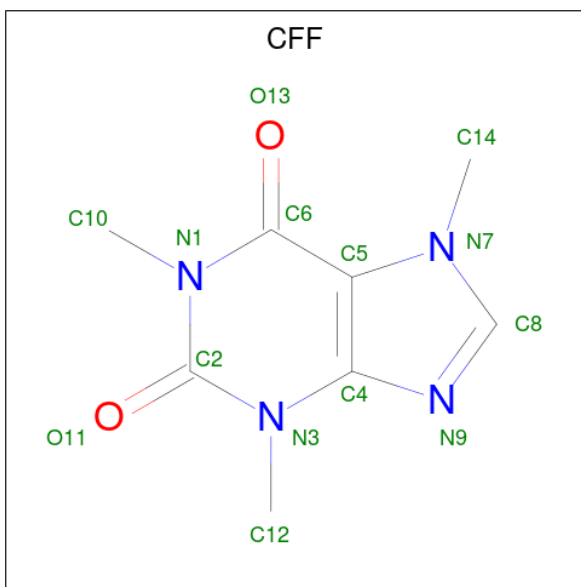
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	
4	E	1	Total	Ca	0
			1	1	
4	G	1	Total	Ca	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 6 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$).

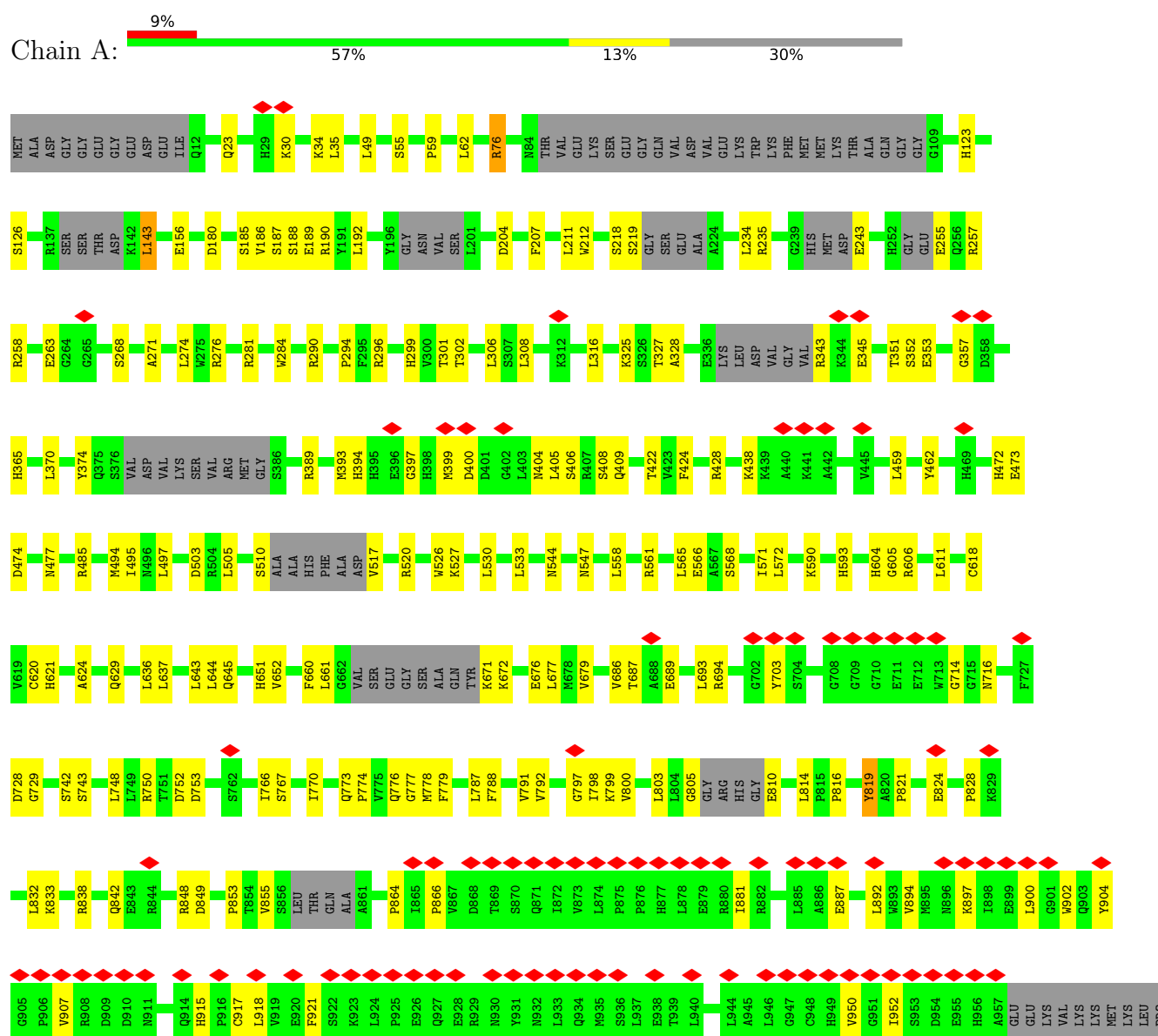


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	4	2	
6	C	1	Total	C	N	O	0
			14	8	4	2	
6	E	1	Total	C	N	O	0
			14	8	4	2	
6	G	1	Total	C	N	O	0
			14	8	4	2	

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

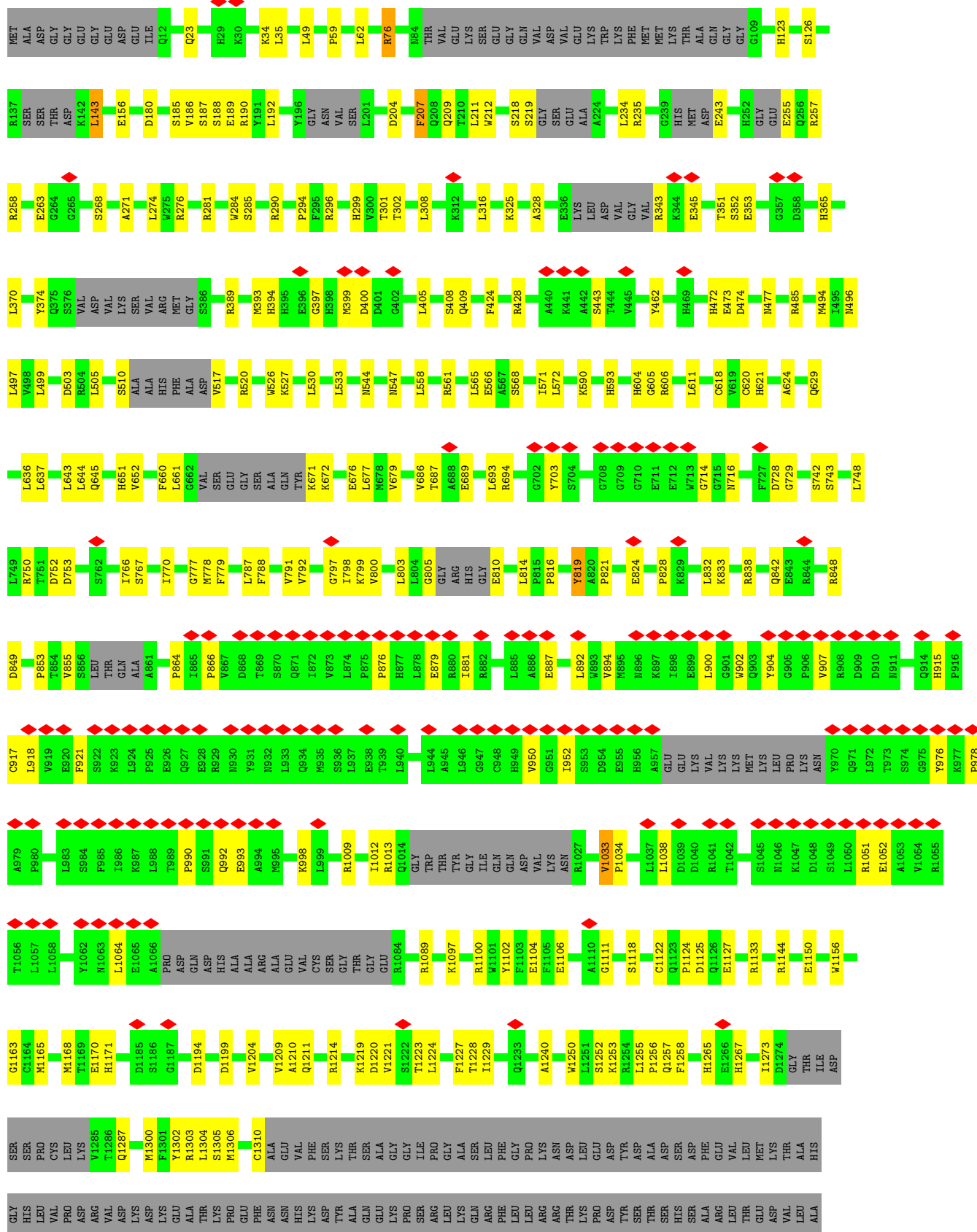






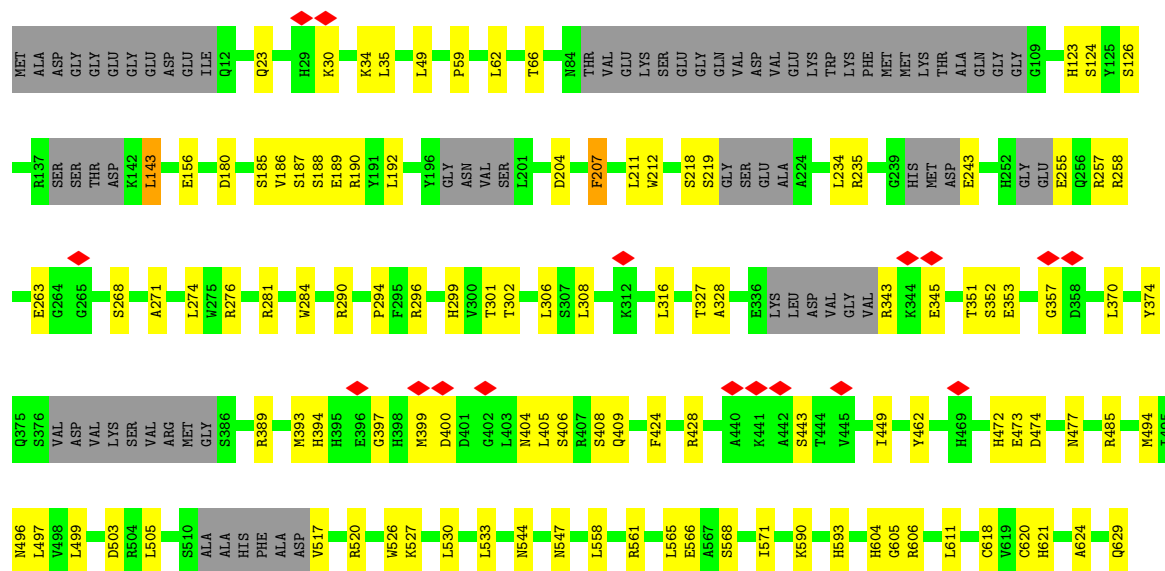
I4868	F4740	ARG	ARG	ARG	GLN	GLY	THR	PHE	LYS	S4055	GLY	S3748	S3628	ARG	ALA	PHE	TYR
M4885	A4741	ILE	ILE	THR	LEU	ASP	GLY	PHE	LYS	H4056	LEU	M3755	W3629	VAL	LEU	LEU	PRO
F4888	L4744	HIS	HIS	SER	ASP	ASP	ASP	SER	PRO	E4065	THR	N3771	H3635	ILE	ASP	THR	ILE
C4892	F4751	ARG	ARG	TRP	GLY	GLY	GLY	TRP	GLY	L4068	GLY	Q3775	L3641	ASN	ARG	THR	ARG
I4894	L4754	TTR	TTR	VAL	GLY	GLY	GLY	VAL	GLY	A4071	GLY	Q3776	I3642	VAL	PHE	PHE	LYS
D4897	I4757	GLY	GLY	PHE	LYS	ARG	ARG	PHE	MET	GLU	THR	K3777	P3648	ASP	SER	SER	ASP
D4900	S4760	GLU	GLU	LEU	GLY	VAL	LEU	LEU	GLY	M4569	ASP	S3793	GLY	PHE	LYS	TYR	TYR
T4901	L4770	VAL	VAL	HIS	GLY	GLY	GLY	HIS	PHE	P4571	ASP	L3794	ALA	ASN	ARG	ARG	ARG
V4902	T4771	GLN	PRO	PHE	PRO	THR	THR	PHE	SER	T4078	GLY	L3797	VAL	ALA	ALA	LYS	LYS
L4911	L4781	LYS	LYS	ALA	LYS	LEU	LEU	ALA	LEU	R4094	ASP	Q3798	PRO	THR	GLY	VAL	THR
N4915	R4791	PHE	PHE	VAL	GLY	SER	GLY	VAL	VAL	I4095	ASP	S3800	GLU	ARG	ARG	VAL	SER
L4916	R4791	TRP	LYS	VAL	GLY	ASP	LEU	VAL	ARG	L4103	GLY	V3803	GLY	GLN	ILE	ALA	PRO
F4922	K4796	LYS	ILE	ARG	LYS	THR	GLY	ARG	LYS	M4110	GLY	F3809	R3661	ARG	LYS	LYS	PRO
L4926	S4797	ILE	ILE	PHE	GLY	ASP	GLY	GLY	TYR	R4115	ASP	N3613	V3662	TYR	ILE	ALA	ALA
V4941	E4798	GLU	A4487	ARG	LEU	LEU	GLY	ILE	ARG	R4145	LEU	G3819	D3663	SER	ARG	LYS	ASP
W4942	G4800	GLY	W4515	GLY	GLY	GLY	GLY	ILE	GLY	W4161	GLY	VAL	Q3667	LEU	GLN	GLY	PHE
Y4945	D4801	MET	L4519	THR	GLY	GLY	GLY	GLY	GLY	Q4165	ASP	GLY	L3670	ARG	LEU	ASP	ARG
C4958	D4804	ASP	V4523	SER	GLY	GLY	GLY	GLY	LEU	E4168	LEU	GLY	L3683	PRO	LEU	VAL	VAL
F4959	M4805	LYS	THR	THR	ASN	GLY	GLY	GLY	LEU	R4171	LEU	GLY	I3695	GLN	GLY	GLY	GLY
Y4963	C4807	ALA	ALA	ALA	LYS	GLY	GLY	GLY	LEU	V3980	GLY	GLY	L3695	ASP	ASP	VAL	SER
E4964	D4808	LEU	VAL	SER	VAL	SER	SER	SER	LEU	V3981	GLY	SER	C3700	LYS	LYS	ILE	ILE
ASP	M4810	PHE	VAL	GLY	VAL	GLY	GLY	GLY	GLY	V3982	ASP	ASP	G3727	ALA	ARG	ARG	ARG
GLN	L4811	SER	GLY	GLY	GLY	GLY	GLY	GLY	LEU	I4174	LEU	ASP	HIS	ALA	TRP	TRP	TRP
LEU	T4812	ASP	GLY	GLY	GLY	GLY	GLY	GLY	SER	E4180	SER	V3630	ASP	VAL	GLN	ILE	TRP
ASN	C4813	ALA	LYS	LYS	LYS	LYS	GLY	GLY	LEU	G4181	LEU	F3641	GLY	HIS	GLN	VAL	SER
	Y4814	ARG	GLU	ALA	ALA	LEU	ALA	ALA	LYS	C4182	GLY	Q3645	ASP	LYS	ALA	ALA	LYS
	M4815	GLY	LEU	LYS	LYS	ASP	LYS	LYS	SER	E4183	SER	Q3652	ASP	LEU	LEU	LEU	HIS
		LYS	PRO	PRO	PRO	LEU	LYS	ILE	LEU	K4184	LEU	N3652	GLY	LEU	ARG	ARG	ASN
	M4818	LYS	THR	ARG	LYS	ASP	LYS	LYS	LYS	I4207	GLY	I3671	LYS	LYS	LYS	LYS	LYS
	Y4819	PRO	ARG	SER	GLY	GLY	VAL	VAL	GLN		SER	T3675	GLY	GLN	LEU	ARG	ARG
	R4823	LYS	SER	SER	GLY	GLY	GLY	GLY	MET	D4026	GLY	L3675	GLY	ARG	PRO	PRO	GLY
	G4826	LYS	SER	GLY	LYS	GLY	GLY	GLY	LYS	T4028	SER	L3680	VAL	LYS	ASN	ILE	ILE
	P4835	ASP	ASN	GLY	GLY	GLY	GLY	GLY	LYS	S4029	ASP	L3881	LYS	ARG	GLY	ASN	GLY
	R4844	SER	ALA	LEU	ALA	LYS	LYS	ASN	LYS	T4032	LEU	R3881	C3744	VAL	THR	ASP	VAL
	I4845	LEU	PHE	ILE	ASN	ILE	MET	GLY	LYS	F4033	GLY	V3882	Q3729	VAL	THR	CYS	VAL
	D4848	ALA	GLY	PRO	PRO	PRO	THR	PRO	THR	Y4036	ARG	Q3883	H3733	ALA	SER	ALA	GLN
	I4858	VAL	SER	ASP	ASP	HIS	ASP	ASP	VAL	S3885	SER	E3884	D3784	PHE	ASP	PRO	ASN
	Y4858	LEU	LEU	LYS	LYS	ASN	PRO	PRO	ARG	S4045	ALA	Y3692	R3735	ARG	PRO	GLY	GLY
	I4862	ASP	ASP	ASP	ASP	ASN	THR	THR	MET	K4051	ASN	K3696	E3739	MET	LYS	GLN	ASN
	T4728	LYS	SER	GLY	GLY	GLY	GLN	GLN	VAL	A4052	LYS		Q3743	ALA	THR	GLY	GLY
		LEU	PRO	LEU	LEU	LEU	VAL	VAL	ALA		SER	D3600		P3608	VAL	LEU	LEU
											GLY			L3609	GLU	VAL	SER

● Molecule 1: RyR2



W2733	P2668	E2540	F2441	CYS	ARG	D2116	E1991	GLU	I1792	G1658	L1570	ASP
S2734	C2669	A2543	Q2442	PHE	GLY	D2116	D2013	G1893	D1808	N1669	F1571	ASP
W2735	A2672	V2553	THR	GLY	SER	L2120	GLU	K1904	P1809	S1678	K1572	ARG
K2737	P2678	TYR	ILE	ALA	L2254	R2128	ASP	L1905	H1679	H1679	E1574	ASP
L2738	PRO	ARG	ALA	LEU	A2257	L2131	LEU	Q1906	V1680	D1681	V1579	ASP
A2739	ASP	LEU	LYS	GLY	L2258	S2132	ASP	M1907	F1682	A1682	P1580	TYR
W2740	SER	SER	GLY	GLY	R2259	V2133	GLY	A1925	Y1687	R1585	R1585	LEU
G2741	MET	ASN	ASN	GLY	E2264	K2141	ASN	S1930	A1688	Q1589	Q1589	GLN
L2742	GLU	VAL	VAL	ASN	K2265	L2142	ASP	D1931	I1689	F1689	F1689	THR
L2743	SER	ILE	VAL	G2343	V2266	L2024	ASP	D1932	I1842	F1690	N1502	ASN
W2744	TYR	CYS	GLU	L2354	V2267	E2138	GLY	D1939	K1840	Y1687	L1505	GLN
G2745	VAL	GLN	ASP	ALA	R2268	K2141	ASP	R1942	I1841	A1688	L1505	GLY
E2746	SER	LEU	GLU	ASP	L2269	L2142	ASP	F1943	I1842	F1689	I1507	THR
G2747	MET	ARG	ASP	GLU	L2270	L2030	LYS	Q1950	F1689	N1601	S1429	GLN
L2747	GLU	P2583	PRO	PRO	A2271	L2030	LYS	L1952	S1849	P1600	V1430	GLN
W2748	LYS	ARG	SER	SER	L2275	G2148	VAL	Q1950	VAL	R1718	R1431	GLY
S2749	GLN	ASP	GLY	ASP	GLN	N2152	LEU	A1951	PHE	R1719	F1434	GLY
L2750	SER	PRO	GLY	GLY	SER	N2153	LYS	L1952	LYS	T1730	F1434	GLN
S2751	MET	SER	SER	PRO	CYS	F2156	LYS	ASN	ALA	E1731	GLY	GLN
S2752	ASP	PRO	THR	PRO	GLN	M2163	GLN	ALA	PRO	T1733	ALA	GLU
G2753	SER	THR	ILE	THR	LEU	M2163	ALA	ALA	GLU	K1734	ALA	PRO
V2754	GLU	SER	SER	SER	VAL	M2168	LYS	LEU	GLU	I1736	ALA	ALA
Q2755	GLY	GLY	GLY	GLY	SER	M2168	VAL	THR	SER	T1737	ALA	ALA
P2756	LYS	SER	SER	SER	TYR	V2175	GLU	ARG	ASP	L1738	ALA	ALA
L2757	GLN	L2598	V2461	ASP	GLY	V2175	GLU	ARG	THR	L1617	ALA	ALA
W2758	SER	L2599	K2466	ASP	PRO	G2181	SER	THR	LEU	L1618	ALA	ALA
K2759	PRO	L2600	V2477	GLY	PRO	GLY	ASP	THR	GLU	V1619	ALA	ALA
P2760	ASP	N2601	ILE	ASP	ILE	GLY	ASP	LYS	ASN	Q1620	ALA	ALA
V2761	THR	GLY	THR	THR	TRP	GLY	LYS	PHE	LYS	C1621	ALA	ALA
L2762	ALA	K2605	ALA	GLY	ASN	GLY	LYS	ARG	ARG	L1622	ALA	ALA
L2763	LEU	V2609	ALA	GLY	P2293	THR	SER	SER	VAL	I1625	ALA	ALA
L2764	SER	G2627	ALA	GLU	R2298	ILE	SER	PRO	GLY	S1629	ALA	ALA
S2765	ALA	TRP	ALA	GLU	D2301	PHE	THR	PRO	GLU	L1630	ALA	ALA
E2766	THR	GLY	T2511	ASP	V2307	P2191	THR	GLN	ASP	H1631	ALA	ALA
K2767	ASN	PHE	D2512	THR	S2313	S2208	GLY	ILE	ARG	P1632	ALA	ALA
E2768	GLY	GLY	M2513	ILE	V2314	R2209	THR	ASN	GLY	E1634	ALA	ALA
K2769	THR	ALA	M2518	THR	E2315	S2209	THR	LEU	LEU	T1755	ALA	ALA
E2770	ALA	ALA	R2519	THR	E2316	K2213	THR	LEU	GLY	S1756	ALA	ALA
L2771	ALA	A2634	Y2520	ALA	E2317	D2217	THR	ALA	ALA	R1757	ALA	ALA
W2772	GLY	D2651	L2521	GLY	N2317	D2217	THR	ALA	GLU	F1763	ALA	ALA
K2773	SER	A2652	L2526	THR	R2323	V2228	GLY	ASP	GLU	S1764	ALA	ALA
L2774	GLN	L2653	L2427	THR	L2324	V2228	GLY	ASP	GLU	T1769	ALA	ALA
P2775	LYS	L2433	L2433	THR	L2325	GLY	GLY	LYS	LYS	Y1779	ALA	ALA
L2776	LYS	ARG	L2436	THR	L2326	ALA	GLY	LYS	GLY	P1780	ALA	ALA
K2777	LYS	CYS	V2436	THR	L2327	ALA	GLY	LYS	GLY	E1781	ALA	ALA
E2778	PRO	ALA	L2439	THR	R2327	ALA	GLY	CYS	LYS	F1782	ALA	ALA
S2779	PRO	ALA	A2440	THR	R2328	ALA	ALA	PRO	ARG	L1659	ALA	ALA
L2780	LYS	L2653	L2439	THR	R2329	ALA	ALA	CYS	PRO	L1660	ALA	ALA
K2781	LYS	L2653	L2439	THR	E2330	ALA	ALA	CYS	LYS	L1667	ALA	ALA
T2782	LYS	L2653	L2439	THR	E2330	ALA	ALA	PRO	LYS			
W2783	LYS	L2653	L2439	THR	E2330	ALA	ALA	PRO	LYS			
L2784	LYS	L2653	L2439	THR	E2330	ALA	ALA	PRO	LYS			
K2785	LYS	L2653	L2439	THR	E2330	ALA	ALA	PRO	LYS			
W2786	LYS	L2653	L2439	THR	E2330	ALA	ALA	PRO	LYS			
K2787	LYS	L2653	L2439	THR	E2330	ALA	ALA	PRO	LYS			
W2788	LYS	L2653	L2439	THR	E2330	ALA	ALA	PRO	LYS			
K2789	LYS	L2653	L2439	THR	E2330	ALA	ALA	PRO	LYS			
L2790	LYS	L2653	L2439	THR	E2330	ALA	ALA	PRO	LYS			
E2791	LYS	L2653	L2439	THR	E2330	ALA	ALA	PRO	LYS			
K2792	LYS	L2653	L2439	THR	E2330	ALA	ALA	PRO	LYS			









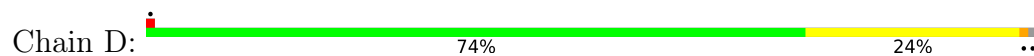








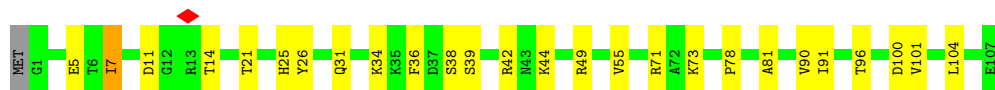
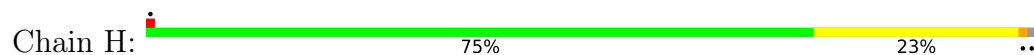
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	149212	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 ($e^-/\text{\AA}^2$)	50	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	0.141	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	436.4, 436.4, 436.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ZN, ATP, 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	0.44	0/26913	0.67	4/36395 (0.0%)
1	C	0.43	0/26913	0.67	5/36395 (0.0%)
1	E	0.43	0/26913	0.67	5/36395 (0.0%)
1	G	0.43	0/26913	0.67	4/36395 (0.0%)
2	B	0.36	0/835	0.65	1/1123 (0.1%)
2	D	0.36	0/835	0.65	1/1123 (0.1%)
2	F	0.36	0/835	0.65	1/1123 (0.1%)
2	H	0.36	0/835	0.65	1/1123 (0.1%)
All	All	0.43	0/110992	0.67	22/150072 (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	15
1	C	0	15
1	E	0	15
1	G	0	15
All	All	0	60

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	4771	THR	N-CA-C	11.30	123.68	111.36
1	C	4771	THR	N-CA-C	11.23	123.60	111.36
1	G	4771	THR	N-CA-C	8.26	121.86	111.69
1	A	4771	THR	N-CA-C	7.54	120.96	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4770	LEU	CB-CA-C	5.24	119.50	110.79
1	E	4770	LEU	CB-CA-C	5.24	119.50	110.79
2	H	7	ILE	N-CA-C	-5.11	106.67	111.48
1	A	1680	VAL	N-CA-C	-5.11	107.85	112.96
1	C	1680	VAL	N-CA-C	-5.11	107.85	112.96
1	E	1680	VAL	N-CA-C	-5.11	107.85	112.96
1	G	1680	VAL	N-CA-C	-5.11	107.85	112.96
2	F	7	ILE	N-CA-C	-5.11	106.68	111.48
2	B	7	ILE	N-CA-C	-5.10	106.69	111.48
2	D	7	ILE	N-CA-C	-5.10	106.69	111.48
1	C	686	VAL	CA-C-N	5.08	131.24	121.54
1	C	686	VAL	C-N-CA	5.08	131.24	121.54
1	A	686	VAL	CA-C-N	5.06	131.20	121.54
1	A	686	VAL	C-N-CA	5.06	131.20	121.54
1	E	686	VAL	CA-C-N	5.06	131.21	121.54
1	E	686	VAL	C-N-CA	5.06	131.21	121.54
1	G	686	VAL	CA-C-N	5.06	131.20	121.54
1	G	686	VAL	C-N-CA	5.06	131.20	121.54

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1127	GLU	Peptide
1	A	1545	ALA	Peptide
1	A	1570	LEU	Peptide
1	A	1579	VAL	Peptide
1	A	1750	GLY	Peptide
1	A	1808	ASP	Peptide
1	A	1809	PRO	Peptide
1	A	1847	GLU	Peptide
1	A	3802	SER	Peptide
1	A	729	GLY	Peptide
1	A	791	VAL	Peptide
1	A	814	LEU	Peptide
1	A	816	PRO	Peptide
1	A	819	TYR	Peptide
1	A	838	ARG	Peptide
1	C	1127	GLU	Peptide
1	C	1545	ALA	Peptide
1	C	1570	LEU	Peptide
1	C	1579	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	C	1750	GLY	Peptide
1	C	1808	ASP	Peptide
1	C	1809	PRO	Peptide
1	C	1847	GLU	Peptide
1	C	3802	SER	Peptide
1	C	729	GLY	Peptide
1	C	791	VAL	Peptide
1	C	814	LEU	Peptide
1	C	816	PRO	Peptide
1	C	819	TYR	Peptide
1	C	838	ARG	Peptide
1	E	1127	GLU	Peptide
1	E	1545	ALA	Peptide
1	E	1570	LEU	Peptide
1	E	1579	VAL	Peptide
1	E	1750	GLY	Peptide
1	E	1808	ASP	Peptide
1	E	1809	PRO	Peptide
1	E	1847	GLU	Peptide
1	E	3802	SER	Peptide
1	E	729	GLY	Peptide
1	E	791	VAL	Peptide
1	E	814	LEU	Peptide
1	E	816	PRO	Peptide
1	E	819	TYR	Peptide
1	E	838	ARG	Peptide
1	G	1127	GLU	Peptide
1	G	1545	ALA	Peptide
1	G	1570	LEU	Peptide
1	G	1579	VAL	Peptide
1	G	1750	GLY	Peptide
1	G	1808	ASP	Peptide
1	G	1809	PRO	Peptide
1	G	1847	GLU	Peptide
1	G	3802	SER	Peptide
1	G	729	GLY	Peptide
1	G	791	VAL	Peptide
1	G	814	LEU	Peptide
1	G	816	PRO	Peptide
1	G	819	TYR	Peptide
1	G	838	ARG	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	26417	0	24909	490	0
1	C	26417	0	24909	500	0
1	E	26417	0	24909	485	0
1	G	26417	0	24909	471	0
2	B	819	0	824	19	0
2	D	819	0	824	19	0
2	F	819	0	824	19	0
2	H	819	0	824	18	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	31	0	12	1	0
5	C	31	0	12	1	0
5	E	31	0	12	1	0
5	G	31	0	12	1	0
6	A	14	0	10	1	0
6	C	14	0	10	1	0
6	E	14	0	10	1	0
6	G	14	0	10	1	0
All	All	109132	0	103020	1803	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 8.

