



## Full wwPDB EM Validation Report ⓘ

Nov 5, 2024 – 05:07 AM EST

PDB ID : 8UXI  
EMDB ID : EMD-42765  
Title : Structure of PKA phosphorylated human RyR2-R420W in the open state in the presence of calcium  
Authors : Miotto, M.C.; Marks, A.R.  
Deposited on : 2023-11-09  
Resolution : 3.29 Å(reported)  
Based on initial model : 7UA5

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

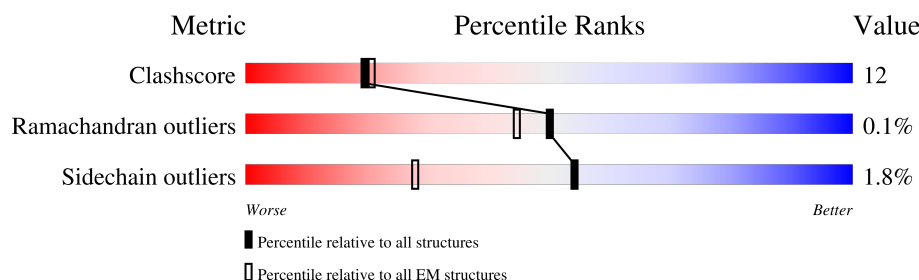
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.29 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	4967	<div> <div>11%</div> <div>58%</div> <div>22%</div> <div>19%</div> </div>
1	B	4967	<div> <div>11%</div> <div>58%</div> <div>22%</div> <div>19%</div> </div>
1	C	4967	<div> <div>11%</div> <div>58%</div> <div>22%</div> <div>19%</div> </div>
1	D	4967	<div> <div>11%</div> <div>58%</div> <div>22%</div> <div>19%</div> </div>
2	E	108	<div> <div>78%</div> <div>19%</div> </div>
2	F	108	<div> <div>78%</div> <div>19%</div> </div>
2	G	108	<div> <div>77%</div> <div>19%</div> </div>
2	H	108	<div> <div>79%</div> <div>18%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 131656 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4004	Total	C	N	O	S	2	0
			32032	20411	5451	5955	215		
1	B	4004	Total	C	N	O	S	2	0
			32032	20411	5451	5955	215		
1	C	4004	Total	C	N	O	S	2	0
			32032	20411	5451	5955	215		
1	D	4004	Total	C	N	O	S	2	0
			32032	20411	5451	5955	215		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	TRP	ARG	variant	UNP Q92736
B	420	TRP	ARG	variant	UNP Q92736
C	420	TRP	ARG	variant	UNP Q92736
D	420	TRP	ARG	variant	UNP Q92736

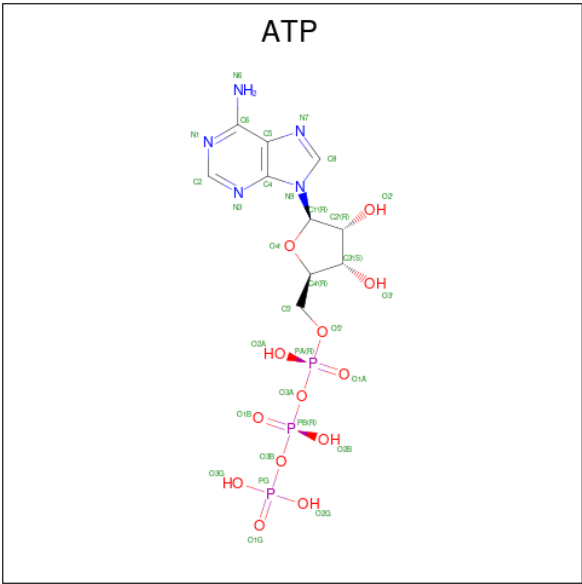
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

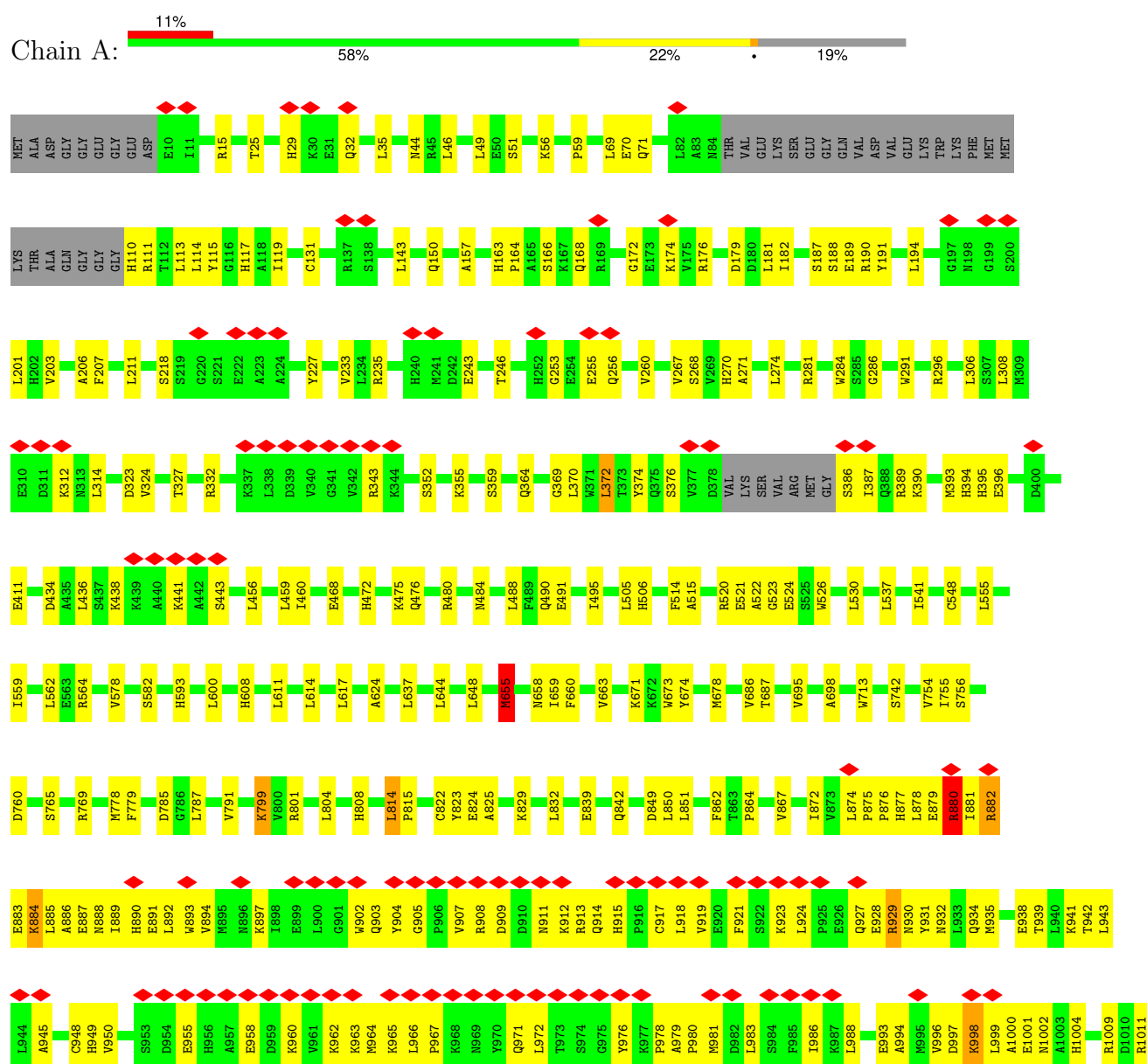
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

### 3 Residue-property plots

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

#### • Molecule 1: Ryanodine receptor 2

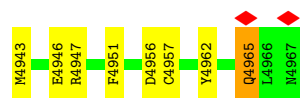




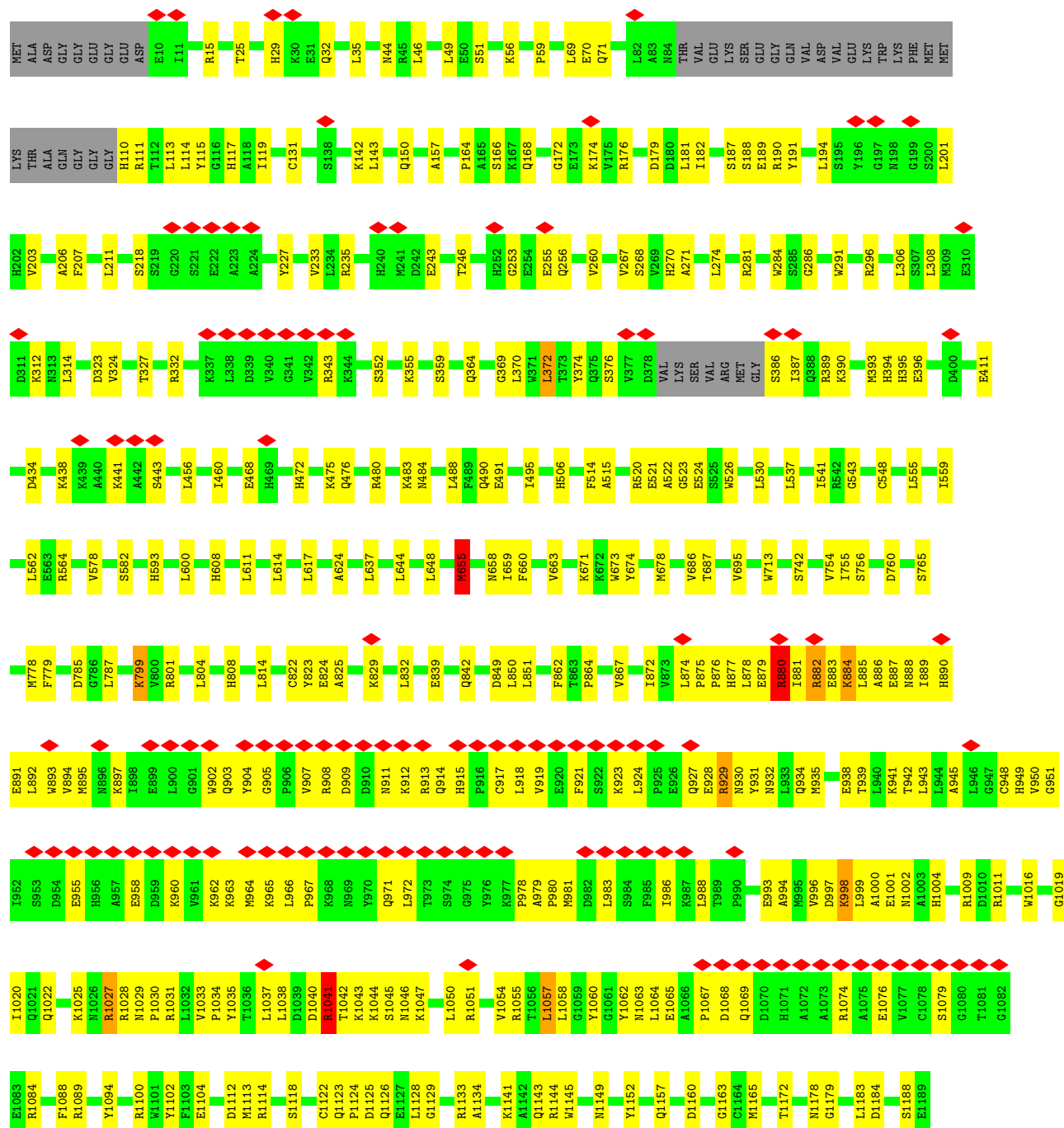






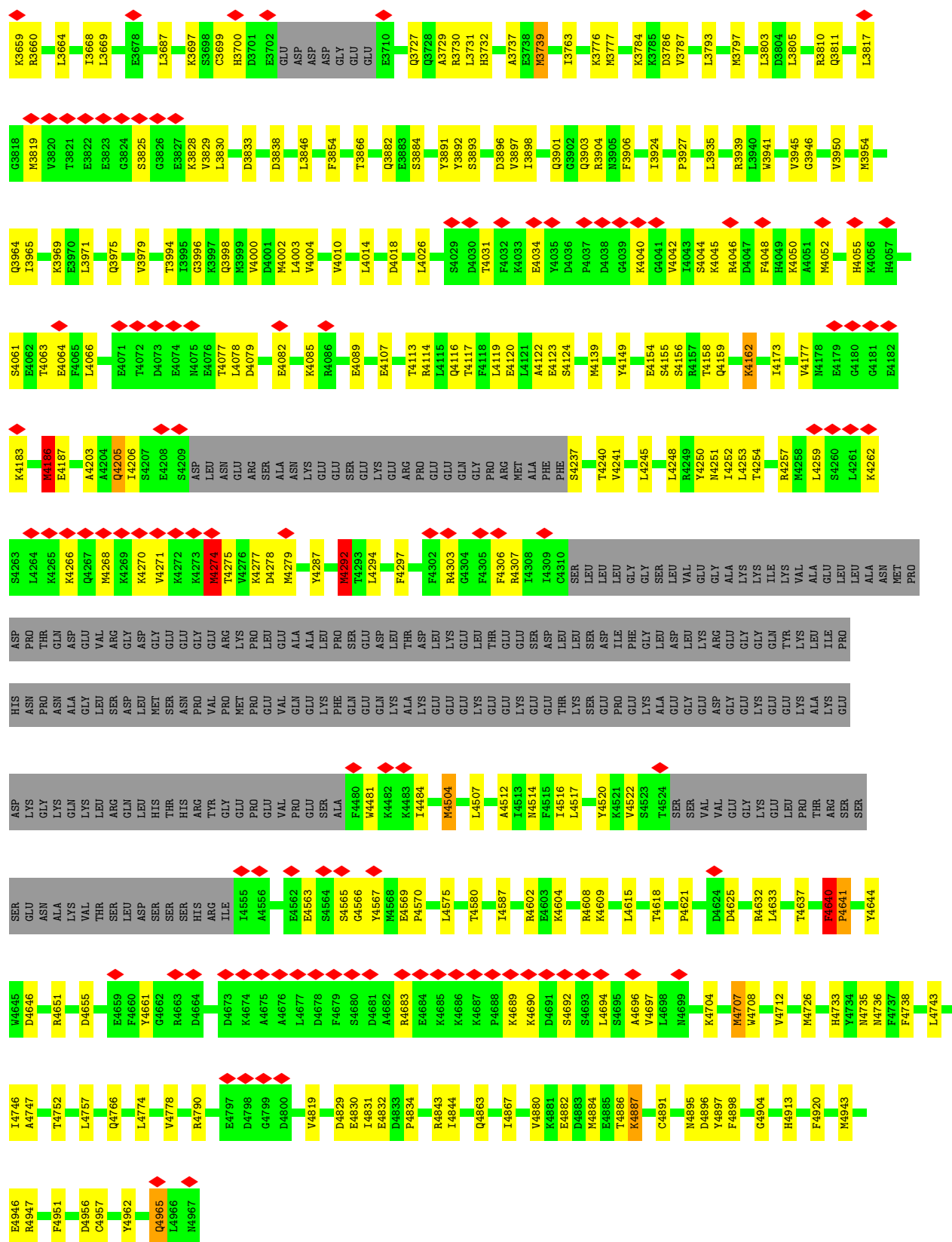


• Molecule 1: Ryanodine receptor 2



L2638	L2525	L2526	L2527	L2534	H2541	A2542	S2543	L2544	I2545	Q2654	K2655	K2656	V2657	E2658	Q2659	F2662	K2663	L2664	A2665	L2666	P2667	C2668	S2670	A2671	V2672	A2673	L2676	V2680	Y2681	E2682	N2684	Y2685	P2686	S2687	K2688	M2689	E2690	K2691	Q2692	S2693	S2694	M2695	D2696	S2697	E2698	G2699	N2700	F2701	N2702	P2703	Q2704	V2706				
L2641	L2642	L2643	L2644	F2649	D2650	A2651	Q2654	K2655	K2656	V2657	E2658	Q2659	F2662	K2663	L2664	A2665	L2666	P2667	C2668	S2670	A2671	V2672	A2673	L2676	V2680	Y2681	E2682	N2684	Y2685	P2686	S2687	K2688	M2689	E2690	K2691	Q2692	S2693	S2694	M2695	D2696	S2697	E2698	G2699	N2700	F2701	N2702	P2703	Q2704	V2706							
L2645	L2646	L2647	L2648	F2649	D2650	A2651	Q2654	K2655	K2656	V2657	E2658	Q2659	F2662	K2663	L2664	A2665	L2666	P2667	C2668	S2670	A2671	V2672	A2673	L2676	V2680	Y2681	E2682	N2684	Y2685	P2686	S2687	K2688	M2689	E2690	K2691	Q2692	S2693	S2694	M2695	D2696	S2697	E2698	G2699	N2700	F2701	N2702	P2703	Q2704	V2706							
L2649	L2650	L2651	L2652	F2653	D2654	A2655	Q2656	K2657	K2658	V2659	E2660	F2661	D2662	K2663	L2664	A2665	L2666	P2667	C2668	S2669	A2670	V2671	A2672	L2673	V2674	Y2675	E2676	N2677	Y2678	P2679	S2680	K2681	M2682	E2683	G2684	H2685	I2686	L2687	V2688	Y2689	F2690	D2691	S2692	E2693	G2694	N2695	F2696	D2697	S2698	E2699	N2700	F2701	N2702	P2703	Q2704	V2706
L2653	L2654	L2655	L2656	F2657	D2658	A2659	Q2660	K2661	K2662	V2663	E2664	F2665	D2666	K2667	L2668	A2669	L2670	P2671	C2672	S2673	A2674	V2675	A2676	L2677	V2678	Y2679	E2680	N2681	Y2682	P2683	S2684	K2685	M2686	E2687	G2688	H2689	I2690	L2691	V2692	Y2693	F2694	D2695	S2696	E2697	G2698	N2699	F2700	D2701	S2702	E2703	N2704	P2705	Q2706	V2707		
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L2729	L2730	L2731	L2732	F2733	D2734	A2735	Q2736	K2737	K2738	V2739	E2740	F2741	D2742	K2743	L2744	A2745	L2746	P2747	C2748	S2749	A2750	V2751	A2752	L2753	V2754	Y2755	E2756	N2757	Y2758	P2759	S2760	K2761	M2762	E2763	G2764	H2765	I2766	L2767	V2768	Y2769	F2770	D2771	S2772	E2773	G2774	N2775	F2776	D2777	S2778	E2779	N2780	P2781	Q2782	V2783		
L2733	L2734	L2735	L2736	F2737	D2738	A2739	Q2740	K2741	K2742	V2743	E2744	F2745	D2746	K2747	L2748	A2749	L2750	P2751	C2752	S																																				





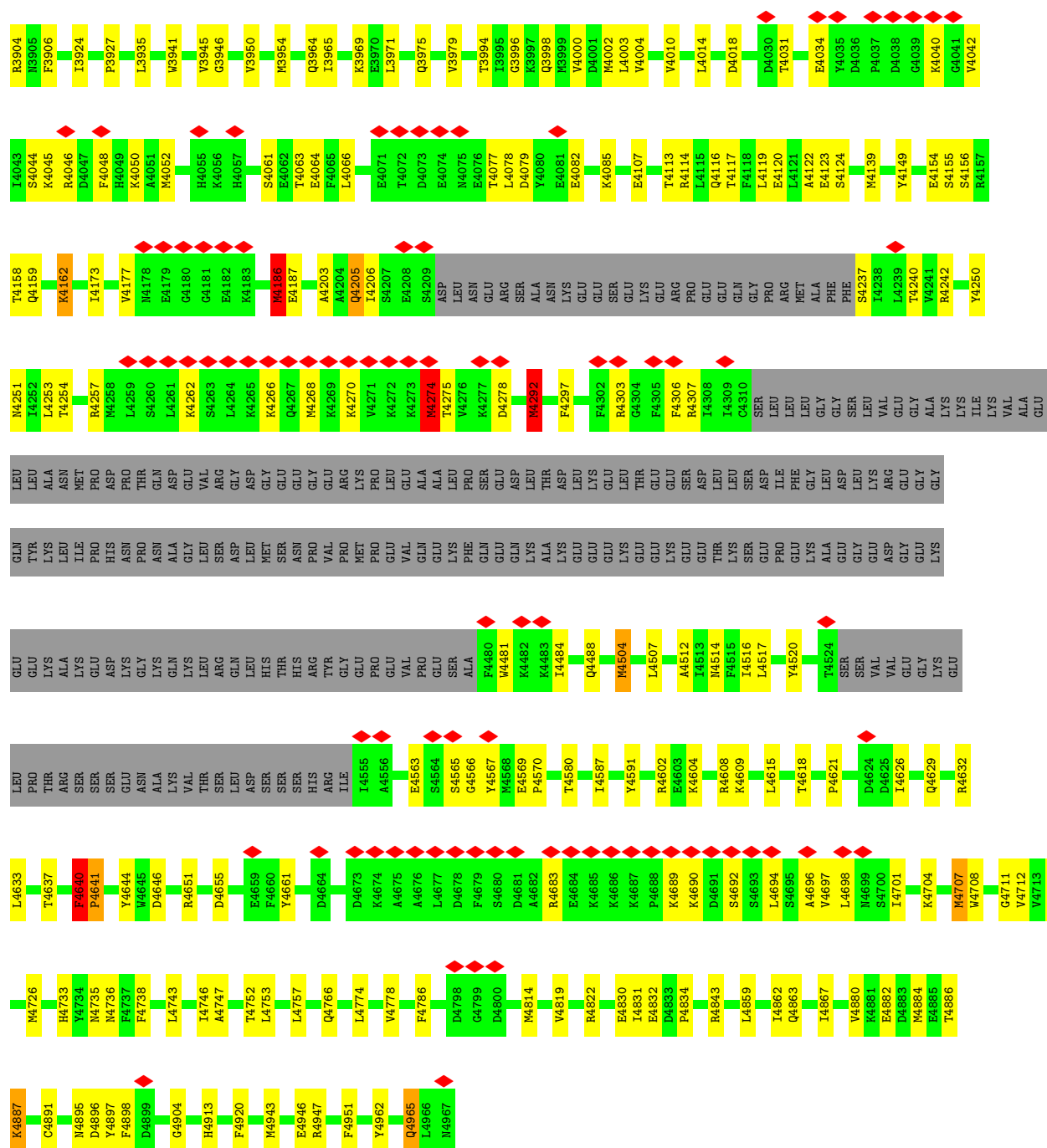
- Molecule 1: Ryanodine receptor 2



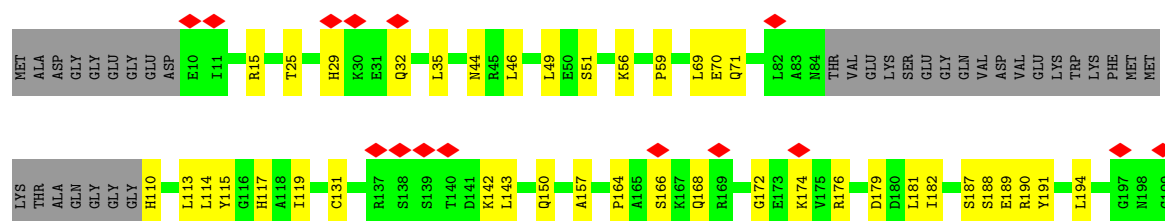
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S2693	S2694	M2695	D2696	S2697	G2698	W2699	G2696	A2632	E2635	L2638	S2641	R2642	K2643	L2644	F2649	D2650	A2651	Q2654	K2655	K2656	Y2657	E2658	Q2659	F2662	K2663	L2664	A2665	L2666	P2667	C2668	L2669	S2670	A2671	V2672	A2673	L2676	P2677	P2678	D2679	Y2680	M2681	E2682	S2683	N2684	Y2685	V2686	S2687	M2688	N2689	E2690	K2691	Q2692					
L2485	L2488	F2492	R2497	C2521	L2525	P2526	L2527	L2534	E2539	H2540	L2541	A2542	S2543	L2544	I2545	L2548	L2555	S2556	K2557	L2561	I2576	L2580	R2581	M2584	Q2585	Q2586	L2587	L2588	L2589	R2590	R2591	L2592	V2593	H2602	A2603	K2604	M2605	P2606	L2607	K2608	L2609	Y2614	K2619	Q2692													
Y2620	L2623	P2624	G2625	G2626	W2627	A2632	E2635	L2638	S2641	R2642	L2643	L2644	F2649	D2650	A2651	Q2654	K2655	K2656	Y2657	E2658	Q2659	F2662	K2663	L2664	A2665	L2666	P2667	C2668	L2669	S2670	A2671	V2672	A2673	L2676	P2677	P2678	D2679	Y2680	M2681	E2682	S2683	N2684	Y2685	V2686	S2687	M2688	N2689	E2690	K2691	Q2692							
P2364	ASN	SER	GLY	SER	SER	SER	THR	LEU	ASP	THR	GLU	GLU	E2377	E2378	D2379	D2380	H2383	M2384	G2385	N2386	D2397	F2301	L2302	R2303	C2308	N2309	N2316	A2317	V2321	F2331	G2332	L2335	R2336	G2337	N2341	G2342	Q2481	D2482	F2483	L2484																	
L2221	L2222	V2227	S2237	D2241	V2247	N2251	L2253	A2254	L2255	A2256	L2257	R2258	E2259	P2260	V2265	C2272	Q2273	Y2285	P2286	W2290	L2291	P2292	R2297	F2301	L2302	R2303	C2308	N2309	N2316	A2317	V2321	F2331	G2332	L2335	R2336	G2337	N2341	G2342	Q2481	D2482	F2483	L2484															
V2074	V2086	L2087	R2090	Q2091	G2096	V2099	L2119	Q2125	L2129	L2130	E2137	E2138	E2139	M2142	I2143	R2144	G2145	L2146	M2150	N2151	N2152	K2153	V2154	T2170	V2171	V2176	G2181	G2182	E2183	S2184	K2185	E2186	M2192	V2193	A2194	F2199	Y2202	I2206	F2215	Y2220																	
E1990	E1991	I1992	I1993	D1994	Q1995	E2010	LEU	ASP	GLU	ASP	GLY	SER	LEU	ASP	GLY	ASN	ASP	LEU	THR	ILE	ARG	GLY	ARG	LEU	LEU	VAL	GLU	LYS	VAL	THR	TYR	LYS	LEU	GLN	GLY	K1961	T1962	F1965	R1966	S1967	Q1972	M1975	L1976	F1979	D1982	K1983	S1984	E1985	C1986	P1987	P1989						
L1829	I1830	M1831	I1833	L1839	I1842	E1847	P1848	S1849	A1853	A1854	ALA	THR	PRO	GLU	GLU	GLU	SER	ASP	THR	ASP	THR	LEU	GLY	LYS	LEU	VAL	ASP	ALA	LYS	LEU	GLN	GLY	ALA	GLY	K1768	V1799	R1807	V1810	L1817	M1828	S1829	L1830	H1831	I1832													
R1482	S1483	N1484	C1485	Y1486	M1487	S1495	P1496	G1497	Q1498	G1499	R1500	N1501	N1502	N1503	G1504	L1505	T1537	K1538	Q1546	S1549	P1550	N1551	V1552	F1553	R1559	I1560	K1561	N1562	M1563	M1564	P1565	S1592	H1593	V1594	F1603	L1604	V1608	Q1615	V1619	Q1620	L1625	M1628	S1629	L1630	H1631	I1632											
LYS	PRO	SER	ARG	LEU	LYS	GLN	ARG	PHE	LEU	LEU	ARG	THR	LYS	PRO	ASP	TYR	SER	THR	HIS	SER	ALA	ARG	LEU	THR	GLU	ASP	VAL	LEU	LEU	ALA	ASP	ASP	R1414	D1415	D1416	Y1417	D1418	F1419	Q1422	I1432	E1437	P1438	N1440	G1444	V1465	D1471	E1472	K1473	G1474	K1475							



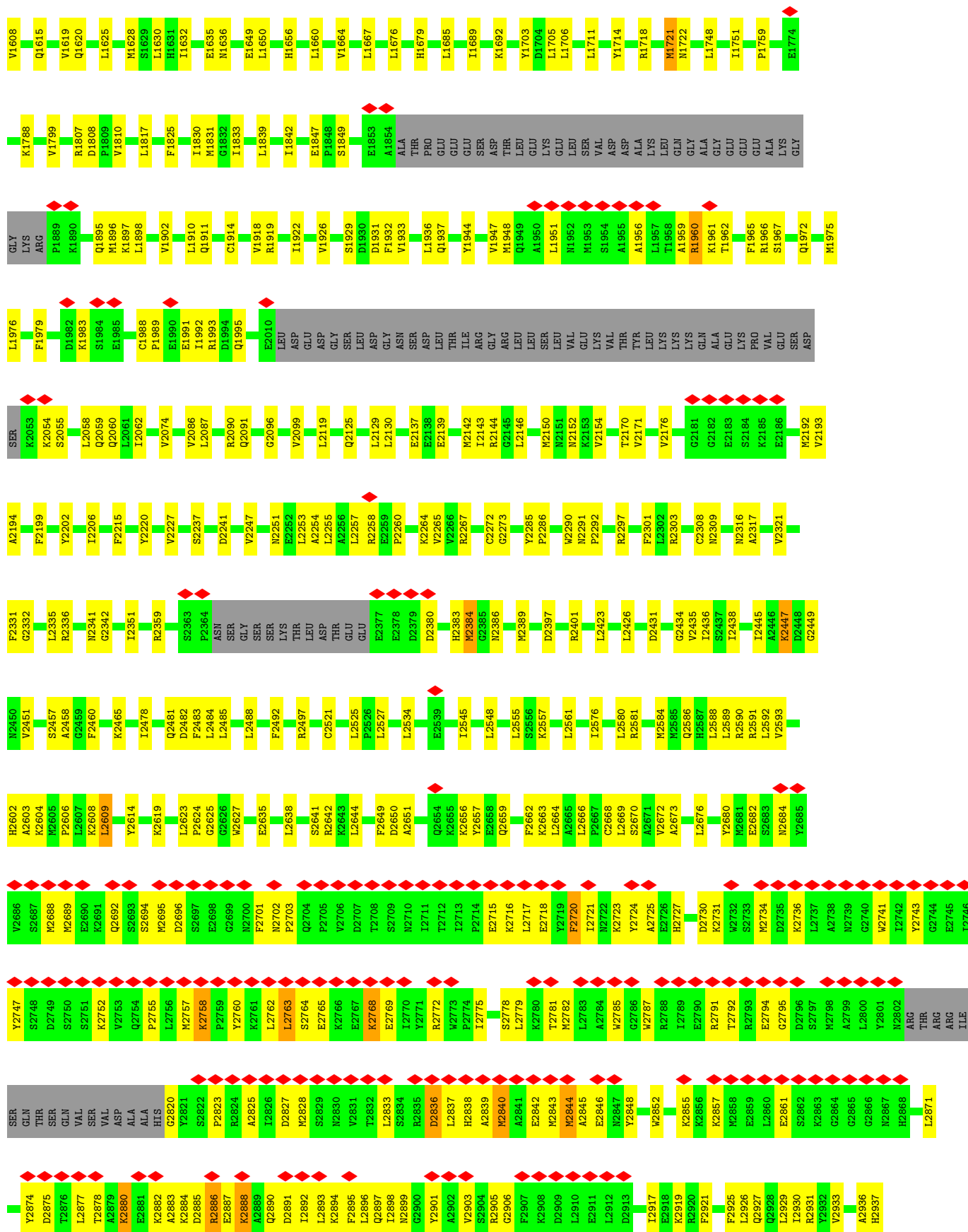




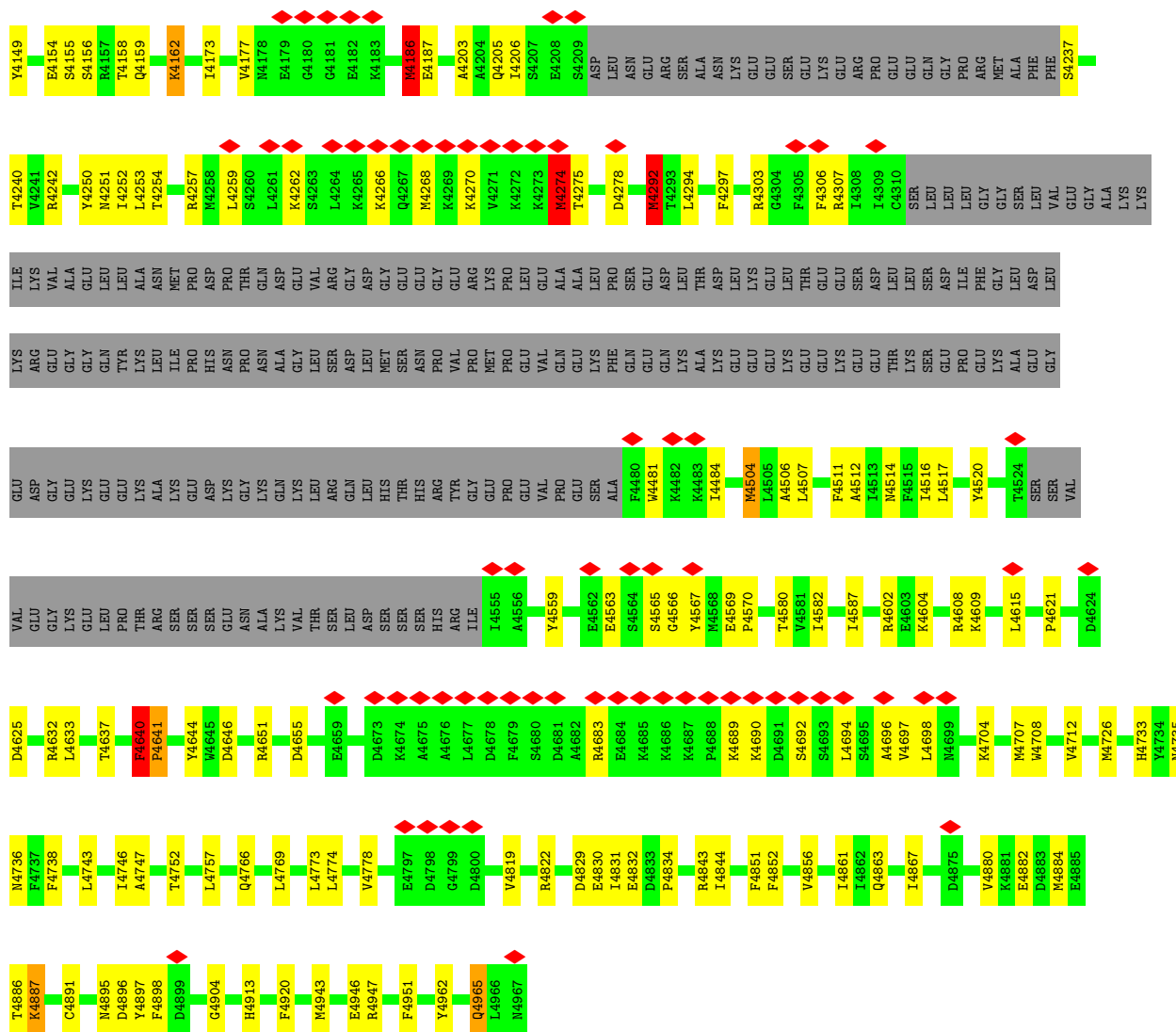
• Molecule 1: Ryanodine receptor 2











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

Chain E: 78% 19%



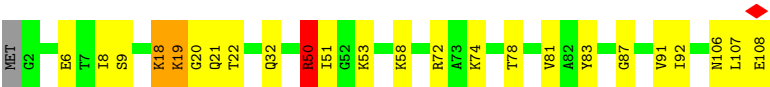
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 78% 19%

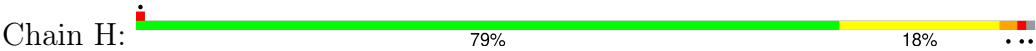


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: 77% 19%



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	149448	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 ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.599	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	431.36, 431.36, 431.36	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8425, 0.8425, 0.8425	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.26	0/32738	0.53	16/44213 (0.0%)
1	B	0.26	0/32738	0.53	16/44213 (0.0%)
1	C	0.26	0/32738	0.53	16/44213 (0.0%)
1	D	0.26	0/32738	0.53	16/44213 (0.0%)
2	E	0.30	0/834	0.61	2/1123 (0.2%)
2	F	0.30	0/834	0.61	2/1123 (0.2%)
2	G	0.30	0/834	0.61	2/1123 (0.2%)
2	H	0.30	0/834	0.61	2/1123 (0.2%)
All	All	0.26	0/134288	0.53	72/181344 (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	4
1	B	0	4
1	C	0	4
1	D	0	4
2	E	0	2
2	F	0	2
2	G	0	2
2	H	0	2
All	All	0	24

There are no bond length outliers.

All (72) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4274	MET	CB-CG-SD	7.23	134.10	112.40
1	B	4274	MET	CB-CG-SD	7.23	134.10	112.40
1	C	4274	MET	CB-CG-SD	7.23	134.09	112.40
1	D	4274	MET	CB-CG-SD	7.23	134.09	112.40
2	F	50	ARG	CA-CB-CG	6.99	128.78	113.40
2	G	50	ARG	CA-CB-CG	6.97	128.73	113.40
2	H	50	ARG	CA-CB-CG	6.96	128.72	113.40
2	E	50	ARG	CA-CB-CG	6.96	128.70	113.40
1	B	2880	LYS	CD-CE-NZ	6.58	126.84	111.70
1	A	2880	LYS	CD-CE-NZ	6.57	126.81	111.70
1	D	2880	LYS	CD-CE-NZ	6.55	126.77	111.70
1	C	2880	LYS	CD-CE-NZ	6.55	126.76	111.70
1	A	4640	PHE	C-N-CD	-6.48	106.34	120.60
1	B	4640	PHE	C-N-CD	-6.48	106.34	120.60
1	C	4640	PHE	C-N-CD	-6.47	106.37	120.60
1	D	4640	PHE	C-N-CD	-6.46	106.40	120.60
1	C	2828	MET	CA-CB-CG	6.43	124.23	113.30
1	B	2828	MET	CA-CB-CG	6.42	124.21	113.30
1	D	2828	MET	CA-CB-CG	6.38	124.15	113.30
1	A	2828	MET	CA-CB-CG	6.38	124.14	113.30
1	A	4292	MET	CB-CG-SD	6.32	131.35	112.40
1	C	4292	MET	CB-CG-SD	6.31	131.34	112.40
1	B	4292	MET	CB-CG-SD	6.31	131.33	112.40
1	D	4292	MET	CB-CG-SD	6.30	131.32	112.40
1	A	1041	ARG	CB-CG-CD	6.27	127.91	111.60
1	B	1041	ARG	CB-CG-CD	6.27	127.90	111.60
1	D	1041	ARG	CB-CG-CD	6.26	127.89	111.60
1	C	1041	ARG	CB-CG-CD	6.26	127.88	111.60
1	B	880	ARG	CA-CB-CG	6.25	127.16	113.40
1	A	880	ARG	CA-CB-CG	6.25	127.15	113.40
1	D	880	ARG	CA-CB-CG	6.24	127.14	113.40
1	C	880	ARG	CA-CB-CG	6.24	127.13	113.40
1	B	1721	MET	CB-CG-SD	6.11	130.72	112.40
1	D	1721	MET	CB-CG-SD	6.10	130.70	112.40
1	A	1721	MET	CB-CG-SD	6.09	130.66	112.40
1	C	1721	MET	CB-CG-SD	6.08	130.64	112.40
1	A	655	MET	CB-CG-SD	5.62	129.28	112.40
1	B	814	LEU	CA-CB-CG	5.62	128.23	115.30
1	D	655	MET	CB-CG-SD	5.62	129.26	112.40
1	C	814	LEU	CA-CB-CG	5.62	128.22	115.30
1	B	655	MET	CB-CG-SD	5.61	129.24	112.40
1	C	655	MET	CB-CG-SD	5.61	129.24	112.40
1	D	814	LEU	CA-CB-CG	5.61	128.20	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2988	ARG	CA-CB-CG	5.61	125.73	113.40
1	B	2988	ARG	CA-CB-CG	5.61	125.73	113.40
1	C	2988	ARG	CA-CB-CG	5.60	125.72	113.40
1	A	2988	ARG	CA-CB-CG	5.59	125.70	113.40
1	A	814	LEU	CA-CB-CG	5.59	128.16	115.30
1	A	372	LEU	CA-CB-CG	5.46	127.86	115.30
1	C	372	LEU	CA-CB-CG	5.45	127.84	115.30
1	B	372	LEU	CA-CB-CG	5.44	127.80	115.30
1	D	372	LEU	CA-CB-CG	5.43	127.80	115.30
1	A	4186	MET	CB-CG-SD	5.40	128.60	112.40
1	D	4186	MET	CB-CG-SD	5.39	128.58	112.40
1	C	4186	MET	CB-CG-SD	5.39	128.58	112.40
1	B	4186	MET	CB-CG-SD	5.37	128.51	112.40
2	H	50	ARG	CB-CG-CD	5.33	125.45	111.60
1	A	2384	MET	CB-CG-SD	5.32	128.36	112.40
1	D	2384	MET	CB-CG-SD	5.32	128.35	112.40
2	E	50	ARG	CB-CG-CD	5.32	125.42	111.60
1	C	2384	MET	CB-CG-SD	5.32	128.35	112.40
2	G	50	ARG	CB-CG-CD	5.31	125.40	111.60
1	B	2384	MET	CB-CG-SD	5.31	128.32	112.40
2	F	50	ARG	CB-CG-CD	5.30	125.38	111.60
1	B	2844	MET	CA-CB-CG	5.24	122.20	113.30
1	A	2844	MET	CA-CB-CG	5.23	122.19	113.30
1	D	2844	MET	CA-CB-CG	5.21	122.16	113.30
1	C	2844	MET	CA-CB-CG	5.20	122.15	113.30
1	C	2763	LEU	CB-CG-CD2	5.18	119.81	111.00
1	B	2763	LEU	CB-CG-CD2	5.17	119.80	111.00
1	D	2763	LEU	CB-CG-CD2	5.17	119.80	111.00
1	A	2763	LEU	CB-CG-CD2	5.15	119.76	111.00

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2827	ASP	Peptide
1	A	4640	PHE	Peptide
1	A	880	ARG	Sidechain,Peptide
1	B	2827	ASP	Peptide
1	B	4640	PHE	Peptide
1	B	880	ARG	Sidechain,Peptide
1	C	2827	ASP	Peptide
1	C	4640	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	C	880	ARG	Sidechain,Peptide
1	D	2827	ASP	Peptide
1	D	4640	PHE	Peptide
1	D	880	ARG	Sidechain,Peptide
2	E	50	ARG	Sidechain,Peptide
2	F	50	ARG	Sidechain,Peptide
2	G	50	ARG	Sidechain,Peptide
2	H	50	ARG	Sidechain,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	32032	0	31689	797	0
1	B	32032	0	31689	795	0
1	C	32032	0	31689	816	0
1	D	32032	0	31689	797	0
2	E	818	0	821	19	0
2	F	818	0	821	17	0
2	G	818	0	821	18	0
2	H	818	0	821	15	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	62	0	24	2	0
4	B	62	0	24	2	0
4	C	62	0	24	2	0
4	D	62	0	24	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	131656	0	130136	3207	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 12.

