



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:27 PM UTC

PDB ID : 8DTZ / pdb_00008dtz
EMDB ID : EMD-27712
Title : Recombinant mouse RyR2 triple phosphonull mutant
S2807A/S2813A/S2030A in complex with FKBP12.6 and nanodisc under closed-state conditions
Authors : Iyer, K.A.; Hu, Y.; Murayama, T.; Samso, M.
Deposited on : 2022-07-26
Resolution : 3.60 Å (reported)
Based on initial model : 6WOU

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

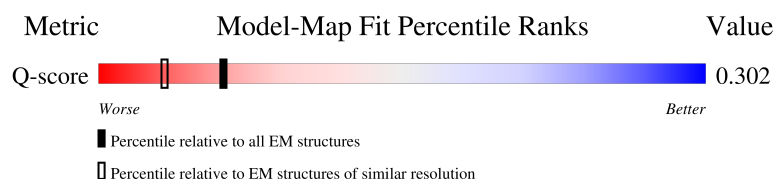
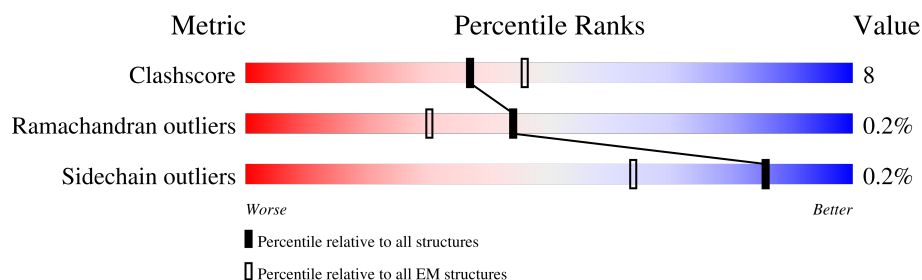
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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

Mol	Chain	Length	Quality of chain
1	A	4966	9% 67% 15% 18%
1	B	4966	9% 67% 15% 18%
1	C	4966	9% 67% 15% 18%
1	D	4966	9% 67% 15% 18%

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Mol	Chain	Length	Quality of chain
2	E	107	 75%25%
2	F	107	 75%25%
2	G	107	 74%26%
2	H	107	 74%26%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 129524 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	4061	Total	C	N	O	S	0	0
			31562	20044	5390	5931	197		
1	B	4061	Total	C	N	O	S	0	0
			31562	20044	5390	5931	197		
1	C	4061	Total	C	N	O	S	0	0
			31562	20044	5390	5931	197		
1	D	4061	Total	C	N	O	S	0	0
			31562	20044	5390	5931	197		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2030	ALA	SER	engineered mutation	UNP E9Q401
A	2807	ALA	SER	engineered mutation	UNP E9Q401
A	2813	ALA	SER	engineered mutation	UNP E9Q401
B	2030	ALA	SER	engineered mutation	UNP E9Q401
B	2807	ALA	SER	engineered mutation	UNP E9Q401
B	2813	ALA	SER	engineered mutation	UNP E9Q401
C	2030	ALA	SER	engineered mutation	UNP E9Q401
C	2807	ALA	SER	engineered mutation	UNP E9Q401
C	2813	ALA	SER	engineered mutation	UNP E9Q401
D	2030	ALA	SER	engineered mutation	UNP E9Q401
D	2807	ALA	SER	engineered mutation	UNP E9Q401
D	2813	ALA	SER	engineered mutation	UNP E9Q401

- 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		

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

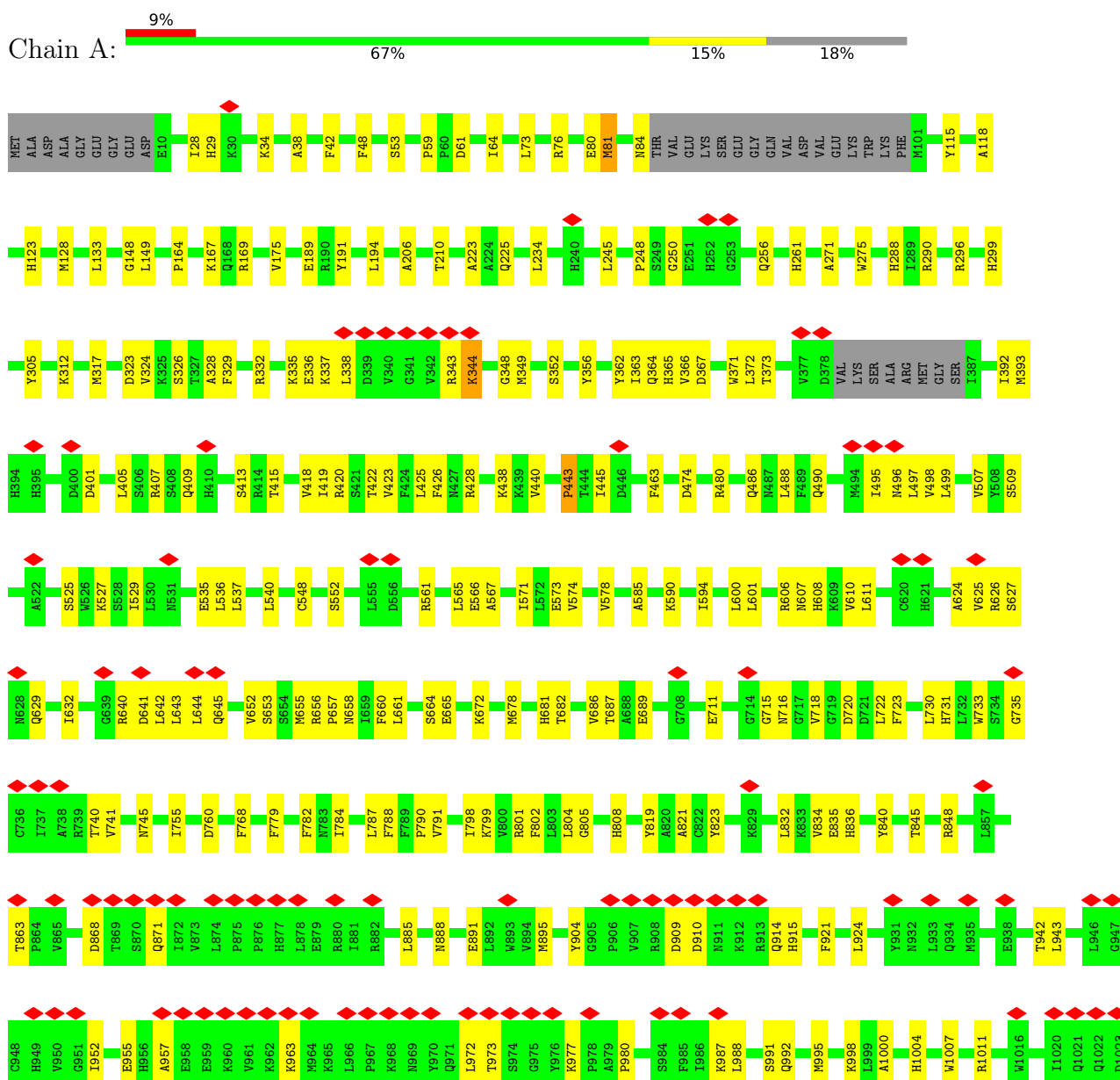
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots

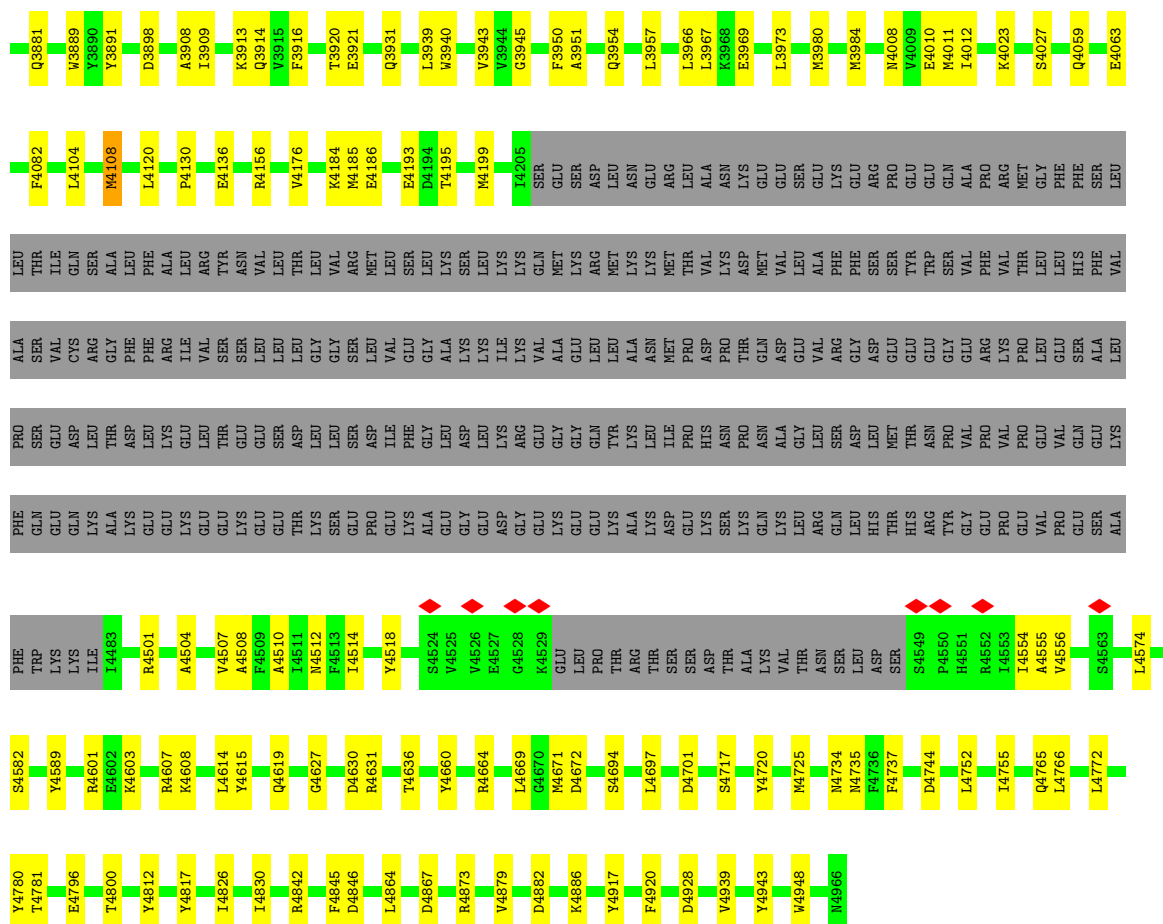
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

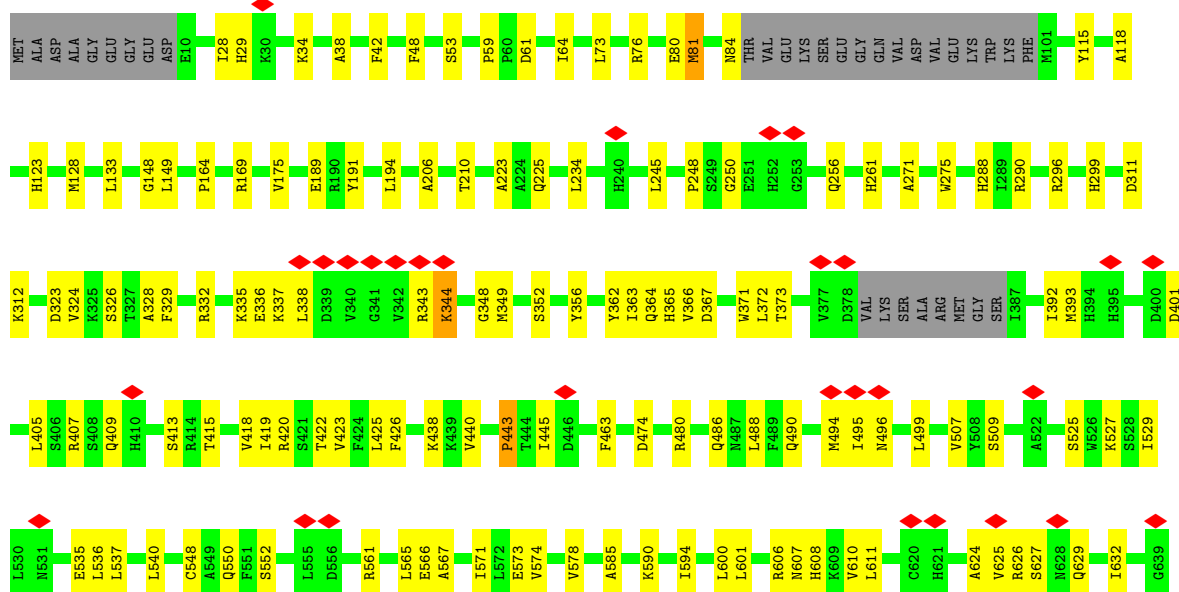


HIS	F2439	L2287	E2168	PRO	L1897	P1781	L1633	A1546	E1418	ARG	GLY	V1024
HIS	Q2440	G2288	T2169	C1987	V1901	P1784	P1634	Q1547	L1126	ILE	THR	K1025
ALA	M2441	W2289	W2170	D1983	M1905	P1784	E1635	Q1548	Y1426	ASP	ILE	
SER	P2442	N2290	E2171	D1983	M1905	I1787	E1636	T1549	Y1427	LYS	ASP	L1032
ILE	THR	C2307	E2172	R2027	L1908	L1796	R1637	S1550	Y1428	LYS	S1279	S1130
ASP	ALA	N2308	W2173	Y2027	L1908	L1796	R1638	N1551	S1429	GLU	D1131	
ASP	ALA	N2308	W2174	Y2027	L1908	L1796	R1638	N1552	I1432	THR	K1283	T1036
LEU	ASP	R2321	W2175	K2039	R1920	P1810	D1641	V1553	I1432	THR	K1284	R1041
LEU	ASP	N2176	N2176	LVS	R1920	P1810	L1642	F1554	P1433	PRO	V1285	
HIS	LVS	LVS	G2180	LVS	V1925	T1814	E1644	LEU	G1435	GLU	S1292	K1044
THR	LVS	LVS	G2181	ALA	V1925	T1815	L1645	GLY	G1153	GLU	V1166	S1045
VAL	L2334	L2334	G2181	GLU	D1929	E1816	T1646	ARG		ASN	T1287	
TYR	R2335	R2335	E2185	LYS	K1934	Y1827	E1647	ILE	G1444	ASN	T1287	D1048
ARG	PRO	R2336	E2186	PRO	R1934	Y1827	E1647	ILE	G1444	ASN	T1287	S1049
LEU	ASP	E2337	E2186	VAL	N1938	P1849	L1651	ASN	I1446	HIS	Y1302	L1050
SER	MET	E2337	E2186	VAL	N1938	P1849	L1651	ASN	I1446	LYS	R1303	R1051
LYS	SER	E2337	E2186	ALA	N1938	P1849	L1651	VAL	D1449	TYR	S1317	E1052
GLY	ALA	G2341	P2189	SER	R1942	VAL	F1654	GLY	F1450	ALA	A1319	A1053
CYS	L2342	L2342	K2190	ASP	Y1943	PHE	H1655	PRO	F1450	GLN	V1189	V1062
SER	L2343	L2343	W2191	SER	N1944	LYS	L1661	LEU	F1457	LYS	A1319	H1063
LEU	F2459	F2459	K2193	ARG	LVS	GLU	L1661	SER	F1457	GLY	A1319	L1064
THR	F2470	S2357	W2194	CYS	Q1948	ALA	S1679	ALA	V1465	GLY	A1319	E1189
ALA	R2473	R2358	C2195	LVS	A1949	ALA	H1680	GLY	V1465	PRO	GLY	L1190
GLN			R2197		L1950	VAL	L1686	LEU	V1465	SER	LEU	L1190
ARG	V2479	S2365	L2217	A2069	M1951	GLU	L1686	PHE	E1472	ARG	PRO	H1063
ASP	F2482	G2366	W2218	L2079	M1952	GLU	E1691	LYS	GLY	LEU	GLY	L1064
SER	L2483	S2366	W2218	M2083	S1953	GLU	E1691	SER	GLY	LYS	ALA	E1065
ILE	L2484	L2370	L2220	M2083	A1954	GLY	N1692	HIS	V1476	ARG	PHE	A1066
VAL	H2485	LEU	N2223	Y2105	L1955	THR	L1699	LYS	V1476	PHE	TYR	P1067
CYS	L2486	ASP	N2223	T2106	L1955	THR	L1699	ASN	R1482	LEU	GLY	D1068
LEU	L2486	ASP	N2223	T2106	L1955	THR	L1699	PRO	S1483	LEU	PRO	Q1069
LEU	L2486	ASP	N2223	T2106	L1955	THR	L1699	VAL	S1483	LYS	ASP	D1070
ILE	P2493	ASP	N2228	S2111	K1960	ILE	L1706	GLN	Y1486	THR	ASP	H1071
C2576		ASP	L2228	S2111	K1960	ILE	L1706	CYS	M1487	LYS	GLU	A1072
L2579	D2502	ASP	P2231	T2115	ARG	SER	I1710	PRO	V1488	PRO	GLU	S1073
R2580	T2503	THR	A2232	R2126	PHE	ILE	I1710	ASP	C1489	TYR	PHE	E1075
	A2504	ILE	N2233	R2126	ARG	GLU	I1710	ARG	A1490	ASP	ASP	R1074
A2505	R2234	HIS	R2234	R2126	ARG	GLU	I1710	GLY	A1490	TYR	ASP	E1075
A2506	T2237					ILE	L1706	PRO	V1488	PRO	GLU	L1224
L2506	R2257					ILE	L1706	PRO	V1488	PRO	GLU	L1224
S2507	R2257					ILE	L1706	PRO	V1488	PRO	GLU	L1224
A2514	E2262					ILE	L1706	PRO	V1488	PRO	GLU	L1224
R2517	L2394	I2395				ILE	L1706	PRO	V1488	PRO	GLU	L1224
	A2402					ILE	L1706	PRO	V1488	PRO	GLU	L1224
L2527	H2406					ILE	L1706	PRO	V1488	PRO	GLU	L1224
THR	ARG					ILE	L1706	PRO	V1488	PRO	GLU	L1224
ARG	CYS					ILE	L1706	PRO	V1488	PRO	GLU	L1224
ALA	L2425					ILE	L1706	PRO	V1488	PRO	GLU	L1224
PRO	L2279					ILE	L1706	PRO	V1488	PRO	GLU	L1224
LEU	W2280					ILE	L1706	PRO	V1488	PRO	GLU	L1224
PRO	K2281					ILE	L1706	PRO	V1488	PRO	GLU	L1224
PHE	K2282					ILE	L1706	PRO	V1488	PRO	GLU	L1224
ALA	G2283					ILE	L1706	PRO	V1488	PRO	GLU	L1224
ALA	G2429					ILE	L1706	PRO	V1488	PRO	GLU	L1224
GLY	P2285					ILE	L1706	PRO	V1488	PRO	GLU	L1224
THR	I2435					ILE	L1706	PRO	V1488	PRO	GLU	L1224
Y2619						ILE	L1706	PRO	V1488	PRO	GLU	L1224
Y2620						ILE	L1706	PRO	V1488	PRO	GLU	L1224



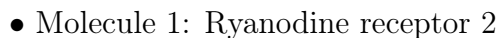


• Molecule 1: Ryanodine receptor 2







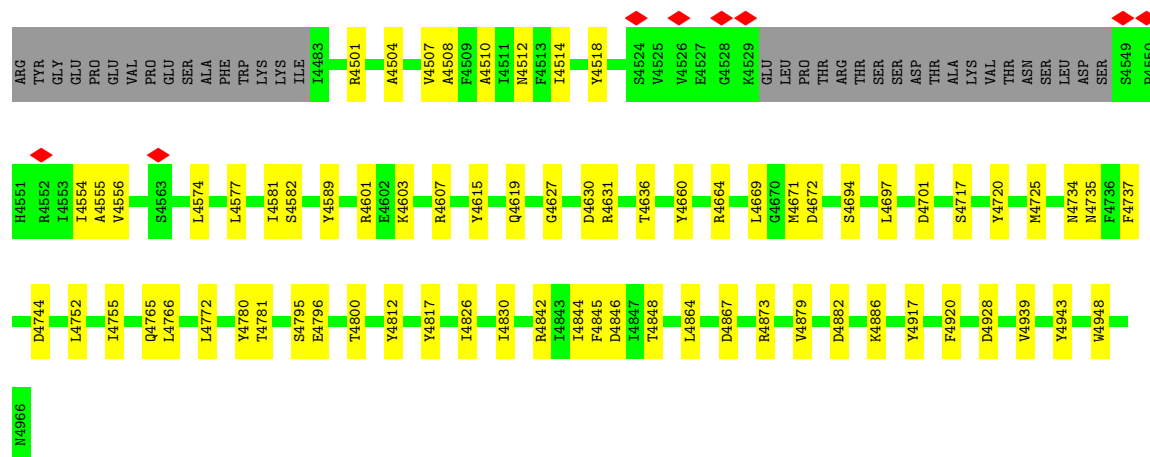


MET	ALA	ASP	ALA	GLY	GLU	GLY	GLU	ASP	E10	I28	H29	K30	K34	A38	F42	F48	S53	P59	P60	D61	T64	L73	R76	E80	M81	N84	THR	VAL	GLU	LYS	SER	GLU	GLN	VAL	ASP	VAL	GLU	LYS	TRP	LYS	PHE	M101	Y115						
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50

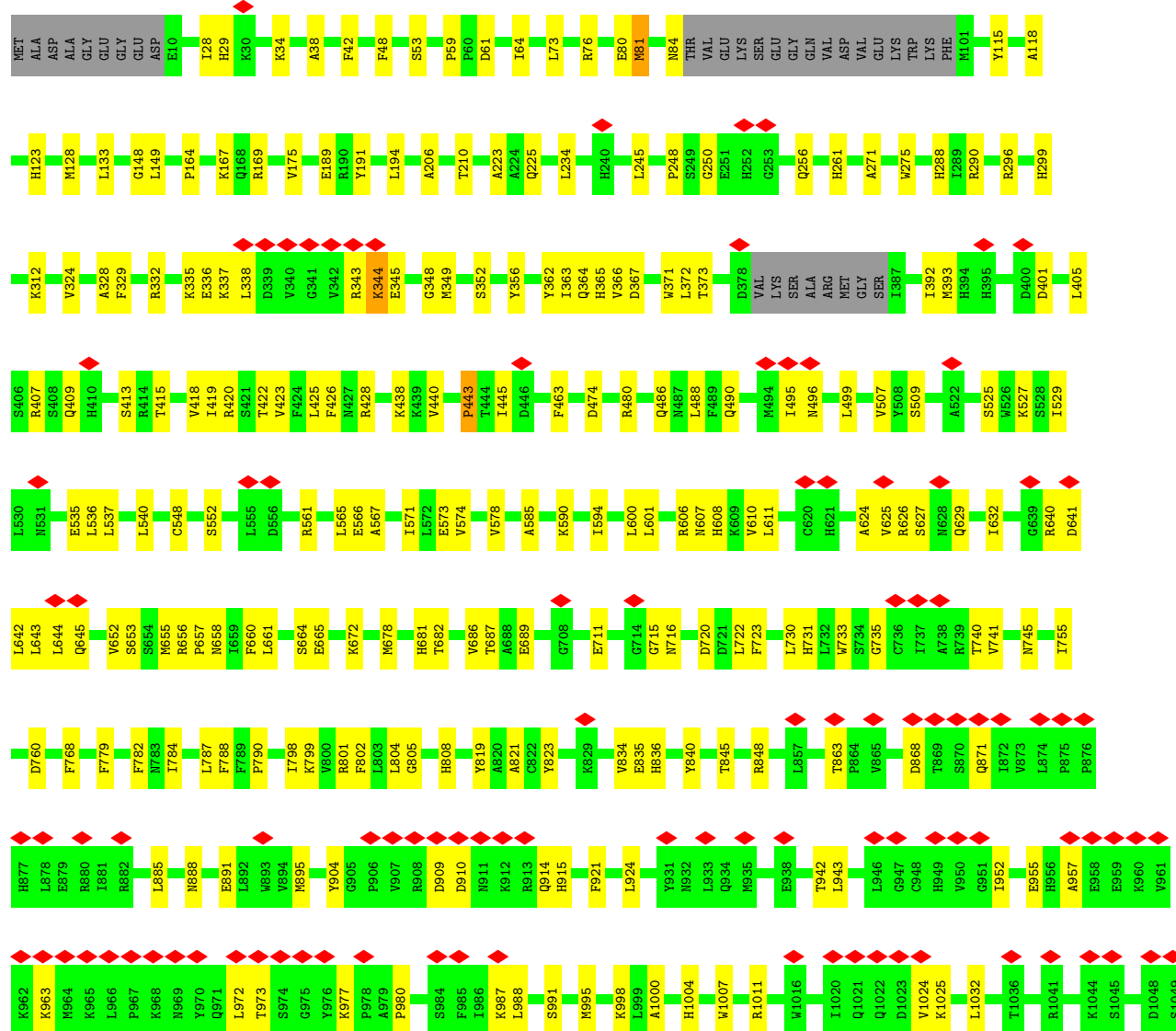


S2898	G2899	Y2900	V2901	V2902	S2903	R2904	GLY	PHE	ASP	LEU	ASP	THR	THR	PRO	SER	ILE	K2854	K2855	K2856	L2857	E2858	L2859	E2860	S2861	K2862	G2863	G2864	G2865	N2866	H2867	P2868	L2869	L2870	V2871	P2872	Y2873	D2874	T2875	L2876	T2877	K2878	E2880	K2881	A2882	K2883	D2884	R2885	E2886	K2887	A2888	Q2889	I2891	F2892	K2893	F2894	Q2896	I2897		
L2776	K2779	T2780	M2781	L2782	A2783	W2784	G2785	W2786	R2787	L2788	E2789	R2790	T2791	R2792	E2793	G2794	D2795	S2796	M2797	A2798	L2799	N2800	N2801	ARG	THR	ARG	ARG	ILE	ALA	GLN	THR	SER	GLN	VAL	ALA	ILE	ASP	A2816	A2817	H2818	G2819	Y2820	S2821	P2822	R2823	A2824	T2825	D2826	M2827	S2828	N2829	V2830	T2831	L2832	S2833	R2834	D2835	L2836	H2837
Y2718	F2719	L2720	N2721	K2722	Y2723	A2724	E2725	H2726	S2727	H2728	D2729	K2730	W2731	S2732	M2733	D2734	K2735	L2736	A2737	N2738	Q2739	W2740	I2741	Y2742	Q2743	E2744	I2745	Y2746	S2747	D2748	S2749	S2750	K2751	L2752	Q2753	P2754	L2755	M2756	K2757	P2758	Y2759	K2760	L2761	L2762	S2763	E2764	K2765	E2766	K2767	E2768	I2769	Y2770	K2771	W2772	P2773	L2774	K2775	E2776	S2777
E2614	Y2619	Y2620	P2623	W2626	S2640	R2641	F2648	S2652	Q2653	K2654	K2655	Y2656	L2660	C2667	L2668	D2678	Y2679	M2680	N2683	M2687	K2690	S2693	MET	ASP	SER	GLN	GLY	ASN	F2700	N2701	P2702	Q2703	P2704	V2705	D2706	T2707	S2708	N2709	I2710	T2711	I2712	P2713	E2714	K2715	L2716	E2717													
Q2440	M2441	P2442	THR	ILE	ALA	LYS	ASP	GLY	LYS	VAL	VAL	GLU	PRO	ASP	MET	SER	ALA	GLY	P2459	K2464	V2468	L2469	F2470	R2473	V2479	F2482	L2483	L2484	H2485	L2486	L2492	P2493	D2502	T2503	A2504	A2505	L2506	S2507	A2514	R2517	L2527	THR	ARG	CYS	ALA	PRO	PHE	ALA											
GLY	THR	GLU	HIS	HIS	ALA	SER	LEU	ILE	ASP	SER	VAL	LEU	HIS	THR	VAL	TYR	ARG	LEU	SER	P2459	K2464	V2468	L2469	F2470	R2473	V2479	F2482	L2483	L2484	H2485	L2486	L2492	P2493	D2502	T2503	A2504	A2505	L2506	S2507	A2514	R2517	L2527	THR	ARG	CYS	ALA	PRO	PHE	ALA										
D2286	L2287	G2288	M2289	N2290	C2307	N2308	R2321	P2332	A2333	L2334	R2335	G2336	E2337	G2341	S2357	R2358	S2365	G2366	T2370	LEU	ASP	ILE	GLU	GLU	GLU	GLU	ASP	ASP	THR	ILE	HIS	M2383	Y2391	L2394	I2395	A2402	H2406	L2425	ILE	PRO	LEU	G2429	V2434	I2435	F2439														
E2168	T2169	M2170	E2171	E2172	M2173	M2174	V2175	N2176	G2180	G2181	E2185	I2186	P2189	K2190	M2191	V2192	A2193	N2194	C2195	R2196	R2197	H2216	L2217	S2218	Y2219	L2220	N2223	S2224	S2225	L2228	P2231	A2232	M2233	R2234	T2237	R2257	E2262	V2265	R2266	M2278	L2279	V2280	S2281	K2282	G2283	Y2284	P2285												
D1993	M1905	R2027	L1908	E1920	V1925	D1929	K1934	N1938	R1942	Y1943	N1944	Q1948	A1949	L1950	N1951	M1952	S1953	A1954	A1955	L1956	T1957	A1958	R1959	K1960	THR	ARG	GLU	PHE	GLU	ASP	ALA	LYS	PRO	PRO	GLN	GLU	GLN	ILE	ASN	MET	LEU	ASN	PHE	LYS	ASP	ASP	LYS	GLU	G1891	L1897	V1901								
H1632	H1633	P1634	E1635	E1636	H1637	R1638	D1641	L1642	L1643	E1644	T1646	E1647	L1651	F1654	H1655	L1661	S1679	H1680	L1686	I1690	E1691	N1692	M1695	P1696	L1699	L1706	I1710	L1720	M1721	M1722	V1728	K1735	S1766	P1767	S1768	F1769	N1774	Y1777	Q1778	Y1779	S1780																		