All (1803) 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:2427:LEU:HD13	1:G:143:LEU:CB	1.41	1.51
1:E:143:LEU:CB	1:G:2427:LEU:HD13	1.41	1.49
1:A:143:LEU:CB	1:C:2427:LEU:HD13	1.41	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:LEU:CB	1:E:2427:LEU:HD13	1.43	1.47
1:A:2427:LEU:CD1	1:G:143:LEU:HB3	1.48	1.42
1:A:143:LEU:HB3	1:C:2427:LEU:CD1	1.48	1.41
1:C:143:LEU:HB3	1:E:2427:LEU:CD1	1.50	1.39
1:E:143:LEU:HB3	1:G:2427:LEU:CD1	1.49	1.39
1:E:4845:ILE:HD12	1:G:4819:TYR:CD1	1.65	1.32
1:C:4845:ILE:HD12	1:E:4819:TYR:CD1	1.65	1.32
1:A:4819:TYR:CD1	1:G:4845:ILE:HD12	1.66	1.28
1:A:4845:ILE:HD12	1:C:4819:TYR:CD1	1.67	1.27
1:G:2327:ARG:O	1:G:2328:ARG:CG	1.83	1.27
1:C:4845:ILE:CD1	1:E:4819:TYR:CD1	2.20	1.25
1:A:2327:ARG:O	1:A:2328:ARG:CG	1.83	1.23
1:A:4819:TYR:O	1:A:4823:ARG:HD3	1.34	1.23
1:A:4819:TYR:CD1	1:G:4845:ILE:CD1	2.22	1.23
1:A:4845:ILE:CD1	1:C:4819:TYR:CD1	2.22	1.22
1:E:4845:ILE:CD1	1:G:4819:TYR:CD1	2.21	1.22
1:G:4819:TYR:O	1:G:4823:ARG:HD3	1.34	1.22
1:C:4819:TYR:O	1:C:4823:ARG:HD3	1.36	1.21
1:A:4862:ILE:HG22	1:C:4868:ILE:HD12	1.30	1.14
1:C:4862:ILE:HG22	1:E:4868:ILE:HD12	1.30	1.13
1:G:2327:ARG:O	1:G:2328:ARG:HG2	0.95	1.13
1:E:4862:ILE:HG22	1:G:4868:ILE:HD12	1.32	1.12
1:A:2327:ARG:O	1:A:2328:ARG:HG2	0.95	1.11
1:C:4845:ILE:HD13	1:E:4819:TYR:CE1	1.86	1.09
1:A:4819:TYR:CE1	1:G:4845:ILE:HD13	1.87	1.08
1:A:4868:ILE:HD12	1:G:4862:ILE:HG22	1.31	1.08
1:E:4845:ILE:HD13	1:G:4819:TYR:CE1	1.86	1.08
1:A:4845:ILE:HD13	1:C:4819:TYR:CE1	1.88	1.07
1:A:2427:LEU:HD13	1:G:143:LEU:CG	1.83	1.06
1:A:4858:ILE:HD12	1:C:4867:ILE:HG21	1.36	1.06
1:A:143:LEU:CG	1:C:2427:LEU:HD13	1.84	1.06
1:C:143:LEU:CG	1:E:2427:LEU:HD13	1.85	1.06
1:C:4858:ILE:HD12	1:E:4867:ILE:HG21	1.38	1.06
1:E:143:LEU:CG	1:G:2427:LEU:HD13	1.83	1.06
1:E:143:LEU:CD2	1:G:2427:LEU:HD13	1.87	1.05
1:A:4867:ILE:HG21	1:G:4858:ILE:HD12	1.36	1.04
1:A:2427:LEU:HD13	1:G:143:LEU:CD2	1.87	1.03
1:C:143:LEU:CD2	1:E:2427:LEU:HD13	1.88	1.03
1:A:143:LEU:CD2	1:C:2427:LEU:HD13	1.88	1.03
1:A:2427:LEU:CD1	1:G:143:LEU:HD22	1.89	1.03
1:E:4858:ILE:HD12	1:G:4867:ILE:HG21	1.36	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:LEU:HD22	1:E:2427:LEU:CD1	1.90	1.01
1:E:143:LEU:HD22	1:G:2427:LEU:CD1	1.89	1.00
1:A:143:LEU:HD22	1:C:2427:LEU:CD1	1.90	1.00
1:C:143:LEU:CB	1:E:2427:LEU:CD1	2.25	0.97
1:A:143:LEU:CB	1:C:2427:LEU:CD1	2.23	0.97
1:A:2427:LEU:CD1	1:G:143:LEU:CB	2.22	0.96
1:A:2427:LEU:HD13	1:G:143:LEU:HB3	0.99	0.96
1:A:143:LEU:HB3	1:C:2427:LEU:HD13	0.98	0.96
1:C:4862:ILE:CG2	1:E:4868:ILE:HD12	1.96	0.96
1:E:143:LEU:HB3	1:G:2427:LEU:HD13	1.00	0.95
1:C:143:LEU:HB3	1:E:2427:LEU:HD13	0.99	0.95
1:A:143:LEU:HD11	1:A:207:PHE:HD2	1.32	0.94
1:A:2427:LEU:CD1	1:G:143:LEU:CD2	2.45	0.94
1:A:143:LEU:CD2	1:C:2427:LEU:CD1	2.45	0.94
1:A:143:LEU:HD22	1:C:2427:LEU:CD2	1.98	0.94
1:A:4862:ILE:CG2	1:C:4868:ILE:HD12	1.96	0.94
1:C:76:ARG:HD3	1:E:3891:TRP:CD2	2.03	0.93
1:C:209:GLN:HE21	1:E:2327:ARG:HH11	1.13	0.93
1:E:143:LEU:CD2	1:G:2427:LEU:CD1	2.44	0.93
1:E:4862:ILE:CG2	1:G:4868:ILE:HD12	1.98	0.93
1:A:143:LEU:HB3	1:C:2427:LEU:HD12	1.51	0.92
1:C:76:ARG:HB3	1:C:76:ARG:HH21	1.33	0.92
1:C:143:LEU:CD2	1:E:2427:LEU:CD1	2.46	0.92
1:E:143:LEU:HD22	1:G:2427:LEU:CD2	1.99	0.92
1:A:76:ARG:HH21	1:A:76:ARG:HG3	1.34	0.92
1:C:143:LEU:HD22	1:E:2427:LEU:CD2	2.00	0.92
1:A:4868:ILE:HD12	1:G:4862:ILE:CG2	1.98	0.92
1:A:2427:LEU:CD2	1:G:143:LEU:HD22	1.99	0.91
1:G:4823:ARG:HB2	1:G:4823:ARG:NH1	1.86	0.90
1:A:2427:LEU:HD12	1:G:143:LEU:HB3	1.51	0.90
1:C:143:LEU:HB3	1:E:2427:LEU:HD12	1.53	0.90
1:C:4823:ARG:HB2	1:C:4823:ARG:NH2	1.87	0.90
1:E:143:LEU:HB3	1:G:2427:LEU:HD12	1.51	0.89
1:A:4819:TYR:CE1	1:G:4845:ILE:CD1	2.52	0.89
1:A:4823:ARG:HB2	1:A:4823:ARG:NH2	1.87	0.89
1:C:2323:ARG:HH21	1:C:2323:ARG:HG3	1.35	0.89
1:E:4845:ILE:CD1	1:G:4819:TYR:CE1	2.50	0.88
1:C:4862:ILE:CG2	1:E:4868:ILE:CD1	2.52	0.88
1:A:4845:ILE:CD1	1:C:4819:TYR:CE1	2.53	0.88
1:E:143:LEU:CB	1:G:2427:LEU:CD1	2.23	0.88
1:A:143:LEU:HD11	1:A:207:PHE:CD2	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4868:ILE:CD1	1:G:4862:ILE:CG2	2.53	0.86
1:A:4862:ILE:CG2	1:C:4868:ILE:CD1	2.52	0.86
1:A:4862:ILE:HD11	1:C:4757:ILE:HD12	1.58	0.86
1:G:4819:TYR:O	1:G:4823:ARG:CD	2.23	0.86
1:E:4862:ILE:HD11	1:G:4757:ILE:HD12	1.58	0.85
1:E:4862:ILE:CD1	1:G:4757:ILE:HD12	2.07	0.84
1:A:4757:ILE:HD12	1:G:4862:ILE:CD1	2.07	0.84
1:A:4862:ILE:CD1	1:C:4757:ILE:HD12	2.08	0.84
1:E:4862:ILE:CG2	1:G:4868:ILE:CD1	2.54	0.84
1:A:4819:TYR:O	1:A:4823:ARG:CD	2.24	0.84
1:A:4757:ILE:HD12	1:G:4862:ILE:HD11	1.58	0.84
1:C:209:GLN:HE21	1:E:2327:ARG:NH1	1.74	0.83
1:C:4862:ILE:HD11	1:E:4757:ILE:HD12	1.60	0.83
1:A:2327:ARG:C	1:A:2328:ARG:HG2	2.03	0.83
1:C:4845:ILE:CD1	1:E:4819:TYR:CE1	2.51	0.82
1:C:4862:ILE:CD1	1:E:4757:ILE:HD12	2.10	0.82
1:C:797:GLY:HA2	1:C:1621:CYS:O	1.82	0.79
1:G:2327:ARG:C	1:G:2328:ARG:HG2	2.03	0.79
1:A:797:GLY:HA2	1:A:1621:CYS:O	1.82	0.79
1:C:76:ARG:HH21	1:C:76:ARG:CB	1.94	0.79
1:E:797:GLY:HA2	1:E:1621:CYS:O	1.82	0.79
1:A:189:GLU:OE2	1:C:2323:ARG:CD	2.32	0.78
1:G:797:GLY:HA2	1:G:1621:CYS:O	1.82	0.78
1:C:2328:ARG:CB	1:C:2328:ARG:HH11	1.97	0.78
1:A:2427:LEU:HD13	1:G:143:LEU:HD22	1.59	0.76
1:A:143:LEU:HD22	1:C:2427:LEU:HD13	1.60	0.76
1:A:1219:LYS:H	1:A:1240:ALA:HB2	1.51	0.76
1:E:2328:ARG:CB	1:E:2328:ARG:HH11	1.99	0.76
1:C:4819:TYR:O	1:C:4823:ARG:CD	2.27	0.75
1:C:143:LEU:HD11	1:C:207:PHE:HD2	1.51	0.75
1:G:143:LEU:HD11	1:G:207:PHE:HD2	1.50	0.75
1:C:1219:LYS:H	1:C:1240:ALA:HB2	1.51	0.75
1:E:1219:LYS:H	1:E:1240:ALA:HB2	1.51	0.75
1:E:143:LEU:HD22	1:G:2427:LEU:HD22	1.70	0.74
1:G:1219:LYS:H	1:G:1240:ALA:HB2	1.51	0.74
1:C:4845:ILE:HD12	1:E:4819:TYR:CG	2.22	0.74
1:G:143:LEU:HD11	1:G:207:PHE:CD2	2.23	0.73
1:C:143:LEU:HD22	1:E:2427:LEU:HD22	1.69	0.73
1:C:143:LEU:HD11	1:C:207:PHE:CD2	2.23	0.73
1:A:143:LEU:HD22	1:C:2427:LEU:HD22	1.69	0.73
1:E:2328:ARG:HH11	1:E:2328:ARG:CA	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:OE2	1:C:2323:ARG:HD3	1.88	0.72
1:C:2328:ARG:HH11	1:C:2328:ARG:CA	2.02	0.72
1:A:76:ARG:HG3	1:A:76:ARG:NH2	1.99	0.72
1:C:842:GLN:HE21	1:C:849:ASP:H	1.36	0.72
1:G:842:GLN:HE21	1:G:849:ASP:H	1.36	0.72
1:A:2427:LEU:HD22	1:G:143:LEU:HD22	1.70	0.72
1:C:76:ARG:CD	1:E:3891:TRP:CG	2.72	0.71
1:E:842:GLN:HE21	1:E:849:ASP:H	1.36	0.71
1:A:842:GLN:HE21	1:A:849:ASP:H	1.36	0.71
1:G:4823:ARG:HB2	1:G:4823:ARG:CZ	2.20	0.71
1:E:4845:ILE:HD12	1:G:4819:TYR:CG	2.24	0.71
1:C:2314:VAL:HG23	1:C:2317:ASN:HB2	1.73	0.71
1:A:728:ASP:HA	1:A:748:LEU:HA	1.72	0.70
1:E:4862:ILE:CD1	1:G:4757:ILE:CD1	2.70	0.70
1:C:728:ASP:HA	1:C:748:LEU:HA	1.72	0.70
1:G:728:ASP:HA	1:G:748:LEU:HA	1.72	0.70
1:C:4845:ILE:CD1	1:E:4819:TYR:CG	2.73	0.70
1:E:2314:VAL:HG23	1:E:2317:ASN:HB2	1.74	0.70
1:A:4757:ILE:CD1	1:G:4862:ILE:CD1	2.70	0.70
1:E:728:ASP:HA	1:E:748:LEU:HA	1.72	0.70
1:E:4845:ILE:CD1	1:G:4819:TYR:CG	2.75	0.69
1:C:4823:ARG:HB2	1:C:4823:ARG:CZ	2.21	0.69
1:A:4823:ARG:HB2	1:A:4823:ARG:CZ	2.20	0.69
1:A:4845:ILE:HD12	1:C:4819:TYR:CG	2.25	0.69
1:A:4862:ILE:CD1	1:C:4757:ILE:CD1	2.70	0.69
1:G:590:LYS:H	1:G:593:HIS:HD2	1.41	0.68
1:A:590:LYS:H	1:A:593:HIS:HD2	1.41	0.68
1:A:4845:ILE:CD1	1:C:4819:TYR:CG	2.76	0.68
1:C:2323:ARG:HG3	1:C:2323:ARG:NH2	2.05	0.68
1:A:4757:ILE:CD1	1:G:4862:ILE:HD12	2.24	0.68
1:A:4862:ILE:HD12	1:C:4757:ILE:CD1	2.24	0.68
1:E:4862:ILE:HD12	1:G:4757:ILE:CD1	2.24	0.68
1:E:1089:ARG:HH22	1:E:1600:PRO:HG3	1.59	0.68
1:A:2427:LEU:HD13	1:G:143:LEU:HB2	1.68	0.68
1:C:1089:ARG:HH22	1:C:1600:PRO:HG3	1.59	0.68
1:C:590:LYS:H	1:C:593:HIS:HD2	1.41	0.68
1:A:4819:TYR:CG	1:G:4845:ILE:HD12	2.24	0.67
1:E:660:PHE:HB3	1:E:787:LEU:HD22	1.77	0.67
1:A:1089:ARG:HH22	1:A:1600:PRO:HG3	1.59	0.67
1:E:4796:LYS:NZ	1:E:4807:CYS:SG	2.68	0.67
1:C:4862:ILE:CD1	1:E:4757:ILE:CD1	2.72	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1089:ARG:HH22	1:G:1600:PRO:HG3	1.59	0.67
1:A:4819:TYR:CG	1:G:4845:ILE:CD1	2.76	0.67
1:G:660:PHE:HB3	1:G:787:LEU:HD22	1.77	0.67
1:E:590:LYS:H	1:E:593:HIS:HD2	1.41	0.66
1:C:143:LEU:HD22	1:E:2427:LEU:HD13	1.59	0.66
1:C:660:PHE:HB3	1:C:787:LEU:HD22	1.77	0.66
1:C:4862:ILE:HD12	1:E:4757:ILE:CD1	2.26	0.65
1:G:4796:LYS:NZ	1:G:4807:CYS:SG	2.68	0.65
1:C:1125:ASP:HA	1:C:1598:ARG:HB2	1.79	0.65
1:A:660:PHE:HB3	1:A:787:LEU:HD22	1.77	0.65
1:G:1125:ASP:HA	1:G:1598:ARG:HB2	1.79	0.65
1:C:4835:PRO:HG3	1:C:4844:ARG:HE	1.62	0.65
1:E:1125:ASP:HA	1:E:1598:ARG:HB2	1.78	0.65
1:A:189:GLU:OE2	1:C:2323:ARG:HD2	1.96	0.65
1:E:4823:ARG:NH2	1:E:4823:ARG:HB3	2.12	0.65
1:G:2314:VAL:HG23	1:G:2317:ASN:HB2	1.79	0.65
1:E:4835:PRO:HG3	1:E:4844:ARG:HE	1.62	0.65
1:A:1125:ASP:HA	1:A:1598:ARG:HB2	1.79	0.65
1:A:2314:VAL:HG23	1:A:2317:ASN:HB2	1.79	0.65
1:A:4796:LYS:NZ	1:A:4807:CYS:SG	2.68	0.64
1:C:207:PHE:CZ	1:E:2326:ILE:CB	2.80	0.64
1:E:4826:GLY:O	1:G:4823:ARG:NH2	2.31	0.64
1:G:4835:PRO:HG3	1:G:4844:ARG:HE	1.62	0.64
1:A:503:ASP:HA	1:A:561:ARG:HH22	1.63	0.64
1:C:4796:LYS:NZ	1:C:4807:CYS:SG	2.68	0.64
1:G:243:GLU:HA	1:G:263:GLU:O	1.98	0.64
1:A:2706:PRO:HB3	1:A:2855:LYS:HG3	1.80	0.64
1:C:503:ASP:HA	1:C:561:ARG:HH22	1.63	0.64
1:E:503:ASP:HA	1:E:561:ARG:HH22	1.63	0.64
1:A:2327:ARG:O	1:A:2328:ARG:CB	2.43	0.64
1:A:4823:ARG:NH1	1:G:4826:GLY:O	2.31	0.64
1:G:503:ASP:HA	1:G:561:ARG:HH22	1.63	0.64
1:E:243:GLU:HA	1:E:263:GLU:O	1.98	0.64
1:A:4835:PRO:HG3	1:A:4844:ARG:HE	1.62	0.63
1:C:1465:VAL:N	1:C:1483:SER:O	2.31	0.63
1:G:123:HIS:HD2	1:G:126:SER:H	1.47	0.63
1:G:1465:VAL:N	1:G:1483:SER:O	2.31	0.63
1:A:123:HIS:HD2	1:A:126:SER:H	1.47	0.63
1:C:1446:ILE:O	1:C:1540:PHE:HB2	1.98	0.63
1:E:2315:GLU:HA	1:E:2315:GLU:OE2	1.97	0.63
1:G:2706:PRO:HB3	1:G:2855:LYS:HG3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ARG:HD2	1:E:3891:TRP:CD1	2.34	0.63
1:E:1446:ILE:O	1:E:1540:PHE:HB2	1.98	0.63
1:C:123:HIS:HD2	1:C:126:SER:H	1.47	0.63
1:C:374:TYR:HB2	1:C:389:ARG:HB3	1.81	0.63
1:E:123:HIS:HD2	1:E:126:SER:H	1.47	0.63
1:E:143:LEU:HB2	1:G:2427:LEU:HD13	1.68	0.63
1:E:374:TYR:HB2	1:E:389:ARG:HB3	1.81	0.63
1:C:243:GLU:HA	1:C:263:GLU:O	1.98	0.62
1:G:374:TYR:HB2	1:G:389:ARG:HB3	1.81	0.62
1:G:4958:CYS:SG	1:G:4959:PHE:N	2.72	0.62
1:A:1465:VAL:N	1:A:1483:SER:O	2.31	0.62
1:E:1465:VAL:N	1:E:1483:SER:O	2.31	0.62
1:E:2706:PRO:HB3	1:E:2855:LYS:HG3	1.80	0.62
1:G:189:GLU:HG2	1:G:189:GLU:O	2.00	0.62
1:G:2327:ARG:O	1:G:2328:ARG:CB	2.43	0.62
1:A:243:GLU:HA	1:A:263:GLU:O	1.98	0.62
1:A:374:TYR:HB2	1:A:389:ARG:HB3	1.81	0.62
1:C:1265:HIS:HD2	1:C:1267:HIS:H	1.48	0.62
1:C:2706:PRO:HB3	1:C:2855:LYS:HG3	1.80	0.62
1:C:4958:CYS:SG	1:C:4959:PHE:N	2.72	0.62
1:G:1446:ILE:O	1:G:1540:PHE:HB2	1.98	0.62
1:A:143:LEU:HD22	1:C:2427:LEU:HD11	1.81	0.62
1:C:4791:ARG:HD2	1:C:4808:ASP:HB3	1.82	0.62
1:C:462:TYR:O	1:C:485:ARG:NH1	2.33	0.62
1:E:4791:ARG:HD2	1:E:4808:ASP:HB3	1.82	0.62
1:A:4845:ILE:HD12	1:C:4819:TYR:HD1	1.57	0.62
1:E:189:GLU:O	1:E:189:GLU:HG2	2.00	0.62
1:G:1265:HIS:HD2	1:G:1267:HIS:H	1.48	0.62
1:C:189:GLU:O	1:C:189:GLU:HG2	2.00	0.62
1:E:143:LEU:HD22	1:G:2427:LEU:HD11	1.81	0.62
1:G:4791:ARG:HD2	1:G:4808:ASP:HB3	1.82	0.62
1:A:462:TYR:O	1:A:485:ARG:NH1	2.33	0.62
1:E:1265:HIS:HD2	1:E:1267:HIS:H	1.48	0.62
1:A:207:PHE:CZ	1:C:2326:ILE:CB	2.82	0.62
1:A:2427:LEU:HD11	1:G:143:LEU:CD2	2.30	0.62
1:A:1265:HIS:HD2	1:A:1267:HIS:H	1.48	0.61
1:A:1446:ILE:O	1:A:1540:PHE:HB2	1.98	0.61
1:A:2427:LEU:HD11	1:G:143:LEU:HD22	1.81	0.61
1:G:462:TYR:O	1:G:485:ARG:NH1	2.33	0.61
1:G:4145:ARG:NH2	1:G:4963:TYR:OH	2.33	0.61
1:A:4791:ARG:HD2	1:A:4808:ASP:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:143:LEU:HD12	1:G:143:LEU:O	2.01	0.61
1:C:143:LEU:HB2	1:E:2427:LEU:HD13	1.69	0.61
1:C:4145:ARG:NH2	1:C:4963:TYR:OH	2.33	0.61
1:E:143:LEU:HD12	1:E:143:LEU:O	2.01	0.61
1:E:4145:ARG:NH2	1:E:4963:TYR:OH	2.33	0.61
1:A:2315:GLU:OE2	1:A:2315:GLU:HA	2.00	0.61
1:E:207:PHE:CZ	1:G:2326:ILE:CB	2.84	0.61
1:E:4005:VAL:HG21	1:E:4115:ARG:HD2	1.83	0.61
1:G:3939:SER:OG	1:G:3940:ARG:N	2.34	0.61
1:A:370:LEU:HB2	1:A:393:MET:HE3	1.83	0.61
1:A:4145:ARG:NH2	1:A:4963:TYR:OH	2.33	0.61
1:C:143:LEU:HD12	1:C:143:LEU:O	2.01	0.61
1:C:4005:VAL:HG21	1:C:4115:ARG:HD2	1.83	0.61
1:E:370:LEU:HB2	1:E:393:MET:HE3	1.83	0.61
1:E:462:TYR:O	1:E:485:ARG:NH1	2.33	0.61
1:A:189:GLU:HG2	1:A:189:GLU:O	2.00	0.61
1:C:370:LEU:HB2	1:C:393:MET:HE3	1.83	0.61
1:A:3939:SER:OG	1:A:3940:ARG:N	2.34	0.61
1:A:4826:GLY:O	1:C:4823:ARG:NH1	2.34	0.61
1:G:370:LEU:HB2	1:G:393:MET:HE3	1.83	0.60
1:A:4868:ILE:CD1	1:G:4862:ILE:HG22	2.15	0.60
1:C:2138:GLU:O	1:C:2141:LYS:NZ	2.34	0.60
1:G:1443:VAL:HG12	1:G:1543:VAL:HG22	1.83	0.60
1:G:2143:MET:HE2	1:G:2175:VAL:HG11	1.83	0.60
1:G:2315:GLU:HA	1:G:2315:GLU:OE2	2.00	0.60
1:A:143:LEU:O	1:A:143:LEU:HD12	2.01	0.60
1:A:4005:VAL:HG21	1:A:4115:ARG:HD2	1.83	0.60
1:A:4848:ASP:OD1	1:C:4823:ARG:NE	2.33	0.60
1:E:4165:GLN:HG2	1:E:4594:LEU:HD11	1.84	0.60
1:G:832:LEU:O	1:G:1614:ARG:NH1	2.35	0.60
1:E:1932:ASP:OD1	1:E:1932:ASP:N	2.35	0.60
1:G:1932:ASP:OD1	1:G:1932:ASP:N	2.35	0.60
1:A:4165:GLN:HG2	1:A:4594:LEU:HD11	1.84	0.60
1:C:4165:GLN:HG2	1:C:4594:LEU:HD11	1.84	0.60
1:E:2328:ARG:HH11	1:E:2328:ARG:HA	1.66	0.60
1:E:3939:SER:OG	1:E:3940:ARG:N	2.34	0.60
1:A:2143:MET:HE2	1:A:2175:VAL:HG11	1.83	0.60
1:C:4791:ARG:HD2	1:C:4808:ASP:CB	2.32	0.60
1:A:832:LEU:O	1:A:1614:ARG:NH1	2.35	0.60
1:G:2893:ILE:HG13	1:G:2894:LEU:HD12	1.84	0.60
1:C:832:LEU:O	1:C:1614:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2893:ILE:HG13	1:C:2894:LEU:HD12	1.84	0.60
1:G:4165:GLN:HG2	1:G:4594:LEU:HD11	1.84	0.60
1:A:2893:ILE:HG13	1:A:2894:LEU:HD12	1.84	0.60
1:C:76:ARG:HD3	1:E:3891:TRP:CG	2.36	0.59
1:E:2893:ILE:HG13	1:E:2894:LEU:HD12	1.84	0.59
1:A:143:LEU:HB2	1:C:2427:LEU:HD13	1.68	0.59
1:E:1224:LEU:HD22	1:E:1227:PHE:HB2	1.84	0.59
1:E:4791:ARG:HD2	1:E:4808:ASP:CB	2.32	0.59
1:G:4005:VAL:HG21	1:G:4115:ARG:HD2	1.83	0.59
1:E:832:LEU:O	1:E:1614:ARG:NH1	2.35	0.59
1:G:3845:GLN:HG3	1:G:3923:GLU:HG3	1.85	0.59
1:A:1443:VAL:HG12	1:A:1543:VAL:HG22	1.83	0.59
1:C:235:ARG:NH1	1:C:268:SER:O	2.36	0.59
1:C:2143:MET:HE2	1:C:2175:VAL:HG11	1.83	0.59
1:C:4515:ASN:ND2	1:C:4740:PHE:O	2.33	0.59
1:G:620:CYS:SG	1:G:621:HIS:N	2.74	0.59
1:G:235:ARG:NH1	1:G:268:SER:O	2.36	0.59
1:A:143:LEU:CD2	1:C:2427:LEU:HD11	2.30	0.59
1:C:4897:ASP:N	1:C:4897:ASP:OD1	2.35	0.59
1:G:4791:ARG:HD2	1:G:4808:ASP:CB	2.32	0.59
1:A:620:CYS:SG	1:A:621:HIS:N	2.74	0.59
1:C:62:LEU:HB3	1:C:276:ARG:HH21	1.68	0.59
1:E:235:ARG:NH1	1:E:268:SER:O	2.36	0.59
1:E:258:ARG:NH1	1:E:316:LEU:O	2.36	0.59
1:C:1224:LEU:HD22	1:C:1227:PHE:HB2	1.84	0.59
1:G:258:ARG:NH1	1:G:316:LEU:O	2.36	0.59
1:A:235:ARG:NH1	1:A:268:SER:O	2.36	0.59
1:C:143:LEU:CD2	1:E:2427:LEU:HD11	2.33	0.59
1:E:1443:VAL:HG12	1:E:1543:VAL:HG22	1.83	0.59
1:E:2143:MET:HE2	1:E:2175:VAL:HG11	1.83	0.59
1:A:3845:GLN:HG3	1:A:3923:GLU:HG3	1.85	0.58
1:E:143:LEU:CD2	1:G:2427:LEU:HD11	2.30	0.58
1:G:2138:GLU:O	1:G:2141:LYS:NZ	2.34	0.58
1:G:4515:ASN:ND2	1:G:4740:PHE:O	2.33	0.58
1:A:188:SER:OG	1:A:190:ARG:NH2	2.35	0.58
1:A:2540:GLU:O	1:A:2543:ALA:HB3	2.03	0.58
1:A:2427:LEU:CG	1:G:143:LEU:HD22	2.34	0.58
1:A:4791:ARG:HD2	1:A:4808:ASP:CB	2.32	0.58
1:C:2540:GLU:O	1:C:2543:ALA:HB3	2.03	0.58
1:E:62:LEU:HB3	1:E:276:ARG:HH21	1.68	0.58
1:E:2540:GLU:O	1:E:2543:ALA:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:GLY:HA2	1:A:810:GLU:HB2	1.85	0.58
1:C:2328:ARG:HH11	1:C:2328:ARG:CG	2.14	0.58
1:E:620:CYS:SG	1:E:621:HIS:N	2.74	0.58
1:G:1224:LEU:HD22	1:G:1227:PHE:HB2	1.84	0.58
1:C:1443:VAL:HG12	1:C:1543:VAL:HG22	1.83	0.58
1:C:1644:LEU:HD23	1:C:1651:LEU:HA	1.86	0.58
1:E:2328:ARG:HH11	1:E:2328:ARG:CG	2.14	0.58
1:A:143:LEU:HD22	1:C:2427:LEU:CG	2.34	0.58
1:A:1224:LEU:HD22	1:A:1227:PHE:HB2	1.84	0.58
1:C:258:ARG:NH1	1:C:316:LEU:O	2.36	0.58
1:E:4958:CYS:SG	1:E:4959:PHE:N	2.72	0.58
1:A:1304:LEU:HB2	1:A:1541:PRO:HG2	1.86	0.58
1:C:1102:TYR:HB2	1:C:1165:MET:HG2	1.86	0.58
1:G:1102:TYR:HB2	1:G:1165:MET:HG2	1.86	0.58
1:G:1304:LEU:HB2	1:G:1541:PRO:HG2	1.86	0.58
1:A:258:ARG:NH1	1:A:316:LEU:O	2.36	0.58
1:E:3845:GLN:HG3	1:E:3923:GLU:HG3	1.85	0.58
1:A:62:LEU:HB3	1:A:276:ARG:HH21	1.68	0.58
1:A:4958:CYS:SG	1:A:4959:PHE:N	2.72	0.58
1:C:4862:ILE:HG23	1:E:4868:ILE:CD1	2.34	0.58
2:F:7:ILE:HB	2:F:71:ARG:HG3	1.86	0.58
1:G:62:LEU:HB3	1:G:276:ARG:HH21	1.68	0.58
1:G:2540:GLU:O	1:G:2543:ALA:HB3	2.03	0.58
1:A:778:MET:SD	1:A:1468:THR:OG1	2.62	0.58
1:A:1682:GLU:HG3	1:A:1782:PHE:HB2	1.85	0.58
2:B:7:ILE:HB	2:B:71:ARG:HG3	1.86	0.58
1:C:3939:SER:OG	1:C:3940:ARG:N	2.34	0.58
1:E:143:LEU:HD22	1:G:2427:LEU:CG	2.33	0.58
1:E:2897:LEU:HB3	1:E:2902:TYR:HB2	1.86	0.58
1:C:778:MET:SD	1:C:1468:THR:OG1	2.62	0.57
1:A:218:SER:OG	1:A:219:SER:N	2.37	0.57
1:E:1682:GLU:HG3	1:E:1782:PHE:HB2	1.85	0.57
1:G:2669:CYS:O	1:G:2672:ALA:HB3	2.04	0.57
2:H:90:VAL:HG23	2:H:91:ILE:HG12	1.86	0.57
1:A:2138:GLU:O	1:A:2141:LYS:NZ	2.34	0.57
1:A:2897:LEU:HB3	1:A:2902:TYR:HB2	1.86	0.57
1:C:1682:GLU:HG3	1:C:1782:PHE:HB2	1.85	0.57
1:E:778:MET:SD	1:E:1468:THR:OG1	2.62	0.57
1:E:1644:LEU:HD23	1:E:1651:LEU:HA	1.86	0.57
1:E:2138:GLU:O	1:E:2141:LYS:NZ	2.34	0.57
1:E:2669:CYS:O	1:E:2672:ALA:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3775:GLN:OE1	1:A:3852:ASN:ND2	2.38	0.57
1:C:3845:GLN:HG3	1:C:3923:GLU:HG3	1.85	0.57
1:E:1102:TYR:HB2	1:E:1165:MET:HG2	1.86	0.57
1:G:218:SER:OG	1:G:219:SER:N	2.37	0.57
1:G:676:GLU:HB2	1:G:803:LEU:HB2	1.87	0.57
1:G:805:GLY:HA2	1:G:810:GLU:HB2	1.85	0.57
1:G:3775:GLN:OE1	1:G:3852:ASN:ND2	2.38	0.57
1:A:1102:TYR:HB2	1:A:1165:MET:HG2	1.86	0.57
1:E:143:LEU:HD22	1:G:2427:LEU:HD13	1.58	0.57
1:E:143:LEU:HD11	1:E:207:PHE:CD2	2.40	0.57
1:E:805:GLY:HA2	1:E:810:GLU:HB2	1.85	0.57
1:C:766:ILE:HB	1:C:779:PHE:HB2	1.87	0.57
1:C:1104:GLU:HA	1:C:1163:GLY:HA2	1.87	0.57
1:C:2669:CYS:O	1:C:2672:ALA:HB3	2.04	0.57
2:D:90:VAL:HG23	2:D:91:ILE:HG12	1.86	0.57
1:G:778:MET:SD	1:G:1468:THR:OG1	2.62	0.57
1:A:1644:LEU:HD23	1:A:1651:LEU:HA	1.86	0.57
1:A:2669:CYS:O	1:A:2672:ALA:HB3	2.04	0.57
2:D:7:ILE:HB	2:D:71:ARG:HG3	1.86	0.57
1:E:3775:GLN:OE1	1:E:3852:ASN:ND2	2.38	0.57
1:G:1714:TYR:OH	1:G:1718:ARG:NH2	2.38	0.57
1:E:1104:GLU:HA	1:E:1163:GLY:HA2	1.87	0.57
1:G:1104:GLU:HA	1:G:1163:GLY:HA2	1.87	0.57
1:G:1736:ILE:HG22	1:G:1738:LEU:H	1.70	0.57
1:G:3667:GLN:HA	1:G:3670:LEU:HB2	1.87	0.57
1:A:766:ILE:HB	1:A:779:PHE:HB2	1.87	0.57
1:A:866:PRO:HG3	1:A:1009:ARG:HD2	1.86	0.57
1:A:1736:ILE:HG22	1:A:1738:LEU:H	1.70	0.57
1:E:4848:ASP:OD1	1:G:4823:ARG:NE	2.35	0.57
1:A:3667:GLN:HA	1:A:3670:LEU:HB2	1.87	0.57
1:A:4862:ILE:HG23	1:C:4868:ILE:CD1	2.34	0.57
1:C:676:GLU:HB2	1:C:803:LEU:HB2	1.87	0.57
1:C:1304:LEU:HB2	1:C:1541:PRO:HG2	1.86	0.57
1:C:2328:ARG:HH11	1:C:2328:ARG:HA	1.68	0.57
1:C:2897:LEU:HB3	1:C:2902:TYR:HB2	1.86	0.57
1:C:3775:GLN:OE1	1:C:3852:ASN:ND2	2.38	0.57
1:E:866:PRO:HG3	1:E:1009:ARG:HD2	1.86	0.57
1:E:1304:LEU:HB2	1:E:1541:PRO:HG2	1.86	0.57
2:H:7:ILE:HB	2:H:71:ARG:HG3	1.86	0.57
1:A:4897:ASP:OD1	1:A:4897:ASP:N	2.35	0.56
1:A:629:GLN:OE1	1:A:1669:ASN:ND2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:866:PRO:HG3	1:C:1009:ARG:HD2	1.86	0.56
1:G:629:GLN:OE1	1:G:1669:ASN:ND2	2.38	0.56
1:G:1682:GLU:HG3	1:G:1782:PHE:HB2	1.85	0.56
1:A:1104:GLU:HA	1:A:1163:GLY:HA2	1.87	0.56
1:C:143:LEU:HD22	1:E:2427:LEU:HD11	1.83	0.56
1:E:748:LEU:HD23	1:E:750:ARG:HG3	1.86	0.56
1:E:766:ILE:HB	1:E:779:PHE:HB2	1.87	0.56
1:E:1009:ARG:O	1:E:1013:ARG:NH2	2.39	0.56
1:G:1644:LEU:HD23	1:G:1651:LEU:HA	1.86	0.56
1:A:1009:ARG:O	1:A:1013:ARG:NH2	2.39	0.56
1:C:1111:GLY:H	1:C:1156:TRP:HZ2	1.54	0.56
1:E:3667:GLN:HA	1:E:3670:LEU:HB2	1.87	0.56
1:E:3729:GLN:O	1:E:3733:HIS:ND1	2.36	0.56
1:G:748:LEU:HD23	1:G:750:ARG:HG3	1.86	0.56
1:G:2897:LEU:HB3	1:G:2902:TYR:HB2	1.86	0.56
1:A:748:LEU:HD23	1:A:750:ARG:HG3	1.86	0.56
1:E:676:GLU:HB2	1:E:803:LEU:HB2	1.87	0.56
1:G:766:ILE:HB	1:G:779:PHE:HB2	1.87	0.56
1:E:1736:ILE:HG22	1:E:1738:LEU:H	1.70	0.56
1:G:1111:GLY:H	1:G:1156:TRP:HZ2	1.54	0.56
1:G:1425:THR:N	1:G:1510:VAL:O	2.39	0.56
1:A:4823:ARG:NE	1:G:4848:ASP:OD1	2.35	0.56
1:C:76:ARG:NE	1:E:3891:TRP:HB3	2.21	0.56
1:C:805:GLY:HA2	1:C:810:GLU:HB2	1.85	0.56
1:E:4862:ILE:HG23	1:G:4868:ILE:CD1	2.36	0.56
1:G:606:ARG:HH22	1:G:1632:ILE:HG23	1.70	0.56
1:G:866:PRO:HG3	1:G:1009:ARG:HD2	1.86	0.56
1:C:1714:TYR:OH	1:C:1718:ARG:NH2	2.38	0.56
2:F:90:VAL:HG23	2:F:91:ILE:HG12	1.86	0.56
1:G:3729:GLN:O	1:G:3733:HIS:ND1	2.36	0.56
1:A:1111:GLY:H	1:A:1156:TRP:HZ2	1.54	0.56
2:B:90:VAL:HG23	2:B:91:ILE:HG12	1.86	0.56
1:C:218:SER:OG	1:C:219:SER:N	2.37	0.56
1:E:218:SER:OG	1:E:219:SER:N	2.37	0.56
1:C:606:ARG:HH22	1:C:1632:ILE:HG23	1.70	0.56
1:C:3667:GLN:HA	1:C:3670:LEU:HB2	1.87	0.56
1:E:1429:SER:HA	1:E:1507:ILE:HG12	1.88	0.56
1:E:2436:VAL:O	1:E:2466:LYS:NZ	2.39	0.56
1:C:143:LEU:HD22	1:E:2427:LEU:CG	2.35	0.55
1:C:1009:ARG:O	1:C:1013:ARG:NH2	2.39	0.55
1:C:1429:SER:HA	1:C:1507:ILE:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1736:ILE:HG22	1:C:1738:LEU:H	1.70	0.55
1:A:993:GLU:OE1	1:A:1051:ARG:NH1	2.39	0.55
1:E:188:SER:OG	1:E:190:ARG:NH2	2.35	0.55
1:E:629:GLN:OE1	1:E:1669:ASN:ND2	2.38	0.55
1:E:3919:ASN:O	1:E:3922:THR:OG1	2.24	0.55
1:G:1009:ARG:O	1:G:1013:ARG:NH2	2.39	0.55
1:G:4897:ASP:OD1	1:G:4897:ASP:N	2.35	0.55
1:A:2712:ILE:O	1:A:2781:LYS:NZ	2.40	0.55
1:A:1144:ARG:NH2	1:A:1150:GLU:OE1	2.40	0.55
2:B:78:PRO:HD3	2:B:96:THR:HG22	1.88	0.55
1:E:624:ALA:HB2	1:E:1667:LEU:HD12	1.88	0.55
1:A:676:GLU:HB2	1:A:803:LEU:HB2	1.87	0.55
1:A:3804:LEU:HD13	1:A:3910:ALA:HB2	1.89	0.55
1:C:624:ALA:HB2	1:C:1667:LEU:HD12	1.88	0.55
2:D:78:PRO:HD3	2:D:96:THR:HG22	1.88	0.55
1:E:606:ARG:HH22	1:E:1632:ILE:HG23	1.70	0.55
1:G:679:VAL:HA	1:G:800:VAL:HG12	1.89	0.55
1:A:624:ALA:HB2	1:A:1667:LEU:HD12	1.88	0.55
1:C:748:LEU:HD23	1:C:750:ARG:HG3	1.86	0.55
1:C:3919:ASN:O	1:C:3922:THR:OG1	2.24	0.55
1:E:1425:THR:N	1:E:1510:VAL:O	2.39	0.55
1:G:4033:PHE:HA	1:G:4036:TYR:HB2	1.88	0.55
1:C:1220:ASP:O	1:C:1224:LEU:N	2.40	0.55
1:C:1425:THR:N	1:C:1510:VAL:O	2.39	0.55
1:A:679:VAL:HA	1:A:800:VAL:HG12	1.89	0.55
1:A:1220:ASP:O	1:A:1224:LEU:N	2.40	0.55
1:C:629:GLN:OE1	1:C:1669:ASN:ND2	2.38	0.55
1:E:993:GLU:OE1	1:E:1051:ARG:NH1	2.39	0.55
1:E:4900:ASP:O	1:E:4902:VAL:N	2.39	0.55
1:G:2712:ILE:O	1:G:2781:LYS:NZ	2.40	0.55
1:G:3804:LEU:HD13	1:G:3910:ALA:HB2	1.89	0.55
1:G:4900:ASP:O	1:G:4902:VAL:N	2.39	0.55
1:A:606:ARG:HH22	1:A:1632:ILE:HG23	1.70	0.55
1:A:1425:THR:N	1:A:1510:VAL:O	2.39	0.55
1:A:4033:PHE:HA	1:A:4036:TYR:HB2	1.88	0.55
1:C:1144:ARG:NH2	1:C:1150:GLU:OE1	2.40	0.55
1:A:1714:TYR:OH	1:A:1718:ARG:NH2	2.38	0.55
1:C:2436:VAL:O	1:C:2466:LYS:NZ	2.39	0.55
1:A:1429:SER:HA	1:A:1507:ILE:HG12	1.88	0.54
1:C:76:ARG:CD	1:E:3891:TRP:CD2	2.83	0.54
1:C:849:ASP:OD2	1:C:1214:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4033:PHE:HA	1:C:4036:TYR:HB2	1.88	0.54
1:C:4823:ARG:CZ	1:C:4823:ARG:CB	2.85	0.54
1:E:1220:ASP:O	1:E:1224:LEU:N	2.40	0.54
1:E:2712:ILE:O	1:E:2781:LYS:NZ	2.40	0.54
1:G:624:ALA:HB2	1:G:1667:LEU:HD12	1.88	0.54
2:H:78:PRO:HD3	2:H:96:THR:HG22	1.88	0.54
1:A:849:ASP:OD2	1:A:1214:ARG:NH2	2.40	0.54
1:E:1111:GLY:H	1:E:1156:TRP:HZ2	1.54	0.54
1:E:2553:VAL:O	1:E:2605:LYS:N	2.41	0.54
1:C:4900:ASP:O	1:C:4902:VAL:N	2.39	0.54
1:C:4630:GLN:OE1	1:C:4633:ARG:NH2	2.41	0.54
1:E:1714:TYR:OH	1:E:1718:ARG:NH2	2.38	0.54
1:E:2328:ARG:HA	1:E:2328:ARG:NH1	2.22	0.54
1:E:4630:GLN:OE1	1:E:4633:ARG:NH2	2.41	0.54
1:A:848:ARG:HD2	1:A:1603:PHE:HE2	1.73	0.54
1:E:4033:PHE:HA	1:E:4036:TYR:HB2	1.88	0.54
1:G:1144:ARG:NH2	1:G:1150:GLU:OE1	2.40	0.54
1:G:1429:SER:HA	1:G:1507:ILE:HG12	1.88	0.54
1:G:3803:VAL:HG13	1:G:3885:SER:HB2	1.90	0.54
1:A:3919:ASN:O	1:A:3922:THR:OG1	2.24	0.54
1:E:1144:ARG:NH2	1:E:1150:GLU:OE1	2.40	0.54
1:E:3803:VAL:HG13	1:E:3885:SER:HB2	1.90	0.54
1:E:4515:ASN:ND2	1:E:4740:PHE:O	2.33	0.54
1:A:4515:ASN:ND2	1:A:4740:PHE:O	2.33	0.54
1:C:993:GLU:OE1	1:C:1051:ARG:NH1	2.39	0.54
1:C:2553:VAL:O	1:C:2605:LYS:N	2.41	0.54
1:G:993:GLU:OE1	1:G:1051:ARG:NH1	2.39	0.54
1:C:1678:SER:OG	2:D:36:PHE:O	2.24	0.54
2:F:78:PRO:HD3	2:F:96:THR:HG22	1.88	0.54
1:G:2307:VAL:HG11	1:G:2321:VAL:HG21	1.90	0.54
1:A:1256:PRO:HB3	1:A:1597:SER:HA	1.90	0.54
1:A:4823:ARG:CZ	1:A:4823:ARG:CB	2.85	0.54
1:C:679:VAL:HA	1:C:800:VAL:HG12	1.89	0.54
1:C:1305:SER:OG	1:C:1306:MET:N	2.41	0.54
1:C:2324:LEU:N	1:C:2324:LEU:HD23	2.22	0.54
1:C:2593:LEU:O	1:C:2597:VAL:N	2.41	0.54
1:E:679:VAL:HA	1:E:800:VAL:HG12	1.89	0.54
1:E:4897:ASP:N	1:E:4897:ASP:OD1	2.35	0.54
1:G:4823:ARG:CZ	1:G:4823:ARG:CB	2.85	0.54
1:A:185:SER:HG	1:A:190:ARG:H	1.56	0.53
1:A:2425:ARG:NH2	1:A:2476:VAL:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1939:ASP:OD1	1:C:1939:ASP:N	2.40	0.53
1:G:1256:PRO:HB3	1:G:1597:SER:HA	1.90	0.53
1:A:2553:VAL:O	1:A:2605:LYS:N	2.41	0.53
1:C:2712:ILE:O	1:C:2781:LYS:NZ	2.40	0.53
1:C:3733:HIS:O	1:C:3777:LYS:NZ	2.41	0.53
1:E:4032:THR:OG1	1:E:4056:HIS:NE2	2.39	0.53
1:G:2425:ARG:NH2	1:G:2476:VAL:O	2.42	0.53
1:G:2593:LEU:O	1:G:2597:VAL:N	2.41	0.53
1:A:4797:SER:OG	1:A:4805:MET:N	2.40	0.53
1:C:753:ASP:HB2	1:C:770:ILE:HD11	1.90	0.53
1:G:2553:VAL:O	1:G:2605:LYS:N	2.41	0.53
1:G:4630:GLN:OE1	1:G:4633:ARG:NH2	2.41	0.53
1:A:2307:VAL:HG11	1:A:2321:VAL:HG21	1.90	0.53
1:A:2782:THR:OG1	1:A:2848:ASN:ND2	2.42	0.53
1:A:4804:ASP:OD1	1:A:4804:ASP:N	2.41	0.53
1:A:4900:ASP:O	1:A:4902:VAL:N	2.39	0.53
1:E:3804:LEU:HD13	1:E:3910:ALA:HB2	1.89	0.53
1:G:1220:ASP:O	1:G:1224:LEU:N	2.40	0.53
1:G:1305:SER:OG	1:G:1306:MET:N	2.41	0.53
1:E:849:ASP:OD2	1:E:1214:ARG:NH2	2.40	0.53
1:E:2425:ARG:NH2	1:E:2476:VAL:O	2.42	0.53
1:E:3733:HIS:O	1:E:3777:LYS:NZ	2.41	0.53
1:G:527:LYS:NZ	1:G:566:GLU:O	2.41	0.53
1:A:3803:VAL:HG13	1:A:3885:SER:HB2	1.90	0.53
1:C:1256:PRO:HB3	1:C:1597:SER:HA	1.90	0.53
1:C:2275:LEU:HB2	1:C:2293:PRO:HG3	1.91	0.53
1:C:3804:LEU:HD13	1:C:3910:ALA:HB2	1.89	0.53
1:C:4725:TRP:HA	1:C:4728:THR:HG22	1.91	0.53
1:G:2275:LEU:HB2	1:G:2293:PRO:HG3	1.91	0.53
1:G:3733:HIS:O	1:G:3777:LYS:NZ	2.41	0.53
1:A:4868:ILE:CD1	1:G:4862:ILE:HG23	2.35	0.53
1:A:4926:LEU:HD13	1:A:4942:TRP:HB2	1.91	0.53
1:G:849:ASP:OD2	1:G:1214:ARG:NH2	2.40	0.53
1:A:752:ASP:N	1:A:752:ASP:OD1	2.41	0.53
1:A:4630:GLN:OE1	1:A:4633:ARG:NH2	2.41	0.53
2:B:26:TYR:N	2:B:39:SER:OG	2.41	0.53
1:C:2323:ARG:HH21	1:C:2323:ARG:CG	2.14	0.53
2:D:31:GLN:NE2	2:D:96:THR:OG1	2.42	0.53
1:E:848:ARG:HD2	1:E:1603:PHE:HE2	1.72	0.53
1:E:4725:TRP:HA	1:E:4728:THR:HG22	1.91	0.53
1:E:4797:SER:OG	1:E:4805:MET:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2593:LEU:O	1:A:2597:VAL:N	2.41	0.53
2:B:31:GLN:NE2	2:B:96:THR:OG1	2.42	0.53
1:C:2425:ARG:NH2	1:C:2476:VAL:O	2.42	0.53
1:C:3803:VAL:HG13	1:C:3885:SER:HB2	1.90	0.53
1:E:1256:PRO:HB3	1:E:1597:SER:HA	1.90	0.53
1:E:1738:LEU:HG	1:E:1925:ALA:HB1	1.90	0.53
1:E:3940:ARG:HG2	1:E:3943:ASP:HB2	1.91	0.53
1:E:4926:LEU:HD13	1:E:4942:TRP:HB2	1.91	0.53
1:G:753:ASP:HB2	1:G:770:ILE:HD11	1.90	0.53
1:G:2782:THR:OG1	1:G:2848:ASN:ND2	2.42	0.53
1:A:672:LYS:N	1:A:819:TYR:O	2.42	0.53
1:A:703:TYR:HA	1:A:1255:LEU:HD21	1.91	0.53
1:C:1738:LEU:HG	1:C:1925:ALA:HB1	1.90	0.53
1:C:1932:ASP:OD1	1:C:1932:ASP:N	2.35	0.53
1:C:2328:ARG:HA	1:C:2328:ARG:NH1	2.24	0.53
1:E:703:TYR:HA	1:E:1255:LEU:HD21	1.91	0.53
1:E:1305:SER:OG	1:E:1306:MET:N	2.41	0.53
1:E:2593:LEU:O	1:E:2597:VAL:N	2.41	0.53
1:E:4845:ILE:HD12	1:G:4819:TYR:HD1	1.55	0.53
1:G:1738:LEU:HG	1:G:1925:ALA:HB1	1.90	0.53
2:H:31:GLN:NE2	2:H:96:THR:OG1	2.42	0.53
1:A:742:SER:OG	1:A:743:SER:N	2.42	0.52
1:A:753:ASP:HB2	1:A:770:ILE:HD11	1.90	0.52
1:A:1738:LEU:HG	1:A:1925:ALA:HB1	1.90	0.52
1:A:2275:LEU:HB2	1:A:2293:PRO:HG3	1.91	0.52