All (3207) 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:B:4237:SER:N	1:B:4240:THR:HG1	1.59	1.01
1:D:4237:SER:N	1:D:4240:THR:HG1	1.59	0.99
1:C:4814:MET:HE1	1:D:4844:ILE:HG21	1.44	0.97
1:A:4237:SER:N	1:A:4240:THR:HG1	1.63	0.96
1:C:4237:SER:N	1:C:4240:THR:HG1	1.61	0.95
1:B:4259:LEU:HD21	1:C:4701:ILE:HG21	1.51	0.91
1:C:3043:ARG:NH2	1:C:3116:GLN:O	2.05	0.89
1:D:3043:ARG:NH2	1:D:3116:GLN:O	2.05	0.89
1:C:2725:ALA:HB1	1:C:2768:LYS:HG3	1.55	0.89
1:C:2581:ARG:HB3	1:C:2584:MET:HG2	1.55	0.88
1:A:2930:ILE:HG12	1:A:3007:LEU:HD21	1.56	0.88
1:B:2581:ARG:HB3	1:B:2584:MET:HG2	1.55	0.88
1:B:3043:ARG:NH2	1:B:3116:GLN:O	2.05	0.88
1:D:2581:ARG:HB3	1:D:2584:MET:HG2	1.55	0.88
1:B:2930:ILE:HG12	1:B:3007:LEU:HD21	1.56	0.88
1:A:2581:ARG:HB3	1:A:2584:MET:HG2	1.55	0.87
1:D:2725:ALA:HB1	1:D:2768:LYS:HG3	1.55	0.87
1:D:2930:ILE:HG12	1:D:3007:LEU:HD21	1.56	0.87
1:A:3043:ARG:NH2	1:A:3116:GLN:O	2.05	0.87
1:B:4962:TYR:HD1	1:B:4965:GLN:HE22	1.23	0.86
1:C:2930:ILE:HG12	1:C:3007:LEU:HD21	1.56	0.86
1:B:2725:ALA:HB1	1:B:2768:LYS:HG3	1.55	0.86
1:D:4962:TYR:HD1	1:D:4965:GLN:HE22	1.23	0.86
1:A:2725:ALA:HB1	1:A:2768:LYS:HG3	1.55	0.85
1:B:4262:LYS:HG3	1:C:4698:LEU:HD22	1.58	0.85
1:C:4962:TYR:HD1	1:C:4965:GLN:HE22	1.23	0.85
1:A:4962:TYR:HD1	1:A:4965:GLN:HE22	1.23	0.85
1:B:3939:ARG:NH2	1:C:172:GLY:O	2.10	0.84
1:C:4481:TRP:HE1	1:C:4692:SER:HA	1.43	0.84
1:A:4481:TRP:HE1	1:A:4692:SER:HA	1.43	0.84
1:B:4481:TRP:HE1	1:B:4692:SER:HA	1.43	0.84
1:A:4766:GLN:HG2	1:D:4752:THR:HG21	1.60	0.84
1:D:4481:TRP:HE1	1:D:4692:SER:HA	1.43	0.83
1:B:2905:ARG:HE	1:B:2906:GLY:H	1.25	0.83
2:F:6:GLU:OE2	2:F:74:LYS:NZ	2.12	0.83
2:H:6:GLU:OE2	2:H:74:LYS:NZ	2.12	0.83
2:G:6:GLU:OE2	2:G:74:LYS:NZ	2.12	0.83
2:E:6:GLU:OE2	2:E:74:LYS:NZ	2.12	0.82
1:A:2720:PHE:HZ	1:A:2896:LEU:HA	1.44	0.82
1:B:4640:PHE:CD2	1:B:4641:PRO:HD3	2.14	0.82
1:C:2720:PHE:HZ	1:C:2896:LEU:HA	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2720:PHE:HZ	1:D:2896:LEU:HA	1.44	0.82
1:D:4640:PHE:CD2	1:D:4641:PRO:HD3	2.14	0.81
1:C:4640:PHE:CD2	1:C:4641:PRO:HD3	2.14	0.81
1:C:2905:ARG:HE	1:C:2906:GLY:H	1.25	0.81
1:D:2591:ARG:HH22	1:D:2875:ASP:HB3	1.45	0.81
1:D:2905:ARG:HE	1:D:2906:GLY:H	1.25	0.81
1:A:2591:ARG:HH22	1:A:2875:ASP:HB3	1.45	0.81
1:B:2720:PHE:HZ	1:B:2896:LEU:HA	1.44	0.81
1:A:2905:ARG:HE	1:A:2906:GLY:H	1.25	0.80
1:A:4640:PHE:CD2	1:A:4641:PRO:HD3	2.14	0.80
1:B:2591:ARG:HH22	1:B:2875:ASP:HB3	1.45	0.80
1:D:890:HIS:HA	1:D:893:TRP:CE3	2.18	0.79
1:C:2591:ARG:HH22	1:C:2875:ASP:HB3	1.45	0.79
1:A:887:GLU:HA	1:A:890:HIS:CD2	2.18	0.79
2:E:50:ARG:NH1	2:E:53:LYS:HG2	1.98	0.79
2:H:50:ARG:NH1	2:H:53:LYS:HG2	1.98	0.79
1:C:887:GLU:HA	1:C:890:HIS:CD2	2.18	0.78
1:D:887:GLU:HA	1:D:890:HIS:CD2	2.18	0.78
1:C:3639:LYS:HA	1:C:4683:ARG:HH22	1.48	0.78
1:C:4863:GLN:HB2	1:D:4856:VAL:HG13	1.65	0.78
1:A:890:HIS:HA	1:A:893:TRP:CE3	2.18	0.78
1:A:678:MET:HG2	1:A:801:ARG:HH21	1.49	0.78
1:B:887:GLU:HA	1:B:890:HIS:CD2	2.18	0.78
1:B:890:HIS:HA	1:B:893:TRP:CE3	2.18	0.78
1:B:3639:LYS:HA	1:B:4683:ARG:HH22	1.48	0.78
1:C:890:HIS:HA	1:C:893:TRP:CE3	2.18	0.78
1:B:678:MET:HG2	1:B:801:ARG:HH21	1.49	0.77
2:G:50:ARG:NH1	2:G:53:LYS:HG2	1.98	0.77
2:F:50:ARG:NH1	2:F:53:LYS:HG2	1.99	0.77
1:D:678:MET:HG2	1:D:801:ARG:HH21	1.49	0.77
1:C:678:MET:HG2	1:C:801:ARG:HH21	1.49	0.77
1:D:996:VAL:HG11	1:D:1054:VAL:HG21	1.67	0.77
1:B:996:VAL:HG11	1:B:1054:VAL:HG21	1.67	0.77
1:A:3639:LYS:HA	1:A:4683:ARG:HH22	1.48	0.77
1:C:996:VAL:HG11	1:C:1054:VAL:HG21	1.67	0.77
1:A:996:VAL:HG11	1:A:1054:VAL:HG21	1.67	0.76
1:B:2731:LYS:HA	1:B:2734:MET:HG2	1.67	0.76
1:C:2731:LYS:HA	1:C:2734:MET:HG2	1.67	0.76
1:D:3639:LYS:HA	1:D:4683:ARG:HH22	1.49	0.76
1:D:930:ASN:O	1:D:934:GLN:NE2	2.19	0.76
1:B:194:LEU:HD11	1:B:201:LEU:HB3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:ASN:O	1:A:934:GLN:NE2	2.19	0.75
1:C:930:ASN:O	1:C:934:GLN:NE2	2.19	0.75
1:C:194:LEU:HD11	1:C:201:LEU:HB3	1.68	0.75
1:B:983:LEU:HD12	1:B:1055:ARG:HB3	1.69	0.75
1:A:555:LEU:HD21	1:A:578:VAL:HG11	1.69	0.75
1:A:983:LEU:HD12	1:A:1055:ARG:HB3	1.69	0.74
1:B:555:LEU:HD21	1:B:578:VAL:HG11	1.69	0.74
1:C:983:LEU:HD12	1:C:1055:ARG:HB3	1.69	0.74
1:A:194:LEU:HD11	1:A:201:LEU:HB3	1.69	0.74
1:D:2731:LYS:HA	1:D:2734:MET:HG2	1.67	0.74
1:B:2308:CYS:SG	1:B:2309:ASN:ND2	2.61	0.74
1:B:930:ASN:O	1:B:934:GLN:NE2	2.20	0.74
1:C:2308:CYS:SG	1:C:2309:ASN:ND2	2.61	0.74
2:E:50:ARG:HH12	2:E:53:LYS:HG2	1.53	0.74
2:G:50:ARG:HH12	2:G:53:LYS:HG2	1.53	0.74
2:H:50:ARG:HH12	2:H:53:LYS:HG2	1.53	0.74
1:D:983:LEU:HD12	1:D:1055:ARG:HB3	1.69	0.74
1:B:878:LEU:HA	1:B:881:ILE:HG22	1.70	0.73
1:D:2129:LEU:HB3	1:D:2142:MET:HE1	1.69	0.73
1:A:2659:GLN:OE1	1:A:2663:LYS:NZ	2.21	0.73
1:D:878:LEU:HA	1:D:881:ILE:HG22	1.70	0.73
1:A:2731:LYS:HA	1:A:2734:MET:HG2	1.67	0.73
2:F:50:ARG:HH12	2:F:53:LYS:HG2	1.53	0.73
1:B:2659:GLN:OE1	1:B:2663:LYS:NZ	2.21	0.73
1:D:194:LEU:HD11	1:D:201:LEU:HB3	1.69	0.73
1:B:864:PRO:O	1:B:1009:ARG:NH2	2.22	0.73
1:D:2308:CYS:SG	1:D:2309:ASN:ND2	2.61	0.73
1:D:2720:PHE:CZ	1:D:2896:LEU:HA	2.24	0.73
1:A:2720:PHE:CZ	1:A:2896:LEU:HA	2.24	0.73
1:D:555:LEU:HD21	1:D:578:VAL:HG11	1.69	0.73
1:D:2659:GLN:OE1	1:D:2663:LYS:NZ	2.21	0.73
1:A:1123:GLN:HG3	1:A:1133:ARG:HH12	1.54	0.73
1:B:921:PHE:HB2	1:B:929:ARG:HG3	1.71	0.73
1:D:921:PHE:HB2	1:D:929:ARG:HG3	1.71	0.73
1:A:878:LEU:HA	1:A:881:ILE:HG22	1.70	0.73
2:F:8:ILE:HD11	2:F:74:LYS:HB2	1.71	0.73
1:B:967:PRO:O	1:B:971:GLN:HB2	1.89	0.73
1:C:555:LEU:HD21	1:C:578:VAL:HG11	1.69	0.73
1:D:1123:GLN:HG3	1:D:1133:ARG:HH12	1.54	0.73
1:A:4641:PRO:HB3	1:A:4644:TYR:HB3	1.70	0.73
2:H:8:ILE:HD11	2:H:74:LYS:HB2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:878:LEU:HA	1:C:881:ILE:HG22	1.70	0.73
2:G:8:ILE:HD11	2:G:74:LYS:HB2	1.71	0.72
1:B:1714:TYR:OH	1:B:1718:ARG:NH2	2.22	0.72
1:A:864:PRO:O	1:A:1009:ARG:NH2	2.22	0.72
1:A:967:PRO:O	1:A:971:GLN:HB2	1.89	0.72
1:A:2308:CYS:SG	1:A:2309:ASN:ND2	2.61	0.72
1:B:1129:GLY:HA3	1:B:1145:TRP:HB3	1.71	0.72
1:C:921:PHE:HB2	1:C:929:ARG:HG3	1.71	0.72
1:C:1129:GLY:HA3	1:C:1145:TRP:HB3	1.71	0.72
1:D:1129:GLY:HA3	1:D:1145:TRP:HB3	1.71	0.72
1:B:2129:LEU:HB3	1:B:2142:MET:HE1	1.70	0.72
1:D:864:PRO:O	1:D:1009:ARG:NH2	2.22	0.72
1:C:967:PRO:O	1:C:971:GLN:HB2	1.89	0.72
1:C:4641:PRO:HB3	1:C:4644:TYR:HB3	1.70	0.72
1:D:967:PRO:O	1:D:971:GLN:HB2	1.89	0.72
2:E:8:ILE:HD11	2:E:74:LYS:HB2	1.71	0.72
1:D:2874:TYR:HA	1:D:2877:LEU:HD13	1.72	0.72
1:B:2720:PHE:CZ	1:B:2896:LEU:HA	2.24	0.72
1:C:864:PRO:O	1:C:1009:ARG:NH2	2.22	0.72
1:C:1714:TYR:OH	1:C:1718:ARG:NH2	2.22	0.72
1:C:2659:GLN:OE1	1:C:2663:LYS:NZ	2.21	0.72
1:C:2720:PHE:CZ	1:C:2896:LEU:HA	2.24	0.72
1:A:799:LYS:HD2	1:A:1620:GLN:HG3	1.72	0.71
1:A:921:PHE:HB2	1:A:929:ARG:HG3	1.71	0.71
1:D:1714:TYR:OH	1:D:1718:ARG:NH2	2.22	0.71
1:D:799:LYS:HD2	1:D:1620:GLN:HG3	1.72	0.71
1:D:4270:LYS:HD3	1:D:4278:ASP:HB3	1.72	0.71
1:A:4270:LYS:HD3	1:A:4278:ASP:HB3	1.72	0.71
1:B:1123:GLN:HG3	1:B:1133:ARG:HH12	1.54	0.71
1:D:4641:PRO:HB3	1:D:4644:TYR:HB3	1.70	0.71
1:A:1714:TYR:OH	1:A:1718:ARG:NH2	2.22	0.71
1:B:308:LEU:HD13	1:B:393:MET:HG3	1.73	0.71
1:C:2874:TYR:HA	1:C:2877:LEU:HD13	1.72	0.71
1:A:308:LEU:HD13	1:A:393:MET:HG3	1.73	0.71
1:B:801:ARG:NH1	1:B:1615:GLN:OE1	2.24	0.71
1:B:4270:LYS:HD3	1:B:4278:ASP:HB3	1.72	0.71
1:C:308:LEU:HD13	1:C:393:MET:HG3	1.73	0.71
1:A:2129:LEU:HB3	1:A:2142:MET:HE1	1.71	0.71
1:B:4641:PRO:HB3	1:B:4644:TYR:HB3	1.70	0.71
1:C:1123:GLN:HG3	1:C:1133:ARG:HH12	1.54	0.71
1:A:1129:GLY:HA3	1:A:1145:TRP:HB3	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:799:LYS:HD2	1:B:1620:GLN:HG3	1.72	0.71
1:D:801:ARG:NH1	1:D:1615:GLN:OE1	2.24	0.71
1:C:799:LYS:HD2	1:C:1620:GLN:HG3	1.72	0.70
1:C:980:PRO:HG2	1:C:983:LEU:HD21	1.73	0.70
1:C:4270:LYS:HD3	1:C:4278:ASP:HB3	1.72	0.70
1:B:2874:TYR:HA	1:B:2877:LEU:HD13	1.72	0.70
1:A:801:ARG:NH1	1:A:1615:GLN:OE1	2.24	0.70
1:D:308:LEU:HD13	1:D:393:MET:HG3	1.73	0.70
1:D:3668:ILE:HG23	1:D:3739:MET:HE2	1.73	0.70
1:D:2386:ASN:ND2	1:D:2457:SER:O	2.24	0.70
1:C:801:ARG:NH1	1:C:1615:GLN:OE1	2.24	0.70
1:A:2874:TYR:HA	1:A:2877:LEU:HD13	1.72	0.70
1:A:1936:LEU:HD21	1:A:1976:LEU:HD13	1.74	0.69
1:B:980:PRO:HG2	1:B:983:LEU:HD21	1.73	0.69
1:B:2727:HIS:CE1	1:B:2731:LYS:HZ1	2.11	0.69
1:A:4052:MET:HG3	1:A:4063:THR:HG23	1.74	0.69
1:C:2727:HIS:CE1	1:C:2731:LYS:HZ1	2.11	0.69
1:D:2717:LEU:O	1:D:2721:ILE:HD12	1.92	0.69
1:A:1960:ARG:HG3	1:A:1961:LYS:N	2.08	0.69
1:B:4052:MET:HG3	1:B:4063:THR:HG23	1.74	0.69
1:C:2717:LEU:O	1:C:2721:ILE:HD12	1.93	0.69
1:B:2717:LEU:O	1:B:2721:ILE:HD12	1.93	0.69
1:B:3668:ILE:HG23	1:B:3739:MET:HE2	1.75	0.69
1:C:1936:LEU:HD21	1:C:1976:LEU:HD13	1.74	0.69
1:B:799:LYS:NZ	1:B:799:LYS:HB3	2.08	0.69
1:C:905:GLY:HA3	1:C:914:GLN:HB3	1.75	0.69
1:D:894:VAL:HA	1:D:897:LYS:HG2	1.75	0.69
1:C:3668:ILE:HG23	1:C:3739:MET:HE2	1.75	0.69
1:D:905:GLY:HA3	1:D:914:GLN:HB3	1.75	0.69
1:D:980:PRO:HG2	1:D:983:LEU:HD21	1.73	0.69
1:A:799:LYS:NZ	1:A:799:LYS:HB3	2.08	0.69
1:A:2959:GLU:N	1:A:2959:GLU:OE2	2.26	0.68
1:B:2386:ASN:ND2	1:B:2457:SER:O	2.24	0.68
1:B:1936:LEU:HD21	1:B:1976:LEU:HD13	1.74	0.68
1:A:2717:LEU:O	1:A:2721:ILE:HD12	1.93	0.68
1:B:1960:ARG:HG3	1:B:1961:LYS:N	2.08	0.68
1:A:897:LYS:HB2	1:A:902:TRP:CD1	2.28	0.68
1:A:905:GLY:HA3	1:A:914:GLN:HB3	1.75	0.68
1:C:799:LYS:NZ	1:C:799:LYS:HB3	2.08	0.68
1:A:980:PRO:HG2	1:A:983:LEU:HD21	1.73	0.68
1:A:4517:LEU:HD23	1:A:4520:TYR:HE2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:897:LYS:HB2	1:B:902:TRP:CD1	2.28	0.68
1:B:4251:ASN:HD22	1:B:4297:PHE:HA	1.59	0.68
1:C:1297:THR:OG1	1:C:1546:GLN:NE2	2.27	0.68
1:C:2386:ASN:ND2	1:C:2457:SER:O	2.24	0.68
1:D:1936:LEU:HD21	1:D:1976:LEU:HD13	1.74	0.68
1:A:1297:THR:OG1	1:A:1546:GLN:NE2	2.27	0.68
1:D:2959:GLU:OE2	1:D:2959:GLU:N	2.26	0.68
1:C:4052:MET:HG3	1:C:4063:THR:HG23	1.74	0.68
1:D:1499:GLY:O	1:D:1502:ASN:ND2	2.27	0.68
1:B:894:VAL:HA	1:B:897:LYS:HG2	1.75	0.68
1:B:905:GLY:HA3	1:B:914:GLN:HB3	1.75	0.68
1:C:1960:ARG:HG3	1:C:1961:LYS:N	2.08	0.68
1:D:4517:LEU:HD23	1:D:4520:TYR:HE2	1.59	0.68
1:A:1499:GLY:O	1:A:1502:ASN:ND2	2.27	0.68
1:A:2763:LEU:HG	1:A:2764:SER:N	2.09	0.68
1:A:3668:ILE:HG23	1:A:3739:MET:HE2	1.76	0.68
1:B:3784:LYS:HE3	1:B:3786:ASP:HB2	1.75	0.68
1:C:2898:ILE:O	1:D:1498:GLN:NE2	2.24	0.68
1:C:897:LYS:HB2	1:C:902:TRP:CD1	2.28	0.67
1:C:1564:MET:HE3	1:C:1565:PRO:HD2	1.76	0.67
1:D:897:LYS:HB2	1:D:902:TRP:CD1	2.29	0.67
1:D:2763:LEU:HG	1:D:2764:SER:N	2.09	0.67
1:B:1297:THR:OG1	1:B:1546:GLN:NE2	2.27	0.67
1:B:2589:LEU:HD23	1:B:2592:LEU:HD12	1.76	0.67
1:C:411:GLU:OE1	1:C:484:ASN:ND2	2.28	0.67
1:D:799:LYS:NZ	1:D:799:LYS:HB3	2.08	0.67
1:D:4052:MET:HG3	1:D:4063:THR:HG23	1.74	0.67
1:A:2589:LEU:HD23	1:A:2592:LEU:HD12	1.76	0.67
1:B:2959:GLU:N	1:B:2959:GLU:OE2	2.26	0.67
1:C:1499:GLY:O	1:C:1502:ASN:ND2	2.27	0.67
1:C:4251:ASN:HD22	1:C:4297:PHE:HA	1.59	0.67
1:D:1297:THR:OG1	1:D:1546:GLN:NE2	2.27	0.67
1:D:3784:LYS:HE3	1:D:3786:ASP:HB2	1.75	0.67
1:D:4251:ASN:HD22	1:D:4297:PHE:HA	1.59	0.67
1:A:4829:ASP:OD1	1:D:4822:ARG:NH1	2.26	0.67
1:B:3016:ARG:O	1:B:3018:ARG:NE	2.20	0.67
1:B:4517:LEU:HD23	1:B:4520:TYR:HE2	1.59	0.67
1:C:2059:GLN:NE2	1:C:2091:GLN:O	2.28	0.67
1:B:1499:GLY:O	1:B:1502:ASN:ND2	2.27	0.67
1:C:993:GLU:OE2	1:C:1051:ARG:NH2	2.28	0.67
1:D:1960:ARG:HG3	1:D:1961:LYS:N	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:GLU:OE1	1:D:484:ASN:ND2	2.28	0.67
1:A:839:GLU:HB3	1:A:851:LEU:HD12	1.76	0.67
1:B:1019:GLY:N	1:B:1029:ASN:O	2.28	0.67
1:D:2927:GLN:HG3	1:D:2930:ILE:HD12	1.77	0.67
1:C:839:GLU:HB3	1:C:851:LEU:HD12	1.76	0.67
1:C:998:LYS:HA	1:C:1001:GLU:HG3	1.77	0.67
1:A:332:ARG:NH1	1:A:364:GLN:OE1	2.28	0.67
1:A:411:GLU:OE1	1:A:484:ASN:ND2	2.28	0.67
1:A:1019:GLY:N	1:A:1029:ASN:O	2.28	0.67
1:A:3784:LYS:HE3	1:A:3786:ASP:HB2	1.75	0.67
1:A:4819:VAL:HG12	1:A:4830:GLU:HG3	1.77	0.67
1:B:332:ARG:NH1	1:B:364:GLN:OE1	2.28	0.67
1:B:993:GLU:OE2	1:B:1051:ARG:NH2	2.28	0.67
1:C:2589:LEU:HD23	1:C:2592:LEU:HD12	1.76	0.67
1:C:3784:LYS:HE3	1:C:3786:ASP:HB2	1.75	0.67
1:C:4517:LEU:HD23	1:C:4520:TYR:HE2	1.59	0.67
1:A:894:VAL:HA	1:A:897:LYS:HG2	1.75	0.67
1:B:839:GLU:HB3	1:B:851:LEU:HD12	1.76	0.67
1:A:548:CYS:HB3	1:A:582:SER:HB2	1.77	0.66
1:A:993:GLU:OE2	1:A:1051:ARG:NH2	2.28	0.66
1:A:2436:ILE:O	1:A:2465:LYS:NZ	2.28	0.66
1:B:998:LYS:HA	1:B:1001:GLU:HG3	1.77	0.66
1:B:4690:LYS:HG3	1:B:4692:SER:H	1.60	0.66
1:C:894:VAL:HA	1:C:897:LYS:HG2	1.75	0.66
1:D:1019:GLY:N	1:D:1029:ASN:O	2.28	0.66
1:D:2059:GLN:NE2	1:D:2091:GLN:O	2.28	0.66
1:D:2589:LEU:HD23	1:D:2592:LEU:HD12	1.76	0.66
1:A:966:LEU:HD12	1:A:978:PRO:HD2	1.78	0.66
1:A:2059:GLN:NE2	1:A:2091:GLN:O	2.28	0.66
1:A:2241:ASP:OD1	1:A:2297:ARG:NH2	2.28	0.66
1:B:2666:LEU:HD13	1:B:2966:VAL:HA	1.78	0.66
1:C:2241:ASP:OD1	1:C:2297:ARG:NH2	2.28	0.66
1:C:2927:GLN:HG3	1:C:2930:ILE:HD12	1.77	0.66
1:D:548:CYS:HB3	1:D:582:SER:HB2	1.77	0.66
1:A:3016:ARG:O	1:A:3018:ARG:NE	2.20	0.66
1:A:4251:ASN:HD22	1:A:4297:PHE:HA	1.59	0.66
1:B:411:GLU:OE1	1:B:484:ASN:ND2	2.28	0.66
1:B:2059:GLN:NE2	1:B:2091:GLN:O	2.28	0.66
1:B:2763:LEU:HG	1:B:2764:SER:N	2.09	0.66
1:C:332:ARG:NH1	1:C:364:GLN:OE1	2.28	0.66
1:A:877:HIS:HD1	1:A:1062:TYR:HE2	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4018:ASP:OD2	1:B:4124:SER:OG	2.09	0.66
1:C:2666:LEU:HD13	1:C:2966:VAL:HA	1.78	0.66
1:A:2608:LYS:HE3	1:A:2664:LEU:HD11	1.78	0.66
1:A:4690:LYS:HG3	1:A:4692:SER:H	1.60	0.66
1:B:2436:ILE:O	1:B:2465:LYS:NZ	2.28	0.66
1:B:2836:ASP:OD1	1:B:2836:ASP:N	2.28	0.66
1:C:2959:GLU:N	1:C:2959:GLU:OE2	2.26	0.66
1:D:332:ARG:NH1	1:D:364:GLN:OE1	2.28	0.66
1:D:839:GLU:HB3	1:D:851:LEU:HD12	1.76	0.66
1:D:2436:ILE:O	1:D:2465:LYS:NZ	2.28	0.66
1:D:4819:VAL:HG12	1:D:4830:GLU:HG3	1.77	0.66
1:A:172:GLY:O	1:D:3939:ARG:NH2	2.28	0.66
1:A:998:LYS:HA	1:A:1001:GLU:HG3	1.77	0.66
1:B:966:LEU:HD12	1:B:978:PRO:HD2	1.78	0.66
1:C:2436:ILE:O	1:C:2465:LYS:NZ	2.28	0.66
1:C:1019:GLY:N	1:C:1029:ASN:O	2.28	0.66
1:C:4819:VAL:HG12	1:C:4830:GLU:HG3	1.77	0.66
1:D:4651:ARG:NH1	1:D:4655:ASP:OD2	2.29	0.66
1:B:2927:GLN:HG3	1:B:2930:ILE:HD12	1.77	0.66
1:A:4651:ARG:NH1	1:A:4655:ASP:OD2	2.29	0.66
1:C:2763:LEU:HG	1:C:2764:SER:N	2.09	0.66
1:C:4651:ARG:NH1	1:C:4655:ASP:OD2	2.29	0.66
1:D:998:LYS:HA	1:D:1001:GLU:HG3	1.77	0.66
1:D:2608:LYS:HE3	1:D:2664:LEU:HD11	1.78	0.66
1:A:2386:ASN:ND2	1:A:2457:SER:O	2.24	0.66
1:D:993:GLU:OE2	1:D:1051:ARG:NH2	2.28	0.66
1:C:3016:ARG:O	1:C:3018:ARG:NE	2.20	0.65
1:D:4690:LYS:HG3	1:D:4692:SER:H	1.60	0.65
1:B:2241:ASP:OD1	1:B:2297:ARG:NH2	2.28	0.65
1:D:1239:PHE:O	1:D:1807:ARG:NH2	2.29	0.65
1:D:2241:ASP:OD1	1:D:2297:ARG:NH2	2.28	0.65
1:D:2666:LEU:HD13	1:D:2966:VAL:HA	1.78	0.65
1:D:3016:ARG:O	1:D:3018:ARG:NE	2.20	0.65
1:A:2666:LEU:HD13	1:A:2966:VAL:HA	1.78	0.65
1:A:2927:GLN:HG3	1:A:2930:ILE:HD12	1.77	0.65
1:B:4819:VAL:HG12	1:B:4830:GLU:HG3	1.77	0.65
1:C:1239:PHE:O	1:C:1807:ARG:NH2	2.29	0.65
1:B:1239:PHE:O	1:B:1807:ARG:NH2	2.29	0.65
1:D:877:HIS:HD1	1:D:1062:TYR:HE2	1.43	0.65
1:C:548:CYS:HB3	1:C:582:SER:HB2	1.77	0.65
1:A:2743:TYR:HB2	1:A:2757:MET:HE3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:HD11	1:B:203:VAL:HG13	1.78	0.65
1:D:966:LEU:HD12	1:D:978:PRO:HD2	1.78	0.65
1:B:548:CYS:HB3	1:B:582:SER:HB2	1.77	0.65
1:B:877:HIS:HD1	1:B:1062:TYR:HE2	1.43	0.65
1:B:4651:ARG:NH1	1:B:4655:ASP:OD2	2.29	0.65
1:C:49:LEU:HD11	1:C:203:VAL:HG13	1.78	0.65
1:C:3042:ALA:HA	1:C:3045:VAL:HG12	1.78	0.65
1:D:2743:TYR:HB2	1:D:2757:MET:HE3	1.78	0.65
1:B:2608:LYS:HE3	1:B:2664:LEU:HD11	1.78	0.65
1:C:4690:LYS:HG3	1:C:4692:SER:H	1.60	0.65
1:C:2608:LYS:HE3	1:C:2664:LEU:HD11	1.78	0.65
1:D:988:LEU:HD13	1:D:1058:LEU:HD11	1.79	0.65
1:A:1239:PHE:O	1:A:1807:ARG:NH2	2.29	0.65
1:A:2445:ILE:HD11	1:A:2449:GLY:HA2	1.79	0.65
1:A:4752:THR:HG21	1:B:4766:GLN:HG2	1.77	0.65
1:C:966:LEU:HD12	1:C:978:PRO:HD2	1.78	0.65
1:A:3042:ALA:HA	1:A:3045:VAL:HG12	1.78	0.64
1:C:988:LEU:HD13	1:C:1058:LEU:HD11	1.79	0.64
1:B:1564:MET:HE3	1:B:1565:PRO:HD2	1.78	0.64
1:B:4287:TYR:HE1	1:C:4591:TYR:CD2	2.16	0.64
1:D:49:LEU:HD11	1:D:203:VAL:HG13	1.78	0.64
1:B:260:VAL:O	1:B:390:LYS:NZ	2.29	0.64
1:D:1245:ARG:NH1	1:D:1692:LYS:O	2.31	0.64
1:D:2590:ARG:NH2	1:D:2875:ASP:OD2	2.31	0.64
1:D:3042:ALA:HA	1:D:3045:VAL:HG12	1.78	0.64
1:D:1040:ASP:OD1	1:D:1044:LYS:NZ	2.25	0.64
1:A:4018:ASP:OD2	1:A:4124:SER:OG	2.09	0.64
1:D:2445:ILE:HD11	1:D:2449:GLY:HA2	1.79	0.64
1:B:1245:ARG:NH1	1:B:1692:LYS:O	2.31	0.64
1:B:3042:ALA:HA	1:B:3045:VAL:HG12	1.78	0.64
1:D:2717:LEU:HD12	1:D:2779:LEU:HD13	1.80	0.64
1:B:2718:GLU:OE2	1:B:2772:ARG:NH1	2.30	0.64
1:C:877:HIS:HD1	1:C:1062:TYR:HE2	1.43	0.64
1:C:1245:ARG:NH1	1:C:1692:LYS:O	2.31	0.64
1:A:49:LEU:HD11	1:A:203:VAL:HG13	1.78	0.63
1:A:2717:LEU:HD12	1:A:2779:LEU:HD13	1.80	0.63
1:C:2590:ARG:NH2	1:C:2875:ASP:OD2	2.31	0.63
1:A:1245:ARG:NH1	1:A:1692:LYS:O	2.31	0.63
1:A:2727:HIS:CE1	1:A:2731:LYS:HZ1	2.16	0.63
1:B:2445:ILE:HD11	1:B:2449:GLY:HA2	1.79	0.63
1:A:2723:LYS:HG2	1:A:2895:PHE:HZ	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3089:GLY:HA2	1:A:3092:GLN:HE21	1.63	0.63
1:A:4514:ASN:HD22	1:A:4517:LEU:HD12	1.64	0.63
1:B:988:LEU:HD13	1:B:1058:LEU:HD11	1.79	0.63
1:C:2337:GLY:HA2	1:D:142:LYS:HD3	1.80	0.63
1:D:4018:ASP:OD2	1:D:4124:SER:OG	2.09	0.63
1:C:808:HIS:HD2	1:C:823:TYR:HB2	1.64	0.63
1:C:2723:LYS:HG2	1:C:2895:PHE:HZ	1.62	0.63
1:D:808:HIS:HD2	1:D:823:TYR:HB2	1.63	0.63
1:C:2717:LEU:HD12	1:C:2779:LEU:HD13	1.80	0.63
1:A:988:LEU:HD13	1:A:1058:LEU:HD11	1.79	0.63
1:B:3089:GLY:HA2	1:B:3092:GLN:HE21	1.63	0.63
1:B:4514:ASN:HD22	1:B:4517:LEU:HD12	1.64	0.63
1:D:2688:MET:HB3	1:D:2689:MET:SD	2.39	0.63
1:B:660:PHE:HB3	1:B:787:LEU:HD23	1.81	0.63
1:B:2723:LYS:HG2	1:B:2895:PHE:HZ	1.62	0.63
1:C:660:PHE:HB3	1:C:787:LEU:HD23	1.81	0.63
1:C:2119:LEU:HB2	1:C:2152:ASN:HD22	1.63	0.63
1:A:2688:MET:HB3	1:A:2689:MET:SD	2.39	0.63
1:C:2445:ILE:HD11	1:C:2449:GLY:HA2	1.79	0.63
1:D:4832:GLU:O	1:D:4843:ARG:NH1	2.32	0.63
1:A:1040:ASP:OD1	1:A:1044:LYS:NZ	2.25	0.62
1:B:2717:LEU:HD12	1:B:2779:LEU:HD13	1.80	0.62
1:B:4752:THR:HG21	1:C:4766:GLN:HG2	1.80	0.62
1:C:1414:ARG:NH1	1:C:1415:ASP:O	2.32	0.62
1:C:3089:GLY:HA2	1:C:3092:GLN:HE21	1.63	0.62
1:A:1414:ARG:NH1	1:A:1415:ASP:O	2.32	0.62
1:A:2119:LEU:HB2	1:A:2152:ASN:HD22	1.64	0.62
1:B:872:ILE:O	1:B:941:LYS:NZ	2.33	0.62
1:B:2688:MET:HB3	1:B:2689:MET:SD	2.39	0.62
1:C:872:ILE:O	1:C:941:LYS:NZ	2.33	0.62
1:C:1685:LEU:HD22	1:C:1706:LEU:HB2	1.81	0.62
1:A:1962:THR:HA	1:A:1965:PHE:HD2	1.64	0.62
1:A:2590:ARG:NH2	1:A:2875:ASP:OD2	2.31	0.62
1:B:2119:LEU:HB2	1:B:2152:ASN:HD22	1.64	0.62
1:D:4514:ASN:HD22	1:D:4517:LEU:HD12	1.63	0.62
1:D:2727:HIS:CE1	1:D:2731:LYS:HZ1	2.17	0.62
1:D:3089:GLY:HA2	1:D:3092:GLN:HE21	1.63	0.62
1:B:1414:ARG:NH1	1:B:1415:ASP:O	2.32	0.62
1:C:1114:ARG:NH1	1:C:1128:LEU:O	2.33	0.62
1:C:2688:MET:HB3	1:C:2689:MET:SD	2.39	0.62
1:C:2917:ILE:HG21	1:C:2999:LYS:HE2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4040:LYS:NZ	1:C:4042:VAL:O	2.33	0.62
1:D:660:PHE:HB3	1:D:787:LEU:HD23	1.81	0.62
1:D:2905:ARG:HE	1:D:2906:GLY:N	1.97	0.62
1:A:660:PHE:HB3	1:A:787:LEU:HD23	1.81	0.62
1:A:1685:LEU:HD22	1:A:1706:LEU:HB2	1.80	0.62
1:B:2590:ARG:NH2	1:B:2875:ASP:OD2	2.31	0.62
1:D:1685:LEU:HD22	1:D:1706:LEU:HB2	1.81	0.62
1:D:2119:LEU:HB2	1:D:2152:ASN:HD22	1.63	0.62
1:D:2723:LYS:HG2	1:D:2895:PHE:HZ	1.62	0.62
1:A:1043:LYS:HA	1:A:1046:ASN:HD21	1.65	0.62
1:B:1074:ARG:HH11	1:B:1076:GLU:HA	1.65	0.62
1:D:1414:ARG:NH1	1:D:1415:ASP:O	2.32	0.62
1:D:2741:TRP:HA	1:D:2752:LYS:HB3	1.82	0.62
1:D:4040:LYS:NZ	1:D:4042:VAL:O	2.33	0.62
1:A:890:HIS:HA	1:A:893:TRP:HE3	1.64	0.62
1:A:2736:LYS:HG2	1:A:2741:TRP:HB2	1.82	0.62
1:B:1043:LYS:HA	1:B:1046:ASN:HD21	1.64	0.62
1:C:4514:ASN:HD22	1:C:4517:LEU:HD12	1.64	0.62
1:D:1896:MET:HB3	1:D:1898:LEU:HD11	1.82	0.62
1:D:2718:GLU:OE2	1:D:2772:ARG:NH1	2.30	0.62
1:A:872:ILE:O	1:A:941:LYS:NZ	2.33	0.62
1:A:4832:GLU:O	1:A:4843:ARG:NH1	2.32	0.62
1:B:1685:LEU:HD22	1:B:1706:LEU:HB2	1.81	0.62
1:C:1896:MET:HB3	1:C:1898:LEU:HD11	1.82	0.62
1:C:1962:THR:HA	1:C:1965:PHE:HD2	1.64	0.62
1:C:2905:ARG:HE	1:C:2906:GLY:N	1.97	0.62
1:D:1564:MET:HE3	1:D:1565:PRO:HD2	1.82	0.62
1:A:2741:TRP:HA	1:A:2752:LYS:HB3	1.82	0.62
1:A:2905:ARG:HE	1:A:2906:GLY:N	1.97	0.62
1:C:4832:GLU:O	1:C:4843:ARG:NH1	2.32	0.62
1:C:2741:TRP:HA	1:C:2752:LYS:HB3	1.82	0.61
1:D:2576:ILE:O	1:D:2580:LEU:HG	2.00	0.61
1:A:888:ASN:ND2	1:A:1060:TYR:OH	2.34	0.61
1:A:2917:ILE:HG21	1:A:2999:LYS:HE2	1.82	0.61
1:C:2576:ILE:O	1:C:2580:LEU:HG	2.00	0.61
1:D:1114:ARG:NH1	1:D:1128:LEU:O	2.33	0.61
1:D:2202:TYR:O	1:D:2206:ILE:HG12	2.01	0.61
1:A:2718:GLU:OE2	1:A:2772:ARG:NH1	2.30	0.61
1:A:4251:ASN:ND2	1:A:4297:PHE:HA	2.16	0.61
1:B:890:HIS:CE1	1:B:921:PHE:HB3	2.36	0.61
1:B:1962:THR:HA	1:B:1965:PHE:HD2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2202:TYR:O	1:B:2206:ILE:HG12	2.01	0.61
1:B:2576:ILE:O	1:B:2580:LEU:HG	2.00	0.61
1:C:2736:LYS:HG2	1:C:2741:TRP:HB2	1.82	0.61
1:D:1937:GLN:HG2	1:D:3609:TYR:HA	1.82	0.61
1:A:808:HIS:HD2	1:A:823:TYR:HB2	1.64	0.61
1:C:4177:VAL:HG21	1:C:4880:VAL:HG13	1.83	0.61
1:D:2642:ARG:NH2	1:D:2682:GLU:OE2	2.34	0.61
1:D:2917:ILE:HG21	1:D:2999:LYS:HE2	1.82	0.61
1:A:1937:GLN:HG2	1:A:3609:TYR:HA	1.82	0.61
1:B:808:HIS:HD2	1:B:823:TYR:HB2	1.64	0.61
1:C:1937:GLN:HG2	1:C:3609:TYR:HA	1.82	0.61
1:C:2497:ARG:HH22	1:C:2878:THR:HB	1.66	0.61
1:D:1962:THR:HA	1:D:1965:PHE:HD2	1.64	0.61
1:D:2736:LYS:HG2	1:D:2741:TRP:HB2	1.82	0.61
1:D:2836:ASP:N	1:D:2836:ASP:OD1	2.28	0.61
1:A:1114:ARG:NH1	1:A:1128:LEU:O	2.33	0.61
1:A:2576:ILE:O	1:A:2580:LEU:HG	2.00	0.61
1:C:888:ASN:ND2	1:C:1060:TYR:OH	2.34	0.61
1:C:2202:TYR:O	1:C:2206:ILE:HG12	2.01	0.61
1:C:2743:TYR:HB2	1:C:2757:MET:HE3	1.82	0.61
1:A:1074:ARG:HH11	1:A:1076:GLU:HA	1.65	0.61
1:A:1896:MET:HB3	1:A:1898:LEU:HD11	1.82	0.61
1:D:2521:CYS:HA	1:D:2525:LEU:HD12	1.83	0.61
1:A:2785:TRP:HB2	1:A:2787:TRP:HZ3	1.66	0.61
1:B:1896:MET:HB3	1:B:1898:LEU:HD11	1.82	0.61
1:C:2642:ARG:NH2	1:C:2682:GLU:OE2	2.34	0.61
1:D:872:ILE:O	1:D:941:LYS:NZ	2.33	0.61
1:A:2792:THR:HG23	1:A:2794:GLU:H	1.66	0.61
1:B:2741:TRP:HA	1:B:2752:LYS:HB3	1.82	0.61
1:D:1043:LYS:HA	1:D:1046:ASN:HD21	1.65	0.61
1:D:2497:ARG:HH22	1:D:2878:THR:HB	1.66	0.61
1:D:2792:THR:HG23	1:D:2794:GLU:H	1.66	0.61
1:A:890:HIS:CE1	1:A:921:PHE:HB3	2.36	0.60
1:A:4040:LYS:NZ	1:A:4042:VAL:O	2.33	0.60
1:C:1074:ARG:HH11	1:C:1076:GLU:HA	1.65	0.60
1:C:4822:ARG:HH12	1:D:4829:ASP:N	1.99	0.60
1:D:888:ASN:ND2	1:D:1060:TYR:OH	2.34	0.60
1:D:1074:ARG:HH11	1:D:1076:GLU:HA	1.65	0.60
1:D:4177:VAL:HG21	1:D:4880:VAL:HG13	1.83	0.60
1:B:888:ASN:ND2	1:B:1060:TYR:OH	2.34	0.60
1:B:890:HIS:HA	1:B:893:TRP:HE3	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4040:LYS:NZ	1:B:4042:VAL:O	2.33	0.60
1:B:4251:ASN:ND2	1:B:4297:PHE:HA	2.16	0.60
1:C:890:HIS:CE1	1:C:921:PHE:HB3	2.36	0.60
1:C:1043:LYS:HA	1:C:1046:ASN:HD21	1.65	0.60
1:D:2785:TRP:HB2	1:D:2787:TRP:HZ3	1.66	0.60
1:B:1114:ARG:NH1	1:B:1128:LEU:O	2.33	0.60
1:B:2130:LEU:HD11	1:B:2170:THR:HG23	1.83	0.60
1:B:2785:TRP:HB2	1:B:2787:TRP:HZ3	1.66	0.60
1:B:2917:ILE:HG21	1:B:2999:LYS:HE2	1.82	0.60
1:B:4832:GLU:O	1:B:4843:ARG:NH1	2.32	0.60
1:C:875:PRO:HD2	1:C:878:LEU:HD12	1.83	0.60
1:D:4251:ASN:ND2	1:D:4297:PHE:HA	2.16	0.60
1:A:2202:TYR:O	1:A:2206:ILE:HG12	2.01	0.60
1:B:904:TYR:HB2	1:B:918:LEU:HB3	1.84	0.60
1:B:2129:LEU:CB	1:B:2142:MET:HE1	2.31	0.60
1:B:2642:ARG:NH2	1:B:2682:GLU:OE2	2.34	0.60
1:C:176:ARG:HB2	1:C:179:ASP:HB2	1.83	0.60
1:C:260:VAL:O	1:C:390:LYS:NZ	2.29	0.60
1:C:4018:ASP:OD2	1:C:4124:SER:OG	2.09	0.60
1:A:1016:TRP:HE3	1:A:1027:ARG:HH11	1.50	0.60
1:A:2642:ARG:NH2	1:A:2682:GLU:OE2	2.34	0.60
1:B:2322:ARG:HH12	1:C:189:GLU:HG2	1.66	0.60
1:C:904:TYR:HB2	1:C:918:LEU:HB3	1.84	0.60
1:C:1001:GLU:O	1:C:1004:HIS:ND1	2.35	0.60
1:C:2792:THR:HG23	1:C:2794:GLU:H	1.66	0.60
1:D:246:THR:HG21	1:D:267:VAL:HG11	1.84	0.60
1:D:890:HIS:HA	1:D:893:TRP:HE3	1.64	0.60
1:A:875:PRO:HD2	1:A:878:LEU:HD12	1.83	0.60
1:A:904:TYR:HB2	1:A:918:LEU:HB3	1.84	0.60
1:B:1937:GLN:HG2	1:B:3609:TYR:HA	1.82	0.60
1:C:2521:CYS:HA	1:C:2525:LEU:HD12	1.83	0.60
1:C:4633:LEU:HB3	1:C:4704:LYS:HZ1	1.67	0.60
1:D:875:PRO:HD2	1:D:878:LEU:HD12	1.84	0.60
1:D:1016:TRP:HE3	1:D:1027:ARG:HH11	1.50	0.60
1:B:2670:SER:HB2	1:B:2973:GLN:HG2	1.84	0.60
1:B:4633:LEU:HB3	1:B:4704:LYS:HZ2	1.66	0.60
1:C:2130:LEU:HD11	1:C:2170:THR:HG23	1.83	0.60
1:D:218:SER:HB2	1:D:286:GLY:HA3	1.84	0.60
1:D:904:TYR:HB2	1:D:918:LEU:HB3	1.84	0.60
1:A:291:TRP:O	1:A:343:ARG:NH1	2.35	0.60
1:A:4707:MET:HG3	1:D:4252:ILE:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2736:LYS:HG2	1:B:2741:TRP:HB2	1.82	0.60
1:C:218:SER:HB2	1:C:286:GLY:HA3	1.84	0.60
1:D:1001:GLU:O	1:D:1004:HIS:ND1	2.35	0.60
1:A:1001:GLU:O	1:A:1004:HIS:ND1	2.35	0.60
1:B:246:THR:HG21	1:B:267:VAL:HG11	1.84	0.60
1:B:875:PRO:HD2	1:B:878:LEU:HD12	1.83	0.60
1:B:2792:THR:HG23	1:B:2794:GLU:H	1.66	0.60
1:B:4569:GLU:HB3	1:B:4570:PRO:HD3	1.84	0.60
1:C:246:THR:HG21	1:C:267:VAL:HG11	1.84	0.60
1:C:907:VAL:HG12	1:C:909:ASP:H	1.67	0.60
1:C:4251:ASN:ND2	1:C:4297:PHE:HA	2.16	0.60
1:D:2119:LEU:HB2	1:D:2152:ASN:ND2	2.17	0.60
1:D:4633:LEU:HB3	1:D:4704:LYS:HZ2	1.67	0.60
1:A:246:THR:HG21	1:A:267:VAL:HG11	1.84	0.60
1:A:2670:SER:HB2	1:A:2973:GLN:HG2	1.84	0.60
1:B:907:VAL:HG12	1:B:909:ASP:H	1.67	0.60
1:B:2497:ARG:HH22	1:B:2878:THR:HB	1.66	0.60
1:B:2743:TYR:HB2	1:B:2757:MET:HE3	1.83	0.60
1:B:2905:ARG:HE	1:B:2906:GLY:N	1.97	0.60
1:C:2129:LEU:HD13	1:C:2142:MET:HE1	1.84	0.60
1:D:907:VAL:HG12	1:D:909:ASP:H	1.67	0.60
1:D:2129:LEU:CB	1:D:2142:MET:HE1	2.32	0.60
1:A:2521:CYS:HA	1:A:2525:LEU:HD12	1.83	0.59
1:A:4177:VAL:HG21	1:A:4880:VAL:HG13	1.83	0.59
1:B:1016:TRP:HE3	1:B:1027:ARG:HH11	1.50	0.59
1:C:1016:TRP:HE3	1:C:1027:ARG:HH11	1.50	0.59
1:A:2130:LEU:HD11	1:A:2170:THR:HG23	1.83	0.59
1:B:1001:GLU:O	1:B:1004:HIS:ND1	2.35	0.59
1:B:4580:THR:OG1	1:B:4733:HIS:NE2	2.33	0.59
1:C:25:THR:OG1	1:C:32:GLN:OE1	2.20	0.59
1:D:25:THR:OG1	1:D:32:GLN:OE1	2.20	0.59
1:D:291:TRP:O	1:D:343:ARG:NH1	2.35	0.59
1:D:890:HIS:CE1	1:D:921:PHE:HB3	2.36	0.59
1:D:4042:VAL:HG12	1:D:4077:THR:HB	1.84	0.59
1:A:2129:LEU:CB	1:A:2142:MET:HE1	2.31	0.59
1:B:4177:VAL:HG21	1:B:4880:VAL:HG13	1.83	0.59
1:C:2670:SER:HB2	1:C:2973:GLN:HG2	1.84	0.59
1:C:2785:TRP:HB2	1:C:2787:TRP:HZ3	1.66	0.59
1:C:4120:GLU:HA	1:C:4123:GLU:HG2	1.84	0.59
1:A:2894:LYS:O	1:A:2898:ILE:HG12	2.02	0.59
1:A:4580:THR:OG1	1:A:4733:HIS:NE2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4042:VAL:HG12	1:C:4077:THR:HB	1.84	0.59
1:C:4569:GLU:HB3	1:C:4570:PRO:HD3	1.84	0.59
1:D:2894:LYS:O	1:D:2898:ILE:HG12	2.02	0.59
1:A:25:THR:OG1	1:A:32:GLN:OE1	2.20	0.59
1:A:1721:MET:HG3	1:A:1759:PRO:HG3	1.85	0.59
1:A:4569:GLU:HB3	1:A:4570:PRO:HD3	1.84	0.59
1:B:114:LEU:HD23	1:B:117:HIS:HE1	1.67	0.59
1:B:2488:LEU:HD11	1:B:2548:LEU:HD22	1.84	0.59
1:D:176:ARG:HB2	1:D:179:ASP:HB2	1.83	0.59
1:A:176:ARG:HB2	1:A:179:ASP:HB2	1.83	0.59
1:A:907:VAL:HG12	1:A:909:ASP:H	1.67	0.59
1:B:176:ARG:HB2	1:B:179:ASP:HB2	1.83	0.59
1:B:2119:LEU:HB2	1:B:2152:ASN:ND2	2.17	0.59
1:C:2488:LEU:HD11	1:C:2548:LEU:HD22	1.84	0.59
1:C:2927:GLN:NE2	1:C:3003:MET:SD	2.76	0.59
1:D:441:LYS:NZ	1:D:443:SER:OG	2.25	0.59
1:B:1040:ASP:OD1	1:B:1044:LYS:NZ	2.26	0.59
1:B:4252:ILE:CG2	1:C:4707:MET:HG3	2.33	0.59
1:C:114:LEU:HD23	1:C:117:HIS:HE1	1.68	0.59
1:B:919:VAL:HB	1:B:923:LYS:HE3	1.84	0.59
1:C:291:TRP:O	1:C:343:ARG:NH1	2.35	0.59
1:D:887:GLU:HA	1:D:890:HIS:NE2	2.18	0.59
1:D:2146:LEU:O	1:D:2150:MET:HG2	2.03	0.59
1:A:887:GLU:HA	1:A:890:HIS:NE2	2.18	0.59
2:F:50:ARG:CZ	2:F:53:LYS:HE3	2.33	0.59
1:B:520:ARG:NH1	1:B:524:GLU:OE1	2.36	0.59
1:B:1962:THR:HG21	1:B:3603:PHE:CG	2.38	0.59
1:B:2521:CYS:HA	1:B:2525:LEU:HD12	1.83	0.59
1:C:4882:GLU:O	1:C:4886:THR:OG1	2.21	0.59
1:D:919:VAL:HB	1:D:923:LYS:HE3	1.84	0.59
1:D:1721:MET:HG3	1:D:1759:PRO:HG3	1.85	0.59
1:D:2670:SER:HB2	1:D:2973:GLN:HG2	1.84	0.59
1:A:4633:LEU:HB3	1:A:4704:LYS:HZ1	1.68	0.59
2:E:50:ARG:CZ	2:E:53:LYS:HE3	2.33	0.59
1:B:948:CYS:HA	1:B:1067:PRO:HD3	1.85	0.59
1:B:1721:MET:HG3	1:B:1759:PRO:HG3	1.85	0.59
1:B:2894:LYS:O	1:B:2898:ILE:HG12	2.02	0.59
1:C:520:ARG:NH1	1:C:524:GLU:OE1	2.36	0.59
1:C:948:CYS:HA	1:C:1067:PRO:HD3	1.85	0.59
1:A:919:VAL:HB	1:A:923:LYS:HE3	1.84	0.58
1:C:143:LEU:HD13	1:C:207:PHE:HE2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:919:VAL:HB	1:C:923:LYS:HE3	1.84	0.58
1:C:4753:LEU:HD22	1:D:4773:LEU:HB2	1.84	0.58
1:D:15:ARG:NH2	1:D:110:HIS:O	2.36	0.58
1:D:4082:GLU:HA	1:D:4085:LYS:HG2	1.85	0.58
1:A:218:SER:HB2	1:A:286:GLY:HA3	1.84	0.58
1:A:882:ARG:HA	1:A:885:LEU:HB3	1.85	0.58
1:A:2497:ARG:HH22	1:A:2878:THR:HB	1.66	0.58
2:H:50:ARG:CZ	2:H:53:LYS:HE3	2.33	0.58
1:B:291:TRP:O	1:B:343:ARG:NH1	2.35	0.58
1:B:1910:LEU:HD22	1:B:2062:ILE:HD11	1.86	0.58
1:A:15:ARG:NH2	1:A:110:HIS:O	2.36	0.58
1:C:1473:LYS:HE3	1:C:1475:LYS:HB2	1.85	0.58
1:D:882:ARG:HA	1:D:885:LEU:HB3	1.85	0.58
1:D:948:CYS:HA	1:D:1067:PRO:HD3	1.85	0.58
1:D:1910:LEU:HD22	1:D:2062:ILE:HD11	1.86	0.58
1:D:1962:THR:HG21	1:D:3603:PHE:CG	2.38	0.58
1:A:948:CYS:HA	1:A:1067:PRO:HD3	1.85	0.58
1:A:2843:MET:HA	1:A:2846:GLU:OE1	2.04	0.58
1:A:4082:GLU:HA	1:A:4085:LYS:HG2	1.85	0.58
1:A:4120:GLU:HA	1:A:4123:GLU:HG2	1.84	0.58
1:A:4882:GLU:O	1:A:4886:THR:OG1	2.21	0.58
1:B:4120:GLU:HA	1:B:4123:GLU:HG2	1.84	0.58
1:C:441:LYS:NZ	1:C:443:SER:OG	2.25	0.58
1:C:1143:GLN:HE21	1:C:1149:ASN:HB2	1.69	0.58
1:C:4082:GLU:HA	1:C:4085:LYS:HG2	1.85	0.58
1:C:4187:GLU:OE2	1:C:4947:ARG:NH2	2.37	0.58
1:D:4120:GLU:HA	1:D:4123:GLU:HG2	1.84	0.58
1:A:1965:PHE:O	1:A:3604:ARG:NH2	2.36	0.58