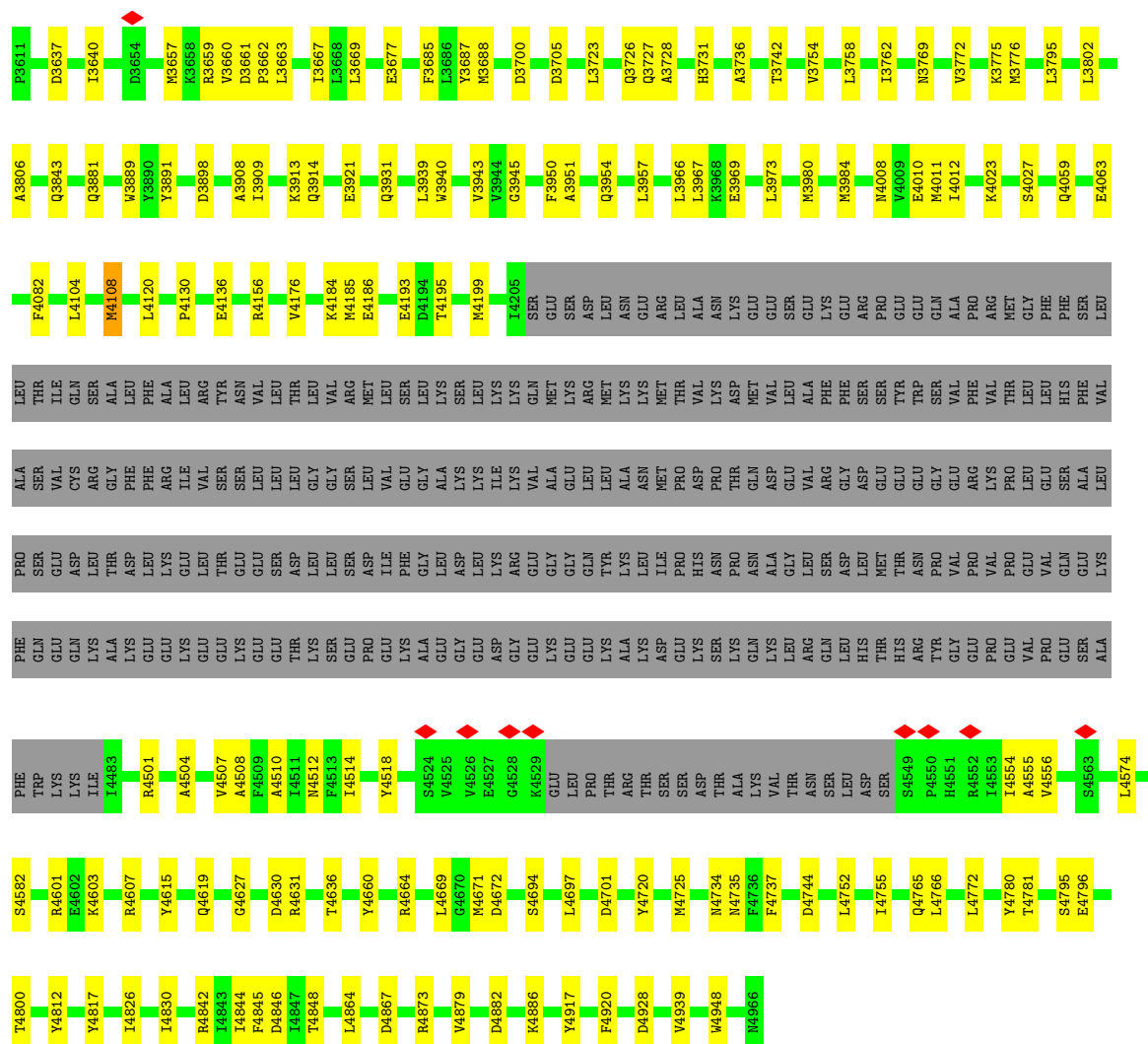


• Molecule 1: Ryanodine receptor 2

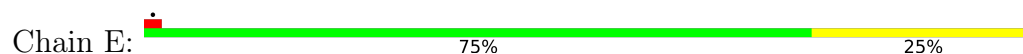




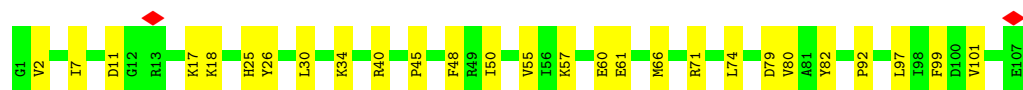
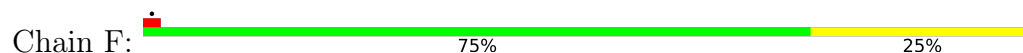




• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

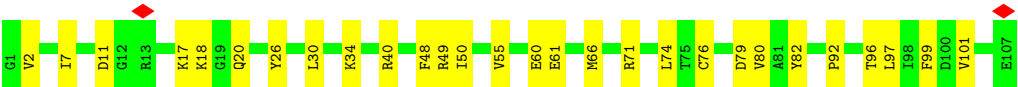


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



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





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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	136874	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.95	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.288	Depositor
Minimum map value	-1.682	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	496.79996, 496.79996, 496.79996	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0799999, 1.0799999, 1.0799999	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

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	0.14	0/32214	0.39	1/43602 (0.0%)
1	B	0.14	0/32214	0.39	1/43602 (0.0%)
1	C	0.14	0/32214	0.39	1/43602 (0.0%)
1	D	0.14	0/32214	0.39	1/43602 (0.0%)
2	E	0.13	0/834	0.39	0/1123
2	F	0.13	0/834	0.39	0/1123
2	G	0.13	0/834	0.39	0/1123
2	H	0.13	0/834	0.39	0/1123
All	All	0.14	0/132192	0.39	4/178900 (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
All	All	0	16

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2189	PRO	CA-N-CD	-6.01	103.58	112.00
1	B	2189	PRO	CA-N-CD	-6.01	103.58	112.00
1	C	2189	PRO	CA-N-CD	-6.01	103.58	112.00
1	D	2189	PRO	CA-N-CD	-6.01	103.58	112.00