1:A:3729:GLN:O	1:A:3733:HIS:ND1	2.36	0.52
1:A:3733:HIS:O	1:A:3777:LYS:NZ	2.41	0.52
1:C:848:ARG:HD2	1:C:1603:PHE:HE2	1.73	0.52
1:E:2275:LEU:HB2	1:E:2293:PRO:HG3	1.91	0.52
1:E:4065:GLU:HA	1:E:4068:LEU:HB2	1.92	0.52
1:A:1305:SER:OG	1:A:1306:MET:N	2.41	0.52
1:C:703:TYR:HA	1:C:1255:LEU:HD21	1.91	0.52
1:C:2782:THR:OG1	1:C:2848:ASN:ND2	2.42	0.52
1:C:4804:ASP:OD1	1:C:4804:ASP:N	2.41	0.52
1:E:527:LYS:NZ	1:E:566:GLU:O	2.41	0.52
1:E:672:LYS:N	1:E:819:TYR:O	2.42	0.52
1:E:1310:CYS:HB2	1:E:1536:SER:HA	1.91	0.52
1:E:2782:THR:OG1	1:E:2848:ASN:ND2	2.42	0.52
1:G:185:SER:HG	1:G:190:ARG:H	1.54	0.52
1:G:703:TYR:HA	1:G:1255:LEU:HD21	1.91	0.52
1:G:848:ARG:HD2	1:G:1603:PHE:HE2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4032:THR:OG1	1:G:4056:HIS:NE2	2.39	0.52
1:G:4926:LEU:HD13	1:G:4942:TRP:HB2	1.91	0.52
1:A:1310:CYS:HB2	1:A:1536:SER:HA	1.91	0.52
1:C:76:ARG:HD3	1:E:3891:TRP:CE2	2.44	0.52
1:C:204:ASP:N	1:C:204:ASP:OD1	2.43	0.52
1:C:1199:ASP:OD2	1:C:1199:ASP:N	2.37	0.52
1:E:143:LEU:HD11	1:E:207:PHE:HD2	1.73	0.52
1:A:1426:TYR:HD2	1:A:1574:GLU:HB2	1.75	0.52
1:A:4065:GLU:HA	1:A:4068:LEU:HB2	1.92	0.52
1:C:3729:GLN:O	1:C:3733:HIS:ND1	2.36	0.52
1:E:752:ASP:OD1	1:E:752:ASP:N	2.41	0.52
1:E:2257:ALA:O	1:E:2259:ARG:NH1	2.43	0.52
2:F:31:GLN:NE2	2:F:96:THR:OG1	2.42	0.52
1:G:3940:ARG:HG2	1:G:3943:ASP:HB2	1.91	0.52
1:A:2436:VAL:O	1:A:2466:LYS:NZ	2.39	0.52
1:E:4804:ASP:N	1:E:4804:ASP:OD1	2.41	0.52
1:G:188:SER:OG	1:G:190:ARG:NH2	2.35	0.52
1:G:565:LEU:HD13	1:G:604:HIS:HE1	1.75	0.52
1:A:3683:LEU:HD22	1:A:3748:SER:HB3	1.92	0.52
1:A:3871:ILE:O	1:A:3875:THR:N	2.42	0.52
1:A:4032:THR:OG1	1:A:4056:HIS:NE2	2.39	0.52
1:C:2328:ARG:CG	1:C:2328:ARG:NH1	2.73	0.52
1:C:3940:ARG:HG2	1:C:3943:ASP:HB2	1.91	0.52
1:C:4823:ARG:HB2	1:C:4823:ARG:HH21	1.71	0.52
1:E:797:GLY:HA2	1:E:1622:LEU:HA	1.92	0.52
1:E:2328:ARG:CG	1:E:2328:ARG:NH1	2.73	0.52
1:G:2436:VAL:O	1:G:2466:LYS:NZ	2.39	0.52
1:C:565:LEU:HD13	1:C:604:HIS:HE1	1.75	0.52
1:C:752:ASP:N	1:C:752:ASP:OD1	2.41	0.52
1:C:3683:LEU:HD22	1:C:3748:SER:HB3	1.92	0.52
1:C:4926:LEU:HD13	1:C:4942:TRP:HB2	1.91	0.52
1:E:4052:ALA:O	1:E:4056:HIS:ND1	2.38	0.52
1:A:4725:TRP:HA	1:A:4728:THR:HG22	1.91	0.52
1:C:2257:ALA:O	1:C:2259:ARG:NH1	2.43	0.52
1:C:4844:ARG:NH2	1:E:4819:TYR:OH	2.43	0.52
1:E:1426:TYR:HD2	1:E:1574:GLU:HB2	1.75	0.52
1:G:3973:MET:HB3	1:G:4095:ILE:HG12	1.92	0.52
1:A:2257:ALA:O	1:A:2259:ARG:NH1	2.43	0.52
1:C:1310:CYS:HB2	1:C:1536:SER:HA	1.91	0.52
1:E:753:ASP:HB2	1:E:770:ILE:HD11	1.90	0.52
1:E:3683:LEU:HD22	1:E:3748:SER:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:742:SER:OG	1:G:743:SER:N	2.42	0.52
1:G:1426:TYR:HD2	1:G:1574:GLU:HB2	1.75	0.52
1:G:4725:TRP:HA	1:G:4728:THR:HG22	1.91	0.52
1:A:204:ASP:OD1	1:A:204:ASP:N	2.43	0.52
1:A:3973:MET:HB3	1:A:4095:ILE:HG12	1.92	0.52
1:E:833:LYS:HA	1:E:1614:ARG:HH12	1.75	0.52
1:E:3956:GLN:NE2	1:E:3973:MET:SD	2.83	0.52
1:E:4823:ARG:HB3	1:E:4823:ARG:HH21	1.74	0.52
2:F:26:TYR:N	2:F:39:SER:OG	2.41	0.52
1:A:3956:GLN:NE2	1:A:3973:MET:SD	2.83	0.51
1:C:188:SER:OG	1:C:190:ARG:NH2	2.35	0.51
1:C:797:GLY:HA2	1:C:1622:LEU:HA	1.92	0.51
1:C:1265:HIS:CD2	1:C:1267:HIS:H	2.28	0.51
1:C:1426:TYR:HD2	1:C:1574:GLU:HB2	1.75	0.51
1:E:742:SER:OG	1:E:743:SER:N	2.42	0.51
1:E:4823:ARG:NH2	1:E:4823:ARG:CB	2.73	0.51
1:E:4823:ARG:CZ	1:E:4823:ARG:HB2	2.40	0.51
1:G:204:ASP:OD1	1:G:204:ASP:N	2.43	0.51
1:G:1642:LEU:O	1:G:1645:THR:OG1	2.26	0.51
1:C:527:LYS:NZ	1:C:566:GLU:O	2.41	0.51
1:C:694:ARG:NH1	1:C:716:ASN:O	2.41	0.51
1:C:1904:LYS:HD2	1:C:2081:LEU:HD21	1.93	0.51
1:C:3956:GLN:NE2	1:C:3973:MET:SD	2.83	0.51
1:E:271:ALA:O	1:E:301:THR:OG1	2.25	0.51
1:E:565:LEU:HD13	1:E:604:HIS:HE1	1.75	0.51
1:E:4823:ARG:CZ	1:E:4823:ARG:CB	2.88	0.51
1:G:3956:GLN:NE2	1:G:3973:MET:SD	2.83	0.51
1:C:742:SER:OG	1:C:743:SER:N	2.42	0.51
1:C:767:SER:HA	1:C:777:GLY:HA3	1.92	0.51
1:C:1431:ARG:HE	1:C:1505:LEU:HD21	1.76	0.51
1:C:1756:SER:OG	1:C:1757:LEU:N	2.44	0.51
1:C:1847:GLU:OE1	1:C:1849:SER:OG	2.29	0.51
2:D:26:TYR:N	2:D:39:SER:OG	2.41	0.51
1:G:833:LYS:HA	1:G:1614:ARG:HH12	1.75	0.51
1:G:2257:ALA:O	1:G:2259:ARG:NH1	2.43	0.51
1:A:343:ARG:NH2	1:A:345:GLU:O	2.44	0.51
1:A:661:LEU:O	1:A:788:PHE:N	2.43	0.51
1:A:3940:ARG:HG2	1:A:3943:ASP:HB2	1.91	0.51
1:C:661:LEU:O	1:C:788:PHE:N	2.43	0.51
1:E:1847:GLU:OE1	1:E:1849:SER:OG	2.28	0.51
1:G:1589:GLN:NE2	1:G:1634:GLU:OE1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:SER:HG	1:C:190:ARG:H	1.56	0.51
1:C:904:TYR:HD1	1:C:918:LEU:HB2	1.76	0.51
1:C:3973:MET:HB3	1:C:4095:ILE:HG12	1.92	0.51
1:C:4065:GLU:HA	1:C:4068:LEU:HB2	1.92	0.51
1:E:694:ARG:NH1	1:E:716:ASN:O	2.41	0.51
1:E:1589:GLN:NE2	1:E:1634:GLU:OE1	2.43	0.51
1:G:4804:ASP:N	1:G:4804:ASP:OD1	2.41	0.51
1:A:693:LEU:HD22	1:A:798:ILE:HD13	1.93	0.51
1:A:904:TYR:HD1	1:A:918:LEU:HB2	1.76	0.51
1:C:209:GLN:NE2	1:E:2327:ARG:NH1	2.54	0.51
1:C:271:ALA:O	1:C:301:THR:OG1	2.25	0.51
1:C:693:LEU:HD22	1:C:798:ILE:HD13	1.93	0.51
1:C:833:LYS:HA	1:C:1614:ARG:HH12	1.75	0.51
1:C:887:GLU:HA	1:C:921:PHE:HB3	1.93	0.51
1:C:1589:GLN:NE2	1:C:1634:GLU:OE1	2.43	0.51
1:E:185:SER:HG	1:E:190:ARG:H	1.55	0.51
1:G:672:LYS:N	1:G:819:TYR:O	2.42	0.51
1:A:767:SER:HA	1:A:777:GLY:HA3	1.92	0.51
1:C:343:ARG:NH2	1:C:345:GLU:O	2.44	0.51
1:E:887:GLU:HA	1:E:921:PHE:HB3	1.93	0.51
1:E:3973:MET:HB3	1:E:4095:ILE:HG12	1.92	0.51
1:G:752:ASP:OD1	1:G:752:ASP:N	2.41	0.51
1:G:1310:CYS:HB2	1:G:1536:SER:HA	1.91	0.51
1:G:3683:LEU:HD22	1:G:3748:SER:HB3	1.92	0.51
1:A:143:LEU:HD22	1:C:2427:LEU:HD21	1.91	0.51
1:C:1718:ARG:HH12	1:C:1758:ARG:HD3	1.76	0.51
1:E:343:ARG:NH2	1:E:345:GLU:O	2.44	0.51
1:E:1431:ARG:HE	1:E:1505:LEU:HD21	1.76	0.51
1:G:887:GLU:HA	1:G:921:PHE:HB3	1.93	0.51
1:G:1556:GLU:O	1:G:1572:LYS:NZ	2.44	0.51
1:A:797:GLY:HA2	1:A:1622:LEU:HA	1.92	0.51
1:A:1589:GLN:NE2	1:A:1634:GLU:OE1	2.43	0.51
1:A:1756:SER:OG	1:A:1757:LEU:N	2.44	0.51
1:E:3683:LEU:HD23	1:E:3755:MET:HG2	1.93	0.51
1:A:1718:ARG:HH12	1:A:1758:ARG:HD3	1.76	0.51
1:E:767:SER:HA	1:E:777:GLY:HA3	1.92	0.51
1:E:2328:ARG:CA	1:E:2328:ARG:NH1	2.73	0.51
1:G:645:GLN:HE22	2:H:34:LYS:HB3	1.76	0.51
1:G:904:TYR:HD1	1:G:918:LEU:HB2	1.76	0.51
1:A:565:LEU:HD13	1:A:604:HIS:HE1	1.75	0.50
1:A:887:GLU:HA	1:A:921:PHE:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1556:GLU:O	1:A:1572:LYS:NZ	2.44	0.50
1:A:1904:LYS:HD2	1:A:2081:LEU:HD21	1.93	0.50
1:C:645:GLN:HE22	2:D:34:LYS:HB3	1.76	0.50
1:C:2314:VAL:HG23	1:C:2314:VAL:O	2.11	0.50
1:E:645:GLN:HE22	2:F:34:LYS:HB3	1.76	0.50
1:E:1712:SER:O	1:E:1712:SER:OG	2.29	0.50
1:G:1718:ARG:HH12	1:G:1758:ARG:HD3	1.76	0.50
1:G:1769:VAL:HG12	2:H:55:VAL:HG23	1.94	0.50
1:G:4065:GLU:HA	1:G:4068:LEU:HB2	1.92	0.50
1:A:645:GLN:HE22	2:B:34:LYS:HB3	1.76	0.50
1:A:694:ARG:NH1	1:A:716:ASN:O	2.41	0.50
1:A:4844:ARG:NH2	1:C:4819:TYR:OH	2.44	0.50
1:C:620:CYS:SG	1:C:621:HIS:N	2.74	0.50
1:G:1763:PHE:HB3	1:G:1781:GLU:HB2	1.93	0.50
1:A:1712:SER:O	1:A:1712:SER:OG	2.29	0.50
1:A:1769:VAL:HG12	2:B:55:VAL:HG23	1.94	0.50
1:A:4094:ASP:OD1	1:A:4094:ASP:N	2.44	0.50
1:E:473:GLU:O	1:E:477:ASN:ND2	2.45	0.50
1:E:1763:PHE:HB3	1:E:1781:GLU:HB2	1.94	0.50
1:E:4094:ASP:N	1:E:4094:ASP:OD1	2.44	0.50
1:G:1678:SER:OG	2:H:36:PHE:O	2.24	0.50
1:A:1431:ARG:HE	1:A:1505:LEU:HD21	1.76	0.50
1:A:4819:TYR:OH	1:G:4844:ARG:NH2	2.45	0.50
1:C:2433:LEU:HA	1:C:2436:VAL:HG12	1.93	0.50
1:E:4663:GLY:H	1:E:4666:ARG:HD3	1.77	0.50
1:G:473:GLU:O	1:G:477:ASN:ND2	2.45	0.50
1:G:797:GLY:HA2	1:G:1622:LEU:HA	1.92	0.50
1:G:1756:SER:OG	1:G:1757:LEU:N	2.44	0.50
1:A:833:LYS:HA	1:A:1614:ARG:HH12	1.75	0.50
1:A:1847:GLU:OE1	1:A:1849:SER:OG	2.29	0.50
1:A:2464:ASP:OD1	1:A:2464:ASP:N	2.44	0.50
1:E:1769:VAL:HG12	2:F:55:VAL:HG23	1.94	0.50
1:E:3729:GLN:OE1	1:E:3771:ASN:ND2	2.45	0.50
2:H:71:ARG:NH2	2:H:100:ASP:OD2	2.43	0.50
1:A:76:ARG:HG2	1:C:3891:TRP:CD2	2.47	0.50
1:A:527:LYS:NZ	1:A:566:GLU:O	2.41	0.50
1:C:473:GLU:O	1:C:477:ASN:ND2	2.45	0.50
1:C:3683:LEU:HD23	1:C:3755:MET:HG2	1.93	0.50
1:C:4032:THR:OG1	1:C:4056:HIS:NE2	2.39	0.50
1:E:693:LEU:HD22	1:E:798:ILE:HD13	1.93	0.50
1:E:904:TYR:HD1	1:E:918:LEU:HB2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1265:HIS:CD2	1:E:1267:HIS:H	2.28	0.50
1:E:2026:ILE:HA	1:E:2029:ARG:HH11	1.76	0.50
1:A:1939:ASP:O	1:A:1943:PHE:N	2.45	0.50
1:A:4858:ILE:HD12	1:C:4867:ILE:CG2	2.26	0.50
1:C:4845:ILE:HD12	1:E:4819:TYR:HD1	1.55	0.50
1:E:2433:LEU:HA	1:E:2436:VAL:HG12	1.93	0.50
1:G:343:ARG:NH2	1:G:345:GLU:O	2.44	0.50
1:G:767:SER:HA	1:G:777:GLY:HA3	1.92	0.50
1:G:4663:GLY:H	1:G:4666:ARG:HD3	1.77	0.50
1:A:473:GLU:O	1:A:477:ASN:ND2	2.45	0.50
1:C:1642:LEU:O	1:C:1645:THR:OG1	2.26	0.50
1:C:2849:TYR:HA	1:C:2852:ILE:HG22	1.94	0.50
1:C:4663:GLY:H	1:C:4666:ARG:HD3	1.77	0.50
1:E:1556:GLU:O	1:E:1572:LYS:NZ	2.44	0.50
1:E:1718:ARG:HH12	1:E:1758:ARG:HD3	1.76	0.50
1:E:2316:GLU:HG2	1:E:3811:ARG:NH2	2.27	0.50
1:E:4844:ARG:NH2	1:G:4819:TYR:OH	2.45	0.50
1:G:271:ALA:O	1:G:301:THR:OG1	2.25	0.50
1:G:1431:ARG:HE	1:G:1505:LEU:HD21	1.76	0.50
1:G:1847:GLU:OE1	1:G:1849:SER:OG	2.29	0.50
1:G:3919:ASN:O	1:G:3922:THR:OG1	2.24	0.50
1:A:1548:THR:OG1	1:A:1549:SER:N	2.45	0.50
1:A:2026:ILE:HA	1:A:2029:ARG:HH11	1.76	0.50
1:A:4770:LEU:O	1:C:4754:LEU:HD21	2.12	0.50
1:E:1939:ASP:O	1:E:1943:PHE:N	2.45	0.50
1:G:694:ARG:NH1	1:G:716:ASN:O	2.41	0.50
1:G:2026:ILE:HA	1:G:2029:ARG:HH11	1.76	0.50
1:G:3683:LEU:HD23	1:G:3755:MET:HG2	1.93	0.50
1:A:4028:THR:HA	1:A:4033:PHE:HD2	1.77	0.49
1:A:4823:ARG:HB2	1:A:4823:ARG:HH21	1.72	0.49
1:C:1556:GLU:O	1:C:1572:LYS:NZ	2.44	0.49
1:C:1769:VAL:HG12	2:D:55:VAL:HG23	1.94	0.49
1:C:2725:TYR:OH	1:C:2892:ASP:OD1	2.30	0.49
1:G:335:LYS:NZ	1:G:398:HIS:O	2.37	0.49
1:G:4028:THR:HA	1:G:4033:PHE:HD2	1.77	0.49
1:A:3800:SER:OG	1:A:3801:CYS:N	2.45	0.49
1:C:2328:ARG:CA	1:C:2328:ARG:NH1	2.73	0.49
1:E:204:ASP:N	1:E:204:ASP:OD1	2.43	0.49
1:G:693:LEU:HD22	1:G:798:ILE:HD13	1.93	0.49
1:G:1904:LYS:HD2	1:G:2081:LEU:HD21	1.93	0.49
1:E:1904:LYS:HD2	1:E:2081:LEU:HD21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2725:TYR:OH	1:E:2892:ASP:OD1	2.30	0.49
1:G:2725:TYR:OH	1:G:2892:ASP:OD1	2.30	0.49
2:H:26:TYR:N	2:H:39:SER:OG	2.41	0.49
1:A:2433:LEU:HA	1:A:2436:VAL:HG12	1.94	0.49
1:C:992:GLN:HB3	1:C:1064:LEU:HD12	1.95	0.49
1:G:1755:THR:O	1:G:1755:THR:OG1	2.29	0.49
1:A:1763:PHE:HB3	1:A:1781:GLU:HB2	1.93	0.49
1:A:2849:TYR:HA	1:A:2852:ILE:HG22	1.94	0.49
1:C:4028:THR:HA	1:C:4033:PHE:HD2	1.77	0.49
1:E:1678:SER:OG	2:F:36:PHE:O	2.24	0.49
1:G:3871:ILE:O	1:G:3875:THR:N	2.42	0.49
1:G:4094:ASP:OD1	1:G:4094:ASP:N	2.44	0.49
1:A:156:GLU:HB3	1:A:186:VAL:HG12	1.95	0.49
1:A:671:LYS:N	1:A:819:TYR:O	2.46	0.49
1:A:1106:GLU:OE2	1:A:1214:ARG:NH1	2.46	0.49
1:A:2725:TYR:OH	1:A:2892:ASP:OD1	2.30	0.49
1:A:4663:GLY:H	1:A:4666:ARG:HD3	1.77	0.49
1:C:530:LEU:HA	1:C:533:LEU:HD12	1.95	0.49
1:C:2026:ILE:HA	1:C:2029:ARG:HH11	1.76	0.49
1:E:651:HIS:HD2	1:E:1625:LEU:HB3	1.78	0.49
2:F:71:ARG:NH2	2:F:100:ASP:OD2	2.43	0.49
1:A:530:LEU:HA	1:A:533:LEU:HD12	1.95	0.49
1:C:35:LEU:HB3	1:C:49:LEU:HD22	1.95	0.49
1:C:651:HIS:HD2	1:C:1625:LEU:HB3	1.78	0.49
1:C:1106:GLU:OE2	1:C:1214:ARG:NH1	2.46	0.49
1:C:1763:PHE:HB3	1:C:1781:GLU:HB2	1.93	0.49
1:C:1939:ASP:O	1:C:1943:PHE:N	2.45	0.49
1:C:2315:GLU:HA	1:C:2315:GLU:OE2	2.11	0.49
1:C:4026:ASP:HA	1:C:4029:SER:HB3	1.94	0.49
1:E:620:CYS:HG	1:E:621:HIS:H	1.59	0.49
1:E:992:GLN:HB3	1:E:1064:LEU:HD12	1.95	0.49
1:E:1106:GLU:OE2	1:E:1214:ARG:NH1	2.46	0.49
1:E:1548:THR:OG1	1:E:1549:SER:N	2.45	0.49
1:E:2156:PHE:HA	1:E:2163:MET:HE3	1.95	0.49
1:G:156:GLU:HB3	1:G:186:VAL:HG12	1.95	0.49
1:G:1548:THR:OG1	1:G:1549:SER:N	2.45	0.49
1:A:1642:LEU:O	1:A:1645:THR:OG1	2.26	0.49
1:A:3729:GLN:OE1	1:A:3771:ASN:ND2	2.45	0.49
1:C:3729:GLN:OE1	1:C:3771:ASN:ND2	2.45	0.49
1:G:651:HIS:HD2	1:G:1625:LEU:HB3	1.78	0.49
1:A:2156:PHE:HA	1:A:2163:MET:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2156:PHE:HA	1:C:2163:MET:HE3	1.95	0.49
1:C:3871:ILE:O	1:C:3875:THR:N	2.42	0.49
1:C:4797:SER:OG	1:C:4805:MET:N	2.40	0.49
1:C:4858:ILE:HD12	1:E:4867:ILE:CG2	2.27	0.49
1:E:530:LEU:HA	1:E:533:LEU:HD12	1.95	0.49
1:E:1209:VAL:N	1:E:1211:GLN:OE1	2.46	0.49
1:E:4028:THR:HA	1:E:4033:PHE:HD2	1.77	0.49
1:G:2433:LEU:HA	1:G:2436:VAL:HG12	1.94	0.49
1:G:4797:SER:OG	1:G:4805:MET:N	2.40	0.49
1:A:1253:LYS:NZ	1:A:1257:GLN:OE1	2.46	0.49
1:A:3683:LEU:HD23	1:A:3755:MET:HG2	1.93	0.49
1:A:4754:LEU:HD21	1:G:4770:LEU:O	2.13	0.49
1:C:4848:ASP:OD1	1:E:4823:ARG:CZ	2.61	0.49
1:E:671:LYS:N	1:E:819:TYR:O	2.46	0.49
1:E:2849:TYR:HA	1:E:2852:ILE:HG22	1.94	0.49
1:E:4026:ASP:HA	1:E:4029:SER:HB3	1.94	0.49
1:E:4174:ILE:HD13	1:E:4885:MET:HE1	1.95	0.49
1:A:1209:VAL:N	1:A:1211:GLN:OE1	2.46	0.48
1:A:4174:ILE:HD13	1:A:4885:MET:HE1	1.95	0.48
1:E:2314:VAL:HG23	1:E:2314:VAL:O	2.12	0.48
1:G:1265:HIS:CD2	1:G:1267:HIS:H	2.28	0.48
1:G:2156:PHE:HA	1:G:2163:MET:HE3	1.95	0.48
1:G:4026:ASP:HA	1:G:4029:SER:HB3	1.94	0.48
1:A:35:LEU:HB3	1:A:49:LEU:HD22	1.95	0.48
1:A:651:HIS:HD2	1:A:1625:LEU:HB3	1.78	0.48
1:E:1199:ASP:OD2	1:E:1199:ASP:N	2.37	0.48
1:G:1106:GLU:OE2	1:G:1214:ARG:NH1	2.46	0.48
1:A:1199:ASP:OD2	1:A:1199:ASP:N	2.37	0.48
1:A:4026:ASP:HA	1:A:4029:SER:HB3	1.94	0.48
1:C:671:LYS:N	1:C:819:TYR:O	2.46	0.48
1:C:2328:ARG:CB	1:C:2329:PRO:CD	2.91	0.48
1:E:306:LEU:O	1:E:327:THR:OG1	2.27	0.48
1:C:1209:VAL:N	1:C:1211:GLN:OE1	2.46	0.48
1:C:3800:SER:OG	1:C:3801:CYS:N	2.45	0.48
1:A:892:LEU:HD13	1:A:1052:GLU:HG3	1.95	0.48
1:C:517:VAL:HG23	1:C:520:ARG:HE	1.79	0.48
1:E:35:LEU:HB3	1:E:49:LEU:HD22	1.95	0.48
1:G:1209:VAL:N	1:G:1211:GLN:OE1	2.46	0.48
1:G:3729:GLN:OE1	1:G:3771:ASN:ND2	2.45	0.48
1:A:4052:ALA:O	1:A:4056:HIS:ND1	2.38	0.48
1:C:156:GLU:HB3	1:C:186:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2737:LYS:HG3	1:C:2758:MET:HE1	1.96	0.48
1:E:3871:ILE:O	1:E:3875:THR:N	2.42	0.48
1:G:517:VAL:HG23	1:G:520:ARG:HE	1.79	0.48
1:G:671:LYS:N	1:G:819:TYR:O	2.46	0.48
1:G:3761:LYS:NZ	1:G:3835:GLU:OE2	2.42	0.48
1:A:517:VAL:HG23	1:A:520:ARG:HE	1.79	0.48
1:A:881:ILE:HD11	1:A:952:ILE:HD13	1.95	0.48
1:A:1932:ASP:OD1	1:A:1932:ASP:N	2.35	0.48
1:A:2737:LYS:HG3	1:A:2758:MET:HE1	1.96	0.48
1:C:797:GLY:CA	1:C:1621:CYS:O	2.59	0.48
1:C:4051:LYS:O	1:C:4055:SER:N	2.46	0.48
1:C:4094:ASP:N	1:C:4094:ASP:OD1	2.44	0.48
1:C:4757:ILE:O	1:C:4760:SER:OG	2.32	0.48
1:G:1253:LYS:NZ	1:G:1257:GLN:OE1	2.46	0.48
1:G:2213:LYS:HA	1:G:2254:LEU:HD21	1.95	0.48
1:G:4174:ILE:HD13	1:G:4885:MET:HE1	1.95	0.48
1:A:1265:HIS:CD2	1:A:1267:HIS:H	2.28	0.48
1:C:892:LEU:HD13	1:C:1052:GLU:HG3	1.94	0.48
1:C:2213:LYS:HA	1:C:2254:LEU:HD21	1.95	0.48
1:E:821:PRO:HG2	1:E:824:GLU:HG2	1.96	0.48
1:E:915:HIS:CE1	1:E:917:CYS:HB2	2.49	0.48
1:E:1426:TYR:HB3	1:E:1571:PHE:HA	1.96	0.48
1:G:35:LEU:HB3	1:G:49:LEU:HD22	1.95	0.48
1:G:2849:TYR:HA	1:G:2852:ILE:HG22	1.94	0.48
1:C:672:LYS:N	1:C:819:TYR:O	2.42	0.48
1:C:1426:TYR:HB3	1:C:1571:PHE:HA	1.96	0.48
1:E:1253:LYS:NZ	1:E:1257:GLN:OE1	2.46	0.48
1:E:3663:ASP:OD2	1:E:3735:ARG:NH2	2.47	0.48
1:G:881:ILE:HD11	1:G:952:ILE:HD13	1.95	0.48
1:A:271:ALA:O	1:A:301:THR:OG1	2.25	0.48
1:A:394:HIS:CD2	1:A:397:GLY:H	2.32	0.48
1:A:821:PRO:HG2	1:A:824:GLU:HG2	1.96	0.48
1:A:992:GLN:HB3	1:A:1064:LEU:HD12	1.95	0.48
1:A:1426:TYR:HB3	1:A:1571:PHE:HA	1.96	0.48
1:A:3663:ASP:OD2	1:A:3735:ARG:NH2	2.47	0.48
1:C:1253:LYS:NZ	1:C:1257:GLN:OE1	2.46	0.48
1:C:4174:ILE:HD13	1:C:4885:MET:HE1	1.95	0.48
1:G:1521:THR:HA	1:G:1526:ASP:HA	1.96	0.48
1:G:3663:ASP:OD2	1:G:3735:ARG:NH2	2.47	0.48
1:A:4754:LEU:HD21	1:G:4770:LEU:C	2.39	0.47
1:E:156:GLU:HB3	1:E:186:VAL:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1303:ARG:HH21	1:E:1595:LEU:HB2	1.79	0.47
1:E:1642:LEU:O	1:E:1645:THR:OG1	2.26	0.47
1:G:992:GLN:HB3	1:G:1064:LEU:HD12	1.95	0.47
1:G:1303:ARG:HH21	1:G:1595:LEU:HB2	1.79	0.47
1:G:1426:TYR:HB3	1:G:1571:PHE:HA	1.96	0.47
1:G:1694:MET:HE2	1:G:1694:MET:HB3	1.81	0.47
1:A:1521:THR:HA	1:A:1526:ASP:HA	1.96	0.47
2:B:71:ARG:NH2	2:B:100:ASP:OD2	2.43	0.47
1:E:517:VAL:HG23	1:E:520:ARG:HE	1.79	0.47
1:E:2213:LYS:HA	1:E:2254:LEU:HD21	1.95	0.47
1:E:4781:LEU:CD1	1:G:4741:ALA:O	2.62	0.47
1:G:530:LEU:HA	1:G:533:LEU:HD12	1.95	0.47
1:A:1930:SER:O	1:A:1930:SER:OG	2.31	0.47
1:A:1942:ARG:NH1	1:A:3609:LEU:H	2.13	0.47
1:A:3799:GLN:O	1:A:3881:ARG:NH2	2.48	0.47
1:A:4741:ALA:O	1:G:4781:LEU:CD1	2.62	0.47
1:A:4770:LEU:HB3	1:C:4754:LEU:CD1	2.44	0.47
1:C:1303:ARG:HH21	1:C:1595:LEU:HB2	1.79	0.47
1:C:3663:ASP:OD2	1:C:3735:ARG:NH2	2.47	0.47
1:C:3799:GLN:O	1:C:3881:ARG:NH2	2.48	0.47
1:G:23:GLN:HE21	1:G:34:LYS:HB3	1.80	0.47
1:C:3900:ASP:OD1	1:C:3900:ASP:N	2.47	0.47
1:G:394:HIS:CD2	1:G:397:GLY:H	2.32	0.47
1:G:4045:SER:HA	1:G:4078:THR:HG22	1.96	0.47
1:A:1303:ARG:HH21	1:A:1595:LEU:HB2	1.79	0.47
1:C:915:HIS:CE1	1:C:917:CYS:HB2	2.49	0.47
1:C:1942:ARG:NH1	1:C:3609:LEU:H	2.13	0.47
1:E:1118:SER:HB2	1:E:1204:VAL:HG11	1.96	0.47
1:E:1655:TYR:OH	1:E:1659:ARG:NH2	2.48	0.47
1:E:2737:LYS:HG3	1:E:2758:MET:HE1	1.96	0.47
1:E:3642:ILE:HD11	1:E:3695:ILE:HG22	1.96	0.47
1:G:1118:SER:HB2	1:G:1204:VAL:HG11	1.96	0.47
1:G:1930:SER:O	1:G:1930:SER:OG	2.31	0.47
1:A:4770:LEU:C	1:C:4754:LEU:HD11	2.39	0.47
1:C:1611:ILE:HG13	1:C:1620:GLN:HB3	1.97	0.47
1:E:1521:THR:HA	1:E:1526:ASP:HA	1.96	0.47
1:E:1611:ILE:HG13	1:E:1620:GLN:HB3	1.97	0.47
1:G:1655:TYR:OH	1:G:1659:ARG:NH2	2.48	0.47
1:G:1942:ARG:NH1	1:G:3609:LEU:H	2.13	0.47
1:G:2737:LYS:HG3	1:G:2758:MET:HE1	1.96	0.47
1:A:1171:HIS:O	1:A:1194:ASP:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2213:LYS:HA	1:A:2254:LEU:HD21	1.95	0.47
1:A:3642:ILE:HD11	1:A:3695:ILE:HG22	1.96	0.47
1:A:4051:LYS:O	1:A:4055:SER:N	2.46	0.47
1:C:881:ILE:HD11	1:C:952:ILE:HD13	1.95	0.47
2:D:71:ARG:NH2	2:D:100:ASP:OD2	2.43	0.47
1:E:568:SER:HA	1:E:571:ILE:HD12	1.97	0.47
1:E:892:LEU:HD13	1:E:1052:GLU:HG3	1.94	0.47
1:G:892:LEU:HD13	1:G:1052:GLU:HG3	1.95	0.47
1:G:1629:SER:OG	1:G:1630:LEU:N	2.48	0.47
1:G:2116:ASP:OD1	1:G:2116:ASP:N	2.46	0.47
1:G:4569:MET:O	1:G:4572:THR:OG1	2.31	0.47
1:A:1655:TYR:OH	1:A:1659:ARG:NH2	2.48	0.47
1:A:4922:PHE:HE2	1:A:4941:VAL:HG11	1.80	0.47
1:C:1430:VAL:HG11	1:C:1443:VAL:HG11	1.97	0.47
1:C:1548:THR:OG1	1:C:1549:SER:N	2.45	0.47
1:C:1629:SER:OG	1:C:1630:LEU:N	2.48	0.47
1:E:1733:THR:HA	1:E:1755:THR:HG21	1.97	0.47
1:G:687:THR:OG1	1:G:689:GLU:O	2.33	0.47
1:G:3799:GLN:O	1:G:3881:ARG:NH2	2.48	0.47
1:A:1118:SER:HB2	1:A:1204:VAL:HG11	1.96	0.47
1:A:3900:ASP:N	1:A:3900:ASP:OD1	2.47	0.47
1:A:3957:MET:O	1:A:3960:SER:OG	2.33	0.47
1:A:4171:ARG:NE	5:A:6002:ATP:O2G	2.41	0.47
2:B:25:HIS:HD2	2:B:104:LEU:HD11	1.80	0.47
1:C:23:GLN:HE21	1:C:34:LYS:HB3	1.80	0.47
1:C:299:HIS:HD2	1:C:302:THR:H	1.63	0.47
1:C:394:HIS:CD2	1:C:397:GLY:H	2.32	0.47
1:C:821:PRO:HG2	1:C:824:GLU:HG2	1.96	0.47
1:C:4922:PHE:HE2	1:C:4941:VAL:HG11	1.80	0.47
1:E:1942:ARG:NH1	1:E:3609:LEU:H	2.13	0.47
1:E:4791:ARG:HH22	1:G:4559:HIS:HE1	1.63	0.47
1:G:66:THR:OG1	1:G:124:SER:OG	2.25	0.47
1:G:661:LEU:O	1:G:788:PHE:N	2.43	0.47
1:G:915:HIS:CE1	1:G:917:CYS:HB2	2.49	0.47
1:G:2996:HIS:O	1:G:3000:LYS:CB	2.63	0.47
1:G:4051:LYS:O	1:G:4055:SER:N	2.46	0.47
1:A:23:GLN:HE21	1:A:34:LYS:HB3	1.80	0.47
1:A:915:HIS:CE1	1:A:917:CYS:HB2	2.49	0.47
1:A:1611:ILE:HG13	1:A:1620:GLN:HB3	1.97	0.47
1:A:2427:LEU:HD21	1:G:143:LEU:HD22	1.91	0.47
1:A:3875:THR:HG21	1:A:3924:TYR:HE2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1221:VAL:HA	1:C:1224:LEU:HB2	1.97	0.47
1:C:2323:ARG:NH2	1:C:2323:ARG:CG	2.73	0.47
1:E:3799:GLN:O	1:E:3881:ARG:NH2	2.48	0.47
1:E:3875:THR:HG21	1:E:3924:TYR:HE2	1.80	0.47
1:E:4810:MET:HB3	1:G:4519:LEU:O	2.15	0.47
1:G:568:SER:HA	1:G:571:ILE:HD12	1.97	0.47
2:H:25:HIS:HD2	2:H:104:LEU:HD11	1.80	0.47
1:A:2324:LEU:HD23	1:A:2324:LEU:N	2.30	0.46
1:A:4045:SER:HA	1:A:4078:THR:HG22	1.96	0.46
1:A:4781:LEU:CD1	1:C:4741:ALA:O	2.63	0.46
1:C:894:VAL:HG13	1:C:918:LEU:HD22	1.97	0.46
1:C:1521:THR:HA	1:C:1526:ASP:HA	1.96	0.46
1:C:2307:VAL:HG12	1:C:2317:ASN:HB3	1.98	0.46
1:C:3980:VAL:HA	1:C:3983:LEU:HG	1.97	0.46
1:E:881:ILE:HD11	1:E:952:ILE:HD13	1.95	0.46
1:E:2996:HIS:O	1:E:3000:LYS:CB	2.63	0.46
2:F:25:HIS:HD2	2:F:104:LEU:HD11	1.80	0.46
1:G:1733:THR:HA	1:G:1755:THR:HG21	1.97	0.46
1:G:1939:ASP:O	1:G:1943:PHE:N	2.45	0.46
1:C:1655:TYR:OH	1:C:1659:ARG:NH2	2.48	0.46
1:C:3875:THR:HG21	1:C:3924:TYR:HE2	1.80	0.46
1:C:4045:SER:HA	1:C:4078:THR:HG22	1.96	0.46
1:E:894:VAL:HG13	1:E:918:LEU:HD22	1.97	0.46
1:E:3980:VAL:HA	1:E:3983:LEU:HG	1.97	0.46
1:E:4045:SER:HA	1:E:4078:THR:HG22	1.96	0.46
1:G:1199:ASP:OD2	1:G:1199:ASP:N	2.37	0.46
1:G:1221:VAL:HA	1:G:1224:LEU:HB2	1.97	0.46
1:G:1611:ILE:HG13	1:G:1620:GLN:HB3	1.97	0.46
1:A:1221:VAL:HA	1:A:1224:LEU:HB2	1.97	0.46
1:A:2226:SER:O	1:A:2226:SER:OG	2.33	0.46
1:C:2996:HIS:O	1:C:3000:LYS:CB	2.63	0.46
1:C:3957:MET:O	1:C:3960:SER:OG	2.33	0.46
1:E:394:HIS:CD2	1:E:397:GLY:H	2.32	0.46
1:E:687:THR:OG1	1:E:689:GLU:O	2.33	0.46
1:E:1756:SER:OG	1:E:1757:LEU:N	2.44	0.46
1:G:4757:ILE:O	1:G:4760:SER:OG	2.32	0.46
1:A:3927:GLY:O	1:A:3929:CYS:N	2.48	0.46
1:C:3642:ILE:HD11	1:C:3695:ILE:HG22	1.96	0.46
1:E:797:GLY:CA	1:E:1621:CYS:O	2.59	0.46
1:E:1764:SER:OG	1:E:1779:SER:O	2.33	0.46
1:G:821:PRO:HG2	1:G:824:GLU:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1440:ASN:N	1:G:1440:ASN:OD1	2.49	0.46
1:G:2324:LEU:N	1:G:2324:LEU:HD23	2.30	0.46
1:A:299:HIS:HD2	1:A:302:THR:H	1.63	0.46
1:A:687:THR:OG1	1:A:689:GLU:O	2.33	0.46
1:A:2996:HIS:O	1:A:3000:LYS:CB	2.63	0.46
1:C:394:HIS:HD2	1:C:397:GLY:H	1.64	0.46
1:C:1118:SER:HB2	1:C:1204:VAL:HG11	1.96	0.46
1:C:1764:SER:OG	1:C:1779:SER:O	2.33	0.46
1:E:605:GLY:HA2	1:E:1589:GLN:HE21	1.81	0.46
1:E:1430:VAL:HG11	1:E:1443:VAL:HG11	1.97	0.46
1:E:4757:ILE:O	1:E:4760:SER:OG	2.32	0.46
1:G:894:VAL:HG13	1:G:918:LEU:HD22	1.97	0.46
1:G:4922:PHE:HE2	1:G:4941:VAL:HG11	1.80	0.46
1:A:1678:SER:OG	2:B:36:PHE:O	2.24	0.46
1:A:4559:HIS:HE1	1:G:4791:ARG:HH22	1.63	0.46
1:E:23:GLN:HE21	1:E:34:LYS:HB3	1.80	0.46
1:E:299:HIS:HD2	1:E:302:THR:H	1.63	0.46
1:E:2110:ASN:OD1	1:E:2113:SER:OG	2.34	0.46
1:E:4922:PHE:HE2	1:E:4941:VAL:HG11	1.80	0.46
1:G:3927:GLY:O	1:G:3929:CYS:N	2.48	0.46
1:A:2116:ASP:N	1:A:2116:ASP:OD1	2.46	0.46
1:C:255:GLU:HB2	1:C:257:ARG:H	1.81	0.46
1:E:394:HIS:HD2	1:E:397:GLY:H	1.64	0.46
1:E:3900:ASP:OD1	1:E:3900:ASP:N	2.47	0.46
1:G:255:GLU:HB2	1:G:257:ARG:H	1.81	0.46
1:G:394:HIS:HD2	1:G:397:GLY:H	1.64	0.46
1:G:3875:THR:HG21	1:G:3924:TYR:HE2	1.80	0.46
1:A:1629:SER:OG	1:A:1630:LEU:N	2.48	0.46
1:A:4757:ILE:O	1:A:4760:SER:OG	2.32	0.46
1:A:4770:LEU:HB3	1:C:4754:LEU:HD13	1.97	0.46
1:C:4168:GLU:OE1	1:C:4595:LYS:NZ	2.46	0.46
1:G:299:HIS:HD2	1:G:302:THR:H	1.63	0.46
1:G:3982:MET:HE2	1:G:3982:MET:HB2	1.84	0.46
1:A:1430:VAL:HG11	1:A:1443:VAL:HG11	1.97	0.46
1:C:568:SER:HA	1:C:571:ILE:HD12	1.97	0.46
1:C:2110:ASN:OD1	1:C:2110:ASN:N	2.49	0.46
1:C:4000:MET:HE3	1:C:4000:MET:HB2	1.80	0.46
2:D:25:HIS:HD2	2:D:104:LEU:HD11	1.80	0.46
1:E:1221:VAL:HA	1:E:1224:LEU:HB2	1.97	0.46
1:E:1629:SER:OG	1:E:1630:LEU:N	2.48	0.46
1:E:2116:ASP:N	1:E:2116:ASP:OD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:605:GLY:HA2	1:G:1589:GLN:HE21	1.81	0.46
1:G:3642:ILE:HD11	1:G:3695:ILE:HG22	1.96	0.46
1:A:394:HIS:HD2	1:A:397:GLY:H	1.64	0.46
1:A:894:VAL:HG13	1:A:918:LEU:HD22	1.97	0.46
1:A:3892:TYR:O	1:A:3896:LYS:NZ	2.40	0.46
1:C:3794:LEU:HD23	1:C:3794:LEU:HA	1.82	0.46
1:E:1033:VAL:HG23	1:E:1038:LEU:HD12	1.98	0.46
1:G:636:LEU:HD21	1:G:643:LEU:HD11	1.98	0.46
1:G:1430:VAL:HG11	1:G:1443:VAL:HG11	1.97	0.46
1:A:568:SER:HA	1:A:571:ILE:HD12	1.97	0.45
1:A:605:GLY:HA2	1:A:1589:GLN:HE21	1.81	0.45
1:A:1733:THR:HA	1:A:1755:THR:HG21	1.97	0.45
1:C:1440:ASN:OD1	1:C:1440:ASN:N	2.49	0.45
1:G:2464:ASP:OD1	1:G:2464:ASP:N	2.44	0.45
1:A:255:GLU:HB2	1:A:257:ARG:H	1.81	0.45
1:A:3793:SER:O	1:A:3797:LEU:N	2.45	0.45
1:C:687:THR:OG1	1:C:689:GLU:O	2.33	0.45
1:C:1220:ASP:HB3	1:C:1223:THR:HB	1.97	0.45
1:C:1221:VAL:HA	1:C:1224:LEU:HD12	1.99	0.45
1:C:1733:THR:HA	1:C:1755:THR:HG21	1.97	0.45
1:E:1221:VAL:HA	1:E:1224:LEU:HD12	1.99	0.45
1:E:2324:LEU:N	1:E:2324:LEU:HD23	2.31	0.45
1:E:4858:ILE:HD12	1:G:4867:ILE:CG2	2.26	0.45
1:G:797:GLY:CA	1:G:1621:CYS:O	2.59	0.45
1:G:1033:VAL:HG23	1:G:1038:LEU:HD12	1.98	0.45
1:A:1100:ARG:HH12	1:A:1170:GLU:H	1.65	0.45
1:A:3794:LEU:HD23	1:A:3794:LEU:HA	1.82	0.45
1:C:4171:ARG:NE	5:C:6002:ATP:O2G	2.41	0.45
1:E:294:PRO:HB2	1:E:328:ALA:HB1	1.99	0.45
1:E:636:LEU:HD21	1:E:643:LEU:HD11	1.99	0.45
1:G:1124:PRO:HB2	1:G:1252:SER:HB2	1.98	0.45
1:G:2173:MET:HE2	1:G:2173:MET:HB2	1.84	0.45
1:G:4823:ARG:HB2	1:G:4823:ARG:HH11	1.71	0.45
1:A:294:PRO:HB2	1:A:328:ALA:HB1	1.99	0.45
1:A:2265:LYS:HA	1:A:2268:ARG:HB2	1.98	0.45
1:A:2326:ILE:CB	1:G:207:PHE:CZ	2.99	0.45
1:A:4819:TYR:HD1	1:G:4845:ILE:HD12	1.56	0.45
1:E:1220:ASP:HB3	1:E:1223:THR:HB	1.98	0.45
1:E:4062:SER:OG	1:E:4063:GLU:OE2	2.32	0.45
1:E:4801:ASP:N	1:E:4801:ASP:OD1	2.49	0.45
1:G:2776:ILE:O	1:G:2779:SER:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3980:VAL:HA	1:G:3983:LEU:HG	1.97	0.45
1:A:1614:ARG:HH11	1:A:1617:TRP:HE1	1.64	0.45
1:A:4519:LEU:O	1:G:4810:MET:HB3	2.17	0.45
1:C:572:LEU:HD12	1:C:572:LEU:HA	1.84	0.45
1:C:1033:VAL:HG23	1:C:1038:LEU:HD12	1.98	0.45
1:C:1124:PRO:HB2	1:C:1252:SER:HB2	1.98	0.45
1:C:4052:ALA:O	1:C:4056:HIS:ND1	2.38	0.45
1:G:1220:ASP:HB3	1:G:1223:THR:HB	1.97	0.45
1:G:2110:ASN:OD1	1:G:2110:ASN:N	2.49	0.45
1:G:2313:SER:OG	1:G:2402:ARG:O	2.33	0.45
1:G:2771:ILE:H	1:G:2771:ILE:HG13	1.63	0.45
1:A:1124:PRO:HB2	1:A:1252:SER:HB2	1.98	0.45
1:A:2314:VAL:HG23	1:A:2314:VAL:O	2.17	0.45
1:C:294:PRO:HB2	1:C:328:ALA:HB1	1.99	0.45
1:C:605:GLY:HA2	1:C:1589:GLN:HE21	1.81	0.45
1:C:4801:ASP:OD1	1:C:4801:ASP:N	2.49	0.45
1:G:1764:SER:OG	1:G:1779:SER:O	2.33	0.45
1:A:1033:VAL:HG23	1:A:1038:LEU:HD12	1.98	0.45
1:A:1220:ASP:HB3	1:A:1223:THR:HB	1.97	0.45
1:A:1221:VAL:HA	1:A:1224:LEU:HD12	1.99	0.45
1:A:2176:MET:HE2	1:A:2176:MET:HB3	1.86	0.45
1:A:2776:ILE:O	1:A:2779:SER:HB3	2.16	0.45
1:C:35:LEU:HD12	1:C:49:LEU:HB3	1.99	0.45
1:C:767:SER:OG	1:C:777:GLY:O	2.35	0.45
1:C:4862:ILE:HG23	1:E:4868:ILE:HD11	1.99	0.45
1:E:2776:ILE:O	1:E:2779:SER:HB3	2.16	0.45
1:E:4051:LYS:O	1:E:4055:SER:N	2.46	0.45
1:G:294:PRO:HB2	1:G:328:ALA:HB1	1.99	0.45
1:G:1100:ARG:HH12	1:G:1170:GLU:H	1.65	0.45
1:G:1171:HIS:O	1:G:1194:ASP:N	2.45	0.45
1:G:2141:LYS:HE2	1:G:2141:LYS:HB2	1.80	0.45
1:G:2208:SER:OG	1:G:2209:ARG:N	2.50	0.45
1:A:3980:VAL:HA	1:A:3983:LEU:HG	1.97	0.45
1:A:4569:MET:O	1:A:4572:THR:OG1	2.31	0.45
1:C:443:SER:O	1:C:443:SER:OG	2.35	0.45
1:C:1171:HIS:O	1:C:1194:ASP:N	2.45	0.45
1:C:2093:TYR:HD2	1:C:3641:LEU:HD22	1.82	0.45
1:C:3927:GLY:O	1:C:3929:CYS:N	2.48	0.45
2:D:26:TYR:HB2	2:D:101:VAL:HG12	1.99	0.45
1:G:1210:ALA:N	1:G:1211:GLN:OE1	2.50	0.45
1:G:3957:MET:O	1:G:3960:SER:OG	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4770:LEU:HD13	1:C:4751:PHE:HD1	1.82	0.45
1:A:4791:ARG:HH22	1:C:4559:HIS:HE1	1.64	0.45
1:A:4867:ILE:CG2	1:G:4858:ILE:HD12	2.26	0.45
1:C:894:VAL:HG22	1:C:918:LEU:HA	1.99	0.45
1:C:1614:ARG:NH1	1:C:1617:TRP:HE1	2.15	0.45
1:C:3893:TYR:OH	1:C:3900:ASP:OD1	2.33	0.45
1:E:661:LEU:O	1:E:788:PHE:N	2.43	0.45
1:E:767:SER:OG	1:E:777:GLY:O	2.35	0.45
1:E:1614:ARG:NH1	1:E:1617:TRP:HE1	2.15	0.45
1:E:2208:SER:OG	1:E:2209:ARG:N	2.50	0.45
1:E:3809:PHE:O	1:E:3813:ASN:N	2.50	0.45
1:G:2265:LYS:HA	1:G:2268:ARG:HB2	1.98	0.45
1:G:4801:ASP:N	1:G:4801:ASP:OD1	2.49	0.45
1:A:767:SER:OG	1:A:777:GLY:O	2.35	0.45
1:A:1210:ALA:N	1:A:1211:GLN:OE1	2.50	0.45
1:E:2265:LYS:HA	1:E:2268:ARG:HB2	1.98	0.45
1:E:4569:MET:O	1:E:4572:THR:OG1	2.31	0.45
1:G:998:LYS:HE3	1:G:998:LYS:HB3	1.82	0.45