1:B:218:SER:HB2	1:B:286:GLY:HA3	1.84	0.58
1:B:2927:GLN:NE2	1:B:3003:MET:SD	2.76	0.58
1:D:2130:LEU:HD11	1:D:2170:THR:HG23	1.83	0.58
1:A:1041:ARG:NH1	1:A:1045:SER:HB3	2.19	0.58
1:A:1910:LEU:HD22	1:A:2062:ILE:HD11	1.86	0.58
2:G:50:ARG:CZ	2:G:53:LYS:HE3	2.33	0.58
1:B:15:ARG:NH2	1:B:110:HIS:O	2.36	0.58
1:B:1473:LYS:HE3	1:B:1475:LYS:HB2	1.85	0.58
1:B:2775:ILE:O	1:B:2779:LEU:HG	2.04	0.58
1:B:4882:GLU:O	1:B:4886:THR:OG1	2.21	0.58
1:C:927:GLN:NE2	1:C:928:GLU:HG3	2.18	0.58
1:C:1041:ARG:NH1	1:C:1045:SER:HB3	2.19	0.58
1:C:2775:ILE:O	1:C:2779:LEU:HG	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2894:LYS:O	1:C:2898:ILE:HG12	2.02	0.58
1:D:520:ARG:NH1	1:D:524:GLU:OE1	2.36	0.58
1:D:1143:GLN:HE21	1:D:1149:ASN:HB2	1.69	0.58
1:D:1965:PHE:O	1:D:3604:ARG:NH2	2.36	0.58
1:D:2775:ILE:O	1:D:2779:LEU:HG	2.04	0.58
1:D:2927:GLN:NE2	1:D:3003:MET:SD	2.76	0.58
1:D:4187:GLU:OE2	1:D:4947:ARG:NH2	2.37	0.58
1:D:4303:ARG:HH11	1:D:4307:ARG:HH22	1.52	0.58
1:D:4569:GLU:HB3	1:D:4570:PRO:HD3	1.84	0.58
1:A:520:ARG:NH1	1:A:524:GLU:OE1	2.36	0.58
1:A:849:ASP:OD1	1:A:1214:ARG:NE	2.37	0.58
1:A:2775:ILE:O	1:A:2779:LEU:HG	2.04	0.58
1:B:25:THR:OG1	1:B:32:GLN:OE1	2.20	0.58
1:B:4303:ARG:HH11	1:B:4307:ARG:HH22	1.52	0.58
1:C:2119:LEU:HB2	1:C:2152:ASN:ND2	2.17	0.58
1:D:1041:ARG:NH1	1:D:1045:SER:HB3	2.19	0.58
1:A:4042:VAL:HG12	1:A:4077:THR:HB	1.84	0.58
1:B:4082:GLU:HA	1:B:4085:LYS:HG2	1.85	0.58
1:C:1040:ASP:OD1	1:C:1044:LYS:NZ	2.25	0.58
1:B:2843:MET:HA	1:B:2846:GLU:OE1	2.04	0.58
1:A:927:GLN:NE2	1:A:928:GLU:HG3	2.19	0.58
1:A:1184:ASP:OD2	1:A:1188:SER:OG	2.22	0.58
1:A:2488:LEU:HD11	1:A:2548:LEU:HD22	1.84	0.58
1:B:143:LEU:HD13	1:B:207:PHE:HE2	1.68	0.58
1:B:927:GLN:NE2	1:B:928:GLU:HG3	2.19	0.58
1:B:1043:LYS:O	1:B:1047:LYS:HG2	2.04	0.58
1:B:1965:PHE:O	1:B:3604:ARG:NH2	2.37	0.58
1:D:927:GLN:NE2	1:D:928:GLU:HG3	2.18	0.58
1:D:2488:LEU:HD11	1:D:2548:LEU:HD22	1.84	0.58
1:A:2119:LEU:HB2	1:A:2152:ASN:ND2	2.17	0.57
1:A:2146:LEU:O	1:A:2150:MET:HG2	2.03	0.57
1:A:4252:ILE:HG21	1:B:4707:MET:HG3	1.86	0.57
1:B:614:LEU:HA	1:B:617:LEU:HD12	1.86	0.57
1:B:2426:LEU:HD23	1:C:143:LEU:HD11	1.86	0.57
1:C:849:ASP:OD1	1:C:1214:ARG:NE	2.37	0.57
1:C:1721:MET:HG3	1:C:1759:PRO:HG3	1.85	0.57
1:C:2142:MET:HB2	1:C:2192:MET:HE1	1.86	0.57
1:C:2718:GLU:OE2	1:C:2772:ARG:NH1	2.30	0.57
1:C:4262:LYS:HG3	1:D:4698:LEU:HD22	1.86	0.57
1:D:114:LEU:HD23	1:D:117:HIS:HE1	1.68	0.57
1:A:1043:LYS:O	1:A:1047:LYS:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1143:GLN:HE21	1:A:1149:ASN:HB2	1.69	0.57
1:B:1143:GLN:HE21	1:B:1149:ASN:HB2	1.69	0.57
1:B:2146:LEU:O	1:B:2150:MET:HG2	2.03	0.57
1:C:1962:THR:HG21	1:C:3603:PHE:CG	2.38	0.57
1:C:4303:ARG:HH11	1:C:4307:ARG:HH22	1.52	0.57
1:D:1722:ASN:O	1:D:1919:ARG:NH2	2.37	0.57
1:D:4882:GLU:O	1:D:4886:THR:OG1	2.21	0.57
1:A:950:VAL:HA	1:A:1064:LEU:HA	1.86	0.57
1:B:1041:ARG:NH1	1:B:1045:SER:HB3	2.19	0.57
1:B:4042:VAL:HG12	1:B:4077:THR:HB	1.84	0.57
1:C:887:GLU:HA	1:C:890:HIS:NE2	2.18	0.57
1:C:1910:LEU:HD22	1:C:2062:ILE:HD11	1.86	0.57
1:C:2146:LEU:O	1:C:2150:MET:HG2	2.03	0.57
1:C:2604:LYS:O	1:C:2608:LYS:HD2	2.04	0.57
1:D:1043:LYS:O	1:D:1047:LYS:HG2	2.04	0.57
1:A:114:LEU:HD23	1:A:117:HIS:HE1	1.68	0.57
1:B:2096:GLY:HA2	1:B:2099:VAL:HG12	1.85	0.57
1:C:2641:SER:HB3	1:C:2676:LEU:HD21	1.87	0.57
1:D:143:LEU:HD13	1:D:207:PHE:HE2	1.68	0.57
1:D:1184:ASP:OD2	1:D:1188:SER:OG	2.22	0.57
1:D:2833:LEU:HB3	1:D:2838[B]:HIS:CE1	2.39	0.57
1:D:2843:MET:HA	1:D:2846:GLU:OE1	2.04	0.57
1:A:1962:THR:HG21	1:A:3603:PHE:CG	2.38	0.57
1:A:2641:SER:HB3	1:A:2676:LEU:HD21	1.87	0.57
1:A:2650:ASP:OD1	1:A:2651:ALA:N	2.38	0.57
1:A:3697:LYS:HA	1:A:3700:HIS:CD2	2.40	0.57
1:A:4303:ARG:HH11	1:A:4307:ARG:HH22	1.52	0.57
1:B:849:ASP:OD1	1:B:1214:ARG:NE	2.37	0.57
1:B:1722:ASN:O	1:B:1919:ARG:NH2	2.37	0.57
1:B:2604:LYS:O	1:B:2608:LYS:HD2	2.04	0.57
1:B:2650:ASP:OD1	1:B:2651:ALA:N	2.38	0.57
1:B:2833:LEU:HD21	1:B:2837:LEU:HD23	1.87	0.57
1:B:3697:LYS:HA	1:B:3700:HIS:CD2	2.40	0.57
1:C:15:ARG:NH2	1:C:110:HIS:O	2.36	0.57
1:C:950:VAL:HA	1:C:1064:LEU:HA	1.86	0.57
1:D:962:LYS:HB3	1:D:981:MET:HB3	1.86	0.57
1:A:614:LEU:HA	1:A:617:LEU:HD12	1.86	0.57
1:A:2096:GLY:HA2	1:A:2099:VAL:HG12	1.86	0.57
1:A:4187:GLU:OE2	1:A:4947:ARG:NH2	2.37	0.57
1:B:887:GLU:HA	1:B:890:HIS:NE2	2.18	0.57
1:C:2273:GLY:O	1:C:2336:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2833:LEU:HD21	1:C:2837:LEU:HD23	1.87	0.57
1:A:4790:ARG:NH2	1:D:4559:TYR:OH	2.36	0.57
1:C:962:LYS:HB3	1:C:981:MET:HB3	1.86	0.57
1:D:2257:LEU:HB2	1:D:2316:ASN:HD21	1.70	0.57
1:D:2641:SER:HB3	1:D:2676:LEU:HD21	1.87	0.57
1:A:1473:LYS:HE3	1:A:1475:LYS:HB2	1.85	0.57
1:A:2273:GLY:O	1:A:2336:ARG:NH2	2.37	0.57
1:A:2604:LYS:O	1:A:2608:LYS:HD2	2.04	0.57
1:C:614:LEU:HA	1:C:617:LEU:HD12	1.86	0.57
1:C:882:ARG:HA	1:C:885:LEU:HB3	1.85	0.57
1:C:2650:ASP:OD1	1:C:2651:ALA:N	2.38	0.57
1:C:4896:ASP:OD1	1:C:4897:TYR:N	2.38	0.57
1:D:2787:TRP:HE1	1:D:2903:VAL:HG23	1.70	0.57
1:B:2273:GLY:O	1:B:2336:ARG:NH2	2.37	0.57
1:B:4896:ASP:OD1	1:B:4897:TYR:N	2.38	0.57
1:C:1965:PHE:O	1:C:3604:ARG:NH2	2.36	0.57
1:D:891:GLU:HB3	1:D:978:PRO:HG3	1.87	0.57
1:D:2604:LYS:O	1:D:2608:LYS:HD2	2.04	0.57
1:A:143:LEU:HD13	1:A:207:PHE:HE2	1.69	0.57
1:A:2927:GLN:NE2	1:A:3003:MET:SD	2.76	0.57
2:E:22:THR:HG22	2:E:50:ARG:HB3	1.87	0.57
1:B:882:ARG:HA	1:B:885:LEU:HB3	1.85	0.57
1:B:4517:LEU:HD21	1:B:4736:ASN:HB3	1.87	0.57
1:C:4517:LEU:HD21	1:C:4736:ASN:HB3	1.87	0.57
1:C:4580:THR:OG1	1:C:4733:HIS:NE2	2.33	0.57
1:D:2650:ASP:OD1	1:D:2651:ALA:N	2.38	0.57
1:D:4517:LEU:HD21	1:D:4736:ASN:HB3	1.87	0.57
1:A:932:ASN:HA	1:A:935:MET:HG2	1.87	0.56
1:B:1604:LEU:HD23	1:B:1625:LEU:HD13	1.87	0.56
1:C:2843:MET:HA	1:C:2846:GLU:OE1	2.04	0.56
1:D:4896:ASP:OD1	1:D:4897:TYR:N	2.38	0.56
2:G:22:THR:HG22	2:G:50:ARG:HB3	1.87	0.56
1:B:1184:ASP:OD2	1:B:1188:SER:OG	2.22	0.56
1:B:2787:TRP:HE1	1:B:2903:VAL:HG23	1.70	0.56
1:C:1604:LEU:HD23	1:C:1625:LEU:HD13	1.87	0.56
1:D:2096:GLY:HA2	1:D:2099:VAL:HG12	1.86	0.56
1:A:2787:TRP:HE1	1:A:2903:VAL:HG23	1.70	0.56
1:A:4896:ASP:OD1	1:A:4897:TYR:N	2.38	0.56
1:B:891:GLU:HB3	1:B:978:PRO:HG3	1.87	0.56
1:B:962:LYS:HB3	1:B:981:MET:HB3	1.86	0.56
1:C:1043:LYS:O	1:C:1047:LYS:HG2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2257:LEU:HB2	1:C:2316:ASN:HD21	1.70	0.56
1:D:614:LEU:HA	1:D:617:LEU:HD12	1.86	0.56
1:D:850:LEU:HD11	1:D:1215:MET:HG3	1.87	0.56
1:D:1473:LYS:HE3	1:D:1475:LYS:HB2	1.85	0.56
1:D:1604:LEU:HD23	1:D:1625:LEU:HD13	1.87	0.56
1:D:3697:LYS:HA	1:D:3700:HIS:CD2	2.40	0.56
1:A:1124:PRO:HD2	1:A:1594:VAL:HG23	1.88	0.56
1:B:850:LEU:HD11	1:B:1215:MET:HG3	1.87	0.56
1:B:894:VAL:HG12	1:B:897:LYS:HZ3	1.71	0.56
1:B:1004:HIS:CE1	1:B:1035:TYR:HB2	2.40	0.56
1:B:2641:SER:HB3	1:B:2676:LEU:HD21	1.87	0.56
1:C:1004:HIS:CE1	1:C:1035:TYR:HB2	2.40	0.56
1:C:1184:ASP:OD2	1:C:1188:SER:OG	2.22	0.56
1:C:2096:GLY:HA2	1:C:2099:VAL:HG12	1.86	0.56
1:C:2787:TRP:HE1	1:C:2903:VAL:HG23	1.70	0.56
1:D:260:VAL:O	1:D:390:LYS:NZ	2.29	0.56
1:D:2833:LEU:HD21	1:D:2837:LEU:HD23	1.87	0.56
1:A:1722:ASN:O	1:A:1919:ARG:NH2	2.38	0.56
1:B:804:LEU:HD13	1:B:832:LEU:HD21	1.87	0.56
1:A:799:LYS:HB3	1:A:799:LYS:HZ3	1.69	0.56
2:E:83:TYR:HB3	2:E:87:GLY:HA2	1.88	0.56
1:C:981:MET:O	1:C:983:LEU:HD22	2.06	0.56
1:D:804:LEU:HD13	1:D:832:LEU:HD21	1.87	0.56
1:D:950:VAL:HA	1:D:1064:LEU:HA	1.86	0.56
1:D:1004:HIS:CE1	1:D:1035:TYR:HB2	2.40	0.56
1:D:1124:PRO:HD2	1:D:1594:VAL:HG23	1.88	0.56
1:B:932:ASN:HA	1:B:935:MET:HG2	1.87	0.56
1:C:890:HIS:HA	1:C:893:TRP:HE3	1.64	0.56
1:C:891:GLU:HB3	1:C:978:PRO:HG3	1.87	0.56
1:A:962:LYS:HB3	1:A:981:MET:HB3	1.86	0.56
1:A:981:MET:O	1:A:983:LEU:HD22	2.06	0.56
2:H:83:TYR:HB3	2:H:87:GLY:HA2	1.88	0.56
1:B:4187:GLU:OE2	1:B:4947:ARG:NH2	2.37	0.56
1:C:3697:LYS:HA	1:C:3700:HIS:CD2	2.40	0.56
1:D:4045:LYS:HD2	1:D:4078:LEU:HD23	1.88	0.56
1:A:2257:LEU:HB2	1:A:2316:ASN:HD21	1.70	0.56
1:A:2833:LEU:HD21	1:A:2837:LEU:HD23	1.87	0.56
1:B:2142:MET:HB2	1:B:2192:MET:HE1	1.86	0.56
1:B:2255:LEU:O	1:B:3810:ARG:NH1	2.38	0.56
1:C:1722:ASN:O	1:C:1919:ARG:NH2	2.37	0.56
1:D:981:MET:O	1:D:983:LEU:HD22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:804:LEU:HD13	1:C:832:LEU:HD21	1.87	0.56
1:C:850:LEU:HD11	1:C:1215:MET:HG3	1.87	0.56
1:C:1124:PRO:HD2	1:C:1594:VAL:HG23	1.88	0.56
1:D:932:ASN:HA	1:D:935:MET:HG2	1.87	0.56
1:A:4517:LEU:HD21	1:A:4736:ASN:HB3	1.87	0.55
1:A:850:LEU:HD11	1:A:1215:MET:HG3	1.88	0.55
1:A:891:GLU:HB3	1:A:978:PRO:HG3	1.87	0.55
1:A:1004:HIS:CE1	1:A:1035:TYR:HB2	2.40	0.55
1:A:2680:TYR:HB3	1:A:2921:PHE:HB2	1.89	0.55
1:C:1788:LYS:HE2	1:C:1833:ILE:HG22	1.88	0.55
1:C:2836:ASP:OD1	1:C:2836:ASP:N	2.28	0.55
1:D:2833:LEU:HB3	1:D:2838[A]:HIS:CE1	2.39	0.55
1:D:3043:ARG:HA	1:D:3046:MET:SD	2.46	0.55
1:A:1604:LEU:HD23	1:A:1625:LEU:HD13	1.87	0.55
1:A:2285:TYR:OH	1:A:2380:ASP:O	2.25	0.55
2:F:22:THR:HG22	2:F:50:ARG:HB3	1.87	0.55
1:B:2833:LEU:HB3	1:B:2838[A]:HIS:CE1	2.41	0.55
1:C:894:VAL:HG12	1:C:897:LYS:HZ3	1.72	0.55
1:C:932:ASN:HA	1:C:935:MET:HG2	1.87	0.55
1:D:364:GLN:NE2	1:D:369:GLY:O	2.38	0.55
1:D:1788:LYS:HE2	1:D:1833:ILE:HG22	1.88	0.55
1:A:364:GLN:NE2	1:A:369:GLY:O	2.38	0.55
1:B:981:MET:O	1:B:983:LEU:HD22	2.06	0.55
1:B:2905:ARG:NE	1:B:2906:GLY:H	2.01	0.55
1:A:804:LEU:HD13	1:A:832:LEU:HD21	1.87	0.55
2:H:22:THR:HG22	2:H:50:ARG:HB3	1.87	0.55
1:C:2769:GLU:HA	1:C:2772:ARG:HB2	1.89	0.55
1:D:1948:MET:HA	1:D:1951:LEU:HD23	1.89	0.55
1:D:2285:TYR:OH	1:D:2380:ASP:O	2.25	0.55
1:A:2769:GLU:HA	1:A:2772:ARG:HB2	1.89	0.55
1:A:4237:SER:N	1:A:4240:THR:OG1	2.36	0.55
2:F:83:TYR:HB3	2:F:87:GLY:HA2	1.88	0.55
1:B:441:LYS:NZ	1:B:443:SER:OG	2.25	0.55
1:B:2257:LEU:HB2	1:B:2316:ASN:HD21	1.70	0.55
1:C:1123:GLN:HG3	1:C:1133:ARG:NH1	2.22	0.55
1:C:3108:LEU:O	1:C:3112:ILE:HG12	2.07	0.55
1:D:2680:TYR:HB3	1:D:2921:PHE:HB2	1.88	0.55
1:A:3043:ARG:HA	1:A:3046:MET:SD	2.46	0.55
1:C:4045:LYS:HD2	1:C:4078:LEU:HD23	1.88	0.55
1:C:4867:ILE:HD12	1:D:4861:ILE:HG13	1.89	0.55
1:D:3031:ASN:HA	1:D:3034:HIS:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1011:ARG:HD2	1:A:1016:TRP:CD1	2.42	0.55
1:A:2781:THR:HB	1:A:2848:TYR:OH	2.07	0.55
1:A:3108:LEU:O	1:A:3112:ILE:HG12	2.07	0.55
1:B:2285:TYR:OH	1:B:2380:ASP:O	2.25	0.55
1:A:4045:LYS:HD2	1:A:4078:LEU:HD23	1.88	0.55
2:G:83:TYR:HB3	2:G:87:GLY:HA2	1.88	0.55
1:B:950:VAL:HA	1:B:1064:LEU:HA	1.86	0.55
1:B:1011:ARG:HD2	1:B:1016:TRP:CD1	2.42	0.55
1:B:1788:LYS:HE2	1:B:1833:ILE:HG22	1.88	0.55
1:B:1967:SER:O	1:B:1972:GLN:NE2	2.31	0.55
1:B:2781:THR:HB	1:B:2848:TYR:OH	2.07	0.55
1:B:4252:ILE:HG21	1:C:4707:MET:HG3	1.88	0.55
1:C:1011:ARG:HD2	1:C:1016:TRP:CD1	2.42	0.55
1:C:3031:ASN:HA	1:C:3034:HIS:CD2	2.42	0.55
1:D:1011:ARG:HD2	1:D:1016:TRP:CD1	2.42	0.55
1:D:1549:SER:OG	1:D:1551:ASN:O	2.26	0.55
1:D:3108:LEU:O	1:D:3112:ILE:HG12	2.07	0.55
1:A:4253:LEU:O	1:A:4257:ARG:HG3	2.07	0.54
1:B:1124:PRO:HD2	1:B:1594:VAL:HG23	1.88	0.54
1:B:2680:TYR:HB3	1:B:2921:PHE:HB2	1.89	0.54
1:D:997:ASP:HA	1:D:1050:LEU:HD11	1.89	0.54
1:B:997:ASP:HA	1:B:1050:LEU:HD11	1.89	0.54
1:B:3108:LEU:O	1:B:3112:ILE:HG12	2.07	0.54
1:C:2760:TYR:HA	1:C:2763:LEU:HB2	1.89	0.54
1:C:2781:THR:HB	1:C:2848:TYR:OH	2.07	0.54
1:C:3043:ARG:HA	1:C:3046:MET:SD	2.46	0.54
1:D:2760:TYR:HA	1:D:2763:LEU:HB2	1.89	0.54
1:A:1948:MET:HA	1:A:1951:LEU:HD23	1.89	0.54
1:A:2087:LEU:O	1:A:2091:GLN:HG2	2.08	0.54
1:A:2874:TYR:HE1	1:A:2882:LYS:CD	2.21	0.54
1:B:4253:LEU:O	1:B:4257:ARG:HG3	2.07	0.54
1:C:997:ASP:HA	1:C:1050:LEU:HD11	1.89	0.54
1:C:1948:MET:HA	1:C:1951:LEU:HD23	1.89	0.54
1:C:4253:LEU:O	1:C:4257:ARG:HG3	2.07	0.54
1:D:2255:LEU:O	1:D:3810:ARG:NH1	2.38	0.54
1:A:611:LEU:HD22	1:A:1660:LEU:HD22	1.90	0.54
1:A:1788:LYS:HE2	1:A:1833:ILE:HG22	1.88	0.54
1:B:113:LEU:HD11	1:B:119:ILE:HD13	1.90	0.54
1:B:842:GLN:HB2	1:B:1603:PHE:HB2	1.89	0.54
1:C:113:LEU:HD11	1:C:119:ILE:HD13	1.90	0.54
1:D:4580:THR:OG1	1:D:4733:HIS:NE2	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:997:ASP:HA	1:A:1050:LEU:HD11	1.89	0.54
1:A:2125:GLN:OE1	1:A:2144:ARG:NH1	2.38	0.54
1:B:3043:ARG:HA	1:B:3046:MET:SD	2.46	0.54
1:C:892:LEU:HD21	1:C:980:PRO:HD3	1.89	0.54
1:C:4587:ILE:HD11	1:C:4726:MET:HB2	1.89	0.54
1:D:113:LEU:HD11	1:D:119:ILE:HD13	1.90	0.54
1:D:611:LEU:HD22	1:D:1660:LEU:HD22	1.90	0.54
1:D:2119:LEU:HD13	1:D:2154:VAL:HG23	1.89	0.54
1:D:2874:TYR:HE1	1:D:2882:LYS:CD	2.21	0.54
1:A:260:VAL:O	1:A:390:LYS:NZ	2.29	0.54
1:A:663:VAL:HG23	1:A:671:LYS:HE3	1.89	0.54
1:A:2142:MET:HB2	1:A:2192:MET:HE1	1.89	0.54
1:A:2836:ASP:N	1:A:2836:ASP:OD1	2.28	0.54
1:A:3031:ASN:HA	1:A:3034:HIS:CD2	2.42	0.54
1:C:908:ARG:NH1	1:C:917:CYS:SG	2.76	0.54
1:C:2255:LEU:O	1:C:3810:ARG:NH1	2.38	0.54
1:A:166:SER:OG	1:A:168:GLN:OE1	2.26	0.54
1:A:2668:CYS:O	1:A:2672:VAL:HG23	2.08	0.54
1:A:4587:ILE:HD11	1:A:4726:MET:HB2	1.89	0.54
1:A:4689:LYS:HE3	1:A:4696:ALA:HB2	1.89	0.54
1:B:394:HIS:CE1	1:B:396:GLU:HB2	2.43	0.54
1:B:2668:CYS:O	1:B:2672:VAL:HG23	2.08	0.54
1:B:4045:LYS:HD2	1:B:4078:LEU:HD23	1.88	0.54
1:C:2285:TYR:OH	1:C:2380:ASP:O	2.25	0.54
1:D:655:MET:HA	1:D:655:MET:HE2	1.90	0.54
1:D:842:GLN:HB2	1:D:1603:PHE:HB2	1.89	0.54
1:D:2273:GLY:O	1:D:2336:ARG:NH2	2.37	0.54
1:A:394:HIS:CE1	1:A:396:GLU:HB2	2.43	0.54
1:A:441:LYS:NZ	1:A:443:SER:OG	2.25	0.54
1:B:3112:ILE:HD13	1:B:3117:PHE:HD2	1.73	0.54
1:C:663:VAL:HG23	1:C:671:LYS:HE3	1.89	0.54
1:C:2680:TYR:HB3	1:C:2921:PHE:HB2	1.88	0.54
1:D:4253:LEU:O	1:D:4257:ARG:HG3	2.07	0.54
1:A:113:LEU:HD11	1:A:119:ILE:HD13	1.90	0.54
1:A:2119:LEU:HD13	1:A:2154:VAL:HG23	1.90	0.54
1:B:1962:THR:HG23	1:B:1966:ARG:HH11	1.73	0.54
1:B:3031:ASN:HA	1:B:3034:HIS:CD2	2.42	0.54
1:C:2725:ALA:CB	1:C:2768:LYS:HG3	2.35	0.54
1:C:3112:ILE:HD13	1:C:3117:PHE:HD2	1.73	0.54
1:C:3729:ALA:HA	1:C:3732:HIS:CD2	2.43	0.54
1:D:2668:CYS:O	1:D:2672:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2781:THR:HB	1:D:2848:TYR:OH	2.07	0.54
1:D:2905:ARG:NE	1:D:2906:GLY:H	2.01	0.54
1:D:3112:ILE:HD13	1:D:3117:PHE:HD2	1.73	0.54
1:A:2255:LEU:O	1:A:3810:ARG:NH1	2.38	0.54
1:A:3112:ILE:HD13	1:A:3117:PHE:HD2	1.73	0.54
1:A:3729:ALA:HA	1:A:3732:HIS:CD2	2.43	0.54
1:B:1123:GLN:HG3	1:B:1133:ARG:NH1	2.22	0.54
1:B:1948:MET:HA	1:B:1951:LEU:HD23	1.89	0.54
1:C:611:LEU:HD22	1:C:1660:LEU:HD22	1.90	0.54
1:C:1444:GLY:HA3	1:C:1487:MET:HA	1.90	0.54
1:C:3608:LEU:HD12	1:C:3611:LEU:HD12	1.90	0.54
1:D:2058:LEU:O	1:D:2062:ILE:HG12	2.08	0.54
1:D:2763:LEU:HG	1:D:2764:SER:H	1.72	0.54
1:D:3729:ALA:HA	1:D:3732:HIS:CD2	2.43	0.54
1:A:2763:LEU:HG	1:A:2764:SER:H	1.72	0.53
1:B:892:LEU:HD21	1:B:980:PRO:HD3	1.89	0.53
1:B:2087:LEU:O	1:B:2091:GLN:HG2	2.08	0.53
1:B:2769:GLU:HA	1:B:2772:ARG:HB2	1.89	0.53
1:B:4279:MET:CE	1:C:4488:GLN:HB2	2.37	0.53
1:B:4689:LYS:HE3	1:B:4696:ALA:HB2	1.89	0.53
1:C:2668:CYS:O	1:C:2672:VAL:HG23	2.08	0.53
1:C:2874:TYR:HE1	1:C:2882:LYS:CD	2.21	0.53
1:C:3607:PRO:HG2	1:C:3610:ASN:HB2	1.90	0.53
1:D:1444:GLY:HA3	1:D:1487:MET:HA	1.90	0.53
1:A:892:LEU:HD21	1:A:980:PRO:HD3	1.89	0.53
1:A:1564:MET:HE3	1:A:1565:PRO:HD2	1.89	0.53
1:A:3608:LEU:HD12	1:A:3611:LEU:HD12	1.90	0.53
1:B:1549:SER:OG	1:B:1551:ASN:O	2.26	0.53
1:B:2833:LEU:HB3	1:B:2838[B]:HIS:CE1	2.41	0.53
1:C:2986:ALA:HB2	1:C:2995:HIS:HB2	1.91	0.53
1:D:394:HIS:CE1	1:D:396:GLU:HB2	2.43	0.53
1:D:1225:LYS:HE3	1:D:1226:TYR:CE2	2.44	0.53
1:D:2087:LEU:O	1:D:2091:GLN:HG2	2.08	0.53
1:D:2986:ALA:HB2	1:D:2995:HIS:HB2	1.90	0.53
1:B:2986:ALA:HB2	1:B:2995:HIS:HB2	1.90	0.53
1:C:1962:THR:HG23	1:C:1966:ARG:HH11	1.73	0.53
1:D:1962:THR:HG23	1:D:1966:ARG:HH11	1.73	0.53
1:D:2769:GLU:HA	1:D:2772:ARG:HB2	1.89	0.53
1:D:2927:GLN:O	1:D:2931:ARG:NE	2.39	0.53
1:A:1225:LYS:HE3	1:A:1226:TYR:CE2	2.43	0.53
1:A:2760:TYR:HA	1:A:2763:LEU:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2785:TRP:HB2	1:A:2787:TRP:CZ3	2.43	0.53
1:B:611:LEU:HD22	1:B:1660:LEU:HD22	1.90	0.53
1:B:2760:TYR:HA	1:B:2763:LEU:HB2	1.89	0.53
1:B:2874:TYR:HE1	1:B:2882:LYS:CD	2.21	0.53
1:B:3003:MET:O	1:B:3007:LEU:HD23	2.08	0.53
1:C:394:HIS:CE1	1:C:396:GLU:HB2	2.43	0.53
1:C:2763:LEU:HG	1:C:2764:SER:H	1.72	0.53
1:C:2979:ARG:H	1:C:2979:ARG:HD3	1.74	0.53
1:D:1123:GLN:HG3	1:D:1133:ARG:NH1	2.22	0.53
1:A:1123:GLN:HG3	1:A:1133:ARG:NH1	2.22	0.53
1:A:1962:THR:HG23	1:A:1966:ARG:HH11	1.73	0.53
1:B:663:VAL:HG23	1:B:671:LYS:HE3	1.89	0.53
1:B:2791:ARG:HD2	1:B:2901:TYR:HE1	1.74	0.53
1:C:1549:SER:OG	1:C:1551:ASN:O	2.25	0.53
1:C:4689:LYS:HE3	1:C:4696:ALA:HB2	1.89	0.53
1:C:4753:LEU:HD21	1:D:4769:LEU:O	2.08	0.53
1:D:663:VAL:HG23	1:D:671:LYS:HE3	1.89	0.53
1:D:892:LEU:HD21	1:D:980:PRO:HD3	1.89	0.53
1:D:2785:TRP:HB2	1:D:2787:TRP:CZ3	2.43	0.53
1:D:4587:ILE:HD11	1:D:4726:MET:HB2	1.89	0.53
1:D:4689:LYS:HE3	1:D:4696:ALA:HB2	1.89	0.53
1:B:1444:GLY:HA3	1:B:1487:MET:HA	1.90	0.53
1:B:2927:GLN:HA	1:B:2930:ILE:HD12	1.91	0.53
1:C:166:SER:OG	1:C:168:GLN:OE1	2.26	0.53
1:C:655:MET:HE2	1:C:655:MET:HA	1.90	0.53
1:C:2905:ARG:NE	1:C:2906:GLY:H	2.02	0.53
1:C:2927:GLN:HA	1:C:2930:ILE:HD12	1.91	0.53
1:C:4752:THR:HG21	1:D:4766:GLN:HG2	1.90	0.53
1:D:2142:MET:HB2	1:D:2192:MET:HE1	1.91	0.53
1:A:908:ARG:NH1	1:A:917:CYS:SG	2.76	0.53
1:A:3003:MET:O	1:A:3007:LEU:HD23	2.08	0.53
1:B:2125:GLN:OE1	1:B:2144:ARG:NH1	2.38	0.53
1:C:2982:PHE:O	1:C:3001:LYS:NZ	2.40	0.53
1:A:3607:PRO:HG2	1:A:3610:ASN:HB2	1.90	0.53
1:B:2119:LEU:HD13	1:B:2154:VAL:HG23	1.90	0.53
1:B:2763:LEU:HG	1:B:2764:SER:H	1.72	0.53
1:B:4587:ILE:HD11	1:B:4726:MET:HB2	1.89	0.53
1:C:842:GLN:HB2	1:C:1603:PHE:HB2	1.90	0.53
1:C:2119:LEU:HD13	1:C:2154:VAL:HG23	1.89	0.53
1:D:908:ARG:NH1	1:D:917:CYS:SG	2.76	0.53
1:D:3003:MET:O	1:D:3007:LEU:HD23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4565:SER:HB2	1:D:4567:TYR:HD1	1.74	0.53
1:A:2986:ALA:HB2	1:A:2995:HIS:HB2	1.91	0.53
1:B:908:ARG:NH1	1:B:917:CYS:SG	2.76	0.53
1:B:2058:LEU:O	1:B:2062:ILE:HG12	2.09	0.53
1:B:2979:ARG:HD3	1:B:2979:ARG:H	1.74	0.53
1:B:3729:ALA:HA	1:B:3732:HIS:CD2	2.43	0.53
1:C:114:LEU:HB3	1:C:117:HIS:CE1	2.44	0.53
1:C:2087:LEU:O	1:C:2091:GLN:HG2	2.08	0.53
1:D:114:LEU:HB3	1:D:117:HIS:CE1	2.44	0.53
1:D:166:SER:OG	1:D:168:GLN:OE1	2.26	0.53
1:D:3607:PRO:HG2	1:D:3610:ASN:HB2	1.90	0.53
1:A:655:MET:HG3	1:A:1619:VAL:HG11	1.91	0.53
1:A:2058:LEU:O	1:A:2062:ILE:HG12	2.09	0.53
1:A:2927:GLN:HA	1:A:2930:ILE:HD12	1.91	0.53
1:B:114:LEU:HB3	1:B:117:HIS:CE1	2.44	0.53
1:B:364:GLN:NE2	1:B:369:GLY:O	2.38	0.53
1:B:1031:ARG:NH2	4:B:5004:ATP:O2G	2.42	0.53
1:B:3607:PRO:HG2	1:B:3610:ASN:HB2	1.90	0.53
1:D:235:ARG:NH1	1:D:268:SER:O	2.42	0.53
1:D:849:ASP:OD1	1:D:1214:ARG:NE	2.37	0.53
1:D:2979:ARG:H	1:D:2979:ARG:HD3	1.74	0.53
1:A:235:ARG:NH1	1:A:268:SER:O	2.42	0.52
1:A:1549:SER:OG	1:A:1551:ASN:O	2.26	0.52
1:B:1225:LYS:HE3	1:B:1226:TYR:CE2	2.43	0.52
1:B:4565:SER:HB2	1:B:4567:TYR:HD1	1.74	0.52
1:C:364:GLN:NE2	1:C:369:GLY:O	2.38	0.52
1:C:686:VAL:HG13	1:C:687:THR:HG23	1.91	0.52
1:C:3003:MET:O	1:C:3007:LEU:HD23	2.08	0.52
1:D:894:VAL:HG12	1:D:897:LYS:HZ3	1.73	0.52
1:D:1102:TYR:HD2	1:D:1165:MET:HG3	1.74	0.52
1:D:2791:ARG:HD2	1:D:2901:TYR:HE1	1.74	0.52
1:A:1444:GLY:HA3	1:A:1487:MET:HA	1.90	0.52
1:B:2778:SER:HA	1:B:2848:TYR:OH	2.10	0.52
1:B:3608:LEU:HD12	1:B:3611:LEU:HD12	1.90	0.52
1:C:2058:LEU:O	1:C:2062:ILE:HG12	2.09	0.52
1:A:191:TYR:N	1:A:206:ALA:O	2.43	0.52
1:A:2791:ARG:HD2	1:A:2901:TYR:HE1	1.74	0.52
1:A:4822:ARG:NH1	1:B:4829:ASP:OD1	2.42	0.52
1:B:2943:PHE:CZ	1:B:2956:TYR:HB2	2.45	0.52
1:C:2423:LEU:HA	1:C:2426:LEU:HD12	1.91	0.52
1:D:191:TYR:N	1:D:206:ALA:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2843:MET:HA	1:D:2846:GLU:CD	2.29	0.52
1:A:114:LEU:HB3	1:A:117:HIS:CE1	2.44	0.52
1:A:842:GLN:HB2	1:A:1603:PHE:HB2	1.90	0.52
1:A:1102:TYR:HD2	1:A:1165:MET:HG3	1.74	0.52
1:A:2943:PHE:CZ	1:A:2956:TYR:HB2	2.45	0.52
1:A:4237:SER:O	1:A:4240:THR:OG1	2.27	0.52
1:B:4237:SER:N	1:B:4240:THR:OG1	2.36	0.52
1:C:2939:TYR:O	1:C:2943:PHE:HD2	1.93	0.52
1:A:1031:ARG:NH2	4:A:5004:ATP:O2G	2.42	0.52
1:A:2478:ILE:HD13	1:A:2527:LEU:HD11	1.92	0.52
1:B:235:ARG:NH1	1:B:268:SER:O	2.42	0.52
1:B:2423:LEU:HA	1:B:2426:LEU:HD12	1.91	0.52
1:B:2927:GLN:O	1:B:2931:ARG:NE	2.39	0.52
1:C:655:MET:HG3	1:C:1619:VAL:HG11	1.91	0.52
1:C:2843:MET:HA	1:C:2846:GLU:CD	2.29	0.52
1:D:2478:ILE:HD13	1:D:2527:LEU:HD11	1.92	0.52
1:A:2642:ARG:HD2	1:A:2680:TYR:HE2	1.75	0.52
1:A:2833:LEU:HB3	1:A:2838[B]:HIS:CE1	2.45	0.52
1:A:2905:ARG:NE	1:A:2906:GLY:H	2.01	0.52
1:A:2966:VAL:O	1:A:2970:LEU:N	2.38	0.52
1:A:4004:VAL:HG21	1:A:4114:ARG:HH11	1.74	0.52
1:B:655:MET:HG3	1:B:1619:VAL:HG11	1.91	0.52
1:B:686:VAL:HG13	1:B:687:THR:HG23	1.92	0.52
1:B:2791:ARG:HH21	1:B:2795:GLY:HA3	1.75	0.52
1:B:4262:LYS:HG3	1:C:4698:LEU:CD2	2.37	0.52
1:C:1102:TYR:HD2	1:C:1165:MET:HG3	1.74	0.52
1:C:2778:SER:HA	1:C:2848:TYR:OH	2.09	0.52
1:C:2943:PHE:CZ	1:C:2956:TYR:HB2	2.45	0.52
1:D:655:MET:HG3	1:D:1619:VAL:HG11	1.91	0.52
1:D:2885:ASP:O	1:D:2888:LYS:HG3	2.10	0.52
1:D:2927:GLN:HA	1:D:2930:ILE:HD12	1.91	0.52
1:D:4237:SER:O	1:D:4240:THR:OG1	2.27	0.52
1:A:2979:ARG:H	1:A:2979:ARG:HD3	1.73	0.52
1:A:4250:TYR:O	1:A:4254:THR:HG23	2.10	0.52
1:A:4565:SER:HB2	1:A:4567:TYR:HD1	1.74	0.52
1:B:166:SER:OG	1:B:168:GLN:OE1	2.26	0.52
1:B:1847:GLU:OE1	1:B:1895:GLN:NE2	2.35	0.52
1:B:2939:TYR:O	1:B:2943:PHE:HD2	1.93	0.52
1:B:3664:LEU:O	1:B:3668:ILE:HG13	2.10	0.52
1:C:674:TYR:HE2	1:C:756:SER:HB2	1.75	0.52
1:C:3699:CYS:SG	1:C:3731:LEU:HD12	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4250:TYR:O	1:C:4254:THR:HG23	2.10	0.52
1:D:686:VAL:HG13	1:D:687:THR:HG23	1.92	0.52
1:D:2778:SER:HA	1:D:2848:TYR:OH	2.10	0.52
1:B:191:TYR:N	1:B:206:ALA:O	2.43	0.52
1:B:4250:TYR:O	1:B:4254:THR:HG23	2.10	0.52
1:C:2785:TRP:HB2	1:C:2787:TRP:CZ3	2.43	0.52
1:C:2791:ARG:HD2	1:C:2901:TYR:HE1	1.74	0.52
1:A:2423:LEU:HA	1:A:2426:LEU:HD12	1.91	0.52
1:A:2843:MET:HA	1:A:2846:GLU:CD	2.29	0.52
1:A:2885:ASP:O	1:A:2888:LYS:HG3	2.10	0.52
1:A:2939:TYR:O	1:A:2943:PHE:HD2	1.93	0.52
1:A:3650:GLU:HB2	1:A:3651:PRO:HD3	1.92	0.52
1:B:3650:GLU:HB2	1:B:3651:PRO:HD3	1.92	0.52
1:B:3846:LEU:HB3	1:B:3854:PHE:CE2	2.45	0.52
1:B:4237:SER:O	1:B:4240:THR:OG1	2.27	0.52
1:C:191:TYR:N	1:C:206:ALA:O	2.43	0.52
1:C:235:ARG:NH1	1:C:268:SER:O	2.42	0.52
1:C:1225:LYS:HE3	1:C:1226:TYR:CE2	2.44	0.52
1:D:2642:ARG:HD2	1:D:2680:TYR:HE2	1.75	0.52
1:D:2791:ARG:HH21	1:D:2795:GLY:HA3	1.75	0.52
1:D:2943:PHE:CZ	1:D:2956:TYR:HB2	2.45	0.52
1:D:3846:LEU:HB3	1:D:3854:PHE:CE2	2.45	0.52
1:A:2725:ALA:CB	1:A:2768:LYS:HG3	2.35	0.52
1:A:3699:CYS:SG	1:A:3731:LEU:HD12	2.50	0.52
1:B:2642:ARG:HD2	1:B:2680:TYR:HE2	1.75	0.52
1:B:2785:TRP:HB2	1:B:2787:TRP:CZ3	2.43	0.52
1:B:2843:MET:HA	1:B:2846:GLU:CD	2.29	0.52
1:B:4004:VAL:HG21	1:B:4114:ARG:HH11	1.74	0.52
1:C:1031:ARG:NH2	4:C:5004:ATP:O2G	2.42	0.52
1:C:1165:MET:HB3	1:C:1236:TYR:CZ	2.45	0.52
1:D:1031:ARG:NH2	4:D:5004:ATP:O2G	2.42	0.52
1:D:3013:VAL:O	1:D:3018:ARG:NH2	2.43	0.52
1:D:3608:LEU:HD12	1:D:3611:LEU:HD12	1.90	0.52
1:A:3664:LEU:O	1:A:3668:ILE:HG13	2.10	0.51
1:B:644:LEU:HD13	1:B:1630:LEU:HD21	1.92	0.51
1:B:1102:TYR:HD2	1:B:1165:MET:HG3	1.74	0.51
1:B:3699:CYS:SG	1:B:3731:LEU:HD12	2.50	0.51
1:D:2939:TYR:O	1:D:2943:PHE:HD2	1.93	0.51
1:A:3697:LYS:HA	1:A:3700:HIS:NE2	2.25	0.51
1:B:1157:GLN:N	1:B:1160:ASP:OD2	2.41	0.51
1:C:644:LEU:HD13	1:C:1630:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3013:VAL:O	1:C:3018:ARG:NH2	2.43	0.51
1:C:4565:SER:HB2	1:C:4567:TYR:HD1	1.74	0.51
1:D:3699:CYS:SG	1:D:3731:LEU:HD12	2.50	0.51
1:D:4250:TYR:O	1:D:4254:THR:HG23	2.10	0.51
1:A:1165:MET:HB3	1:A:1236:TYR:CZ	2.45	0.51
1:D:2423:LEU:HA	1:D:2426:LEU:HD12	1.91	0.51
1:B:1432:ILE:O	1:B:1500:ARG:NH2	2.44	0.51
1:B:1718:ARG:HD2	1:B:1830:ILE:O	2.11	0.51
1:C:1799:VAL:O	1:C:1896:MET:HE1	2.11	0.51
1:C:4004:VAL:HG21	1:C:4114:ARG:HH11	1.74	0.51
1:A:2642:ARG:NH1	1:A:2921:PHE:HD1	2.09	0.51
1:A:2791:ARG:HH21	1:A:2795:GLY:HA3	1.75	0.51
1:C:2885:ASP:O	1:C:2888:LYS:HG3	2.10	0.51
1:C:3846:LEU:HB3	1:C:3854:PHE:CE2	2.45	0.51
1:D:1165:MET:HB3	1:D:1236:TYR:CZ	2.45	0.51
1:D:4004:VAL:HG21	1:D:4114:ARG:HH11	1.74	0.51
1:A:686:VAL:HG13	1:A:687:THR:HG23	1.92	0.51
1:A:2176:VAL:HG22	1:A:2220:TYR:CZ	2.46	0.51
1:A:3095:ASN:O	1:A:3099:VAL:HG22	2.11	0.51
1:B:3650:GLU:HA	1:B:3660:ARG:HH22	1.75	0.51
1:C:2731:LYS:HA	1:C:2734:MET:CG	2.38	0.51
1:C:3095:ASN:O	1:C:3099:VAL:HG22	2.11	0.51
1:C:3697:LYS:HA	1:C:3700:HIS:NE2	2.25	0.51
1:C:4237:SER:O	1:C:4240:THR:OG1	2.27	0.51
1:A:1564:MET:HE3	1:A:1578:PRO:HA	1.93	0.51
1:A:2778:SER:HA	1:A:2848:TYR:OH	2.10	0.51
1:A:2874:TYR:CE1	1:A:2882:LYS:HD3	2.46	0.51
1:B:3095:ASN:O	1:B:3099:VAL:HG22	2.11	0.51
1:B:3697:LYS:HA	1:B:3700:HIS:NE2	2.25	0.51
1:B:674:TYR:HE2	1:B:756:SER:HB2	1.75	0.51
1:B:2731:LYS:HA	1:B:2734:MET:CG	2.38	0.51
1:B:2874:TYR:CE1	1:B:2882:LYS:HD3	2.46	0.51
1:B:2885:ASP:O	1:B:2888:LYS:HG3	2.10	0.51
1:B:4154:GLU:O	1:B:4158:THR:HG23	2.11	0.51
1:C:1718:ARG:HD2	1:C:1830:ILE:O	2.11	0.51
1:C:2833:LEU:HB3	1:C:2838[A]:HIS:CE1	2.46	0.51
1:D:3697:LYS:HA	1:D:3700:HIS:NE2	2.25	0.51
1:A:131:CYS:SG	1:A:150:GLN:HB2	2.51	0.51
1:A:644:LEU:HD13	1:A:1630:LEU:HD21	1.92	0.51
1:A:2833:LEU:HB3	1:A:2838[A]:HIS:CE1	2.45	0.51
1:A:3846:LEU:HB3	1:A:3854:PHE:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3882:GLN:NE2	1:A:3946:GLY:HA3	2.26	0.51
1:B:876:PRO:O	1:B:880:ARG:HD2	2.11	0.51
1:B:1165:MET:HB3	1:B:1236:TYR:CZ	2.45	0.51
1:B:2478:ILE:HD13	1:B:2527:LEU:HD11	1.92	0.51
1:B:2715:GLU:HA	1:B:2718:GLU:HB2	1.93	0.51
1:C:876:PRO:O	1:C:880:ARG:HD2	2.11	0.51
1:C:2478:ILE:HD13	1:C:2527:LEU:HD11	1.92	0.51
1:C:2791:ARG:HH21	1:C:2795:GLY:HA3	1.75	0.51
1:C:2846:GLU:CB	1:C:2874:TYR:HD2	2.24	0.51
1:C:2927:GLN:O	1:C:2931:ARG:NE	2.39	0.51
1:C:3650:GLU:HB2	1:C:3651:PRO:HD3	1.92	0.51
1:D:3664:LEU:O	1:D:3668:ILE:HG13	2.10	0.51
1:D:4481:TRP:NE1	1:D:4692:SER:HA	2.21	0.51
1:A:876:PRO:O	1:A:880:ARG:HD2	2.11	0.51
1:A:1718:ARG:HD2	1:A:1830:ILE:O	2.11	0.51
1:A:2927:GLN:O	1:A:2931:ARG:NE	2.39	0.51
1:A:3043:ARG:HH11	1:A:3047:LYS:HZ2	1.58	0.51
1:B:3013:VAL:O	1:B:3018:ARG:NH2	2.43	0.51
1:B:4863:GLN:O	1:B:4867:ILE:HG12	2.11	0.51
1:C:2055:SER:HB2	1:C:2060:GLN:HB3	1.93	0.51
1:C:2957:GLU:HA	1:C:2960:ILE:HG12	1.93	0.51
1:C:3664:LEU:O	1:C:3668:ILE:HG13	2.10	0.51
1:C:4481:TRP:HE3	1:C:4484:ILE:HD11	1.76	0.51
1:D:674:TYR:HE2	1:D:756:SER:HB2	1.75	0.51
1:D:876:PRO:O	1:D:880:ARG:HD2	2.11	0.51
1:D:1847:GLU:OE1	1:D:1895:GLN:NE2	2.35	0.51
1:D:2055:SER:HB2	1:D:2060:GLN:HB3	1.93	0.51
1:D:2731:LYS:HA	1:D:2734:MET:CG	2.38	0.51
1:D:2874:TYR:CE1	1:D:2882:LYS:HD3	2.46	0.51
1:D:3650:GLU:HA	1:D:3660:ARG:HH22	1.75	0.51
1:D:4863:GLN:O	1:D:4867:ILE:HG12	2.11	0.51
1:A:1432:ILE:O	1:A:1500:ARG:NH2	2.44	0.50
1:A:2055:SER:HB2	1:A:2060:GLN:HB3	1.93	0.50
1:A:4154:GLU:O	1:A:4158:THR:HG23	2.11	0.50
1:A:4863:GLN:O	1:A:4867:ILE:HG12	2.11	0.50
1:C:131:CYS:SG	1:C:150:GLN:HB2	2.51	0.50
1:C:2125:GLN:OE1	1:C:2144:ARG:NH1	2.38	0.50
1:C:2642:ARG:NH1	1:C:2921:PHE:HD1	2.09	0.50
1:C:3901:GLN:OE1	1:C:3904:ARG:NH1	2.45	0.50
1:D:2642:ARG:NH1	1:D:2921:PHE:HD1	2.09	0.50
1:A:3013:VAL:O	1:A:3018:ARG:NH2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3901:GLN:OE1	1:A:3904:ARG:NH1	2.44	0.50
1:B:3901:GLN:OE1	1:B:3904:ARG:NH1	2.44	0.50
1:C:2176:VAL:HG22	1:C:2220:TYR:CZ	2.46	0.50
1:C:4863:GLN:O	1:C:4867:ILE:HG12	2.11	0.50
1:D:253:GLY:HA3	1:D:256:GLN:NE2	2.27	0.50
1:D:1718:ARG:HD2	1:D:1830:ILE:O	2.10	0.50
1:D:1799:VAL:O	1:D:1896:MET:HE1	2.11	0.50
1:D:3043:ARG:HH11	1:D:3047:LYS:HZ2	1.60	0.50
1:D:3650:GLU:HB2	1:D:3651:PRO:HD3	1.92	0.50
1:A:939:THR:HG23	1:A:999:LEU:HD21	1.94	0.50
1:A:2846:GLU:CB	1:A:2874:TYR:HD2	2.24	0.50
1:B:2176:VAL:HG22	1:B:2220:TYR:CZ	2.46	0.50
1:B:4481:TRP:NE1	1:B:4692:SER:HA	2.21	0.50
1:C:2715:GLU:HA	1:C:2718:GLU:HB2	1.93	0.50
1:D:713:TRP:HH2	1:D:1251:LEU:HD21	1.76	0.50
1:D:2846:GLU:CB	1:D:2874:TYR:HD2	2.24	0.50
1:D:2926:LEU:O	1:D:2930:ILE:HG13	2.12	0.50
1:A:386:SER:OG	1:A:387:ILE:N	2.44	0.50
1:A:713:TRP:HH2	1:A:1251:LEU:HD21	1.76	0.50
1:A:4559:TYR:OH	1:B:4790:ARG:NH2	2.45	0.50
1:B:131:CYS:SG	1:B:150:GLN:HB2	2.51	0.50
1:B:4271:VAL:HG11	1:C:4481:TRP:CZ3	2.46	0.50
1:B:4481:TRP:HE3	1:B:4484:ILE:HD11	1.76	0.50
1:C:253:GLY:HA3	1:C:256:GLN:NE2	2.26	0.50
1:C:3650:GLU:HA	1:C:3660:ARG:HH22	1.75	0.50
1:C:4274:MET:HE2	1:C:4274:MET:H	1.76	0.50
1:D:644:LEU:HD13	1:D:1630:LEU:HD21	1.92	0.50
1:D:1172:THR:OG1	1:D:1190:LEU:HD22	2.12	0.50
1:A:674:TYR:HE2	1:A:756:SER:HB2	1.75	0.50
1:B:2846:GLU:CB	1:B:2874:TYR:HD2	2.24	0.50
1:C:2642:ARG:HD2	1:C:2680:TYR:HE2	1.75	0.50
1:D:879:GLU:HA	1:D:882:ARG:HD2	1.93	0.50
1:A:2715:GLU:HA	1:A:2718:GLU:HB2	1.93	0.50
1:A:2926:LEU:O	1:A:2930:ILE:HG13	2.12	0.50
1:A:3650:GLU:HA	1:A:3660:ARG:HH22	1.75	0.50
1:B:1922:ILE:O	1:B:1926:VAL:HG23	2.12	0.50
1:B:2055:SER:HB2	1:B:2060:GLN:HB3	1.93	0.50
1:B:2482:ASP:OD1	1:B:2483:PHE:N	2.45	0.50
1:B:2642:ARG:NH1	1:B:2921:PHE:HD1	2.09	0.50
1:B:3882:GLN:NE2	1:B:3946:GLY:HA3	2.26	0.50
1:C:2874:TYR:CE1	1:C:2882:LYS:HD3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1432:ILE:O	1:D:1500:ARG:NH2	2.44	0.50
1:D:2957:GLU:HA	1:D:2960:ILE:HG12	1.93	0.50
1:A:1799:VAL:O	1:A:1896:MET:HE1	2.12	0.50
1:B:386:SER:OG	1:B:387:ILE:N	2.44	0.50
1:B:713:TRP:HH2	1:B:1251:LEU:HD21	1.76	0.50
1:B:1172:THR:OG1	1:B:1190:LEU:HD22	2.12	0.50
1:B:1799:VAL:O	1:B:1896:MET:HE1	2.10	0.50
1:B:4507:LEU:HD21	1:B:4746:ILE:HG22	1.94	0.50
1:C:271:ALA:HB2	1:C:488:LEU:HD22	1.94	0.50
1:C:4507:LEU:HD21	1:C:4746:ILE:HG22	1.94	0.50
1:D:131:CYS:SG	1:D:150:GLN:HB2	2.51	0.50
1:D:2176:VAL:HG22	1:D:2220:TYR:CZ	2.46	0.50
1:D:2482:ASP:OD1	1:D:2483:PHE:N	2.45	0.50
1:A:1157:GLN:N	1:A:1160:ASP:OD2	2.41	0.50