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1777	TYR	Peptide
1	A	4023	LYS	Peptide
1	A	443	PRO	Peptide
1	A	4555	ALA	Peptide
1	B	1777	TYR	Peptide
1	B	4023	LYS	Peptide
1	B	443	PRO	Peptide
1	B	4555	ALA	Peptide
1	C	1777	TYR	Peptide
1	C	4023	LYS	Peptide
1	C	443	PRO	Peptide
1	C	4555	ALA	Peptide
1	D	1777	TYR	Peptide
1	D	4023	LYS	Peptide
1	D	443	PRO	Peptide
1	D	4555	ALA	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	31562	0	30401	470	0
1	B	31562	0	30401	471	0
1	C	31562	0	30401	478	0
1	D	31562	0	30401	472	0
2	E	818	0	824	20	0
2	F	818	0	824	21	0
2	G	818	0	824	21	0
2	H	818	0	824	21	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
All	All	129524	0	124900	1930	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1930) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3951:ALA:HB1	1:A:4011:MET:HE1	1.55	0.88
1:B:3951:ALA:HB1	1:B:4011:MET:HE1	1.55	0.87
1:C:3951:ALA:HB1	1:C:4011:MET:HE1	1.55	0.86
1:D:3951:ALA:HB1	1:D:4011:MET:HE1	1.55	0.86
1:B:329:PHE:HB3	1:B:363:ILE:HD11	1.67	0.76
1:D:329:PHE:HB3	1:D:363:ILE:HD11	1.67	0.76
1:A:329:PHE:HB3	1:A:363:ILE:HD11	1.67	0.75
1:C:329:PHE:HB3	1:C:363:ILE:HD11	1.67	0.75
1:C:1954:ALA:HA	1:C:1958:ALA:HB3	1.69	0.75
1:D:1954:ALA:HA	1:D:1958:ALA:HB3	1.69	0.74
1:B:2626:TRP:HE1	1:B:2641:ARG:HE	1.36	0.74
1:A:1954:ALA:HA	1:A:1958:ALA:HB3	1.69	0.73
1:B:1954:ALA:HA	1:B:1958:ALA:HB3	1.69	0.73
1:D:2626:TRP:HE1	1:D:2641:ARG:HE	1.36	0.73
1:A:2626:TRP:HE1	1:A:2641:ARG:HE	1.36	0.73
1:C:1695:MET:HE3	1:C:1696:PRO:HD2	1.71	0.73
1:D:1695:MET:HE3	1:D:1696:PRO:HD2	1.71	0.73
1:A:1695:MET:HE3	1:A:1696:PRO:HD2	1.71	0.73
1:B:731:HIS:HB2	1:B:740:THR:HA	1.70	0.73
1:B:2987:ARG:HH11	1:B:2997:ASN:HB3	1.54	0.72
1:B:1695:MET:HE3	1:B:1696:PRO:HD2	1.71	0.72
1:C:2626:TRP:HE1	1:C:2641:ARG:HE	1.36	0.72
1:A:2987:ARG:HH11	1:A:2997:ASN:HB3	1.54	0.72
1:D:731:HIS:HB2	1:D:740:THR:HA	1.70	0.72
1:A:731:HIS:HB2	1:A:740:THR:HA	1.70	0.71
1:C:731:HIS:HB2	1:C:740:THR:HA	1.70	0.71
1:C:2987:ARG:HH11	1:C:2997:ASN:HB3	1.54	0.71
1:B:672:LYS:HB3	1:B:819:TYR:HA	1.72	0.71
1:A:3843:GLN:HG3	1:A:3921:GLU:HG3	1.72	0.71
1:D:2987:ARG:HH11	1:D:2997:ASN:HB3	1.54	0.71
1:B:3843:GLN:HG3	1:B:3921:GLU:HG3	1.72	0.71
1:C:3843:GLN:HG3	1:C:3921:GLU:HG3	1.72	0.71
1:D:3843:GLN:HG3	1:D:3921:GLU:HG3	1.72	0.70
1:A:672:LYS:HB3	1:A:819:TYR:HA	1.72	0.70
1:D:672:LYS:HB3	1:D:819:TYR:HA	1.72	0.70
1:C:672:LYS:HB3	1:C:819:TYR:HA	1.72	0.70
2:F:50:ILE:HD12	2:F:60:GLU:HG3	1.74	0.70
2:E:50:ILE:HD12	2:E:60:GLU:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:957:ALA:HB1	1:A:963:LYS:H	1.57	0.69
1:B:1655:HIS:HD2	1:B:1699:LEU:HD11	1.58	0.69
1:C:3769:ASN:HB3	1:C:3772:VAL:HG12	1.75	0.69
1:C:1655:HIS:HD2	1:C:1699:LEU:HD11	1.58	0.69
2:G:50:ILE:HD12	2:G:60:GLU:HG3	1.74	0.69
2:H:50:ILE:HD12	2:H:60:GLU:HG3	1.74	0.69
1:C:957:ALA:HB1	1:C:963:LYS:H	1.57	0.69
1:B:722:LEU:HD13	1:B:735:GLY:HA3	1.75	0.68
1:D:957:ALA:HB1	1:D:963:LYS:H	1.57	0.68
1:A:3280:LEU:HG	1:A:3282:ILE:HG22	1.75	0.68
1:B:957:ALA:HB1	1:B:963:LYS:H	1.57	0.68
1:B:3280:LEU:HG	1:B:3282:ILE:HG22	1.75	0.68
1:C:722:LEU:HD13	1:C:735:GLY:HA3	1.75	0.68
1:D:3769:ASN:HB3	1:D:3772:VAL:HG12	1.75	0.68
1:A:3769:ASN:HB3	1:A:3772:VAL:HG12	1.75	0.67
1:B:3769:ASN:HB3	1:B:3772:VAL:HG12	1.75	0.67
1:D:1655:HIS:HD2	1:D:1699:LEU:HD11	1.58	0.67
1:D:3280:LEU:HG	1:D:3282:ILE:HG22	1.75	0.67
1:A:2514:ALA:HA	1:A:2517:ARG:HE	1.60	0.67
1:A:1655:HIS:HD2	1:A:1699:LEU:HD11	1.58	0.67
1:C:3280:LEU:HG	1:C:3282:ILE:HG22	1.75	0.67
2:F:17:LYS:HE3	2:F:18:LYS:H	1.60	0.66
1:D:722:LEU:HD13	1:D:735:GLY:HA3	1.75	0.66
2:E:17:LYS:HE3	2:E:18:LYS:H	1.60	0.66
2:G:17:LYS:HE3	2:G:18:LYS:H	1.60	0.66
1:A:722:LEU:HD13	1:A:735:GLY:HA3	1.75	0.66
1:C:418:VAL:O	1:C:422:THR:OG1	2.12	0.66
1:D:645:GLN:HE22	2:H:34:LYS:HB3	1.60	0.66
1:D:1117:TRP:HE1	1:D:1166:VAL:HG22	1.61	0.66
1:B:418:VAL:O	1:B:422:THR:OG1	2.12	0.66
1:D:2514:ALA:HA	1:D:2517:ARG:HE	1.60	0.66
2:H:17:LYS:HE3	2:H:18:LYS:H	1.60	0.66
1:C:1117:TRP:HE1	1:C:1166:VAL:HG22	1.61	0.66
1:D:1090:ALA:HA	1:D:1249:MET:HA	1.78	0.66
1:A:1090:ALA:HA	1:A:1249:MET:HA	1.78	0.66
1:C:645:GLN:HE22	2:G:34:LYS:HB3	1.60	0.66
1:C:1090:ALA:HA	1:C:1249:MET:HA	1.78	0.65
1:D:1267:HIS:HB3	1:D:1292:SER:HA	1.79	0.65
1:A:645:GLN:HE22	2:E:34:LYS:HB3	1.60	0.65
1:A:1267:HIS:HB3	1:A:1292:SER:HA	1.79	0.65
1:B:645:GLN:HE22	2:F:34:LYS:HB3	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1267:HIS:HB3	1:C:1292:SER:HA	1.79	0.65
1:C:2514:ALA:HA	1:C:2517:ARG:HE	1.60	0.65
1:D:644:LEU:O	1:D:1680:HIS:ND1	2.30	0.65
1:B:1090:ALA:HA	1:B:1249:MET:HA	1.78	0.65
1:B:2514:ALA:HA	1:B:2517:ARG:HE	1.60	0.65
1:B:1117:TRP:HE1	1:B:1166:VAL:HG22	1.61	0.65
1:B:1267:HIS:HB3	1:B:1292:SER:HA	1.79	0.65
1:C:715:GLY:HA3	1:C:720:ASP:HB3	1.78	0.65
1:A:1117:TRP:HE1	1:A:1166:VAL:HG22	1.61	0.65
1:B:715:GLY:HA3	1:B:720:ASP:HB3	1.78	0.65
1:C:644:LEU:O	1:C:1680:HIS:ND1	2.30	0.65
1:D:1434:PRO:HG2	1:D:1504:ASN:HB3	1.79	0.65
1:D:2441:MET:HB3	1:D:2492:LEU:HD13	1.79	0.65
1:A:1434:PRO:HG2	1:A:1504:ASN:HB3	1.79	0.65
1:C:2441:MET:HB3	1:C:2492:LEU:HD13	1.79	0.65
1:D:715:GLY:HA3	1:D:720:ASP:HB3	1.78	0.65
1:D:3931:GLN:NE2	1:D:3984:MET:O	2.30	0.64
1:A:715:GLY:HA3	1:A:720:ASP:HB3	1.78	0.64
1:A:4830:ILE:HB	1:A:4842:ARG:HH21	1.62	0.64
1:B:2678:ASP:OD2	1:B:2679:TYR:N	2.31	0.64
1:C:3931:GLN:NE2	1:C:3984:MET:O	2.30	0.64
1:A:418:VAL:O	1:A:422:THR:OG1	2.12	0.64
1:A:3931:GLN:NE2	1:A:3984:MET:O	2.30	0.64
1:B:4830:ILE:HB	1:B:4842:ARG:HH21	1.62	0.64
1:C:4518:TYR:OH	1:C:4735:ASN:ND2	2.31	0.64
2:H:66:MET:HE1	2:H:101:VAL:HG13	1.80	0.64
1:A:4518:TYR:OH	1:A:4735:ASN:ND2	2.31	0.64
1:B:1434:PRO:HG2	1:B:1504:ASN:HB3	1.79	0.64
1:B:2441:MET:HB3	1:B:2492:LEU:HD13	1.79	0.64
1:C:2678:ASP:OD2	1:C:2679:TYR:N	2.31	0.64
2:E:66:MET:HE1	2:E:101:VAL:HG13	1.80	0.64
1:C:2196:CYS:SG	1:C:2197:ARG:N	2.71	0.64
1:C:3018:ILE:HG22	1:C:3020:LEU:H	1.63	0.64
1:C:4830:ILE:HB	1:C:4842:ARG:HH21	1.62	0.64
1:B:644:LEU:O	1:B:1680:HIS:ND1	2.30	0.64
1:A:3018:ILE:HG22	1:A:3020:LEU:H	1.63	0.64
1:C:2576:CYS:N	1:C:2613:TYR:O	2.31	0.64
1:D:2576:CYS:N	1:D:2613:TYR:O	2.31	0.64
1:A:2441:MET:HB3	1:A:2492:LEU:HD13	1.79	0.63
1:A:2678:ASP:OD2	1:A:2679:TYR:N	2.31	0.63
1:B:2576:CYS:N	1:B:2613:TYR:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3931:GLN:NE2	1:B:3984:MET:O	2.30	0.63
1:B:4518:TYR:OH	1:B:4735:ASN:ND2	2.31	0.63
1:C:1434:PRO:HG2	1:C:1504:ASN:HB3	1.79	0.63
2:F:66:MET:HE1	2:F:101:VAL:HG13	1.80	0.63
1:A:324:VAL:O	1:A:328:ALA:HB2	1.99	0.63
1:D:2678:ASP:OD2	1:D:2679:TYR:N	2.31	0.63
1:D:3018:ILE:HG22	1:D:3020:LEU:H	1.63	0.63
1:D:4830:ILE:HB	1:D:4842:ARG:HH21	1.62	0.63
2:G:66:MET:HE1	2:G:101:VAL:HG13	1.80	0.63
1:A:644:LEU:O	1:A:1680:HIS:ND1	2.30	0.63
1:B:419:ILE:O	1:B:423:VAL:HG22	1.99	0.63
1:D:4518:TYR:OH	1:D:4735:ASN:ND2	2.31	0.63
1:A:419:ILE:O	1:A:423:VAL:HG22	1.99	0.63
1:A:2196:CYS:SG	1:A:2197:ARG:N	2.71	0.63
1:A:2576:CYS:N	1:A:2613:TYR:O	2.31	0.63
1:C:419:ILE:O	1:C:423:VAL:HG22	1.99	0.63
1:C:2587:LEU:HD11	1:C:2603:LYS:HB3	1.81	0.63
1:C:3349:GLU:HA	1:C:3352:LEU:HD23	1.81	0.63
1:B:2196:CYS:SG	1:B:2197:ARG:N	2.71	0.63
1:D:1104:GLU:HG3	1:D:1224:LEU:HD22	1.81	0.63
1:D:2587:LEU:HD11	1:D:2603:LYS:HB3	1.81	0.63
1:C:1104:GLU:HG3	1:C:1224:LEU:HD22	1.81	0.63
1:D:2196:CYS:SG	1:D:2197:ARG:N	2.71	0.63
1:B:3018:ILE:HG22	1:B:3020:LEU:H	1.63	0.62
1:B:3349:GLU:HA	1:B:3352:LEU:HD23	1.81	0.62
1:C:802:PHE:HB2	1:C:1618:TRP:HB2	1.81	0.62
1:D:537:LEU:HD23	1:D:540:LEU:HD13	1.82	0.62
1:D:324:VAL:O	1:D:328:ALA:HB2	1.99	0.62
1:D:802:PHE:HB2	1:D:1618:TRP:HB2	1.81	0.62
1:D:895:MET:HE3	1:D:980:PRO:HB3	1.81	0.62
1:A:363:ILE:HG23	1:A:372:LEU:HD13	1.82	0.62
1:A:802:PHE:HB2	1:A:1618:TRP:HB2	1.81	0.62
1:A:3349:GLU:HA	1:A:3352:LEU:HD23	1.81	0.62
1:B:802:PHE:HB2	1:B:1618:TRP:HB2	1.81	0.62
1:B:1091:GLU:HG2	1:B:1250:TRP:HE1	1.65	0.62
1:C:1091:GLU:HG2	1:C:1250:TRP:HE1	1.65	0.62
1:D:419:ILE:O	1:D:423:VAL:HG22	1.99	0.62
1:B:324:VAL:O	1:B:328:ALA:HB2	1.99	0.62
1:D:3349:GLU:HA	1:D:3352:LEU:HD23	1.81	0.62
1:C:324:VAL:O	1:C:328:ALA:HB2	1.99	0.62
1:D:3891:TYR:HE2	1:D:3898:ASP:H	1.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2587:LEU:HD11	1:B:2603:LYS:HB3	1.81	0.62
1:C:537:LEU:HD23	1:C:540:LEU:HD13	1.82	0.62
1:A:2587:LEU:HD11	1:A:2603:LYS:HB3	1.81	0.62
1:B:1432:ILE:HD13	1:B:1546:ALA:HB2	1.82	0.62
1:C:3000:LYS:HG2	1:C:3070:THR:HG22	1.82	0.62
1:D:1432:ILE:HD13	1:D:1546:ALA:HB2	1.82	0.62
1:A:2185:GLU:HG2	1:A:2186:ILE:HG12	1.82	0.61
1:A:3891:TYR:HE2	1:A:3898:ASP:H	1.48	0.61
1:B:895:MET:HE3	1:B:980:PRO:HB3	1.81	0.61
1:D:1091:GLU:HG2	1:D:1250:TRP:HE1	1.65	0.61
1:A:1091:GLU:HG2	1:A:1250:TRP:HE1	1.65	0.61
1:B:537:LEU:HD23	1:B:540:LEU:HD13	1.82	0.61
1:A:653:SER:HB2	1:A:1611:ARG:HH12	1.65	0.61
1:A:1104:GLU:HG3	1:A:1224:LEU:HD22	1.81	0.61
1:C:2185:GLU:HG2	1:C:2186:ILE:HG12	1.82	0.61
1:D:2307:CYS:SG	1:D:2308:ASN:N	2.73	0.61
1:D:2185:GLU:HG2	1:D:2186:ILE:HG12	1.82	0.61
1:A:3025:ALA:HB3	1:A:3029:VAL:HB	1.82	0.61
1:B:1104:GLU:HG3	1:B:1224:LEU:HD22	1.81	0.61
1:C:895:MET:HE3	1:C:980:PRO:HB3	1.81	0.61
1:C:1432:ILE:HG12	1:C:1554:PHE:HB2	1.83	0.61
1:D:653:SER:HB2	1:D:1611:ARG:HH12	1.65	0.61
1:D:363:ILE:HG23	1:D:372:LEU:HD13	1.82	0.61
1:A:189:GLU:OE1	1:D:2321:ARG:NH1	2.34	0.61
1:C:678:MET:HB3	1:C:801:ARG:HB2	1.83	0.61
1:D:3000:LYS:HG2	1:D:3070:THR:HG22	1.82	0.61
1:B:363:ILE:HG23	1:B:372:LEU:HD13	1.82	0.61
1:B:653:SER:HB2	1:B:1611:ARG:HH12	1.65	0.61
1:B:1432:ILE:HG12	1:B:1554:PHE:HB2	1.83	0.61
1:B:3000:LYS:HG2	1:B:3070:THR:HG22	1.82	0.61
1:C:271:ALA:HB2	1:C:488:LEU:HD11	1.83	0.61
1:C:1129:GLY:HA3	1:C:1145:TRP:HB3	1.82	0.61
1:D:3025:ALA:HB3	1:D:3029:VAL:HB	1.82	0.61
1:D:4781:THR:HG21	1:D:4812:TYR:HA	1.83	0.61
1:A:895:MET:HE3	1:A:980:PRO:HB3	1.81	0.61
1:A:1129:GLY:HA3	1:A:1145:TRP:HB3	1.82	0.61
1:B:271:ALA:HB2	1:B:488:LEU:HD11	1.83	0.61
1:A:271:ALA:HB2	1:A:488:LEU:HD11	1.83	0.60
1:A:537:LEU:HD23	1:A:540:LEU:HD13	1.82	0.60
1:B:678:MET:HB3	1:B:801:ARG:HB2	1.83	0.60
1:A:644:LEU:HD11	1:A:1634:PRO:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:644:LEU:HD11	1:C:1634:PRO:HG3	1.84	0.60
1:C:2161:MET:H	1:C:2161:MET:HE2	1.66	0.60
1:A:4781:THR:HG21	1:A:4812:TYR:HA	1.83	0.60
1:B:2648:PHE:O	1:B:2652:SER:CB	2.50	0.60
1:D:271:ALA:HB2	1:D:488:LEU:HD11	1.83	0.60
1:A:1633:ILE:HG13	1:A:1651:LEU:HD11	1.83	0.60
1:A:3000:LYS:HG2	1:A:3070:THR:HG22	1.82	0.60
1:B:2185:GLU:HG2	1:B:2186:ILE:HG12	1.82	0.60
1:C:653:SER:HB2	1:C:1611:ARG:HH12	1.65	0.60
1:D:678:MET:HB3	1:D:801:ARG:HB2	1.83	0.60
1:C:1920:ARG:NH2	1:C:2039:LYS:O	2.34	0.60
1:A:678:MET:HB3	1:A:801:ARG:HB2	1.83	0.60
1:A:1432:ILE:HG12	1:A:1554:PHE:HB2	1.83	0.60
1:B:644:LEU:HD11	1:B:1634:PRO:HG3	1.84	0.60
1:D:1129:GLY:HA3	1:D:1145:TRP:HB3	1.82	0.60
1:A:1432:ILE:HD13	1:A:1546:ALA:HB2	1.82	0.60
1:A:2648:PHE:O	1:A:2652:SER:CB	2.50	0.60
1:B:1633:ILE:HG13	1:B:1651:LEU:HD11	1.83	0.60
1:C:1432:ILE:HD13	1:C:1546:ALA:HB2	1.82	0.60
1:C:2281:SER:OG	1:C:2282:LYS:NZ	2.35	0.60
1:C:3891:TYR:HE2	1:C:3898:ASP:H	1.48	0.60
1:C:4781:THR:HG21	1:C:4812:TYR:HA	1.83	0.60
1:D:1920:ARG:NH2	1:D:2039:LYS:O	2.34	0.60
1:C:438:LYS:HG3	1:C:440:VAL:HG23	1.84	0.60
1:D:2281:SER:OG	1:D:2282:LYS:NZ	2.35	0.60
1:D:3195:SER:O	1:D:3199:ASN:N	2.35	0.60
1:B:2161:MET:HE2	1:B:2161:MET:H	1.66	0.60
1:B:3025:ALA:HB3	1:B:3029:VAL:HB	1.82	0.60
1:B:1129:GLY:HA3	1:B:1145:TRP:HB3	1.82	0.59
1:C:2648:PHE:O	1:C:2652:SER:CB	2.50	0.59
1:D:644:LEU:HD11	1:D:1634:PRO:HG3	1.84	0.59
1:D:2648:PHE:O	1:D:2652:SER:CB	2.50	0.59
1:A:1444:GLY:HA3	1:A:1488:VAL:HA	1.84	0.59
1:B:34:LYS:H	1:B:53:SER:HB3	1.67	0.59
1:B:2321:ARG:NH1	1:C:189:GLU:OE1	2.34	0.59
1:B:3891:TYR:HE2	1:B:3898:ASP:H	1.48	0.59
1:C:363:ILE:HG23	1:C:372:LEU:HD13	1.82	0.59
1:C:1245:ARG:NH1	1:C:1810:PRO:O	2.36	0.59
1:C:3025:ALA:HB3	1:C:3029:VAL:HB	1.82	0.59
1:C:3195:SER:O	1:C:3199:ASN:N	2.35	0.59
1:A:1920:ARG:NH2	1:A:2039:LYS:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1633:ILE:HG13	1:C:1651:LEU:HD11	1.83	0.59
1:A:1190:LEU:HD21	1:A:1193:LYS:HB2	1.85	0.59
1:B:438:LYS:HG3	1:B:440:VAL:HG23	1.84	0.59
1:C:1441:VAL:HG21	1:C:1546:ALA:HA	1.85	0.59
1:C:1444:GLY:HA3	1:C:1488:VAL:HA	1.84	0.59
1:B:4781:THR:HG21	1:B:4812:TYR:HA	1.83	0.59
1:C:2648:PHE:O	1:C:2652:SER:HB2	2.03	0.59
1:D:438:LYS:HG3	1:D:440:VAL:HG23	1.84	0.59
1:B:607:ASN:O	1:B:608:HIS:ND1	2.36	0.59
1:A:34:LYS:H	1:A:53:SER:HB3	1.67	0.59
1:A:2161:MET:H	1:A:2161:MET:HE2	1.66	0.59
1:B:1441:VAL:HG21	1:B:1546:ALA:HA	1.85	0.59
1:C:4601:ARG:NH1	1:C:4630:ASP:OD1	2.35	0.59
1:D:1432:ILE:HG12	1:D:1554:PHE:HB2	1.83	0.59
1:D:1633:ILE:HG13	1:D:1651:LEU:HD11	1.83	0.59
1:D:2161:MET:H	1:D:2161:MET:HE2	1.66	0.59
1:D:3700:ASP:OD2	1:D:3726:GLN:NE2	2.36	0.59
1:A:438:LYS:HG3	1:A:440:VAL:HG23	1.84	0.59
1:B:1258:PHE:O	1:B:1303:ARG:NH1	2.36	0.59
1:B:2281:SER:OG	1:B:2282:LYS:NZ	2.35	0.59
1:B:2648:PHE:O	1:B:2652:SER:HB2	2.03	0.59
1:C:1258:PHE:O	1:C:1303:ARG:NH1	2.36	0.59
1:C:2307:CYS:SG	1:C:2308:ASN:N	2.73	0.59
1:C:2321:ARG:NH1	1:D:189:GLU:OE1	2.34	0.59
1:C:3957:LEU:HB3	1:C:3967:LEU:HD12	1.85	0.59
1:D:1444:GLY:HA3	1:D:1488:VAL:HA	1.84	0.59
1:B:1444:GLY:HA3	1:B:1488:VAL:HA	1.84	0.59
1:C:34:LYS:H	1:C:53:SER:HB3	1.67	0.59
1:C:607:ASN:O	1:C:608:HIS:ND1	2.36	0.59
1:C:942:THR:O	1:C:998:LYS:NZ	2.36	0.59
1:A:2281:SER:OG	1:A:2282:LYS:NZ	2.35	0.58
1:D:463:PHE:HB3	1:D:536:LEU:HD12	1.85	0.58
1:A:942:THR:O	1:A:998:LYS:NZ	2.36	0.58
1:A:1258:PHE:O	1:A:1303:ARG:NH1	2.36	0.58
1:A:2321:ARG:NH1	1:B:189:GLU:OE1	2.34	0.58
1:A:2334:LEU:HD12	1:A:2341:GLY:HA3	1.85	0.58
1:B:1920:ARG:NH2	1:B:2039:LYS:O	2.34	0.58
1:B:2334:LEU:HD12	1:B:2341:GLY:HA3	1.85	0.58
1:C:2334:LEU:HD12	1:C:2341:GLY:HA3	1.85	0.58
1:D:418:VAL:O	1:D:422:THR:OG1	2.12	0.58
1:D:2334:LEU:HD12	1:D:2341:GLY:HA3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1245:ARG:NH1	1:A:1810:PRO:O	2.36	0.58
1:B:1190:LEU:HD21	1:B:1193:LYS:HB2	1.85	0.58
1:A:4010:GLU:HG2	1:A:4120:LEU:HD13	1.86	0.58
1:C:245:LEU:HB2	1:C:275:TRP:HH2	1.68	0.58
1:D:4010:GLU:HG2	1:D:4120:LEU:HD13	1.86	0.58
1:A:607:ASN:O	1:A:608:HIS:ND1	2.36	0.58
1:A:2648:PHE:O	1:A:2652:SER:HB2	2.03	0.58
1:B:1144:ARG:NH1	1:B:1191:ALA:O	2.37	0.58
1:B:1245:ARG:NH1	1:B:1810:PRO:O	2.36	0.58
1:B:1780:SER:HB2	1:B:1781:PRO:HD3	1.85	0.58
1:B:4619:GLN:OE1	1:B:4631:ARG:NH1	2.36	0.58
1:D:1144:ARG:NH1	1:D:1191:ALA:O	2.37	0.58
1:D:1190:LEU:HD21	1:D:1193:LYS:HB2	1.85	0.58
1:D:1441:VAL:HG21	1:D:1546:ALA:HA	1.85	0.58
1:A:3195:SER:O	1:A:3199:ASN:N	2.35	0.58
1:A:3700:ASP:OD2	1:A:3726:GLN:NE2	2.36	0.58
1:A:4601:ARG:NH1	1:A:4630:ASP:OD1	2.35	0.58
1:C:3700:ASP:OD2	1:C:3726:GLN:NE2	2.36	0.58
1:D:34:LYS:H	1:D:53:SER:HB3	1.67	0.58
1:A:245:LEU:HB2	1:A:275:TRP:HH2	1.68	0.58
1:A:1144:ARG:NH1	1:A:1191:ALA:O	2.37	0.58
1:B:463:PHE:HB3	1:B:536:LEU:HD12	1.85	0.58
1:D:3957:LEU:HB3	1:D:3967:LEU:HD12	1.85	0.58
1:A:463:PHE:HB3	1:A:536:LEU:HD12	1.85	0.58
1:A:1780:SER:HB2	1:A:1781:PRO:HD3	1.85	0.58
1:A:4619:GLN:OE1	1:A:4631:ARG:NH1	2.36	0.58
1:B:942:THR:O	1:B:998:LYS:NZ	2.36	0.58
1:B:3700:ASP:OD2	1:B:3726:GLN:NE2	2.36	0.58
1:D:607:ASN:O	1:D:608:HIS:ND1	2.36	0.58
1:D:942:THR:O	1:D:998:LYS:NZ	2.36	0.58
2:F:30:LEU:HB3	2:F:34:LYS:HB2	1.86	0.58
1:A:1441:VAL:HG21	1:A:1546:ALA:HA	1.85	0.58
1:A:2307:CYS:SG	1:A:2308:ASN:N	2.73	0.58
1:B:3195:SER:O	1:B:3199:ASN:N	2.35	0.58
1:D:4601:ARG:NH1	1:D:4630:ASP:OD1	2.35	0.58
1:A:3939:LEU:HD11	1:A:3980:MET:HE1	1.86	0.57
1:B:1119:ARG:NH2	1:B:1196:ASP:O	2.37	0.57
1:B:4601:ARG:NH1	1:B:4630:ASP:OD1	2.35	0.57
1:D:1258:PHE:O	1:D:1303:ARG:NH1	2.36	0.57
1:D:1780:SER:HB2	1:D:1781:PRO:HD3	1.85	0.57
1:B:245:LEU:HB2	1:B:275:TRP:HH2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:PHE:HB3	1:C:536:LEU:HD12	1.85	0.57
1:C:1083:GLU:OE1	1:C:1084:ARG:NH1	2.38	0.57
1:D:548:CYS:O	1:D:552:SER:OG	2.22	0.57
1:D:904:TYR:O	1:D:914:GLN:NE2	2.37	0.57
1:C:904:TYR:O	1:C:914:GLN:NE2	2.37	0.57
1:D:711:GLU:HG3	1:D:1259:LEU:HD21	1.86	0.57
1:D:1245:ARG:NH1	1:D:1810:PRO:O	2.36	0.57
1:D:2648:PHE:O	1:D:2652:SER:HB2	2.03	0.57
1:B:904:TYR:O	1:B:914:GLN:NE2	2.37	0.57
1:B:3957:LEU:HB3	1:B:3967:LEU:HD12	1.85	0.57
1:C:1144:ARG:NH1	1:C:1191:ALA:O	2.37	0.57
1:C:1190:LEU:HD21	1:C:1193:LYS:HB2	1.85	0.57
2:E:30:LEU:HB3	2:E:34:LYS:HB2	1.86	0.57
1:B:527:LYS:NZ	1:B:566:GLU:OE1	2.32	0.57
1:A:1119:ARG:NH2	1:A:1196:ASP:O	2.37	0.57
1:B:3939:LEU:HD11	1:B:3980:MET:HE1	1.86	0.57
1:B:4589:TYR:OH	1:B:4717:SER:OG	2.22	0.57
1:C:711:GLU:HG3	1:C:1259:LEU:HD21	1.86	0.57
1:C:1780:SER:HB2	1:C:1781:PRO:HD3	1.85	0.57
1:C:3913:LYS:HG3	1:C:3973:LEU:HD13	1.86	0.57
1:D:245:LEU:HB2	1:D:275:TRP:HH2	1.68	0.57
1:D:1119:ARG:NH2	1:D:1196:ASP:O	2.37	0.57
1:A:3957:LEU:HB3	1:A:3967:LEU:HD12	1.85	0.57
1:D:3754:VAL:HG11	1:D:3795:LEU:HD21	1.86	0.57
1:A:1735:LYS:NZ	1:A:1929:ASP:OD2	2.38	0.57
1:B:4010:GLU:HG2	1:B:4120:LEU:HD13	1.86	0.57
2:G:30:LEU:HB3	2:G:34:LYS:HB2	1.86	0.57
1:A:711:GLU:HG3	1:A:1259:LEU:HD21	1.86	0.57
1:A:904:TYR:O	1:A:914:GLN:NE2	2.37	0.57
1:C:1119:ARG:NH2	1:C:1196:ASP:O	2.37	0.57
1:B:1299:ILE:HG12	1:B:1457:PHE:HE1	1.70	0.57
1:B:3913:LYS:HG3	1:B:3973:LEU:HD13	1.86	0.57
1:D:81:MET:N	1:D:81:MET:SD	2.78	0.57
1:B:2307:CYS:SG	1:B:2308:ASN:N	2.73	0.56
1:B:3754:VAL:HG11	1:B:3795:LEU:HD21	1.86	0.56
1:B:3950:PHE:HZ	1:B:3973:LEU:HG	1.69	0.56
1:C:527:LYS:NZ	1:C:566:GLU:OE1	2.32	0.56
1:C:4010:GLU:HG2	1:C:4120:LEU:HD13	1.86	0.56
1:D:3939:LEU:HD11	1:D:3980:MET:HE1	1.86	0.56
1:B:4130:PRO:O	1:B:4156:ARG:NH2	2.39	0.56
1:C:81:MET:N	1:C:81:MET:SD	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3754:VAL:HG11	1:C:3795:LEU:HD21	1.86	0.56
1:C:3939:LEU:HD11	1:C:3980:MET:HE1	1.86	0.56
1:C:3950:PHE:HZ	1:C:3973:LEU:HG	1.69	0.56
1:D:2219:TYR:O	1:D:2223:ASN:ND2	2.39	0.56
1:D:4130:PRO:O	1:D:4156:ARG:NH2	2.39	0.56
2:H:30:LEU:HB3	2:H:34:LYS:HB2	1.86	0.56
1:A:3754:VAL:HG11	1:A:3795:LEU:HD21	1.86	0.56
1:B:1083:GLU:OE1	1:B:1084:ARG:NH1	2.38	0.56
1:B:3013:LEU:HD13	1:B:3032:LEU:H	1.71	0.56
1:C:4589:TYR:OH	1:C:4717:SER:OG	2.22	0.56
1:D:3950:PHE:HZ	1:D:3973:LEU:HG	1.69	0.56
1:A:527:LYS:NZ	1:A:566:GLU:OE1	2.32	0.56
1:A:2219:TYR:O	1:A:2223:ASN:ND2	2.39	0.56
1:A:3913:LYS:HG3	1:A:3973:LEU:HD13	1.86	0.56
1:D:672:LYS:NZ	1:D:760:ASP:OD2	2.36	0.56
1:D:1299:ILE:HG12	1:D:1457:PHE:HE1	1.70	0.56
1:B:711:GLU:HG3	1:B:1259:LEU:HD21	1.86	0.56
1:C:1283:LEU:HD21	1:C:1427:TYR:HB3	1.88	0.56
1:A:2680:MET:HB3	1:A:2683:ASN:HB2	1.88	0.56
1:D:527:LYS:NZ	1:D:566:GLU:OE1	2.32	0.56
1:D:3913:LYS:HG3	1:D:3973:LEU:HD13	1.86	0.56
1:A:81:MET:N	1:A:81:MET:SD	2.78	0.56
1:A:871:GLN:HE22	1:A:998:LYS:HD3	1.71	0.56
1:A:1299:ILE:HG12	1:A:1457:PHE:HE1	1.70	0.56
1:A:4130:PRO:O	1:A:4156:ARG:NH2	2.39	0.56
1:C:871:GLN:HE22	1:C:998:LYS:HD3	1.71	0.56
1:C:4619:GLN:OE1	1:C:4631:ARG:NH1	2.36	0.56
1:B:81:MET:SD	1:B:81:MET:N	2.78	0.56
1:B:689:GLU:OE2	2:F:71:ARG:NH1	2.39	0.56
1:B:910:ASP:OD2	1:B:915:HIS:NE2	2.39	0.56
1:B:2219:TYR:O	1:B:2223:ASN:ND2	2.39	0.56
1:C:548:CYS:O	1:C:552:SER:OG	2.22	0.56
1:C:1299:ILE:HG12	1:C:1457:PHE:HE1	1.70	0.56
1:C:2357:SER:OG	1:C:2358:ARG:N	2.39	0.56
1:C:4130:PRO:O	1:C:4156:ARG:NH2	2.39	0.56
1:D:2680:MET:HB3	1:D:2683:ASN:HB2	1.88	0.56
1:A:3013:LEU:HD13	1:A:3032:LEU:H	1.71	0.56
1:A:3950:PHE:HZ	1:A:3973:LEU:HG	1.69	0.56
1:C:3013:LEU:HD13	1:C:3032:LEU:H	1.71	0.56
1:A:1283:LEU:HD21	1:A:1427:TYR:HB3	1.88	0.55
1:B:2286:ASP:OD1	1:B:2286:ASP:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3015:ARG:HH22	1:C:3080:THR:HB	1.71	0.55
1:D:1283:LEU:HD21	1:D:1427:TYR:HB3	1.88	0.55
2:G:74:LEU:HB3	2:G:99:PHE:HB2	1.88	0.55
1:A:910:ASP:OD2	1:A:915:HIS:NE2	2.39	0.55
1:A:1429:SER:HB2	1:A:1508:ILE:HA	1.88	0.55
1:B:1283:LEU:HD21	1:B:1427:TYR:HB3	1.88	0.55
1:D:784:ILE:HA	1:D:788:PHE:HZ	1.72	0.55
1:D:3015:ARG:HH22	1:D:3080:THR:HB	1.71	0.55
1:A:2286:ASP:OD1	1:A:2286:ASP:N	2.39	0.55
1:A:3015:ARG:HH22	1:A:3080:THR:HB	1.71	0.55
1:C:910:ASP:OD2	1:C:915:HIS:NE2	2.39	0.55
1:C:2219:TYR:O	1:C:2223:ASN:ND2	2.39	0.55
1:D:910:ASP:OD2	1:D:915:HIS:NE2	2.39	0.55
1:D:1083:GLU:OE1	1:D:1084:ARG:NH1	2.38	0.55
1:B:474:ASP:OD2	1:B:474:ASP:N	2.39	0.55
1:B:548:CYS:O	1:B:552:SER:OG	2.22	0.55
1:B:784:ILE:HA	1:B:788:PHE:HZ	1.72	0.55
1:D:1735:LYS:NZ	1:D:1929:ASP:OD2	2.38	0.55
1:A:784:ILE:HA	1:A:788:PHE:HZ	1.72	0.55
1:D:871:GLN:HE22	1:D:998:LYS:HD3	1.71	0.55
1:D:4619:GLN:OE1	1:D:4631:ARG:NH1	2.36	0.55
2:F:48:PHE:HD1	2:F:55:VAL:HG11	1.72	0.55
1:C:343:ARG:HG2	1:C:344:LYS:H	1.72	0.55
1:C:2680:MET:HB3	1:C:2683:ASN:HB2	1.88	0.55
1:D:343:ARG:HG2	1:D:344:LYS:H	1.72	0.55
1:D:689:GLU:OE2	2:H:71:ARG:NH1	2.39	0.55
2:E:74:LEU:HB3	2:E:99:PHE:HB2	1.88	0.55
1:C:689:GLU:OE2	2:G:71:ARG:NH1	2.39	0.55
1:C:1429:SER:HB2	1:C:1508:ILE:HA	1.88	0.55
1:C:3504:VAL:HA	1:C:3507:ILE:HD12	1.89	0.55
2:F:74:LEU:HB3	2:F:99:PHE:HB2	1.88	0.55
2:G:48:PHE:HD1	2:G:55:VAL:HG11	1.72	0.55
1:B:343:ARG:HG2	1:B:344:LYS:H	1.72	0.55
1:B:4755:ILE:HD11	1:C:4765:GLN:HB3	1.89	0.55
1:D:2357:SER:OG	1:D:2358:ARG:N	2.39	0.55
1:A:343:ARG:HG2	1:A:344:LYS:H	1.72	0.54
2:E:48:PHE:HD1	2:E:55:VAL:HG11	1.72	0.54
1:B:3015:ARG:HH22	1:B:3080:THR:HB	1.71	0.54
1:C:2286:ASP:OD1	1:C:2286:ASP:N	2.39	0.54
1:C:4755:ILE:HD11	1:D:4765:GLN:HB3	1.89	0.54
1:A:3265:THR:HB	1:A:3342:GLU:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4765:GLN:HB3	1:D:4755:ILE:HD11	1.89	0.54
1:B:2357:SER:OG	1:B:2358:ARG:N	2.39	0.54
1:B:2680:MET:HB3	1:B:2683:ASN:HB2	1.88	0.54
1:B:3265:THR:HB	1:B:3342:GLU:HG3	1.90	0.54
1:C:2391:TYR:O	1:C:2395:ILE:HD12	2.07	0.54
1:D:3013:LEU:HD13	1:D:3032:LEU:H	1.71	0.54
1:A:2441:MET:HG2	1:A:2493:PRO:HD3	1.90	0.54
1:B:3504:VAL:HA	1:B:3507:ILE:HD12	1.89	0.54
1:C:784:ILE:HA	1:C:788:PHE:HZ	1.72	0.54
1:D:1429:SER:HB2	1:D:1508:ILE:HA	1.88	0.54
1:A:4672:ASP:OD1	1:A:4672:ASP:N	2.41	0.54
1:C:1000:ALA:O	1:C:1004:HIS:ND1	2.37	0.54
1:C:1735:LYS:NZ	1:C:1929:ASP:OD2	2.38	0.54
1:D:3265:THR:HB	1:D:3342:GLU:HG3	1.90	0.54
2:H:74:LEU:HB3	2:H:99:PHE:HB2	1.88	0.54
1:A:1083:GLU:OE1	1:A:1084:ARG:NH1	2.38	0.54
1:A:2391:TYR:O	1:A:2395:ILE:HD12	2.07	0.54
1:A:4615:TYR:OH	1:A:4627:GLY:O	2.24	0.54
1:B:2391:TYR:O	1:B:2395:ILE:HD12	2.07	0.54
1:B:2441:MET:HG2	1:B:2493:PRO:HD3	1.90	0.54
1:C:3685:PHE:HA	1:C:3688:MET:HE3	1.90	0.54
1:A:2357:SER:OG	1:A:2358:ARG:N	2.39	0.54
1:C:991:SER:O	1:C:995:MET:HG2	2.08	0.54
1:C:1510:CYS:O	1:C:1520:THR:OG1	2.26	0.54
1:C:4615:TYR:OH	1:C:4627:GLY:O	2.24	0.54
1:D:1000:ALA:O	1:D:1004:HIS:ND1	2.37	0.54
1:D:2391:TYR:O	1:D:2395:ILE:HD12	2.07	0.54
1:A:689:GLU:OE2	2:E:71:ARG:NH1	2.39	0.54
1:A:2701:ASN:O	1:A:2849:ASN:ND2	2.41	0.54
1:A:4755:ILE:HD11	1:B:4765:GLN:HB3	1.89	0.54
1:B:871:GLN:HE22	1:B:998:LYS:HD3	1.71	0.54
1:B:991:SER:O	1:B:995:MET:HG2	2.08	0.54
1:D:1993:ASP:OD1	1:D:1993:ASP:N	2.41	0.54
1:D:3909:ILE:HG21	1:D:3969:GLU:HG2	1.90	0.54
1:A:372:LEU:HA	1:A:393:MET:HE1	1.90	0.54
1:A:3909:ILE:HG21	1:A:3969:GLU:HG2	1.90	0.54
1:B:372:LEU:HA	1:B:393:MET:HE1	1.90	0.54
1:C:2991:THR:HA	1:C:2994:HIS:HB3	1.90	0.54
1:D:1722:MET:SD	1:D:2126:ARG:NH2	2.81	0.54
1:D:2701:ASN:O	1:D:2849:ASN:ND2	2.41	0.54
1:D:3504:VAL:HA	1:D:3507:ILE:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3685:PHE:HA	1:D:3688:MET:HE3	1.90	0.54
2:H:48:PHE:HD1	2:H:55:VAL:HG11	1.72	0.54
1:A:548:CYS:O	1:A:552:SER:OG	2.22	0.54
1:A:1722:MET:SD	1:A:2126:ARG:NH2	2.81	0.54
1:A:3504:VAL:HA	1:A:3507:ILE:HD12	1.89	0.54
1:B:1429:SER:OG	1:B:1506:LEU:O	2.24	0.54
1:B:3685:PHE:HA	1:B:3688:MET:HE3	1.90	0.54
1:C:3265:THR:HB	1:C:3342:GLU:HG3	1.90	0.54
1:D:2872:PRO:O	1:D:2875:THR:OG1	2.26	0.54
1:B:1722:MET:SD	1:B:2126:ARG:NH2	2.81	0.53
1:D:4672:ASP:OD1	1:D:4672:ASP:N	2.41	0.53
1:C:2872:PRO:O	1:C:2875:THR:OG1	2.26	0.53
1:D:372:LEU:HA	1:D:393:MET:HE1	1.90	0.53
1:D:1429:SER:OG	1:D:1506:LEU:O	2.24	0.53
1:D:2619:TYR:HB3	1:D:2623:PRO:HG3	1.90	0.53
1:B:1735:LYS:NZ	1:B:1929:ASP:OD2	2.38	0.53
1:B:2159:ASN:OD1	1:B:2162:ARG:NH2	2.41	0.53
1:B:2872:PRO:O	1:B:2875:THR:OG1	2.26	0.53
1:C:1445:TRP:HB2	1:C:1487:MET:HE2	1.90	0.53
1:D:2286:ASP:OD1	1:D:2286:ASP:N	2.39	0.53
1:A:1000:ALA:O	1:A:1004:HIS:ND1	2.37	0.53
1:A:4660:TYR:O	1:A:4664:ARG:NH2	2.42	0.53
1:D:2159:ASN:OD1	1:D:2162:ARG:NH2	2.41	0.53
1:D:3843:GLN:OE1	1:D:3914:GLN:NE2	2.41	0.53
1:A:2619:TYR:HB3	1:A:2623:PRO:HG3	1.90	0.53
1:B:1174:MET:HE1	1:B:1176:THR:HG23	1.91	0.53
1:B:1429:SER:HB2	1:B:1508:ILE:HA	1.88	0.53
1:B:2145:LEU:HD23	1:B:2148:ILE:HD11	1.91	0.53
1:C:1174:MET:HE1	1:C:1176:THR:HG23	1.91	0.53
1:C:1722:MET:SD	1:C:2126:ARG:NH2	2.81	0.53
1:C:3843:GLN:OE1	1:C:3914:GLN:NE2	2.41	0.53
1:C:3909:ILE:HG21	1:C:3969:GLU:HG2	1.90	0.53
1:C:4672:ASP:N	1:C:4672:ASP:OD1	2.41	0.53
1:A:672:LYS:NZ	1:A:760:ASP:OD2	2.36	0.53
1:A:1445:TRP:HB2	1:A:1487:MET:HE2	1.90	0.53
1:A:2145:LEU:HD23	1:A:2148:ILE:HD11	1.91	0.53
1:A:2159:ASN:OD1	1:A:2162:ARG:NH2	2.41	0.53
1:A:2262:GLU:O	1:A:2266:ARG:HG2	2.09	0.53
1:A:2872:PRO:O	1:A:2875:THR:OG1	2.26	0.53
1:B:535:GLU:HG2	1:B:573:GLU:HG3	1.91	0.53
1:B:4059:GLN:HA	1:B:4063:GLU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4615:TYR:OH	1:B:4627:GLY:O	2.24	0.53
1:C:2159:ASN:OD1	1:C:2162:ARG:NH2	2.41	0.53
1:C:2441:MET:HG2	1:C:2493:PRO:HD3	1.90	0.53
1:D:2262:GLU:O	1:D:2266:ARG:HG2	2.09	0.53
1:A:474:ASP:OD2	1:A:474:ASP:N	2.39	0.53
1:B:2217:LEU:HA	1:B:2220:LEU:HB2	1.91	0.53
1:C:372:LEU:HA	1:C:393:MET:HE1	1.90	0.53
1:D:2991:THR:HA	1:D:2994:HIS:HB3	1.90	0.53
1:D:3418:PHE:O	1:D:3422:ASN:ND2	2.35	0.53
1:D:4660:TYR:O	1:D:4664:ARG:NH2	2.42	0.53
1:A:3685:PHE:HA	1:A:3688:MET:HE3	1.90	0.53
1:A:3687:TYR:HE2	1:A:3742:THR:HG21	1.74	0.53
1:A:4507:VAL:HG23	1:A:4574:LEU:HD22	1.91	0.53
1:B:4660:TYR:O	1:B:4664:ARG:NH2	2.42	0.53
1:C:2703:GLN:HE22	1:C:2853:LYS:HD3	1.74	0.53
1:C:4507:VAL:HG23	1:C:4574:LEU:HD22	1.91	0.53
1:D:2703:GLN:HE22	1:D:2853:LYS:HD3	1.74	0.53
1:A:1450:PHE:HD1	1:A:1485:CYS:HB3	1.74	0.53
1:B:3909:ILE:HG21	1:B:3969:GLU:HG2	1.90	0.53
1:C:535:GLU:HG2	1:C:573:GLU:HG3	1.91	0.53
1:C:4660:TYR:O	1:C:4664:ARG:NH2	2.42	0.53
1:D:2217:LEU:HA	1:D:2220:LEU:HB2	1.91	0.53
1:D:3687:TYR:HE2	1:D:3742:THR:HG21	1.74	0.53
1:A:2991:THR:HA	1:A:2994:HIS:HB3	1.90	0.53
1:B:1445:TRP:HB2	1:B:1487:MET:HE2	1.90	0.53
1:B:1450:PHE:HD1	1:B:1485:CYS:HB3	1.74	0.53
1:C:3452:LYS:NZ	1:C:3553:ILE:O	2.42	0.53
1:A:535:GLU:HG2	1:A:573:GLU:HG3	1.91	0.52
1:A:4554:ILE:HG12	1:A:4556:VAL:HA	1.91	0.52
1:B:288:HIS:CD2	1:B:352:SER:H	2.28	0.52
1:B:2619:TYR:HB3	1:B:2623:PRO:HG3	1.90	0.52
1:B:3687:TYR:HE2	1:B:3742:THR:HG21	1.74	0.52
1:B:4554:ILE:HG12	1:B:4556:VAL:HA	1.91	0.52
1:C:1784:PRO:HB2	1:C:1787:ILE:HG12	1.91	0.52
1:D:1445:TRP:HB2	1:D:1487:MET:HE2	1.90	0.52
1:D:2441:MET:HG2	1:D:2493:PRO:HD3	1.90	0.52
1:D:2892:PHE:O	1:D:2896:GLN:HB2	2.10	0.52
1:D:3095:TYR:OH	1:D:3219:GLU:OE1	2.27	0.52
1:A:288:HIS:CD2	1:A:352:SER:H	2.28	0.52
1:A:991:SER:O	1:A:995:MET:HG2	2.08	0.52
1:A:3434:THR:O	1:A:3440:LYS:NZ	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2069:ALA:HB1	1:B:3662:PRO:HB3	1.92	0.52
1:B:2991:THR:HA	1:B:2994:HIS:HB3	1.90	0.52
1:C:2145:LEU:HD23	1:C:2148:ILE:HD11	1.91	0.52
1:C:2892:PHE:O	1:C:2896:GLN:HB2	2.10	0.52
1:C:4059:GLN:HA	1:C:4063:GLU:HB2	1.91	0.52
1:D:991:SER:O	1:D:995:MET:HG2	2.08	0.52
1:B:3843:GLN:OE1	1:B:3914:GLN:NE2	2.41	0.52
1:C:1429:SER:OG	1:C:1506:LEU:O	2.24	0.52
1:C:1450:PHE:HD1	1:C:1485:CYS:HB3	1.74	0.52
1:D:288:HIS:CD2	1:D:352:SER:H	2.28	0.52
1:A:1174:MET:HE1	1:A:1176:THR:HG23	1.91	0.52
1:C:730:LEU:HG	2:G:7:ILE:HG22	1.92	0.52
1:C:2619:TYR:HB3	1:C:2623:PRO:HG3	1.90	0.52
1:B:640:ARG:H	1:B:643:LEU:HD12	1.75	0.52
1:B:1000:ALA:O	1:B:1004:HIS:ND1	2.37	0.52
1:B:3452:LYS:NZ	1:B:3553:ILE:O	2.42	0.52
1:B:4672:ASP:N	1:B:4672:ASP:OD1	2.41	0.52
1:B:4694:SER:HA	1:B:4697:LEU:HD13	1.91	0.52
1:C:288:HIS:CD2	1:C:352:SER:H	2.28	0.52
1:C:2069:ALA:HB1	1:C:3662:PRO:HB3	1.92	0.52
1:C:2217:LEU:HA	1:C:2220:LEU:HB2	1.91	0.52
1:C:2262:GLU:O	1:C:2266:ARG:HG2	2.09	0.52
1:D:1174:MET:HE1	1:D:1176:THR:HG23	1.91	0.52
1:D:1784:PRO:HB2	1:D:1787:ILE:HG12	1.91	0.52
1:B:1126:LEU:HD12	1:B:1127:GLU:H	1.75	0.52
1:B:2262:GLU:O	1:B:2266:ARG:HG2	2.09	0.52
1:D:1450:PHE:HD1	1:D:1485:CYS:HB3	1.74	0.52
1:D:2069:ALA:HB1	1:D:3662:PRO:HB3	1.92	0.52
1:C:3663:LEU:O	1:C:3667:ILE:HG12	2.10	0.52
1:A:1128:LEU:HD23	1:A:1206:SER:HB2	1.92	0.52
1:A:3843:GLN:OE1	1:A:3914:GLN:NE2	2.41	0.52
1:A:4694:SER:HA	1:A:4697:LEU:HD13	1.91	0.52
1:B:61:ASP:OD1	1:B:61:ASP:N	2.42	0.52
1:B:1510:CYS:O	1:B:1520:THR:OG1	2.26	0.52
1:C:1126:LEU:HD12	1:C:1127:GLU:H	1.75	0.52
1:C:4694:SER:HA	1:C:4697:LEU:HD13	1.91	0.52
1:D:730:LEU:HG	2:H:7:ILE:HG22	1.92	0.52
1:A:1784:PRO:HB2	1:A:1787:ILE:HG12	1.91	0.52
1:B:2148:ILE:HD12	1:B:2166:MET:SD	2.50	0.52
1:B:2892:PHE:O	1:B:2896:GLN:HB2	2.10	0.52
1:B:4669:LEU:HB3	1:B:4671:MET:HE1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3095:TYR:OH	1:C:3219:GLU:OE1	2.27	0.52
1:C:3687:TYR:HE2	1:C:3742:THR:HG21	1.74	0.52
1:D:1126:LEU:HD12	1:D:1127:GLU:H	1.75	0.52
1:A:656:ARG:HG3	1:A:835:GLU:HB3	1.92	0.52
1:A:2069:ALA:HB1	1:A:3662:PRO:HB3	1.92	0.52
1:B:656:ARG:HG3	1:B:835:GLU:HB3	1.92	0.52
1:B:4501:ARG:NH2	1:B:4744:ASP:OD1	2.43	0.52
1:D:4501:ARG:NH2	1:D:4744:ASP:OD1	2.43	0.52
1:A:194:LEU:HD13	1:A:210:THR:HG21	1.92	0.51
1:A:2217:LEU:HA	1:A:2220:LEU:HB2	1.91	0.51
1:A:3555:ASN:O	1:A:3559:HIS:NE2	2.44	0.51
1:B:1953:SER:HA	1:B:1956:LEU:HD12	1.92	0.51
1:B:2701:ASN:O	1:B:2849:ASN:ND2	2.41	0.51
1:C:804:LEU:HB2	1:C:808:HIS:HE2	1.76	0.51
1:D:474:ASP:OD2	1:D:474:ASP:N	2.39	0.51
1:D:535:GLU:HG2	1:D:573:GLU:HG3	1.91	0.51
1:D:2145:LEU:HD23	1:D:2148:ILE:HD11	1.91	0.51
1:D:2148:ILE:HD12	1:D:2166:MET:SD	2.50	0.51
1:D:4059:GLN:HA	1:D:4063:GLU:HB2	1.91	0.51
1:D:4554:ILE:HG12	1:D:4556:VAL:HA	1.91	0.51
1:A:606:ARG:HE	1:A:1633:ILE:HG21	1.75	0.51