1:A:494:MET:HA	1:A:497:LEU:HB2	2.00	0.44
1:A:1718:ARG:NH1	1:A:1758:ARG:HD3	2.33	0.44
1:C:2776:ILE:O	1:C:2779:SER:HB3	2.16	0.44
1:E:1718:ARG:NH1	1:E:1758:ARG:HD3	2.33	0.44
1:E:2110:ASN:OD1	1:E:2110:ASN:N	2.49	0.44
1:G:2314:VAL:HG23	1:G:2314:VAL:O	2.17	0.44
1:A:35:LEU:HD12	1:A:49:LEU:HB3	1.99	0.44
1:A:306:LEU:O	1:A:327:THR:OG1	2.27	0.44
1:C:1602:GLN:HB2	1:C:1643:GLU:HG2	1.99	0.44
1:C:4781:LEU:CD1	1:E:4741:ALA:O	2.65	0.44
1:E:1124:PRO:HB2	1:E:1252:SER:HB2	1.98	0.44
1:E:1210:ALA:N	1:E:1211:GLN:OE1	2.50	0.44
1:E:2093:TYR:HD2	1:E:3641:LEU:HD22	1.82	0.44
1:E:2168:MET:HE3	1:E:2168:MET:HB2	1.70	0.44
1:E:3957:MET:O	1:E:3960:SER:OG	2.33	0.44
1:G:1221:VAL:HA	1:G:1224:LEU:HD12	1.99	0.44
1:G:1718:ARG:NH1	1:G:1758:ARG:HD3	2.33	0.44
1:G:1849:SER:OG	1:G:1849:SER:O	2.35	0.44
1:A:636:LEU:HD21	1:A:643:LEU:HD11	1.99	0.44
1:A:2208:SER:OG	1:A:2209:ARG:N	2.50	0.44
2:B:78:PRO:HA	2:B:81:ALA:HB3	2.00	0.44
1:C:290:ARG:HA	1:C:353:GLU:HG2	1.99	0.44
1:C:544:ASN:HB2	1:C:547:ASN:HD22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1718:ARG:NH1	1:C:1758:ARG:HD3	2.33	0.44
1:C:1930:SER:O	1:C:1930:SER:OG	2.31	0.44
1:C:2141:LYS:HE2	1:C:2141:LYS:HB2	1.80	0.44
2:D:78:PRO:HA	2:D:81:ALA:HB3	2.00	0.44
1:E:1440:ASN:OD1	1:E:1440:ASN:N	2.49	0.44
1:E:1614:ARG:HH11	1:E:1617:TRP:HE1	1.64	0.44
1:E:2264:GLU:HG2	1:E:2324:LEU:CD1	2.47	0.44
1:E:3927:GLY:O	1:E:3929:CYS:N	2.48	0.44
2:F:57:LYS:HD2	2:F:57:LYS:HA	1.69	0.44
1:G:290:ARG:HA	1:G:353:GLU:HG2	1.99	0.44
2:H:78:PRO:HA	2:H:81:ALA:HB3	2.00	0.44
1:A:1614:ARG:HA	1:A:1614:ARG:HD3	1.86	0.44
1:A:4168:GLU:OE1	1:A:4595:LYS:NZ	2.46	0.44
1:C:408:SER:OG	1:C:409:GLN:N	2.50	0.44
1:C:1210:ALA:N	1:C:1211:GLN:OE1	2.50	0.44
1:C:2110:ASN:OD1	1:C:2113:SER:OG	2.34	0.44
1:C:2265:LYS:HA	1:C:2268:ARG:HB2	1.98	0.44
1:C:2771:ILE:H	1:C:2771:ILE:HG13	1.63	0.44
2:F:26:TYR:HB2	2:F:101:VAL:HG12	1.99	0.44
2:F:78:PRO:HA	2:F:81:ALA:HB3	2.00	0.44
1:A:2110:ASN:OD1	1:A:2113:SER:OG	2.34	0.44
2:B:21:THR:HG22	2:B:49:ARG:HE	1.83	0.44
1:C:2208:SER:OG	1:C:2209:ARG:N	2.50	0.44
2:D:21:THR:HG22	2:D:49:ARG:HE	1.83	0.44
1:E:1939:ASP:OD1	1:E:1939:ASP:N	2.40	0.44
1:E:2307:VAL:HG12	1:E:2317:ASN:HB3	1.99	0.44
1:E:4168:GLU:OE1	1:E:4595:LYS:NZ	2.46	0.44
1:A:243:GLU:OE2	1:A:389:ARG:NH2	2.51	0.44
1:A:1440:ASN:OD1	1:A:1440:ASN:N	2.49	0.44
1:A:1811:GLY:HA3	1:A:1816:PHE:HB2	2.00	0.44
1:A:2093:TYR:HD2	1:A:3641:LEU:HD22	1.82	0.44
1:C:494:MET:HA	1:C:497:LEU:HB2	2.00	0.44
1:C:3809:PHE:O	1:C:3813:ASN:N	2.50	0.44
1:E:35:LEU:HD12	1:E:49:LEU:HB3	1.99	0.44
1:E:243:GLU:OE2	1:E:389:ARG:NH2	2.51	0.44
1:E:255:GLU:HB2	1:E:257:ARG:H	1.81	0.44
1:E:544:ASN:HB2	1:E:547:ASN:HD22	1.83	0.44
1:E:1930:SER:O	1:E:1930:SER:OG	2.31	0.44
1:G:408:SER:OG	1:G:409:GLN:N	2.50	0.44
1:G:494:MET:HA	1:G:497:LEU:HB2	1.99	0.44
1:G:894:VAL:HG22	1:G:918:LEU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1614:ARG:NH1	1:G:1617:TRP:HE1	2.15	0.44
1:G:1614:ARG:HH11	1:G:1617:TRP:HE1	1.64	0.44
1:G:4052:ALA:O	1:G:4056:HIS:ND1	2.38	0.44
1:G:4062:SER:OG	1:G:4063:GLU:OE2	2.32	0.44
1:A:4751:PHE:HD1	1:G:4770:LEU:HD13	1.82	0.44
1:C:636:LEU:HD21	1:C:643:LEU:HD11	1.99	0.44
1:E:1811:GLY:HA3	1:E:1816:PHE:HB2	2.00	0.44
1:E:3962:ASP:HB2	1:E:3965:GLN:HE22	1.83	0.44
1:G:544:ASN:HB2	1:G:547:ASN:HD22	1.83	0.44
1:G:1602:GLN:HB2	1:G:1643:GLU:HG2	1.99	0.44
1:G:2110:ASN:OD1	1:G:2113:SER:OG	2.34	0.44
1:G:2148:GLY:O	1:G:2152:ASN:ND2	2.51	0.44
1:C:76:ARG:HD2	1:E:3891:TRP:CG	2.45	0.44
1:C:243:GLU:OE2	1:C:389:ARG:NH2	2.51	0.44
1:C:1614:ARG:HH11	1:C:1617:TRP:HE1	1.64	0.44
1:E:2141:LYS:HE2	1:E:2141:LYS:HB2	1.80	0.44
1:E:4045:SER:OG	1:E:4048:ASP:N	2.48	0.44
1:G:234:LEU:HD13	1:G:405:LEU:HD22	2.00	0.44
1:G:611:LEU:HD22	1:G:1660:LEU:HD22	1.99	0.44
1:G:3900:ASP:N	1:G:3900:ASP:OD1	2.47	0.44
2:H:21:THR:HG22	2:H:49:ARG:HE	1.83	0.44
1:A:290:ARG:HA	1:A:353:GLU:HG2	1.99	0.44
1:A:408:SER:OG	1:A:409:GLN:N	2.50	0.44
1:A:1009:ARG:HA	1:A:1012:ILE:HG12	2.00	0.44
2:B:57:LYS:HA	2:B:57:LYS:HD2	1.69	0.44
1:C:1687:TYR:OH	1:C:1691:ASN:ND2	2.51	0.44
1:C:2148:GLY:O	1:C:2152:ASN:ND2	2.51	0.44
1:C:4045:SER:OG	1:C:4048:ASP:N	2.48	0.44
1:C:4945:TYR:OH	6:C:6003:CFF:H81	2.18	0.44
2:F:21:THR:HG22	2:F:49:ARG:HE	1.83	0.44
1:G:767:SER:OG	1:G:777:GLY:O	2.35	0.44
1:A:652:VAL:HG21	1:A:714:GLY:HA3	2.00	0.43
1:A:4810:MET:HB3	1:C:4519:LEU:O	2.18	0.43
1:C:652:VAL:HG21	1:C:714:GLY:HA3	2.00	0.43
1:C:1572:LYS:HD2	1:C:1585:ARG:H	1.83	0.43
1:C:3892:TYR:O	1:C:3896:LYS:NZ	2.40	0.43
1:C:4569:MET:O	1:C:4572:THR:OG1	2.31	0.43
1:E:1687:TYR:OH	1:E:1691:ASN:ND2	2.51	0.43
1:E:2148:GLY:O	1:E:2152:ASN:ND2	2.51	0.43
1:G:35:LEU:HD12	1:G:49:LEU:HB3	1.99	0.43
1:A:1572:LYS:HD2	1:A:1585:ARG:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1614:ARG:NH1	1:A:1617:TRP:HE1	2.15	0.43
1:A:2120:LEU:HD13	1:A:2153:ASN:HD22	1.83	0.43
1:A:2313:SER:OG	1:A:2402:ARG:O	2.33	0.43
2:B:26:TYR:HB2	2:B:101:VAL:HG12	1.99	0.43
1:C:1009:ARG:HA	1:C:1012:ILE:HG12	2.00	0.43
1:C:1100:ARG:HH12	1:C:1170:GLU:H	1.65	0.43
1:C:1811:GLY:HA3	1:C:1816:PHE:HB2	2.00	0.43
1:E:234:LEU:HD13	1:E:405:LEU:HD22	2.00	0.43
1:E:443:SER:O	1:E:443:SER:OG	2.35	0.43
1:E:652:VAL:HG21	1:E:714:GLY:HA3	2.00	0.43
1:E:1694:MET:HB3	1:E:1694:MET:HE2	1.81	0.43
1:E:2103:LEU:HD23	1:E:2103:LEU:HA	1.81	0.43
1:G:652:VAL:HG21	1:G:714:GLY:HA3	2.00	0.43
1:G:1687:TYR:OH	1:G:1691:ASN:ND2	2.51	0.43
1:G:1811:GLY:HA3	1:G:1816:PHE:HB2	2.00	0.43
1:G:2093:TYR:HD2	1:G:3641:LEU:HD22	1.82	0.43
1:G:2226:SER:O	1:G:2226:SER:OG	2.33	0.43
1:G:3809:PHE:O	1:G:3813:ASN:N	2.50	0.43
1:A:544:ASN:HB2	1:A:547:ASN:HD22	1.83	0.43
1:A:611:LEU:HD22	1:A:1660:LEU:HD22	1.99	0.43
1:A:2771:ILE:H	1:A:2771:ILE:HG13	1.63	0.43
1:C:1755:THR:O	1:C:1755:THR:OG1	2.29	0.43
1:E:494:MET:HA	1:E:497:LEU:HB2	2.00	0.43
1:E:894:VAL:HG22	1:E:918:LEU:HA	1.99	0.43
1:E:1100:ARG:HH12	1:E:1170:GLU:H	1.65	0.43
1:E:1602:GLN:HB2	1:E:1643:GLU:HG2	1.99	0.43
1:E:4945:TYR:OH	6:E:6003:CFF:H81	2.18	0.43
1:G:3962:ASP:HB2	1:G:3965:GLN:HE22	1.83	0.43
1:A:406:SER:O	1:A:406:SER:OG	2.35	0.43
1:A:797:GLY:CA	1:A:1621:CYS:O	2.59	0.43
1:A:894:VAL:HG22	1:A:918:LEU:HA	1.99	0.43
1:A:1823:LYS:HB2	1:A:1823:LYS:HE3	1.88	0.43
1:A:2088:LEU:HD12	1:A:2088:LEU:HA	1.84	0.43
1:C:2298:ARG:O	1:C:2301:ASP:HB3	2.19	0.43
1:E:1009:ARG:HA	1:E:1012:ILE:HG12	2.00	0.43
1:G:243:GLU:OE2	1:G:389:ARG:NH2	2.51	0.43
1:G:308:LEU:HD22	1:G:393:MET:HE2	2.01	0.43
1:G:1009:ARG:HA	1:G:1012:ILE:HG12	2.00	0.43
1:G:3794:LEU:HD23	1:G:3794:LEU:HA	1.82	0.43
1:A:1694:MET:HB3	1:A:1694:MET:HE2	1.81	0.43
1:A:3982:MET:HE2	1:A:3982:MET:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4862:ILE:HG23	1:C:4868:ILE:HD11	1.99	0.43
1:C:399:MET:N	1:C:399:MET:SD	2.92	0.43
1:C:2876:ASP:OD1	1:C:2876:ASP:N	2.47	0.43
1:C:4810:MET:HB3	1:E:4519:LEU:O	2.18	0.43
2:D:57:LYS:HD2	2:D:57:LYS:HA	1.69	0.43
1:E:30:LYS:HD3	1:E:30:LYS:HA	1.69	0.43
1:E:408:SER:OG	1:E:409:GLN:N	2.50	0.43
1:G:976:TYR:CZ	1:G:978:PRO:HB3	2.53	0.43
1:G:2120:LEU:HD13	1:G:2153:ASN:HD22	1.83	0.43
2:H:26:TYR:HB2	2:H:101:VAL:HG12	1.99	0.43
1:A:1228:THR:OG1	1:A:1229:ILE:N	2.52	0.43
1:A:4523:VAL:CG1	1:G:4808:ASP:HB2	2.49	0.43
1:C:611:LEU:HD22	1:C:1660:LEU:HD22	1.99	0.43
1:C:976:TYR:CZ	1:C:978:PRO:HB3	2.53	0.43
1:C:2168:MET:HE3	1:C:2168:MET:HB2	1.70	0.43
1:E:308:LEU:HD22	1:E:393:MET:HE2	2.01	0.43
1:E:2270:LEU:HA	1:E:2270:LEU:HD23	1.81	0.43
1:G:1228:THR:OG1	1:G:1229:ILE:N	2.52	0.43
1:G:1572:LYS:HD2	1:G:1585:ARG:H	1.83	0.43
1:G:1610:ARG:HE	1:G:1610:ARG:HB3	1.64	0.43
1:G:2298:ARG:O	1:G:2301:ASP:HB3	2.19	0.43
1:G:3984:LEU:HD23	1:G:3984:LEU:HA	1.87	0.43
1:G:4945:TYR:OH	6:G:6003:CFF:H81	2.18	0.43
1:A:399:MET:N	1:A:399:MET:SD	2.92	0.43
1:A:1687:TYR:OH	1:A:1691:ASN:ND2	2.51	0.43
1:A:2298:ARG:O	1:A:2301:ASP:HB3	2.19	0.43
1:A:2323:ARG:HD2	1:G:189:GLU:OE2	2.18	0.43
1:C:180:ASP:HB3	1:C:211:LEU:HD12	2.01	0.43
1:C:374:TYR:HE1	1:C:400:ASP:HB2	1.84	0.43
1:C:3962:ASP:HB2	1:C:3965:GLN:HE22	1.83	0.43
1:E:66:THR:OG1	1:E:124:SER:OG	2.25	0.43
1:E:611:LEU:HD22	1:E:1660:LEU:HD22	1.99	0.43
1:E:1228:THR:OG1	1:E:1229:ILE:N	2.52	0.43
1:E:1572:LYS:HD2	1:E:1585:ARG:H	1.83	0.43
1:E:2313:SER:OG	1:E:2402:ARG:O	2.33	0.43
1:E:4892:CYS:HB3	1:E:4894:ILE:HG12	2.01	0.43
1:G:1211:GLN:OE1	1:G:1211:GLN:N	2.52	0.43
1:G:1630:LEU:HD22	1:G:1641:ILE:HG13	2.01	0.43
1:G:1907:MET:HE3	1:G:1907:MET:HB2	1.77	0.43
1:A:897:LYS:HE3	1:A:897:LYS:HB3	1.92	0.43
1:A:976:TYR:CZ	1:A:978:PRO:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1211:GLN:OE1	1:A:1211:GLN:N	2.52	0.43
1:C:1211:GLN:OE1	1:C:1211:GLN:N	2.52	0.43
1:C:1840:LYS:O	1:C:1844:GLN:NE2	2.52	0.43
1:C:4892:CYS:HB3	1:C:4894:ILE:HG12	2.01	0.43
1:E:374:TYR:HE1	1:E:400:ASP:HB2	1.84	0.43
1:E:3892:TYR:O	1:E:3896:LYS:NZ	2.40	0.43
1:E:4000:MET:HB2	1:E:4000:MET:HE3	1.80	0.43
1:G:374:TYR:HE1	1:G:400:ASP:HB2	1.84	0.43
1:G:572:LEU:HD12	1:G:572:LEU:HA	1.84	0.43
1:G:2397:ILE:HD13	1:G:2397:ILE:HA	1.90	0.43
1:G:4171:ARG:NE	5:G:6002:ATP:O2G	2.41	0.43
1:A:1602:GLN:HB2	1:A:1643:GLU:HG2	1.99	0.43
1:A:4868:ILE:HD11	1:G:4862:ILE:HG23	2.00	0.43
2:B:42:ARG:HG3	2:B:44:LYS:HB2	2.01	0.43
1:C:156:GLU:HB2	1:C:187:SER:HB3	2.01	0.43
1:C:644:LEU:HB3	1:C:1630:LEU:HD12	2.01	0.43
1:C:4791:ARG:HH22	1:E:4559:HIS:HE1	1.66	0.43
1:E:3829:LYS:HB3	1:E:3829:LYS:HE3	1.86	0.43
2:F:38:SER:OG	2:F:39:SER:N	2.52	0.43
1:A:374:TYR:HE1	1:A:400:ASP:HB2	1.84	0.43
1:A:4744:LEU:HD23	1:A:4744:LEU:HA	1.78	0.43
1:C:900:LEU:HD23	1:C:902:TRP:HE1	1.84	0.43
1:C:2267:VAL:HG21	1:C:2324:LEU:HB3	2.00	0.43
1:E:290:ARG:HA	1:E:353:GLU:HG2	1.99	0.43
1:E:4770:LEU:HD13	1:G:4751:PHE:HD1	1.83	0.43
1:A:59:PRO:HB3	1:A:296:ARG:CZ	2.49	0.42
1:A:180:ASP:HB3	1:A:211:LEU:HD12	2.01	0.42
1:A:2148:GLY:O	1:A:2152:ASN:ND2	2.51	0.42
1:A:3962:ASP:HB2	1:A:3965:GLN:HE22	1.83	0.42
1:A:4945:TYR:OH	6:A:6003:CFF:H81	2.18	0.42
2:B:11:ASP:OD2	2:B:14:THR:OG1	2.35	0.42
1:C:2120:LEU:HD13	1:C:2153:ASN:HD22	1.83	0.42
2:D:11:ASP:OD2	2:D:14:THR:OG1	2.35	0.42
1:E:399:MET:N	1:E:399:MET:SD	2.92	0.42
1:E:2298:ARG:O	1:E:2301:ASP:HB3	2.19	0.42
1:E:4858:ILE:CD1	1:G:4867:ILE:HG21	2.27	0.42
1:A:572:LEU:HD12	1:A:572:LEU:HA	1.84	0.42
1:A:864:PRO:HG3	1:A:1034:PRO:HB3	2.01	0.42
1:A:1445:TRP:H	1:A:1487:MET:HG2	1.84	0.42
1:A:2270:LEU:HD23	1:A:2270:LEU:HA	1.81	0.42
1:C:2271:ALA:HB2	1:C:2328:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:ASP:OD1	2:D:11:ASP:N	2.52	0.42
1:E:474:ASP:HA	1:E:477:ASN:HD22	1.84	0.42
1:E:976:TYR:CZ	1:E:978:PRO:HB3	2.53	0.42
1:E:1211:GLN:OE1	1:E:1211:GLN:N	2.52	0.42
1:E:2271:ALA:HB2	1:E:2328:ARG:HD3	2.01	0.42
1:E:3857:ASN:OD1	1:E:3860:ARG:NH1	2.52	0.42
1:E:4808:ASP:HB2	1:G:4523:VAL:CG1	2.50	0.42
1:G:3880:LEU:HD21	1:G:3940:ARG:HD2	2.01	0.42
2:H:42:ARG:HG3	2:H:44:LYS:HB2	2.01	0.42
1:A:1840:LYS:O	1:A:1844:GLN:NE2	2.52	0.42
1:C:234:LEU:HD13	1:C:405:LEU:HD22	2.00	0.42
1:C:998:LYS:HB3	1:C:998:LYS:HE3	1.82	0.42
1:C:4823:ARG:H	1:C:4823:ARG:HG3	1.55	0.42
1:E:900:LEU:HD23	1:E:902:TRP:HE1	1.84	0.42
1:E:1250:TRP:HE1	1:E:1602:GLN:HG3	1.84	0.42
1:E:4894:ILE:HD13	1:E:4894:ILE:HA	1.94	0.42
1:G:3857:ASN:OD1	1:G:3860:ARG:NH1	2.52	0.42
2:H:38:SER:OG	2:H:39:SER:N	2.52	0.42
1:A:156:GLU:HB2	1:A:187:SER:HB3	2.01	0.42
1:A:1630:LEU:HD22	1:A:1641:ILE:HG13	2.01	0.42
1:A:4589:ILE:HD13	1:A:4589:ILE:HA	1.92	0.42
1:C:1228:THR:OG1	1:C:1229:ILE:N	2.52	0.42
1:C:3880:LEU:HD21	1:C:3940:ARG:HD2	2.01	0.42
1:E:1823:LYS:HB2	1:E:1823:LYS:HE3	1.88	0.42
1:E:1828:LEU:HD12	1:E:1828:LEU:HA	1.87	0.42
1:E:1840:LYS:O	1:E:1844:GLN:NE2	2.52	0.42
2:F:30:LEU:HD23	2:F:30:LEU:HA	1.90	0.42
1:G:192:LEU:O	1:G:212:TRP:NE1	2.47	0.42
1:G:399:MET:SD	1:G:399:MET:N	2.92	0.42
1:G:2168:MET:HE3	1:G:2168:MET:HB2	1.70	0.42
1:G:4045:SER:OG	1:G:4048:ASP:N	2.48	0.42
1:A:308:LEU:HD22	1:A:393:MET:HE2	2.01	0.42
1:A:2168:MET:HB2	1:A:2168:MET:HE3	1.70	0.42
1:A:3880:LEU:HD21	1:A:3940:ARG:HD2	2.01	0.42
1:A:4892:CYS:HB3	1:A:4894:ILE:HG12	2.01	0.42
1:E:143:LEU:HD22	1:G:2427:LEU:HD21	1.92	0.42
1:E:189:GLU:OE2	1:G:2323:ARG:HD2	2.19	0.42
1:E:406:SER:O	1:E:406:SER:OG	2.35	0.42
1:E:449:ILE:HD13	1:E:449:ILE:HA	1.88	0.42
1:G:1250:TRP:NE1	1:G:1643:GLU:OE2	2.53	0.42
1:G:3844:LEU:HA	1:G:3844:LEU:HD23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:5:GLU:HB3	2:H:73:LYS:HB3	2.02	0.42
1:A:234:LEU:HD13	1:A:405:LEU:HD22	2.00	0.42
1:A:677:LEU:HD11	1:A:792:VAL:HG21	2.02	0.42
1:A:3609:LEU:HD12	1:A:3609:LEU:HA	1.86	0.42
1:C:59:PRO:HB3	1:C:296:ARG:CZ	2.49	0.42
1:C:864:PRO:HG3	1:C:1034:PRO:HB3	2.01	0.42
1:C:1250:TRP:HE1	1:C:1602:GLN:HG3	1.84	0.42
1:C:2030:LEU:HD23	1:C:2030:LEU:HA	1.90	0.42
1:E:59:PRO:HB3	1:E:296:ARG:CZ	2.50	0.42
1:E:351:THR:OG1	1:E:352:SER:N	2.53	0.42
1:E:1445:TRP:H	1:E:1487:MET:HG2	1.84	0.42
1:E:1610:ARG:HE	1:E:1610:ARG:HB3	1.64	0.42
1:E:3609:LEU:HD12	1:E:3609:LEU:HA	1.86	0.42
1:A:900:LEU:HD23	1:A:902:TRP:HE1	1.84	0.42
1:A:2518:ASN:HA	1:A:2521:LEU:HD12	2.02	0.42
1:A:4801:ASP:N	1:A:4801:ASP:OD1	2.49	0.42
1:A:4808:ASP:HB2	1:C:4523:VAL:HG11	2.02	0.42
1:C:351:THR:OG1	1:C:352:SER:N	2.53	0.42
1:C:1785:ASP:OD1	1:C:1785:ASP:N	2.53	0.42
1:C:1792:ILE:HG12	1:C:1842:ILE:HD11	2.01	0.42
1:C:1907:MET:HB2	1:C:1907:MET:HE3	1.77	0.42
1:C:3793:SER:O	1:C:3797:LEU:N	2.45	0.42
1:C:4770:LEU:HD13	1:E:4751:PHE:HD1	1.85	0.42
1:E:156:GLU:HB2	1:E:187:SER:HB3	2.01	0.42
1:E:357:GLY:O	1:E:404:ASN:ND2	2.46	0.42
1:E:505:LEU:HD23	1:E:505:LEU:HA	1.83	0.42
1:E:677:LEU:HD11	1:E:792:VAL:HG21	2.02	0.42
1:E:4862:ILE:HG23	1:G:4868:ILE:HD11	2.01	0.42
1:G:59:PRO:HB3	1:G:296:ARG:CZ	2.49	0.42
1:G:1658:LEU:HD23	1:G:1658:LEU:HA	1.80	0.42
1:G:1840:LYS:O	1:G:1844:GLN:NE2	2.52	0.42
1:G:2163:MET:N	1:G:2163:MET:SD	2.93	0.42
1:G:3892:TYR:O	1:G:3896:LYS:NZ	2.40	0.42
1:A:1250:TRP:NE1	1:A:1643:GLU:OE2	2.53	0.42
1:A:1258:PHE:HA	1:A:1595:LEU:HA	2.02	0.42
1:A:2163:MET:SD	1:A:2163:MET:N	2.93	0.42
1:A:4818:MET:HE2	1:A:4818:MET:HB2	1.84	0.42
2:B:38:SER:OG	2:B:39:SER:N	2.52	0.42
1:C:308:LEU:HD22	1:C:393:MET:HE2	2.00	0.42
1:C:1445:TRP:H	1:C:1487:MET:HG2	1.84	0.42
1:C:1730:THR:O	1:C:1733:THR:OG1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:42:ARG:HG3	2:D:44:LYS:HB2	2.01	0.42
1:E:1258:PHE:HA	1:E:1595:LEU:HA	2.02	0.42
1:E:2845:MET:HE3	1:E:2845:MET:HB3	1.92	0.42
1:G:156:GLU:HB2	1:G:187:SER:HB3	2.01	0.42
1:G:180:ASP:HB3	1:G:211:LEU:HD12	2.01	0.42
1:G:1445:TRP:H	1:G:1487:MET:HG2	1.84	0.42
1:G:2518:ASN:HA	1:G:2521:LEU:HD12	2.02	0.42
1:G:3991:VAL:HG12	1:G:4145:ARG:NH2	2.35	0.42
1:A:325:LYS:O	1:A:365:HIS:NE2	2.53	0.42
1:A:357:GLY:O	1:A:404:ASN:ND2	2.46	0.42
1:A:472:HIS:ND1	1:A:472:HIS:O	2.53	0.42
1:A:644:LEU:HB3	1:A:1630:LEU:HD12	2.01	0.42
1:A:1273:ILE:HD11	1:A:1287:GLN:HB2	2.02	0.42
1:C:274:LEU:HD23	1:C:274:LEU:HA	1.90	0.42
1:C:1258:PHE:HA	1:C:1595:LEU:HA	2.02	0.42
2:D:38:SER:OG	2:D:39:SER:N	2.52	0.42
1:E:274:LEU:HD23	1:E:274:LEU:HA	1.90	0.42
1:E:1273:ILE:HD11	1:E:1287:GLN:HB2	2.02	0.42
1:E:2120:LEU:HD13	1:E:2153:ASN:HD22	1.83	0.42
1:E:2771:ILE:H	1:E:2771:ILE:HG13	1.63	0.42
1:G:474:ASP:HA	1:G:477:ASN:HD22	1.84	0.42
1:G:1250:TRP:HE1	1:G:1602:GLN:HG3	1.84	0.42
1:G:1792:ILE:HG12	1:G:1842:ILE:HD11	2.01	0.42
1:A:1764:SER:OG	1:A:1779:SER:O	2.33	0.42
1:C:2316:GLU:HG2	1:C:3811:ARG:NH2	2.35	0.42
1:C:3630:ILE:HD13	1:C:3630:ILE:HA	1.93	0.42
1:E:1630:LEU:HD22	1:E:1641:ILE:HG13	2.01	0.42
1:G:1258:PHE:HA	1:G:1595:LEU:HA	2.02	0.42
1:G:1273:ILE:HD11	1:G:1287:GLN:HB2	2.02	0.42
1:G:1911:LEU:HD23	1:G:1911:LEU:HA	1.92	0.42
1:A:3991:VAL:HG12	1:A:4145:ARG:NH2	2.35	0.41
1:A:4867:ILE:HG21	1:G:4858:ILE:CD1	2.27	0.41
2:B:5:GLU:HB3	2:B:73:LYS:HB3	2.02	0.41
1:C:1273:ILE:HD11	1:C:1287:GLN:HB2	2.02	0.41
1:C:2103:LEU:HD23	1:C:2103:LEU:HA	1.81	0.41
1:C:3920:THR:O	1:C:3920:THR:OG1	2.38	0.41
1:E:180:ASP:HB3	1:E:211:LEU:HD12	2.01	0.41
1:E:799:LYS:HA	1:E:1619:VAL:O	2.20	0.41
1:E:1171:HIS:O	1:E:1194:ASP:N	2.45	0.41
1:E:1250:TRP:NE1	1:E:1643:GLU:OE2	2.53	0.41
1:E:4770:LEU:C	1:G:4754:LEU:HD21	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4849:ILE:HD12	1:E:4849:ILE:HA	1.92	0.41
1:G:438:LYS:HA	1:G:438:LYS:HD3	1.88	0.41
1:G:677:LEU:HD11	1:G:792:VAL:HG21	2.02	0.41
1:G:900:LEU:HD23	1:G:902:TRP:HE1	1.84	0.41
1:G:1526:ASP:N	1:G:1526:ASP:OD1	2.52	0.41
1:G:2402:ARG:HA	1:G:2402:ARG:HD3	1.86	0.41
1:G:4892:CYS:HB3	1:G:4894:ILE:HG12	2.01	0.41
1:A:1250:TRP:HE1	1:A:1602:GLN:HG3	1.84	0.41
1:A:1300:MET:HB3	1:A:1302:TYR:CZ	2.55	0.41
1:A:1792:ILE:HG12	1:A:1842:ILE:HD11	2.01	0.41
1:A:1828:LEU:HD12	1:A:1828:LEU:HA	1.87	0.41
1:C:76:ARG:CB	1:C:76:ARG:NH2	2.73	0.41
1:C:1300:MET:HB3	1:C:1302:TYR:CZ	2.54	0.41
1:E:2328:ARG:CB	1:E:2329:PRO:CD	2.97	0.41
1:G:325:LYS:O	1:G:365:HIS:NE2	2.53	0.41
1:G:351:THR:OG1	1:G:352:SER:N	2.53	0.41
1:G:864:PRO:HG3	1:G:1034:PRO:HB3	2.01	0.41
1:G:2270:LEU:HD23	1:G:2270:LEU:HA	1.81	0.41
1:A:438:LYS:HD3	1:A:438:LYS:HA	1.87	0.41
1:A:1689:ILE:HD11	1:A:1706:LEU:HD22	2.02	0.41
1:A:3841:PHE:HB3	1:A:3920:THR:HG21	2.02	0.41
1:C:1570:LEU:HD23	1:C:1570:LEU:HA	1.95	0.41
1:C:1689:ILE:HD11	1:C:1706:LEU:HD22	2.02	0.41
1:C:2116:ASP:OD1	1:C:2116:ASP:N	2.46	0.41
1:E:1300:MET:HB3	1:E:1302:TYR:CZ	2.55	0.41
1:E:2099:LEU:HD12	1:E:2099:LEU:HA	1.92	0.41
1:E:3880:LEU:HD21	1:E:3940:ARG:HD2	2.01	0.41
1:E:3991:VAL:HG12	1:E:4145:ARG:NH2	2.35	0.41
1:E:4811:LEU:HD11	1:E:4815:MET:HE3	2.01	0.41
1:E:4819:TYR:O	1:E:4823:ARG:NE	2.53	0.41
1:G:1300:MET:HB3	1:G:1302:TYR:CZ	2.55	0.41
1:A:2073:GLU:H	1:A:2073:GLU:HG2	1.66	0.41
1:A:4523:VAL:HG11	1:G:4808:ASP:HB2	2.02	0.41
1:C:677:LEU:HD11	1:C:792:VAL:HG21	2.02	0.41
1:C:2128:ARG:O	1:C:2131:LEU:HB2	2.20	0.41
1:C:2270:LEU:HA	1:C:2270:LEU:HD23	1.81	0.41
1:E:281:ARG:NH2	1:E:284:TRP:O	2.54	0.41
1:E:1785:ASP:N	1:E:1785:ASP:OD1	2.53	0.41
1:E:1792:ILE:HG12	1:E:1842:ILE:HD11	2.01	0.41
1:E:1907:MET:HE3	1:E:1907:MET:HB2	1.77	0.41
2:F:42:ARG:HG3	2:F:44:LYS:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:281:ARG:NH2	1:G:284:TRP:O	2.54	0.41
1:G:1842:ILE:HD13	1:G:1842:ILE:HA	1.91	0.41
1:A:505:LEU:HD22	1:A:526:TRP:CD1	2.56	0.41
1:A:1942:ARG:HH12	1:A:3609:LEU:H	1.69	0.41
1:A:4808:ASP:HB2	1:C:4523:VAL:CG1	2.50	0.41
1:C:474:ASP:HA	1:C:477:ASN:HD22	1.85	0.41
1:C:2141:LYS:H	1:C:2141:LYS:HG3	1.74	0.41
1:E:505:LEU:HD22	1:E:526:TRP:CD1	2.56	0.41
1:E:3628:SER:OG	1:E:3629:TRP:N	2.54	0.41
1:G:644:LEU:HB3	1:G:1630:LEU:HD12	2.01	0.41
1:G:3663:ASP:HB2	1:G:3666:HIS:HB2	2.02	0.41
1:G:3841:PHE:HB3	1:G:3920:THR:HG21	2.02	0.41
1:G:4168:GLU:OE1	1:G:4595:LYS:NZ	2.46	0.41
1:G:4811:LEU:HD11	1:G:4815:MET:HE3	2.01	0.41
2:H:11:ASP:OD2	2:H:14:THR:OG1	2.35	0.41
1:A:1685:LEU:HD23	1:A:1685:LEU:HA	1.93	0.41
1:A:2834:LEU:HD13	1:A:2839:HIS:HB3	2.03	0.41
1:C:505:LEU:HD22	1:C:526:TRP:CD1	2.56	0.41
1:C:1250:TRP:NE1	1:C:1643:GLU:OE2	2.53	0.41
1:C:1731:GLU:O	1:C:1735:SER:OG	2.37	0.41
1:C:1906:GLN:HE21	1:C:1906:GLN:HB3	1.67	0.41
1:C:2071:ALA:HB2	1:C:2085:MET:HE1	2.03	0.41
1:C:2313:SER:OG	1:C:2402:ARG:O	2.33	0.41
1:C:2518:ASN:HA	1:C:2521:LEU:HD12	2.02	0.41
1:C:4770:LEU:C	1:E:4754:LEU:HD21	2.46	0.41
1:E:192:LEU:O	1:E:212:TRP:NE1	2.47	0.41
1:E:2067:MET:HE3	1:E:2085:MET:HG2	2.03	0.41
1:E:2834:LEU:HD13	1:E:2839:HIS:HB3	2.03	0.41
1:E:3663:ASP:HB2	1:E:3666:HIS:HB2	2.02	0.41
1:G:618:CYS:HB2	1:G:629:GLN:HG2	2.02	0.41
1:G:1614:ARG:HA	1:G:1614:ARG:HD3	1.86	0.41
2:H:11:ASP:OD1	2:H:11:ASP:N	2.52	0.41
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.90	0.41
1:A:558:LEU:HD23	1:A:558:LEU:HA	1.87	0.41
1:A:1757:LEU:HA	1:A:1757:LEU:HD12	1.89	0.41
1:A:3663:ASP:HB2	1:A:3666:HIS:HB2	2.02	0.41
1:A:4809:ASP:O	1:A:4813:CYS:N	2.49	0.41
1:C:1122:CYS:HA	1:C:1133:ARG:HD3	2.03	0.41
1:C:1630:LEU:HD22	1:C:1641:ILE:HG13	2.01	0.41
1:C:2067:MET:HE3	1:C:2085:MET:HG2	2.03	0.41
1:C:3993:ASN:HD22	1:C:4110:MET:HG3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4561:VAL:HG11	1:C:4570:GLU:HB3	2.03	0.41
1:C:4811:LEU:HD11	1:C:4815:MET:HE3	2.01	0.41
1:E:644:LEU:HB3	1:E:1630:LEU:HD12	2.01	0.41
1:E:1122:CYS:HA	1:E:1133:ARG:HD3	2.03	0.41
1:E:2071:ALA:HB2	1:E:2085:MET:HE1	2.02	0.41
1:E:2853:TRP:HA	1:E:2856:LYS:HB2	2.03	0.41
1:E:3844:LEU:HD23	1:E:3844:LEU:HA	1.84	0.41
1:E:3993:ASN:HD22	1:E:4110:MET:HG3	1.86	0.41
1:G:799:LYS:HA	1:G:1619:VAL:O	2.20	0.41
1:A:35:LEU:HD13	1:A:35:LEU:HA	1.96	0.41
1:A:618:CYS:HB2	1:A:629:GLN:HG2	2.02	0.41
1:A:2128:ARG:O	1:A:2131:LEU:HB2	2.20	0.41
1:C:2163:MET:N	1:C:2163:MET:SD	2.93	0.41
1:E:1097:LYS:HA	1:E:1168:MET:HE2	2.03	0.41
1:E:2518:ASN:HA	1:E:2521:LEU:HD12	2.02	0.41
2:F:5:GLU:HB3	2:F:73:LYS:HB3	2.02	0.41
1:G:505:LEU:HD22	1:G:526:TRP:CD1	2.56	0.41
1:G:1942:ARG:HH12	1:G:3609:LEU:H	1.69	0.41
1:G:2067:MET:HE3	1:G:2085:MET:HG2	2.03	0.41
1:G:3739:GLU:O	1:G:3743:GLN:N	2.53	0.41
1:A:55:SER:O	1:A:296:ARG:NH2	2.45	0.41
1:A:424:PHE:HB3	1:A:428:ARG:HH21	1.86	0.41
1:A:1526:ASP:OD1	1:A:1526:ASP:N	2.52	0.41
1:A:1907:MET:HB2	1:A:1907:MET:HE3	1.77	0.41
1:A:1939:ASP:OD1	1:A:1939:ASP:N	2.40	0.41
1:A:2110:ASN:OD1	1:A:2110:ASN:N	2.49	0.41
1:A:3739:GLU:O	1:A:3743:GLN:N	2.53	0.41
1:A:3883:GLN:HE21	1:A:3947:GLY:HA3	1.86	0.41
1:A:4103:LEU:HD23	1:A:4103:LEU:HA	1.94	0.41
1:C:424:PHE:HB3	1:C:428:ARG:HH21	1.86	0.41
1:C:424:PHE:HB3	1:C:428:ARG:NH2	2.36	0.41
1:C:618:CYS:HB2	1:C:629:GLN:HG2	2.02	0.41
1:C:1610:ARG:HE	1:C:1610:ARG:HB3	1.64	0.41
1:C:1614:ARG:HD3	1:C:1614:ARG:HA	1.86	0.41
1:C:1658:LEU:HD23	1:C:1658:LEU:HA	1.80	0.41
1:C:2099:LEU:HD12	1:C:2099:LEU:HA	1.92	0.41
1:C:2264:GLU:HG2	1:C:2324:LEU:CD1	2.51	0.41
1:C:3844:LEU:HD23	1:C:3844:LEU:HA	1.84	0.41
1:C:3991:VAL:HG12	1:C:4145:ARG:NH2	2.35	0.41
1:C:4108:GLU:OE1	1:C:4136:ARG:NH2	2.54	0.41
1:E:424:PHE:HB3	1:E:428:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:472:HIS:O	1:E:472:HIS:ND1	2.53	0.41
1:E:558:LEU:HD22	1:E:571:ILE:HG23	2.03	0.41
1:E:864:PRO:HG3	1:E:1034:PRO:HB3	2.01	0.41
1:E:2163:MET:N	1:E:2163:MET:SD	2.93	0.41
1:E:3739:GLU:O	1:E:3743:GLN:N	2.53	0.41
1:G:422:THR:HG21	1:G:459:LEU:HD11	2.03	0.41
1:G:2128:ARG:O	1:G:2131:LEU:HB2	2.20	0.41
1:G:2328:ARG:HA	1:G:2328:ARG:HD3	1.91	0.41
1:G:2834:LEU:HD13	1:G:2839:HIS:HB3	2.03	0.41
1:G:3829:LYS:HE3	1:G:3829:LYS:HB3	1.86	0.41
1:G:3883:GLN:HE21	1:G:3947:GLY:HA3	1.86	0.41
1:G:4561:VAL:HG11	1:G:4570:GLU:HB3	2.03	0.41
1:G:4791:ARG:HD2	1:G:4808:ASP:HB2	2.03	0.41
1:A:510:SER:HA	1:A:520:ARG:NH2	2.36	0.41
1:A:773:GLN:HA	1:A:774:PRO:HD3	1.94	0.41
1:A:799:LYS:HA	1:A:1619:VAL:O	2.20	0.41
1:A:2210:GLN:H	1:A:2210:GLN:HG2	1.74	0.41
1:A:4770:LEU:HD13	1:C:4751:PHE:CD1	2.56	0.41
1:C:3841:PHE:HB3	1:C:3920:THR:HG21	2.02	0.41
2:D:5:GLU:HB3	2:D:73:LYS:HB3	2.02	0.41
1:E:618:CYS:HB2	1:E:629:GLN:HG2	2.02	0.41
1:E:3841:PHE:HB3	1:E:3920:THR:HG21	2.02	0.41
1:E:4171:ARG:NE	5:E:6002:ATP:O2G	2.41	0.41
1:E:4561:VAL:HG11	1:E:4570:GLU:HB3	2.03	0.41
1:G:1785:ASP:OD1	1:G:1785:ASP:N	2.53	0.41
1:G:3991:VAL:HG23	1:G:3992:VAL:H	1.87	0.41
1:A:235:ARG:HE	1:A:274:LEU:HD21	1.86	0.40
1:A:424:PHE:HB3	1:A:428:ARG:NH2	2.36	0.40
1:A:474:ASP:HA	1:A:477:ASN:HD22	1.85	0.40
1:A:776:GLN:HB3	1:A:778:MET:HE3	2.03	0.40
1:A:1122:CYS:HA	1:A:1133:ARG:HD3	2.03	0.40
1:A:2103:LEU:HD23	1:A:2103:LEU:HA	1.81	0.40
1:A:3809:PHE:O	1:A:3813:ASN:N	2.50	0.40
1:C:143:LEU:HD22	1:E:2427:LEU:HD21	1.93	0.40
1:C:281:ARG:O	1:C:285:SER:OG	2.37	0.40
1:C:799:LYS:HA	1:C:1619:VAL:O	2.20	0.40
1:C:1719:LEU:HA	1:C:1719:LEU:HD23	1.87	0.40
1:C:4845:ILE:HD13	1:C:4845:ILE:HA	1.90	0.40
1:E:776:GLN:HB3	1:E:778:MET:HE3	2.03	0.40
1:E:1942:ARG:HH12	1:E:3609:LEU:H	1.69	0.40
1:E:2327:ARG:HA	1:E:2327:ARG:HD2	1.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3991:VAL:HG23	1:E:3992:VAL:H	1.87	0.40
1:E:4570:GLU:HG3	1:E:4571:PRO:HD3	2.03	0.40
1:G:235:ARG:HE	1:G:274:LEU:HD21	1.86	0.40
1:G:1097:LYS:HA	1:G:1168:MET:HE2	2.03	0.40
1:G:2853:TRP:HA	1:G:2856:LYS:HB2	2.03	0.40
1:G:3628:SER:OG	1:G:3629:TRP:N	2.54	0.40
1:G:3793:SER:O	1:G:3797:LEU:N	2.45	0.40
1:A:30:LYS:HA	1:A:30:LYS:HD3	1.69	0.40
1:A:2067:MET:HE3	1:A:2085:MET:HG2	2.03	0.40
1:A:2071:ALA:HB2	1:A:2085:MET:HE1	2.03	0.40
1:C:325:LYS:O	1:C:365:HIS:NE2	2.53	0.40
1:C:496:ASN:HA	1:C:499:LEU:HD12	2.04	0.40
1:C:3628:SER:OG	1:C:3629:TRP:N	2.54	0.40
1:C:4721:LEU:HD23	1:C:4721:LEU:HA	1.87	0.40
1:C:4782:TYR:HD1	1:C:4782:TYR:HA	1.78	0.40
1:E:496:ASN:HA	1:E:499:LEU:HD12	2.04	0.40
1:E:544:ASN:HB3	1:E:547:ASN:H	1.86	0.40
1:E:3883:GLN:HE21	1:E:3947:GLY:HA3	1.86	0.40
1:E:4791:ARG:HH22	1:G:4559:HIS:CE1	2.39	0.40
1:A:351:THR:OG1	1:A:352:SER:N	2.53	0.40
1:A:558:LEU:HD22	1:A:571:ILE:HG23	2.03	0.40
1:A:4811:LEU:HD11	1:A:4815:MET:HE3	2.01	0.40
1:A:4823:ARG:H	1:A:4823:ARG:HG3	1.55	0.40
1:C:281:ARG:NH2	1:C:284:TRP:O	2.54	0.40
1:C:558:LEU:HD22	1:C:571:ILE:HG23	2.03	0.40
1:C:876:PRO:HA	1:C:879:GLU:HB3	2.04	0.40
1:C:1482:ARG:HD2	1:C:1531:TYR:HA	2.03	0.40
1:C:2402:ARG:HA	1:C:2402:ARG:HD3	1.86	0.40
1:C:3921:LEU:HA	1:C:3921:LEU:HD23	1.88	0.40
1:C:4809:ASP:O	1:C:4813:CYS:N	2.49	0.40
1:E:876:PRO:HA	1:E:879:GLU:HB3	2.04	0.40
1:E:1102:TYR:HA	1:E:1164:CYS:O	2.22	0.40
1:E:2128:ARG:O	1:E:2131:LEU:HB2	2.20	0.40
1:E:2141:LYS:H	1:E:2141:LYS:HG3	1.74	0.40
1:G:544:ASN:HB3	1:G:547:ASN:H	1.86	0.40
1:G:1122:CYS:HA	1:G:1133:ARG:HD3	2.03	0.40
1:G:2071:ALA:HB2	1:G:2085:MET:HE1	2.02	0.40
1:G:4845:ILE:HD13	1:G:4845:ILE:HA	1.90	0.40
1:A:281:ARG:NH2	1:A:284:TRP:O	2.54	0.40
1:A:422:THR:HG21	1:A:459:LEU:HD11	2.03	0.40
1:A:495:ILE:H	1:A:495:ILE:HG13	1.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1102:TYR:HA	1:A:1164:CYS:O	2.22	0.40
1:A:2845:MET:HE3	1:A:2845:MET:HB3	1.92	0.40
1:A:3628:SER:OG	1:A:3629:TRP:N	2.54	0.40
2:B:103:LEU:HD11	2:B:106:LEU:HD21	2.03	0.40
1:C:510:SER:HA	1:C:520:ARG:NH2	2.36	0.40
1:C:1097:LYS:HA	1:C:1168:MET:HE2	2.03	0.40
1:C:2088:LEU:HA	1:C:2088:LEU:HD12	1.84	0.40
1:C:3714:SER:O	1:C:3714:SER:OG	2.34	0.40
1:C:3857:ASN:OD1	1:C:3860:ARG:NH1	2.52	0.40
1:E:424:PHE:HB3	1:E:428:ARG:HH21	1.86	0.40
1:E:1849:SER:OG	1:E:1849:SER:O	2.35	0.40
1:E:2322:VAL:HG11	1:E:2420:ILE:HG22	2.02	0.40
1:E:4596:VAL:HA	1:E:4599:VAL:HG12	2.04	0.40
1:E:4791:ARG:HD2	1:E:4808:ASP:HB2	2.03	0.40
1:G:424:PHE:HB3	1:G:428:ARG:NH2	2.36	0.40
1:G:558:LEU:HD22	1:G:571:ILE:HG23	2.03	0.40
1:G:3959:LEU:HD13	1:G:3968:LEU:HD22	2.04	0.40
1:G:4828:ILE:HD12	1:G:4828:ILE:HA	1.86	0.40
1:A:192:LEU:O	1:A:212:TRP:NE1	2.47	0.40
1:A:1591:LEU:HD23	1:A:1591:LEU:HA	1.92	0.40
1:A:1658:LEU:HD23	1:A:1658:LEU:HA	1.80	0.40
1:A:1785:ASP:N	1:A:1785:ASP:OD1	2.53	0.40
1:A:2853:TRP:HA	1:A:2856:LYS:HB2	2.03	0.40
1:A:3993:ASN:HD22	1:A:4110:MET:HG3	1.86	0.40
1:A:4561:VAL:HG11	1:A:4570:GLU:HB3	2.03	0.40
1:A:4888:LYS:HB3	1:A:4888:LYS:HE2	1.93	0.40
1:A:4911:LEU:HA	1:A:4915:ASN:HD22	1.87	0.40
1:C:192:LEU:O	1:C:212:TRP:NE1	2.47	0.40
1:C:472:HIS:ND1	1:C:472:HIS:O	2.53	0.40
1:C:1842:ILE:HD13	1:C:1842:ILE:HA	1.91	0.40
1:C:2513:MET:HE2	1:C:2513:MET:HB3	1.95	0.40
1:C:2834:LEU:HD13	1:C:2839:HIS:HB3	2.03	0.40
1:E:2226:SER:O	1:E:2226:SER:OG	2.33	0.40
2:F:11:ASP:OD2	2:F:14:THR:OG1	2.35	0.40
1:G:424:PHE:HB3	1:G:428:ARG:HH21	1.86	0.40
1:G:3714:SER:O	1:G:3714:SER:OG	2.35	0.40
1:G:3993:ASN:HD22	1:G:4110:MET:HG3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3336/4968 (67%)	2981 (89%)	347 (10%)	8 (0%)	43	74
1	C	3336/4968 (67%)	2982 (89%)	345 (10%)	9 (0%)	36	69
1	E	3336/4968 (67%)	2980 (89%)	347 (10%)	9 (0%)	36	69
1	G	3336/4968 (67%)	2980 (89%)	348 (10%)	8 (0%)	43	74
2	B	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	D	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	F	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	H	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
All	All	13764/20304 (68%)	12323 (90%)	1407 (10%)	34 (0%)	44	74