1:A:1172:THR:OG1	1:A:1190:LEU:HD22	2.12	0.50
1:A:2891:ASP:OD1	1:A:2892:ILE:N	2.45	0.50
2:F:19:LYS:HD3	2:F:20:GLY:H	1.77	0.50
1:B:271:ALA:HB2	1:B:488:LEU:HD22	1.94	0.50
1:B:939:THR:HG23	1:B:999:LEU:HD21	1.94	0.50
1:C:824:GLU:CD	1:C:1028:ARG:HH22	2.16	0.50
1:C:879:GLU:HA	1:C:882:ARG:HD2	1.94	0.50
1:C:1113:MET:HE3	1:C:1211:GLN:HB3	1.94	0.50
1:C:1144:ARG:NH2	1:C:1184:ASP:OD1	2.45	0.50
1:D:1144:ARG:NH2	1:D:1184:ASP:OD1	2.45	0.50
1:D:2891:ASP:OD1	1:D:2892:ILE:N	2.45	0.50
1:D:3095:ASN:O	1:D:3099:VAL:HG22	2.11	0.50
1:A:243:GLU:OE1	1:A:389:ARG:NH2	2.45	0.50
1:A:2999:LYS:HA	1:A:3002:GLU:HG3	1.94	0.50
1:A:4701:ILE:HG21	1:D:4259:LEU:HD21	1.94	0.50
2:H:19:LYS:HD3	2:H:20:GLY:H	1.77	0.50
1:B:879:GLU:HA	1:B:882:ARG:HD2	1.93	0.50
1:B:1144:ARG:NH2	1:B:1184:ASP:OD1	2.45	0.50
1:B:2957:GLU:HA	1:B:2960:ILE:HG12	1.93	0.50
1:B:4252:ILE:HG21	1:C:4707:MET:HA	1.93	0.50
1:B:4962:TYR:HD1	1:B:4965:GLN:NE2	2.02	0.50
1:C:1922:ILE:O	1:C:1926:VAL:HG23	2.12	0.50
1:C:2481:GLN:HE22	1:C:2485:LEU:HD11	1.77	0.50
1:C:3924:ILE:HG21	1:C:3935:LEU:HD22	1.94	0.50
1:C:4859:LEU:HD21	1:D:4851:PHE:CZ	2.46	0.50
1:D:939:THR:HG23	1:D:999:LEU:HD21	1.94	0.50
1:D:4237:SER:N	1:D:4240:THR:OG1	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:VAL:HG12	1:A:897:LYS:HZ3	1.77	0.49
1:A:1144:ARG:NH2	1:A:1184:ASP:OD1	2.45	0.49
1:A:2482:ASP:OD1	1:A:2483:PHE:N	2.45	0.49
1:A:2588:LEU:O	1:A:2592:LEU:HG	2.12	0.49
1:A:3924:ILE:HG21	1:A:3935:LEU:HD22	1.94	0.49
1:C:1172:THR:OG1	1:C:1190:LEU:HD22	2.12	0.49
1:C:1432:ILE:O	1:C:1500:ARG:NH2	2.44	0.49
1:C:2603:ALA:C	1:C:2606:PRO:HD2	2.32	0.49
1:C:2999:LYS:HA	1:C:3002:GLU:HG3	1.94	0.49
1:C:3882:GLN:NE2	1:C:3946:GLY:HA3	2.26	0.49
1:C:4046:ARG:HB3	1:C:4050:LYS:NZ	2.27	0.49
1:D:886:ALA:HA	1:D:889:ILE:HG12	1.94	0.49
1:D:2125:GLN:OE1	1:D:2144:ARG:NH1	2.38	0.49
1:D:3811:GLN:HE22	1:D:3829:VAL:HG13	1.77	0.49
1:A:879:GLU:HA	1:A:882:ARG:HD2	1.93	0.49
2:E:58:LYS:HG3	2:E:81:VAL:HB	1.94	0.49
2:H:58:LYS:HG3	2:H:81:VAL:HB	1.94	0.49
1:C:2247:VAL:HG11	1:C:2257:LEU:HD21	1.94	0.49
1:C:2926:LEU:O	1:C:2930:ILE:HG13	2.12	0.49
1:C:4237:SER:N	1:C:4240:THR:OG1	2.36	0.49
1:D:441:LYS:HZ2	1:D:443:SER:HG	1.53	0.49
1:D:515:ALA:HB2	1:D:523:GLY:HA3	1.94	0.49
1:D:3012:GLY:O	1:D:3016:ARG:HG3	2.12	0.49
1:D:4481:TRP:HE3	1:D:4484:ILE:HD11	1.76	0.49
1:A:1967:SER:O	1:A:1972:GLN:NE2	2.31	0.49
1:A:2603:ALA:C	1:A:2606:PRO:HD2	2.32	0.49
1:A:3811:GLN:HE22	1:A:3829:VAL:HG13	1.77	0.49
1:B:515:ALA:HB2	1:B:523:GLY:HA3	1.94	0.49
1:B:1685:LEU:HB3	1:B:1706:LEU:HD12	1.94	0.49
1:B:2891:ASP:OD1	1:B:2892:ILE:N	2.45	0.49
1:C:2657:TYR:HA	1:C:2662:PHE:CE1	2.48	0.49
1:C:2833:LEU:HB3	1:C:2838[B]:HIS:CE1	2.46	0.49
1:C:3012:GLY:O	1:C:3016:ARG:HG3	2.13	0.49
1:C:4154:GLU:O	1:C:4158:THR:HG23	2.11	0.49
1:D:3882:GLN:NE2	1:D:3946:GLY:HA3	2.26	0.49
1:A:490:GLN:HG2	1:A:495:ILE:HD12	1.95	0.49
1:A:559:ILE:HD13	1:A:593:HIS:HB3	1.95	0.49
1:A:1685:LEU:HB3	1:A:1706:LEU:HD12	1.94	0.49
1:A:1922:ILE:O	1:A:1926:VAL:HG23	2.12	0.49
2:E:19:LYS:HD3	2:E:20:GLY:H	1.77	0.49
1:B:1685:LEU:O	1:B:1689:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2657:TYR:HA	1:B:2662:PHE:CE1	2.48	0.49
1:C:1685:LEU:O	1:C:1689:ILE:HG12	2.12	0.49
1:C:2891:ASP:OD1	1:C:2892:ILE:N	2.45	0.49
1:C:3996:GLY:O	1:C:4000:VAL:HG23	2.13	0.49
1:D:2999:LYS:HA	1:D:3002:GLU:HG3	1.94	0.49
1:D:3901:GLN:OE1	1:D:3904:ARG:NH1	2.45	0.49
1:D:3996:GLY:O	1:D:4000:VAL:HG23	2.13	0.49
1:A:515:ALA:HB2	1:A:523:GLY:HA3	1.94	0.49
1:B:490:GLN:HG2	1:B:495:ILE:HD12	1.95	0.49
1:B:3924:ILE:HG21	1:B:3935:LEU:HD22	1.94	0.49
1:B:3996:GLY:O	1:B:4000:VAL:HG23	2.13	0.49
1:C:2588:LEU:O	1:C:2592:LEU:HG	2.12	0.49
1:C:3787:VAL:HG21	1:C:3866:THR:HB	1.95	0.49
1:D:559:ILE:HD13	1:D:593:HIS:HB3	1.95	0.49
1:D:1922:ILE:O	1:D:1926:VAL:HG23	2.12	0.49
1:D:3924:ILE:HG21	1:D:3935:LEU:HD22	1.94	0.49
1:A:1685:LEU:O	1:A:1689:ILE:HG12	2.12	0.49
1:A:2957:GLU:HA	1:A:2960:ILE:HG12	1.93	0.49
1:A:4834:PRO:HB3	1:A:4843:ARG:HG2	1.94	0.49
2:G:58:LYS:HG3	2:G:81:VAL:HB	1.94	0.49
1:B:824:GLU:CD	1:B:1028:ARG:HH22	2.16	0.49
1:B:2725:ALA:CB	1:B:2768:LYS:HG3	2.35	0.49
1:B:4046:ARG:HB3	1:B:4050:LYS:NZ	2.27	0.49
1:C:243:GLU:OE1	1:C:389:ARG:NH2	2.45	0.49
1:D:2715:GLU:HA	1:D:2718:GLU:HB2	1.93	0.49
1:A:824:GLU:CD	1:A:1028:ARG:HH22	2.16	0.49
1:A:2968:LEU:HD21	1:A:3029:ILE:HA	1.95	0.49
1:B:2247:VAL:HG11	1:B:2257:LEU:HD21	1.94	0.49
1:B:2603:ALA:C	1:B:2606:PRO:HD2	2.32	0.49
1:B:4279:MET:HE1	1:C:4488:GLN:HB2	1.94	0.49
1:C:1157:GLN:N	1:C:1160:ASP:OD2	2.41	0.49
1:C:1847:GLU:OE1	1:C:1895:GLN:NE2	2.35	0.49
1:C:3811:GLN:HE22	1:C:3829:VAL:HG13	1.77	0.49
1:D:3097:THR:HG23	1:D:3101:LEU:HD12	1.94	0.49
1:D:4154:GLU:O	1:D:4158:THR:HG23	2.11	0.49
1:A:4698:LEU:HD22	1:D:4262:LYS:HG3	1.94	0.49
2:H:19:LYS:HE2	2:H:51:ILE:HG22	1.94	0.49
1:B:253:GLY:HA3	1:B:256:GLN:NE2	2.26	0.49
1:B:2988:ARG:H	1:B:2989:PRO:CD	2.26	0.49
1:B:2999:LYS:HA	1:B:3002:GLU:HG3	1.94	0.49
1:C:939:THR:HG23	1:C:999:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4481:TRP:NE1	1:C:4692:SER:HA	2.21	0.49
1:C:4814:MET:HE2	1:D:4844:ILE:HD13	1.94	0.49
1:D:490:GLN:HG2	1:D:495:ILE:HD12	1.95	0.49
1:D:2603:ALA:C	1:D:2606:PRO:HD2	2.32	0.49
1:D:4637:THR:HG22	1:D:4704:LYS:HG2	1.95	0.49
1:B:624:ALA:HB2	1:B:1667:LEU:HD12	1.94	0.49
1:B:903:GLN:HB2	1:B:913:ARG:O	2.13	0.49
1:B:2481:GLN:HE22	1:B:2485:LEU:HD11	1.77	0.49
1:C:490:GLN:HG2	1:C:495:ILE:HD12	1.95	0.49
1:C:515:ALA:HB2	1:C:523:GLY:HA3	1.94	0.49
1:C:559:ILE:HD13	1:C:593:HIS:HB3	1.95	0.49
1:C:1298:ASP:N	1:C:1546:GLN:HE22	2.11	0.49
1:C:2482:ASP:OD1	1:C:2483:PHE:N	2.45	0.49
1:D:243:GLU:OE1	1:D:389:ARG:NH2	2.45	0.49
1:D:624:ALA:HB2	1:D:1667:LEU:HD12	1.95	0.49
1:D:824:GLU:CD	1:D:1028:ARG:HH22	2.16	0.49
1:D:2588:LEU:O	1:D:2592:LEU:HG	2.12	0.49
1:D:2657:TYR:HA	1:D:2662:PHE:CE1	2.48	0.49
1:D:2682:GLU:OE1	1:D:2919:LYS:HA	2.13	0.49
1:A:903:GLN:HB2	1:A:913:ARG:O	2.13	0.49
1:A:1298:ASP:N	1:A:1546:GLN:HE22	2.11	0.49
1:A:4046:ARG:HB3	1:A:4050:LYS:NZ	2.27	0.49
1:A:4481:TRP:HE3	1:A:4484:ILE:HD11	1.76	0.49
2:E:78:THR:O	2:E:81:VAL:HG22	2.13	0.49
2:F:19:LYS:HE2	2:F:51:ILE:HG22	1.94	0.49
1:B:1298:ASP:N	1:B:1546:GLN:HE22	2.11	0.49
1:B:4522:VAL:HG23	1:C:4786:PHE:CZ	2.48	0.49
1:C:713:TRP:HH2	1:C:1251:LEU:HD21	1.76	0.49
1:C:2878:THR:C	1:C:2882:LYS:HE2	2.33	0.49
1:C:4274:MET:H	1:C:4274:MET:CE	2.26	0.49
1:D:271:ALA:HB2	1:D:488:LEU:HD22	1.94	0.49
1:D:2481:GLN:HE22	1:D:2485:LEU:HD11	1.77	0.49
1:A:253:GLY:HA3	1:A:256:GLN:NE2	2.26	0.48
1:A:271:ALA:HB2	1:A:488:LEU:HD22	1.94	0.48
1:A:2768:LYS:O	1:A:2772:ARG:N	2.36	0.48
2:G:19:LYS:HD3	2:G:20:GLY:H	1.77	0.48
1:B:243:GLU:OE1	1:B:389:ARG:NH2	2.45	0.48
1:B:2682:GLU:OE1	1:B:2919:LYS:HA	2.13	0.48
1:B:2878:THR:C	1:B:2882:LYS:HE2	2.33	0.48
1:B:3008:PHE:CD1	1:B:3036:LEU:HB3	2.48	0.48
1:B:3811:GLN:HE22	1:B:3829:VAL:HG13	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:903:GLN:HB2	1:C:913:ARG:O	2.13	0.48
1:C:1035:TYR:HA	1:C:1038:LEU:HB2	1.96	0.48
1:C:1967:SER:O	1:C:1972:GLN:NE2	2.31	0.48
1:D:1495:SER:OG	1:D:1496:PRO:HD3	2.13	0.48
1:D:1967:SER:O	1:D:1972:GLN:NE2	2.31	0.48
1:D:4834:PRO:HB3	1:D:4843:ARG:HG2	1.94	0.48
1:A:624:ALA:HB2	1:A:1667:LEU:HD12	1.94	0.48
1:A:2988:ARG:H	1:A:2989:PRO:CD	2.26	0.48
1:A:4014:LEU:HD13	1:A:4122:ALA:HB2	1.96	0.48
2:F:58:LYS:HG3	2:F:81:VAL:HB	1.94	0.48
2:F:78:THR:O	2:F:81:VAL:HG22	2.13	0.48
2:G:78:THR:O	2:G:81:VAL:HG22	2.13	0.48
2:H:78:THR:O	2:H:81:VAL:HG22	2.13	0.48
1:B:1035:TYR:HA	1:B:1038:LEU:HB2	1.95	0.48
1:B:3097:THR:HG23	1:B:3101:LEU:HD12	1.94	0.48
1:B:4139:MET:HB3	1:B:4951:PHE:HA	1.96	0.48
1:B:4274:MET:H	1:B:4274:MET:CE	2.26	0.48
1:C:1500:ARG:HG3	1:C:1505:LEU:HB2	1.95	0.48
1:C:2682:GLU:OE1	1:C:2919:LYS:HA	2.13	0.48
1:D:1500:ARG:HG3	1:D:1505:LEU:HB2	1.95	0.48
1:D:2758:LYS:NZ	1:D:2762:LEU:O	2.36	0.48
1:D:3008:PHE:CD1	1:D:3036:LEU:HB3	2.48	0.48
1:D:4046:ARG:HB3	1:D:4050:LYS:NZ	2.27	0.48
1:A:2139:GLU:HA	1:A:2192:MET:HE3	1.95	0.48
1:A:2682:GLU:OE1	1:A:2919:LYS:HA	2.13	0.48
1:A:4507:LEU:HD21	1:A:4746:ILE:HG22	1.94	0.48
1:B:2588:LEU:O	1:B:2592:LEU:HG	2.12	0.48
1:B:3012:GLY:O	1:B:3016:ARG:HG3	2.12	0.48
1:B:3787:VAL:HG21	1:B:3866:THR:HB	1.95	0.48
1:C:1495:SER:OG	1:C:1496:PRO:HD3	2.14	0.48
1:C:3008:PHE:CD1	1:C:3036:LEU:HB3	2.48	0.48
1:D:2878:THR:C	1:D:2882:LYS:HE2	2.34	0.48
1:D:4014:LEU:HD13	1:D:4122:ALA:HB2	1.95	0.48
1:D:4139:MET:HB3	1:D:4951:PHE:HA	1.95	0.48
1:A:3996:GLY:O	1:A:4000:VAL:HG23	2.13	0.48
2:G:19:LYS:HE2	2:G:51:ILE:HG22	1.94	0.48
1:B:785:ASP:OD2	1:B:785:ASP:N	2.46	0.48
1:B:949:HIS:HB2	1:B:1065:GLU:HG2	1.96	0.48
1:B:1495:SER:OG	1:B:1496:PRO:HD3	2.13	0.48
1:C:308:LEU:CD1	1:C:393:MET:HG3	2.43	0.48
1:C:661:LEU:O	1:C:788:PHE:N	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1944:TYR:HA	1:C:1947:VAL:HG12	1.95	0.48
1:C:4514:ASN:HA	1:C:4517:LEU:HD12	1.96	0.48
1:D:1685:LEU:O	1:D:1689:ILE:HG12	2.12	0.48
1:D:4274:MET:CE	1:D:4274:MET:H	2.26	0.48
1:A:1495:SER:OG	1:A:1496:PRO:HD3	2.14	0.48
1:A:2731:LYS:HA	1:A:2734:MET:CG	2.38	0.48
1:A:3012:GLY:O	1:A:3016:ARG:HG3	2.13	0.48
1:A:3097:THR:HG23	1:A:3101:LEU:HD12	1.94	0.48
1:A:4139:MET:HB3	1:A:4951:PHE:HA	1.96	0.48
1:B:2139:GLU:HA	1:B:2192:MET:HE3	1.95	0.48
1:C:2139:GLU:HA	1:C:2192:MET:HE3	1.95	0.48
1:C:4637:THR:HG22	1:C:4704:LYS:HG2	1.95	0.48
1:D:903:GLN:HB2	1:D:913:ARG:O	2.13	0.48
1:D:2247:VAL:HG11	1:D:2257:LEU:HD21	1.94	0.48
1:D:2725:ALA:CB	1:D:2768:LYS:HG3	2.35	0.48
1:D:4507:LEU:HD21	1:D:4746:ILE:HG22	1.94	0.48
1:A:2317:ALA:O	1:A:2321:VAL:HG23	2.14	0.48
1:A:2481:GLN:HE22	1:A:2485:LEU:HD11	1.77	0.48
1:A:2657:TYR:HA	1:A:2662:PHE:CE1	2.48	0.48
1:A:3805:LEU:HD21	1:A:3891:TYR:HB2	1.96	0.48
1:B:3805:LEU:HD21	1:B:3891:TYR:HB2	1.96	0.48
1:C:1079:SER:OG	1:C:1084:ARG:NH2	2.43	0.48
1:C:4139:MET:HB3	1:C:4951:PHE:HA	1.96	0.48
1:D:661:LEU:O	1:D:788:PHE:N	2.33	0.48
1:D:963:LYS:HD2	1:D:980:PRO:HA	1.96	0.48
1:D:3805:LEU:HD21	1:D:3891:TYR:HB2	1.96	0.48
1:A:949:HIS:HB2	1:A:1065:GLU:HG2	1.96	0.48
1:A:1944:TYR:HA	1:A:1947:VAL:HG12	1.95	0.48
1:A:2878:THR:C	1:A:2882:LYS:HE2	2.34	0.48
1:A:3008:PHE:CD1	1:A:3036:LEU:HB3	2.48	0.48
1:A:3787:VAL:HG21	1:A:3866:THR:HB	1.95	0.48
1:A:4962:TYR:HD1	1:A:4965:GLN:NE2	2.02	0.48
2:E:19:LYS:HE2	2:E:51:ILE:HG22	1.94	0.48
1:B:886:ALA:HA	1:B:889:ILE:HG12	1.94	0.48
1:B:2758:LYS:HZ1	1:B:2764:SER:N	2.12	0.48
1:B:2926:LEU:O	1:B:2930:ILE:HG13	2.12	0.48
1:B:2966:VAL:O	1:B:2970:LEU:N	2.38	0.48
1:C:2968:LEU:HD21	1:C:3029:ILE:HA	1.95	0.48
1:C:2988:ARG:H	1:C:2989:PRO:CD	2.26	0.48
1:C:3805:LEU:HD21	1:C:3891:TYR:HB2	1.96	0.48
1:C:4014:LEU:HD13	1:C:4122:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4834:PRO:HB3	1:C:4843:ARG:HG2	1.94	0.48
1:D:386:SER:OG	1:D:387:ILE:N	2.44	0.48
1:D:799:LYS:HB3	1:D:799:LYS:HZ3	1.79	0.48
1:D:1035:TYR:HA	1:D:1038:LEU:HB2	1.95	0.48
1:D:1944:TYR:HA	1:D:1947:VAL:HG12	1.95	0.48
1:D:3072:MET:C	1:D:3076:LYS:HZ2	2.17	0.48
1:A:1143:GLN:HG2	1:A:1149:ASN:HB2	1.96	0.48
1:A:2247:VAL:HG11	1:A:2257:LEU:HD21	1.94	0.48
1:A:2937:HIS:CE1	1:A:3014:LEU:HB2	2.49	0.48
1:A:4274:MET:CE	1:A:4274:MET:H	2.26	0.48
1:A:4637:THR:HG22	1:A:4704:LYS:HG2	1.95	0.48
1:A:4714:PHE:CD1	1:D:4294:LEU:HD12	2.48	0.48
1:D:785:ASP:OD2	1:D:785:ASP:N	2.47	0.48
1:D:1298:ASP:N	1:D:1546:GLN:HE22	2.11	0.48
1:D:2139:GLU:HA	1:D:2192:MET:HE3	1.95	0.48
1:D:2837:LEU:HA	1:D:2840:MET:HB2	1.96	0.48
1:D:2966:VAL:O	1:D:2970:LEU:N	2.38	0.48
1:D:3787:VAL:HG21	1:D:3866:THR:HB	1.95	0.48
1:D:3817:LEU:HD22	1:D:3819:MET:HG2	1.96	0.48
1:A:1035:TYR:HA	1:A:1038:LEU:HB2	1.95	0.48
1:A:1500:ARG:HG3	1:A:1505:LEU:HB2	1.95	0.48
1:B:1944:TYR:HA	1:B:1947:VAL:HG12	1.95	0.48
1:B:2837:LEU:HA	1:B:2840:MET:HB2	1.96	0.48
1:C:1685:LEU:HB3	1:C:1706:LEU:HD12	1.94	0.48
1:C:3072:MET:C	1:C:3076:LYS:HZ2	2.17	0.48
1:C:4107:GLU:OE1	1:C:4149:TYR:OH	2.24	0.48
1:D:1160:ASP:OD1	1:D:1178:ASN:ND2	2.47	0.48
1:D:1685:LEU:HB3	1:D:1706:LEU:HD12	1.94	0.48
1:A:874:LEU:HB3	1:A:879:GLU:OE2	2.14	0.48
1:A:886:ALA:HA	1:A:889:ILE:HG12	1.94	0.48
1:A:1962:THR:HA	1:A:1965:PHE:CD2	2.48	0.48
1:A:2194:ALA:HA	1:A:2237:SER:HB3	1.96	0.48
1:A:2837:LEU:HA	1:A:2840:MET:HB2	1.96	0.48
1:B:559:ILE:HD13	1:B:593:HIS:HB3	1.95	0.48
1:B:874:LEU:HB3	1:B:879:GLU:OE2	2.14	0.48
1:B:927:GLN:HE22	1:B:928:GLU:HG3	1.79	0.48
1:B:1094:TYR:OH	1:B:1808:ASP:OD2	2.29	0.48
1:B:2194:ALA:HA	1:B:2237:SER:HB3	1.96	0.48
1:B:2317:ALA:O	1:B:2321:VAL:HG23	2.14	0.48
1:B:2968:LEU:HD21	1:B:3029:ILE:HA	1.95	0.48
1:B:4834:PRO:HB3	1:B:4843:ARG:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:949:HIS:HB2	1:C:1065:GLU:HG2	1.96	0.48
1:C:1118:SER:HB3	1:C:1204:VAL:HG11	1.96	0.48
1:C:2649:PHE:HD1	1:C:2669:LEU:HD21	1.79	0.48
1:C:2937:HIS:CE1	1:C:3014:LEU:HB2	2.49	0.48
1:C:3817:LEU:HD22	1:C:3819:MET:HG2	1.96	0.48
1:D:306:LEU:HD11	1:D:314:LEU:HD12	1.96	0.48
1:D:927:GLN:HE22	1:D:928:GLU:HG3	1.79	0.48
1:D:1088:PHE:HB2	1:D:1205:CYS:SG	2.54	0.48
1:D:4514:ASN:HA	1:D:4517:LEU:HD12	1.96	0.48
1:D:4831:ILE:HG13	1:D:4843:ARG:NH2	2.29	0.48
1:A:306:LEU:HD11	1:A:314:LEU:HD12	1.96	0.47
1:A:2701:PHE:CD2	1:A:2703:PRO:HG3	2.50	0.47
2:G:9:SER:HB3	2:G:72:ARG:HB3	1.96	0.47
1:B:2937:HIS:CE1	1:B:3014:LEU:HB2	2.49	0.47
1:B:4014:LEU:HD13	1:B:4122:ALA:HB2	1.96	0.47
1:C:2455:ASP:OD2	1:C:2457:SER:OG	2.21	0.47
1:C:3097:THR:HG23	1:C:3101:LEU:HD12	1.94	0.47
1:C:4831:ILE:HG13	1:C:4843:ARG:NH2	2.29	0.47
1:D:915:HIS:CD2	1:D:917:CYS:HB2	2.49	0.47
1:D:2649:PHE:HD1	1:D:2669:LEU:HD21	1.79	0.47
1:D:2937:HIS:CE1	1:D:3014:LEU:HB2	2.49	0.47
1:A:1100:ARG:HG3	1:A:1236:TYR:HA	1.96	0.47
1:A:1847:GLU:OE1	1:A:1895:GLN:NE2	2.35	0.47
2:G:18:LYS:O	2:G:21:GLN:HB2	2.15	0.47
1:B:267:VAL:HA	1:B:270:HIS:HB2	1.96	0.47
1:B:1500:ARG:HG3	1:B:1505:LEU:HB2	1.95	0.47
1:B:4155:SER:O	1:B:4159:GLN:HG2	2.14	0.47
1:B:4274:MET:H	1:B:4274:MET:HE2	1.79	0.47
1:C:4155:SER:O	1:C:4159:GLN:HG2	2.14	0.47
1:D:756:SER:OG	1:D:769:ARG:O	2.32	0.47
1:D:949:HIS:HB2	1:D:1065:GLU:HG2	1.96	0.47
1:D:2701:PHE:CD2	1:D:2703:PRO:HG3	2.50	0.47
1:D:2968:LEU:HD21	1:D:3029:ILE:HA	1.95	0.47
1:D:2988:ARG:H	1:D:2989:PRO:CD	2.26	0.47
1:A:915:HIS:CD2	1:A:917:CYS:HB2	2.49	0.47
1:A:2341:ASN:OD1	1:A:2342:GLY:N	2.48	0.47
1:A:4155:SER:O	1:A:4159:GLN:HG2	2.14	0.47
2:H:18:LYS:O	2:H:21:GLN:HB2	2.14	0.47
1:B:799:LYS:HB3	1:B:799:LYS:HZ3	1.79	0.47
1:B:4514:ASN:HA	1:B:4517:LEU:HD12	1.96	0.47
1:C:884:LYS:HA	1:C:887:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1143:GLN:HG2	1:C:1149:ASN:HB2	1.96	0.47
1:D:1143:GLN:HG2	1:D:1149:ASN:HB2	1.96	0.47
1:D:1979:PHE:HE1	1:D:1988:CYS:HB3	1.79	0.47
1:A:267:VAL:HA	1:A:270:HIS:HB2	1.96	0.47
2:E:18:LYS:O	2:E:21:GLN:HB2	2.15	0.47
1:B:994:ALA:O	1:B:998:LYS:HD3	2.15	0.47
1:B:3965:ILE:HG22	1:B:3969:LYS:NZ	2.30	0.47
1:C:1088:PHE:HB2	1:C:1205:CYS:SG	2.54	0.47
1:C:2317:ALA:O	1:C:2321:VAL:HG23	2.14	0.47
1:D:323:ASP:O	1:D:327:THR:OG1	2.24	0.47
1:D:2341:ASN:OD1	1:D:2342:GLY:N	2.48	0.47
1:A:308:LEU:CD1	1:A:393:MET:HG3	2.43	0.47
1:A:1144:ARG:HE	1:A:1152:TYR:HB2	1.79	0.47
1:A:1266:GLU:OE2	1:A:1267:HIS:ND1	2.44	0.47
1:A:4275:THR:HG23	1:A:4278:ASP:H	1.80	0.47
1:B:884:LYS:HA	1:B:887:GLU:HG3	1.96	0.47
1:B:1088:PHE:HB2	1:B:1205:CYS:SG	2.54	0.47
1:B:1160:ASP:OD1	1:B:1178:ASN:ND2	2.46	0.47
1:B:2701:PHE:CD2	1:B:2703:PRO:HG3	2.50	0.47
1:B:4637:THR:HG22	1:B:4704:LYS:HG2	1.95	0.47
1:B:4831:ILE:HG13	1:B:4843:ARG:NH2	2.29	0.47
1:B:4887:LYS:HB2	1:B:4887:LYS:HE3	1.58	0.47
1:C:386:SER:OG	1:C:387:ILE:N	2.44	0.47
1:C:624:ALA:HB2	1:C:1667:LEU:HD12	1.94	0.47
1:C:886:ALA:HA	1:C:889:ILE:HG12	1.94	0.47
1:C:2194:ALA:HA	1:C:2237:SER:HB3	1.96	0.47
1:C:2341:ASN:OD1	1:C:2342:GLY:N	2.48	0.47
1:C:3006:SER:HB3	1:C:3053:VAL:HG13	1.97	0.47
1:D:1440:ASN:HB3	1:D:1546:GLN:HB3	1.97	0.47
1:D:4155:SER:O	1:D:4159:GLN:HG2	2.14	0.47
1:A:3006:SER:HB3	1:A:3053:VAL:HG13	1.97	0.47
1:B:306:LEU:HD11	1:B:314:LEU:HD12	1.96	0.47
1:B:963:LYS:HD2	1:B:980:PRO:HA	1.96	0.47
1:B:3006:SER:HB3	1:B:3053:VAL:HG13	1.97	0.47
1:C:765:SER:HB2	1:C:778:MET:HE1	1.97	0.47
1:C:2193:VAL:HG11	1:C:2227:VAL:HG11	1.97	0.47
1:C:2701:PHE:CD2	1:C:2703:PRO:HG3	2.50	0.47
1:D:1144:ARG:HE	1:D:1152:TYR:HB2	1.79	0.47
1:A:1440:ASN:HB3	1:A:1546:GLN:HB3	1.97	0.47
1:A:1768:PHE:O	2:E:83:TYR:OH	2.26	0.47
1:A:1979:PHE:HE1	1:A:1988:CYS:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2171:VAL:HG21	1:A:2199:PHE:CE2	2.50	0.47
1:A:2649:PHE:HD1	1:A:2669:LEU:HD21	1.79	0.47
1:A:2925:PHE:O	1:A:2929:LEU:HG	2.15	0.47
1:A:3817:LEU:HD22	1:A:3819:MET:HG2	1.96	0.47
1:A:3965:ILE:HG22	1:A:3969:LYS:NZ	2.30	0.47
2:F:18:LYS:O	2:F:21:GLN:HB2	2.15	0.47
2:H:9:SER:HB3	2:H:72:ARG:HB3	1.96	0.47
1:B:1100:ARG:HG3	1:B:1236:TYR:HA	1.96	0.47
1:B:2193:VAL:HG11	1:B:2227:VAL:HG11	1.97	0.47
1:B:4107:GLU:OE1	1:B:4149:TYR:OH	2.24	0.47
1:B:4522:VAL:HG23	1:C:4786:PHE:CE1	2.49	0.47
1:C:434:ASP:O	1:C:438:LYS:HG2	2.15	0.47
1:C:874:LEU:HB3	1:C:879:GLU:OE2	2.14	0.47
1:C:927:GLN:HE22	1:C:928:GLU:HG3	1.79	0.47
1:C:963:LYS:HD2	1:C:980:PRO:HA	1.96	0.47
1:C:2826:ILE:HG21	1:D:1501:ASN:HB2	1.96	0.47
1:C:4173:ILE:HD12	1:C:4884:MET:HE1	1.97	0.47
1:D:874:LEU:HB3	1:D:879:GLU:OE2	2.14	0.47
1:D:1100:ARG:HG3	1:D:1236:TYR:HA	1.96	0.47
1:D:1415:ASP:OD2	1:D:1559:ARG:NH2	2.43	0.47
1:D:1898:LEU:HD23	1:D:1902:VAL:HG11	1.97	0.47
1:D:2317:ALA:O	1:D:2321:VAL:HG23	2.14	0.47
1:D:3950:VAL:O	1:D:3954:MET:HB2	2.15	0.47
1:A:994:ALA:O	1:A:998:LYS:HD3	2.15	0.47
1:A:1141:LYS:O	1:A:1141:LYS:HD3	2.15	0.47
1:B:1042:THR:O	1:B:1046:ASN:ND2	2.48	0.47
1:B:1118:SER:HB3	1:B:1204:VAL:HG11	1.96	0.47
1:B:1897:LYS:O	1:B:1897:LYS:HD3	2.15	0.47
1:B:2939:TYR:HB3	1:B:2943:PHE:HE2	1.80	0.47
1:C:306:LEU:HD11	1:C:314:LEU:HD12	1.96	0.47
1:C:1042:THR:O	1:C:1046:ASN:ND2	2.48	0.47
1:C:1141:LYS:O	1:C:1141:LYS:HD3	2.15	0.47
1:D:1118:SER:HB3	1:D:1204:VAL:HG11	1.96	0.47
1:D:2484:LEU:HD13	1:D:2534:LEU:HD23	1.97	0.47
1:D:2846:GLU:HB3	1:D:2874:TYR:HD2	1.80	0.47
1:A:434:ASP:O	1:A:438:LYS:HG2	2.15	0.47
1:A:1088:PHE:HB2	1:A:1205:CYS:SG	2.54	0.47
1:A:1825:PHE:CE1	1:A:1842:ILE:HD12	2.50	0.47
1:A:2882:LYS:HB2	1:A:2886:ARG:CZ	2.45	0.47
1:A:2939:TYR:HB3	1:A:2943:PHE:HE2	1.80	0.47
1:A:3950:VAL:O	1:A:3954:MET:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:673:TRP:CZ3	1:B:825:ALA:HB2	2.50	0.47
1:B:1141:LYS:O	1:B:1141:LYS:HD3	2.15	0.47
1:B:1144:ARG:HE	1:B:1152:TYR:HB2	1.80	0.47
1:B:2332:GLY:O	1:B:2336:ARG:HG3	2.15	0.47
1:B:2716:LYS:HB3	1:B:2901:TYR:OH	2.15	0.47
1:B:3817:LEU:HD22	1:B:3819:MET:HG2	1.96	0.47
1:C:1303:ARG:NH2	1:C:1635:GLU:OE1	2.48	0.47
1:C:3950:VAL:O	1:C:3954:MET:HB2	2.15	0.47
1:C:4186:MET:HA	1:C:4186:MET:CE	2.45	0.47
1:D:2194:ALA:HA	1:D:2237:SER:HB3	1.96	0.47
1:A:2193:VAL:HG11	1:A:2227:VAL:HG11	1.97	0.47
1:A:3732:HIS:O	1:A:3776:LYS:NZ	2.47	0.47
1:A:4186:MET:HA	1:A:4186:MET:CE	2.45	0.47
1:B:915:HIS:CD2	1:B:917:CYS:HB2	2.49	0.47
1:B:1143:GLN:HG2	1:B:1149:ASN:HB2	1.96	0.47
1:B:2778:SER:O	1:B:2848:TYR:OH	2.33	0.47
1:B:2882:LYS:HB2	1:B:2886:ARG:CZ	2.45	0.47
1:C:267:VAL:HA	1:C:270:HIS:HB2	1.96	0.47
1:C:2837:LEU:HA	1:C:2840:MET:HB2	1.96	0.47
1:C:3090:VAL:HA	1:C:3093:ILE:HG22	1.97	0.47
1:C:4004:VAL:HG21	1:C:4114:ARG:HD2	1.96	0.47
1:D:3732:HIS:O	1:D:3776:LYS:NZ	2.47	0.47
1:D:4186:MET:HA	1:D:4186:MET:CE	2.45	0.47
1:A:756:SER:OG	1:A:769:ARG:O	2.32	0.46
1:A:2484:LEU:HD13	1:A:2534:LEU:HD23	1.97	0.46
1:A:2758:LYS:HZ1	1:A:2764:SER:N	2.13	0.46
1:A:3793:LEU:O	1:A:3797:MET:HG3	2.15	0.46
1:A:4831:ILE:HG13	1:A:4843:ARG:NH2	2.29	0.46
1:A:4887:LYS:HE3	1:A:4887:LYS:HB2	1.58	0.46
2:E:9:SER:HB3	2:E:72:ARG:HB3	1.96	0.46
1:B:1047:LYS:O	1:B:1051:ARG:HG2	2.16	0.46
1:B:3732:HIS:O	1:B:3776:LYS:NZ	2.47	0.46
1:B:3950:VAL:O	1:B:3954:MET:HB2	2.15	0.46
1:C:2171:VAL:HG21	1:C:2199:PHE:CE2	2.50	0.46
1:C:2925:PHE:O	1:C:2929:LEU:HG	2.15	0.46
1:D:3042:ALA:HB3	1:D:3117:PHE:CD2	2.51	0.46
1:D:4275:THR:HG23	1:D:4278:ASP:H	1.80	0.46
1:A:1079:SER:OG	1:A:1084:ARG:NH2	2.43	0.46
1:A:1898:LEU:HD23	1:A:1902:VAL:HG11	1.97	0.46
1:A:4514:ASN:HA	1:A:4517:LEU:HD12	1.96	0.46
1:B:2290:TRP:CZ3	1:B:2292:PRO:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2484:LEU:HD13	1:B:2534:LEU:HD23	1.97	0.46
1:B:2936:ALA:O	1:B:2940:ILE:HG12	2.15	0.46
1:B:3042:ALA:HB3	1:B:3117:PHE:CD2	2.50	0.46
1:B:4186:MET:HA	1:B:4186:MET:CE	2.45	0.46
1:C:1100:ARG:HG3	1:C:1236:TYR:HA	1.96	0.46
1:C:2778:SER:HA	1:C:2848:TYR:CE2	2.50	0.46
1:D:1141:LYS:O	1:D:1141:LYS:HD3	2.15	0.46
1:D:1157:GLN:N	1:D:1160:ASP:OD2	2.41	0.46
1:D:1303:ARG:NH2	1:D:1635:GLU:OE1	2.48	0.46
1:D:1825:PHE:CE1	1:D:1842:ILE:HD12	2.50	0.46
1:D:2290:TRP:CZ3	1:D:2292:PRO:HB3	2.51	0.46
1:D:2778:SER:HA	1:D:2848:TYR:CE2	2.51	0.46
1:D:3965:ILE:HG22	1:D:3969:LYS:HZ3	1.80	0.46
1:D:4173:ILE:HD12	1:D:4884:MET:HE1	1.97	0.46
1:A:785:ASP:OD2	1:A:785:ASP:N	2.46	0.46
1:A:884:LYS:HA	1:A:887:GLU:HG3	1.96	0.46
1:A:963:LYS:HD2	1:A:980:PRO:HA	1.96	0.46
1:A:2692:GLN:HA	1:A:2695:MET:HG3	1.98	0.46
1:A:2778:SER:O	1:A:2848:TYR:OH	2.33	0.46
1:B:308:LEU:CD1	1:B:393:MET:HG3	2.43	0.46
1:B:2649:PHE:HD1	1:B:2669:LEU:HD21	1.79	0.46
1:B:2893:LEU:HD12	1:B:2894:LYS:N	2.31	0.46
1:B:3090:VAL:HA	1:B:3093:ILE:HG22	1.97	0.46
1:B:3622:GLN:HB3	1:B:3626:LYS:NZ	2.30	0.46
1:B:3793:LEU:O	1:B:3797:MET:HG3	2.15	0.46
1:C:1440:ASN:HB3	1:C:1546:GLN:HB3	1.97	0.46
1:C:1898:LEU:HD23	1:C:1902:VAL:HG11	1.97	0.46
1:C:3042:ALA:HB3	1:C:3117:PHE:CD2	2.50	0.46
1:C:3622:GLN:HB3	1:C:3626:LYS:NZ	2.30	0.46
1:C:3793:LEU:O	1:C:3797:MET:HG3	2.15	0.46
1:D:267:VAL:HA	1:D:270:HIS:HB2	1.96	0.46
1:D:434:ASP:O	1:D:438:LYS:HG2	2.15	0.46
1:D:2171:VAL:HG21	1:D:2199:PHE:CE2	2.50	0.46
1:D:2988:ARG:HD2	1:D:2989:PRO:CD	2.46	0.46
1:D:4962:TYR:HD1	1:D:4965:GLN:NE2	2.02	0.46
1:A:182:ILE:HD12	1:A:191:TYR:HE1	1.81	0.46
1:A:2982:PHE:O	1:A:3001:LYS:NZ	2.40	0.46
1:B:182:ILE:HD12	1:B:191:TYR:HE1	1.80	0.46
1:B:1440:ASN:HB3	1:B:1546:GLN:HB3	1.97	0.46
1:B:2171:VAL:HG21	1:B:2199:PHE:CE2	2.50	0.46
1:B:2778:SER:HA	1:B:2848:TYR:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3072:MET:C	1:B:3076:LYS:HZ2	2.18	0.46
1:C:1825:PHE:CE1	1:C:1842:ILE:HD12	2.50	0.46
1:C:2290:TRP:CZ3	1:C:2292:PRO:HB3	2.51	0.46
1:C:2716:LYS:HB3	1:C:2901:TYR:OH	2.15	0.46
1:C:2758:LYS:NZ	1:C:2762:LEU:O	2.36	0.46
1:C:2826:ILE:CG2	1:D:1501:ASN:HB2	2.46	0.46
1:C:2882:LYS:HB2	1:C:2886:ARG:CZ	2.45	0.46
1:C:2936:ALA:O	1:C:2940:ILE:HG12	2.15	0.46
1:C:4962:TYR:HD1	1:C:4965:GLN:NE2	2.02	0.46
1:D:69:LEU:HD22	1:D:119:ILE:HG12	1.97	0.46
1:D:476:GLN:HB3	1:D:480:ARG:NH1	2.30	0.46
1:D:2692:GLN:HA	1:D:2695:MET:HG3	1.98	0.46
1:D:2982:PHE:O	1:D:3001:LYS:NZ	2.40	0.46
1:D:3006:SER:HB3	1:D:3053:VAL:HG13	1.97	0.46
1:D:4004:VAL:HG21	1:D:4114:ARG:HD2	1.96	0.46
1:D:4116:GLN:HA	1:D:4119:LEU:HD12	1.97	0.46
1:A:1047:LYS:O	1:A:1051:ARG:HG2	2.16	0.46
1:A:1089:ARG:O	1:A:1250:TRP:N	2.46	0.46
1:A:1160:ASP:OD1	1:A:1178:ASN:ND2	2.47	0.46
1:A:3042:ALA:HB3	1:A:3117:PHE:CD2	2.50	0.46
2:F:9:SER:HB3	2:F:72:ARG:HB3	1.96	0.46
1:B:189:GLU:OE1	1:B:189:GLU:N	2.49	0.46
1:B:270:HIS:CE1	1:B:491:GLU:HG3	2.51	0.46
1:B:829:LYS:NZ	1:B:1037:LEU:HD23	2.31	0.46
1:B:1825:PHE:CE1	1:B:1842:ILE:HD12	2.50	0.46
1:B:2341:ASN:OD1	1:B:2342:GLY:N	2.48	0.46
1:B:2724:TYR:HB2	1:B:2895:PHE:CE2	2.51	0.46
1:B:2846:GLU:HB3	1:B:2874:TYR:HD2	1.80	0.46
1:B:3067:ASP:HA	1:B:3070:LYS:HE3	1.98	0.46
1:B:3830:LEU:HB3	1:B:3833:ASP:OD2	2.16	0.46
1:C:673:TRP:CZ3	1:C:825:ALA:HB2	2.50	0.46
1:C:994:ALA:O	1:C:998:LYS:HD3	2.15	0.46
1:C:1979:PHE:HE1	1:C:1988:CYS:HB3	1.79	0.46
1:C:2332:GLY:O	1:C:2336:ARG:HG3	2.15	0.46
1:C:2484:LEU:HD13	1:C:2534:LEU:HD23	1.97	0.46
1:C:2692:GLN:HA	1:C:2695:MET:HG3	1.98	0.46
1:C:2926:LEU:HD11	1:C:3003:MET:SD	2.56	0.46
1:C:2988:ARG:HD2	1:C:2989:PRO:CD	2.46	0.46
1:C:3965:ILE:HG22	1:C:3969:LYS:NZ	2.30	0.46
1:D:884:LYS:HA	1:D:887:GLU:HG3	1.96	0.46
1:D:1047:LYS:O	1:D:1051:ARG:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1113:MET:HE3	1:D:1211:GLN:HB3	1.97	0.46
1:D:2724:TYR:HB2	1:D:2895:PHE:CE2	2.51	0.46
1:D:2882:LYS:HB2	1:D:2886:ARG:CZ	2.45	0.46
1:D:2925:PHE:O	1:D:2929:LEU:HG	2.15	0.46
1:D:2926:LEU:HD11	1:D:3003:MET:SD	2.56	0.46
1:D:4965:GLN:N	1:D:4965:GLN:OE1	2.49	0.46
1:A:157:ALA:HA	1:A:187:SER:HB3	1.98	0.46
1:A:270:HIS:CE1	1:A:491:GLU:HG3	2.51	0.46
1:A:673:TRP:CZ3	1:A:825:ALA:HB2	2.50	0.46
1:A:1118:SER:HB3	1:A:1204:VAL:HG11	1.96	0.46
1:A:1303:ARG:NH2	1:A:1635:GLU:OE1	2.48	0.46
1:A:2926:LEU:HD11	1:A:3003:MET:SD	2.56	0.46
1:A:3067:ASP:HA	1:A:3070:LYS:HE3	1.98	0.46
1:B:374:TYR:CD2	1:B:376:SER:HB3	2.51	0.46
1:B:2723:LYS:HD3	1:B:2899:ASN:ND2	2.31	0.46
1:B:4116:GLN:HA	1:B:4119:LEU:HD12	1.98	0.46
1:B:4641:PRO:HG2	1:B:4646:ASP:O	2.16	0.46
1:C:915:HIS:CD2	1:C:917:CYS:HB2	2.49	0.46
1:C:1047:LYS:O	1:C:1051:ARG:HG2	2.16	0.46
1:C:1160:ASP:OD1	1:C:1178:ASN:ND2	2.47	0.46
1:C:2893:LEU:HD12	1:C:2894:LYS:N	2.31	0.46
1:C:3830:LEU:HB3	1:C:3833:ASP:OD2	2.16	0.46
1:C:3975:GLN:O	1:C:3979:VAL:HG23	2.16	0.46
1:D:1079:SER:OG	1:D:1084:ARG:NH2	2.43	0.46
1:D:2768:LYS:O	1:D:2772:ARG:N	2.36	0.46
1:D:2778:SER:O	1:D:2848:TYR:OH	2.33	0.46
1:D:2936:ALA:O	1:D:2940:ILE:HG12	2.15	0.46
1:D:3965:ILE:HG22	1:D:3969:LYS:NZ	2.30	0.46
1:D:4274:MET:H	1:D:4274:MET:HE2	1.81	0.46
1:A:829:LYS:NZ	1:A:1037:LEU:HD23	2.31	0.46
1:A:1897:LYS:O	1:A:1897:LYS:HD3	2.15	0.46
1:A:2936:ALA:O	1:A:2940:ILE:HG12	2.15	0.46
1:A:3072:MET:C	1:A:3076:LYS:HZ2	2.19	0.46
1:A:4563:GLU:CG	1:A:4566:GLY:H	2.29	0.46
1:B:35:LEU:HD23	1:B:51:SER:HA	1.98	0.46
1:B:434:ASP:O	1:B:438:LYS:HG2	2.15	0.46
1:B:1303:ARG:NH2	1:B:1635:GLU:OE1	2.48	0.46
1:B:2925:PHE:O	1:B:2929:LEU:HG	2.15	0.46
1:B:4004:VAL:HG21	1:B:4114:ARG:HD2	1.96	0.46
1:B:4159:GLN:O	1:B:4162:LYS:HB2	2.16	0.46
1:B:4275:THR:HG23	1:B:4278:ASP:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ALA:HA	1:C:187:SER:HB3	1.98	0.46
1:C:235:ARG:HE	1:C:274:LEU:HD23	1.81	0.46
1:C:374:TYR:CD2	1:C:376:SER:HB3	2.51	0.46
1:C:2778:SER:O	1:C:2848:TYR:OH	2.33	0.46
1:D:189:GLU:OE1	1:D:189:GLU:N	2.49	0.46
1:D:994:ALA:O	1:D:998:LYS:HD3	2.15	0.46
1:D:1042:THR:O	1:D:1046:ASN:ND2	2.48	0.46
1:D:1144:ARG:HH22	1:D:1184:ASP:CG	2.19	0.46
1:A:374:TYR:CD2	1:A:376:SER:HB3	2.51	0.46
1:A:938:GLU:OE2	1:A:942:THR:OG1	2.34	0.46
1:A:2431:ASP:O	1:A:2435:VAL:HG23	2.16	0.46
1:A:2716:LYS:HB3	1:A:2901:TYR:OH	2.15	0.46
1:A:2723:LYS:HD3	1:A:2899:ASN:ND2	2.31	0.46
1:A:2988:ARG:HD2	1:A:2989:PRO:CD	2.46	0.46
1:A:4004:VAL:HG21	1:A:4114:ARG:HD2	1.96	0.46
1:B:2988:ARG:HD2	1:B:2989:PRO:CD	2.46	0.46
1:B:3975:GLN:O	1:B:3979:VAL:HG23	2.16	0.46
1:B:4965:GLN:OE1	1:B:4965:GLN:N	2.49	0.46
1:C:69:LEU:HD22	1:C:119:ILE:HG12	1.97	0.46
1:C:1144:ARG:HE	1:C:1152:TYR:HB2	1.79	0.46
1:C:1897:LYS:O	1:C:1897:LYS:HD3	2.15	0.46
1:C:2431:ASP:O	1:C:2435:VAL:HG23	2.16	0.46
1:C:2939:TYR:HB3	1:C:2943:PHE:HE2	1.80	0.46
1:C:3965:ILE:HG22	1:C:3969:LYS:HZ3	1.81	0.46
1:C:4116:GLN:HA	1:C:4119:LEU:HD12	1.98	0.46
1:C:4743:LEU:O	1:C:4746:ILE:HG12	2.16	0.46
1:D:374:TYR:CD2	1:D:376:SER:HB3	2.51	0.46
1:D:673:TRP:CZ3	1:D:825:ALA:HB2	2.50	0.46
1:D:765:SER:HA	1:D:779:PHE:O	2.16	0.46
1:D:1564:MET:HE3	1:D:1578:PRO:HA	1.97	0.46
1:A:323:ASP:O	1:A:327:THR:OG1	2.24	0.46
1:A:765:SER:HA	1:A:779:PHE:O	2.16	0.46
1:A:2724:TYR:HB2	1:A:2895:PHE:CE2	2.51	0.46
1:A:2846:GLU:HB3	1:A:2874:TYR:HD2	1.80	0.46
1:A:3830:LEU:HB3	1:A:3833:ASP:OD2	2.16	0.46
1:B:1020:ILE:C	1:B:1030:PRO:HB3	2.36	0.46
1:B:1179:GLY:HA3	1:B:1229:ILE:HD11	1.98	0.46
1:B:1898:LEU:HD23	1:B:1902:VAL:HG11	1.97	0.46
1:B:1962:THR:HA	1:B:1965:PHE:CD2	2.48	0.46
1:B:2614:TYR:CD2	1:B:2672:VAL:HG22	2.51	0.46
1:C:938:GLU:OE2	1:C:942:THR:OG1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2614:TYR:CD2	1:C:2672:VAL:HG22	2.51	0.46
1:D:1020:ILE:C	1:D:1030:PRO:HB3	2.36	0.46
1:D:1179:GLY:HA3	1:D:1229:ILE:HD11	1.98	0.46
1:D:2939:TYR:HB3	1:D:2943:PHE:HE2	1.80	0.46
1:D:4018:ASP:OD1	1:D:4022:LYS:NZ	2.42	0.46
1:A:2694:SER:HA	1:A:2702:ASN:HB3	1.98	0.46
1:B:2431:ASP:O	1:B:2435:VAL:HG23	2.16	0.46
1:B:4563:GLU:CG	1:B:4566:GLY:H	2.29	0.46
1:C:1911:GLN:OE1	1:C:2090:ARG:NH1	2.49	0.46
1:C:2723:LYS:HD3	1:C:2899:ASN:ND2	2.31	0.46
1:C:4275:THR:HG23	1:C:4278:ASP:H	1.80	0.46
1:D:270:HIS:CE1	1:D:491:GLU:HG3	2.51	0.46
1:D:308:LEU:CD1	1:D:393:MET:HG3	2.43	0.46
1:D:938:GLU:OE2	1:D:942:THR:OG1	2.34	0.46
1:D:2193:VAL:HG11	1:D:2227:VAL:HG11	1.97	0.46
1:A:189:GLU:OE1	1:A:189:GLU:N	2.49	0.45
1:A:1042:THR:O	1:A:1046:ASN:ND2	2.48	0.45
1:A:1911:GLN:OE1	1:A:2090:ARG:NH1	2.49	0.45
1:A:2332:GLY:O	1:A:2336:ARG:HG3	2.15	0.45
1:A:2642:ARG:HH12	1:A:2921:PHE:HA	1.82	0.45
1:A:3622:GLN:HB3	1:A:3626:LYS:NZ	2.30	0.45
1:B:938:GLU:OE2	1:B:942:THR:OG1	2.34	0.45
1:C:189:GLU:N	1:C:189:GLU:OE1	2.49	0.45
1:C:2966:VAL:O	1:C:2970:LEU:N	2.38	0.45
1:C:3017:HIS:O	1:C:3018:ARG:HD3	2.16	0.45
1:C:3043:ARG:HH11	1:C:3047:LYS:HZ2	1.64	0.45
1:D:59:PRO:HG3	1:D:296:ARG:CZ	2.46	0.45
1:D:182:ILE:HD12	1:D:191:TYR:HE1	1.81	0.45
1:D:235:ARG:HE	1:D:274:LEU:HD23	1.81	0.45
1:D:2893:LEU:HD12	1:D:2894:LYS:N	2.31	0.45
1:D:3090:VAL:HA	1:D:3093:ILE:HG22	1.97	0.45
1:D:4743:LEU:O	1:D:4746:ILE:HG12	2.16	0.45
1:D:4898:PHE:O	1:D:4904:GLY:HA3	2.17	0.45
1:A:59:PRO:HG3	1:A:296:ARG:CZ	2.47	0.45
1:A:927:GLN:HE22	1:A:928:GLU:HG3	1.79	0.45
1:A:2434:GLY:O	1:A:2438:ILE:HG13	2.17	0.45
1:A:2833:LEU:HD11	1:A:2837:LEU:HD23	1.97	0.45
1:A:2893:LEU:HD12	1:A:2894:LYS:N	2.31	0.45
1:A:4116:GLN:HA	1:A:4119:LEU:HD12	1.98	0.45
1:A:4965:GLN:N	1:A:4965:GLN:OE1	2.49	0.45
1:B:765:SER:HB2	1:B:778:MET:HE1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1911:GLN:OE1	1:B:2090:ARG:NH1	2.49	0.45
1:B:1979:PHE:HE1	1:B:1988:CYS:HB3	1.79	0.45
1:B:2642:ARG:HH12	1:B:2921:PHE:HA	1.82	0.45
1:B:2857:LYS:O	1:B:2861:GLU:OE1	2.35	0.45