1:A:1766:SER:O	1:A:1774:ASN:ND2	2.44	0.51
1:A:2148:ILE:HD12	1:A:2166:MET:SD	2.50	0.51
1:A:2892:PHE:O	1:A:2896:GLN:HB2	2.10	0.51
1:B:1489:CYS:SG	1:B:1490:ALA:N	2.84	0.51
1:B:2703:GLN:HE22	1:B:2853:LYS:HD3	1.74	0.51
1:B:4507:VAL:HG23	1:B:4574:LEU:HD22	1.91	0.51
1:C:194:LEU:HD13	1:C:210:THR:HG21	1.92	0.51
1:C:640:ARG:H	1:C:643:LEU:HD12	1.75	0.51
1:C:2148:ILE:HD12	1:C:2166:MET:SD	2.50	0.51
1:D:1128:LEU:HD23	1:D:1206:SER:HB2	1.92	0.51
1:D:1953:SER:HA	1:D:1956:LEU:HD12	1.92	0.51
1:A:730:LEU:HG	2:E:7:ILE:HG22	1.92	0.51
1:A:1489:CYS:SG	1:A:1490:ALA:N	2.84	0.51
1:C:1549:THR:C	1:C:1551:PRO:HD3	2.36	0.51
1:D:606:ARG:HE	1:D:1633:ILE:HG21	1.75	0.51
1:A:4669:LEU:HB3	1:A:4671:MET:HE1	1.92	0.51
1:B:3095:TYR:OH	1:B:3219:GLU:OE1	2.27	0.51
1:A:1510:CYS:O	1:A:1520:THR:OG1	2.26	0.51
1:A:4501:ARG:NH2	1:A:4744:ASP:OD1	2.43	0.51
1:B:3555:ASN:O	1:B:3559:HIS:NE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:ARG:HE	1:C:1633:ILE:HG21	1.75	0.51
1:C:972:LEU:HD12	1:C:977:LYS:HB2	1.92	0.51
1:C:1766:SER:O	1:C:1774:ASN:ND2	2.44	0.51
1:C:4501:ARG:NH2	1:C:4744:ASP:OD1	2.43	0.51
1:C:4669:LEU:HB3	1:C:4671:MET:HE1	1.92	0.51
1:D:1489:CYS:SG	1:D:1490:ALA:N	2.84	0.51
1:B:1449:ASP:OD1	1:B:1449:ASP:N	2.44	0.51
1:B:1766:SER:O	1:B:1774:ASN:ND2	2.44	0.51
1:D:2234:ARG:NH2	1:D:2281:SER:OG	2.44	0.51
1:A:640:ARG:H	1:A:643:LEU:HD12	1.75	0.51
1:A:1302:TYR:HE2	1:A:1546:ALA:HB3	1.76	0.51
1:A:2234:ARG:NH2	1:A:2281:SER:OG	2.44	0.51
1:A:2703:GLN:HE22	1:A:2853:LYS:HD3	1.74	0.51
1:A:4059:GLN:HA	1:A:4063:GLU:HB2	1.91	0.51
1:B:804:LEU:HB2	1:B:808:HIS:HE2	1.76	0.51
1:B:1784:PRO:HB2	1:B:1787:ILE:HG12	1.91	0.51
1:B:1905:MET:SD	1:B:1905:MET:N	2.81	0.51
1:C:4554:ILE:HG12	1:C:4556:VAL:HA	1.91	0.51
1:D:640:ARG:H	1:D:643:LEU:HD12	1.75	0.51
1:D:804:LEU:HB2	1:D:808:HIS:HE2	1.76	0.51
1:D:4507:VAL:HG23	1:D:4574:LEU:HD22	1.91	0.51
1:D:4636:THR:OG1	1:D:4701:ASP:OD2	2.29	0.51
1:B:606:ARG:HE	1:B:1633:ILE:HG21	1.75	0.51
1:B:730:LEU:HG	2:F:7:ILE:HG22	1.92	0.51
1:C:656:ARG:HG3	1:C:835:GLU:HB3	1.92	0.51
1:C:1489:CYS:SG	1:C:1490:ALA:N	2.84	0.51
1:C:1897:LEU:HD22	1:C:1901:VAL:HG11	1.93	0.51
1:C:1905:MET:SD	1:C:1905:MET:N	2.81	0.51
1:D:656:ARG:HG3	1:D:835:GLU:HB3	1.92	0.51
1:D:1302:TYR:HE2	1:D:1546:ALA:HB3	1.76	0.51
1:D:1549:THR:C	1:D:1551:PRO:HD3	2.36	0.51
1:D:2587:LEU:HD23	1:D:2607:LYS:HB2	1.92	0.51
1:D:4694:SER:HA	1:D:4697:LEU:HD13	1.91	0.51
1:A:1126:LEU:HD12	1:A:1127:GLU:H	1.75	0.51
1:D:194:LEU:HD13	1:D:210:THR:HG21	1.92	0.51
1:D:3555:ASN:O	1:D:3559:HIS:NE2	2.44	0.51
1:D:3663:LEU:O	1:D:3667:ILE:HG12	2.10	0.51
1:A:1905:MET:SD	1:A:1905:MET:N	2.81	0.51
1:B:1128:LEU:HD23	1:B:1206:SER:HB2	1.92	0.51
1:B:3663:LEU:O	1:B:3667:ILE:HG12	2.10	0.51
1:C:3555:ASN:O	1:C:3559:HIS:NE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:731:HIS:CE1	1:D:733:TRP:HB3	2.46	0.51
1:D:4882:ASP:OD1	1:D:4886:LYS:NZ	2.44	0.51
1:A:245:LEU:HB2	1:A:275:TRP:CH2	2.47	0.50
1:A:1449:ASP:OD1	1:A:1449:ASP:N	2.44	0.50
1:A:3802:LEU:HD21	1:A:3908:ALA:HB2	1.93	0.50
1:A:4882:ASP:OD1	1:A:4886:LYS:NZ	2.44	0.50
1:B:245:LEU:HB2	1:B:275:TRP:CH2	2.47	0.50
1:B:1302:TYR:HE2	1:B:1546:ALA:HB3	1.76	0.50
1:B:1769:PHE:O	2:F:82:TYR:OH	2.29	0.50
1:B:1897:LEU:HD22	1:B:1901:VAL:HG11	1.93	0.50
1:B:2648:PHE:O	1:B:2652:SER:OG	2.29	0.50
1:C:1302:TYR:HE2	1:C:1546:ALA:HB3	1.76	0.50
1:C:2587:LEU:HD23	1:C:2607:LYS:HB2	1.92	0.50
1:C:2648:PHE:O	1:C:2652:SER:OG	2.29	0.50
1:D:1766:SER:O	1:D:1774:ASN:ND2	2.44	0.50
1:D:1897:LEU:HD22	1:D:1901:VAL:HG11	1.93	0.50
1:D:972:LEU:HD12	1:D:977:LYS:HB2	1.92	0.50
1:A:804:LEU:HB2	1:A:808:HIS:HE2	1.76	0.50
1:A:972:LEU:HD12	1:A:977:LYS:HB2	1.92	0.50
1:A:4636:THR:OG1	1:A:4701:ASP:OD2	2.29	0.50
1:B:972:LEU:HD12	1:B:977:LYS:HB2	1.92	0.50
1:C:61:ASP:OD1	1:C:61:ASP:N	2.42	0.50
1:C:686:VAL:HG13	1:C:687:THR:HG23	1.94	0.50
1:C:1953:SER:HA	1:C:1956:LEU:HD12	1.92	0.50
1:D:1769:PHE:O	2:H:82:TYR:OH	2.29	0.50
1:A:3663:LEU:O	1:A:3667:ILE:HG12	2.10	0.50
1:A:4589:TYR:HH	1:A:4717:SER:HG	1.48	0.50
1:B:2174:MET:HE2	1:B:2191:MET:HG2	1.94	0.50
1:C:1128:LEU:HD23	1:C:1206:SER:HB2	1.92	0.50
1:D:723:PHE:HB3	1:D:1465:VAL:HG21	1.94	0.50
1:A:2587:LEU:HD23	1:A:2607:LYS:HB2	1.92	0.50
1:B:4636:THR:OG1	1:B:4701:ASP:OD2	2.29	0.50
1:C:731:HIS:CE1	1:C:733:TRP:HB3	2.46	0.50
1:D:4669:LEU:HB3	1:D:4671:MET:HE1	1.92	0.50
1:D:4720:TYR:OH	1:D:4744:ASP:OD1	2.26	0.50
1:A:723:PHE:HB3	1:A:1465:VAL:HG21	1.94	0.50
1:A:731:HIS:CE1	1:A:733:TRP:HB3	2.46	0.50
1:A:1549:THR:C	1:A:1551:PRO:HD3	2.36	0.50
1:A:1953:SER:HA	1:A:1956:LEU:HD12	1.92	0.50
1:A:2585:GLN:HA	1:A:2588:LEU:HD12	1.93	0.50
1:C:2174:MET:HE2	1:C:2191:MET:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4636:THR:OG1	1:C:4701:ASP:OD2	2.29	0.50
1:A:1897:LEU:HD22	1:A:1901:VAL:HG11	1.93	0.50
1:A:3418:PHE:O	1:A:3422:ASN:ND2	2.35	0.50
1:B:191:TYR:N	1:B:206:ALA:O	2.38	0.50
1:B:323:ASP:OD1	1:B:326:SER:OG	2.28	0.50
1:B:1549:THR:C	1:B:1551:PRO:HD3	2.36	0.50
1:C:245:LEU:HB2	1:C:275:TRP:CH2	2.47	0.50
1:C:3802:LEU:HD21	1:C:3908:ALA:HB2	1.93	0.50
1:D:1510:CYS:O	1:D:1520:THR:OG1	2.26	0.50
1:A:419:ILE:HG13	1:A:420:ARG:N	2.27	0.50
1:B:194:LEU:HD13	1:B:210:THR:HG21	1.92	0.50
1:B:723:PHE:HB3	1:B:1465:VAL:HG21	1.94	0.50
1:B:2587:LEU:HD23	1:B:2607:LYS:HB2	1.92	0.50
1:C:723:PHE:HB3	1:C:1465:VAL:HG21	1.94	0.50
1:C:1952:MET:HE3	1:C:1953:SER:N	2.27	0.50
1:C:2585:GLN:HA	1:C:2588:LEU:HD12	1.93	0.50
1:B:332:ARG:NE	1:B:364:GLN:OE1	2.44	0.50
1:B:686:VAL:HG13	1:B:687:THR:HG23	1.94	0.50
1:B:1952:MET:HE3	1:B:1953:SER:N	2.27	0.50
1:B:2234:ARG:NH2	1:B:2281:SER:OG	2.44	0.50
1:B:3731:HIS:O	1:B:3775:LYS:NZ	2.41	0.50
1:B:4795:SER:OG	1:B:4800:THR:OG1	2.30	0.50
1:C:288:HIS:HD2	1:C:352:SER:H	1.58	0.50
1:C:474:ASP:OD2	1:C:474:ASP:N	2.39	0.50
1:C:1449:ASP:OD1	1:C:1449:ASP:N	2.44	0.50
1:C:2105:TYR:HE1	1:C:2159:ASN:HB2	1.76	0.50
1:C:2701:ASN:O	1:C:2849:ASN:ND2	2.41	0.50
1:A:288:HIS:HD2	1:A:352:SER:H	1.58	0.49
1:B:288:HIS:HD2	1:B:352:SER:H	1.58	0.49
1:B:2105:TYR:HE1	1:B:2159:ASN:HB2	1.76	0.49
1:C:2234:ARG:NH2	1:C:2281:SER:OG	2.44	0.49
1:D:245:LEU:HB2	1:D:275:TRP:CH2	2.47	0.49
1:D:419:ILE:HG13	1:D:420:ARG:N	2.27	0.49
1:D:3731:HIS:O	1:D:3775:LYS:NZ	2.41	0.49
1:D:4615:TYR:OH	1:D:4627:GLY:O	2.24	0.49
1:A:1024:VAL:HG13	1:A:1025:LYS:HG2	1.94	0.49
1:A:1769:PHE:O	2:E:82:TYR:OH	2.29	0.49
1:D:288:HIS:HD2	1:D:352:SER:H	1.58	0.49
1:C:1769:PHE:O	2:G:82:TYR:OH	2.29	0.49
1:D:681:HIS:HB3	1:D:799:LYS:HG2	1.95	0.49
1:D:2585:GLN:HA	1:D:2588:LEU:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:OE1	1:A:84:ASN:ND2	2.42	0.49
1:A:952:ILE:HD11	1:A:955:GLU:HA	1.95	0.49
1:A:2231:PRO:HG2	1:A:2233:MET:HG2	1.94	0.49
1:B:419:ILE:HG13	1:B:420:ARG:N	2.27	0.49
1:B:731:HIS:CE1	1:B:733:TRP:HB3	2.46	0.49
1:B:868:ASP:OD1	1:B:868:ASP:N	2.46	0.49
1:C:393:MET:HE2	1:C:393:MET:HA	1.94	0.49
1:C:480:ARG:NH1	1:C:3677:GLU:OE2	2.45	0.49
1:C:681:HIS:HB3	1:C:799:LYS:HG2	1.95	0.49
1:D:419:ILE:HG13	1:D:420:ARG:H	1.76	0.49
1:D:2174:MET:HE2	1:D:2191:MET:HG2	1.94	0.49
1:A:2174:MET:HE2	1:A:2191:MET:HG2	1.94	0.49
1:A:3452:LYS:NZ	1:A:3553:ILE:O	2.42	0.49
1:D:1905:MET:HA	1:D:1908:LEU:HB2	1.94	0.49
1:D:2231:PRO:HG2	1:D:2233:MET:HG2	1.94	0.49
1:D:2648:PHE:O	1:D:2652:SER:OG	2.29	0.49
1:D:3727:GLN:O	1:D:3731:HIS:ND1	2.44	0.49
1:A:288:HIS:CD2	1:A:349:MET:HB3	2.47	0.49
1:A:480:ARG:NH1	1:A:3677:GLU:OE2	2.45	0.49
1:B:480:ARG:NH1	1:B:3677:GLU:OE2	2.45	0.49
1:B:681:HIS:HB3	1:B:799:LYS:HG2	1.95	0.49
1:B:2585:GLN:HA	1:B:2588:LEU:HD12	1.93	0.49
1:B:4882:ASP:OD1	1:B:4886:LYS:NZ	2.44	0.49
1:C:419:ILE:HG13	1:C:420:ARG:N	2.27	0.49
1:C:561:ARG:HH22	1:C:567:ALA:H	1.61	0.49
1:D:288:HIS:CD2	1:D:349:MET:HB3	2.47	0.49
1:D:480:ARG:NH1	1:D:3677:GLU:OE2	2.45	0.49
1:D:868:ASP:N	1:D:868:ASP:OD1	2.46	0.49
1:A:419:ILE:HG13	1:A:420:ARG:H	1.76	0.49
1:A:681:HIS:HB3	1:A:799:LYS:HG2	1.95	0.49
1:A:686:VAL:HG13	1:A:687:THR:HG23	1.94	0.49
1:B:332:ARG:N	1:B:362:TYR:O	2.44	0.49
1:B:952:ILE:HD11	1:B:955:GLU:HA	1.95	0.49
1:B:3436:SER:O	1:B:3439:SER:N	2.45	0.49
1:C:1905:MET:HA	1:C:1908:LEU:HB2	1.94	0.49
1:D:61:ASP:OD1	1:D:61:ASP:N	2.42	0.49
1:D:2105:TYR:HE1	1:D:2159:ASN:HB2	1.76	0.49
1:A:1993:ASP:OD1	1:A:1993:ASP:N	2.41	0.49
1:A:4720:TYR:OH	1:A:4744:ASP:OD1	2.26	0.49
1:B:80:GLU:OE1	1:B:84:ASN:ND2	2.42	0.49
1:B:419:ILE:HG13	1:B:420:ARG:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:821:ALA:HB3	1:B:823:TYR:HE1	1.78	0.49
1:B:2795:ASP:N	1:B:2795:ASP:OD1	2.46	0.49
1:B:4104:LEU:O	1:B:4108:MET:HB2	2.13	0.49
1:C:288:HIS:CD2	1:C:349:MET:HB3	2.47	0.49
1:C:1944:ASN:OD1	1:C:1944:ASN:N	2.46	0.49
1:C:2231:PRO:HG2	1:C:2233:MET:HG2	1.94	0.49
1:D:191:TYR:N	1:D:206:ALA:O	2.38	0.49
1:D:686:VAL:HG13	1:D:687:THR:HG23	1.94	0.49
1:D:3436:SER:O	1:D:3439:SER:N	2.45	0.49
1:A:372:LEU:H	1:A:372:LEU:HD12	1.78	0.49
1:A:868:ASP:N	1:A:868:ASP:OD1	2.46	0.49
1:A:1944:ASN:OD1	1:A:1944:ASN:N	2.46	0.49
1:C:1024:VAL:HG13	1:C:1025:LYS:HG2	1.94	0.49
1:D:1024:VAL:HG13	1:D:1025:LYS:HG2	1.94	0.49
1:D:1952:MET:HE3	1:D:1953:SER:N	2.27	0.49
1:A:393:MET:HE2	1:A:393:MET:HA	1.94	0.49
1:A:1434:PRO:HD3	1:A:1506:LEU:HD23	1.95	0.49
1:A:1728:VAL:HG11	1:A:1925:VAL:HG11	1.95	0.49
1:B:234:LEU:HD12	1:B:405:LEU:HD22	1.95	0.49
1:B:288:HIS:CD2	1:B:349:MET:HB3	2.47	0.49
1:B:1517:GLY:O	1:B:1533:GLN:NE2	2.46	0.49
1:B:3802:LEU:HD21	1:B:3908:ALA:HB2	1.93	0.49
1:C:1153:GLY:HA2	1:C:1182:LEU:HD12	1.95	0.49
1:C:2713:PRO:HD2	1:C:2782:LEU:HD13	1.95	0.49
1:D:1153:GLY:HA2	1:D:1182:LEU:HD12	1.95	0.49
1:D:3802:LEU:HD21	1:D:3908:ALA:HB2	1.93	0.49
1:B:372:LEU:HD12	1:B:372:LEU:H	1.78	0.48
1:C:3727:GLN:O	1:C:3731:HIS:ND1	2.44	0.48
1:D:561:ARG:HH22	1:D:567:ALA:H	1.61	0.48
1:A:234:LEU:HD12	1:A:405:LEU:HD22	1.95	0.48
1:A:921:PHE:HA	1:A:924:LEU:HD12	1.96	0.48
1:A:1952:MET:HE3	1:A:1953:SER:N	2.27	0.48
1:A:2105:TYR:HE1	1:A:2159:ASN:HB2	1.76	0.48
1:A:3731:HIS:O	1:A:3775:LYS:NZ	2.41	0.48
1:B:393:MET:HE2	1:B:393:MET:HA	1.94	0.48
1:C:419:ILE:HG13	1:C:420:ARG:H	1.76	0.48
1:C:486:GLN:HG2	1:C:540:LEU:HG	1.96	0.48
1:C:4104:LEU:O	1:C:4108:MET:HB2	2.13	0.48
1:D:393:MET:HE2	1:D:393:MET:HA	1.94	0.48
1:D:578:VAL:HG11	1:D:585:ALA:H	1.79	0.48
1:D:4104:LEU:O	1:D:4108:MET:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:TYR:N	1:A:206:ALA:O	2.38	0.48
1:A:332:ARG:N	1:A:362:TYR:O	2.44	0.48
1:B:561:ARG:HH22	1:B:567:ALA:H	1.61	0.48
1:B:578:VAL:HG11	1:B:585:ALA:H	1.79	0.48
1:B:1317:SER:OG	1:B:1318:VAL:N	2.46	0.48
1:B:1993:ASP:OD1	1:B:1993:ASP:N	2.41	0.48
1:C:578:VAL:HG11	1:C:585:ALA:H	1.79	0.48
1:D:2713:PRO:HD2	1:D:2782:LEU:HD13	1.95	0.48
1:D:3434:THR:O	1:D:3440:LYS:NZ	2.31	0.48
1:A:1938:ASN:HB3	1:A:1942:ARG:HH12	1.79	0.48
1:A:2713:PRO:HD2	1:A:2782:LEU:HD13	1.95	0.48
1:B:921:PHE:HA	1:B:924:LEU:HD12	1.96	0.48
1:B:1605:LEU:HD21	1:B:1608:ASP:HA	1.96	0.48
1:C:290:ARG:HH22	1:C:349:MET:HA	1.79	0.48
1:C:3436:SER:O	1:C:3439:SER:N	2.45	0.48
1:C:3460:MET:SD	1:C:3460:MET:N	2.87	0.48
1:C:3731:HIS:O	1:C:3775:LYS:NZ	2.41	0.48
1:C:4186:GLU:OE1	1:C:4948:TRP:NE1	2.42	0.48
1:D:1517:GLY:O	1:D:1533:GLN:NE2	2.46	0.48
1:D:1605:LEU:HD21	1:D:1608:ASP:HA	1.96	0.48
1:D:1728:VAL:HG11	1:D:1925:VAL:HG11	1.95	0.48
2:G:2:VAL:HG11	2:G:61:GLU:HB3	1.95	0.48
1:A:578:VAL:HG11	1:A:585:ALA:H	1.79	0.48
1:A:1153:GLY:HA2	1:A:1182:LEU:HD12	1.95	0.48
1:A:1905:MET:HA	1:A:1908:LEU:HB2	1.94	0.48
1:A:2168:GLU:O	1:A:2172:GLU:HG3	2.14	0.48
1:A:2648:PHE:O	1:A:2652:SER:OG	2.29	0.48
1:B:1024:VAL:HG13	1:B:1025:LYS:HG2	1.94	0.48
1:B:2168:GLU:O	1:B:2172:GLU:HG3	2.14	0.48
1:B:2191:MET:SD	1:B:2191:MET:N	2.85	0.48
1:C:1605:LEU:HD21	1:C:1608:ASP:HA	1.96	0.48
1:D:1938:ASN:HB3	1:D:1942:ARG:HH12	1.79	0.48
1:A:561:ARG:HH22	1:A:567:ALA:H	1.61	0.48
1:A:1487:MET:HG2	1:A:1487:MET:O	2.14	0.48
1:A:3436:SER:O	1:A:3439:SER:N	2.45	0.48
1:A:4104:LEU:O	1:A:4108:MET:HB2	2.13	0.48
1:B:1938:ASN:HB3	1:B:1942:ARG:HH12	1.79	0.48
1:B:2713:PRO:HD2	1:B:2782:LEU:HD13	1.95	0.48
1:C:3198:ALA:HB2	1:C:3248:TRP:CE2	2.49	0.48
1:C:4882:ASP:OD1	1:C:4886:LYS:NZ	2.44	0.48
1:D:290:ARG:HH22	1:D:349:MET:HA	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:LEU:H	1:D:372:LEU:HD12	1.78	0.48
1:D:952:ILE:HD11	1:D:955:GLU:HA	1.95	0.48
1:D:3452:LYS:NZ	1:D:3553:ILE:O	2.42	0.48
2:H:2:VAL:HG11	2:H:61:GLU:HB3	1.95	0.48
1:A:1605:LEU:HD21	1:A:1608:ASP:HA	1.96	0.48
1:A:3095:TYR:OH	1:A:3219:GLU:OE1	2.27	0.48
1:A:4752:LEU:HD11	1:B:4772:LEU:HD11	1.96	0.48
1:A:4846:ASP:OD2	1:D:4817:TYR:OH	2.27	0.48
1:B:1434:PRO:HD3	1:B:1506:LEU:HD23	1.95	0.48
1:C:290:ARG:NH1	1:C:349:MET:O	2.38	0.48
1:C:821:ALA:HB3	1:C:823:TYR:HE1	1.78	0.48
1:D:234:LEU:HD12	1:D:405:LEU:HD22	1.95	0.48
1:D:821:ALA:HB3	1:D:823:TYR:HE1	1.78	0.48
1:A:64:ILE:O	1:A:123:HIS:NE2	2.47	0.48
1:B:486:GLN:HG2	1:B:540:LEU:HG	1.96	0.48
1:B:1153:GLY:HA2	1:B:1182:LEU:HD12	1.95	0.48
1:C:234:LEU:HD12	1:C:405:LEU:HD22	1.95	0.48
1:C:3556:VAL:O	1:C:3557:LEU:HD13	2.14	0.48
1:D:1434:PRO:HD3	1:D:1506:LEU:HD23	1.95	0.48
2:E:11:ASP:OD1	2:E:11:ASP:N	2.47	0.48
1:A:73:LEU:O	1:A:118:ALA:N	2.46	0.48
1:A:248:PRO:HD3	1:A:261:HIS:CD2	2.49	0.48
1:A:821:ALA:HB3	1:A:823:TYR:HE1	1.78	0.48
1:A:2660:LEU:HD13	1:A:2693:SER:H	1.79	0.48
1:B:1487:MET:O	1:B:1487:MET:HG2	2.14	0.48
1:B:4752:LEU:HD11	1:C:4772:LEU:HD11	1.96	0.48
1:C:952:ILE:HD11	1:C:955:GLU:HA	1.95	0.48
1:D:248:PRO:HD3	1:D:261:HIS:CD2	2.49	0.48
1:D:1944:ASN:N	1:D:1944:ASN:OD1	2.46	0.48
1:A:290:ARG:HH22	1:A:349:MET:HA	1.79	0.48
1:A:1317:SER:OG	1:A:1318:VAL:N	2.46	0.48
1:A:3025:ALA:N	1:A:3029:VAL:O	2.46	0.48
1:A:4734:ASN:HB3	1:A:4737:PHE:HD2	1.79	0.48
1:B:73:LEU:O	1:B:118:ALA:N	2.46	0.48
1:B:248:PRO:HD3	1:B:261:HIS:CD2	2.49	0.48
1:B:490:GLN:HG3	1:B:540:LEU:CD2	2.44	0.48
1:B:1905:MET:HA	1:B:1908:LEU:HB2	1.94	0.48
1:B:1944:ASN:OD1	1:B:1944:ASN:N	2.46	0.48
1:B:3198:ALA:HB2	1:B:3248:TRP:CE2	2.49	0.48
1:C:248:PRO:HD3	1:C:261:HIS:CD2	2.49	0.48
1:C:2660:LEU:HD13	1:C:2693:SER:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3418:PHE:O	1:C:3422:ASN:ND2	2.35	0.48
1:D:486:GLN:HG2	1:D:540:LEU:HG	1.96	0.48
1:C:1487:MET:O	1:C:1487:MET:HG2	2.14	0.47
1:D:490:GLN:HG3	1:D:540:LEU:CD2	2.44	0.47
1:D:921:PHE:HA	1:D:924:LEU:HD12	1.96	0.47
1:A:490:GLN:HG3	1:A:540:LEU:CD2	2.44	0.47
1:B:1728:VAL:HG11	1:B:1925:VAL:HG11	1.95	0.47
1:B:2231:PRO:HG2	1:B:2233:MET:HG2	1.94	0.47
1:B:3418:PHE:O	1:B:3422:ASN:ND2	2.35	0.47
1:B:4582:SER:C	1:B:4725:MET:HE1	2.39	0.47
1:C:921:PHE:HA	1:C:924:LEU:HD12	1.96	0.47
1:C:4582:SER:C	1:C:4725:MET:HE1	2.39	0.47
1:C:4752:LEU:HD11	1:D:4772:LEU:HD11	1.96	0.47
1:D:1433:PHE:HB2	1:D:1553:VAL:HA	1.96	0.47
1:A:845:THR:O	1:A:848:ARG:NH2	2.47	0.47
1:A:1517:GLY:O	1:A:1533:GLN:NE2	2.46	0.47
1:A:3460:MET:N	1:A:3460:MET:SD	2.87	0.47
1:A:3556:VAL:O	1:A:3557:LEU:HD13	2.14	0.47
1:B:3460:MET:N	1:B:3460:MET:SD	2.87	0.47
1:C:372:LEU:H	1:C:372:LEU:HD12	1.78	0.47
1:D:332:ARG:N	1:D:362:TYR:O	2.44	0.47
1:D:3556:VAL:O	1:D:3557:LEU:HD13	2.14	0.47
1:A:2278:MET:SD	1:A:2279:LEU:N	2.88	0.47
1:A:4582:SER:C	1:A:4725:MET:HE1	2.39	0.47
1:B:164:PRO:HB3	1:B:169:ARG:HB2	1.96	0.47
1:B:336:GLU:HG3	1:B:338:LEU:HD22	1.97	0.47
1:B:840:TYR:OH	1:B:1086:ARG:NH1	2.37	0.47
1:B:909:ASP:OD1	1:B:909:ASP:N	2.48	0.47
1:B:2278:MET:SD	1:B:2279:LEU:HB2	2.55	0.47
1:C:323:ASP:OD1	1:C:326:SER:OG	2.28	0.47
1:C:332:ARG:N	1:C:362:TYR:O	2.44	0.47
1:C:490:GLN:HG3	1:C:540:LEU:CD2	2.44	0.47
1:C:1434:PRO:HD3	1:C:1506:LEU:HD23	1.95	0.47
1:C:2168:GLU:O	1:C:2172:GLU:HG3	2.14	0.47
1:D:2168:GLU:O	1:D:2172:GLU:HG3	2.14	0.47
1:D:2655:LYS:HB3	1:D:2655:LYS:HE3	1.77	0.47
1:D:2660:LEU:HD13	1:D:2693:SER:H	1.79	0.47
1:D:3460:MET:N	1:D:3460:MET:SD	2.87	0.47
1:D:4734:ASN:HB3	1:D:4737:PHE:HD2	1.79	0.47
1:D:4795:SER:OG	1:D:4800:THR:OG1	2.30	0.47
2:E:2:VAL:HG11	2:E:61:GLU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2:VAL:HG11	2:F:61:GLU:HB3	1.95	0.47
1:A:640:ARG:HB3	2:E:92:PRO:HB3	1.97	0.47
1:A:909:ASP:N	1:A:909:ASP:OD1	2.48	0.47
1:B:290:ARG:HH22	1:B:349:MET:HA	1.79	0.47
1:B:787:LEU:HD11	1:B:863:THR:H	1.80	0.47
1:B:1433:PHE:HB2	1:B:1553:VAL:HA	1.96	0.47
1:B:4720:TYR:OH	1:B:4744:ASP:OD1	2.26	0.47
1:C:73:LEU:O	1:C:118:ALA:N	2.46	0.47
1:C:332:ARG:NE	1:C:364:GLN:OE1	2.44	0.47
1:D:1646:THR:HG23	1:D:1647:GLU:HG3	1.97	0.47
1:D:2504:ALA:HB3	1:D:2507:SER:HB2	1.96	0.47
1:D:3025:ALA:N	1:D:3029:VAL:O	2.46	0.47
2:E:60:GLU:OE1	2:E:60:GLU:N	2.45	0.47
1:A:336:GLU:HG3	1:A:338:LEU:HD22	1.97	0.47
1:A:499:LEU:HD21	1:A:537:LEU:HD22	1.97	0.47
1:B:672:LYS:NZ	1:B:760:ASP:OD2	2.36	0.47
1:C:164:PRO:HB3	1:C:169:ARG:HB2	1.96	0.47
1:C:640:ARG:HB3	2:G:92:PRO:HB3	1.97	0.47
1:C:787:LEU:HD11	1:C:863:THR:H	1.80	0.47
1:C:1433:PHE:HB2	1:C:1553:VAL:HA	1.96	0.47
1:C:1728:VAL:HG11	1:C:1925:VAL:HG11	1.95	0.47
1:C:2402:ALA:O	1:C:2473:ARG:NH2	2.44	0.47
1:C:2504:ALA:HB3	1:C:2507:SER:HB2	1.96	0.47
1:D:2278:MET:SD	1:D:2279:LEU:N	2.88	0.47
1:A:486:GLN:HG2	1:A:540:LEU:HG	1.96	0.47
1:A:787:LEU:HD11	1:A:863:THR:H	1.80	0.47
1:A:2228:LEU:HG	1:A:2231:PRO:HD2	1.97	0.47
1:A:3198:ALA:HB2	1:A:3248:TRP:CE2	2.49	0.47
1:A:4176:VAL:HG11	1:A:4879:VAL:HA	1.96	0.47
1:A:4186:GLU:OE1	1:A:4948:TRP:NE1	2.42	0.47
1:A:4772:LEU:HD11	1:D:4752:LEU:HD11	1.96	0.47
1:B:499:LEU:HD21	1:B:537:LEU:HD22	1.97	0.47
1:B:845:THR:O	1:B:848:ARG:NH2	2.47	0.47
1:C:845:THR:O	1:C:848:ARG:NH2	2.47	0.47
1:C:868:ASP:OD1	1:C:868:ASP:N	2.46	0.47
1:C:1938:ASN:HB3	1:C:1942:ARG:HH12	1.79	0.47
1:D:73:LEU:O	1:D:118:ALA:N	2.46	0.47
1:D:644:LEU:HD21	1:D:1634:PRO:HD3	1.97	0.47
1:D:787:LEU:HD11	1:D:863:THR:H	1.80	0.47
1:D:1487:MET:HG2	1:D:1487:MET:O	2.14	0.47
1:D:3881:GLN:NE2	1:D:3945:GLY:HA3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4582:SER:C	1:D:4725:MET:HE1	2.39	0.47
1:A:2504:ALA:HB3	1:A:2507:SER:HB2	1.96	0.47
1:B:660:PHE:HZ	1:B:787:LEU:HD23	1.80	0.47
1:C:644:LEU:HD21	1:C:1634:PRO:HD3	1.97	0.47
1:C:4817:TYR:OH	1:D:4846:ASP:OD2	2.27	0.47
1:D:640:ARG:HB3	2:H:92:PRO:HB3	1.97	0.47
1:D:2228:LEU:HG	1:D:2231:PRO:HD2	1.97	0.47
1:B:2111:SER:O	1:B:2115:THR:OG1	2.33	0.47
1:B:2504:ALA:HB3	1:B:2507:SER:HB2	1.96	0.47
1:C:191:TYR:N	1:C:206:ALA:O	2.38	0.47
1:C:1317:SER:OG	1:C:1318:VAL:N	2.46	0.47
1:C:2278:MET:SD	1:C:2279:LEU:HB2	2.55	0.47
1:D:290:ARG:NH1	1:D:349:MET:O	2.38	0.47
1:D:332:ARG:NE	1:D:364:GLN:OE1	2.44	0.47
1:D:845:THR:O	1:D:848:ARG:NH2	2.47	0.47
1:D:909:ASP:OD1	1:D:909:ASP:N	2.48	0.47
1:D:1449:ASP:OD1	1:D:1449:ASP:N	2.44	0.47
1:D:3198:ALA:HB2	1:D:3248:TRP:CE2	2.49	0.47
2:F:11:ASP:N	2:F:11:ASP:OD1	2.47	0.47
1:A:644:LEU:HD21	1:A:1634:PRO:HD3	1.97	0.47
1:B:2228:LEU:HG	1:B:2231:PRO:HD2	1.97	0.47
1:B:3556:VAL:O	1:B:3557:LEU:HD13	2.14	0.47
1:B:3657:MET:HE1	1:B:3660:VAL:H	1.80	0.47
1:C:2228:LEU:HG	1:C:2231:PRO:HD2	1.97	0.47
1:C:2278:MET:SD	1:C:2279:LEU:N	2.88	0.47
1:C:3657:MET:HE1	1:C:3660:VAL:H	1.80	0.47
1:C:4734:ASN:HB3	1:C:4737:PHE:HD2	1.79	0.47
1:D:3657:MET:HE1	1:D:3660:VAL:H	1.80	0.47
1:D:4176:VAL:HG11	1:D:4879:VAL:HA	1.96	0.47
1:A:3657:MET:HE1	1:A:3660:VAL:H	1.80	0.46
1:A:3881:GLN:NE2	1:A:3945:GLY:HA3	2.30	0.46
1:B:1113:MET:HG2	1:B:1207:LEU:HD23	1.97	0.46
1:C:336:GLU:HG3	1:C:338:LEU:HD22	1.97	0.46
1:C:499:LEU:HD21	1:C:537:LEU:HD22	1.97	0.46
1:C:1646:THR:HG23	1:C:1647:GLU:HG3	1.97	0.46
1:C:2606:LEU:O	1:C:2610:THR:OG1	2.31	0.46
1:D:336:GLU:HG3	1:D:338:LEU:HD22	1.97	0.46
1:D:2278:MET:SD	1:D:2279:LEU:HB2	2.55	0.46
2:H:60:GLU:OE1	2:H:60:GLU:N	2.45	0.46
1:A:61:ASP:OD1	1:A:61:ASP:N	2.42	0.46
1:A:1646:THR:HG23	1:A:1647:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2278:MET:SD	1:A:2279:LEU:HB2	2.55	0.46
1:B:644:LEU:HD21	1:B:1634:PRO:HD3	1.97	0.46
1:B:657:PRO:HA	1:B:834:VAL:HA	1.97	0.46
1:B:2660:LEU:HD13	1:B:2693:SER:H	1.79	0.46
1:B:4136:GLU:O	1:B:4917:TYR:OH	2.31	0.46
1:C:2171:MET:O	1:C:2175:VAL:HG23	2.15	0.46
1:C:4176:VAL:HG11	1:C:4879:VAL:HA	1.96	0.46
1:D:499:LEU:HD21	1:D:537:LEU:HD22	1.97	0.46
1:D:1113:MET:HG2	1:D:1207:LEU:HD23	1.97	0.46
2:F:60:GLU:OE1	2:F:60:GLU:N	2.45	0.46
1:A:164:PRO:HB3	1:A:169:ARG:HB2	1.96	0.46
1:A:657:PRO:HA	1:A:834:VAL:HA	1.97	0.46
1:C:3954:GLN:H	1:C:3954:GLN:HG2	1.57	0.46
1:A:1113:MET:HG2	1:A:1207:LEU:HD23	1.97	0.46
1:A:1433:PHE:HB2	1:A:1553:VAL:HA	1.96	0.46
1:B:611:LEU:HD22	1:B:1661:LEU:HD22	1.97	0.46
1:B:640:ARG:HB3	2:F:92:PRO:HB3	1.97	0.46
1:B:2171:MET:O	1:B:2175:VAL:HG23	2.15	0.46
1:B:4176:VAL:HG11	1:B:4879:VAL:HA	1.96	0.46
1:B:4734:ASN:HB3	1:B:4737:PHE:HD2	1.79	0.46
1:C:2687:MET:HB3	1:C:2690:LYS:HE2	1.97	0.46
1:C:3881:GLN:NE2	1:C:3945:GLY:HA3	2.30	0.46
1:D:164:PRO:HB3	1:D:169:ARG:HB2	1.96	0.46
1:D:1905:MET:N	1:D:1905:MET:SD	2.81	0.46
1:B:3727:GLN:O	1:B:3731:HIS:ND1	2.44	0.46
1:D:2171:MET:O	1:D:2175:VAL:HG23	2.15	0.46
1:D:3351:GLU:HG2	1:D:3354:ILE:HB	1.98	0.46
1:D:4186:GLU:OE1	1:D:4948:TRP:NE1	2.42	0.46
2:H:48:PHE:CD1	2:H:55:VAL:HG11	2.50	0.46
1:B:1646:THR:HG23	1:B:1647:GLU:HG3	1.97	0.46
1:B:2278:MET:SD	1:B:2279:LEU:N	2.88	0.46
1:B:4781:THR:HG21	1:B:4812:TYR:HD1	1.81	0.46
1:C:1257:GLN:HB2	1:C:1260:GLN:HE22	1.81	0.46
1:C:1645:LEU:HD11	1:C:1651:LEU:HD23	1.98	0.46
2:G:11:ASP:OD1	2:G:11:ASP:N	2.47	0.46
2:H:11:ASP:OD1	2:H:11:ASP:N	2.47	0.46
1:A:1429:SER:OG	1:A:1506:LEU:O	2.24	0.46
1:A:3351:GLU:HG2	1:A:3354:ILE:HB	1.98	0.46
1:B:2189:PRO:O	1:B:2192:VAL:HG12	2.16	0.46
1:B:3881:GLN:NE2	1:B:3945:GLY:HA3	2.30	0.46
1:D:344:LYS:HB3	1:D:345:GLU:H	1.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:48:PHE:CD1	2:E:55:VAL:HG11	2.50	0.46
2:G:60:GLU:OE1	2:G:60:GLU:N	2.45	0.46
1:A:973:THR:HG22	1:A:977:LYS:HG3	1.98	0.46
1:B:356:TYR:CZ	1:B:407:ARG:HB3	2.51	0.46
1:B:973:THR:HG22	1:B:977:LYS:HG3	1.98	0.46
1:B:4920:PHE:HE2	1:B:4939:VAL:HG11	1.81	0.46
1:C:356:TYR:CZ	1:C:407:ARG:HB3	2.51	0.46
1:C:4781:THR:HG21	1:C:4812:TYR:HD1	1.81	0.46
2:E:76:CYS:O	2:E:96:THR:OG1	2.29	0.46
1:A:625:VAL:HG12	1:A:627:SER:H	1.81	0.46
1:A:660:PHE:HZ	1:A:787:LEU:HD23	1.80	0.46
1:A:1257:GLN:HB2	1:A:1260:GLN:HE22	1.81	0.46
1:A:1638:ARG:NH2	1:A:1651:LEU:HD22	2.31	0.46
1:A:2189:PRO:O	1:A:2192:VAL:HG12	2.16	0.46
1:A:4136:GLU:O	1:A:4917:TYR:OH	2.31	0.46
1:B:1257:GLN:HB2	1:B:1260:GLN:HE22	1.81	0.46
1:C:1113:MET:HG2	1:C:1207:LEU:HD23	1.97	0.46
1:D:657:PRO:HA	1:D:834:VAL:HA	1.97	0.46
1:D:2502:ASP:N	1:D:2502:ASP:OD1	2.49	0.46
1:D:3660:VAL:HG13	1:D:3661:ASP:H	1.81	0.46
1:A:611:LEU:HD22	1:A:1661:LEU:HD22	1.97	0.46
1:A:840:TYR:OH	1:A:1086:ARG:NH1	2.37	0.46
1:A:2687:MET:HB3	1:A:2690:LYS:HE2	1.97	0.46
1:A:3657:MET:SD	1:A:3659:ARG:N	2.83	0.46
1:B:3351:GLU:HG2	1:B:3354:ILE:HB	1.98	0.46
1:C:660:PHE:HZ	1:C:787:LEU:HD23	1.80	0.46
1:C:2079:LEU:O	1:C:2083:MET:HG3	2.16	0.46
1:C:4184:LYS:HG2	1:C:4185:MET:HE2	1.98	0.46
1:C:4795:SER:OG	1:C:4800:THR:OG1	2.30	0.46
1:D:64:ILE:O	1:D:123:HIS:NE2	2.47	0.46
1:D:2079:LEU:O	1:D:2083:MET:HG3	2.16	0.46
1:D:2402:ALA:O	1:D:2473:ARG:NH2	2.44	0.46
1:A:256:GLN:H	1:A:256:GLN:CD	2.24	0.45
1:A:4781:THR:HG21	1:A:4812:TYR:HD1	1.81	0.45
1:D:973:THR:HG22	1:D:977:LYS:HG3	1.98	0.45
1:D:4781:THR:HG21	1:D:4812:TYR:HD1	1.81	0.45
1:A:1089:ARG:HE	1:A:1092:LYS:NZ	2.14	0.45
1:A:1237:GLU:HB3	1:A:1241:VAL:HG11	1.98	0.45
1:A:2171:MET:O	1:A:2175:VAL:HG23	2.15	0.45
1:B:1237:GLU:HB3	1:B:1241:VAL:HG11	1.98	0.45
1:C:657:PRO:HA	1:C:834:VAL:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:660:PHE:HZ	1:D:787:LEU:HD23	1.80	0.45
1:D:2111:SER:O	1:D:2115:THR:OG1	2.33	0.45
1:D:2189:PRO:O	1:D:2192:VAL:HG12	2.16	0.45
1:D:4184:LYS:HG2	1:D:4185:MET:HE2	1.98	0.45
1:A:3660:VAL:HG13	1:A:3661:ASP:H	1.81	0.45
1:A:4184:LYS:HG2	1:A:4185:MET:HE2	1.98	0.45
1:A:4867:ASP:OD1	1:D:4873:ARG:NE	2.43	0.45
1:B:256:GLN:CD	1:B:256:GLN:H	2.24	0.45
1:B:1638:ARG:NH2	1:B:1651:LEU:HD22	2.31	0.45
1:B:2655:LYS:HE3	1:B:2655:LYS:HB3	1.77	0.45
1:B:3015:ARG:NH2	1:B:3080:THR:O	2.50	0.45
1:B:3660:VAL:HG13	1:B:3661:ASP:H	1.81	0.45
1:C:373:THR:OG1	1:C:392:ILE:O	2.34	0.45
1:C:611:LEU:HD22	1:C:1661:LEU:HD22	1.97	0.45
1:C:1237:GLU:HB3	1:C:1241:VAL:HG11	1.98	0.45
1:C:2189:PRO:O	1:C:2192:VAL:HG12	2.16	0.45
1:C:3025:ALA:N	1:C:3029:VAL:O	2.46	0.45
1:C:3728:ALA:HA	1:C:3731:HIS:CE1	2.51	0.45
1:D:1257:GLN:HB2	1:D:1260:GLN:HE22	1.81	0.45
1:D:3015:ARG:NH2	1:D:3080:THR:O	2.50	0.45
2:F:48:PHE:CD1	2:F:55:VAL:HG11	2.50	0.45
1:A:1645:LEU:HD11	1:A:1651:LEU:HD23	1.98	0.45
1:A:3015:ARG:NH2	1:A:3080:THR:O	2.50	0.45
1:B:2492:LEU:H	1:B:2492:LEU:HD12	1.81	0.45
1:B:3728:ALA:HA	1:B:3731:HIS:CE1	2.51	0.45
1:C:256:GLN:H	1:C:256:GLN:CD	2.24	0.45
1:C:2502:ASP:OD1	1:C:2502:ASP:N	2.49	0.45
1:D:2492:LEU:H	1:D:2492:LEU:HD12	1.81	0.45
1:A:332:ARG:NE	1:A:364:GLN:OE1	2.44	0.45
1:A:4826:ILE:HG13	1:A:4830:ILE:HD11	1.99	0.45
1:C:3015:ARG:NH2	1:C:3080:THR:O	2.50	0.45
1:C:4826:ILE:HG13	1:C:4830:ILE:HD11	1.99	0.45
1:D:256:GLN:H	1:D:256:GLN:CD	2.24	0.45
1:D:1317:SER:OG	1:D:1318:VAL:N	2.46	0.45
2:G:76:CYS:O	2:G:96:THR:OG1	2.29	0.45
1:A:290:ARG:NH2	1:A:348:GLY:O	2.50	0.45
1:A:3954:GLN:H	1:A:3954:GLN:HG2	1.57	0.45
1:B:2687:MET:HB3	1:B:2690:LYS:HE2	1.97	0.45
1:B:3025:ALA:N	1:B:3029:VAL:O	2.46	0.45
1:C:1293:GLN:O	1:C:1550:SER:OG	2.27	0.45
1:C:2492:LEU:HD12	1:C:2492:LEU:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4920:PHE:HE2	1:C:4939:VAL:HG11	1.81	0.45
1:D:611:LEU:HD22	1:D:1661:LEU:HD22	1.97	0.45
1:D:1118:SER:OG	1:D:1119:ARG:N	2.50	0.45
1:D:1638:ARG:NH2	1:D:1651:LEU:HD22	2.31	0.45
1:A:323:ASP:OD1	1:A:326:SER:OG	2.28	0.45
1:A:1118:SER:OG	1:A:1119:ARG:N	2.50	0.45
1:B:1645:LEU:HD11	1:B:1651:LEU:HD23	1.98	0.45
1:C:1089:ARG:HE	1:C:1092:LYS:NZ	2.14	0.45
1:C:2435:ILE:HG12	1:C:2486:LEU:HD11	1.99	0.45
1:D:373:THR:OG1	1:D:392:ILE:O	2.34	0.45
1:D:1089:ARG:HE	1:D:1092:LYS:NZ	2.14	0.45
1:D:1641:ASP:OD1	1:D:1644:GLU:N	2.47	0.45
2:H:76:CYS:O	2:H:96:THR:OG1	2.29	0.45
1:A:1731:THR:O	1:A:1734:THR:OG1	2.33	0.45
1:A:2777:SER:O	1:A:2780:THR:OG1	2.29	0.45
1:B:290:ARG:NH2	1:B:348:GLY:O	2.50	0.45
1:B:625:VAL:HG12	1:B:627:SER:H	1.81	0.45
1:B:4184:LYS:HG2	1:B:4185:MET:HE2	1.98	0.45
1:C:1686:LEU:O	1:C:1690:ILE:HG12	2.17	0.45
1:C:3660:VAL:HG13	1:C:3661:ASP:H	1.81	0.45
1:C:4734:ASN:HB3	1:C:4737:PHE:CD2	2.52	0.45
1:A:2228:LEU:HA	1:A:2237:THR:HB	1.99	0.45
1:A:4734:ASN:HB3	1:A:4737:PHE:CD2	2.52	0.45
1:B:1089:ARG:HE	1:B:1092:LYS:NZ	2.14	0.45
1:B:1641:ASP:OD1	1:B:1644:GLU:N	2.47	0.45
1:B:1686:LEU:O	1:B:1690:ILE:HG12	2.17	0.45
1:B:4186:GLU:OE1	1:B:4948:TRP:NE1	2.42	0.45
1:C:625:VAL:HG12	1:C:627:SER:H	1.81	0.45
1:C:909:ASP:OD1	1:C:909:ASP:N	2.48	0.45
1:C:1634:PRO:HD2	1:C:1654:PHE:HE2	1.82	0.45
1:C:3351:GLU:HG2	1:C:3354:ILE:HB	1.98	0.45
1:D:356:TYR:CZ	1:D:407:ARG:HB3	2.51	0.45
1:D:1645:LEU:HD11	1:D:1651:LEU:HD23	1.98	0.45
1:D:1692:ASN:HB3	1:D:1695:MET:HG2	1.99	0.45
1:A:731:HIS:HA	1:A:741:VAL:HG12	1.99	0.45
1:A:2079:LEU:O	1:A:2083:MET:HG3	2.16	0.45
1:B:1634:PRO:HD2	1:B:1654:PHE:HE2	1.82	0.45
1:B:1810:PRO:HG2	1:B:1814:THR:HA	1.99	0.45
1:C:973:THR:HG22	1:C:977:LYS:HG3	1.98	0.45
1:C:1810:PRO:HG2	1:C:1814:THR:HA	1.99	0.45
1:D:625:VAL:HG12	1:D:627:SER:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:755:ILE:HD11	1:D:768:PHE:HB3	1.99	0.45
1:D:3728:ALA:HA	1:D:3731:HIS:CE1	2.51	0.45
1:D:4826:ILE:HG13	1:D:4830:ILE:HD11	1.99	0.45
1:A:373:THR:OG1	1:A:392:ILE:O	2.34	0.44
1:A:1089:ARG:HB3	1:A:1204:VAL:HG23	2.00	0.44
1:A:1487:MET:HG3	1:A:1532:TYR:HB2	1.99	0.44
1:A:2492:LEU:H	1:A:2492:LEU:HD12	1.81	0.44
1:A:3728:ALA:HA	1:A:3731:HIS:CE1	2.51	0.44
1:A:4920:PHE:HE2	1:A:4939:VAL:HG11	1.81	0.44
1:B:2079:LEU:O	1:B:2083:MET:HG3	2.16	0.44
1:B:3954:GLN:H	1:B:3954:GLN:HG2	1.57	0.44
1:B:4734:ASN:HB3	1:B:4737:PHE:CD2	2.52	0.44
1:C:64:ILE:O	1:C:123:HIS:NE2	2.47	0.44
1:C:324:VAL:O	1:C:328:ALA:CB	2.65	0.44
1:C:641:ASP:OD1	1:C:642:LEU:N	2.49	0.44
1:C:840:TYR:OH	1:C:1086:ARG:NH1	2.37	0.44
1:C:1638:ARG:NH2	1:C:1651:LEU:HD22	2.31	0.44
1:C:4873:ARG:NE	1:D:4867:ASP:OD1	2.43	0.44
1:D:324:VAL:O	1:D:328:ALA:CB	2.65	0.44
1:D:1237:GLU:HB3	1:D:1241:VAL:HG11	1.98	0.44
1:D:2435:ILE:HG12	1:D:2486:LEU:HD11	1.99	0.44
1:D:4734:ASN:HB3	1:D:4737:PHE:CD2	2.52	0.44
1:A:324:VAL:O	1:A:328:ALA:CB	2.65	0.44
1:A:1686:LEU:O	1:A:1690:ILE:HG12	2.17	0.44
1:A:3250:GLU:OE1	1:A:3280:LEU:N	2.51	0.44
1:B:1089:ARG:HB3	1:B:1204:VAL:HG23	2.00	0.44
1:B:4826:ILE:HG13	1:B:4830:ILE:HD11	1.99	0.44
1:C:290:ARG:NH2	1:C:348:GLY:O	2.50	0.44
1:C:805:GLY:HA3	1:C:823:TYR:CD1	2.53	0.44
1:C:1118:SER:OG	1:C:1119:ARG:N	2.50	0.44
1:C:1641:ASP:OD1	1:C:1644:GLU:N	2.47	0.44
1:C:2619:TYR:HB3	1:C:2623:PRO:CG	2.48	0.44
1:C:2795:ASP:OD1	1:C:2795:ASP:N	2.46	0.44
1:D:805:GLY:HA3	1:D:823:TYR:CD1	2.53	0.44
1:D:840:TYR:OH	1:D:1086:ARG:NH1	2.37	0.44
1:D:2228:LEU:HA	1:D:2237:THR:HB	1.99	0.44
1:A:805:GLY:HA3	1:A:823:TYR:CD1	2.53	0.44
1:A:1692:ASN:HB3	1:A:1695:MET:HG2	1.99	0.44
1:B:223:ALA:HB1	1:B:225:GLN:HE22	1.83	0.44
1:B:805:GLY:HA3	1:B:823:TYR:CD1	2.53	0.44
1:B:3246:SER:HB2	1:B:3280:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4193:GLU:CD	1:B:4607:ARG:HH22	2.26	0.44
1:C:332:ARG:HH22	1:C:366:VAL:HG22	1.82	0.44
1:C:1517:GLY:O	1:C:1533:GLN:NE2	2.46	0.44
1:C:2234:ARG:HH21	1:C:2281:SER:HG	1.66	0.44
1:C:4136:GLU:O	1:C:4917:TYR:OH	2.31	0.44
1:C:4720:TYR:OH	1:C:4744:ASP:OD1	2.26	0.44
1:D:2687:MET:HB3	1:D:2690:LYS:HE2	1.97	0.44
1:A:133:LEU:HD22	1:A:148:GLY:HA3	2.00	0.44
1:A:682:THR:HA	1:A:798:ILE:HD13	1.99	0.44
1:A:755:ILE:HD11	1:A:768:PHE:HB3	1.99	0.44
1:A:1634:PRO:HD2	1:A:1654:PHE:HE2	1.82	0.44
1:A:1641:ASP:OD1	1:A:1644:GLU:N	2.47	0.44
1:A:2619:TYR:HB3	1:A:2623:PRO:CG	2.48	0.44
1:B:28:ILE:HG12	1:B:29:HIS:CE1	2.53	0.44
1:B:133:LEU:HD22	1:B:148:GLY:HA3	2.00	0.44
1:B:682:THR:HA	1:B:798:ILE:HD13	1.99	0.44
1:B:2107:ILE:HG13	1:B:2157:HIS:CE1	2.53	0.44
1:B:2619:TYR:HB3	1:B:2623:PRO:CG	2.48	0.44
1:C:223:ALA:HB1	1:C:225:GLN:HE22	1.83	0.44
1:C:1993:ASP:OD1	1:C:1993:ASP:N	2.41	0.44