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2328	ARG
1	A	4901	THR
1	C	2328	ARG
1	C	4901	THR
1	E	2328	ARG
1	E	4901	THR
1	G	2328	ARG
1	G	4901	THR
1	C	2329	PRO
1	E	2329	PRO
1	A	1580	PRO
1	C	1580	PRO
1	E	1580	PRO
1	G	1580	PRO
1	A	853	PRO
1	A	4916	LEU
1	C	853	PRO

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Mol	Chain	Res	Type
1	C	4916	LEU
1	E	853	PRO
1	E	4916	LEU
1	G	853	PRO
1	G	4916	LEU
1	A	1848	PRO
1	C	1848	PRO
1	E	1848	PRO
1	G	1848	PRO
1	A	1535	PRO
1	C	1535	PRO
1	E	1535	PRO
1	G	1535	PRO
1	A	828	PRO
1	C	828	PRO
1	E	828	PRO
1	G	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	2650/4355 (61%)	2629 (99%)	21 (1%)	73	77
1	C	2650/4355 (61%)	2625 (99%)	25 (1%)	70	75
1	E	2648/4355 (61%)	2623 (99%)	25 (1%)	70	75
1	G	2650/4355 (61%)	2629 (99%)	21 (1%)	73	77
2	B	88/89 (99%)	88 (100%)	0	100	100
2	D	88/89 (99%)	88 (100%)	0	100	100
2	F	88/89 (99%)	88 (100%)	0	100	100
2	H	88/89 (99%)	88 (100%)	0	100	100
All	All	10950/17776 (62%)	10858 (99%)	92 (1%)	70	77