1:B:4173:ILE:HD12	1:B:4884:MET:HE1	1.98	0.45
1:C:59:PRO:HG3	1:C:296:ARG:CZ	2.47	0.45
1:C:912:LYS:HZ3	1:C:914:GLN:HG3	1.82	0.45
1:C:2434:GLY:O	1:C:2438:ILE:HG13	2.17	0.45
1:C:4159:GLN:O	1:C:4162:LYS:HB2	2.16	0.45
1:C:4747:ALA:HB1	1:C:4757:LEU:HD11	1.99	0.45
1:D:355:LYS:O	1:D:359:SER:OG	2.26	0.45
1:D:1118:SER:HA	1:D:1134:ALA:HA	1.98	0.45
1:D:1266:GLU:OE2	1:D:1267:HIS:ND1	2.44	0.45
1:D:2332:GLY:O	1:D:2336:ARG:HG3	2.15	0.45
1:D:3067:ASP:HA	1:D:3070:LYS:HE3	1.98	0.45
1:A:2778:SER:HA	1:A:2848:TYR:CE2	2.51	0.45
1:A:4173:ILE:HD12	1:A:4884:MET:HE1	1.97	0.45
1:A:4898:PHE:O	1:A:4904:GLY:HA3	2.17	0.45
1:B:69:LEU:HD22	1:B:119:ILE:HG12	1.97	0.45
1:B:157:ALA:HA	1:B:187:SER:HB3	1.98	0.45
1:B:476:GLN:HB3	1:B:480:ARG:NH1	2.30	0.45
1:B:1944:TYR:CZ	1:B:3604:ARG:HD2	2.52	0.45
1:B:3017:HIS:O	1:B:3018:ARG:HD3	2.16	0.45
1:C:270:HIS:CE1	1:C:491:GLU:HG3	2.51	0.45
1:C:2724:TYR:HB2	1:C:2895:PHE:CE2	2.51	0.45
1:C:4162:LYS:HD3	1:C:4162:LYS:HA	1.58	0.45
1:C:4965:GLN:OE1	1:C:4965:GLN:N	2.49	0.45
1:D:35:LEU:HD23	1:D:51:SER:HA	1.98	0.45
1:D:157:ALA:HA	1:D:187:SER:HB3	1.98	0.45
1:D:2431:ASP:O	1:D:2435:VAL:HG23	2.16	0.45
1:D:2642:ARG:HH12	1:D:2921:PHE:HA	1.81	0.45
1:D:2758:LYS:HZ1	1:D:2764:SER:N	2.13	0.45
1:D:3793:LEU:O	1:D:3797:MET:HG3	2.15	0.45
1:D:4563:GLU:CG	1:D:4566:GLY:H	2.29	0.45
1:D:4887:LYS:HE3	1:D:4887:LYS:HB2	1.58	0.45
1:A:235:ARG:HE	1:A:274:LEU:HD23	1.81	0.45
1:A:476:GLN:HB3	1:A:480:ARG:NH1	2.30	0.45
1:A:4641:PRO:HG2	1:A:4646:ASP:O	2.15	0.45
1:B:59:PRO:HG3	1:B:296:ARG:CZ	2.47	0.45
1:B:765:SER:HA	1:B:779:PHE:O	2.16	0.45
1:C:476:GLN:HB3	1:C:480:ARG:NH1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:765:SER:HA	1:C:779:PHE:O	2.16	0.45
1:C:1020:ILE:C	1:C:1030:PRO:HB3	2.36	0.45
1:C:1975:MET:HB3	1:C:1975:MET:HE3	1.73	0.45
1:C:2623:LEU:HG	1:C:2625:GLY:H	1.81	0.45
1:C:2694:SER:HA	1:C:2702:ASN:HB3	1.98	0.45
1:C:2830:ASN:ND2	1:D:1435:GLY:HA3	2.32	0.45
1:C:2975:PHE:CE2	1:C:3036:LEU:HD11	2.52	0.45
1:C:4641:PRO:HG2	1:C:4646:ASP:O	2.15	0.45
1:D:2723:LYS:HD3	1:D:2899:ASN:ND2	2.31	0.45
1:D:3830:LEU:HB3	1:D:3833:ASP:OD2	2.16	0.45
1:A:35:LEU:HD23	1:A:51:SER:HA	1.98	0.45
1:A:456:LEU:O	1:A:460:ILE:HG12	2.17	0.45
1:A:514:PHE:CD2	1:A:526:TRP:HB2	2.52	0.45
1:A:1849:SER:O	1:A:2054:LYS:NZ	2.34	0.45
1:A:1944:TYR:CZ	1:A:3604:ARG:HD2	2.52	0.45
1:A:2846:GLU:HB3	1:A:2874:TYR:CD2	2.52	0.45
1:A:4159:GLN:O	1:A:4162:LYS:HB2	2.16	0.45
1:A:4743:LEU:O	1:A:4746:ILE:HG12	2.16	0.45
1:B:235:ARG:HE	1:B:274:LEU:HD23	1.81	0.45
1:B:912:LYS:HZ3	1:B:914:GLN:HG3	1.82	0.45
1:B:2619:LYS:HB3	1:B:2627:TRP:CH2	2.52	0.45
1:B:2692:GLN:HA	1:B:2695:MET:HG3	1.97	0.45
1:B:2975:PHE:CE2	1:B:3036:LEU:HD11	2.52	0.45
1:C:948:CYS:SG	1:C:1064:LEU:HD13	2.57	0.45
1:C:1415:ASP:OD2	1:C:1559:ARG:NH2	2.43	0.45
1:C:2758:LYS:HZ1	1:C:2764:SER:N	2.15	0.45
1:C:2846:GLU:HB3	1:C:2874:TYR:HD2	1.80	0.45
1:C:2999:LYS:O	1:C:3002:GLU:HG3	2.17	0.45
1:C:4563:GLU:CG	1:C:4566:GLY:H	2.29	0.45
1:D:1911:GLN:OE1	1:D:2090:ARG:NH1	2.50	0.45
1:D:4641:PRO:HG2	1:D:4646:ASP:O	2.16	0.45
1:D:4747:ALA:HB1	1:D:4757:LEU:HD11	1.99	0.45
1:A:2290:TRP:CZ3	1:A:2292:PRO:HB3	2.51	0.45
1:A:4886:THR:O	1:A:4895:ASN:HB3	2.17	0.45
1:B:2846:GLU:HB3	1:B:2874:TYR:CD2	2.52	0.45
1:B:2926:LEU:HD11	1:B:3003:MET:SD	2.56	0.45
1:C:514:PHE:CD2	1:C:526:TRP:HB2	2.52	0.45
1:C:785:ASP:OD2	1:C:785:ASP:N	2.46	0.45
1:C:931:TYR:O	1:C:935:MET:HG2	2.17	0.45
1:C:2129:LEU:HB3	1:C:2142:MET:HE3	1.99	0.45
1:C:2833:LEU:HD11	1:C:2837:LEU:HD23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4814:MET:CE	1:D:4844:ILE:HD13	2.46	0.45
1:D:456:LEU:O	1:D:460:ILE:HG12	2.17	0.45
1:D:829:LYS:NZ	1:D:1037:LEU:HD23	2.31	0.45
1:D:1979:PHE:CE1	1:D:1988:CYS:HB3	2.52	0.45
1:D:2614:TYR:CD2	1:D:2672:VAL:HG22	2.51	0.45
1:D:3622:GLN:HB3	1:D:3626:LYS:NZ	2.30	0.45
1:D:4079:ASP:O	1:D:4082:GLU:HG3	2.17	0.45
1:A:2975:PHE:CE2	1:A:3036:LEU:HD11	2.52	0.45
1:A:3090:VAL:HA	1:A:3093:ILE:HG22	1.98	0.45
1:A:4079:ASP:O	1:A:4082:GLU:HG3	2.17	0.45
1:B:2623:LEU:HG	1:B:2625:GLY:H	1.81	0.45
1:B:2694:SER:HA	1:B:2702:ASN:HB3	1.98	0.45
1:B:4079:ASP:O	1:B:4082:GLU:HG3	2.17	0.45
1:C:35:LEU:HD23	1:C:51:SER:HA	1.98	0.45
1:C:1144:ARG:HH22	1:C:1184:ASP:CG	2.19	0.45
1:C:1561:LYS:HE3	1:C:1562:ASN:OD1	2.17	0.45
1:C:2555:LEU:O	1:C:2561:LEU:HD11	2.17	0.45
1:C:2954:PHE:O	1:C:2957:GLU:HG3	2.17	0.45
1:D:1561:LYS:HE3	1:D:1562:ASN:OD1	2.17	0.45
1:D:2555:LEU:O	1:D:2561:LEU:HD11	2.16	0.45
1:D:2857:LYS:O	1:D:2861:GLU:OE1	2.35	0.45
1:D:3017:HIS:O	1:D:3018:ARG:HD3	2.16	0.45
1:D:4159:GLN:O	1:D:4162:LYS:HB2	2.16	0.45
1:A:1000:ALA:HB2	1:A:1050:LEU:HD12	1.99	0.45
1:B:472:HIS:O	1:B:475:LYS:HB2	2.17	0.45
1:C:2623:LEU:HD12	1:C:2624:PRO:HD2	1.99	0.45
1:C:2642:ARG:HH12	1:C:2921:PHE:HA	1.82	0.45
1:C:4079:ASP:O	1:C:4082:GLU:HG3	2.17	0.45
1:C:4898:PHE:O	1:C:4904:GLY:HA3	2.17	0.45
1:D:472:HIS:O	1:D:475:LYS:HB2	2.17	0.45
1:D:514:PHE:CD2	1:D:526:TRP:HB2	2.52	0.45
1:D:2878:THR:O	1:D:2882:LYS:HG3	2.17	0.45
1:D:2885:ASP:HB2	1:D:2888:LYS:HE3	1.99	0.45
1:A:1144:ARG:HH22	1:A:1184:ASP:CG	2.20	0.45
1:A:1931:ASP:OD1	1:A:1932:PHE:N	2.50	0.45
1:A:2555:LEU:O	1:A:2561:LEU:HD11	2.17	0.45
1:A:2623:LEU:HD12	1:A:2624:PRO:HD2	1.99	0.45
1:A:4747:ALA:HB1	1:A:4757:LEU:HD11	1.99	0.45
1:B:174:LYS:HB2	1:B:176:ARG:NH2	2.32	0.45
1:B:1931:ASP:OD1	1:B:1932:PHE:N	2.50	0.45
1:B:2758:LYS:HA	1:B:2759:PRO:HD3	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2999:LYS:O	1:B:3002:GLU:HG3	2.17	0.45
1:B:4886:THR:O	1:B:4895:ASN:HB3	2.17	0.45
1:C:182:ILE:HD12	1:C:191:TYR:HE1	1.80	0.45
1:C:1266:GLU:OE2	1:C:1267:HIS:ND1	2.44	0.45
1:C:2878:THR:O	1:C:2882:LYS:HG3	2.17	0.45
1:C:3067:ASP:HA	1:C:3070:LYS:HE3	1.98	0.45
1:D:2331:PHE:HB3	1:D:2335:LEU:HB2	1.99	0.45
1:D:2623:LEU:HG	1:D:2625:GLY:H	1.81	0.45
1:D:2954:PHE:O	1:D:2957:GLU:HG3	2.17	0.45
1:D:2999:LYS:O	1:D:3002:GLU:HG3	2.17	0.45
1:D:4565:SER:HB2	1:D:4567:TYR:CD1	2.52	0.45
1:A:894:VAL:HA	1:A:897:LYS:HZ3	1.82	0.45
1:A:2623:LEU:HG	1:A:2625:GLY:H	1.81	0.45
1:A:3811:GLN:HG2	1:A:3825:SER:HB2	1.99	0.45
1:B:1079:SER:OG	1:B:1084:ARG:NH2	2.43	0.45
1:B:2555:LEU:O	1:B:2561:LEU:HD11	2.17	0.45
1:B:2839:ALA:O	1:B:2842:GLU:HG3	2.17	0.45
1:B:4156:SER:HB3	1:B:4920:PHE:CE1	2.52	0.45
1:B:4743:LEU:O	1:B:4746:ILE:HG12	2.16	0.45
1:C:456:LEU:O	1:C:460:ILE:HG12	2.17	0.45
1:C:829:LYS:NZ	1:C:1037:LEU:HD23	2.31	0.45
1:C:1000:ALA:HB2	1:C:1050:LEU:HD12	1.99	0.45
1:C:2885:ASP:HB2	1:C:2888:LYS:HE3	1.99	0.45
1:D:174:LYS:HB2	1:D:176:ARG:NH2	2.32	0.45
1:D:1000:ALA:HB2	1:D:1050:LEU:HD12	1.99	0.45
1:D:1944:TYR:CZ	1:D:3604:ARG:HD2	2.51	0.45
1:D:4882:GLU:OE1	1:D:4886:THR:OG1	2.35	0.45
1:D:4886:THR:O	1:D:4895:ASN:HB3	2.17	0.45
1:A:69:LEU:HD22	1:A:119:ILE:HG12	1.97	0.44
1:A:355:LYS:O	1:A:359:SER:OG	2.26	0.44
1:A:948:CYS:SG	1:A:1064:LEU:HD13	2.57	0.44
1:A:1179:GLY:HA3	1:A:1229:ILE:HD11	1.98	0.44
1:A:2286:PRO:HG3	1:A:2359:ARG:HA	1.99	0.44
1:A:2839:ALA:O	1:A:2842:GLU:HG3	2.17	0.44
1:A:2999:LYS:O	1:A:3002:GLU:HG3	2.17	0.44
1:B:456:LEU:O	1:B:460:ILE:HG12	2.17	0.44
1:B:1144:ARG:HH22	1:B:1184:ASP:CG	2.19	0.44
1:B:2592:LEU:CD1	1:B:2609:LEU:HD21	2.47	0.44
1:B:2768:LYS:O	1:B:2772:ARG:N	2.36	0.44
1:B:2833:LEU:HD11	1:B:2837:LEU:HD23	1.98	0.44
1:B:2878:THR:O	1:B:2882:LYS:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2933:VAL:HG12	1:B:3010:LYS:HZ2	1.82	0.44
1:B:2954:PHE:O	1:B:2957:GLU:HG3	2.17	0.44
1:C:2286:PRO:HG3	1:C:2359:ARG:HA	1.99	0.44
1:C:2933:VAL:HG12	1:C:3010:LYS:HZ2	1.82	0.44
1:D:1897:LYS:O	1:D:1897:LYS:HD3	2.15	0.44
1:D:2592:LEU:CD1	1:D:2609:LEU:HD21	2.48	0.44
1:D:2623:LEU:HD12	1:D:2624:PRO:HD2	1.99	0.44
1:D:2716:LYS:HB3	1:D:2901:TYR:OH	2.15	0.44
1:A:441:LYS:HZ2	1:A:443:SER:HG	1.55	0.44
1:A:867:VAL:HG12	1:A:1002:ASN:HD21	1.82	0.44
1:A:1020:ILE:C	1:A:1030:PRO:HB3	2.36	0.44
1:A:2614:TYR:CD2	1:A:2672:VAL:HG22	2.51	0.44
1:A:3975:GLN:O	1:A:3979:VAL:HG23	2.16	0.44
1:A:4565:SER:HB2	1:A:4567:TYR:CD1	2.52	0.44
1:A:4708:TRP:O	1:A:4712:VAL:HG23	2.18	0.44
1:A:4882:GLU:OE1	1:A:4886:THR:OG1	2.35	0.44
1:B:655:MET:HE2	1:B:655:MET:HA	1.98	0.44
1:B:2623:LEU:HD12	1:B:2624:PRO:HD2	1.99	0.44
1:B:4046:ARG:NE	1:B:4046:ARG:HA	2.33	0.44
1:C:2331:PHE:HB3	1:C:2335:LEU:HB2	2.00	0.44
1:C:2787:TRP:HE1	1:C:2903:VAL:CG2	2.30	0.44
1:C:2972:ASP:HB2	1:C:3032:CYS:SG	2.57	0.44
1:C:3811:GLN:HG2	1:C:3825:SER:HB2	1.99	0.44
1:D:1564:MET:CE	1:D:1565:PRO:HD2	2.47	0.44
1:D:2434:GLY:O	1:D:2438:ILE:HG13	2.17	0.44
1:D:2846:GLU:HB3	1:D:2874:TYR:CD2	2.52	0.44
1:D:2972:ASP:HB2	1:D:3032:CYS:SG	2.57	0.44
1:D:3975:GLN:O	1:D:3979:VAL:HG23	2.16	0.44
1:D:3994:THR:O	1:D:3998:GLN:HG3	2.18	0.44
1:A:912:LYS:HZ3	1:A:914:GLN:HG3	1.82	0.44
1:A:1011:ARG:HA	1:A:1011:ARG:HD3	1.80	0.44
1:A:1118:SER:HA	1:A:1134:ALA:HA	1.98	0.44
1:A:1592:SER:OG	1:A:1594:VAL:HG12	2.18	0.44
1:A:2619:LYS:HB3	1:A:2627:TRP:CH2	2.52	0.44
1:A:2720:PHE:HE1	1:A:2895:PHE:CE2	2.36	0.44
1:B:948:CYS:SG	1:B:1064:LEU:HD13	2.57	0.44
1:B:1118:SER:HA	1:B:1134:ALA:HA	1.98	0.44
1:B:1592:SER:OG	1:B:1594:VAL:HG12	2.18	0.44
1:B:4708:TRP:O	1:B:4712:VAL:HG23	2.18	0.44
1:C:1179:GLY:HA3	1:C:1229:ILE:HD11	1.98	0.44
1:C:1931:ASP:OD1	1:C:1932:PHE:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2592:LEU:CD1	1:C:2609:LEU:HD21	2.47	0.44
1:C:2620:TYR:OH	1:C:2632:ALA:O	2.34	0.44
1:C:2857:LYS:O	1:C:2861:GLU:OE1	2.35	0.44
1:D:867:VAL:HG12	1:D:1002:ASN:HD21	1.82	0.44
1:D:1592:SER:OG	1:D:1594:VAL:HG12	2.17	0.44
1:D:2694:SER:HA	1:D:2702:ASN:HB3	1.98	0.44
1:D:2833:LEU:HD11	1:D:2837:LEU:HD23	1.97	0.44
1:D:3811:GLN:NE2	1:D:3828:LYS:HB2	2.33	0.44
1:A:655:MET:HA	1:A:655:MET:HE2	2.00	0.44
1:A:1183:LEU:HD23	1:A:1183:LEU:H	1.83	0.44
1:A:1561:LYS:HE3	1:A:1562:ASN:OD1	2.17	0.44
1:A:3017:HIS:O	1:A:3018:ARG:HD3	2.16	0.44
1:B:983:LEU:CD1	1:B:1055:ARG:HB3	2.45	0.44
1:B:1016:TRP:HE1	1:B:1029:ASN:ND2	2.16	0.44
1:B:1183:LEU:HD23	1:B:1183:LEU:H	1.83	0.44
1:B:4898:PHE:O	1:B:4904:GLY:HA3	2.17	0.44
1:C:472:HIS:O	1:C:475:LYS:HB2	2.17	0.44
1:C:678:MET:SD	1:C:754:VAL:HG22	2.58	0.44
1:C:1118:SER:HA	1:C:1134:ALA:HA	1.98	0.44
1:C:1592:SER:OG	1:C:1594:VAL:HG12	2.18	0.44
1:C:1944:TYR:CZ	1:C:3604:ARG:HD2	2.52	0.44
1:C:2619:LYS:HB3	1:C:2627:TRP:CH2	2.52	0.44
1:C:2839:ALA:O	1:C:2842:GLU:HG3	2.17	0.44
1:C:3811:GLN:NE2	1:C:3828:LYS:HB2	2.33	0.44
1:D:912:LYS:HZ3	1:D:914:GLN:HG3	1.82	0.44
1:D:1896:MET:HB3	1:D:1898:LEU:CD1	2.48	0.44
1:D:2619:LYS:HB3	1:D:2627:TRP:CH2	2.52	0.44
1:D:2727:HIS:CG	1:D:2731:LYS:HZ3	2.36	0.44
1:D:2747:TYR:CD1	1:D:2755:PRO:HD3	2.53	0.44
1:A:174:LYS:HB2	1:A:176:ARG:NH2	2.32	0.44
1:A:931:TYR:O	1:A:935:MET:HG2	2.17	0.44
1:A:1144:ARG:HH21	1:A:1152:TYR:HB2	1.82	0.44
1:A:2331:PHE:HB3	1:A:2335:LEU:HB2	1.99	0.44
1:A:2878:THR:O	1:A:2882:LYS:HG3	2.17	0.44
1:A:3954:MET:HB3	1:A:3971:LEU:HD21	2.00	0.44
1:B:678:MET:SD	1:B:754:VAL:HG22	2.58	0.44
1:B:1561:LYS:HE3	1:B:1562:ASN:OD1	2.17	0.44
1:B:2703:PRO:HD3	1:B:2857:LYS:HE3	2.00	0.44
1:B:2972:ASP:HB2	1:B:3032:CYS:SG	2.57	0.44
1:B:4565:SER:HB2	1:B:4567:TYR:CD1	2.52	0.44
1:C:1144:ARG:HH21	1:C:1152:TYR:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1979:PHE:CE1	1:C:1988:CYS:HB3	2.52	0.44
1:C:2747:TYR:CD1	1:C:2755:PRO:HD3	2.53	0.44
1:C:3954:MET:HB3	1:C:3971:LEU:HD21	2.00	0.44
1:A:505:LEU:HD23	1:A:505:LEU:HA	1.85	0.44
1:A:1016:TRP:HE1	1:A:1029:ASN:ND2	2.16	0.44
1:A:3811:GLN:NE2	1:A:3828:LYS:HB2	2.33	0.44
1:A:4156:SER:HB3	1:A:4920:PHE:CE1	2.52	0.44
1:B:1979:PHE:CE1	1:B:1988:CYS:HB3	2.52	0.44
1:B:2434:GLY:O	1:B:2438:ILE:HG13	2.17	0.44
1:B:3994:THR:O	1:B:3998:GLN:HG3	2.17	0.44
1:C:1125:ASP:OD1	1:C:1126:GLN:N	2.51	0.44
1:D:678:MET:SD	1:D:754:VAL:HG22	2.58	0.44
1:D:948:CYS:SG	1:D:1064:LEU:HD13	2.57	0.44
1:D:1975:MET:HE3	1:D:1975:MET:HB3	1.73	0.44
1:D:2720:PHE:HE1	1:D:2895:PHE:CE2	2.36	0.44
1:D:2975:PHE:CE2	1:D:3036:LEU:HD11	2.52	0.44
1:D:3954:MET:HB3	1:D:3971:LEU:HD21	2.00	0.44
1:A:921:PHE:HA	1:A:924:LEU:HG	2.00	0.44
1:A:2885:ASP:HB2	1:A:2888:LYS:HE3	1.99	0.44
1:A:4903:HIS:N	1:B:4183:LYS:HZ2	2.16	0.44
2:E:51:ILE:O	2:E:53:LYS:NZ	2.36	0.44
1:B:514:PHE:CD2	1:B:526:TRP:HB2	2.52	0.44
1:B:931:TYR:O	1:B:935:MET:HG2	2.17	0.44
1:B:3965:ILE:HG22	1:B:3969:LYS:HZ3	1.81	0.44
1:B:4003:LEU:HD22	1:B:4010:VAL:HG21	2.00	0.44
1:B:4747:ALA:HB1	1:B:4757:LEU:HD11	1.98	0.44
1:C:1989:PRO:O	1:C:1993:ARG:HG3	2.18	0.44
1:C:2846:GLU:HB3	1:C:2874:TYR:CD2	2.52	0.44
1:D:1016:TRP:HE1	1:D:1029:ASN:ND2	2.16	0.44
1:D:3811:GLN:HG2	1:D:3825:SER:HB2	1.99	0.44
1:D:4048:PHE:O	1:D:4052:MET:HG2	2.18	0.44
1:A:760:ASP:HB3	1:A:765:SER:OG	2.18	0.44
1:A:862:PHE:CD1	1:A:1034:PRO:HG3	2.53	0.44
1:A:1979:PHE:CE1	1:A:1988:CYS:HB3	2.52	0.44
1:A:2972:ASP:HB2	1:A:3032:CYS:SG	2.57	0.44
1:A:4003:LEU:HD22	1:A:4010:VAL:HG21	2.00	0.44
2:G:106:ASN:OD1	2:G:107:LEU:N	2.51	0.44
1:B:760:ASP:HB3	1:B:765:SER:OG	2.18	0.44
1:B:964:MET:HB2	1:B:979:ALA:HB1	2.00	0.44
1:B:1437:GLU:HA	1:B:1438:PRO:HD3	1.82	0.44
1:B:1979:PHE:HB2	1:B:3628:TRP:HZ2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1989:PRO:O	1:B:1993:ARG:HG3	2.18	0.44
1:B:2286:PRO:HG3	1:B:2359:ARG:HA	1.99	0.44
1:B:2303:ARG:HE	1:B:2401:ARG:NE	2.16	0.44
1:B:2758:LYS:NZ	1:B:2762:LEU:O	2.36	0.44
1:B:2787:TRP:HE1	1:B:2903:VAL:CG2	2.30	0.44
1:B:3811:GLN:NE2	1:B:3828:LYS:HB2	2.33	0.44
1:C:1979:PHE:HB2	1:C:3628:TRP:HZ2	1.83	0.44
1:C:4003:LEU:HD22	1:C:4010:VAL:HG21	2.00	0.44
1:C:4044:SER:HA	1:C:4077:THR:HA	2.00	0.44
1:D:760:ASP:HB3	1:D:765:SER:OG	2.18	0.44
1:D:2593:VAL:HG12	1:D:2644:LEU:HB2	2.00	0.44
1:D:4107:GLU:OE1	1:D:4149:TYR:OH	2.24	0.44
1:A:1564:MET:CE	1:A:1565:PRO:HD2	2.47	0.44
1:A:1914:CYS:O	1:A:1918:VAL:HG23	2.18	0.44
1:A:2215:PHE:CG	1:A:2253:LEU:HD22	2.53	0.44
1:A:2592:LEU:CD1	1:A:2609:LEU:HD21	2.47	0.44
1:B:1956:ALA:O	1:B:1959:ALA:HB3	2.18	0.44
1:B:2720:PHE:HE1	1:B:2895:PHE:CE2	2.36	0.44
1:B:3954:MET:HB3	1:B:3971:LEU:HD21	2.00	0.44
1:C:174:LYS:HB2	1:C:176:ARG:NH2	2.32	0.44
1:C:527:LYS:HE2	1:C:527:LYS:HB2	1.82	0.44
1:C:1057:LEU:HD11	1:C:1064:LEU:HD23	2.00	0.44
1:C:1896:MET:HB3	1:C:1898:LEU:CD1	2.48	0.44
1:C:2720:PHE:HE1	1:C:2895:PHE:CE2	2.36	0.44
1:C:4173:ILE:O	1:C:4177:VAL:HG22	2.18	0.44
1:C:4886:THR:O	1:C:4895:ASN:HB3	2.17	0.44
1:D:862:PHE:CD1	1:D:1034:PRO:HG3	2.53	0.44
1:D:1144:ARG:HH21	1:D:1152:TYR:HB2	1.82	0.44
1:D:2286:PRO:HG3	1:D:2359:ARG:HA	1.99	0.44
1:D:2787:TRP:HE1	1:D:2903:VAL:CG2	2.30	0.44
1:D:4203:ALA:HA	1:D:4206:ILE:HG12	2.00	0.44
1:A:765:SER:HB2	1:A:778:MET:HE1	2.00	0.43
1:A:1979:PHE:HB2	1:A:3628:TRP:HZ2	1.83	0.43
1:A:1992:ILE:HA	1:A:1995:GLN:OE1	2.19	0.43
1:A:2593:VAL:HG12	1:A:2644:LEU:HB2	2.00	0.43
1:A:4046:ARG:NE	1:A:4046:ARG:HA	2.32	0.43
1:B:921:PHE:HA	1:B:924:LEU:HG	2.00	0.43
1:B:998:LYS:HB2	1:B:998:LYS:HE2	1.86	0.43
1:B:2720:PHE:CD2	1:B:2901:TYR:CE2	3.06	0.43
1:C:3803:LEU:HB2	1:C:3884:SER:HB2	2.00	0.43
1:C:3994:THR:O	1:C:3998:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4708:TRP:O	1:C:4712:VAL:HG23	2.18	0.43
1:D:921:PHE:HA	1:D:924:LEU:HG	2.00	0.43
1:D:1057:LEU:HD11	1:D:1064:LEU:HD23	2.00	0.43
1:D:1979:PHE:HB2	1:D:3628:TRP:HZ2	1.83	0.43
1:D:2215:PHE:CG	1:D:2253:LEU:HD22	2.53	0.43
1:D:2397:ASP:O	1:D:2401:ARG:HG3	2.18	0.43
1:A:537:LEU:O	1:A:541:ILE:HG12	2.18	0.43
1:A:1125:ASP:OD1	1:A:1126:GLN:N	2.51	0.43
1:A:2703:PRO:HD3	1:A:2857:LYS:HE3	2.00	0.43
1:A:2857:LYS:O	1:A:2861:GLU:OE1	2.35	0.43
2:H:106:ASN:OD1	2:H:107:LEU:N	2.51	0.43
1:B:1089:ARG:O	1:B:1250:TRP:N	2.46	0.43
1:B:2303:ARG:HG2	1:B:2401:ARG:HD2	2.01	0.43
1:B:2747:TYR:CD1	1:B:2755:PRO:HD3	2.53	0.43
1:C:281:ARG:NH1	1:C:284:TRP:O	2.51	0.43
1:C:468:GLU:C	1:C:475:LYS:HZ1	2.20	0.43
1:C:1016:TRP:HE1	1:C:1029:ASN:ND2	2.16	0.43
1:C:1089:ARG:O	1:C:1250:TRP:N	2.46	0.43
1:C:1183:LEU:HD23	1:C:1183:LEU:H	1.83	0.43
1:C:2678:PRO:O	1:C:2922:ALA:N	2.42	0.43
1:D:1125:ASP:OD1	1:D:1126:GLN:N	2.51	0.43
1:D:1962:THR:HA	1:D:1965:PHE:CD2	2.48	0.43
1:D:4708:TRP:O	1:D:4712:VAL:HG23	2.18	0.43
1:D:4735:ASN:HB3	1:D:4738:PHE:HD2	1.83	0.43
1:A:70:GLU:HG2	1:A:71:GLN:CD	2.39	0.43
1:A:468:GLU:HA	1:A:475:LYS:HE3	2.01	0.43
1:A:562:LEU:HG	1:A:600:LEU:HD13	2.00	0.43
1:A:695:VAL:HG11	1:A:755:ILE:HG21	2.00	0.43
1:A:1415:ASP:OD2	1:A:1559:ARG:NH2	2.43	0.43
1:A:2954:PHE:O	1:A:2957:GLU:HG3	2.17	0.43
1:A:4292:MET:HA	1:A:4292:MET:CE	2.48	0.43
1:B:1125:ASP:OD1	1:B:1126:GLN:N	2.51	0.43
1:B:2734:MET:SD	1:B:2825:ALA:HB2	2.59	0.43
1:B:2833:LEU:HD11	1:B:2837:LEU:CD2	2.49	0.43
1:B:4173:ILE:O	1:B:4177:VAL:HG22	2.18	0.43
1:B:4292:MET:HA	1:B:4292:MET:CE	2.49	0.43
1:C:862:PHE:CD1	1:C:1034:PRO:HG3	2.53	0.43
1:C:921:PHE:HA	1:C:924:LEU:HG	2.00	0.43
1:C:964:MET:HB2	1:C:979:ALA:HB1	2.00	0.43
1:C:2215:PHE:CG	1:C:2253:LEU:HD22	2.53	0.43
1:C:4156:SER:HB3	1:C:4920:PHE:CE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:931:TYR:O	1:D:935:MET:HG2	2.17	0.43
1:D:1931:ASP:OD1	1:D:1932:PHE:N	2.50	0.43
1:D:1956:ALA:O	1:D:1959:ALA:HB3	2.18	0.43
1:D:2890:GLN:OE1	1:D:2890:GLN:HA	2.18	0.43
1:D:4044:SER:HA	1:D:4077:THR:HA	2.00	0.43
1:D:4156:SER:HB3	1:D:4920:PHE:CE1	2.52	0.43
1:A:472:HIS:O	1:A:475:LYS:HB2	2.17	0.43
1:A:874:LEU:HG	1:A:878:LEU:HB2	2.01	0.43
1:A:964:MET:HB2	1:A:979:ALA:HB1	2.00	0.43
1:A:1538:LYS:HD2	1:A:1636:ASN:ND2	2.33	0.43
1:A:1649:GLU:HG2	1:A:1650:LEU:N	2.34	0.43
1:A:2258:ARG:HB3	1:A:2260:PRO:HD2	2.00	0.43
1:A:2303:ARG:HE	1:A:2401:ARG:NE	2.16	0.43
1:A:2890:GLN:OE1	1:A:2890:GLN:HA	2.18	0.43
1:A:3803:LEU:HB2	1:A:3884:SER:HB2	2.00	0.43
2:F:106:ASN:OD1	2:F:107:LEU:N	2.51	0.43
1:B:874:LEU:HG	1:B:878:LEU:HB2	2.01	0.43
1:B:1057:LEU:HD11	1:B:1064:LEU:HD23	2.00	0.43
1:B:1144:ARG:HH21	1:B:1152:TYR:HB2	1.82	0.43
1:B:1896:MET:HB3	1:B:1898:LEU:CD1	2.48	0.43
1:B:2331:PHE:HB3	1:B:2335:LEU:HB2	2.00	0.43
1:B:2846:GLU:HA	1:B:2874:TYR:CD2	2.53	0.43
1:B:2885:ASP:HB2	1:B:2888:LYS:HE3	1.99	0.43
1:B:2890:GLN:OE1	1:B:2890:GLN:HA	2.18	0.43
1:B:3803:LEU:HB2	1:B:3884:SER:HB2	2.00	0.43
1:B:3893:SER:OG	1:C:80:GLU:OE2	2.36	0.43
1:C:1649:GLU:HG2	1:C:1650:LEU:N	2.34	0.43
1:C:2545:ILE:HD11	1:C:2580:LEU:HD22	2.00	0.43
1:C:2833:LEU:HD11	1:C:2837:LEU:CD2	2.48	0.43
1:C:2890:GLN:OE1	1:C:2890:GLN:HA	2.18	0.43
1:C:4046:ARG:HA	1:C:4046:ARG:NE	2.33	0.43
1:C:4048:PHE:O	1:C:4052:MET:HG2	2.18	0.43
1:C:4774:LEU:O	1:C:4778:VAL:HG23	2.19	0.43
1:D:537:LEU:O	1:D:541:ILE:HG12	2.18	0.43
1:D:1183:LEU:HD23	1:D:1183:LEU:H	1.83	0.43
1:D:1437:GLU:HA	1:D:1438:PRO:HD3	1.82	0.43
1:D:2846:GLU:HA	1:D:2874:TYR:CD2	2.53	0.43
1:D:4162:LYS:HD3	1:D:4162:LYS:HA	1.58	0.43
1:A:2303:ARG:HG2	1:A:2401:ARG:HD2	2.01	0.43
1:A:2734:MET:SD	1:A:2825:ALA:HB2	2.59	0.43
1:A:2933:VAL:HG12	1:A:3010:LYS:HZ2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3903:GLN:HE21	1:A:3964:GLN:HE21	1.67	0.43
1:B:70:GLU:HG2	1:B:71:GLN:CD	2.39	0.43
1:B:867:VAL:HG12	1:B:1002:ASN:HD21	1.82	0.43
1:B:1649:GLU:HG2	1:B:1650:LEU:N	2.33	0.43
1:B:2724:TYR:HB2	1:B:2895:PHE:HE2	1.84	0.43
1:B:3088:LYS:HG3	1:B:3090:VAL:HG12	2.01	0.43
1:B:3811:GLN:HG2	1:B:3825:SER:HB2	1.99	0.43
1:C:114:LEU:HD11	1:C:172:GLY:O	2.19	0.43
1:C:468:GLU:HA	1:C:475:LYS:HE3	2.01	0.43
1:C:4048:PHE:CD2	1:C:4078:LEU:HD21	2.54	0.43
1:C:4735:ASN:HB3	1:C:4738:PHE:HD2	1.83	0.43
1:D:70:GLU:HG2	1:D:71:GLN:CD	2.38	0.43
1:D:695:VAL:HG11	1:D:755:ILE:HG21	2.00	0.43
1:D:2589:LEU:O	1:D:2593:VAL:HG13	2.19	0.43
1:D:2839:ALA:O	1:D:2842:GLU:HG3	2.17	0.43
1:D:4046:ARG:NE	1:D:4046:ARG:HA	2.33	0.43
1:A:281:ARG:NH1	1:A:284:TRP:O	2.51	0.43
1:A:678:MET:SD	1:A:754:VAL:HG22	2.58	0.43
1:A:2724:TYR:HB2	1:A:2895:PHE:HE2	1.84	0.43
1:A:2846:GLU:HA	1:A:2874:TYR:CD2	2.53	0.43
1:A:3088:LYS:HG3	1:A:3090:VAL:HG12	2.01	0.43
1:A:3994:THR:O	1:A:3998:GLN:HG3	2.18	0.43
1:A:4203:ALA:HA	1:A:4206:ILE:HG12	2.00	0.43
1:A:4707:MET:HG3	1:D:4252:ILE:CG2	2.48	0.43
1:B:44:ASN:HD21	1:B:46:LEU:HB2	1.84	0.43
1:B:468:GLU:HA	1:B:475:LYS:HE3	2.01	0.43
1:B:1266:GLU:OE2	1:B:1267:HIS:ND1	2.44	0.43
1:B:1689:ILE:HG23	1:B:1703:TYR:CZ	2.54	0.43
1:B:2619:LYS:NZ	1:B:2623:LEU:HD22	2.34	0.43
1:B:3805:LEU:HD23	1:C:76:ARG:NH2	2.33	0.43
1:B:3903:GLN:HE21	1:B:3964:GLN:HE21	1.67	0.43
1:B:4621:PRO:HD2	1:B:4632:ARG:HH22	1.84	0.43
1:C:233:VAL:HG12	1:C:274:LEU:HD22	2.01	0.43
1:C:874:LEU:HG	1:C:878:LEU:HB2	2.01	0.43
1:C:883:GLU:OE2	1:C:929:ARG:NH2	2.51	0.43
1:C:1310:CYS:HB2	1:C:1537:THR:H	1.84	0.43
1:C:2589:LEU:O	1:C:2593:VAL:HG13	2.19	0.43
1:D:44:ASN:HD21	1:D:46:LEU:HB2	1.84	0.43
1:D:1989:PRO:O	1:D:1993:ARG:HG3	2.18	0.43
1:D:2143:ILE:HG13	1:D:2192:MET:HE1	2.00	0.43
1:D:2254:ALA:O	1:D:2316:ASN:ND2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2303:ARG:HE	1:D:2401:ARG:NE	2.16	0.43
1:D:2724:TYR:HB2	1:D:2895:PHE:HE2	1.84	0.43
1:D:2833:LEU:HD11	1:D:2837:LEU:CD2	2.49	0.43
1:D:3803:LEU:HB2	1:D:3884:SER:HB2	2.00	0.43
1:A:70:GLU:HG2	1:A:71:GLN:NE2	2.34	0.43
1:A:2397:ASP:O	1:A:2401:ARG:HG3	2.18	0.43
1:A:2684:ASN:OD1	1:A:2919:LYS:NZ	2.45	0.43
1:A:4621:PRO:HD2	1:A:4632:ARG:HH22	1.84	0.43
1:B:233:VAL:HG12	1:B:274:LEU:HD22	2.01	0.43
1:B:883:GLU:OE2	1:B:929:ARG:NH2	2.51	0.43
1:B:1016:TRP:CE3	1:B:1027:ARG:NH1	2.87	0.43
1:B:1929:SER:O	1:B:1933:VAL:HG12	2.19	0.43
1:B:1992:ILE:HA	1:B:1995:GLN:OE1	2.19	0.43
1:B:4162:LYS:HA	1:B:4162:LYS:HD3	1.58	0.43
1:C:760:ASP:HB3	1:C:765:SER:OG	2.18	0.43
1:C:1016:TRP:CE3	1:C:1027:ARG:NH1	2.87	0.43
1:C:1538:LYS:HD2	1:C:1636:ASN:ND2	2.33	0.43
1:C:1962:THR:HA	1:C:1965:PHE:CD2	2.48	0.43
1:C:2703:PRO:HD3	1:C:2857:LYS:HE3	2.00	0.43
1:C:4061:SER:O	1:C:4064:GLU:HG3	2.19	0.43
1:C:4292:MET:CE	1:C:4292:MET:HA	2.48	0.43
1:C:4621:PRO:HD2	1:C:4632:ARG:HH22	1.84	0.43
1:D:115:TYR:HE1	1:D:181:LEU:HD21	1.84	0.43
1:D:1689:ILE:HG23	1:D:1703:TYR:CZ	2.54	0.43
1:D:1914:CYS:O	1:D:1918:VAL:HG23	2.18	0.43
1:D:4173:ILE:O	1:D:4177:VAL:HG22	2.18	0.43
1:A:2426:LEU:HD23	1:B:143:LEU:HD11	2.00	0.43
1:A:2833:LEU:HD11	1:A:2837:LEU:CD2	2.49	0.43
1:A:4048:PHE:CD2	1:A:4078:LEU:HD21	2.54	0.43
1:A:4048:PHE:O	1:A:4052:MET:HG2	2.18	0.43
1:A:4061:SER:O	1:A:4064:GLU:HG3	2.19	0.43
2:G:83:TYR:OH	1:C:1768:PHE:O	2.30	0.43
1:B:56:LYS:HD3	1:B:324:VAL:HG11	2.01	0.43
1:B:70:GLU:HG2	1:B:71:GLN:NE2	2.34	0.43
1:B:862:PHE:CD1	1:B:1034:PRO:HG3	2.53	0.43
1:B:1000:ALA:HB2	1:B:1050:LEU:HD12	1.99	0.43
1:B:2215:PHE:CG	1:B:2253:LEU:HD22	2.53	0.43
1:B:2251:ASN:HB2	1:B:3819:MET:HE1	2.01	0.43
1:B:2842:GLU:O	1:B:2845:ALA:HB3	2.19	0.43
1:C:44:ASN:HD21	1:C:46:LEU:HB2	1.84	0.43
1:C:1122:CYS:HA	1:C:1133:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2397:ASP:O	1:C:2401:ARG:HG3	2.18	0.43
1:C:4565:SER:HB2	1:C:4567:TYR:CD1	2.52	0.43
1:D:2684:ASN:OD1	1:D:2919:LYS:NZ	2.45	0.43
1:D:4003:LEU:HD22	1:D:4010:VAL:HG21	2.00	0.43
1:A:115:TYR:HE1	1:A:181:LEU:HD21	1.84	0.43
1:A:1112:ASP:OD1	1:A:1208:GLY:HA3	2.19	0.43
1:A:2090:ARG:HE	1:A:2090:ARG:HB3	1.64	0.43
1:A:2956:TYR:HA	1:A:2959:GLU:OE2	2.19	0.43
1:A:4814:MET:HE1	1:B:4844:ILE:HG21	2.01	0.43
1:B:537:LEU:O	1:B:541:ILE:HG12	2.18	0.43
1:B:1564:MET:CE	1:B:1565:PRO:HD2	2.47	0.43
1:B:1975:MET:HB3	1:B:1975:MET:HE3	1.74	0.43
1:B:2397:ASP:O	1:B:2401:ARG:HG3	2.18	0.43
1:B:2545:ILE:HD11	1:B:2580:LEU:HD22	2.00	0.43
1:C:2724:TYR:HB2	1:C:2895:PHE:HE2	1.84	0.43
1:D:637:LEU:HD22	1:D:1679:HIS:CD2	2.54	0.43
1:D:2757:MET:HA	1:D:2820:GLY:HA3	2.01	0.43
1:D:2933:VAL:HG12	1:D:3010:LYS:HZ2	1.84	0.43
1:A:1011:ARG:NH2	4:A:5004:ATP:O1G	2.52	0.43
1:A:2142:MET:HB2	1:A:2192:MET:CE	2.49	0.43
1:A:2720:PHE:CD2	1:A:2901:TYR:CE2	3.06	0.43
1:A:3015:VAL:HG21	1:A:3033:LEU:HD11	2.01	0.43
2:E:106:ASN:OD1	2:E:107:LEU:N	2.51	0.43
1:B:114:LEU:HD11	1:B:172:GLY:O	2.19	0.43
1:B:281:ARG:NH1	1:B:284:TRP:O	2.51	0.43
1:B:506:HIS:HB3	1:B:564:ARG:HH12	1.84	0.43
1:B:1031:ARG:O	1:B:1033:VAL:HG12	2.19	0.43
1:B:4048:PHE:CD2	1:B:4078:LEU:HD21	2.54	0.43
1:B:4061:SER:O	1:B:4064:GLU:HG3	2.19	0.43
1:B:4203:ALA:HA	1:B:4206:ILE:HG12	2.00	0.43
1:B:4774:LEU:O	1:B:4778:VAL:HG23	2.19	0.43
1:B:4882:GLU:OE1	1:B:4886:THR:OG1	2.35	0.43
1:C:70:GLU:HG2	1:C:71:GLN:NE2	2.34	0.43
1:C:562:LEU:HG	1:C:600:LEU:HD13	2.00	0.43
1:C:637:LEU:HD22	1:C:1679:HIS:CD2	2.54	0.43
1:C:867:VAL:HG12	1:C:1002:ASN:HD21	1.82	0.43
1:C:2086:VAL:HG22	1:C:3687:LEU:HD13	2.01	0.43
1:C:2303:ARG:HE	1:C:2401:ARG:NE	2.16	0.43
1:C:2593:VAL:HG12	1:C:2644:LEU:HB2	2.00	0.43
1:C:2720:PHE:CD2	1:C:2901:TYR:CE2	3.06	0.43
1:C:2734:MET:SD	1:C:2825:ALA:HB2	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3892:TYR:HD2	1:C:3906:PHE:HE2	1.67	0.43
1:D:468:GLU:HA	1:D:475:LYS:HE3	2.01	0.43
1:D:964:MET:HB2	1:D:979:ALA:HB1	2.00	0.43
1:D:2258:ARG:HB3	1:D:2260:PRO:HD2	2.00	0.43
1:D:2724:TYR:HA	1:D:2727:HIS:HB3	2.01	0.43
1:D:3015:VAL:HG21	1:D:3033:LEU:HD11	2.01	0.43
1:A:114:LEU:HD11	1:A:172:GLY:O	2.19	0.42
1:A:115:TYR:HB3	1:A:164:PRO:HD3	2.01	0.42
1:A:1689:ILE:HG23	1:A:1703:TYR:CZ	2.54	0.42
1:A:1929:SER:O	1:A:1933:VAL:HG12	2.19	0.42
1:A:1960:ARG:HH21	1:A:1960:ARG:HD2	1.69	0.42
1:A:2747:TYR:CD1	1:A:2755:PRO:HD3	2.53	0.42
1:A:2787:TRP:HE1	1:A:2903:VAL:CG2	2.30	0.42
1:A:4044:SER:HA	1:A:4077:THR:HA	2.00	0.42
1:A:4173:ILE:O	1:A:4177:VAL:HG22	2.18	0.42
1:A:4604:LYS:O	1:A:4608:ARG:HG2	2.20	0.42
1:A:4774:LEU:O	1:A:4778:VAL:HG23	2.19	0.42
1:B:562:LEU:HG	1:B:600:LEU:HD13	2.00	0.42
1:B:801:ARG:HE	1:B:801:ARG:HB2	1.69	0.42
1:B:1310:CYS:HB2	1:B:1537:THR:H	1.84	0.42
1:B:2254:ALA:O	1:B:2316:ASN:ND2	2.52	0.42
1:B:4044:SER:HA	1:B:4077:THR:HA	2.00	0.42
1:C:56:LYS:HD3	1:C:324:VAL:HG11	2.01	0.42
1:C:70:GLU:HG2	1:C:71:GLN:CD	2.38	0.42
1:C:1068:ASP:OD1	1:C:1069:GLN:N	2.52	0.42
1:C:2303:ARG:HG2	1:C:2401:ARG:HD2	2.01	0.42
1:C:3032:CYS:HA	1:C:3035:ILE:HG12	2.01	0.42
1:D:1011:ARG:NH2	4:D:5004:ATP:O1G	2.52	0.42
1:D:1992:ILE:HA	1:D:1995:GLN:OE1	2.19	0.42
1:D:2383:HIS:ND1	1:D:2458:ALA:HB2	2.34	0.42
1:D:2389:MET:HE1	1:D:2460:PHE:HA	2.00	0.42
1:D:2720:PHE:CD2	1:D:2901:TYR:CE2	3.06	0.42
1:D:4292:MET:HA	1:D:4292:MET:CE	2.49	0.42
1:A:227:TYR:CD1	1:A:352:SER:HB3	2.54	0.42
1:A:227:TYR:CG	1:A:352:SER:HB3	2.55	0.42
1:A:637:LEU:HD22	1:A:1679:HIS:CD2	2.54	0.42
1:A:1057:LEU:HD11	1:A:1064:LEU:HD23	2.00	0.42
1:A:1896:MET:HB3	1:A:1898:LEU:CD1	2.48	0.42
1:A:2589:LEU:O	1:A:2593:VAL:HG13	2.19	0.42
1:A:2678:PRO:O	1:A:2922:ALA:N	2.42	0.42
1:A:2727:HIS:CG	1:A:2731:LYS:HZ3	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3639:LYS:HE2	1:A:3639:LYS:HB2	1.92	0.42
1:A:4602:ARG:NH1	1:A:4712:VAL:HG22	2.35	0.42
1:B:892:LEU:HD11	1:B:980:PRO:HG3	2.01	0.42
1:B:1112:ASP:OD1	1:B:1208:GLY:HA3	2.19	0.42
1:B:1538:LYS:HD2	1:B:1636:ASN:ND2	2.33	0.42
1:B:2086:VAL:HG22	1:B:3687:LEU:HD13	2.01	0.42
1:B:2890:GLN:O	1:B:2893:LEU:HG	2.19	0.42
1:B:4604:LYS:O	1:B:4608:ARG:HG2	2.20	0.42
1:C:227:TYR:CD1	1:C:352:SER:HB3	2.54	0.42
1:C:2619:LYS:NZ	1:C:2623:LEU:HD22	2.34	0.42
1:C:2757:MET:HA	1:C:2820:GLY:HA3	2.01	0.42
1:C:2846:GLU:HA	1:C:2874:TYR:CD2	2.53	0.42
1:C:2890:GLN:O	1:C:2893:LEU:HG	2.19	0.42
1:D:70:GLU:HG2	1:D:71:GLN:NE2	2.34	0.42
1:D:114:LEU:HD11	1:D:172:GLY:O	2.19	0.42
1:D:874:LEU:HG	1:D:878:LEU:HB2	2.01	0.42
1:D:883:GLU:OE2	1:D:929:ARG:NH2	2.51	0.42
1:D:1089:ARG:O	1:D:1250:TRP:N	2.46	0.42
1:D:2137:GLU:H	1:D:2137:GLU:CD	2.23	0.42
1:D:2703:PRO:HD3	1:D:2857:LYS:HE3	2.00	0.42
1:D:2956:TYR:HA	1:D:2959:GLU:OE2	2.19	0.42
1:D:3903:GLN:HE21	1:D:3964:GLN:HE21	1.67	0.42
1:A:56:LYS:HD3	1:A:324:VAL:HG11	2.01	0.42
1:A:233:VAL:HG12	1:A:274:LEU:HD22	2.01	0.42
1:A:608:HIS:HB2	1:A:1656:HIS:CD2	2.55	0.42
1:A:972:LEU:HD23	1:A:972:LEU:H	1.84	0.42
1:A:1031:ARG:O	1:A:1033:VAL:HG12	2.19	0.42
1:A:1956:ALA:O	1:A:1959:ALA:HB3	2.18	0.42
1:A:2619:LYS:NZ	1:A:2623:LEU:HD22	2.34	0.42
1:A:2757:MET:HA	1:A:2820:GLY:HA3	2.01	0.42
1:A:4563:GLU:OE1	1:A:4563:GLU:N	2.53	0.42
2:H:91:VAL:HB	2:H:92:ILE:HD12	2.02	0.42
1:B:227:TYR:CD1	1:B:352:SER:HB3	2.54	0.42
1:B:227:TYR:CG	1:B:352:SER:HB3	2.55	0.42
1:B:1011:ARG:NH2	4:B:5004:ATP:O1G	2.52	0.42
1:B:1122:CYS:HA	1:B:1133:ARG:HG2	2.00	0.42
1:B:1564:MET:HE3	1:B:1578:PRO:HA	2.01	0.42
1:B:2593:VAL:HG12	1:B:2644:LEU:HB2	2.00	0.42
1:B:2956:TYR:HA	1:B:2959:GLU:OE2	2.19	0.42
1:B:4048:PHE:O	1:B:4052:MET:HG2	2.18	0.42
1:C:240:HIS:CG	1:D:168:GLN:HE21	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:LEU:HD23	1:C:274:LEU:HA	1.85	0.42
1:C:867:VAL:HG12	1:C:1002:ASN:ND2	2.35	0.42
1:C:1031:ARG:O	1:C:1033:VAL:HG12	2.19	0.42
1:C:1829:LEU:HD12	1:C:1829:LEU:HA	1.91	0.42
1:C:1914:CYS:O	1:C:1918:VAL:HG23	2.18	0.42
1:C:4504:MET:HA	1:C:4504:MET:CE	2.50	0.42
1:C:4604:LYS:O	1:C:4608:ARG:HG2	2.19	0.42
1:D:233:VAL:HG12	1:D:274:LEU:HD22	2.01	0.42
1:D:281:ARG:NH1	1:D:284:TRP:O	2.51	0.42
1:D:882:ARG:NH1	1:D:883:GLU:HB2	2.35	0.42
1:D:972:LEU:HD23	1:D:972:LEU:H	1.84	0.42
1:D:1810:VAL:HB	1:D:1817:LEU:HD13	2.02	0.42
1:D:2545:ILE:HD11	1:D:2580:LEU:HD22	2.00	0.42
1:D:2734:MET:SD	1:D:2825:ALA:HB2	2.59	0.42
1:D:3737:ALA:HB1	1:D:3777:MET:HG3	2.02	0.42
1:D:4061:SER:O	1:D:4064:GLU:HG3	2.19	0.42
1:D:4602:ARG:NH1	1:D:4712:VAL:HG22	2.35	0.42
1:A:883:GLU:OE2	1:A:929:ARG:NH2	2.52	0.42
1:A:1608:VAL:HG12	1:A:1619:VAL:HG22	2.01	0.42
1:A:1989:PRO:O	1:A:1993:ARG:HG3	2.18	0.42
1:A:2254:ALA:O	1:A:2316:ASN:ND2	2.52	0.42
1:A:2545:ILE:HD11	1:A:2580:LEU:HD22	2.00	0.42
1:A:2758:LYS:NZ	1:A:2762:LEU:O	2.36	0.42
2:E:91:VAL:HB	2:E:92:ILE:HD12	2.02	0.42
1:B:308:LEU:HD11	1:B:312:LYS:HA	2.02	0.42
1:B:1697:LEU:HD23	1:B:1697:LEU:HA	1.93	0.42
1:B:1914:CYS:O	1:B:1918:VAL:HG23	2.18	0.42
1:B:4294:LEU:HD12	1:C:4714:PHE:CD1	2.54	0.42
1:B:4504:MET:HA	1:B:4504:MET:CE	2.50	0.42
1:C:505:LEU:HA	1:C:505:LEU:HD23	1.85	0.42
1:C:1011:ARG:NH2	4:C:5004:ATP:O1G	2.52	0.42
1:C:1112:ASP:OD1	1:C:1208:GLY:HA3	2.19	0.42
1:C:1810:VAL:HB	1:C:1817:LEU:HD13	2.01	0.42
1:C:2137:GLU:H	1:C:2137:GLU:CD	2.23	0.42
1:C:2142:MET:HB2	1:C:2192:MET:CE	2.49	0.42