1:C:2107:ILE:HG13	1:C:2157:HIS:CE1	2.53	0.44
1:C:2228:LEU:HA	1:C:2237:THR:HB	1.99	0.44
1:D:1487:MET:HG3	1:D:1532:TYR:HB2	1.99	0.44
1:D:4920:PHE:HE2	1:D:4939:VAL:HG11	1.81	0.44
1:A:356:TYR:CZ	1:A:407:ARG:HB3	2.51	0.44
1:A:2584:MET:N	1:A:2584:MET:SD	2.91	0.44
1:A:3727:GLN:O	1:A:3731:HIS:ND1	2.44	0.44
1:A:4873:ARG:NE	1:B:4867:ASP:OD1	2.43	0.44
1:B:409:GLN:O	1:B:413:SER:N	2.51	0.44
1:B:1692:ASN:HB3	1:B:1695:MET:HG2	1.99	0.44
1:B:4108:MET:HE2	1:B:4108:MET:HA	1.99	0.44
1:C:28:ILE:HG12	1:C:29:HIS:CE1	2.53	0.44
1:C:2279:LEU:HD22	1:C:2288:GLY:HA2	2.00	0.44
1:D:731:HIS:HA	1:D:741:VAL:HG12	1.99	0.44
2:G:20:GLN:O	2:G:49:ARG:NH2	2.40	0.44
2:G:48:PHE:CD1	2:G:55:VAL:HG11	2.50	0.44
2:H:79:ASP:OD1	2:H:80:VAL:N	2.50	0.44
1:A:4008:ASN:O	1:A:4012:ILE:HG12	2.18	0.44
1:A:4796:GLU:HG2	1:A:4800:THR:HG21	2.00	0.44
1:B:373:THR:OG1	1:B:392:ILE:O	2.34	0.44
1:B:2584:MET:N	1:B:2584:MET:SD	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1089:ARG:HB3	1:C:1204:VAL:HG23	2.00	0.44
1:C:2149:MET:HE3	1:C:2194:ASN:HB2	2.00	0.44
1:C:2223:ASN:O	1:C:2225:SER:N	2.51	0.44
1:D:290:ARG:NH2	1:D:348:GLY:O	2.50	0.44
1:D:2107:ILE:HG13	1:D:2157:HIS:CE1	2.53	0.44
1:D:2584:MET:N	1:D:2584:MET:SD	2.91	0.44
1:D:2619:TYR:HB3	1:D:2623:PRO:CG	2.48	0.44
1:D:4008:ASN:O	1:D:4012:ILE:HG12	2.18	0.44
1:B:332:ARG:HH22	1:B:366:VAL:HG22	1.82	0.44
1:B:1779:TYR:CE2	1:B:1781:PRO:HD2	2.53	0.44
1:B:2502:ASP:OD1	1:B:2502:ASP:N	2.49	0.44
1:B:3250:GLU:OE1	1:B:3280:LEU:N	2.51	0.44
1:C:250:GLY:HA3	1:C:256:GLN:OE1	2.18	0.44
1:C:2584:MET:SD	1:C:2584:MET:N	2.91	0.44
1:C:3250:GLU:OE1	1:C:3280:LEU:N	2.51	0.44
1:C:4008:ASN:O	1:C:4012:ILE:HG12	2.18	0.44
1:D:133:LEU:HD22	1:D:148:GLY:HA3	2.00	0.44
1:D:288:HIS:CG	1:D:349:MET:HB3	2.53	0.44
1:D:332:ARG:HH22	1:D:366:VAL:HG22	1.82	0.44
1:D:409:GLN:O	1:D:413:SER:N	2.51	0.44
1:D:664:SER:OG	1:D:665:GLU:N	2.50	0.44
1:D:885:LEU:HA	1:D:888:ASN:HD21	1.83	0.44
2:F:79:ASP:OD1	2:F:80:VAL:N	2.50	0.44
2:G:79:ASP:OD1	2:G:80:VAL:N	2.50	0.44
1:A:223:ALA:HB1	1:A:225:GLN:HE22	1.83	0.44
1:A:661:LEU:HD13	1:A:790:PRO:HD3	2.00	0.44
1:A:885:LEU:HA	1:A:888:ASN:HD21	1.83	0.44
1:A:2223:ASN:O	1:A:2225:SER:N	2.51	0.44
1:A:2290:ASN:OD1	1:A:2290:ASN:N	2.51	0.44
1:B:2228:LEU:HA	1:B:2237:THR:HB	1.99	0.44
1:C:2728:HIS:CD2	1:C:2762:LEU:HD11	2.53	0.44
1:C:3246:SER:HB2	1:C:3280:LEU:HD22	1.99	0.44
1:D:495:ILE:HG23	1:D:496:ASN:H	1.83	0.44
1:D:1089:ARG:HB3	1:D:1204:VAL:HG23	2.00	0.44
1:D:3250:GLU:OE1	1:D:3280:LEU:N	2.51	0.44
1:D:4108:MET:HA	1:D:4108:MET:HE2	1.99	0.44
1:A:28:ILE:HG12	1:A:29:HIS:CE1	2.53	0.44
1:A:1779:TYR:CE2	1:A:1781:PRO:HD2	2.53	0.44
1:A:2435:ILE:HG12	1:A:2486:LEU:HD11	1.99	0.44
1:A:3246:SER:HB2	1:A:3280:LEU:HD22	1.99	0.44
1:B:661:LEU:HD13	1:B:790:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2149:MET:HE3	1:B:2194:ASN:HB2	2.00	0.44
1:B:4008:ASN:O	1:B:4012:ILE:HG12	2.18	0.44
1:C:664:SER:OG	1:C:665:GLU:N	2.50	0.44
1:C:2781:MET:HA	1:C:2784:TRP:HE3	1.83	0.44
1:C:4193:GLU:CD	1:C:4607:ARG:HH22	2.26	0.44
1:C:4504:ALA:HA	1:C:4507:VAL:HG12	2.00	0.44
1:D:1686:LEU:O	1:D:1690:ILE:HG12	2.17	0.44
1:A:332:ARG:HH22	1:A:366:VAL:HG22	1.82	0.43
1:B:324:VAL:O	1:B:328:ALA:CB	2.65	0.43
1:B:885:LEU:HA	1:B:888:ASN:HD21	1.83	0.43
1:B:2279:LEU:HD22	1:B:2288:GLY:HA2	2.00	0.43
1:B:4508:ALA:O	1:B:4512:ASN:ND2	2.51	0.43
1:C:755:ILE:HD11	1:C:768:PHE:HB3	1.99	0.43
1:C:1779:TYR:CE2	1:C:1781:PRO:HD2	2.53	0.43
1:C:4844:ILE:O	1:C:4848:THR:OG1	2.36	0.43
1:D:1810:PRO:HG2	1:D:1814:THR:HA	1.99	0.43
1:D:2223:ASN:O	1:D:2225:SER:N	2.51	0.43
1:D:2279:LEU:HD22	1:D:2288:GLY:HA2	2.00	0.43
1:D:2795:ASP:N	1:D:2795:ASP:OD1	2.46	0.43
1:D:4193:GLU:CD	1:D:4607:ARG:HH22	2.26	0.43
1:D:4504:ALA:HA	1:D:4507:VAL:HG12	2.00	0.43
1:A:1810:PRO:HG2	1:A:1814:THR:HA	1.99	0.43
1:A:2107:ILE:HG13	1:A:2157:HIS:CE1	2.53	0.43
1:A:4193:GLU:CD	1:A:4607:ARG:HH22	2.26	0.43
1:A:4508:ALA:O	1:A:4512:ASN:ND2	2.51	0.43
1:B:288:HIS:CG	1:B:349:MET:HB3	2.53	0.43
1:B:335:LYS:HD3	1:B:362:TYR:CE2	2.54	0.43
1:B:987:LYS:NZ	1:B:988:LEU:O	2.42	0.43
1:B:2435:ILE:HG12	1:B:2486:LEU:HD11	1.99	0.43
1:C:335:LYS:HD3	1:C:362:TYR:CE2	2.54	0.43
1:C:943:LEU:HD13	1:C:995:MET:HE3	2.01	0.43
1:C:1487:MET:HG3	1:C:1532:TYR:HB2	1.99	0.43
1:C:2165:GLY:O	1:C:2169:THR:HG23	2.19	0.43
1:D:1634:PRO:HD2	1:D:1654:PHE:HE2	1.82	0.43
1:D:2161:MET:HG3	1:D:2166:MET:HE3	2.01	0.43
1:D:2728:HIS:CD2	1:D:2762:LEU:HD11	2.53	0.43
1:D:2781:MET:HA	1:D:2784:TRP:HE3	1.83	0.43
2:G:97:LEU:HD23	2:G:97:LEU:HA	1.83	0.43
2:H:17:LYS:HE3	2:H:18:LYS:N	2.32	0.43
1:A:290:ARG:NH1	1:A:349:MET:O	2.38	0.43
1:A:2662:LYS:HA	1:A:2662:LYS:HD2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4752:LEU:HD12	1:A:4752:LEU:HA	1.80	0.43
1:A:4817:TYR:OH	1:B:4846:ASP:OD2	2.27	0.43
1:B:38:ALA:HB1	1:B:64:ILE:HD12	2.00	0.43
1:B:64:ILE:O	1:B:123:HIS:NE2	2.47	0.43
1:B:943:LEU:HD13	1:B:995:MET:HE3	2.01	0.43
1:B:2223:ASN:O	1:B:2225:SER:N	2.51	0.43
1:B:3736:ALA:HB1	1:B:3776:MET:HG2	2.00	0.43
1:C:133:LEU:HD22	1:C:148:GLY:HA3	2.00	0.43
1:C:409:GLN:O	1:C:413:SER:N	2.51	0.43
1:C:4508:ALA:O	1:C:4512:ASN:ND2	2.51	0.43
1:D:28:ILE:HG12	1:D:29:HIS:CE1	2.53	0.43
1:D:223:ALA:HB1	1:D:225:GLN:HE22	1.83	0.43
1:D:250:GLY:HA3	1:D:256:GLN:OE1	2.18	0.43
1:D:2191:MET:SD	1:D:2191:MET:N	2.85	0.43
1:A:288:HIS:CG	1:A:349:MET:HB3	2.53	0.43
1:A:409:GLN:O	1:A:413:SER:N	2.51	0.43
1:A:664:SER:OG	1:A:665:GLU:N	2.50	0.43
1:A:2502:ASP:OD1	1:A:2502:ASP:N	2.49	0.43
1:A:2728:HIS:CD2	1:A:2762:LEU:HD11	2.53	0.43
1:A:4108:MET:HA	1:A:4108:MET:HE2	1.99	0.43
1:B:2165:GLY:O	1:B:2169:THR:HG23	2.19	0.43
1:B:2290:ASN:OD1	1:B:2290:ASN:N	2.51	0.43
1:B:4796:GLU:HG2	1:B:4800:THR:HG21	2.00	0.43
1:C:42:PHE:HB2	1:C:425:LEU:HD12	2.01	0.43
1:C:288:HIS:CG	1:C:349:MET:HB3	2.53	0.43
1:C:311:ASP:OD1	1:C:311:ASP:N	2.47	0.43
1:D:661:LEU:HD13	1:D:790:PRO:HD3	2.00	0.43
1:D:1629:MET:HG3	1:D:1642:ILE:HG12	2.01	0.43
1:D:3736:ALA:HB1	1:D:3776:MET:HG2	2.00	0.43
1:A:250:GLY:HA3	1:A:256:GLN:OE1	2.18	0.43
1:A:2149:MET:HE3	1:A:2194:ASN:HB2	2.00	0.43
1:A:2716:LEU:HD23	1:A:2716:LEU:H	1.83	0.43
1:B:311:ASP:OD1	1:B:311:ASP:N	2.47	0.43
1:B:755:ILE:HD11	1:B:768:PHE:HB3	1.99	0.43
1:B:4195:THR:HG22	1:B:4199:MET:HE2	2.00	0.43
1:B:4504:ALA:HA	1:B:4507:VAL:HG12	2.00	0.43
1:C:415:THR:O	1:C:419:ILE:HG12	2.19	0.43
1:C:682:THR:HA	1:C:798:ILE:HD13	1.99	0.43
1:C:1692:ASN:HB3	1:C:1695:MET:HG2	1.99	0.43
1:C:2111:SER:O	1:C:2115:THR:OG1	2.33	0.43
1:C:4796:GLU:HG2	1:C:4800:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2640:SER:OG	1:D:2641:ARG:NH1	2.52	0.43
1:D:4508:ALA:O	1:D:4512:ASN:ND2	2.51	0.43
1:D:4796:GLU:HG2	1:D:4800:THR:HG21	2.00	0.43
2:H:26:TYR:N	2:H:40:ARG:HH12	2.17	0.43
1:A:495:ILE:HG23	1:A:496:ASN:H	1.83	0.43
1:A:1706:LEU:O	1:A:1710:ILE:HG13	2.19	0.43
1:B:664:SER:OG	1:B:665:GLU:N	2.50	0.43
1:B:1118:SER:OG	1:B:1119:ARG:N	2.50	0.43
1:B:1487:MET:HG3	1:B:1532:TYR:HB2	1.99	0.43
1:B:1706:LEU:O	1:B:1710:ILE:HG13	2.19	0.43
1:C:495:ILE:HG23	1:C:496:ASN:H	1.83	0.43
1:C:4108:MET:HE2	1:C:4108:MET:HA	1.99	0.43
1:D:3246:SER:HB2	1:D:3280:LEU:HD22	1.99	0.43
1:D:3637:ASP:HA	1:D:3640:ILE:HG22	2.01	0.43
1:D:4752:LEU:HD12	1:D:4752:LEU:HA	1.80	0.43
2:G:26:TYR:N	2:G:40:ARG:HH12	2.17	0.43
1:A:38:ALA:HB1	1:A:64:ILE:HD12	2.00	0.43
1:A:335:LYS:HD3	1:A:362:TYR:CE2	2.54	0.43
1:A:2165:GLY:O	1:A:2169:THR:HG23	2.19	0.43
1:A:2257:ARG:HH21	1:A:3806:ALA:HB1	1.84	0.43
1:A:2640:SER:OG	1:A:2641:ARG:NH1	2.52	0.43
1:B:2161:MET:HG3	1:B:2166:MET:HE3	2.01	0.43
1:B:4873:ARG:NE	1:C:4867:ASP:OD1	2.43	0.43
1:C:3736:ALA:HB1	1:C:3776:MET:HG2	2.00	0.43
1:D:624:ALA:HB3	1:D:2131:VAL:HG12	2.01	0.43
1:D:1779:TYR:CE2	1:D:1781:PRO:HD2	2.53	0.43
1:D:2149:MET:HE3	1:D:2194:ASN:HB2	2.00	0.43
1:D:4027:SER:HB2	1:D:4082:PHE:HD1	1.83	0.43
2:F:97:LEU:HD23	2:F:97:LEU:HA	1.83	0.43
1:A:3736:ALA:HB1	1:A:3776:MET:HG2	2.00	0.43
1:A:4195:THR:HG22	1:A:4199:MET:HE2	2.00	0.43
1:B:2781:MET:HA	1:B:2784:TRP:HE3	1.83	0.43
1:B:4027:SER:HB2	1:B:4082:PHE:HD1	1.83	0.43
1:C:1131:ASP:OD1	1:C:1131:ASP:N	2.52	0.43
1:C:2171:MET:SD	1:C:2216:HIS:ND1	2.88	0.43
1:C:3637:ASP:HA	1:C:3640:ILE:HG22	2.01	0.43
1:D:48:PHE:H	1:D:48:PHE:HD2	1.67	0.43
1:D:365:HIS:HE1	1:D:367:ASP:HB2	1.84	0.43
1:D:682:THR:HA	1:D:798:ILE:HD13	1.99	0.43
1:D:943:LEU:HD13	1:D:995:MET:HE3	2.01	0.43
1:D:1435:GLY:HA3	1:D:1502:ASN:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2395:ILE:HD12	1:D:2395:ILE:H	1.84	0.43
2:E:79:ASP:OD1	2:E:80:VAL:N	2.50	0.43
1:A:365:HIS:HE1	1:A:367:ASP:HB2	1.84	0.43
1:A:4928:ASP:OD1	1:A:4928:ASP:N	2.52	0.43
1:B:275:TRP:HE1	1:B:299:HIS:HD2	1.67	0.43
1:B:495:ILE:HG23	1:B:496:ASN:H	1.83	0.43
1:B:731:HIS:HA	1:B:741:VAL:HG12	1.99	0.43
1:B:1435:GLY:HA3	1:B:1502:ASN:HA	2.01	0.43
1:B:1934:LYS:HD2	1:B:2027:ARG:HH21	1.84	0.43
1:B:3637:ASP:HA	1:B:3640:ILE:HG22	2.01	0.43
1:C:2716:LEU:HD23	1:C:2716:LEU:H	1.83	0.43
1:C:4928:ASP:N	1:C:4928:ASP:OD1	2.52	0.43
1:D:2290:ASN:OD1	1:D:2290:ASN:N	2.51	0.43
1:D:2855:LYS:HE3	1:D:2870:LEU:HB2	2.01	0.43
1:A:1629:MET:HG3	1:A:1642:ILE:HG12	2.01	0.43
1:A:1934:LYS:HD2	1:A:2027:ARG:HH21	1.84	0.43
1:A:2279:LEU:HD22	1:A:2288:GLY:HA2	2.00	0.43
1:A:3940:TRP:HA	1:A:3943:VAL:HG12	2.01	0.43
1:A:4504:ALA:HA	1:A:4507:VAL:HG12	2.00	0.43
1:B:250:GLY:HA3	1:B:256:GLN:OE1	2.18	0.43
1:B:3940:TRP:HA	1:B:3943:VAL:HG12	2.01	0.43
1:C:1641:ASP:OD1	1:C:1642:ILE:N	2.52	0.43
1:C:1706:LEU:O	1:C:1710:ILE:HG13	2.19	0.43
1:C:2257:ARG:HH21	1:C:3806:ALA:HB1	1.84	0.43
1:C:2855:LYS:HE3	1:C:2870:LEU:HB2	2.01	0.43
1:C:3957:LEU:HD11	1:C:3966:LEU:HD22	2.01	0.43
1:C:4027:SER:HB2	1:C:4082:PHE:HD1	1.83	0.43
1:D:2662:LYS:HA	1:D:2662:LYS:HD2	1.82	0.43
1:A:943:LEU:HD13	1:A:995:MET:HE3	2.01	0.42
1:A:1641:ASP:OD1	1:A:1642:ILE:N	2.52	0.42
1:A:2161:MET:HG3	1:A:2166:MET:HE3	2.01	0.42
1:C:275:TRP:HE1	1:C:299:HIS:HD2	1.67	0.42
1:C:624:ALA:HB3	1:C:2131:VAL:HG12	2.01	0.42
1:C:624:ALA:HB1	1:C:629:GLN:OE1	2.19	0.42
1:C:661:LEU:HD13	1:C:790:PRO:HD3	2.00	0.42
1:C:731:HIS:HA	1:C:741:VAL:HG12	1.99	0.42
1:C:2161:MET:HG3	1:C:2166:MET:HE3	2.01	0.42
1:C:2655:LYS:HE3	1:C:2655:LYS:HB3	1.77	0.42
1:D:275:TRP:HE1	1:D:299:HIS:HD2	1.67	0.42
1:D:415:THR:O	1:D:419:ILE:HG12	2.19	0.42
1:D:3940:TRP:HA	1:D:3943:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:THR:O	1:A:419:ILE:HG12	2.19	0.42
1:A:490:GLN:NE2	1:A:540:LEU:O	2.52	0.42
1:A:624:ALA:HB3	1:A:2131:VAL:HG12	2.01	0.42
1:A:1131:ASP:N	1:A:1131:ASP:OD1	2.52	0.42
1:A:1435:GLY:HA3	1:A:1502:ASN:HA	2.01	0.42
1:A:2278:MET:O	1:A:2279:LEU:HD12	2.20	0.42
1:A:2781:MET:HA	1:A:2784:TRP:HE3	1.83	0.42
1:B:2716:LEU:H	1:B:2716:LEU:HD23	1.83	0.42
1:B:2728:HIS:CD2	1:B:2762:LEU:HD11	2.53	0.42
1:B:3723:LEU:O	1:B:3727:GLN:HG2	2.19	0.42
1:C:48:PHE:H	1:C:48:PHE:HD2	1.67	0.42
1:C:490:GLN:NE2	1:C:540:LEU:O	2.52	0.42
1:D:1641:ASP:OD1	1:D:1642:ILE:N	2.52	0.42
1:D:2257:ARG:HH21	1:D:3806:ALA:HB1	1.84	0.42
1:D:3957:LEU:HD11	1:D:3966:LEU:HD22	2.01	0.42
2:H:97:LEU:HD23	2:H:97:LEU:HA	1.83	0.42
1:A:626:ARG:HG2	1:A:2131:VAL:HB	2.01	0.42
1:B:42:PHE:HB2	1:B:425:LEU:HD12	2.01	0.42
1:B:731:HIS:NE2	1:B:733:TRP:HB3	2.35	0.42
1:B:3657:MET:SD	1:B:3659:ARG:N	2.83	0.42
1:C:38:ALA:HB1	1:C:64:ILE:HD12	2.00	0.42
1:C:571:ILE:HA	1:C:574:VAL:HG12	2.01	0.42
1:C:731:HIS:NE2	1:C:733:TRP:HB3	2.35	0.42
1:C:1435:GLY:HA3	1:C:1502:ASN:HA	2.01	0.42
1:C:1633:ILE:HD13	1:C:1633:ILE:HA	1.84	0.42
1:C:2667:CYS:SG	1:C:2668:LEU:N	2.93	0.42
1:D:42:PHE:HB2	1:D:425:LEU:HD12	2.01	0.42
1:D:641:ASP:OD1	1:D:642:LEU:N	2.49	0.42
1:D:1706:LEU:O	1:D:1710:ILE:HG13	2.19	0.42
1:D:4928:ASP:OD1	1:D:4928:ASP:N	2.52	0.42
2:F:26:TYR:N	2:F:40:ARG:HH12	2.17	0.42
1:A:2111:SER:O	1:A:2115:THR:OG1	2.33	0.42
1:A:2173:VAL:HA	1:A:2176:ASN:HD21	1.85	0.42
1:A:2391:TYR:O	1:A:2394:LEU:N	2.53	0.42
1:A:2395:ILE:HD12	1:A:2395:ILE:H	1.84	0.42
1:A:4027:SER:HB2	1:A:4082:PHE:HD1	1.83	0.42
1:B:658:ASN:HA	1:B:835:GLU:HB2	2.02	0.42
1:B:1641:ASP:OD1	1:B:1642:ILE:N	2.52	0.42
1:B:1840:LEU:HD12	1:B:1840:LEU:HA	1.91	0.42
1:B:3957:LEU:HD11	1:B:3966:LEU:HD22	2.01	0.42
1:C:885:LEU:HA	1:C:888:ASN:HD21	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1629:MET:HG3	1:C:1642:ILE:HG12	2.01	0.42
1:C:4195:THR:HG22	1:C:4199:MET:HE2	2.00	0.42
1:D:335:LYS:HD3	1:D:362:TYR:CE2	2.54	0.42
1:D:422:THR:O	1:D:426:PHE:HB3	2.20	0.42
1:D:658:ASN:HA	1:D:835:GLU:HB2	2.02	0.42
1:D:1827:TYR:HD1	1:D:1908:LEU:HD23	1.85	0.42
1:D:1934:LYS:HD2	1:D:2027:ARG:HH21	1.84	0.42
2:E:26:TYR:N	2:E:40:ARG:HH12	2.17	0.42
1:A:624:ALA:HB1	1:A:629:GLN:OE1	2.19	0.42
1:A:779:PHE:CZ	1:A:782:PHE:HB3	2.54	0.42
1:A:1511:VAL:HG23	1:A:1519:LEU:HD12	2.01	0.42
1:A:2606:LEU:O	1:A:2610:THR:OG1	2.31	0.42
1:A:2614:GLU:HG2	1:A:2619:TYR:HE1	1.85	0.42
1:B:490:GLN:NE2	1:B:540:LEU:O	2.52	0.42
1:B:1297:THR:HA	1:B:1548:ALA:HB3	2.02	0.42
1:B:2257:ARG:HH21	1:B:3806:ALA:HB1	1.84	0.42
1:C:652:VAL:HG22	1:C:716:ASN:HB3	2.02	0.42
1:C:1934:LYS:HD2	1:C:2027:ARG:HH21	1.84	0.42
1:C:2278:MET:O	1:C:2279:LEU:HD12	2.20	0.42
1:D:891:GLU:O	1:D:895:MET:HG2	2.20	0.42
1:D:2165:GLY:O	1:D:2169:THR:HG23	2.19	0.42
1:D:2667:CYS:SG	1:D:2668:LEU:N	2.93	0.42
1:A:275:TRP:HE1	1:A:299:HIS:HD2	1.67	0.42
1:A:565:LEU:HB3	1:A:600:LEU:HD12	2.02	0.42
1:A:658:ASN:HA	1:A:835:GLU:HB2	2.02	0.42
1:A:731:HIS:NE2	1:A:733:TRP:HB3	2.35	0.42
1:A:987:LYS:NZ	1:A:988:LEU:O	2.42	0.42
1:A:1679:SER:HB2	1:A:1769:PHE:CE2	2.55	0.42
1:A:3637:ASP:HA	1:A:3640:ILE:HG22	2.01	0.42
1:B:415:THR:HA	1:B:418:VAL:HG12	2.02	0.42
1:B:415:THR:O	1:B:419:ILE:HG12	2.19	0.42
1:B:652:VAL:HG22	1:B:716:ASN:HB3	2.02	0.42
1:B:2278:MET:O	1:B:2279:LEU:HD12	2.20	0.42
1:B:3705:ASP:OD1	1:B:3705:ASP:N	2.53	0.42
1:C:1297:THR:HA	1:C:1548:ALA:HB3	2.02	0.42
1:C:1511:VAL:HG23	1:C:1519:LEU:HD12	2.01	0.42
1:C:2640:SER:OG	1:C:2641:ARG:NH1	2.52	0.42
1:C:4104:LEU:HD12	1:C:4104:LEU:HA	1.92	0.42
1:C:4176:VAL:HG21	1:C:4879:VAL:HG23	2.02	0.42
1:C:4603:LYS:O	1:C:4607:ARG:HG3	2.20	0.42
1:D:565:LEU:HB3	1:D:600:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1297:THR:HA	1:D:1548:ALA:HB3	2.02	0.42
1:D:2716:LEU:HD23	1:D:2716:LEU:H	1.83	0.42
1:A:891:GLU:O	1:A:895:MET:HG2	2.20	0.42
1:A:1297:THR:HA	1:A:1548:ALA:HB3	2.02	0.42
1:B:1679:SER:HB2	1:B:1769:PHE:CE2	2.55	0.42
1:B:2173:VAL:HA	1:B:2176:ASN:HD21	1.85	0.42
1:C:422:THR:O	1:C:426:PHE:HB3	2.20	0.42
1:C:1679:SER:HB2	1:C:1769:PHE:CE2	2.55	0.42
1:C:2391:TYR:O	1:C:2394:LEU:N	2.53	0.42
1:C:4193:GLU:OE2	1:C:4943:TYR:OH	2.28	0.42
1:D:490:GLN:NE2	1:D:540:LEU:O	2.52	0.42
1:D:779:PHE:CZ	1:D:782:PHE:HB3	2.54	0.42
1:D:2434:VAL:HG21	1:D:2470:PHE:HD2	1.85	0.42
1:A:415:THR:HA	1:A:418:VAL:HG12	2.02	0.42
1:A:3705:ASP:OD1	1:A:3705:ASP:N	2.53	0.42
1:B:422:THR:O	1:B:426:PHE:HB3	2.20	0.42
1:B:2667:CYS:SG	1:B:2668:LEU:N	2.93	0.42
1:C:1827:TYR:HD1	1:C:1908:LEU:HD23	1.85	0.42
1:C:2395:ILE:HD12	1:C:2395:ILE:H	1.84	0.42
1:D:626:ARG:HG2	1:D:2131:VAL:HB	2.01	0.42
1:D:731:HIS:NE2	1:D:733:TRP:HB3	2.35	0.42
1:D:3723:LEU:O	1:D:3727:GLN:HG2	2.19	0.42
1:D:4136:GLU:O	1:D:4917:TYR:OH	2.31	0.42
1:D:4176:VAL:HG21	1:D:4879:VAL:HG23	2.02	0.42
1:D:4603:LYS:O	1:D:4607:ARG:HG3	2.20	0.42
1:A:422:THR:O	1:A:426:PHE:HB3	2.20	0.42
1:A:2795:ASP:N	1:A:2795:ASP:OD1	2.46	0.42
1:A:3654:ASP:OD1	1:A:3654:ASP:N	2.48	0.42
1:A:3957:LEU:HD11	1:A:3966:LEU:HD22	2.01	0.42
1:B:655:MET:HE1	1:B:836:HIS:CG	2.55	0.42
1:B:779:PHE:CZ	1:B:782:PHE:HB3	2.54	0.42
1:B:891:GLU:O	1:B:895:MET:HG2	2.20	0.42
1:B:2391:TYR:O	1:B:2394:LEU:N	2.53	0.42
1:B:2614:GLU:HG2	1:B:2619:TYR:HE1	1.85	0.42
1:B:4176:VAL:HG21	1:B:4879:VAL:HG23	2.02	0.42
1:C:655:MET:HE1	1:C:836:HIS:CG	2.55	0.42
1:C:2290:ASN:N	1:C:2290:ASN:OD1	2.51	0.42
1:C:3723:LEU:O	1:C:3727:GLN:HG2	2.19	0.42
1:D:652:VAL:HG22	1:D:716:ASN:HB3	2.02	0.42
1:D:1731:THR:O	1:D:1734:THR:OG1	2.33	0.42
1:D:2171:MET:SD	1:D:2216:HIS:ND1	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2173:VAL:HA	1:D:2176:ASN:HD21	1.85	0.42
1:D:2278:MET:O	1:D:2279:LEU:HD12	2.20	0.42
1:D:3000:LYS:HE3	1:D:3070:THR:HA	2.02	0.42
1:D:4195:THR:HG22	1:D:4199:MET:HE2	2.00	0.42
1:A:42:PHE:HB2	1:A:425:LEU:HD12	2.01	0.42
1:A:571:ILE:HA	1:A:574:VAL:HG12	2.01	0.42
1:A:1827:TYR:HD1	1:A:1908:LEU:HD23	1.85	0.42
1:A:2667:CYS:SG	1:A:2668:LEU:N	2.93	0.42
1:A:3000:LYS:HE3	1:A:3070:THR:HA	2.02	0.42
1:B:624:ALA:HB3	1:B:2131:VAL:HG12	2.01	0.42
1:B:4603:LYS:O	1:B:4607:ARG:HG3	2.20	0.42
1:B:4928:ASP:N	1:B:4928:ASP:OD1	2.52	0.42
1:C:80:GLU:OE1	1:C:84:ASN:ND2	2.42	0.42
1:C:312:LYS:HG2	1:C:393:MET:HB2	2.02	0.42
1:C:672:LYS:NZ	1:C:760:ASP:OD2	2.36	0.42
1:C:1011:ARG:HH12	1:C:1032:LEU:N	2.18	0.42
1:D:80:GLU:OE1	1:D:84:ASN:ND2	2.42	0.42
1:D:2234:ARG:HH21	1:D:2281:SER:HG	1.68	0.42
1:D:2777:SER:O	1:D:2780:THR:OG1	2.29	0.42
1:A:652:VAL:HG22	1:A:716:ASN:HB3	2.02	0.41
1:A:2402:ALA:O	1:A:2473:ARG:NH2	2.44	0.41
1:A:4603:LYS:O	1:A:4607:ARG:HG3	2.20	0.41
1:B:312:LYS:HG2	1:B:393:MET:HB2	2.02	0.41
1:B:571:ILE:HA	1:B:574:VAL:HG12	2.01	0.41
1:B:626:ARG:HG2	1:B:2131:VAL:HB	2.01	0.41
1:B:1629:MET:HG3	1:B:1642:ILE:HG12	2.01	0.41
1:B:4039:LYS:HE2	1:B:4039:LYS:HB2	1.91	0.41
1:C:365:HIS:HE1	1:C:367:ASP:HB2	1.84	0.41
1:C:2173:VAL:HA	1:C:2176:ASN:HD21	1.85	0.41
1:D:128:MET:HB3	1:D:149:LEU:HB3	2.02	0.41
1:D:601:LEU:HG	1:D:610:VAL:HG11	2.02	0.41
1:D:655:MET:HE1	1:D:836:HIS:CG	2.55	0.41
1:D:1679:SER:HB2	1:D:1769:PHE:CE2	2.55	0.41
1:A:525:SER:O	1:A:529:ILE:HG22	2.20	0.41
1:A:590:LYS:O	1:A:594:ILE:HG12	2.20	0.41
1:A:601:LEU:HG	1:A:610:VAL:HG11	2.02	0.41
1:A:2855:LYS:HE3	1:A:2870:LEU:HB2	2.01	0.41
1:A:3723:LEU:O	1:A:3727:GLN:HG2	2.19	0.41
1:A:4193:GLU:OE2	1:A:4943:TYR:OH	2.28	0.41
1:B:59:PRO:HB3	1:B:296:ARG:CZ	2.50	0.41
1:B:507:VAL:O	1:B:509:SER:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:ALA:HB1	1:B:629:GLN:OE1	2.19	0.41
1:B:2855:LYS:HE3	1:B:2870:LEU:HB2	2.01	0.41
1:B:4817:TYR:OH	1:C:4846:ASP:OD2	2.27	0.41
1:C:115:TYR:CZ	1:C:175:VAL:HG22	2.55	0.41
1:C:128:MET:HB3	1:C:149:LEU:HB3	2.02	0.41
1:C:590:LYS:O	1:C:594:ILE:HG12	2.20	0.41
1:C:658:ASN:HA	1:C:835:GLU:HB2	2.02	0.41
1:C:779:PHE:CZ	1:C:782:PHE:HB3	2.54	0.41
1:D:38:ALA:HB1	1:D:64:ILE:HD12	2.00	0.41
1:D:2614:GLU:HG2	1:D:2619:TYR:HE1	1.85	0.41
1:D:3705:ASP:OD1	1:D:3705:ASP:N	2.53	0.41
1:D:4780:TYR:HD1	1:D:4845:PHE:CE1	2.38	0.41
2:F:17:LYS:HE3	2:F:18:LYS:N	2.32	0.41
1:A:48:PHE:H	1:A:48:PHE:HD2	1.67	0.41
1:A:59:PRO:HB3	1:A:296:ARG:CZ	2.50	0.41
1:A:463:PHE:HB3	1:A:536:LEU:CD1	2.50	0.41
1:B:48:PHE:H	1:B:48:PHE:HD2	1.67	0.41
1:B:365:HIS:HE1	1:B:367:ASP:HB2	1.84	0.41
1:B:463:PHE:HB3	1:B:536:LEU:CD1	2.50	0.41
1:B:601:LEU:HG	1:B:610:VAL:HG11	2.02	0.41
1:B:4780:TYR:HD1	1:B:4845:PHE:CE1	2.38	0.41
1:C:59:PRO:HB3	1:C:296:ARG:CZ	2.50	0.41
1:C:565:LEU:HB3	1:C:600:LEU:HD12	2.02	0.41
1:C:1720:LEU:HD12	1:C:1720:LEU:HA	1.96	0.41
1:C:3940:TRP:HA	1:C:3943:VAL:HG12	2.01	0.41
1:D:1987:CYS:HA	1:D:1988:PRO:HD3	1.94	0.41
1:A:537:LEU:HD23	1:A:540:LEU:CD1	2.49	0.41
1:A:2434:VAL:HG21	1:A:2470:PHE:HD2	1.85	0.41
1:A:3758:LEU:O	1:A:3762:ILE:HG23	2.21	0.41
1:A:3889:TRP:HB2	1:B:76:ARG:HE	1.85	0.41
1:B:290:ARG:NH1	1:B:349:MET:O	2.38	0.41
1:B:590:LYS:O	1:B:594:ILE:HG12	2.20	0.41
1:B:1131:ASP:N	1:B:1131:ASP:OD1	2.52	0.41
1:B:1302:TYR:CE2	1:B:1546:ALA:HB3	2.56	0.41
1:B:2157:HIS:O	1:B:2161:MET:HE1	2.21	0.41
1:B:2832:LEU:HB3	1:B:2837:HIS:CE1	2.56	0.41
1:B:4193:GLU:OE2	1:B:4607:ARG:NH2	2.52	0.41
1:C:891:GLU:O	1:C:895:MET:HG2	2.20	0.41
1:C:1183:LEU:HD11	1:C:1189:GLU:HG2	2.03	0.41
1:C:1642:ILE:HG23	1:C:1643:LEU:HD22	2.03	0.41
1:C:2434:VAL:HG21	1:C:2470:PHE:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4752:LEU:HD12	1:C:4752:LEU:HA	1.80	0.41
1:D:312:LYS:HG2	1:D:393:MET:HB2	2.02	0.41
1:D:1131:ASP:OD1	1:D:1131:ASP:N	2.52	0.41
1:D:2391:TYR:O	1:D:2394:LEU:N	2.53	0.41
2:G:17:LYS:HE3	2:G:18:LYS:N	2.32	0.41
1:A:133:LEU:HB2	1:A:148:GLY:H	1.86	0.41
1:A:655:MET:HE1	1:A:836:HIS:CG	2.55	0.41
1:B:115:TYR:CZ	1:B:175:VAL:HG22	2.55	0.41
1:B:1446:ILE:HA	1:B:1486:TYR:HA	2.02	0.41
1:B:3000:LYS:HE3	1:B:3070:THR:HA	2.02	0.41
1:B:3758:LEU:O	1:B:3762:ILE:HG23	2.21	0.41
1:C:507:VAL:O	1:C:509:SER:N	2.53	0.41
1:C:601:LEU:HG	1:C:610:VAL:HG11	2.02	0.41
1:C:1446:ILE:HA	1:C:1486:TYR:HA	2.02	0.41
1:C:2101:LEU:HD23	1:C:2101:LEU:HA	1.89	0.41
1:D:571:ILE:HA	1:D:574:VAL:HG12	2.01	0.41
1:D:2832:LEU:HB3	1:D:2837:HIS:CE1	2.56	0.41
1:D:4735:ASN:OD1	1:D:4735:ASN:N	2.53	0.41
1:A:115:TYR:CZ	1:A:175:VAL:HG22	2.55	0.41
1:A:167:LYS:HA	1:A:167:LYS:HD3	1.89	0.41
1:A:1011:ARG:HH12	1:A:1032:LEU:N	2.18	0.41
1:A:1426:TYR:HB2	1:A:1511:VAL:HG12	2.03	0.41
1:A:2167:HIS:CE1	1:A:2168:GLU:HG2	2.56	0.41
1:A:3015:ARG:NH2	1:A:3080:THR:HB	2.35	0.41
1:A:4176:VAL:HG21	1:A:4879:VAL:HG23	2.02	0.41
1:B:525:SER:O	1:B:529:ILE:HG22	2.20	0.41
1:B:1511:VAL:HG23	1:B:1519:LEU:HD12	2.01	0.41
1:B:1814:THR:OG1	1:B:1815:THR:N	2.54	0.41
1:B:2395:ILE:HD12	1:B:2395:ILE:H	1.84	0.41
1:B:2434:VAL:HG21	1:B:2470:PHE:HD2	1.85	0.41
1:B:2640:SER:OG	1:B:2641:ARG:NH1	2.52	0.41
1:B:3310:LYS:HG3	1:B:3311:PRO:HD3	2.02	0.41
1:B:4019:PHE:O	1:B:4027:SER:OG	2.33	0.41
1:C:626:ARG:HG2	1:C:2131:VAL:HB	2.01	0.41
1:C:2080:VAL:HG13	1:C:3669:LEU:HD22	2.03	0.41
1:C:3310:LYS:HG3	1:C:3311:PRO:HD3	2.02	0.41
1:C:3916:PHE:O	1:C:3920:THR:HG23	2.21	0.41
1:D:507:VAL:O	1:D:509:SER:N	2.53	0.41
1:D:1011:ARG:HH12	1:D:1032:LEU:N	2.18	0.41
1:D:1183:LEU:HD11	1:D:1189:GLU:HG2	2.03	0.41
1:D:2101:LEU:HD23	1:D:2101:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3657:MET:SD	1:D:3659:ARG:N	2.83	0.41
1:A:443:PRO:HA	1:A:445:ILE:HG22	2.02	0.41
1:A:507:VAL:O	1:A:509:SER:N	2.53	0.41
1:A:2832:LEU:HB3	1:A:2837:HIS:CE1	2.56	0.41
1:A:4510:ALA:O	1:A:4514:ILE:HG12	2.21	0.41
1:B:443:PRO:HA	1:B:445:ILE:HG22	2.02	0.41
1:B:1011:ARG:HH12	1:B:1032:LEU:N	2.18	0.41
1:B:1183:LEU:HD11	1:B:1189:GLU:HG2	2.03	0.41
1:B:1633:ILE:HD13	1:B:1633:ILE:HA	1.84	0.41
1:B:2101:LEU:HD23	1:B:2101:LEU:HA	1.89	0.41
1:C:337:LYS:NZ	1:C:371:TRP:HE1	2.18	0.41
1:C:497:LEU:HB3	1:C:498:VAL:H	1.63	0.41
1:C:718:VAL:HG11	1:C:791:VAL:HG11	2.02	0.41
1:C:2614:GLU:HG2	1:C:2619:TYR:HE1	1.85	0.41
1:C:3705:ASP:OD1	1:C:3705:ASP:N	2.53	0.41
1:C:3758:LEU:O	1:C:3762:ILE:HG23	2.21	0.41
1:D:115:TYR:CZ	1:D:175:VAL:HG22	2.55	0.41
1:D:133:LEU:HB2	1:D:148:GLY:H	1.86	0.41
1:D:624:ALA:HB1	1:D:629:GLN:OE1	2.19	0.41
1:D:1511:VAL:HG23	1:D:1519:LEU:HD12	2.01	0.41
1:D:3758:LEU:O	1:D:3762:ILE:HG23	2.21	0.41
2:E:17:LYS:HE3	2:E:18:LYS:N	2.32	0.41
1:A:337:LYS:NZ	1:A:371:TRP:HE1	2.18	0.41
1:A:497:LEU:HB3	1:A:498:VAL:H	1.63	0.41
1:A:641:ASP:OD1	1:A:642:LEU:N	2.49	0.41
1:A:3916:PHE:O	1:A:3920:THR:HG23	2.21	0.41
1:B:537:LEU:HD23	1:B:540:LEU:CD1	2.49	0.41
1:B:1642:ILE:HG23	1:B:1643:LEU:HD22	2.03	0.41
1:B:3916:PHE:O	1:B:3920:THR:HG23	2.21	0.41
1:C:525:SER:O	1:C:529:ILE:HG22	2.20	0.41
1:C:1814:THR:OG1	1:C:1815:THR:N	2.54	0.41
1:C:2157:HIS:O	1:C:2161:MET:HE1	2.21	0.41
1:C:2777:SER:O	1:C:2780:THR:OG1	2.29	0.41
1:C:3491:ALA:HA	1:C:3494:ARG:HD2	2.03	0.41
1:C:4577:LEU:HG	1:C:4581:ILE:HD11	2.02	0.41
1:D:415:THR:HA	1:D:418:VAL:HG12	2.02	0.41
1:D:525:SER:O	1:D:529:ILE:HG22	2.20	0.41
1:D:1426:TYR:HB2	1:D:1511:VAL:HG12	2.03	0.41
1:D:1720:LEU:HD12	1:D:1720:LEU:HA	1.96	0.41
1:D:2189:PRO:HA	1:D:2191:MET:SD	2.61	0.41
1:D:3491:ALA:HA	1:D:3494:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4510:ALA:O	1:D:4514:ILE:HG12	2.21	0.41
1:A:76:ARG:HE	1:D:3889:TRP:HB2	1.85	0.41
1:A:128:MET:HB3	1:A:149:LEU:HB3	2.02	0.41
1:A:312:LYS:HG2	1:A:393:MET:HB2	2.02	0.41
1:A:362:TYR:OH	1:A:401:ASP:HB3	2.21	0.41
1:A:1068:ASP:OD1	1:A:1068:ASP:N	2.50	0.41
1:A:4735:ASN:OD1	1:A:4735:ASN:N	2.53	0.41
1:B:1814:THR:HG23	1:B:1816:GLU:HG2	2.03	0.41
1:B:1827:TYR:HD1	1:B:1908:LEU:HD23	1.85	0.41
1:B:2189:PRO:HA	1:B:2191:MET:SD	2.61	0.41
1:B:2796:SER:HB3	1:B:2897:ILE:HG22	2.03	0.41
1:B:3889:TRP:HB2	1:C:76:ARG:HE	1.85	0.41
1:B:4735:ASN:OD1	1:B:4735:ASN:N	2.53	0.41
1:C:133:LEU:HB2	1:C:148:GLY:H	1.86	0.41
1:C:300:VAL:HG21	1:C:419:ILE:HD12	2.03	0.41
1:C:362:TYR:OH	1:C:401:ASP:HB3	2.21	0.41
1:C:1302:TYR:CE2	1:C:1546:ALA:HB3	2.56	0.41
1:C:2189:PRO:HA	1:C:2191:MET:SD	2.61	0.41
1:C:2654:LYS:HG3	1:C:2656:TYR:H	1.86	0.41
1:C:3000:LYS:HE3	1:C:3070:THR:HA	2.02	0.41
1:C:3015:ARG:NH2	1:C:3080:THR:HB	2.35	0.41
1:C:3098:VAL:HA	1:C:3101:LEU:HD13	2.03	0.41
1:C:3370:PRO:HA	1:C:3373:ILE:HB	2.03	0.41
1:C:3889:TRP:HB2	1:D:76:ARG:HE	1.85	0.41
1:C:4056:HIS:O	1:C:4062:THR:OG1	2.33	0.41
1:C:4780:TYR:HD1	1:C:4845:PHE:CE1	2.38	0.41
1:D:59:PRO:HB3	1:D:296:ARG:CZ	2.50	0.41
1:D:590:LYS:O	1:D:594:ILE:HG12	2.20	0.41
1:D:1302:TYR:CE2	1:D:1546:ALA:HB3	2.56	0.41
1:D:1796:LEU:HD23	1:D:1796:LEU:HA	1.90	0.41
1:D:1814:THR:HG23	1:D:1816:GLU:HG2	2.03	0.41
1:D:2167:HIS:CE1	1:D:2168:GLU:HG2	2.56	0.41
1:D:2796:SER:HB3	1:D:2897:ILE:HG22	2.03	0.41
1:D:3098:VAL:HA	1:D:3101:LEU:HD13	2.03	0.41
1:D:4844:ILE:O	1:D:4848:THR:OG1	2.36	0.41
1:A:718:VAL:HG11	1:A:791:VAL:HG11	2.02	0.41
1:A:723:PHE:HE1	1:A:1482:ARG:HB3	1.86	0.41
1:A:988:LEU:HD11	1:A:992:GLN:HG2	2.03	0.41
1:A:1446:ILE:HA	1:A:1486:TYR:HA	2.02	0.41
1:B:133:LEU:HB2	1:B:148:GLY:H	1.86	0.41
1:B:362:TYR:OH	1:B:401:ASP:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:LEU:HB3	1:B:600:LEU:HD12	2.02	0.41
1:B:4018:MET:C	1:B:4020:LEU:H	2.29	0.41
1:C:443:PRO:HA	1:C:445:ILE:HG22	2.02	0.41
1:C:723:PHE:HE1	1:C:1482:ARG:HB3	1.86	0.41
1:C:1461:ARG:O	1:C:1463:ARG:N	2.51	0.41
1:D:337:LYS:NZ	1:D:371:TRP:HE1	2.18	0.41
1:D:362:TYR:OH	1:D:401:ASP:HB3	2.21	0.41
1:D:3954:GLN:H	1:D:3954:GLN:HG2	1.57	0.41
1:D:4766:LEU:HD12	1:D:4864:LEU:HD13	2.03	0.41
1:A:1814:THR:HG23	1:A:1816:GLU:HG2	2.03	0.40
1:A:2157:HIS:O	1:A:2161:MET:HE1	2.21	0.40
1:A:3098:VAL:HA	1:A:3101:LEU:HD13	2.03	0.40
1:A:4766:LEU:HD12	1:A:4864:LEU:HD13	2.03	0.40
1:B:337:LYS:NZ	1:B:371:TRP:HE1	2.18	0.40
1:B:723:PHE:HE1	1:B:1482:ARG:HB3	1.86	0.40
1:B:858:THR:OG1	1:B:861:ALA:O	2.32	0.40
1:B:1524:ASN:OD1	1:B:1524:ASN:N	2.54	0.40
1:B:2080:VAL:HG13	1:B:3669:LEU:HD22	2.03	0.40
1:B:2654:LYS:HG3	1:B:2656:TYR:H	1.86	0.40
1:B:3491:ALA:HA	1:B:3494:ARG:HD2	2.03	0.40
1:B:4577:LEU:HG	1:B:4581:ILE:HD11	2.02	0.40
1:C:2832:LEU:HB3	1:C:2837:HIS:CE1	2.56	0.40
1:D:745:ASN:O	1:D:745:ASN:ND2	2.55	0.40
1:D:1814:THR:OG1	1:D:1815:THR:N	2.54	0.40
1:B:2113:GLU:OE2	1:B:2113:GLU:N	2.54	0.40
1:B:3098:VAL:HA	1:B:3101:LEU:HD13	2.03	0.40
1:B:3370:PRO:HA	1:B:3373:ILE:HB	2.03	0.40
1:C:988:LEU:HD11	1:C:992:GLN:HG2	2.03	0.40
1:C:4510:ALA:O	1:C:4514:ILE:HG12	2.21	0.40
1:C:4766:LEU:HD12	1:C:4864:LEU:HD13	2.03	0.40
1:D:428:ARG:NH1	1:D:428:ARG:O	2.54	0.40
1:D:537:LEU:HD23	1:D:540:LEU:CD1	2.49	0.40
1:D:1446:ILE:HA	1:D:1486:TYR:HA	2.02	0.40
1:A:745:ASN:O	1:A:745:ASN:ND2	2.55	0.40
1:A:808:HIS:CE1	1:A:832:LEU:HD11	2.57	0.40
1:A:4608:LYS:HD3	1:A:4614:LEU:HD22	2.03	0.40
1:B:2167:HIS:CE1	1:B:2168:GLU:HG2	2.56	0.40
1:B:3202:ASP:HA	1:B:3207:ILE:HD13	2.04	0.40
1:C:405:LEU:HD23	1:C:405:LEU:HA	1.86	0.40
1:C:415:THR:HA	1:C:418:VAL:HG12	2.02	0.40
1:C:537:LEU:HD23	1:C:540:LEU:CD1	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1426:TYR:HB2	1:C:1511:VAL:HG12	2.03	0.40
1:C:1438:PRO:HG2	1:C:1547:GLN:HB3	2.04	0.40
1:C:2167:HIS:CE1	1:C:2168:GLU:HG2	2.56	0.40
1:C:2464:LYS:O	1:C:2468:VAL:HG13	2.22	0.40
1:D:405:LEU:HD23	1:D:405:LEU:HA	1.86	0.40
1:D:443:PRO:HA	1:D:445:ILE:HG22	2.02	0.40
1:D:723:PHE:HE1	1:D:1482:ARG:HB3	1.86	0.40
1:D:987:LYS:NZ	1:D:988:LEU:O	2.42	0.40
1:D:2080:VAL:HG13	1:D:3669:LEU:HD22	2.03	0.40
1:D:2101:LEU:O	1:D:2104:THR:HG22	2.22	0.40
1:A:428:ARG:NH1	1:A:428:ARG:O	2.54	0.40
1:A:1183:LEU:HD11	1:A:1189:GLU:HG2	2.03	0.40
1:A:1796:LEU:HD23	1:A:1796:LEU:HA	1.90	0.40
1:A:1814:THR:OG1	1:A:1815:THR:N	2.54	0.40
1:A:2654:LYS:HG3	1:A:2656:TYR:H	1.86	0.40
1:A:2796:SER:HB3	1:A:2897:ILE:HG22	2.03	0.40
1:A:4780:TYR:HD1	1:A:4845:PHE:CE1	2.38	0.40
1:B:128:MET:HB3	1:B:149:LEU:HB3	2.02	0.40
1:B:494:MET:HB3	1:B:550:GLN:HB3	2.04	0.40
1:B:641:ASP:OD1	1:B:642:LEU:N	2.49	0.40
1:B:808:HIS:CE1	1:B:832:LEU:HD11	2.57	0.40
1:B:2723:TYR:CE2	1:B:2898:SER:HB3	2.57	0.40
1:C:1631:LEU:HD12	1:C:1633:ILE:HG12	2.04	0.40
1:C:2171:MET:HE1	1:C:2216:HIS:HB2	2.04	0.40
1:D:167:LYS:HD3	1:D:167:LYS:HA	1.89	0.40
1:D:2157:HIS:O	1:D:2161:MET:HE1	2.21	0.40
1:D:2464:LYS:O	1:D:2468:VAL:HG13	2.22	0.40
1:D:2723:TYR:CE2	1:D:2898:SER:HB3	2.57	0.40
1:D:4193:GLU:OE2	1:D:4607:ARG:NH2	2.52	0.40
2:E:25:HIS:CD2	2:E:45:PRO:HB3	2.56	0.40
2:F:25:HIS:CD2	2:F:45:PRO:HB3	2.56	0.40
1:A:305:TYR:N	1:A:317:MET:O	2.42	0.40
1:A:1637:ASN:OD1	1:A:1637:ASN:N	2.55	0.40
1:A:2191:MET:SD	1:A:2191:MET:N	2.85	0.40
1:A:2723:TYR:CE2	1:A:2898:SER:HB3	2.57	0.40
1:A:3491:ALA:HA	1:A:3494:ARG:HD2	2.03	0.40
1:B:718:VAL:HG11	1:B:791:VAL:HG11	2.02	0.40
1:B:1426:TYR:HB2	1:B:1511:VAL:HG12	2.03	0.40
1:B:1461:ARG:O	1:B:1463:ARG:N	2.51	0.40
1:C:494:MET:HB3	1:C:550:GLN:HB3	2.04	0.40
1:C:2723:TYR:CE2	1:C:2898:SER:HB3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2796:SER:HB3	1:C:2897:ILE:HG22	2.03	0.40
1:D:1642:ILE:HG23	1:D:1643:LEU:HD22	2.03	0.40
1:D:3310:LYS:HG3	1:D:3311:PRO:HD3	2.02	0.40
1:D:3370:PRO:HA	1:D:3373:ILE:HB	2.03	0.40
2:F:57:LYS:H	2:F:57:LYS:HG2	1.70	0.40
2:H:25:HIS:CD2	2:H:45:PRO:HB3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4011/4966 (81%)	3600 (90%)	404 (10%)	7 (0%)	43	72
1	B	4011/4966 (81%)	3600 (90%)	404 (10%)	7 (0%)	43	72
1	C	4011/4966 (81%)	3600 (90%)	404 (10%)	7 (0%)	43	72
1	D	4011/4966 (81%)	3600 (90%)	404 (10%)	7 (0%)	43	72
2	E	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
2	F	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
2	G	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
2	H	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
All	All	16464/20292 (81%)	14804 (90%)	1632 (10%)	28 (0%)	44	72