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ARG
1	A	143	LEU
1	A	637	LEU
1	A	855	VAL
1	A	907	VAL
1	A	950	VAL
1	A	990	PRO
1	A	1033	VAL
1	A	1466	THR
1	A	1611	ILE
1	A	1932	ASP
1	A	2217	ASP
1	A	2315	GLU
1	A	2324	LEU
1	A	2832	VAL
1	A	2877	THR
1	A	3803	VAL
1	A	3992	VAL
1	A	4014	ILE
1	A	4161	TRP
1	A	4823	ARG
1	C	76	ARG
1	C	143	LEU
1	C	207	PHE
1	C	637	LEU
1	C	855	VAL
1	C	907	VAL
1	C	950	VAL
1	C	990	PRO
1	C	1033	VAL
1	C	1466	THR
1	C	1611	ILE
1	C	1932	ASP
1	C	2217	ASP
1	C	2315	GLU
1	C	2323	ARG
1	C	2324	LEU
1	C	2327	ARG
1	C	2328	ARG
1	C	2832	VAL
1	C	2877	THR
1	C	3803	VAL
1	C	3992	VAL

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Mol	Chain	Res	Type
1	C	4014	ILE
1	C	4161	TRP
1	C	4823	ARG
1	E	143	LEU
1	E	207	PHE
1	E	637	LEU
1	E	855	VAL
1	E	907	VAL
1	E	990	PRO
1	E	1033	VAL
1	E	1466	THR
1	E	1611	ILE
1	E	1932	ASP
1	E	2217	ASP
1	E	2315	GLU
1	E	2320	VAL
1	E	2323	ARG
1	E	2324	LEU
1	E	2327	ARG
1	E	2328	ARG
1	E	2832	VAL
1	E	2877	THR
1	E	3618	VAL
1	E	3803	VAL
1	E	3992	VAL
1	E	4014	ILE
1	E	4161	TRP
1	E	4823	ARG
1	G	143	LEU
1	G	207	PHE
1	G	637	LEU
1	G	855	VAL
1	G	907	VAL
1	G	950	VAL
1	G	990	PRO
1	G	1033	VAL
1	G	1466	THR
1	G	1611	ILE
1	G	1932	ASP
1	G	2217	ASP
1	G	2315	GLU
1	G	2324	LEU