1:C:2842:GLU:O	1:C:2845:ALA:HB3	2.19	0.42
1:C:3903:GLN:HE21	1:C:3964:GLN:HE21	1.67	0.42
1:C:4609:LYS:HD2	1:C:4615:LEU:HD13	2.02	0.42
1:C:4694:LEU:HA	1:C:4697:VAL:HG12	2.02	0.42
1:D:1016:TRP:CE3	1:D:1027:ARG:NH1	2.87	0.42
1:D:1649:GLU:HG2	1:D:1650:LEU:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2272:CYS:O	1:D:2291:ASN:N	2.51	0.42
1:A:1016:TRP:CE3	1:A:1027:ARG:NH1	2.87	0.42
1:A:1711:LEU:HB3	1:A:1831:MET:SD	2.60	0.42
1:A:2137:GLU:H	1:A:2137:GLU:CD	2.23	0.42
1:A:2604:LYS:HB3	1:A:2608:LYS:NZ	2.35	0.42
1:A:2930:ILE:CG1	1:A:3007:LEU:HD21	2.39	0.42
1:A:3614:HIS:CD2	1:A:3615:ARG:HG2	2.55	0.42
1:A:3892:TYR:HD2	1:A:3906:PHE:HE2	1.67	0.42
1:B:637:LEU:HD22	1:B:1679:HIS:CD2	2.54	0.42
1:B:2258:ARG:HB3	1:B:2260:PRO:HD2	2.00	0.42
1:B:3737:ALA:HB1	1:B:3777:MET:HG3	2.02	0.42
1:B:3892:TYR:HD2	1:B:3906:PHE:HE2	1.67	0.42
1:C:608:HIS:HB2	1:C:1656:HIS:CD2	2.55	0.42
1:C:972:LEU:HD23	1:C:972:LEU:H	1.84	0.42
1:C:2074:VAL:HG23	1:C:3660:ARG:HG2	2.02	0.42
1:C:2258:ARG:HB3	1:C:2260:PRO:HD2	2.00	0.42
1:C:2673:ALA:HB1	1:C:2974:TYR:HD1	1.84	0.42
1:C:2943:PHE:HZ	1:C:2956:TYR:HB2	1.84	0.42
1:C:2956:TYR:HA	1:C:2959:GLU:OE2	2.19	0.42
1:C:3896:ASP:OD1	1:C:3897:VAL:N	2.53	0.42
1:C:4563:GLU:HG2	1:C:4566:GLY:H	1.85	0.42
1:D:483:LYS:NZ	1:D:543:GLY:O	2.51	0.42
1:D:521:GLU:HG2	1:D:522:ALA:N	2.35	0.42
1:D:2303:ARG:HG2	1:D:2401:ARG:HD2	2.01	0.42
1:D:2557:LYS:NZ	1:D:2602:HIS:HB3	2.35	0.42
1:D:2673:ALA:HB1	1:D:2974:TYR:HD1	1.84	0.42
1:D:4621:PRO:HD2	1:D:4632:ARG:HH22	1.84	0.42
1:A:308:LEU:HD11	1:A:312:LYS:HA	2.02	0.42
1:A:395:HIS:NE2	1:A:396:GLU:OE2	2.53	0.42
1:A:966:LEU:HD23	1:A:966:LEU:HA	1.86	0.42
1:A:1042:THR:O	1:A:1045:SER:OG	2.26	0.42
1:A:3737:ALA:HB1	1:A:3777:MET:HG3	2.02	0.42
1:A:3896:ASP:OD1	1:A:3897:VAL:N	2.53	0.42
1:B:2137:GLU:H	1:B:2137:GLU:CD	2.23	0.42
1:B:3614:HIS:CD2	1:B:3615:ARG:HG2	2.55	0.42
1:B:3669:LEU:HD23	1:B:3669:LEU:HA	1.92	0.42
1:C:678:MET:HG2	1:C:801:ARG:NH2	2.27	0.42
1:C:799:LYS:HB3	1:C:799:LYS:HZ2	1.81	0.42
1:C:998:LYS:HB2	1:C:998:LYS:HE2	1.86	0.42
1:C:1956:ALA:O	1:C:1959:ALA:HB3	2.18	0.42
1:C:2337:GLY:HA2	1:D:142:LYS:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3088:LYS:HG3	1:C:3090:VAL:HG12	2.01	0.42
1:C:4242:ARG:HA	1:C:4242:ARG:HD2	1.92	0.42
1:D:867:VAL:HG12	1:D:1002:ASN:ND2	2.34	0.42
1:D:951:GLY:N	1:D:1063:ASN:O	2.45	0.42
1:D:1310:CYS:HB2	1:D:1537:THR:H	1.84	0.42
1:D:1538:LYS:HD2	1:D:1636:ASN:ND2	2.33	0.42
1:D:2142:MET:HB2	1:D:2192:MET:CE	2.49	0.42
1:D:2604:LYS:HB3	1:D:2608:LYS:NZ	2.34	0.42
1:D:2975:PHE:HD2	1:D:3036:LEU:HD21	1.85	0.42
1:D:3892:TYR:HD2	1:D:3906:PHE:HE2	1.67	0.42
1:D:4609:LYS:HD2	1:D:4615:LEU:HD13	2.02	0.42
1:D:4774:LEU:O	1:D:4778:VAL:HG23	2.19	0.42
1:A:659:ILE:HD13	1:A:822:CYS:HB3	2.02	0.42
1:A:2251:ASN:HB2	1:A:3819:MET:HE1	2.01	0.42
1:A:2557:LYS:NZ	1:A:2602:HIS:HB3	2.35	0.42
1:A:2724:TYR:HA	1:A:2727:HIS:HB3	2.01	0.42
1:A:2976:LYS:O	1:A:2979:ARG:NH1	2.51	0.42
1:B:695:VAL:HG11	1:B:755:ILE:HG21	2.00	0.42
1:B:972:LEU:HD23	1:B:972:LEU:H	1.84	0.42
1:B:2251:ASN:HD22	1:B:3817:LEU:HD11	1.84	0.42
1:B:2589:LEU:O	1:B:2593:VAL:HG13	2.19	0.42
1:B:2673:ALA:HB1	1:B:2974:TYR:HD1	1.84	0.42
1:B:2724:TYR:HA	1:B:2727:HIS:HB3	2.01	0.42
1:B:2757:MET:HA	1:B:2820:GLY:HA3	2.01	0.42
1:B:3015:VAL:HG21	1:B:3033:LEU:HD11	2.01	0.42
1:B:3642:GLU:HG3	1:B:3646:LYS:NZ	2.35	0.42
1:B:3896:ASP:OD1	1:B:3897:VAL:N	2.53	0.42
1:B:4694:LEU:HA	1:B:4697:VAL:HG12	2.02	0.42
1:C:395:HIS:NE2	1:C:396:GLU:OE2	2.53	0.42
1:C:882:ARG:NH1	1:C:883:GLU:HB2	2.35	0.42
1:C:1689:ILE:HG23	1:C:1703:TYR:CZ	2.54	0.42
1:C:1748:LEU:HB3	1:C:1751:ILE:HD13	2.02	0.42
1:C:2251:ASN:HD22	1:C:3817:LEU:HD11	1.84	0.42
1:C:2557:LYS:NZ	1:C:2602:HIS:HB3	2.35	0.42
1:C:2945:GLY:HA2	1:C:2948:ARG:HH21	1.84	0.42
1:D:188:SER:HB2	1:D:190:ARG:HH11	1.85	0.42
1:D:395:HIS:NE2	1:D:396:GLU:OE2	2.53	0.42
1:D:648:LEU:HD23	1:D:1628:MET:HB2	2.02	0.42
1:D:892:LEU:HD11	1:D:980:PRO:HG3	2.01	0.42
1:D:998:LYS:HB2	1:D:998:LYS:HE2	1.86	0.42
1:D:1608:VAL:HG12	1:D:1619:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2090:ARG:HE	1:D:2090:ARG:HB3	1.64	0.42
1:D:2251:ASN:HD22	1:D:3817:LEU:HD11	1.84	0.42
1:D:2619:LYS:NZ	1:D:2623:LEU:HD22	2.34	0.42
1:D:4048:PHE:CD2	1:D:4078:LEU:HD21	2.54	0.42
1:A:44:ASN:HD21	1:A:46:LEU:HB2	1.84	0.42
1:A:188:SER:HB2	1:A:190:ARG:HH11	1.85	0.42
1:A:882:ARG:NH1	1:A:883:GLU:HB2	2.35	0.42
1:A:983:LEU:CD1	1:A:1055:ARG:HB3	2.45	0.42
1:A:1122:CYS:HA	1:A:1133:ARG:HG2	2.00	0.42
1:A:1310:CYS:HB2	1:A:1537:THR:H	1.84	0.42
1:A:1894:LEU:HD23	1:A:1894:LEU:HA	1.89	0.42
2:F:91:VAL:HB	2:F:92:ILE:HD12	2.02	0.42
1:B:188:SER:HB2	1:B:190:ARG:HH11	1.85	0.42
1:B:867:VAL:HG12	1:B:1002:ASN:ND2	2.34	0.42
1:B:882:ARG:NH1	1:B:883:GLU:HB2	2.35	0.42
1:B:1068:ASP:OD1	1:B:1069:GLN:N	2.52	0.42
1:B:1960:ARG:HH21	1:B:1960:ARG:HD2	1.69	0.42
1:B:2265:VAL:HG21	1:B:2301:PHE:CE2	2.55	0.42
1:B:2383:HIS:ND1	1:B:2458:ALA:HB2	2.34	0.42
1:B:3650:GLU:HG3	1:B:3659:LYS:HE2	2.02	0.42
1:B:3846:LEU:HD13	1:B:3854:PHE:CZ	2.55	0.42
1:B:4248:LEU:HD22	1:C:4711:GLY:HA2	2.02	0.42
1:B:4563:GLU:HG2	1:B:4566:GLY:H	1.85	0.42
1:B:4735:ASN:HB3	1:B:4738:PHE:HD2	1.84	0.42
1:C:227:TYR:CG	1:C:352:SER:HB3	2.54	0.42
1:C:506:HIS:HB3	1:C:564:ARG:HH12	1.84	0.42
1:C:521:GLU:HG2	1:C:522:ALA:N	2.35	0.42
1:C:537:LEU:O	1:C:541:ILE:HG12	2.18	0.42
1:C:1711:LEU:HB3	1:C:1831:MET:SD	2.60	0.42
1:C:1929:SER:O	1:C:1933:VAL:HG12	2.19	0.42
1:C:1979:PHE:HE1	1:C:1986:CYS:HG	1.65	0.42
1:C:2265:VAL:HG21	1:C:2301:PHE:CE2	2.55	0.42
1:C:2975:PHE:HD2	1:C:3036:LEU:HD21	1.85	0.42
1:D:56:LYS:HD3	1:D:324:VAL:HG11	2.01	0.42
1:D:1031:ARG:O	1:D:1033:VAL:HG12	2.19	0.42
1:D:1419:PHE:HD2	1:D:1562:ASN:ND2	2.18	0.42
1:D:2943:PHE:HZ	1:D:2956:TYR:HB2	1.84	0.42
1:D:3832:ASP:HB2	1:D:3835:PHE:HB3	2.02	0.42
1:D:4031:THR:HA	1:D:4034:GLU:OE1	2.20	0.42
1:D:4604:LYS:O	1:D:4608:ARG:HG2	2.20	0.42
1:A:2890:GLN:O	1:A:2893:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2975:PHE:HD2	1:A:3036:LEU:HD21	1.85	0.42
1:A:4609:LYS:HD2	1:A:4615:LEU:HD13	2.02	0.42
2:G:32:GLN:HG2	1:C:1312:GLU:OE1	2.20	0.42
1:B:2557:LYS:NZ	1:B:2602:HIS:HB3	2.35	0.42
1:B:2604:LYS:HB3	1:B:2608:LYS:NZ	2.35	0.42
1:B:2943:PHE:HZ	1:B:2956:TYR:HB2	1.84	0.42
1:B:2975:PHE:HD2	1:B:3036:LEU:HD21	1.85	0.42
1:B:4602:ARG:NH1	1:B:4712:VAL:HG22	2.35	0.42
1:B:4609:LYS:HD2	1:B:4615:LEU:HD13	2.02	0.42
1:C:323:ASP:O	1:C:327:THR:OG1	2.24	0.42
1:C:2383:HIS:ND1	1:C:2458:ALA:HB2	2.34	0.42
1:C:2543:SER:HB2	1:C:2879:ALA:HB2	2.02	0.42
1:C:2604:LYS:HB3	1:C:2608:LYS:NZ	2.34	0.42
1:C:3015:VAL:HG21	1:C:3033:LEU:HD11	2.01	0.42
1:C:3071:THR:HG21	1:C:3097:THR:OG1	2.20	0.42
1:C:3650:GLU:HG3	1:C:3659:LYS:HE2	2.02	0.42
1:D:227:TYR:CD1	1:D:352:SER:HB3	2.54	0.42
1:D:3650:GLU:HG3	1:D:3659:LYS:HE2	2.02	0.42
1:D:3896:ASP:OD1	1:D:3897:VAL:N	2.53	0.42
1:D:3954:MET:HB3	1:D:3971:LEU:CD2	2.50	0.42
1:A:521:GLU:HG2	1:A:522:ALA:N	2.35	0.42
1:A:1068:ASP:OD1	1:A:1069:GLN:N	2.52	0.42
1:A:1113:MET:HE3	1:A:1211:GLN:HB3	2.02	0.42
1:A:2074:VAL:HG23	1:A:3660:ARG:HG2	2.02	0.42
1:A:2086:VAL:HG22	1:A:3687:LEU:HD13	2.01	0.42
1:A:2445:ILE:HA	1:A:2451:VAL:HA	2.02	0.42
1:A:2447:LYS:H	1:A:2447:LYS:HG2	1.68	0.42
1:A:2620:TYR:OH	1:A:2632:ALA:O	2.34	0.42
1:A:2666:LEU:CD1	1:A:2966:VAL:HA	2.49	0.42
1:A:2937:HIS:CD2	1:A:3014:LEU:HD12	2.55	0.42
1:A:2945:GLY:HA2	1:A:2948:ARG:HH21	1.84	0.42
1:A:2988:ARG:HD2	1:A:2989:PRO:N	2.35	0.42
1:A:3644:LEU:HD23	1:A:3644:LEU:HA	1.94	0.42
1:A:3832:ASP:HB2	1:A:3835:PHE:HB3	2.02	0.42
1:A:3846:LEU:HD13	1:A:3854:PHE:CZ	2.55	0.42
1:A:4274:MET:H	1:A:4274:MET:HE2	1.84	0.42
1:A:4735:ASN:HB3	1:A:4738:PHE:HD2	1.83	0.42
2:F:19:LYS:HB2	2:F:19:LYS:HE3	1.87	0.42
1:B:115:TYR:HB3	1:B:164:PRO:HD3	2.01	0.42
1:B:211:LEU:H	1:B:211:LEU:HD23	1.85	0.42
1:B:1947:VAL:HG23	1:B:1961:LYS:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:801:ARG:HE	1:C:801:ARG:HB2	1.69	0.42
1:C:892:LEU:HD11	1:C:980:PRO:HG3	2.01	0.42
1:C:943:LEU:O	1:C:948:CYS:HB3	2.20	0.42
1:C:1465:VAL:HG12	1:C:1482:ARG:HB3	2.02	0.42
1:C:1608:VAL:HG12	1:C:1619:VAL:HG22	2.01	0.42
1:C:1992:ILE:HA	1:C:1995:GLN:OE1	2.19	0.42
1:C:2758:LYS:HA	1:C:2759:PRO:HD3	1.84	0.42
1:C:3737:ALA:HB1	1:C:3777:MET:HG3	2.02	0.42
1:C:4563:GLU:OE1	1:C:4563:GLU:N	2.53	0.42
1:D:562:LEU:HG	1:D:600:LEU:HD13	2.00	0.42
1:D:659:ILE:HD13	1:D:822:CYS:HB3	2.02	0.42
1:D:1068:ASP:OD1	1:D:1069:GLN:N	2.52	0.42
1:D:1304:LEU:HD23	1:D:1304:LEU:HA	1.89	0.42
1:D:2265:VAL:HG21	1:D:2301:PHE:CE2	2.55	0.42
1:D:2727:HIS:CE1	1:D:2731:LYS:NZ	2.87	0.42
1:D:2842:GLU:O	1:D:2845:ALA:HB3	2.19	0.42
1:D:3614:HIS:CD2	1:D:3615:ARG:HG2	2.55	0.42
1:A:15:ARG:HH21	1:A:111:ARG:HA	1.85	0.41
1:A:506:HIS:HB3	1:A:564:ARG:HH12	1.84	0.41
1:A:648:LEU:HD23	1:A:1628:MET:HB2	2.02	0.41
1:A:1244:ASN:OD1	1:A:1245:ARG:N	2.53	0.41
1:A:1484:ASN:OD1	1:A:1485:CYS:N	2.53	0.41
1:A:2337:GLY:HA2	1:B:142:LYS:HD3	2.01	0.41
1:A:2842:GLU:O	1:A:2845:ALA:HB3	2.19	0.41
1:A:2943:PHE:HZ	1:A:2956:TYR:HB2	1.84	0.41
1:A:3650:GLU:HG3	1:A:3659:LYS:HE2	2.02	0.41
1:B:648:LEU:HD23	1:B:1628:MET:HB2	2.02	0.41
1:B:1622:LEU:HD23	1:B:1622:LEU:HA	1.88	0.41
1:B:2937:HIS:CD2	1:B:3014:LEU:HD12	2.55	0.41
1:B:3071:THR:HG21	1:B:3097:THR:OG1	2.20	0.41
1:C:344:LYS:NZ	1:C:345:GLU:O	2.42	0.41
1:C:827:LEU:HD23	1:C:827:LEU:HA	1.88	0.41
1:C:2768:LYS:O	1:C:2772:ARG:N	2.36	0.41
1:C:2976:LYS:O	1:C:2979:ARG:NH1	2.51	0.41
1:C:4887:LYS:HE3	1:C:4887:LYS:HB2	1.58	0.41
1:D:115:TYR:HB3	1:D:164:PRO:HD3	2.01	0.41
1:D:227:TYR:CG	1:D:352:SER:HB3	2.54	0.41
1:D:983:LEU:CD1	1:D:1055:ARG:HB3	2.45	0.41
1:D:1112:ASP:OD1	1:D:1208:GLY:HA3	2.19	0.41
1:D:1122:CYS:HA	1:D:1133:ARG:HG2	2.00	0.41
1:D:1438:PRO:HG2	1:D:1494:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2086:VAL:HG22	1:D:3687:LEU:HD13	2.01	0.41
1:D:3032:CYS:HA	1:D:3035:ILE:HG12	2.02	0.41
1:D:4116:GLN:O	1:D:4120:GLU:OE1	2.38	0.41
1:D:4563:GLU:OE1	1:D:4563:GLU:N	2.53	0.41
1:A:892:LEU:HD11	1:A:980:PRO:HG3	2.01	0.41
1:A:1419:PHE:HD2	1:A:1562:ASN:ND2	2.18	0.41
1:A:1419:PHE:HD1	1:A:1422:GLN:HE21	1.68	0.41
1:A:1748:LEU:HB3	1:A:1751:ILE:HD13	2.02	0.41
1:A:2383:HIS:ND1	1:A:2458:ALA:HB2	2.34	0.41
1:A:3642:GLU:HG3	1:A:3646:LYS:NZ	2.35	0.41
2:E:19:LYS:HB2	2:E:19:LYS:HE3	1.86	0.41
1:B:15:ARG:HH21	1:B:111:ARG:HA	1.85	0.41
1:B:115:TYR:HE1	1:B:181:LEU:HD21	1.84	0.41
1:B:521:GLU:HG2	1:B:522:ALA:N	2.35	0.41
1:B:1608:VAL:HG12	1:B:1619:VAL:HG22	2.01	0.41
1:B:2620:TYR:OH	1:B:2632:ALA:O	2.34	0.41
1:B:2684:ASN:OD1	1:B:2919:LYS:NZ	2.45	0.41
1:B:2945:GLY:HA2	1:B:2948:ARG:HH21	1.84	0.41
1:B:2988:ARG:HD2	1:B:2989:PRO:N	2.35	0.41
1:B:4245:LEU:HD11	1:C:4629:GLN:HB2	2.01	0.41
1:C:695:VAL:HG11	1:C:755:ILE:HG21	2.00	0.41
1:C:2730:ASP:OD1	1:C:2823:PRO:HB3	2.20	0.41
1:C:2988:ARG:HD2	1:C:2989:PRO:N	2.35	0.41
1:C:4203:ALA:HA	1:C:4206:ILE:HG12	2.01	0.41
1:C:4859:LEU:HD21	1:D:4851:PHE:HZ	1.85	0.41
1:D:505:LEU:HD23	1:D:505:LEU:HA	1.85	0.41
1:D:1465:VAL:HG12	1:D:1482:ARG:HB3	2.02	0.41
1:D:1929:SER:O	1:D:1933:VAL:HG12	2.19	0.41
1:D:2840:MET:O	1:D:2843:MET:HG3	2.21	0.41
1:D:2890:GLN:O	1:D:2893:LEU:HG	2.19	0.41
1:D:2897:GLN:OE1	1:D:2897:GLN:N	2.50	0.41
1:D:3071:THR:HG21	1:D:3097:THR:OG1	2.20	0.41
1:A:867:VAL:HG12	1:A:1002:ASN:ND2	2.35	0.41
1:A:872:ILE:HG13	1:A:945:ALA:HB2	2.02	0.41
1:A:1810:VAL:HB	1:A:1817:LEU:HD13	2.02	0.41
1:A:2720:PHE:HD2	1:A:2901:TYR:CE2	2.38	0.41
1:A:3054:LYS:HB3	1:A:3058:ARG:NH1	2.35	0.41
1:A:3965:ILE:HG22	1:A:3969:LYS:HZ3	1.85	0.41
1:A:4563:GLU:HG2	1:A:4566:GLY:H	1.85	0.41
1:B:608:HIS:HB2	1:B:1656:HIS:CD2	2.55	0.41
1:B:943:LEU:O	1:B:948:CYS:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2840:MET:O	1:B:2843:MET:HG3	2.21	0.41
1:B:4279:MET:HE2	1:C:4488:GLN:HB2	2.03	0.41
1:C:308:LEU:HD11	1:C:312:LYS:HA	2.02	0.41
1:C:370:LEU:CD2	1:C:395:HIS:HB3	2.51	0.41
1:C:1104:GLU:HA	1:C:1163:GLY:HA3	2.02	0.41
1:C:2222:LEU:HD23	1:C:2222:LEU:HA	1.92	0.41
1:C:3017:HIS:HB3	1:C:3093:ILE:HG13	2.03	0.41
1:C:3614:HIS:CD2	1:C:3615:ARG:HG2	2.55	0.41
1:C:3846:LEU:HD13	1:C:3854:PHE:CZ	2.55	0.41
1:C:3892:TYR:CE2	1:C:3898:ILE:HG23	2.56	0.41
1:C:3954:MET:HB3	1:C:3971:LEU:CD2	2.50	0.41
1:C:4113:THR:O	1:C:4117:THR:HG23	2.21	0.41
1:C:4116:GLN:O	1:C:4120:GLU:OE1	2.38	0.41
1:D:1484:ASN:OD1	1:D:1485:CYS:N	2.53	0.41
1:D:1849:SER:O	1:D:2054:LYS:NZ	2.34	0.41
1:D:2730:ASP:OD1	1:D:2823:PRO:HB3	2.20	0.41
1:D:4002:MET:HE2	1:D:4002:MET:HB3	1.87	0.41
1:A:1975:MET:HE3	1:A:1975:MET:HB3	1.75	0.41
1:A:2143:ILE:HG13	1:A:2192:MET:HE1	2.01	0.41
1:A:2251:ASN:HD22	1:A:3817:LEU:HD11	1.84	0.41
1:A:2673:ALA:HB1	1:A:2974:TYR:HD1	1.84	0.41
1:A:2727:HIS:CE1	1:A:2731:LYS:NZ	2.87	0.41
1:A:2840:MET:O	1:A:2843:MET:HG3	2.21	0.41
1:A:3954:MET:HB3	1:A:3971:LEU:CD2	2.50	0.41
2:G:91:VAL:HB	2:G:92:ILE:HD12	2.02	0.41
1:B:1113:MET:HE3	1:B:1211:GLN:HB3	2.02	0.41
1:B:1484:ASN:OD1	1:B:1485:CYS:N	2.53	0.41
1:B:2730:ASP:OD1	1:B:2823:PRO:HB3	2.20	0.41
1:B:4113:THR:O	1:B:4117:THR:HG23	2.21	0.41
1:B:4735:ASN:HB3	1:B:4738:PHE:CD2	2.56	0.41
1:B:4956:ASP:OD1	1:B:4957:CYS:N	2.54	0.41
1:C:115:TYR:HE1	1:C:181:LEU:HD21	1.84	0.41
1:C:255:GLU:HG2	1:C:256:GLN:OE1	2.21	0.41
1:C:877:HIS:CA	1:C:880:ARG:HH11	2.34	0.41
1:C:1947:VAL:HG23	1:C:1961:LYS:HE2	2.02	0.41
1:C:2724:TYR:HA	1:C:2727:HIS:HB3	2.01	0.41
1:C:2897:GLN:OE1	1:C:2897:GLN:N	2.50	0.41
1:C:2937:HIS:CD2	1:C:3014:LEU:HD12	2.55	0.41
1:C:3941:TRP:O	1:C:3945:VAL:HG23	2.20	0.41
1:D:308:LEU:HD11	1:D:312:LYS:HA	2.02	0.41
1:D:895:MET:HE3	1:D:972:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1711:LEU:HB3	1:D:1831:MET:SD	2.60	0.41
1:D:2720:PHE:HD2	1:D:2901:TYR:CE2	2.39	0.41
1:D:2945:GLY:HA2	1:D:2948:ARG:HH21	1.84	0.41
1:D:3088:LYS:HG3	1:D:3090:VAL:HG12	2.01	0.41
1:D:3941:TRP:O	1:D:3945:VAL:HG23	2.20	0.41
1:D:4694:LEU:HA	1:D:4697:VAL:HG12	2.02	0.41
1:A:459:LEU:HD23	1:A:459:LEU:HA	1.92	0.41
1:A:2541:HIS:HB3	1:A:2544:LEU:HD21	2.03	0.41
1:A:2758:LYS:HA	1:A:2759:PRO:HD3	1.83	0.41
1:A:3939:ARG:NH2	1:B:172:GLY:O	2.53	0.41
2:E:108:GLU:N	2:E:108:GLU:OE2	2.54	0.41
1:B:4031:THR:HA	1:B:4034:GLU:OE1	2.20	0.41
1:C:2254:ALA:O	1:C:2316:ASN:ND2	2.52	0.41
1:C:3732:HIS:O	1:C:3776:LYS:NZ	2.47	0.41
1:C:4602:ARG:NH1	1:C:4712:VAL:HG22	2.35	0.41
1:D:943:LEU:O	1:D:948:CYS:HB3	2.20	0.41
1:D:1991:GLU:HG2	1:D:1992:ILE:N	2.36	0.41
1:D:3846:LEU:HD13	1:D:3854:PHE:CZ	2.55	0.41
1:D:4242:ARG:HA	1:D:4242:ARG:HD2	1.92	0.41
1:D:4504:MET:HA	1:D:4504:MET:CE	2.50	0.41
1:A:255:GLU:HG2	1:A:256:GLN:OE1	2.21	0.41
1:A:678:MET:HG2	1:A:801:ARG:NH2	2.27	0.41
1:A:814:LEU:HA	1:A:815:PRO:HD3	1.94	0.41
1:A:971:GLN:HG2	1:A:972:LEU:HD23	2.03	0.41
1:A:1552:VAL:HG12	1:A:1553:PHE:HD1	1.86	0.41
1:A:2822:SER:HA	1:A:2823:PRO:HD3	1.92	0.41
1:A:3071:THR:HG21	1:A:3097:THR:OG1	2.20	0.41
1:A:4162:LYS:HA	1:A:4162:LYS:HD3	1.58	0.41
1:A:4504:MET:HA	1:A:4504:MET:CE	2.50	0.41
1:B:1104:GLU:HA	1:B:1163:GLY:HA3	2.02	0.41
1:B:1415:ASP:OD2	1:B:1559:ARG:NH2	2.43	0.41
1:B:1419:PHE:HD2	1:B:1562:ASN:ND2	2.18	0.41
1:B:1552:VAL:HG12	1:B:1553:PHE:HD1	1.86	0.41
1:B:2541:HIS:HB3	1:B:2544:LEU:HD21	2.03	0.41
1:B:3032:CYS:HA	1:B:3035:ILE:HG12	2.01	0.41
1:B:3892:TYR:CE2	1:B:3898:ILE:HG23	2.56	0.41
1:B:4116:GLN:O	1:B:4120:GLU:OE1	2.38	0.41
1:C:648:LEU:HD23	1:C:1628:MET:HB2	2.02	0.41
1:C:1419:PHE:HD2	1:C:1562:ASN:ND2	2.18	0.41
1:C:1484:ASN:OD1	1:C:1485:CYS:N	2.53	0.41
1:C:1894:LEU:HD23	1:C:1894:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3642:GLU:HG3	1:C:3646:LYS:NZ	2.35	0.41
1:C:3763:ILE:HD11	1:C:3838:ASP:O	2.21	0.41
1:D:506:HIS:HB3	1:D:564:ARG:HH12	1.84	0.41
1:D:608:HIS:HB2	1:D:1656:HIS:CD2	2.55	0.41
1:D:2447:LYS:H	1:D:2447:LYS:HG2	1.68	0.41
1:D:2937:HIS:CD2	1:D:3014:LEU:HD12	2.55	0.41
1:D:3017:HIS:HB3	1:D:3093:ILE:HG13	2.02	0.41
1:D:4735:ASN:HB3	1:D:4738:PHE:CD2	2.56	0.41
1:A:1991:GLU:HG2	1:A:1992:ILE:N	2.36	0.41
1:A:4694:LEU:HA	1:A:4697:VAL:HG12	2.02	0.41
1:B:483:LYS:NZ	1:B:543:GLY:O	2.51	0.41
1:B:955:GLU:HG2	1:B:958:GLU:OE2	2.21	0.41
1:B:986:ILE:HD12	1:B:1058:LEU:HB2	2.02	0.41
1:B:1244:ASN:OD1	1:B:1245:ARG:N	2.53	0.41
1:B:1283:LEU:HB2	1:B:1555:PHE:HB2	2.03	0.41
1:B:1810:VAL:HB	1:B:1817:LEU:HD13	2.02	0.41
1:B:1988:CYS:HA	1:B:1989:PRO:HD3	1.95	0.41
1:B:2445:ILE:HA	1:B:2451:VAL:HA	2.02	0.41
1:B:2543:SER:HB2	1:B:2879:ALA:HB2	2.02	0.41
1:B:2883:ALA:O	1:B:2887:GLU:OE1	2.39	0.41
1:B:3043:ARG:HH11	1:B:3047:LYS:HZ2	1.69	0.41
1:B:4205:GLN:HE21	1:B:4205:GLN:HB3	1.73	0.41
1:B:4563:GLU:N	1:B:4563:GLU:OE1	2.52	0.41
1:C:506:HIS:CE1	1:C:530:LEU:HD21	2.56	0.41
1:C:911:ASN:OD1	1:C:912:LYS:N	2.54	0.41
1:C:3832:ASP:HB2	1:C:3835:PHE:HB3	2.02	0.41
1:C:4862:ILE:HG22	1:D:4852:PHE:HE1	1.86	0.41
1:D:986:ILE:HD12	1:D:1058:LEU:HB2	2.02	0.41
1:D:1419:PHE:HD1	1:D:1422:GLN:HE21	1.68	0.41
1:D:1748:LEU:HB3	1:D:1751:ILE:HD13	2.02	0.41
1:D:3054:LYS:HB3	1:D:3058:ARG:NH1	2.35	0.41
1:A:877:HIS:CA	1:A:880:ARG:HH11	2.34	0.41
1:A:911:ASN:OD1	1:A:912:LYS:N	2.54	0.41
1:A:955:GLU:HG2	1:A:958:GLU:OE2	2.21	0.41
1:A:986:ILE:HD12	1:A:1058:LEU:HB2	2.02	0.41
1:A:2272:CYS:O	1:A:2291:ASN:N	2.51	0.41
1:A:2389:MET:HE1	1:A:2460:PHE:HA	2.02	0.41
1:A:3892:TYR:CE2	1:A:3898:ILE:HG23	2.56	0.41
1:A:4107:GLU:OE1	1:A:4149:TYR:OH	2.24	0.41
1:A:4116:GLN:O	1:A:4120:GLU:OE1	2.38	0.41
1:B:877:HIS:CA	1:B:880:ARG:HH11	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:SER:HB2	1:C:190:ARG:HH11	1.85	0.41
1:C:658:ASN:HB2	1:C:832:LEU:HD12	2.02	0.41
1:C:1849:SER:O	1:C:2054:LYS:NZ	2.34	0.41
1:C:1991:GLU:HG2	1:C:1992:ILE:N	2.36	0.41
1:C:2720:PHE:HD2	1:C:2901:TYR:CE2	2.39	0.41
1:C:4882:GLU:OE1	1:C:4886:THR:OG1	2.35	0.41
1:D:1283:LEU:HB2	1:D:1555:PHE:HB2	2.03	0.41
1:D:2662:PHE:HE2	1:D:2962:PHE:HD1	1.69	0.41
1:D:2727:HIS:CD2	1:D:2731:LYS:NZ	2.89	0.41
1:D:4625:ASP:OD1	1:D:4625:ASP:N	2.47	0.41
1:A:211:LEU:HD23	1:A:211:LEU:H	1.85	0.41
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.85	0.41
1:A:1721:MET:HA	1:A:1721:MET:HE3	2.03	0.41
1:A:2265:VAL:HG21	1:A:2301:PHE:CE2	2.55	0.41
1:A:2543:SER:HB2	1:A:2879:ALA:HB2	2.02	0.41
1:A:2586:GLN:O	1:A:2590:ARG:HG3	2.21	0.41
1:A:2883:ALA:O	1:A:2887:GLU:OE1	2.39	0.41
1:A:2887:GLU:HG2	1:A:2888:LYS:N	2.36	0.41
1:A:3019:ILE:HB	1:A:3096:TYR:HD1	1.86	0.41
1:A:3763:ILE:HD11	1:A:3838:ASP:O	2.21	0.41
1:A:3941:TRP:O	1:A:3945:VAL:HG23	2.20	0.41
1:A:4046:ARG:HB3	1:A:4050:LYS:HZ1	1.85	0.41
1:A:4511:PHE:HD2	1:A:4743:LEU:HD21	1.86	0.41
1:A:4618:THR:HG22	1:A:4661:TYR:CE2	2.56	0.41
1:A:4899:ASP:OD1	1:B:4183:LYS:NZ	2.53	0.41
2:F:108:GLU:N	2:F:108:GLU:OE2	2.54	0.41
2:G:108:GLU:N	2:G:108:GLU:OE2	2.54	0.41
1:B:29:HIS:O	1:B:29:HIS:ND1	2.54	0.41
1:B:323:ASP:O	1:B:327:THR:OG1	2.24	0.41
1:B:370:LEU:CD2	1:B:395:HIS:HB3	2.51	0.41
1:B:395:HIS:NE2	1:B:396:GLU:OE2	2.53	0.41
1:B:506:HIS:CE1	1:B:530:LEU:HD21	2.55	0.41
1:B:658:ASN:HB2	1:B:832:LEU:HD12	2.02	0.41
1:B:895:MET:HE3	1:B:972:LEU:HD22	2.03	0.41
1:B:911:ASN:OD1	1:B:912:LYS:N	2.54	0.41
1:B:951:GLY:N	1:B:1063:ASN:O	2.45	0.41
1:B:1664:VAL:HG23	1:B:1676:LEU:HD11	2.02	0.41
1:B:1711:LEU:HB3	1:B:1831:MET:SD	2.60	0.41
1:B:1748:LEU:HB3	1:B:1751:ILE:HD13	2.02	0.41
1:B:2074:VAL:HG23	1:B:3660:ARG:HG2	2.02	0.41
1:B:2142:MET:HB2	1:B:2192:MET:CE	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2662:PHE:HE2	1:B:2962:PHE:HD1	1.69	0.41
1:B:3639:LYS:HE2	1:B:3639:LYS:HB2	1.92	0.41
1:B:3954:MET:HB3	1:B:3971:LEU:CD2	2.50	0.41
1:B:4618:THR:HG22	1:B:4661:TYR:CE2	2.56	0.41
1:C:115:TYR:HB3	1:C:164:PRO:HD3	2.01	0.41
1:C:483:LYS:NZ	1:C:543:GLY:O	2.51	0.41
1:C:551:PHE:HE2	1:C:558:LEU:HD22	1.86	0.41
1:C:872:ILE:HG13	1:C:945:ALA:HB2	2.02	0.41
1:C:895:MET:HE3	1:C:972:LEU:HD22	2.02	0.41
1:C:955:GLU:HG2	1:C:958:GLU:OE2	2.21	0.41
1:C:983:LEU:CD1	1:C:1055:ARG:HB3	2.45	0.41
1:C:1089:ARG:HB3	1:C:1204:VAL:HG23	2.03	0.41
1:C:1839:LEU:HD12	1:C:1842:ILE:HD11	2.02	0.41
1:C:2684:ASN:OD1	1:C:2919:LYS:NZ	2.45	0.41
1:C:2696:ASP:OD1	1:C:2696:ASP:N	2.54	0.41
1:C:2826:ILE:HD13	1:D:1501:ASN:ND2	2.36	0.41
1:C:2883:ALA:O	1:C:2887:GLU:OE1	2.39	0.41
1:C:3019:ILE:HB	1:C:3096:TYR:HD1	1.86	0.41
1:C:3054:LYS:HB3	1:C:3058:ARG:NH1	2.35	0.41
1:C:4031:THR:HA	1:C:4034:GLU:OE1	2.20	0.41
1:C:4205:GLN:HE21	1:C:4205:GLN:HB3	1.73	0.41
1:C:4512:ALA:O	1:C:4516:ILE:HG13	2.21	0.41
1:C:4943:MET:HA	1:C:4946:GLU:HG2	2.03	0.41
1:D:29:HIS:ND1	1:D:29:HIS:O	2.54	0.41
1:D:211:LEU:HD23	1:D:211:LEU:H	1.85	0.41
1:D:370:LEU:CD2	1:D:395:HIS:HB3	2.51	0.41
1:D:658:ASN:HB2	1:D:832:LEU:HD12	2.02	0.41
1:D:971:GLN:HG2	1:D:972:LEU:HD23	2.03	0.41
1:D:1089:ARG:HB3	1:D:1204:VAL:HG23	2.03	0.41
1:D:1705:LEU:HD12	1:D:1705:LEU:HA	1.93	0.41
1:D:2074:VAL:HG23	1:D:3660:ARG:HG2	2.02	0.41
1:D:2488:LEU:HA	1:D:2492:PHE:HB2	2.03	0.41
1:D:3642:GLU:HG3	1:D:3646:LYS:NZ	2.35	0.41
1:D:3892:TYR:CE2	1:D:3898:ILE:HG23	2.56	0.41
1:D:4891:CYS:HB3	1:D:4913:HIS:CE1	2.56	0.41
1:A:658:ASN:HB2	1:A:832:LEU:HD12	2.02	0.41
1:A:698:ALA:HB2	1:A:791:VAL:HG11	2.03	0.41
1:A:1089:ARG:HB3	1:A:1204:VAL:HG23	2.03	0.41
1:A:1437:GLU:HA	1:A:1438:PRO:HD3	1.82	0.41
1:A:2727:HIS:CD2	1:A:2731:LYS:NZ	2.89	0.41
1:A:4031:THR:HA	1:A:4034:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4113:THR:O	1:A:4117:THR:HG23	2.21	0.41
1:B:611:LEU:HD23	1:B:611:LEU:HA	1.93	0.41
1:B:678:MET:HG2	1:B:801:ARG:NH2	2.27	0.41
1:B:1089:ARG:HB3	1:B:1204:VAL:HG23	2.03	0.41
1:B:2488:LEU:HA	1:B:2492:PHE:HB2	2.03	0.41
1:B:2841:ALA:HB1	1:B:2889:ALA:HB1	2.03	0.41
1:B:4026:LEU:HB2	1:B:4055:HIS:ND1	2.36	0.41
1:B:4575:LEU:HD23	1:B:4575:LEU:HA	1.97	0.41
1:B:4891:CYS:HB3	1:B:4913:HIS:CE1	2.56	0.41
1:C:29:HIS:ND1	1:C:29:HIS:O	2.54	0.41
1:C:211:LEU:H	1:C:211:LEU:HD23	1.85	0.41
1:C:756:SER:OG	1:C:769:ARG:O	2.32	0.41
1:C:2272:CYS:O	1:C:2291:ASN:N	2.51	0.41
1:C:2541:HIS:HB3	1:C:2544:LEU:HD21	2.03	0.41
1:C:2662:PHE:HE2	1:C:2962:PHE:HD1	1.69	0.41
1:D:480:ARG:NH2	1:D:3676:LEU:O	2.54	0.41
1:D:551:PHE:HE2	1:D:558:LEU:HD22	1.86	0.41
1:D:606:ARG:NH2	1:D:1632:ILE:HG23	2.36	0.41
1:D:949:HIS:O	1:D:1065:GLU:N	2.51	0.41
1:D:1011:ARG:HB3	1:D:1016:TRP:HD1	1.86	0.41
1:D:1947:VAL:HG23	1:D:1961:LYS:HE2	2.02	0.41
1:D:3019:ILE:HB	1:D:3096:TYR:HD1	1.86	0.41
1:D:3042:ALA:O	1:D:3045:VAL:HG12	2.21	0.41
1:D:4105:LEU:HD23	1:D:4105:LEU:HA	1.96	0.41
1:D:4511:PHE:HD2	1:D:4743:LEU:HD21	1.86	0.41
1:D:4943:MET:HA	1:D:4946:GLU:HG2	2.03	0.41
1:A:370:LEU:CD2	1:A:395:HIS:HB3	2.51	0.40
1:A:480:ARG:NH2	1:A:3676:LEU:O	2.55	0.40
1:A:506:HIS:CE1	1:A:530:LEU:HD21	2.56	0.40
1:A:1104:GLU:HA	1:A:1163:GLY:HA3	2.02	0.40
1:A:2351:ILE:HD11	1:A:2460:PHE:HB2	2.03	0.40
1:A:2662:PHE:HE2	1:A:2962:PHE:HD1	1.69	0.40
1:A:2696:ASP:OD1	1:A:2696:ASP:N	2.54	0.40
1:A:2727:HIS:O	1:A:2730:ASP:HB2	2.21	0.40
1:A:2730:ASP:OD1	1:A:2823:PRO:HB3	2.20	0.40
1:A:2946:GLY:HA3	1:A:2954:PHE:HZ	1.86	0.40
1:A:3032:CYS:HA	1:A:3035:ILE:HG12	2.02	0.40
1:B:255:GLU:HG2	1:B:256:GLN:OE1	2.21	0.40
1:B:1011:ARG:HB3	1:B:1016:TRP:HD1	1.86	0.40
1:B:1304:LEU:HD23	1:B:1304:LEU:HA	1.89	0.40
1:B:1465:VAL:HG12	1:B:1482:ARG:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1839:LEU:HA	1:B:1842:ILE:HG12	2.03	0.40
1:B:1839:LEU:HD12	1:B:1842:ILE:HD11	2.02	0.40
1:B:1991:GLU:HG2	1:B:1992:ILE:N	2.36	0.40
1:B:2720:PHE:HD2	1:B:2901:TYR:CE2	2.39	0.40
1:B:2887:GLU:HG2	1:B:2888:LYS:N	2.36	0.40
1:B:3017:HIS:HB3	1:B:3093:ILE:HG13	2.02	0.40
1:B:3019:ILE:HB	1:B:3096:TYR:HD1	1.86	0.40
1:B:3054:LYS:HB3	1:B:3058:ARG:NH1	2.35	0.40
1:B:3111:HIS:HA	1:B:3114:GLN:HG2	2.03	0.40
1:B:3763:ILE:HD11	1:B:3838:ASP:O	2.21	0.40
1:B:4089:GLU:OE1	1:B:4089:GLU:N	2.54	0.40
1:B:4625:ASP:OD1	1:B:4625:ASP:N	2.47	0.40
1:C:235:ARG:HE	1:C:274:LEU:CD2	2.34	0.40
1:C:1244:ASN:OD1	1:C:1245:ARG:N	2.53	0.40
1:C:1437:GLU:HA	1:C:1438:PRO:HD3	1.82	0.40
1:C:2251:ASN:HB2	1:C:3819:MET:HE1	2.02	0.40
1:C:2887:GLU:HG2	1:C:2888:LYS:N	2.36	0.40
1:C:3042:ALA:O	1:C:3045:VAL:HG12	2.21	0.40
1:C:4640:PHE:CG	1:C:4641:PRO:HD3	2.55	0.40
1:D:235:ARG:HE	1:D:274:LEU:CD2	2.34	0.40
1:D:911:ASN:OD1	1:D:912:LYS:N	2.54	0.40
1:D:1664:VAL:HG23	1:D:1676:LEU:HD11	2.02	0.40
1:D:1839:LEU:HD12	1:D:1842:ILE:HD11	2.03	0.40
1:D:2351:ILE:HD11	1:D:2460:PHE:HB2	2.03	0.40
1:D:2696:ASP:OD1	1:D:2696:ASP:N	2.54	0.40
1:D:4563:GLU:HG2	1:D:4566:GLY:H	1.85	0.40
1:A:29:HIS:ND1	1:A:29:HIS:O	2.54	0.40
1:A:436:LEU:HD23	1:A:436:LEU:HA	1.94	0.40
1:A:808:HIS:O	1:A:1616:GLY:HA2	2.21	0.40
1:A:1438:PRO:HG2	1:A:1494:MET:HE1	2.02	0.40
1:A:1446:ILE:HG12	1:A:1542:ALA:HB2	2.03	0.40
1:A:2841:ALA:HB1	1:A:2889:ALA:HB1	2.03	0.40
1:A:4512:ALA:O	1:A:4516:ILE:HG13	2.21	0.40
1:A:4891:CYS:HB3	1:A:4913:HIS:CE1	2.56	0.40
1:B:659:ILE:HD13	1:B:822:CYS:HB3	2.02	0.40
1:B:966:LEU:HD23	1:B:966:LEU:HA	1.86	0.40
1:B:3941:TRP:O	1:B:3945:VAL:HG23	2.20	0.40
1:B:4277:LYS:HD3	1:B:4277:LYS:HA	1.84	0.40
1:C:480:ARG:NH2	1:C:3676:LEU:O	2.54	0.40
1:C:659:ILE:HD13	1:C:822:CYS:HB3	2.02	0.40
1:C:1011:ARG:HB3	1:C:1016:TRP:HD1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1103:PHE:CE2	1:C:1164:CYS:HB2	2.57	0.40
1:C:1552:VAL:HG12	1:C:1553:PHE:HD1	1.86	0.40
1:C:1564:MET:CE	1:C:1565:PRO:HD2	2.47	0.40
1:C:2087:LEU:HD12	1:C:2087:LEU:HA	1.95	0.40
1:C:2445:ILE:HA	1:C:2451:VAL:HA	2.02	0.40
1:C:2840:MET:O	1:C:2843:MET:HG3	2.20	0.40
1:C:2926:LEU:HD21	1:C:3000:GLU:HG3	2.02	0.40
1:C:2943:PHE:HA	1:C:2954:PHE:HE2	1.86	0.40
1:D:255:GLU:HG2	1:D:256:GLN:OE1	2.21	0.40
1:D:506:HIS:CE1	1:D:530:LEU:HD21	2.56	0.40
1:D:765:SER:HB2	1:D:778:MET:HE1	2.02	0.40
1:D:877:HIS:CA	1:D:880:ARG:HH11	2.34	0.40
1:D:2887:GLU:HG2	1:D:2888:LYS:N	2.36	0.40
1:D:2988:ARG:HD2	1:D:2989:PRO:N	2.35	0.40
1:D:4026:LEU:HB2	1:D:4055:HIS:ND1	2.36	0.40
1:D:4512:ALA:O	1:D:4516:ILE:HG13	2.21	0.40
1:A:1103:PHE:CE2	1:A:1164:CYS:HB2	2.57	0.40
1:A:1839:LEU:HD12	1:A:1842:ILE:HD11	2.03	0.40
1:A:2926:LEU:HD21	1:A:3000:GLU:HG3	2.02	0.40
1:A:3042:ALA:O	1:A:3045:VAL:HG12	2.21	0.40
1:A:4735:ASN:HB3	1:A:4738:PHE:CD2	2.55	0.40
1:B:2635:GLU:HA	1:B:2638:LEU:HB2	2.04	0.40
1:B:2696:ASP:N	1:B:2696:ASP:OD1	2.54	0.40
1:B:2727:HIS:O	1:B:2730:ASP:HB2	2.21	0.40
1:C:143:LEU:HB3	1:C:190:ARG:HH21	1.86	0.40
1:C:606:ARG:NH2	1:C:1632:ILE:HG23	2.36	0.40
1:C:1664:VAL:HG23	1:C:1676:LEU:HD11	2.02	0.40
1:C:1719:LEU:HD21	1:C:1830:ILE:HD12	2.03	0.40
1:C:2586:GLN:HE21	1:C:2586:GLN:HB2	1.74	0.40
1:C:2635:GLU:HA	1:C:2638:LEU:HB2	2.04	0.40
1:D:143:LEU:HB3	1:D:190:ARG:HH21	1.86	0.40
1:D:1094:TYR:OH	1:D:1808:ASP:OD2	2.29	0.40
1:D:1104:GLU:HA	1:D:1163:GLY:HA3	2.02	0.40
1:D:1446:ILE:HG12	1:D:1542:ALA:HB2	2.03	0.40
1:D:1839:LEU:HA	1:D:1842:ILE:HG12	2.03	0.40
1:D:2445:ILE:HA	1:D:2451:VAL:HA	2.02	0.40
1:D:2852:TRP:HA	1:D:2855:LYS:NZ	2.37	0.40
1:D:2883:ALA:O	1:D:2887:GLU:OE1	2.39	0.40
1:D:4113:THR:O	1:D:4117:THR:HG23	2.21	0.40
1:D:4640:PHE:CG	1:D:4641:PRO:HD3	2.55	0.40
1:A:163:HIS:HB2	1:A:182:ILE:HG13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2243:ALA:O	1:A:2247:VAL:HG22	2.22	0.40
1:A:2244:ALA:O	1:A:2248:MET:HB2	2.22	0.40
1:A:2264:LYS:HG2	1:A:2267:ARG:NH2	2.37	0.40
1:A:4026:LEU:HB2	1:A:4055:HIS:ND1	2.37	0.40
1:A:4943:MET:HA	1:A:4946:GLU:HG2	2.03	0.40
1:B:872:ILE:HG13	1:B:945:ALA:HB2	2.02	0.40
1:B:1419:PHE:HD1	1:B:1422:GLN:HE21	1.68	0.40
1:B:2325:ILE:HD12	1:C:207:PHE:CE1	2.56	0.40
1:B:2852:TRP:HA	1:B:2855:LYS:NZ	2.37	0.40
1:B:2926:LEU:HD21	1:B:3000:GLU:HG3	2.02	0.40
1:B:2932:TYR:OH	1:B:2962:PHE:HD2	2.05	0.40
1:B:4512:ALA:O	1:B:4516:ILE:HG13	2.21	0.40
1:B:4943:MET:HA	1:B:4946:GLU:HG2	2.03	0.40
1:C:2488:LEU:HA	1:C:2492:PHE:HB2	2.03	0.40
1:C:2586:GLN:O	1:C:2590:ARG:HG3	2.21	0.40
1:C:2727:HIS:O	1:C:2730:ASP:HB2	2.21	0.40
1:C:2727:HIS:CD2	1:C:2731:LYS:NZ	2.89	0.40
1:C:4618:THR:HG22	1:C:4661:TYR:CE2	2.56	0.40
1:C:4891:CYS:HB3	1:C:4913:HIS:CE1	2.56	0.40
1:D:955:GLU:HG2	1:D:958:GLU:OE2	2.21	0.40
1:D:1244:ASN:OD1	1:D:1245:ARG:N	2.53	0.40
1:D:1960:ARG:HH21	1:D:1960:ARG:HD2	1.69	0.40
1:D:2264:LYS:HG2	1:D:2267:ARG:NH2	2.37	0.40
1:D:2635:GLU:HA	1:D:2638:LEU:HB2	2.04	0.40
1:D:2926:LEU:HD21	1:D:3000:GLU:HG3	2.02	0.40
1:D:3111:HIS:HA	1:D:3114:GLN:HG2	2.03	0.40
1:A:943:LEU:O	1:A:948:CYS:HB3	2.20	0.40
1:A:976:TYR:O	1:A:978:PRO:HD3	2.22	0.40
1:A:1465:VAL:HG12	1:A:1482:ARG:HB3	2.02	0.40
1:A:2943:PHE:HA	1:A:2954:PHE:HE2	1.86	0.40
1:A:3017:HIS:HB3	1:A:3093:ILE:HG13	2.02	0.40
1:A:4506:ALA:HB2	1:A:4582:ILE:HG22	2.04	0.40
1:A:4956:ASP:OD1	1:A:4957:CYS:N	2.53	0.40
1:B:355:LYS:O	1:B:359:SER:OG	2.26	0.40
1:B:949:HIS:O	1:B:1065:GLU:N	2.51	0.40
1:B:1298:ASP:OD1	1:B:1299:ILE:N	2.54	0.40
1:B:2638:LEU:HD23	1:B:2638:LEU:HA	1.92	0.40
1:B:3042:ALA:O	1:B:3045:VAL:HG12	2.21	0.40
1:B:3727:GLN:HG2	1:B:3730:ARG:NH2	2.37	0.40
1:B:4241:VAL:HG13	1:C:4626:ILE:HB	2.04	0.40
1:C:986:ILE:HD12	1:C:1058:LEU:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1419:PHE:HD1	1:C:1422:GLN:HE21	1.68	0.40
1:C:1471:ASP:OD1	1:C:1475:LYS:HB3	2.22	0.40
1:C:2650:ASP:O	1:C:2654:GLN:OE1	2.40	0.40
1:C:2932:TYR:OH	1:C:2962:PHE:HD2	2.05	0.40
1:C:3111:HIS:HA	1:C:3114:GLN:HG2	2.03	0.40
1:C:4735:ASN:HB3	1:C:4738:PHE:CD2	2.55	0.40
1:D:814:LEU:HA	1:D:815:PRO:HD3	1.94	0.40
1:D:2976:LYS:O	1:D:2979:ARG:NH1	2.51	0.40
1:D:4506:ALA:HB2	1:D:4582:ILE:HG22	2.04	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	3978/4967 (80%)	3852 (97%)	123 (3%)	3 (0%)	48	76
1	B	3978/4967 (80%)	3852 (97%)	123 (3%)	3 (0%)	48	76
1	C	3978/4967 (80%)	3851 (97%)	124 (3%)	3 (0%)	48	76
1	D	3978/4967 (80%)	3850 (97%)	125 (3%)	3 (0%)	48	76
2	E	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	F	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	G	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	H	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
All	All	16332/20300 (80%)	15805 (97%)	515 (3%)	12 (0%)	50	76