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	LYS
1	A	1484	ASN
1	A	3253	PRO
1	B	344	LYS

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Mol	Chain	Res	Type
1	B	1484	ASN
1	B	3253	PRO
1	C	344	LYS
1	C	1484	ASN
1	C	3253	PRO
1	D	344	LYS
1	D	1484	ASN
1	D	3253	PRO
1	A	1768	SER
1	B	1768	SER
1	C	1768	SER
1	D	1768	SER
1	A	1285	VAL
1	B	1285	VAL
1	C	1285	VAL
1	D	1285	VAL
1	A	1299	ILE
1	A	2988	PRO
1	B	1299	ILE
1	B	2988	PRO
1	C	1299	ILE
1	C	2988	PRO
1	D	1299	ILE
1	D	2988	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	3319/4352 (76%)	3313 (100%)	6 (0%)	87	85
1	B	3319/4352 (76%)	3313 (100%)	6 (0%)	87	85
1	C	3319/4352 (76%)	3313 (100%)	6 (0%)	87	85
1	D	3319/4352 (76%)	3313 (100%)	6 (0%)	87	85
2	E	88/88 (100%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	88/88 (100%)	88 (100%)	0	100	100
2	G	88/88 (100%)	88 (100%)	0	100	100
2	H	88/88 (100%)	88 (100%)	0	100	100
All	All	13628/17760 (77%)	13604 (100%)	24 (0%)	85	85