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Mol	Chain	Res	Type
1	G	2832	VAL
1	G	2877	THR
1	G	3803	VAL
1	G	3992	VAL
1	G	4014	ILE
1	G	4161	TRP
1	G	4823	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (204) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	123	HIS
1	A	394	HIS
1	A	476	GLN
1	A	477	ASN
1	A	490	GLN
1	A	496	ASN
1	A	593	HIS
1	A	604	HIS
1	A	628	ASN
1	A	651	HIS
1	A	692	HIS
1	A	771	ASN
1	A	890	HIS
1	A	914	GLN
1	A	915	HIS
1	A	1004	HIS
1	A	1005	ASN
1	A	1265	HIS
1	A	1293	GLN
1	A	1503	ASN
1	A	1589	GLN
1	A	1636	ASN
1	A	1691	ASN
1	A	1805	HIS
1	A	1836	ASN
1	A	1906	GLN
1	A	1918	GLN
1	A	1940	ASN
1	A	2119	ASN
1	A	2152	ASN

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Mol	Chain	Res	Type
1	A	2317	ASN
1	A	2848	ASN
1	A	2851	ASN
1	A	3852	ASN
1	A	3916	GLN
1	A	3956	GLN
1	A	3961	GLN
1	A	3993	ASN
1	A	4490	GLN
1	A	4494	ASN
1	A	4559	HIS
1	A	4621	GLN
1	A	4880	GLN
1	A	4904	HIS
1	A	4915	ASN
1	A	4934	HIS
1	A	4937	GLN
2	B	25	HIS
2	B	31	GLN
1	C	23	GLN
1	C	123	HIS
1	C	209	GLN
1	C	394	HIS
1	C	476	GLN
1	C	477	ASN
1	C	490	GLN
1	C	496	ASN
1	C	593	HIS
1	C	604	HIS
1	C	628	ASN
1	C	651	HIS
1	C	692	HIS
1	C	771	ASN
1	C	890	HIS
1	C	903	GLN
1	C	914	GLN
1	C	915	HIS
1	C	1005	ASN
1	C	1265	HIS
1	C	1293	GLN
1	C	1440	ASN
1	C	1452	GLN

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Mol	Chain	Res	Type
1	C	1503	ASN
1	C	1589	GLN
1	C	1636	ASN
1	C	1691	ASN
1	C	1805	HIS
1	C	1836	ASN
1	C	1906	GLN
1	C	1918	GLN
1	C	1940	ASN
1	C	2119	ASN
1	C	2152	ASN
1	C	2317	ASN
1	C	2848	ASN
1	C	2851	ASN
1	C	3852	ASN
1	C	3916	GLN
1	C	3956	GLN
1	C	3961	GLN
1	C	3990	ASN
1	C	3993	ASN
1	C	4490	GLN
1	C	4559	HIS
1	C	4621	GLN
1	C	4880	GLN
1	C	4904	HIS
1	C	4915	ASN
1	C	4934	HIS
1	C	4937	GLN
2	D	25	HIS
2	D	31	GLN
1	E	23	GLN
1	E	123	HIS
1	E	209	GLN
1	E	394	HIS
1	E	476	GLN
1	E	477	ASN
1	E	490	GLN
1	E	496	ASN
1	E	593	HIS
1	E	604	HIS
1	E	628	ASN
1	E	651	HIS

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Mol	Chain	Res	Type
1	E	692	HIS
1	E	771	ASN
1	E	890	HIS
1	E	914	GLN
1	E	915	HIS
1	E	1005	ASN
1	E	1265	HIS
1	E	1293	GLN
1	E	1452	GLN
1	E	1503	ASN
1	E	1589	GLN
1	E	1626	GLN
1	E	1636	ASN
1	E	1691	ASN
1	E	1805	HIS
1	E	1836	ASN
1	E	1906	GLN
1	E	1918	GLN
1	E	1940	ASN
1	E	2119	ASN
1	E	2152	ASN
1	E	2317	ASN
1	E	2319	ASN
1	E	2848	ASN
1	E	2851	ASN
1	E	3852	ASN
1	E	3916	GLN
1	E	3956	GLN
1	E	3961	GLN
1	E	3990	ASN
1	E	3993	ASN
1	E	4490	GLN
1	E	4494	ASN
1	E	4559	HIS
1	E	4621	GLN
1	E	4880	GLN
1	E	4904	HIS
1	E	4915	ASN
1	E	4934	HIS
1	E	4937	GLN
2	F	25	HIS
2	F	31	GLN

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Mol	Chain	Res	Type
1	G	23	GLN
1	G	123	HIS
1	G	394	HIS
1	G	410	HIS
1	G	477	ASN
1	G	490	GLN
1	G	496	ASN
1	G	593	HIS
1	G	604	HIS
1	G	628	ASN
1	G	651	HIS
1	G	771	ASN
1	G	890	HIS
1	G	914	GLN
1	G	915	HIS
1	G	1005	ASN
1	G	1265	HIS
1	G	1293	GLN
1	G	1452	GLN
1	G	1589	GLN
1	G	1636	ASN
1	G	1691	ASN
1	G	1805	HIS
1	G	1836	ASN
1	G	1906	GLN
1	G	1918	GLN
1	G	1940	ASN
1	G	2119	ASN
1	G	2152	ASN
1	G	2317	ASN
1	G	2848	ASN
1	G	2851	ASN
1	G	3852	ASN
1	G	3916	GLN
1	G	3961	GLN
1	G	3993	ASN
1	G	4490	GLN
1	G	4494	ASN
1	G	4559	HIS
1	G	4621	GLN
1	G	4880	GLN
1	G	4904	HIS

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Mol	Chain	Res	Type
1	G	4915	ASN
1	G	4934	HIS
1	G	4937	GLN
2	H	25	HIS
2	H	31	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 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	$\# Z > 2$
5	ATP	A	6002	-	32,33,33	1.34	4 (12%)	48,52,52	1.67	8 (16%)
6	CFF	G	6003	-	15,15,15	2.28	8 (53%)	23,23,23	2.80	9 (39%)
5	ATP	E	6002	-	32,33,33	1.34	4 (12%)	48,52,52	1.67	8 (16%)
5	ATP	C	6002	-	32,33,33	1.34	4 (12%)	48,52,52	1.68	8 (16%)
6	CFF	E	6003	-	15,15,15	2.28	8 (53%)	23,23,23	2.80	10 (43%)
5	ATP	G	6002	-	32,33,33	1.34	4 (12%)	48,52,52	1.67	8 (16%)
6	CFF	A	6003	-	15,15,15	2.28	8 (53%)	23,23,23	2.80	9 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CFF	C	6003	-	15,15,15	2.28	8 (53%)	23,23,23	2.79	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
5	ATP	A	6002	-	-	5/22/38/38	0/3/3/3
6	CFF	G	6003	-	-	-	0/2/2/2
5	ATP	E	6002	-	-	5/22/38/38	0/3/3/3
5	ATP	C	6002	-	-	5/22/38/38	0/3/3/3
6	CFF	E	6003	-	-	-	0/2/2/2
5	ATP	G	6002	-	-	5/22/38/38	0/3/3/3
6	CFF	A	6003	-	-	-	0/2/2/2
6	CFF	C	6003	-	-	-	0/2/2/2

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	6003	CFF	C6-N1	-4.13	1.31	1.40
6	C	6003	CFF	C6-N1	-4.13	1.31	1.40
6	G	6003	CFF	C6-N1	-4.13	1.31	1.40
6	E	6003	CFF	C6-N1	-4.12	1.31	1.40
5	A	6002	ATP	C5-N7	-3.94	1.31	1.39
5	C	6002	ATP	C5-N7	-3.94	1.31	1.39
5	E	6002	ATP	C5-N7	-3.94	1.31	1.39
5	G	6002	ATP	C5-N7	-3.94	1.31	1.39
6	E	6003	CFF	C4-N3	-3.60	1.32	1.38
6	A	6003	CFF	C4-N3	-3.57	1.32	1.38
6	C	6003	CFF	C4-N3	-3.57	1.32	1.38
6	G	6003	CFF	C4-N3	-3.57	1.32	1.38
5	A	6002	ATP	C5-C4	3.47	1.45	1.39
5	C	6002	ATP	C5-C4	3.47	1.45	1.39
5	E	6002	ATP	C5-C4	3.47	1.45	1.39
5	G	6002	ATP	C5-C4	3.47	1.45	1.39
6	A	6003	CFF	C5-N7	-2.92	1.33	1.38
6	C	6003	CFF	C5-N7	-2.92	1.33	1.38
6	E	6003	CFF	C5-N7	-2.92	1.33	1.38
6	G	6003	CFF	C5-N7	-2.92	1.33	1.38
5	E	6002	ATP	C4-N9	-2.80	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	6002	ATP	C4-N9	-2.79	1.31	1.37
5	C	6002	ATP	C4-N9	-2.79	1.31	1.37
5	G	6002	ATP	C4-N9	-2.79	1.31	1.37
6	A	6003	CFF	C5-C6	-2.52	1.36	1.43
6	C	6003	CFF	C5-C6	-2.52	1.36	1.43
6	E	6003	CFF	C5-C6	-2.52	1.36	1.43
6	G	6003	CFF	C5-C6	-2.52	1.36	1.43
6	E	6003	CFF	C2-N3	-2.45	1.34	1.39
6	A	6003	CFF	C2-N3	-2.43	1.34	1.39
6	C	6003	CFF	C2-N3	-2.43	1.34	1.39
6	G	6003	CFF	C2-N3	-2.43	1.34	1.39
6	A	6003	CFF	O13-C6	-2.41	1.18	1.23
6	C	6003	CFF	O13-C6	-2.41	1.18	1.23
6	E	6003	CFF	O13-C6	-2.41	1.18	1.23
6	G	6003	CFF	O13-C6	-2.41	1.18	1.23
5	A	6002	ATP	C8-N9	-2.35	1.33	1.37
5	C	6002	ATP	C8-N9	-2.35	1.33	1.37
5	E	6002	ATP	C8-N9	-2.35	1.33	1.37
5	G	6002	ATP	C8-N9	-2.35	1.33	1.37
6	A	6003	CFF	C2-N1	-2.35	1.34	1.39
6	C	6003	CFF	C2-N1	-2.35	1.34	1.39
6	E	6003	CFF	C2-N1	-2.35	1.34	1.39
6	G	6003	CFF	C2-N1	-2.35	1.34	1.39
6	A	6003	CFF	O11-C2	-2.21	1.18	1.22
6	E	6003	CFF	O11-C2	-2.21	1.18	1.22
6	G	6003	CFF	O11-C2	-2.21	1.18	1.22
6	C	6003	CFF	O11-C2	-2.20	1.18	1.22

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	6003	CFF	C14-N7-C8	-7.81	111.67	126.28
6	G	6003	CFF	C14-N7-C8	-7.81	111.67	126.28
6	C	6003	CFF	C14-N7-C8	-7.79	111.70	126.28
6	E	6003	CFF	C14-N7-C8	-7.78	111.73	126.28
5	C	6002	ATP	C5-C4-N3	-5.37	119.32	126.72
5	A	6002	ATP	C5-C4-N3	-5.35	119.34	126.72
5	E	6002	ATP	C5-C4-N3	-5.35	119.34	126.72
5	G	6002	ATP	C5-C4-N3	-5.35	119.34	126.72
6	A	6003	CFF	C14-N7-C5	5.29	140.37	127.77
6	C	6003	CFF	C14-N7-C5	5.29	140.37	127.77
6	E	6003	CFF	C14-N7-C5	5.29	140.37	127.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	6003	CFF	C14-N7-C5	5.29	140.37	127.77
5	C	6002	ATP	N3-C4-N9	4.93	135.55	127.17
5	A	6002	ATP	N3-C4-N9	4.91	135.53	127.17
5	G	6002	ATP	N3-C4-N9	4.91	135.53	127.17
5	E	6002	ATP	N3-C4-N9	4.90	135.49	127.17
6	E	6003	CFF	C5-C6-N1	4.35	120.02	112.06
6	A	6003	CFF	C5-C6-N1	4.33	119.99	112.06
6	C	6003	CFF	C5-C6-N1	4.33	119.99	112.06
6	G	6003	CFF	C5-C6-N1	4.33	119.99	112.06
5	A	6002	ATP	N3-C2-N1	-3.68	123.01	128.58
5	G	6002	ATP	N3-C2-N1	-3.68	123.01	128.58
5	C	6002	ATP	N3-C2-N1	-3.67	123.02	128.58
5	E	6002	ATP	N3-C2-N1	-3.66	123.04	128.58
6	E	6003	CFF	C6-N1-C2	-3.44	120.07	125.66
5	C	6002	ATP	C2-N3-C4	3.43	120.20	111.83
5	A	6002	ATP	C2-N3-C4	3.42	120.18	111.83
5	G	6002	ATP	C2-N3-C4	3.42	120.18	111.83
6	A	6003	CFF	C6-N1-C2	-3.42	120.10	125.66
6	C	6003	CFF	C6-N1-C2	-3.42	120.10	125.66
6	G	6003	CFF	C6-N1-C2	-3.42	120.10	125.66
5	E	6002	ATP	C2-N3-C4	3.41	120.16	111.83
6	A	6003	CFF	O13-C6-C5	-3.06	120.10	126.38
6	C	6003	CFF	O13-C6-C5	-3.06	120.10	126.38
6	E	6003	CFF	O13-C6-C5	-3.06	120.10	126.38
6	G	6003	CFF	O13-C6-C5	-3.06	120.10	126.38
6	A	6003	CFF	N7-C8-N9	-2.95	108.14	113.48
6	G	6003	CFF	N7-C8-N9	-2.95	108.14	113.48
6	C	6003	CFF	N7-C8-N9	-2.93	108.17	113.48
6	E	6003	CFF	N7-C8-N9	-2.91	108.20	113.48
6	E	6003	CFF	C6-C5-C4	-2.80	119.39	122.92
6	A	6003	CFF	C6-C5-C4	-2.77	119.43	122.92
6	C	6003	CFF	C6-C5-C4	-2.77	119.43	122.92
6	G	6003	CFF	C6-C5-C4	-2.77	119.43	122.92
5	E	6002	ATP	N6-C6-N1	2.74	124.49	118.38
5	A	6002	ATP	N6-C6-N1	2.73	124.45	118.38
5	C	6002	ATP	N6-C6-N1	2.73	124.45	118.38
5	G	6002	ATP	N6-C6-N1	2.73	124.45	118.38
6	E	6003	CFF	N3-C4-N9	2.72	130.55	126.27
6	A	6003	CFF	N3-C4-N9	2.68	130.49	126.27
6	G	6003	CFF	N3-C4-N9	2.68	130.49	126.27
6	C	6003	CFF	N3-C4-N9	2.67	130.47	126.27
5	C	6002	ATP	C2'-C1'-N9	-2.44	107.24	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	6002	ATP	C2'-C1'-N9	-2.43	107.26	113.30
5	E	6002	ATP	C2'-C1'-N9	-2.43	107.26	113.30
5	G	6002	ATP	C2'-C1'-N9	-2.43	107.26	113.30
5	E	6002	ATP	C5-C6-N6	-2.42	117.29	123.29
5	A	6002	ATP	C5-C6-N6	-2.42	117.30	123.29
5	C	6002	ATP	C5-C6-N6	-2.42	117.30	123.29
5	G	6002	ATP	C5-C6-N6	-2.42	117.30	123.29
5	A	6002	ATP	C4-N9-C8	2.27	108.12	105.74
5	C	6002	ATP	C4-N9-C8	2.27	108.12	105.74
5	G	6002	ATP	C4-N9-C8	2.27	108.12	105.74
5	E	6002	ATP	C4-N9-C8	2.24	108.09	105.74
6	E	6003	CFF	C12-N3-C2	2.19	121.14	117.33
6	A	6003	CFF	C12-N3-C2	2.18	121.14	117.33
6	C	6003	CFF	C12-N3-C2	2.18	121.14	117.33
6	G	6003	CFF	C12-N3-C2	2.18	121.14	117.33
6	E	6003	CFF	C10-N1-C6	2.02	120.78	117.64

There are no chirality outliers.

All (20) torsion outliers are listed below:

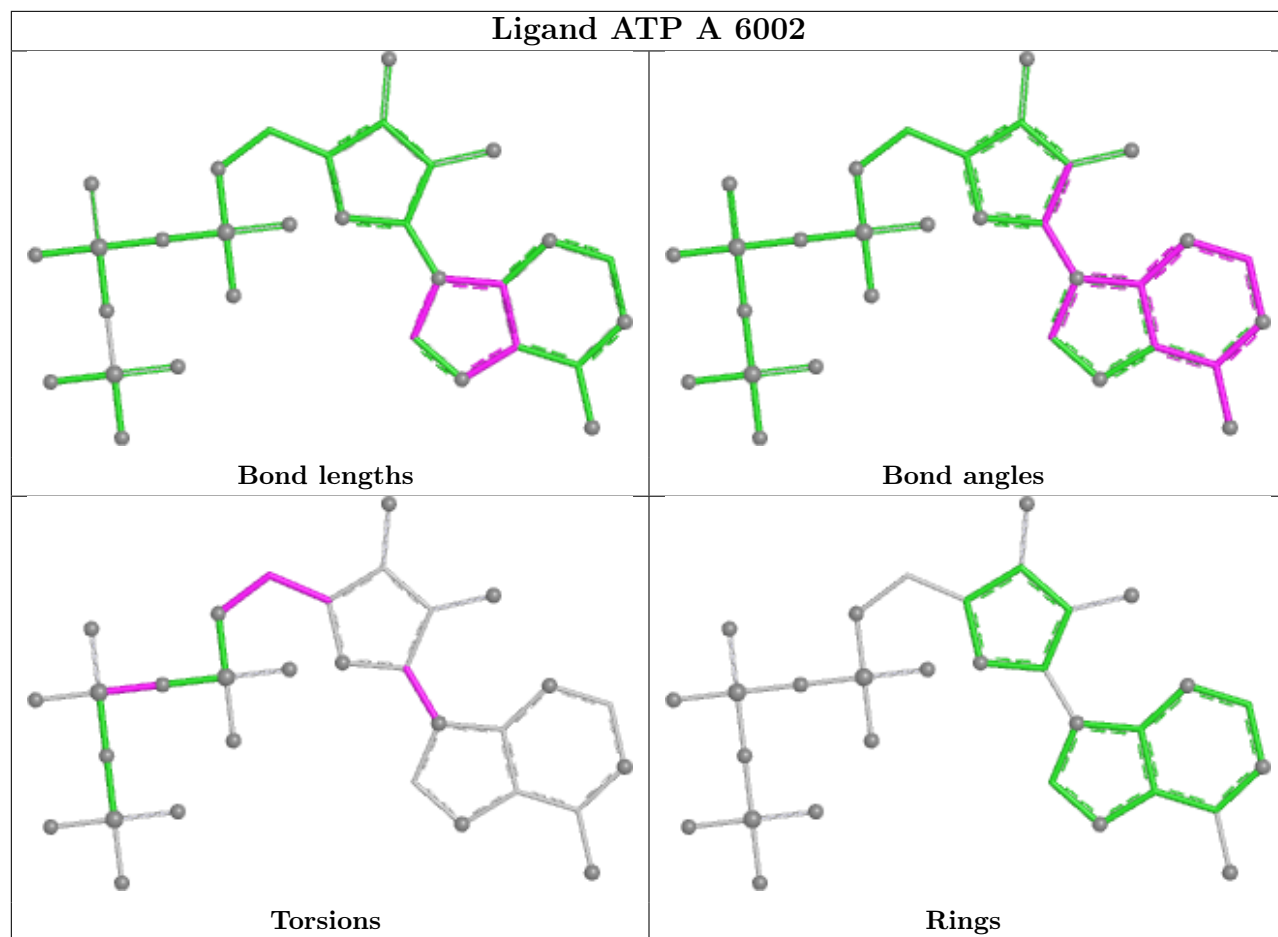
Mol	Chain	Res	Type	Atoms
5	A	6002	ATP	C3'-C4'-C5'-O5'
5	C	6002	ATP	C3'-C4'-C5'-O5'
5	E	6002	ATP	C3'-C4'-C5'-O5'
5	G	6002	ATP	C3'-C4'-C5'-O5'
5	A	6002	ATP	O4'-C4'-C5'-O5'
5	C	6002	ATP	O4'-C4'-C5'-O5'
5	E	6002	ATP	O4'-C4'-C5'-O5'
5	G	6002	ATP	O4'-C4'-C5'-O5'
5	A	6002	ATP	PA-O3A-PB-O1B
5	C	6002	ATP	PA-O3A-PB-O1B
5	E	6002	ATP	PA-O3A-PB-O1B
5	G	6002	ATP	PA-O3A-PB-O1B
5	A	6002	ATP	C4'-C5'-O5'-PA
5	C	6002	ATP	C4'-C5'-O5'-PA
5	E	6002	ATP	C4'-C5'-O5'-PA
5	G	6002	ATP	C4'-C5'-O5'-PA
5	C	6002	ATP	O4'-C1'-N9-C8
5	A	6002	ATP	O4'-C1'-N9-C8
5	E	6002	ATP	O4'-C1'-N9-C8
5	G	6002	ATP	O4'-C1'-N9-C8

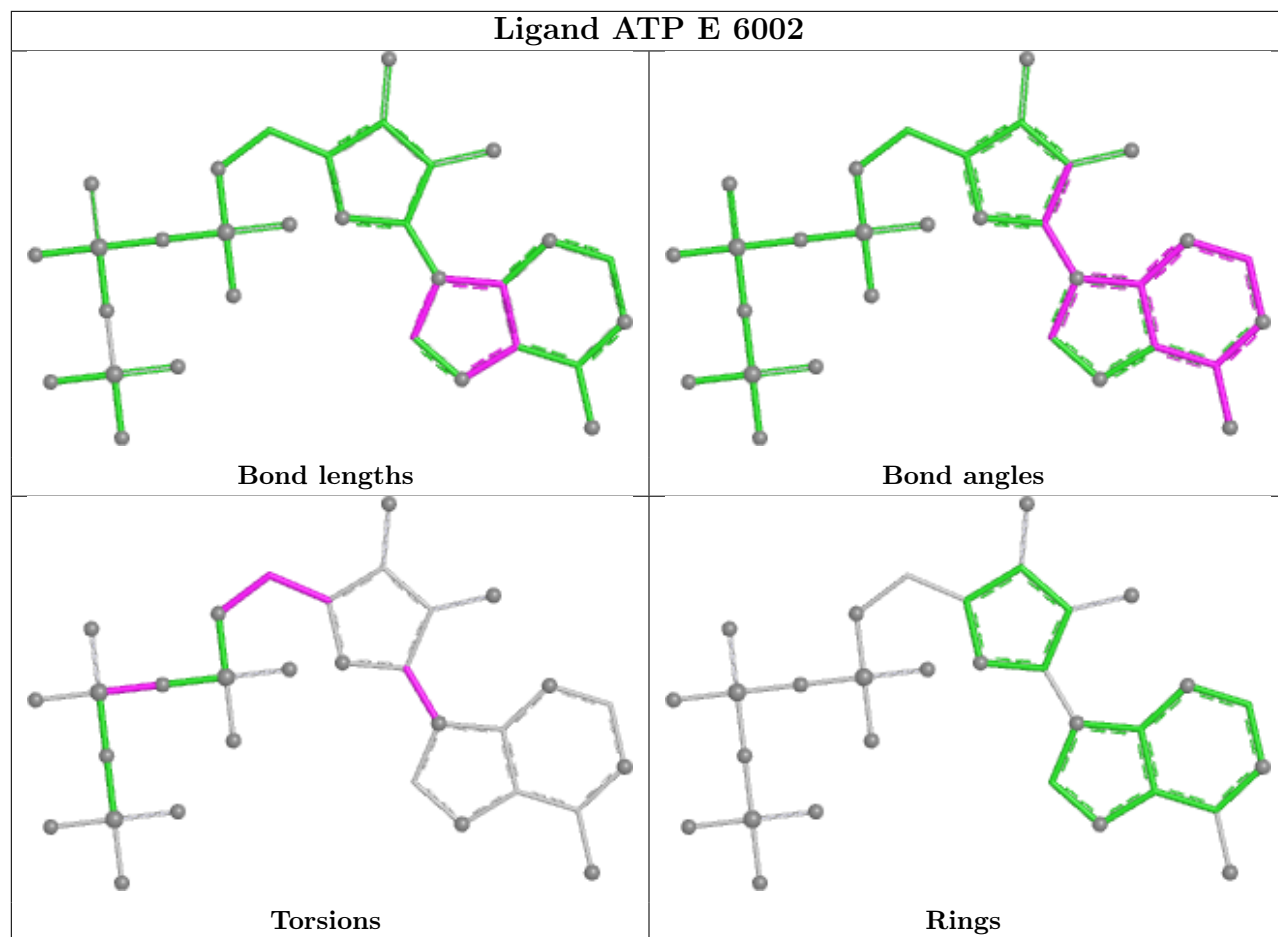
There are no ring outliers.

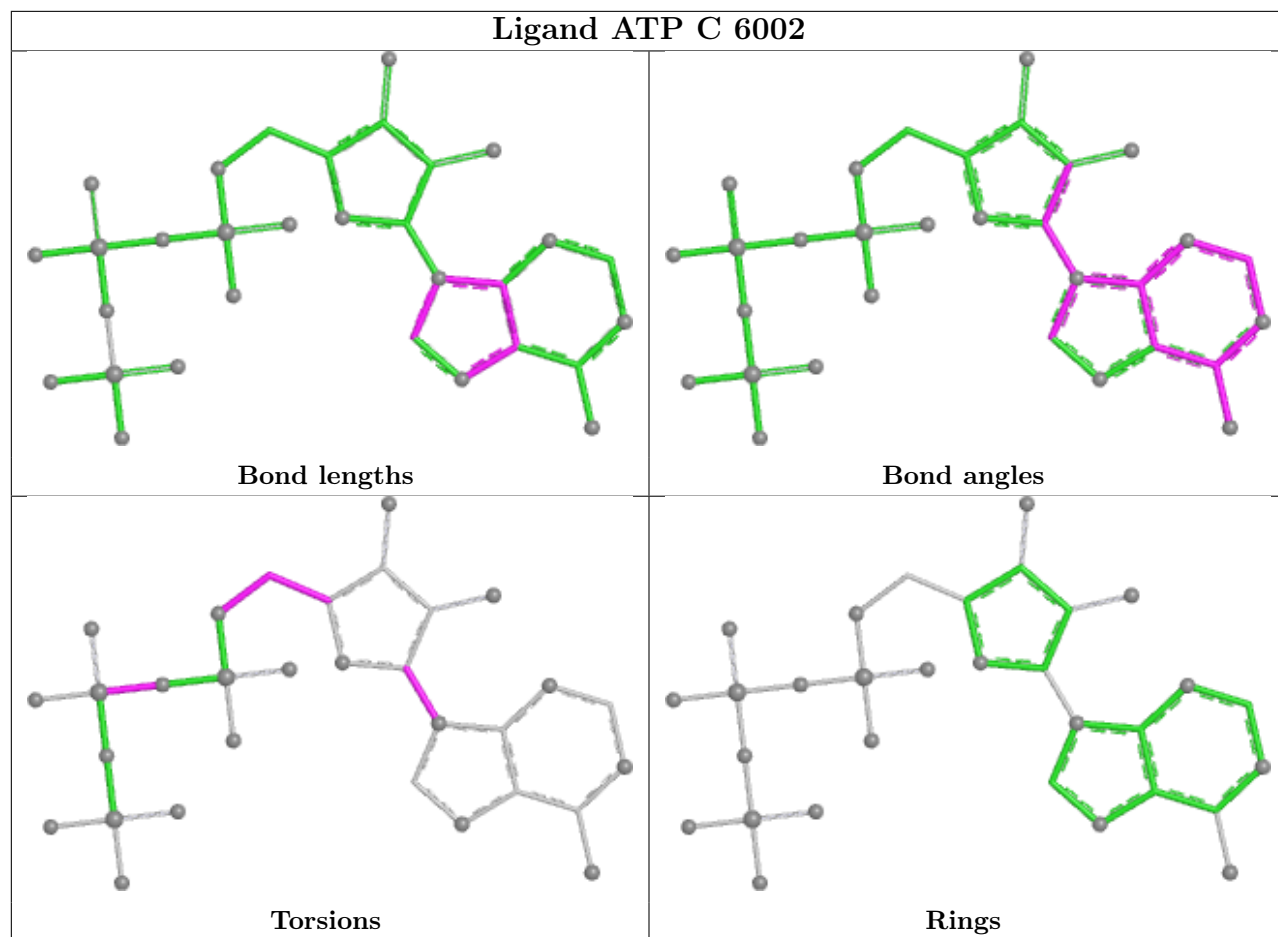
8 monomers are involved in 8 short contacts:

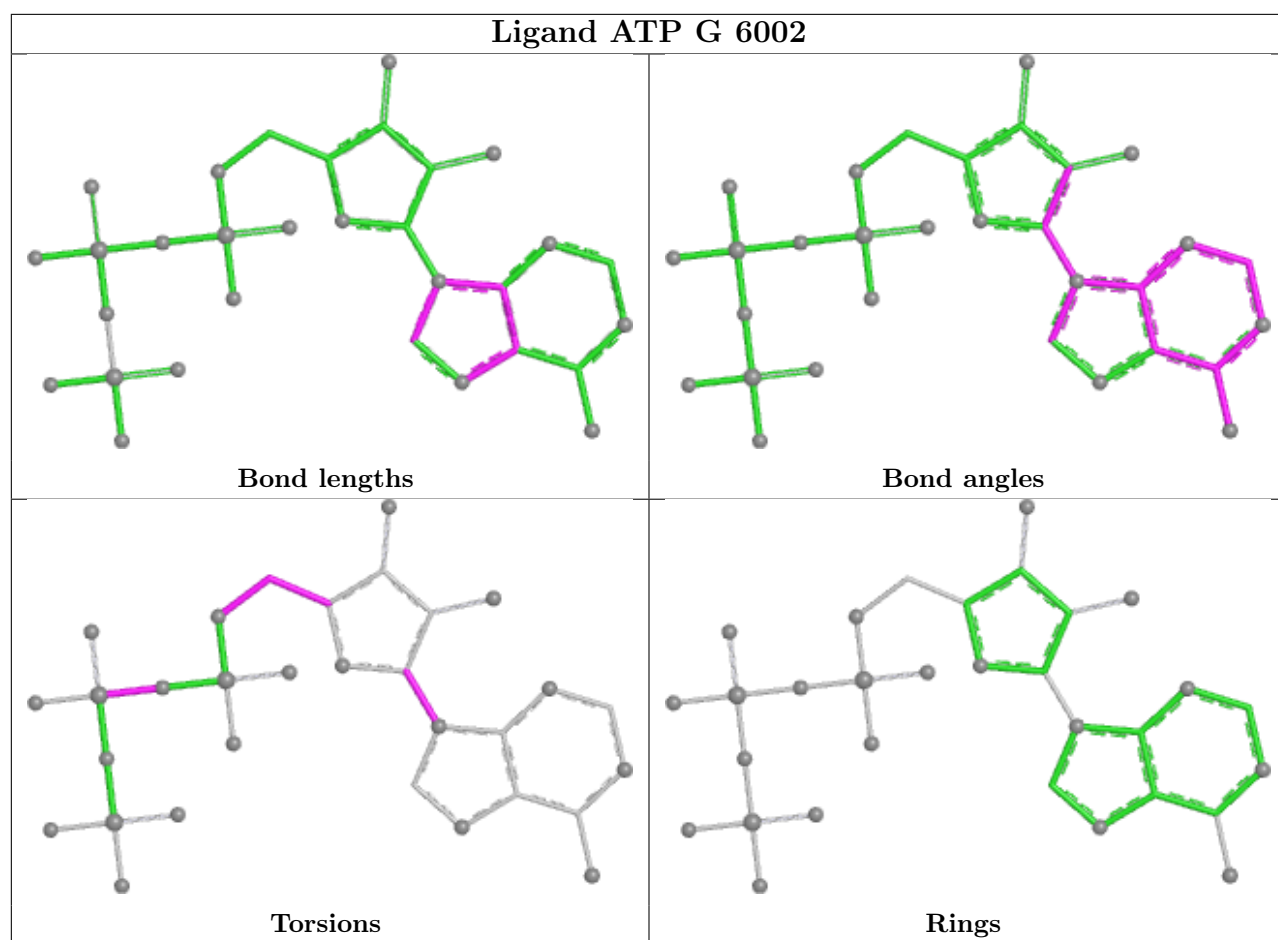
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	6002	ATP	1	0
6	G	6003	CFF	1	0
5	E	6002	ATP	1	0
5	C	6002	ATP	1	0
6	E	6003	CFF	1	0
5	G	6002	ATP	1	0
6	A	6003	CFF	1	0
6	C	6003	CFF	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

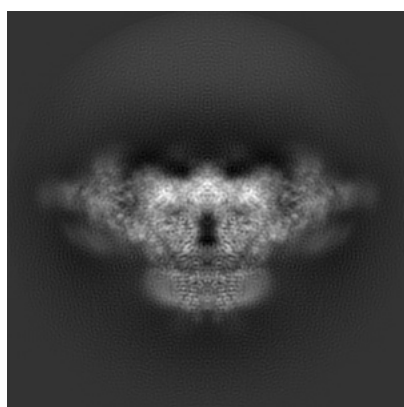
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9879. These allow visual inspection of the internal detail of the map and identification of artifacts.