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2988	ARG

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Mol	Chain	Res	Type
1	A	3927	PRO
1	A	4641	PRO
1	B	2988	ARG
1	B	3927	PRO
1	B	4641	PRO
1	C	2988	ARG
1	C	3927	PRO
1	C	4641	PRO
1	D	2988	ARG
1	D	3927	PRO
1	D	4641	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	3513/4358 (81%)	3452 (98%)	61 (2%)	56	74
1	B	3513/4358 (81%)	3452 (98%)	61 (2%)	56	74
1	C	3513/4358 (81%)	3452 (98%)	61 (2%)	56	74
1	D	3513/4358 (81%)	3452 (98%)	61 (2%)	56	74
2	E	88/89 (99%)	85 (97%)	3 (3%)	32	59
2	F	88/89 (99%)	85 (97%)	3 (3%)	32	59
2	G	88/89 (99%)	85 (97%)	3 (3%)	32	59
2	H	88/89 (99%)	85 (97%)	3 (3%)	32	59
All	All	14404/17788 (81%)	14148 (98%)	256 (2%)	54	74

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	372	LEU
1	A	655	MET
1	A	742	SER
1	A	799	LYS

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Mol	Chain	Res	Type
1	A	880	ARG
1	A	882	ARG
1	A	884	LYS
1	A	929	ARG
1	A	960	LYS
1	A	965	LYS
1	A	998	LYS
1	A	1022	GLN
1	A	1025	LYS
1	A	1027	ARG
1	A	1041	ARG
1	A	1057	LEU
1	A	1202	ILE
1	A	1473	LYS
1	A	1960	ARG
1	A	1983	LYS
1	A	2384	MET
1	A	2447	LYS
1	A	2586	GLN
1	A	2609	LEU
1	A	2656	LYS
1	A	2720	PHE
1	A	2758	LYS
1	A	2765	GLU
1	A	2768	LYS
1	A	2782	MET
1	A	2836	ASP
1	A	2840	MET
1	A	2844	MET
1	A	2871	LEU
1	A	2880	LYS
1	A	2884	LYS
1	A	2886	ARG
1	A	2888	LYS
1	A	2979	ARG
1	A	2988	ARG
1	A	3007	LEU
1	A	3018	ARG
1	A	3021	LEU
1	A	3033	LEU
1	A	3051	GLU
1	A	3600	VAL

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Mol	Chain	Res	Type
1	A	3739	MET
1	A	4002	MET
1	A	4066	LEU
1	A	4162	LYS
1	A	4186	MET
1	A	4205	GLN
1	A	4266	LYS
1	A	4268	MET
1	A	4274	MET
1	A	4292	MET
1	A	4306	PHE
1	A	4504	MET
1	A	4707	MET
1	A	4887	LYS
1	A	4965	GLN
2	E	18	LYS
2	E	19	LYS
2	E	50	ARG
2	F	18	LYS
2	F	19	LYS
2	F	50	ARG
2	G	18	LYS
2	G	19	LYS
2	G	50	ARG
2	H	18	LYS
2	H	19	LYS
2	H	50	ARG
1	B	372	LEU
1	B	655	MET
1	B	742	SER
1	B	799	LYS
1	B	880	ARG
1	B	882	ARG
1	B	884	LYS
1	B	929	ARG
1	B	960	LYS
1	B	965	LYS
1	B	998	LYS
1	B	1022	GLN
1	B	1025	LYS
1	B	1027	ARG
1	B	1041	ARG

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Mol	Chain	Res	Type
1	B	1057	LEU
1	B	1202	ILE
1	B	1473	LYS
1	B	1960	ARG
1	B	1983	LYS
1	B	2384	MET
1	B	2447	LYS
1	B	2586	GLN
1	B	2609	LEU
1	B	2656	LYS
1	B	2720	PHE
1	B	2758	LYS
1	B	2765	GLU
1	B	2768	LYS
1	B	2782	MET
1	B	2836	ASP
1	B	2840	MET
1	B	2844	MET
1	B	2871	LEU
1	B	2880	LYS
1	B	2884	LYS
1	B	2886	ARG
1	B	2888	LYS
1	B	2979	ARG
1	B	2988	ARG
1	B	3007	LEU
1	B	3018	ARG
1	B	3021	LEU
1	B	3033	LEU
1	B	3051	GLU
1	B	3600	VAL
1	B	3739	MET
1	B	4002	MET
1	B	4066	LEU
1	B	4162	LYS
1	B	4186	MET
1	B	4205	GLN
1	B	4266	LYS
1	B	4268	MET
1	B	4274	MET
1	B	4292	MET
1	B	4306	PHE

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Mol	Chain	Res	Type
1	B	4504	MET
1	B	4707	MET
1	B	4887	LYS
1	B	4965	GLN
1	C	372	LEU
1	C	655	MET
1	C	742	SER
1	C	799	LYS
1	C	880	ARG
1	C	882	ARG
1	C	884	LYS
1	C	929	ARG
1	C	960	LYS
1	C	965	LYS
1	C	998	LYS
1	C	1022	GLN
1	C	1025	LYS
1	C	1027	ARG
1	C	1041	ARG
1	C	1057	LEU
1	C	1202	ILE
1	C	1473	LYS
1	C	1960	ARG
1	C	1983	LYS
1	C	2384	MET
1	C	2447	LYS
1	C	2586	GLN
1	C	2609	LEU
1	C	2656	LYS
1	C	2720	PHE
1	C	2758	LYS
1	C	2765	GLU
1	C	2768	LYS
1	C	2782	MET
1	C	2836	ASP
1	C	2840	MET
1	C	2844	MET
1	C	2871	LEU
1	C	2880	LYS
1	C	2884	LYS
1	C	2886	ARG
1	C	2888	LYS

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Mol	Chain	Res	Type
1	C	2979	ARG
1	C	2988	ARG
1	C	3007	LEU
1	C	3018	ARG
1	C	3021	LEU
1	C	3033	LEU
1	C	3051	GLU
1	C	3600	VAL
1	C	3739	MET
1	C	4002	MET
1	C	4066	LEU
1	C	4162	LYS
1	C	4186	MET
1	C	4205	GLN
1	C	4266	LYS
1	C	4268	MET
1	C	4274	MET
1	C	4292	MET
1	C	4306	PHE
1	C	4504	MET
1	C	4707	MET
1	C	4887	LYS
1	C	4965	GLN
1	D	372	LEU
1	D	655	MET
1	D	742	SER
1	D	799	LYS
1	D	880	ARG
1	D	882	ARG
1	D	884	LYS
1	D	929	ARG
1	D	960	LYS
1	D	965	LYS
1	D	998	LYS
1	D	1022	GLN
1	D	1025	LYS
1	D	1027	ARG
1	D	1041	ARG
1	D	1057	LEU
1	D	1202	ILE
1	D	1473	LYS
1	D	1960	ARG

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Mol	Chain	Res	Type
1	D	1983	LYS
1	D	2384	MET
1	D	2447	LYS
1	D	2586	GLN
1	D	2609	LEU
1	D	2656	LYS
1	D	2720	PHE
1	D	2758	LYS
1	D	2765	GLU
1	D	2768	LYS
1	D	2782	MET
1	D	2836	ASP
1	D	2840	MET
1	D	2844	MET
1	D	2871	LEU
1	D	2880	LYS
1	D	2884	LYS
1	D	2886	ARG
1	D	2888	LYS
1	D	2979	ARG
1	D	2988	ARG
1	D	3007	LEU
1	D	3018	ARG
1	D	3021	LEU
1	D	3033	LEU
1	D	3051	GLU
1	D	3600	VAL
1	D	3739	MET
1	D	4002	MET
1	D	4066	LEU
1	D	4162	LYS
1	D	4186	MET
1	D	4205	GLN
1	D	4266	LYS
1	D	4268	MET
1	D	4274	MET
1	D	4292	MET
1	D	4306	PHE
1	D	4504	MET
1	D	4707	MET
1	D	4887	LYS
1	D	4965	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	HIS
1	A	198	ASN
1	A	544	ASN
1	A	888	ASN
1	A	890	HIS
1	A	915	HIS
1	A	927	GLN
1	A	934	GLN
1	A	1046	ASN
1	A	1452	GLN
1	A	1546	GLN
1	A	2309	ASN
1	A	3811	GLN
1	A	3903	GLN
1	A	3931	ASN
1	A	4514	ASN
1	B	117	HIS
1	B	544	ASN
1	B	888	ASN
1	B	890	HIS
1	B	915	HIS
1	B	927	GLN
1	B	934	GLN
1	B	1046	ASN
1	B	1452	GLN
1	B	1546	GLN
1	B	2309	ASN
1	B	2540	HIS
1	B	3811	GLN
1	B	3903	GLN
1	B	3931	ASN
1	B	4514	ASN
1	C	117	HIS
1	C	198	ASN
1	C	544	ASN
1	C	888	ASN
1	C	890	HIS
1	C	915	HIS
1	C	927	GLN
1	C	934	GLN
1	C	1046	ASN

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Mol	Chain	Res	Type
1	C	1452	GLN
1	C	1546	GLN
1	C	2309	ASN
1	C	3811	GLN
1	C	3903	GLN
1	C	3931	ASN
1	C	4514	ASN
1	D	117	HIS
1	D	544	ASN
1	D	888	ASN
1	D	915	HIS
1	D	927	GLN
1	D	934	GLN
1	D	1046	ASN
1	D	1452	GLN
1	D	1546	GLN
1	D	2309	ASN
1	D	3811	GLN
1	D	3903	GLN
1	D	3931	ASN
1	D	4514	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [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
4	ATP	A	5002	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
4	ATP	D	5004	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
4	ATP	C	5004	-	28,33,33	0.63	0	34,52,52	0.58	1 (2%)
4	ATP	A	5004	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
4	ATP	D	5002	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
4	ATP	B	5002	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
4	ATP	C	5002	-	28,33,33	0.63	0	34,52,52	0.58	1 (2%)
4	ATP	B	5004	-	28,33,33	0.64	0	34,52,52	0.58	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	5002	-	-	10/18/38/38	0/3/3/3
4	ATP	D	5004	-	-	6/18/38/38	0/3/3/3
4	ATP	C	5004	-	-	6/18/38/38	0/3/3/3
4	ATP	A	5004	-	-	6/18/38/38	0/3/3/3
4	ATP	D	5002	-	-	10/18/38/38	0/3/3/3
4	ATP	B	5002	-	-	10/18/38/38	0/3/3/3
4	ATP	C	5002	-	-	10/18/38/38	0/3/3/3
4	ATP	B	5004	-	-	6/18/38/38	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	5004	ATP	C5-C6-N6	2.35	123.90	120.31
4	A	5004	ATP	C5-C6-N6	2.33	123.86	120.31
4	D	5002	ATP	C5-C6-N6	2.32	123.85	120.31
4	B	5004	ATP	C5-C6-N6	2.32	123.85	120.31
4	B	5002	ATP	C5-C6-N6	2.32	123.84	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	A	5002	ATP	C5-C6-N6	2.32	123.84	120.31
4	C	5002	ATP	C5-C6-N6	2.29	123.80	120.31
4	C	5004	ATP	C5-C6-N6	2.28	123.78	120.31

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	PB-O3A-PA-O5'
4	A	5002	ATP	C5'-O5'-PA-O1A
4	A	5002	ATP	C5'-O5'-PA-O2A
4	A	5002	ATP	C5'-O5'-PA-O3A
4	B	5002	ATP	PB-O3A-PA-O5'
4	B	5002	ATP	C5'-O5'-PA-O1A
4	B	5002	ATP	C5'-O5'-PA-O2A
4	B	5002	ATP	C5'-O5'-PA-O3A
4	C	5002	ATP	PB-O3A-PA-O5'
4	C	5002	ATP	C5'-O5'-PA-O1A
4	C	5002	ATP	C5'-O5'-PA-O2A
4	C	5002	ATP	C5'-O5'-PA-O3A
4	D	5002	ATP	PB-O3A-PA-O5'
4	D	5002	ATP	C5'-O5'-PA-O1A
4	D	5002	ATP	C5'-O5'-PA-O2A
4	D	5002	ATP	C5'-O5'-PA-O3A
4	A	5002	ATP	C3'-C4'-C5'-O5'
4	B	5002	ATP	C3'-C4'-C5'-O5'
4	C	5002	ATP	C3'-C4'-C5'-O5'
4	D	5002	ATP	C3'-C4'-C5'-O5'
4	A	5002	ATP	O4'-C4'-C5'-O5'
4	B	5002	ATP	O4'-C4'-C5'-O5'
4	C	5002	ATP	O4'-C4'-C5'-O5'
4	D	5002	ATP	O4'-C4'-C5'-O5'
4	A	5004	ATP	PB-O3B-PG-O1G
4	B	5004	ATP	PB-O3B-PG-O1G
4	C	5004	ATP	PB-O3B-PG-O1G
4	D	5004	ATP	PB-O3B-PG-O1G
4	A	5002	ATP	PG-O3B-PB-O3A
4	B	5002	ATP	PG-O3B-PB-O3A
4	C	5002	ATP	PG-O3B-PB-O3A
4	D	5002	ATP	PG-O3B-PB-O3A
4	A	5004	ATP	C5'-O5'-PA-O1A
4	A	5004	ATP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
4	A	5004	ATP	C5'-O5'-PA-O3A
4	B	5004	ATP	C5'-O5'-PA-O1A
4	B	5004	ATP	C5'-O5'-PA-O2A
4	B	5004	ATP	C5'-O5'-PA-O3A
4	C	5004	ATP	C5'-O5'-PA-O1A
4	C	5004	ATP	C5'-O5'-PA-O2A
4	C	5004	ATP	C5'-O5'-PA-O3A
4	D	5004	ATP	C5'-O5'-PA-O1A
4	D	5004	ATP	C5'-O5'-PA-O2A
4	D	5004	ATP	C5'-O5'-PA-O3A
4	A	5004	ATP	PB-O3B-PG-O2G
4	A	5004	ATP	PB-O3B-PG-O3G
4	B	5004	ATP	PB-O3B-PG-O2G
4	B	5004	ATP	PB-O3B-PG-O3G
4	C	5004	ATP	PB-O3B-PG-O2G
4	C	5004	ATP	PB-O3B-PG-O3G
4	D	5004	ATP	PB-O3B-PG-O2G
4	D	5004	ATP	PB-O3B-PG-O3G
4	A	5002	ATP	PG-O3B-PB-O2B
4	A	5002	ATP	PB-O3A-PA-O1A
4	A	5002	ATP	PB-O3A-PA-O2A
4	B	5002	ATP	PG-O3B-PB-O2B
4	B	5002	ATP	PB-O3A-PA-O1A
4	B	5002	ATP	PB-O3A-PA-O2A
4	C	5002	ATP	PG-O3B-PB-O2B
4	C	5002	ATP	PB-O3A-PA-O1A
4	C	5002	ATP	PB-O3A-PA-O2A
4	D	5002	ATP	PG-O3B-PB-O2B
4	D	5002	ATP	PB-O3A-PA-O1A
4	D	5002	ATP	PB-O3A-PA-O2A

There are no ring outliers.

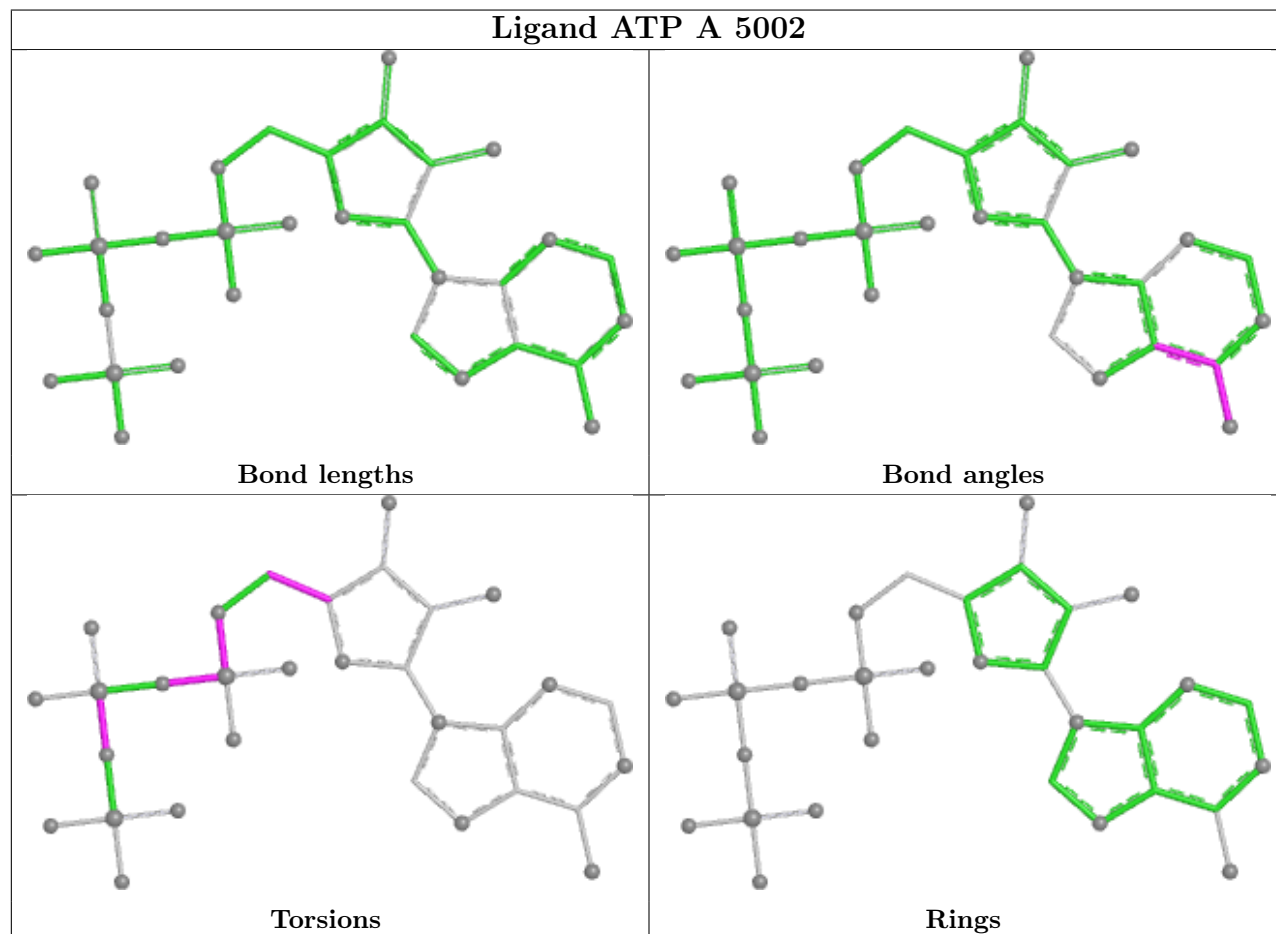
4 monomers are involved in 8 short contacts:

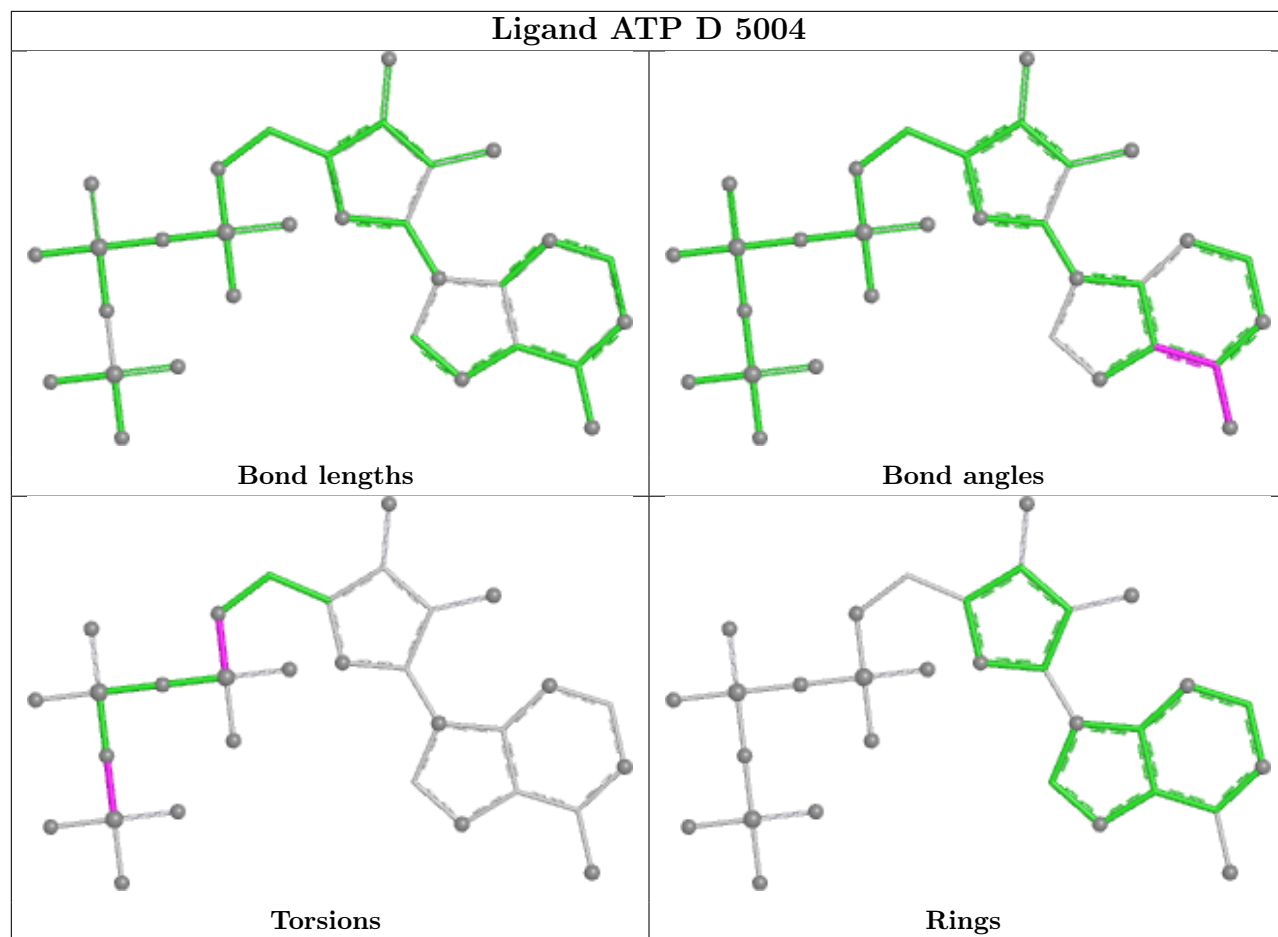
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5004	ATP	2	0
4	C	5004	ATP	2	0
4	A	5004	ATP	2	0
4	B	5004	ATP	2	0