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	MET
1	A	632	ILE
1	A	1007	TRP
1	A	2265	VAL
1	A	3002	MET
1	A	4108	MET
1	B	81	MET
1	B	632	ILE
1	B	1007	TRP
1	B	2265	VAL
1	B	3002	MET
1	B	4108	MET
1	C	81	MET
1	C	632	ILE
1	C	1007	TRP
1	C	2265	VAL
1	C	3002	MET
1	C	4108	MET
1	D	81	MET
1	D	632	ILE
1	D	1007	TRP
1	D	2265	VAL
1	D	3002	MET
1	D	4108	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (185) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	HIS
1	A	288	HIS
1	A	464	HIS
1	A	645	GLN

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Mol	Chain	Res	Type
1	A	871	GLN
1	A	888	ASN
1	A	890	HIS
1	A	914	GLN
1	A	971	GLN
1	A	992	GLN
1	A	1002	ASN
1	A	1244	ASN
1	A	1657	HIS
1	A	1837	ASN
1	A	1845	GLN
1	A	1904	GLN
1	A	2058	GLN
1	A	2070	GLN
1	A	2090	GLN
1	A	2151	ASN
1	A	2176	ASN
1	A	2223	ASN
1	A	2703	GLN
1	A	2738	ASN
1	A	2753	GLN
1	A	2889	GLN
1	A	3016	HIS
1	A	3078	GLN
1	A	3307	ASN
1	A	3410	ASN
1	A	3513	HIS
1	A	3790	GLN
1	A	3881	GLN
1	A	3924	GLN
1	A	3948	HIS
1	A	3974	GLN
1	A	4126	ASN
1	A	4200	GLN
1	A	4735	ASN
1	A	4761	HIS
1	A	4786	ASN
1	A	4793	ASN
1	A	4964	GLN
1	B	261	HIS
1	B	288	HIS
1	B	464	HIS