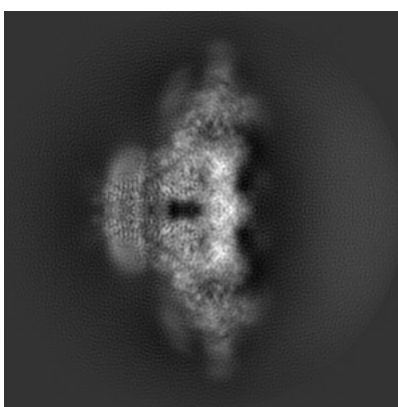
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

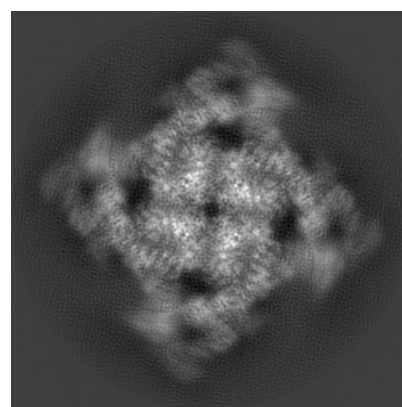
6.1.1 Primary map



X



Y

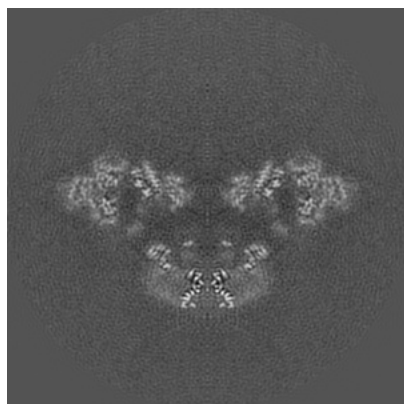


Z

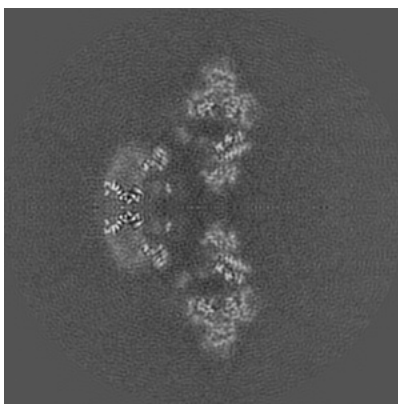
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

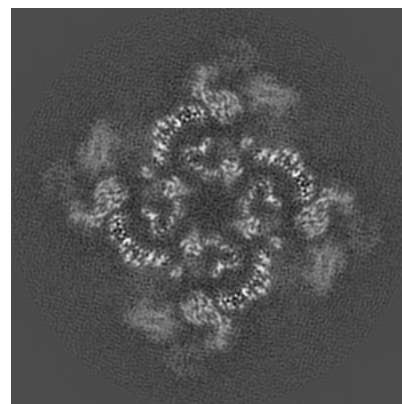
6.2.1 Primary map



X Index: 200



Y Index: 200

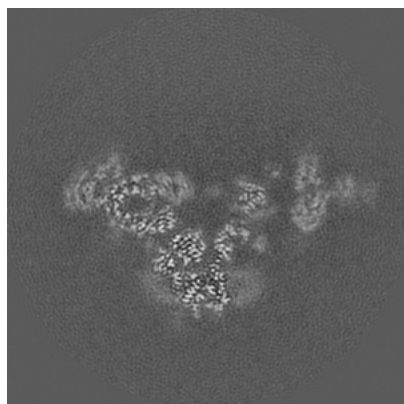


Z Index: 200

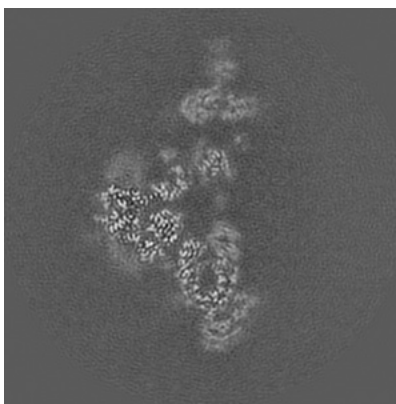
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

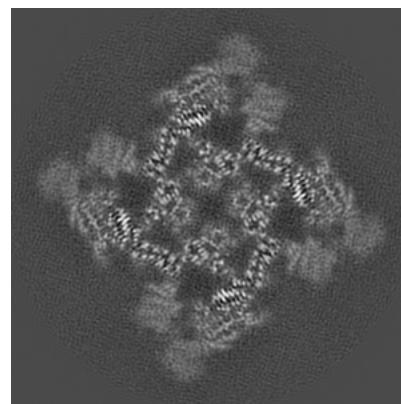
6.3.1 Primary map



X Index: 213



Y Index: 187

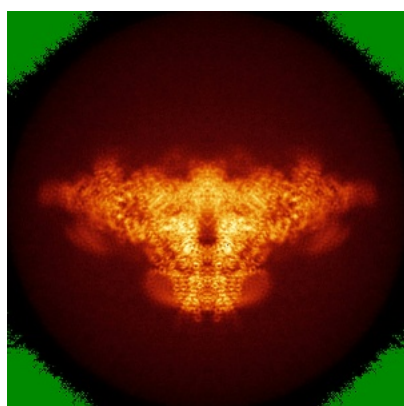


Z Index: 211

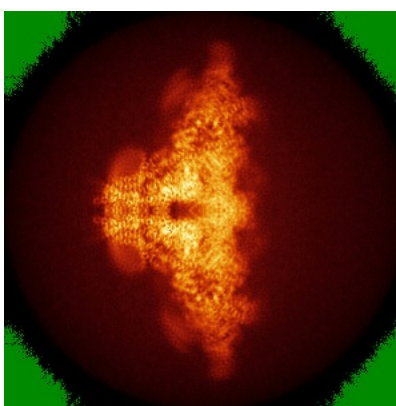
The images above show the largest variance slices of the map in three orthogonal directions.

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

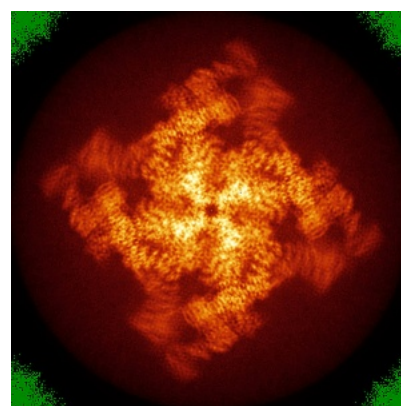
6.4.1 Primary map



X



Y

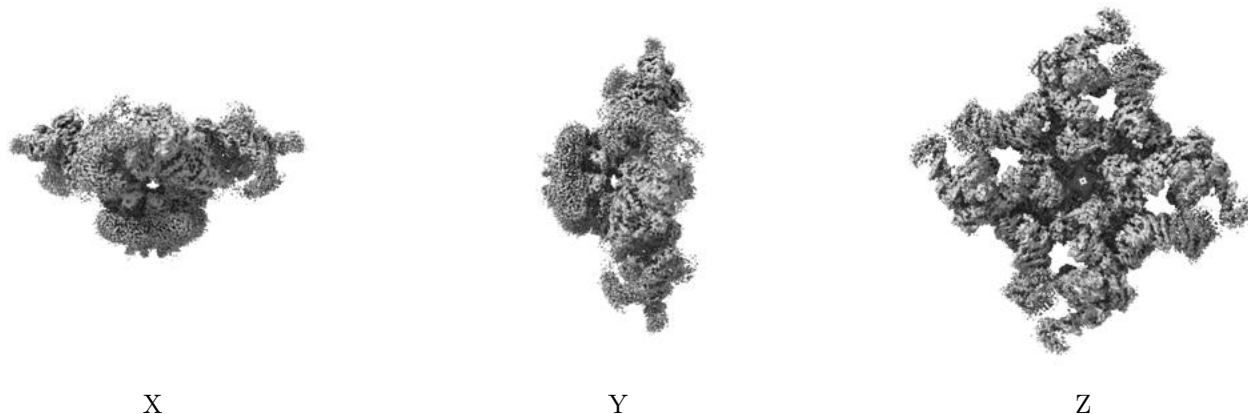


Z

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 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

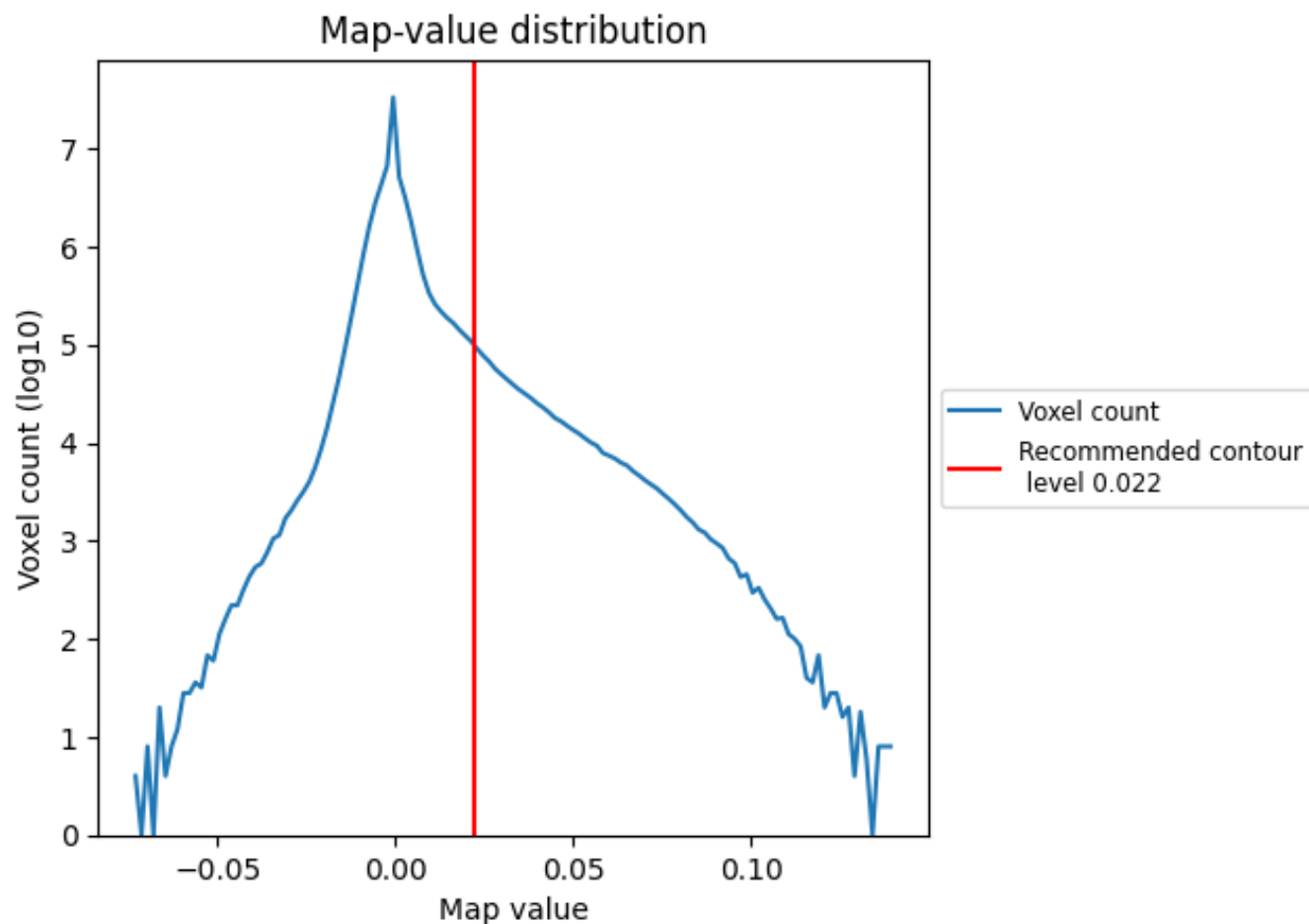
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

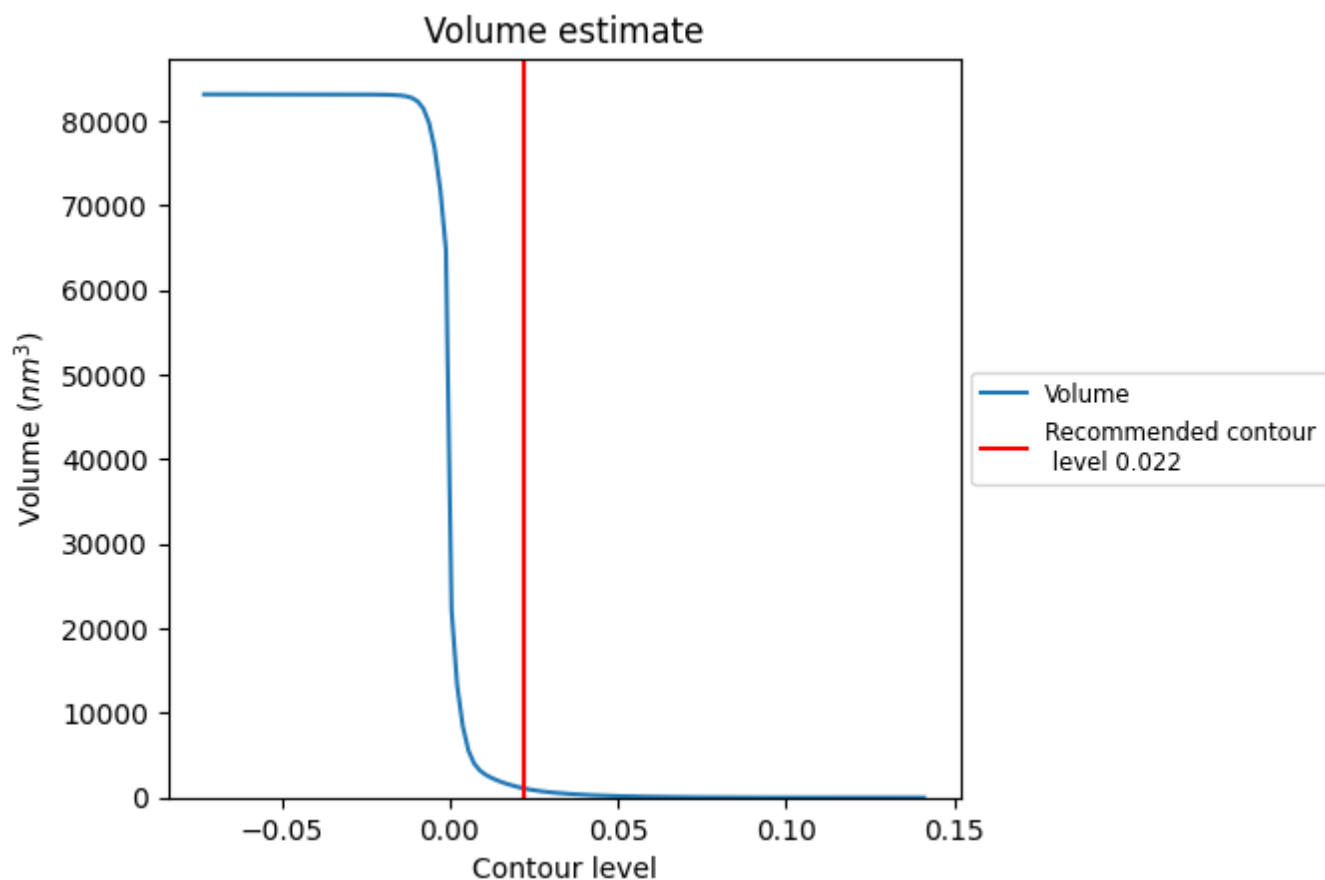
This section contains the results of statistical analysis of the map.

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.

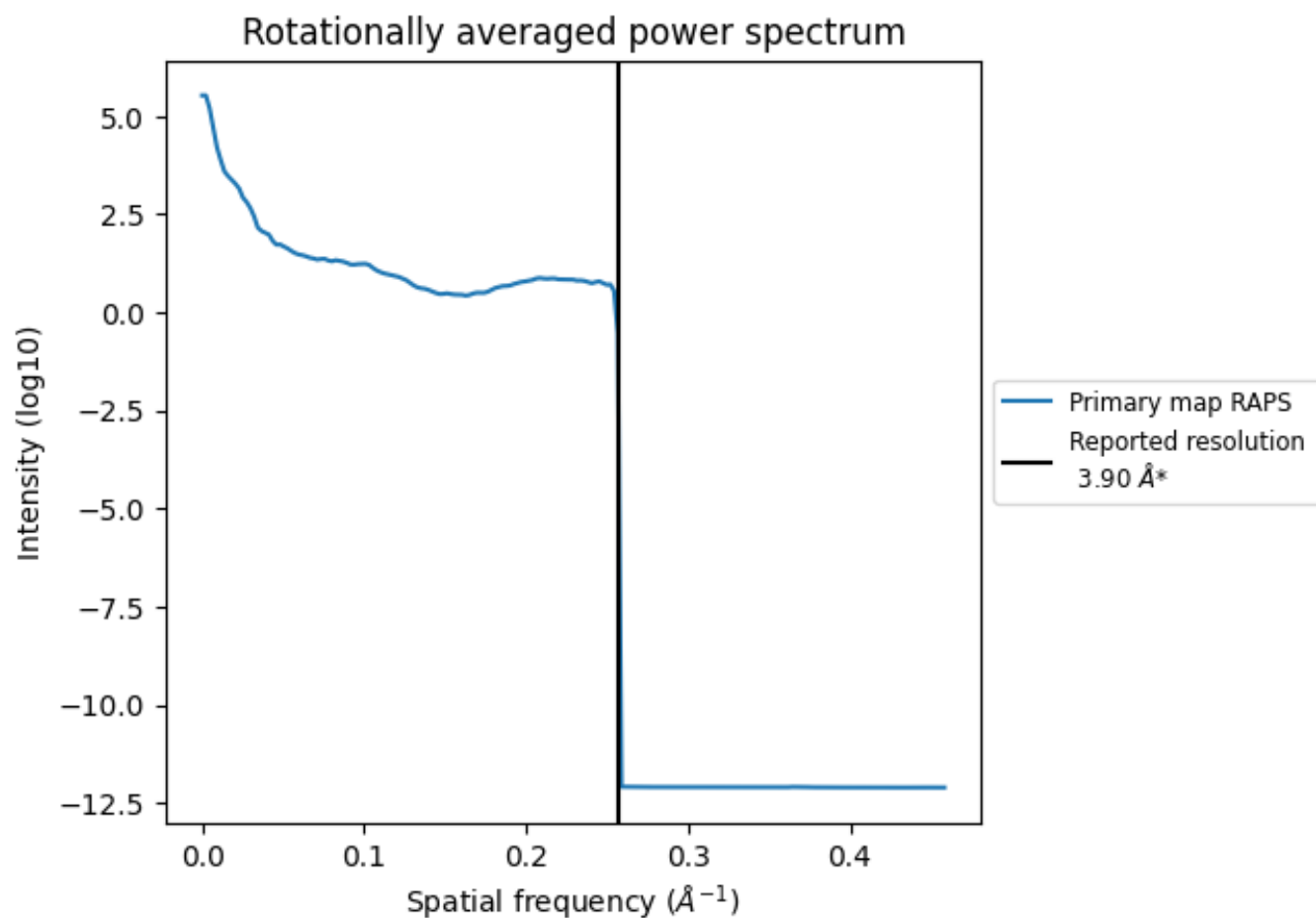
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1096 nm³; this corresponds to an approximate mass of 990 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 ⓘ

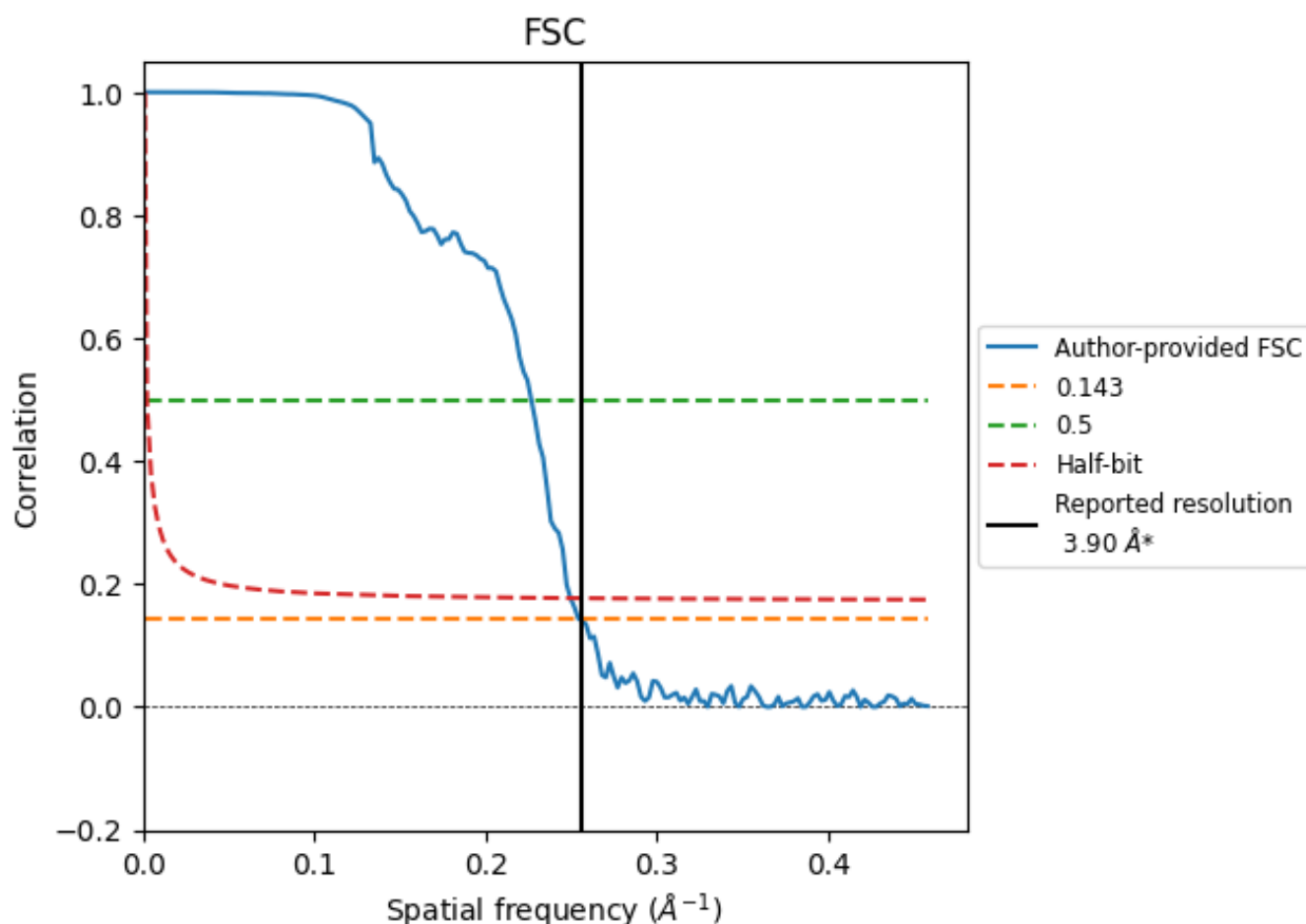


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.93	4.41	4.00
Unmasked-calculated*	-	-	-

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

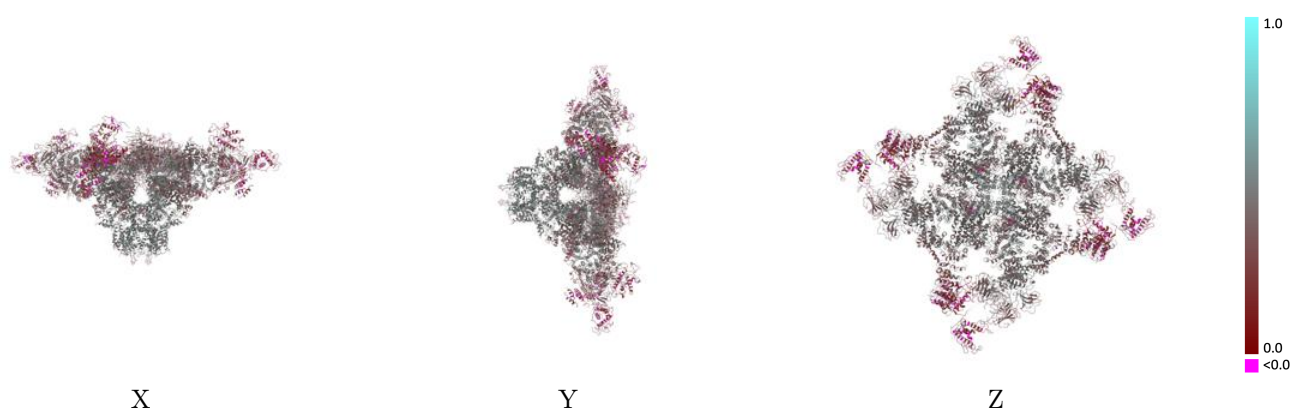
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9879 and PDB model 6JRR. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

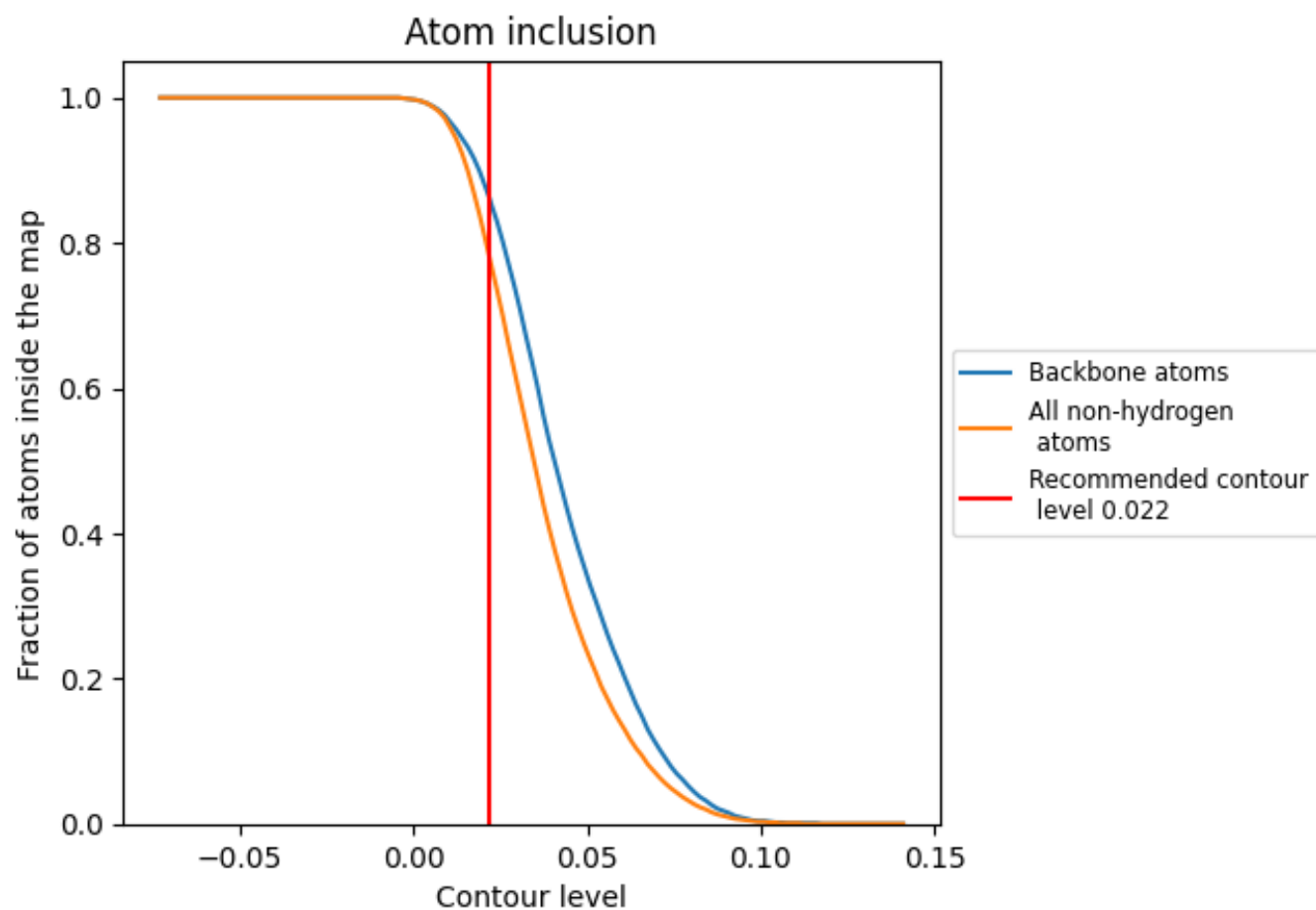


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 78% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7780	0.3900
A	0.7770	0.3900
B	0.8140	0.4170
C	0.7770	0.3890
D	0.8150	0.4160
E	0.7770	0.3890
F	0.8180	0.4170
G	0.7770	0.3890
H	0.8150	0.4160

1.0

0.0

<0.0