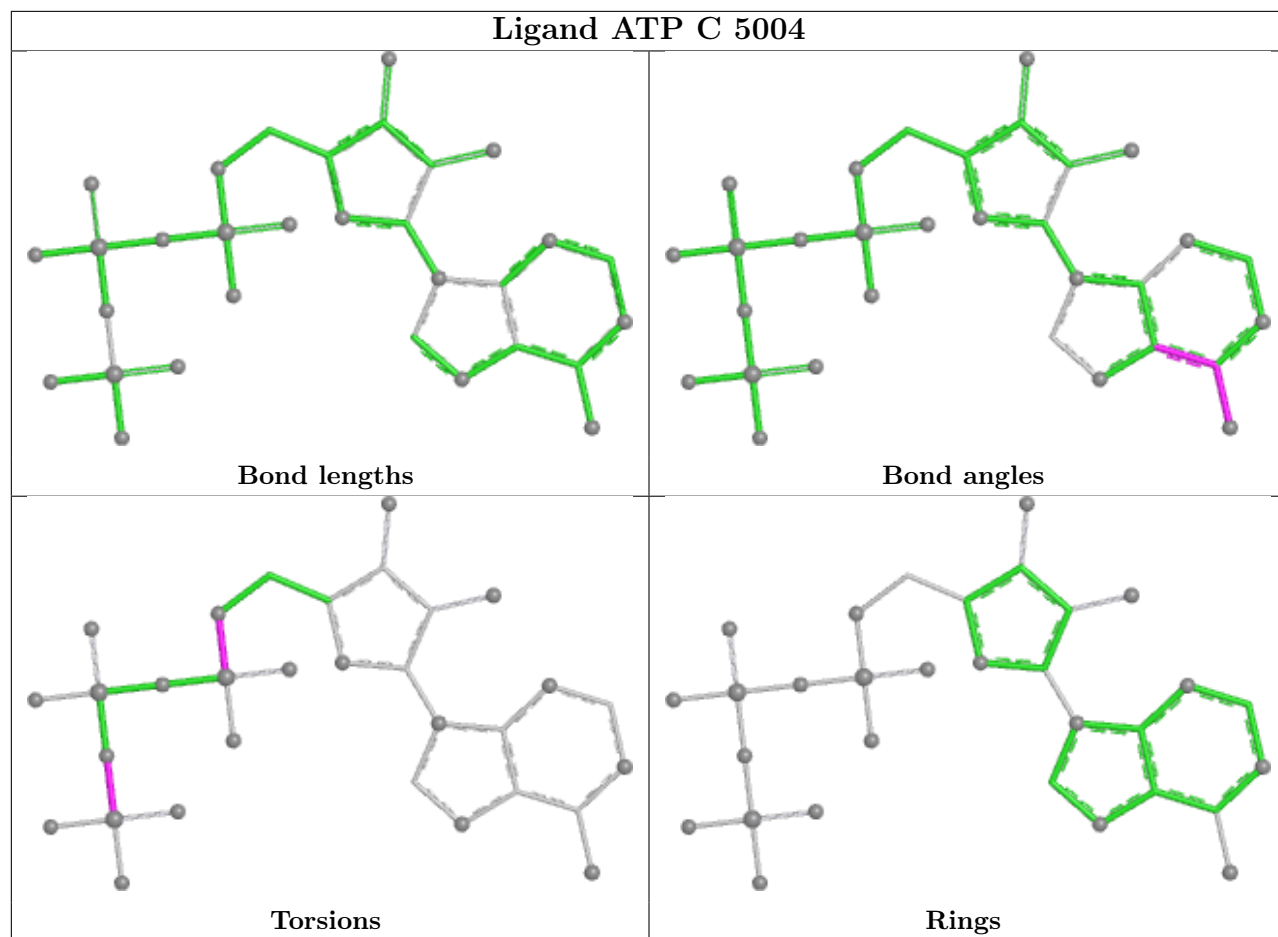
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

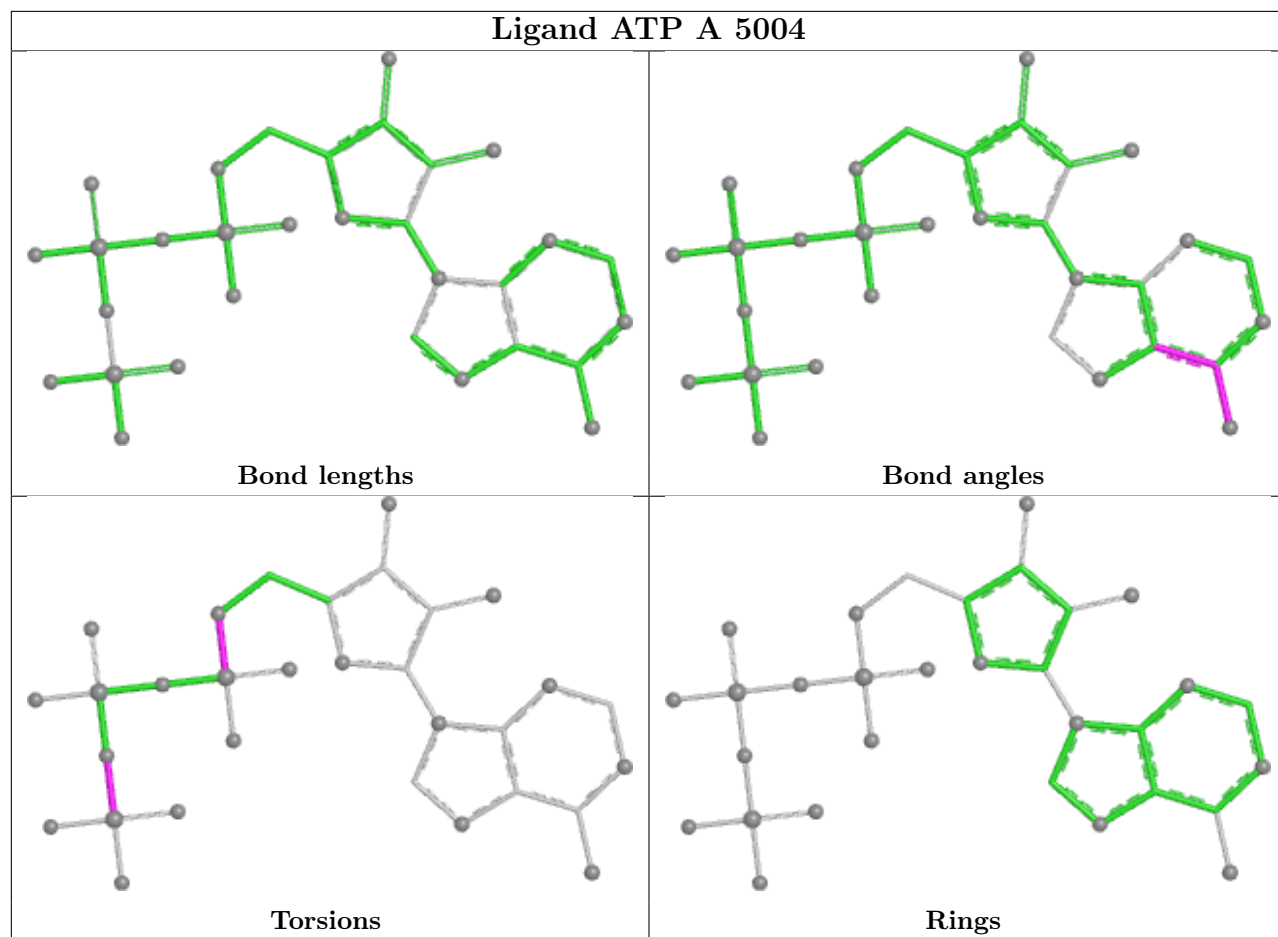


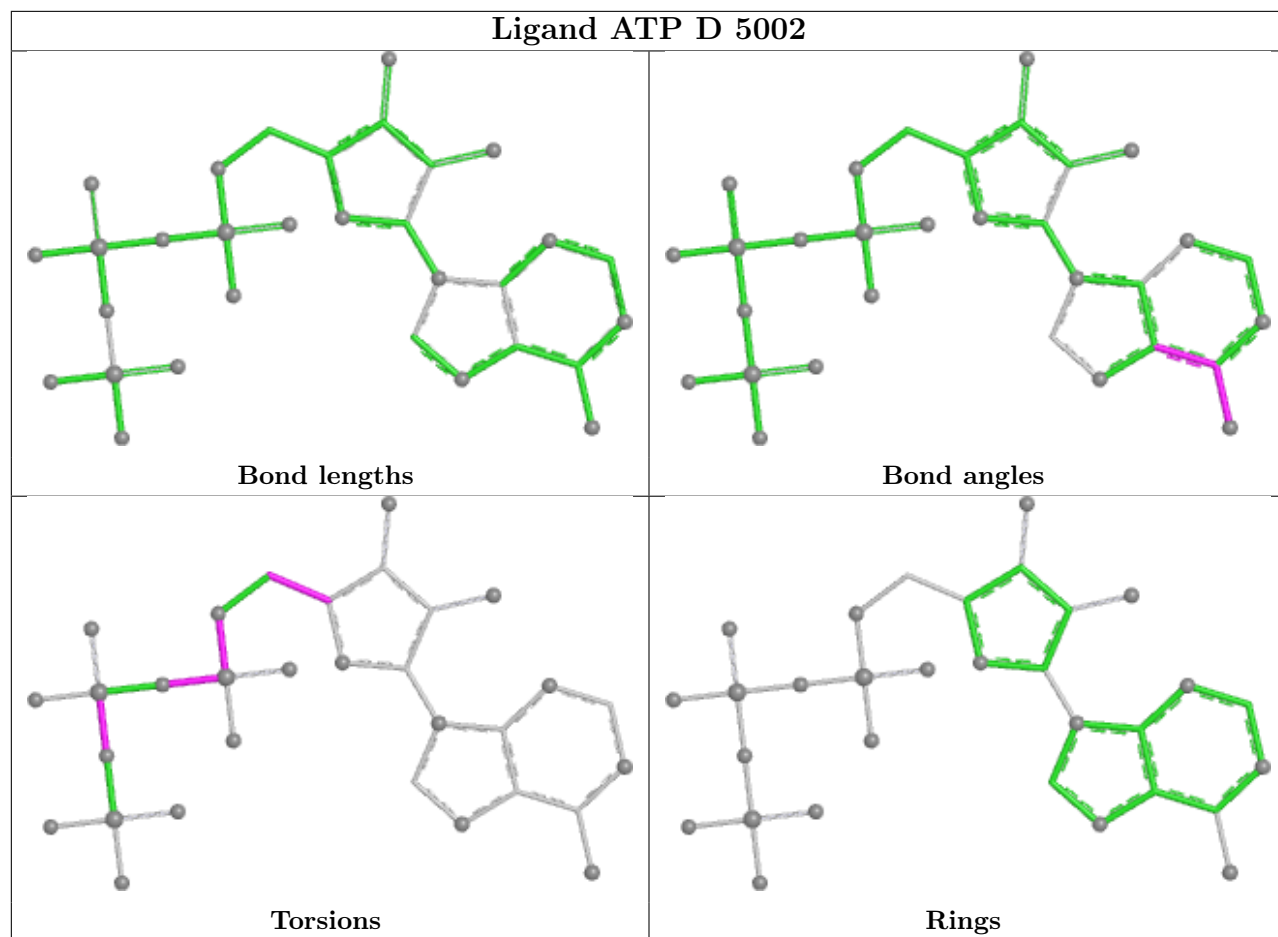
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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

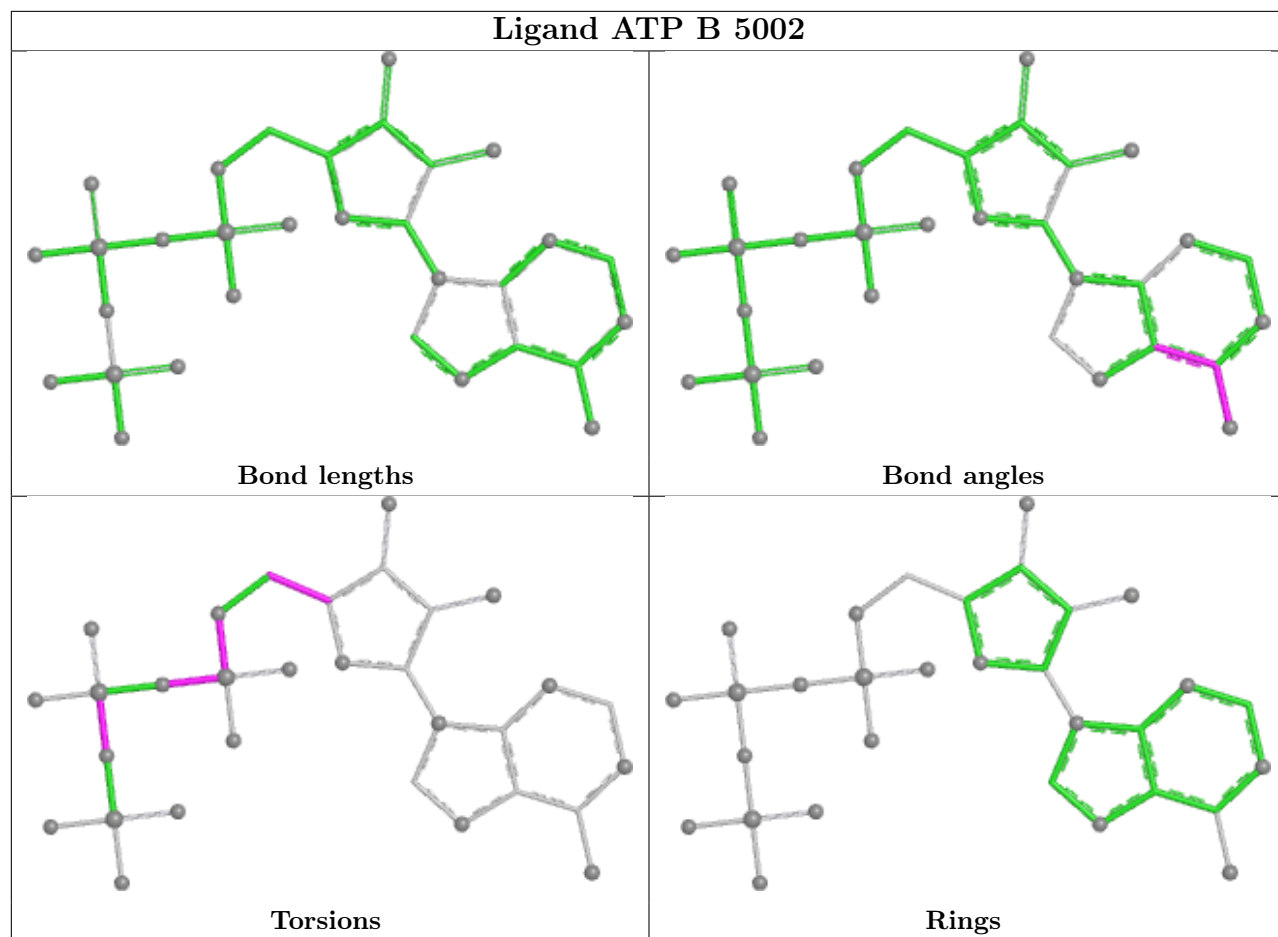


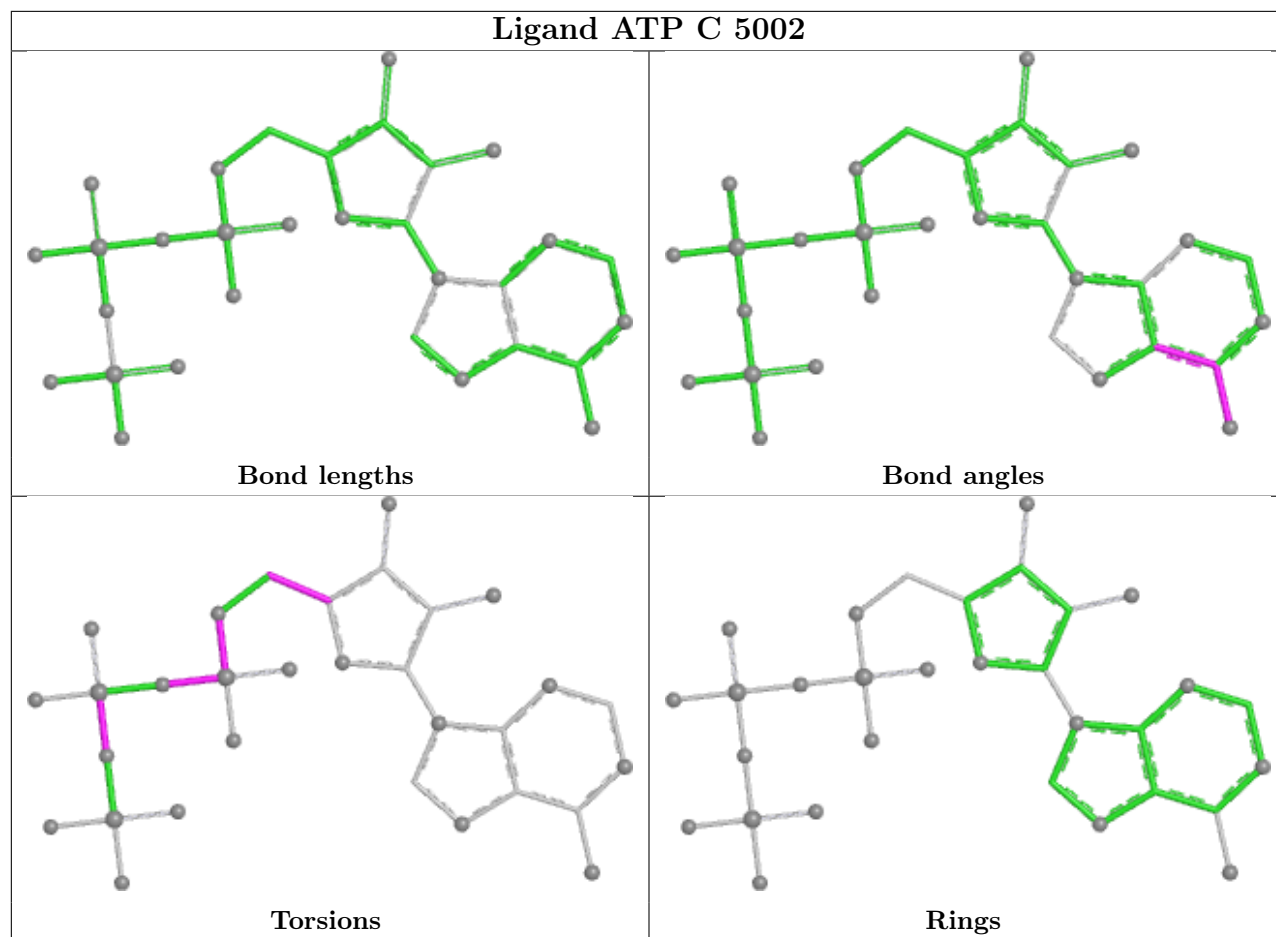


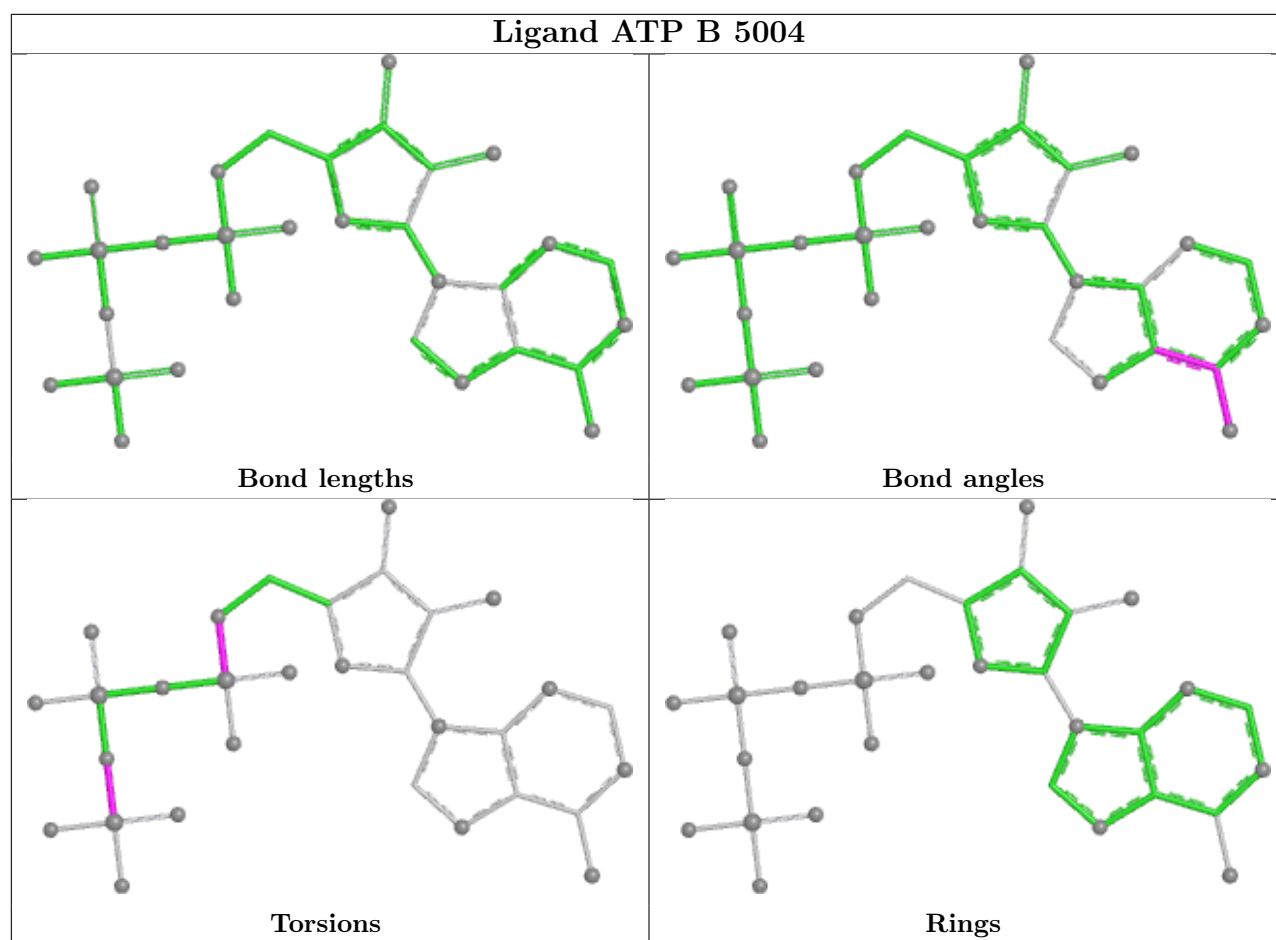












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



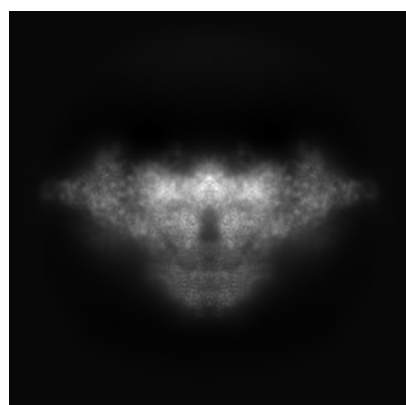
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42765. These allow visual inspection of the internal detail of the map and identification of artifacts.

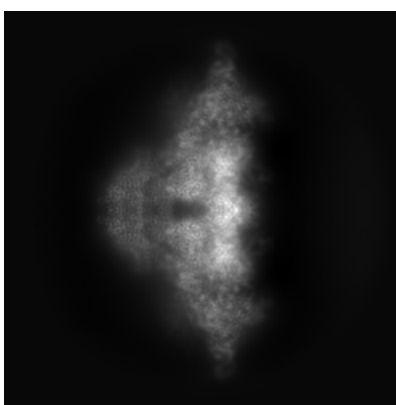
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

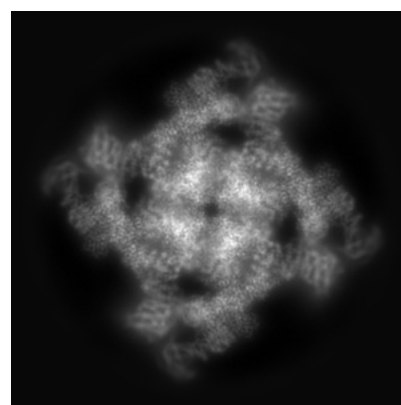
#### 6.1.1 Primary map



X



Y

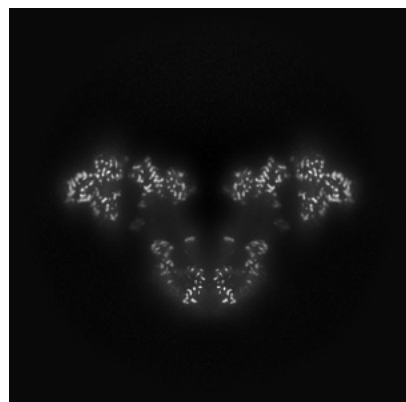


Z

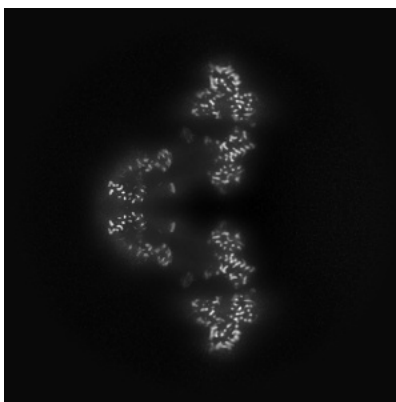
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

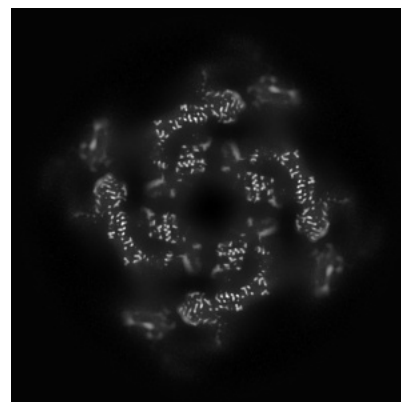
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

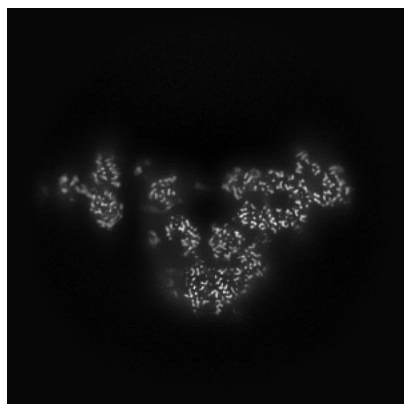


Z Index: 256

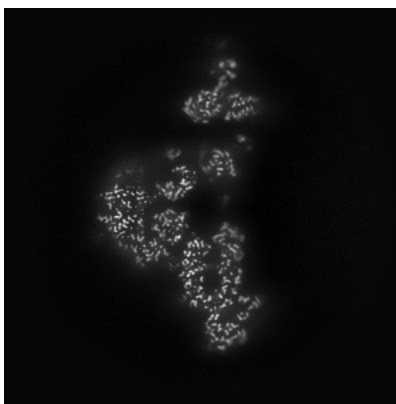
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

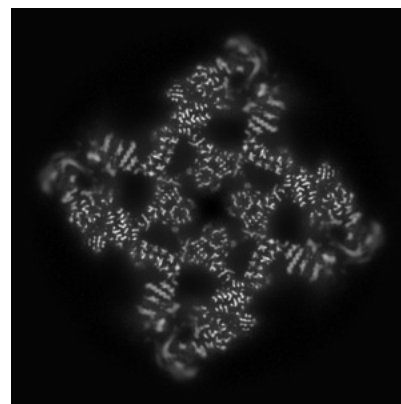
### 6.3.1 Primary map



X Index: 239



Y Index: 239

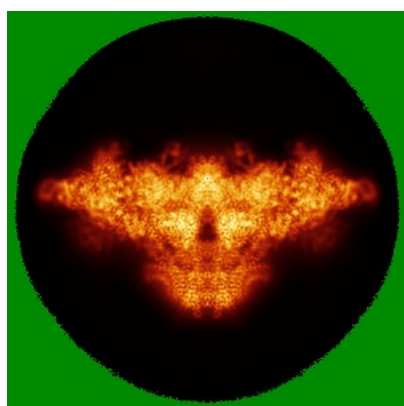


Z Index: 277

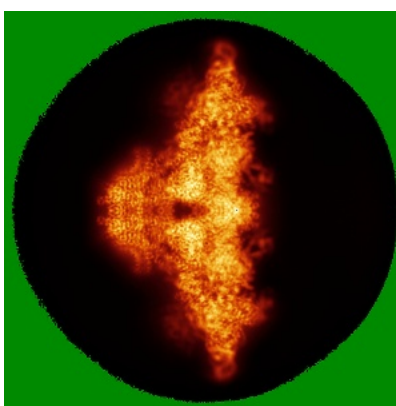
The images above show the largest variance slices of the map in three orthogonal directions.

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

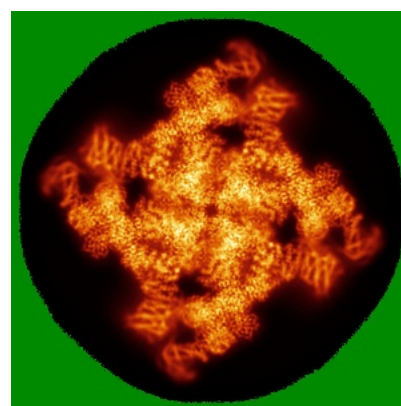
### 6.4.1 Primary map



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

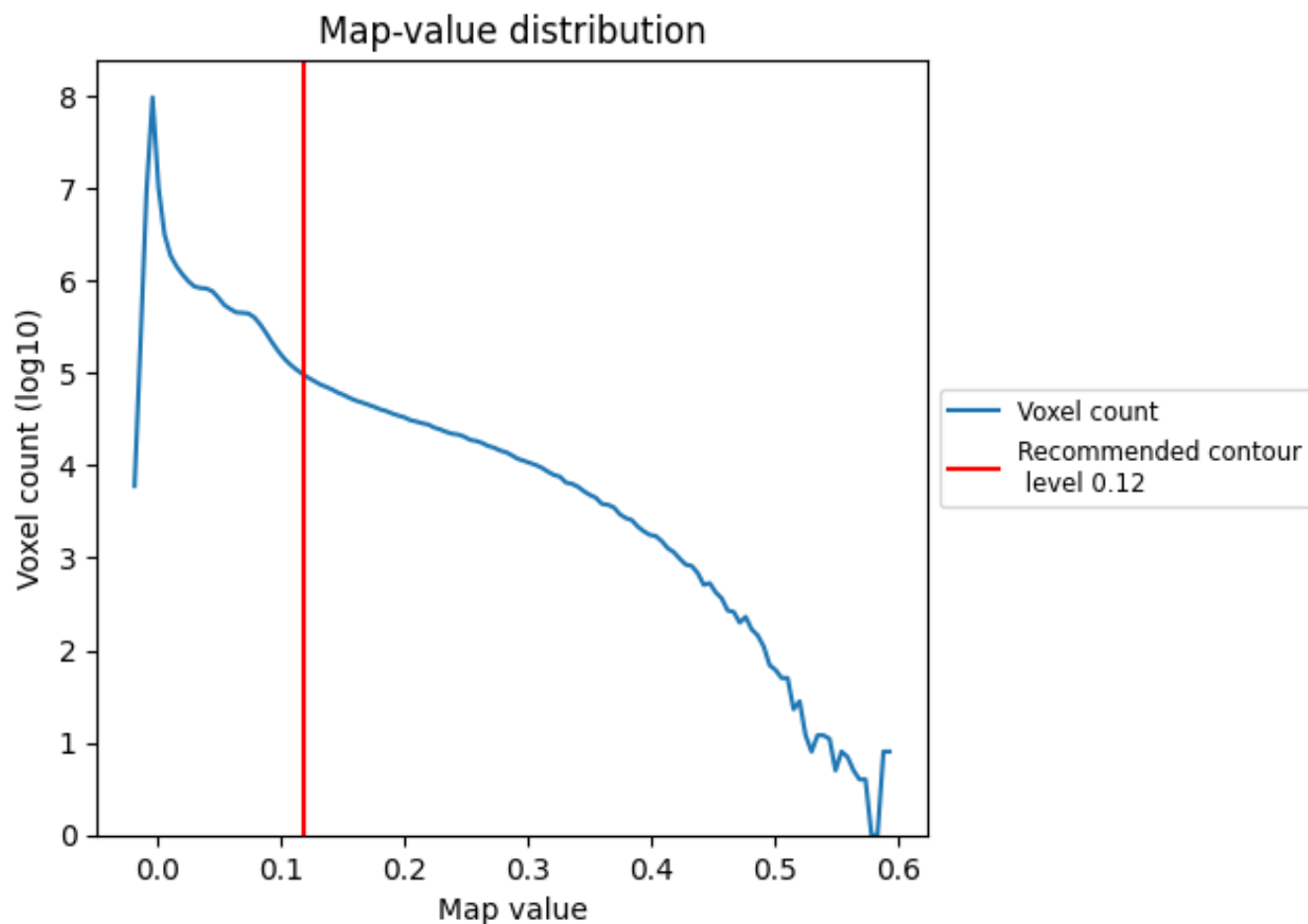
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

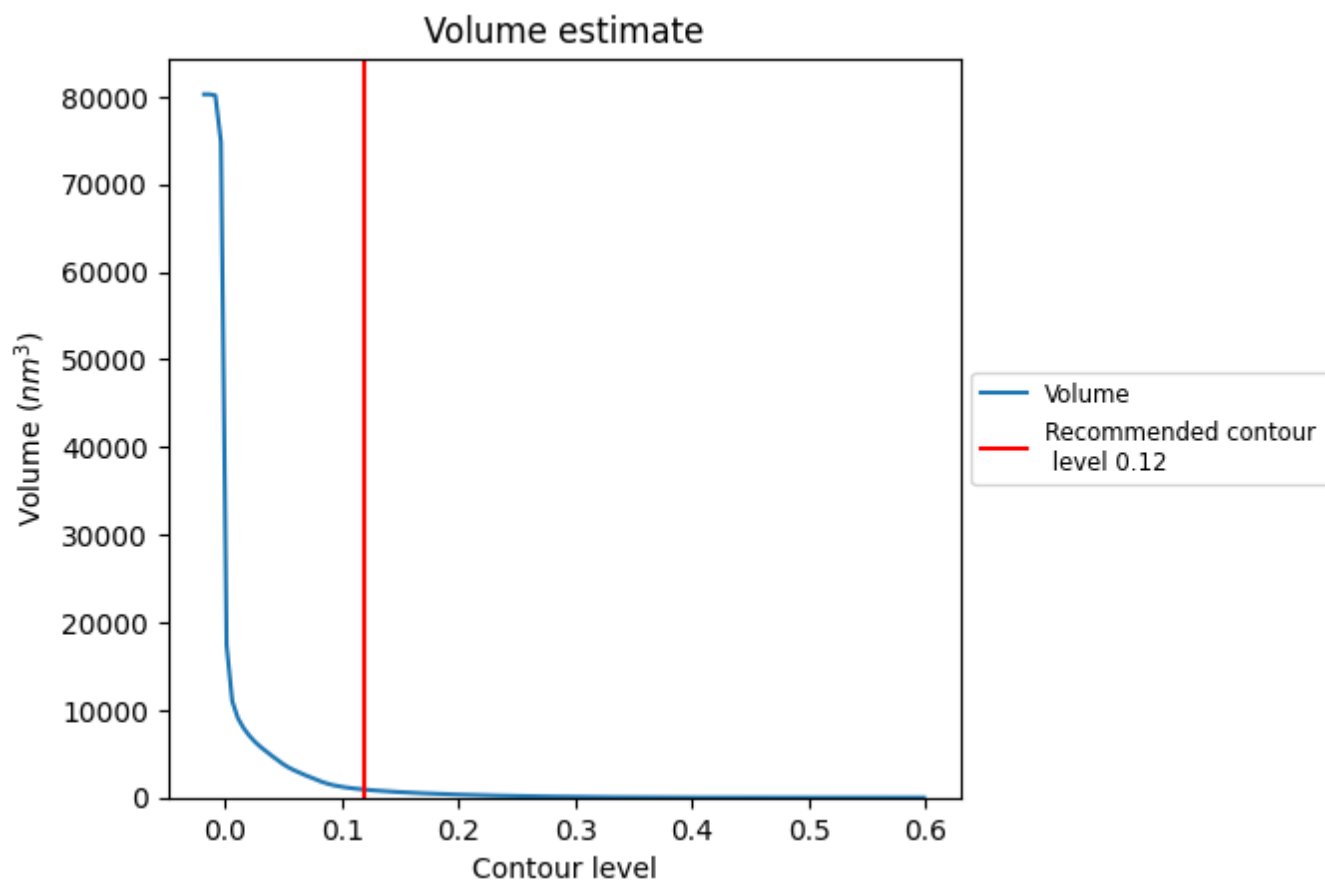
This section contains the results of statistical analysis of the map.

### 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.

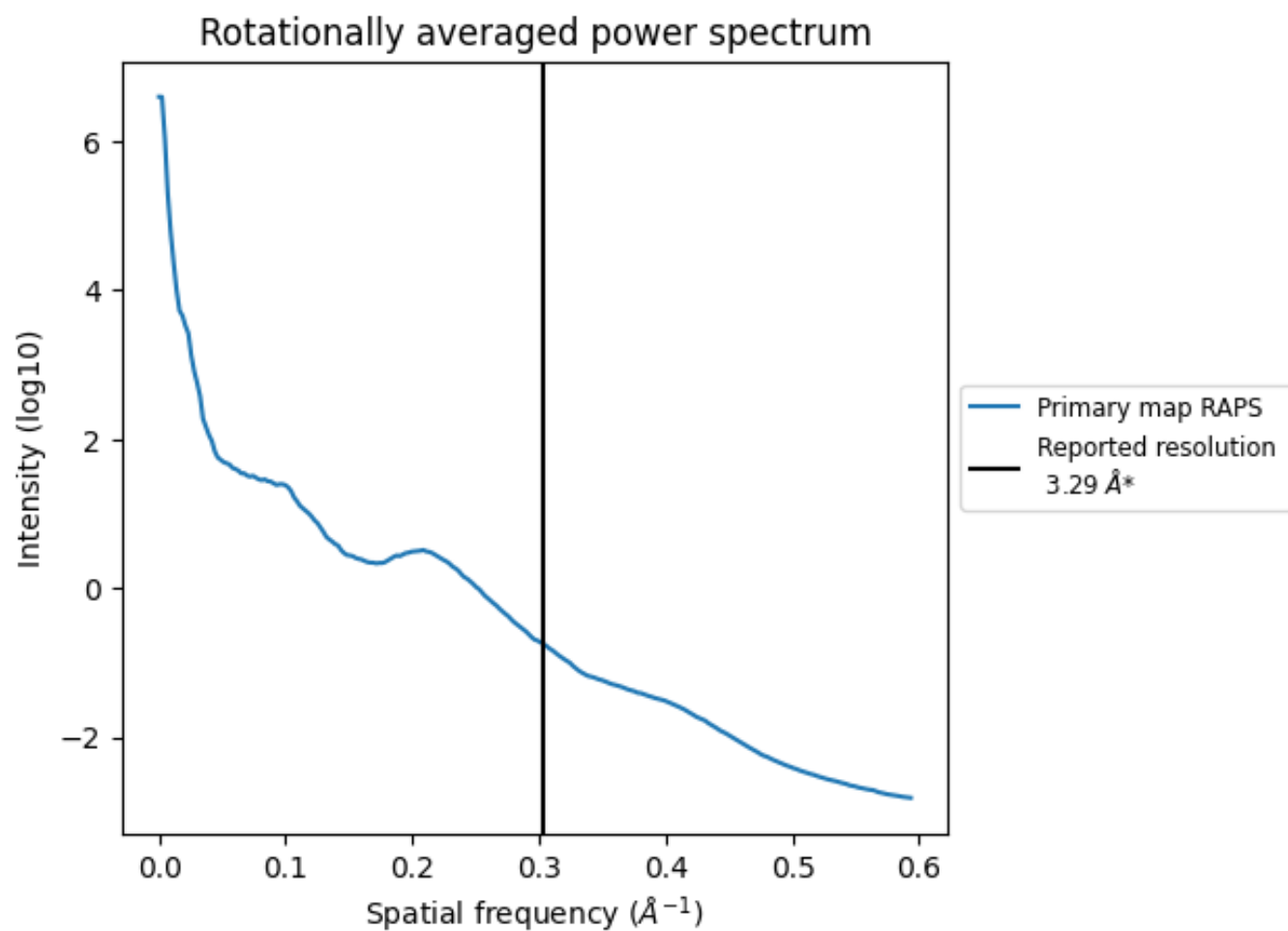
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 906 nm<sup>3</sup>; this corresponds to an approximate mass of 818 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 0.304 Å<sup>-1</sup>

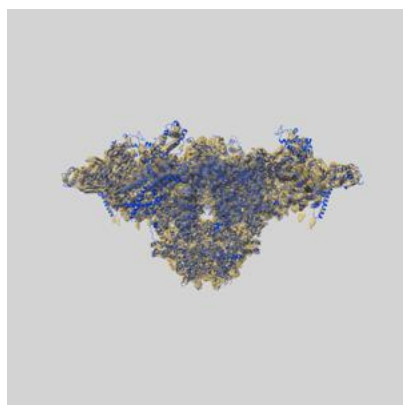
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

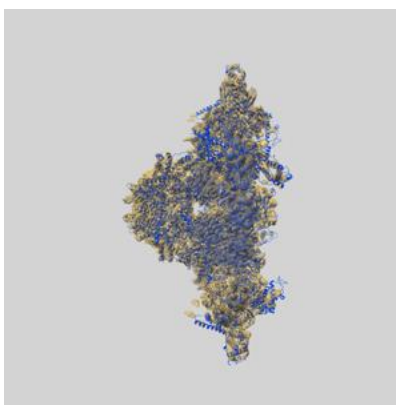
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42765 and PDB model 8UXI. Per-residue inclusion information can be found in section [3](#) on page [6](#).

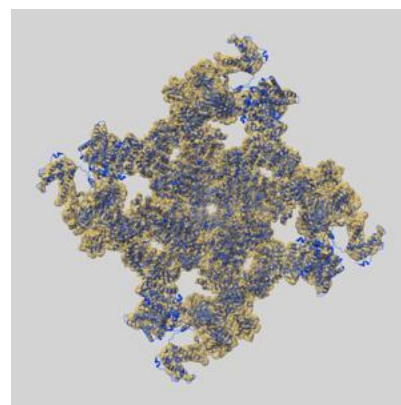
### 9.1 Map-model overlay [i](#)



X



Y

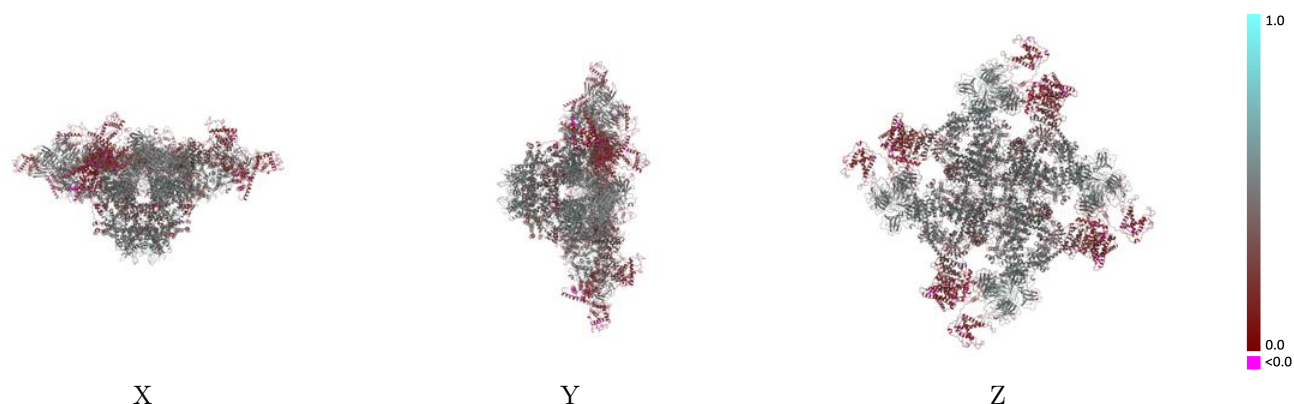


Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

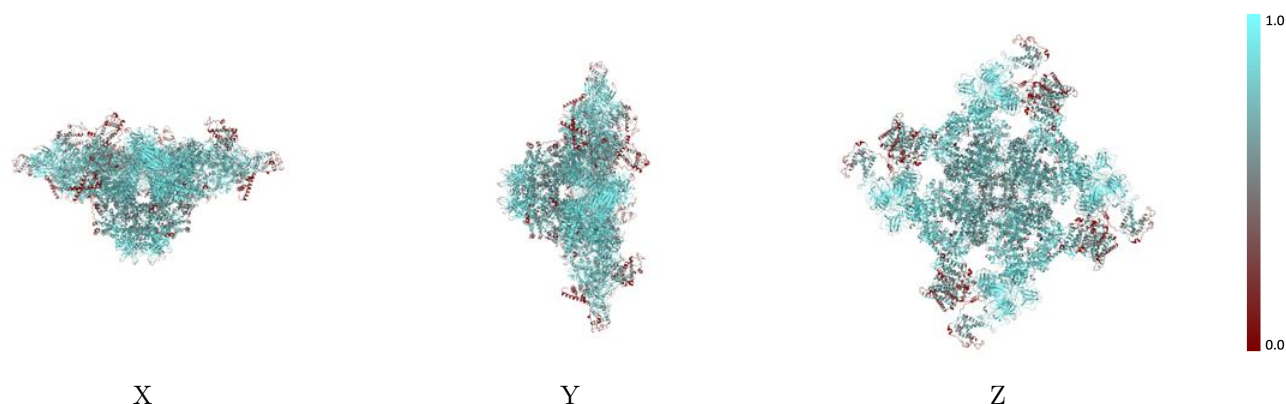


## 9.2 Q-score mapped to coordinate model [i](#)



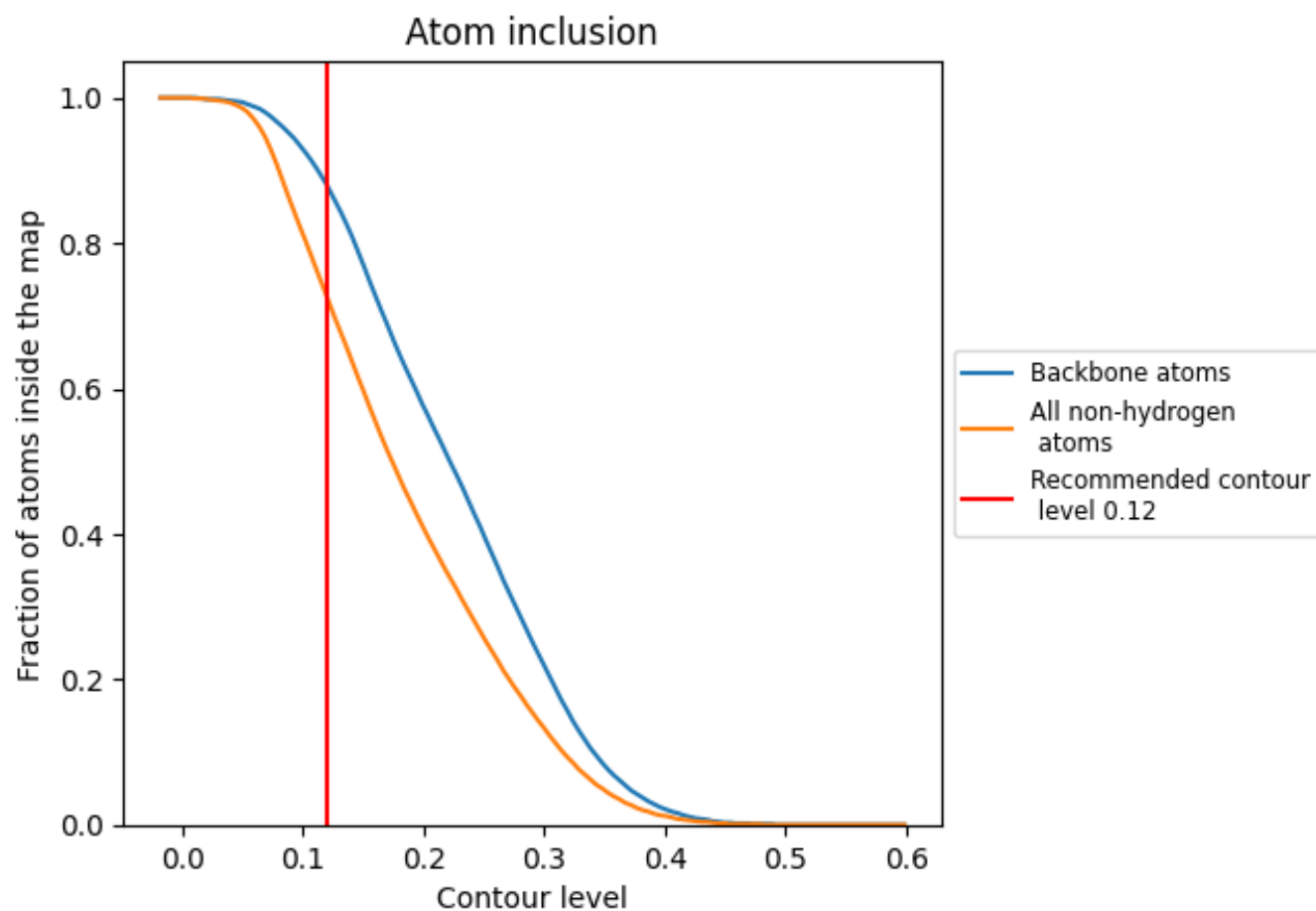
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 73% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7260	<div></div> 0.3900
A	<div></div> 0.7250	<div></div> 0.3900
B	<div></div> 0.7210	<div></div> 0.3840
C	<div></div> 0.7290	<div></div> 0.3950
D	<div></div> 0.7170	<div></div> 0.3790
E	<div></div> 0.8420	<div></div> 0.4870
F	<div></div> 0.8340	<div></div> 0.4830
G	<div></div> 0.8420	<div></div> 0.4880
H	<div></div> 0.8510	<div></div> 0.4860