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Mol	Chain	Res	Type
1	B	487	ASN
1	B	645	GLN
1	B	871	GLN
1	B	888	ASN
1	B	890	HIS
1	B	896	ASN
1	B	971	GLN
1	B	992	GLN
1	B	1002	ASN
1	B	1657	HIS
1	B	1837	ASN
1	B	1845	GLN
1	B	1904	GLN
1	B	2058	GLN
1	B	2070	GLN
1	B	2090	GLN
1	B	2151	ASN
1	B	2176	ASN
1	B	2223	ASN
1	B	2703	GLN
1	B	2738	ASN
1	B	2753	GLN
1	B	2889	GLN
1	B	3016	HIS
1	B	3078	GLN
1	B	3307	ASN
1	B	3410	ASN
1	B	3417	ASN
1	B	3513	HIS
1	B	3790	GLN
1	B	3881	GLN
1	B	3924	GLN
1	B	3948	HIS
1	B	3974	GLN
1	B	4126	ASN
1	B	4200	GLN
1	B	4635	ASN
1	B	4735	ASN
1	B	4761	HIS
1	B	4786	ASN
1	B	4793	ASN
1	B	4964	GLN

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Mol	Chain	Res	Type
1	C	225	GLN
1	C	261	HIS
1	C	288	HIS
1	C	464	HIS
1	C	487	ASN
1	C	645	GLN
1	C	871	GLN
1	C	888	ASN
1	C	890	HIS
1	C	896	ASN
1	C	914	GLN
1	C	971	GLN
1	C	992	GLN
1	C	1002	ASN
1	C	1657	HIS
1	C	1837	ASN
1	C	1845	GLN
1	C	1904	GLN
1	C	2058	GLN
1	C	2070	GLN
1	C	2090	GLN
1	C	2151	ASN
1	C	2176	ASN
1	C	2223	ASN
1	C	2703	GLN
1	C	2738	ASN
1	C	2753	GLN
1	C	2889	GLN
1	C	3016	HIS
1	C	3078	GLN
1	C	3307	ASN
1	C	3410	ASN
1	C	3513	HIS
1	C	3790	GLN
1	C	3881	GLN
1	C	3924	GLN
1	C	3948	HIS
1	C	3974	GLN
1	C	4126	ASN
1	C	4735	ASN
1	C	4761	HIS
1	C	4786	ASN

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Mol	Chain	Res	Type
1	C	4793	ASN
1	C	4964	GLN
1	D	225	GLN
1	D	261	HIS
1	D	288	HIS
1	D	464	HIS
1	D	645	GLN
1	D	871	GLN
1	D	888	ASN
1	D	890	HIS
1	D	896	ASN
1	D	914	GLN
1	D	971	GLN
1	D	992	GLN
1	D	1002	ASN
1	D	1014	GLN
1	D	1657	HIS
1	D	1837	ASN
1	D	1845	GLN
1	D	1904	GLN
1	D	2058	GLN
1	D	2070	GLN
1	D	2090	GLN
1	D	2151	ASN
1	D	2176	ASN
1	D	2223	ASN
1	D	2703	GLN
1	D	2738	ASN
1	D	2753	GLN
1	D	2889	GLN
1	D	3016	HIS
1	D	3078	GLN
1	D	3307	ASN
1	D	3410	ASN
1	D	3513	HIS
1	D	3790	GLN
1	D	3881	GLN
1	D	3924	GLN
1	D	3948	HIS
1	D	3974	GLN
1	D	4126	ASN
1	D	4200	GLN

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Mol	Chain	Res	Type
1	D	4735	ASN
1	D	4761	HIS
1	D	4786	ASN
1	D	4793	ASN
1	D	4964	GLN
2	E	43	ASN
2	E	105	ASN
2	F	43	ASN
2	F	105	ASN
2	G	43	ASN
2	G	105	ASN
2	H	43	ASN
2	H	105	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

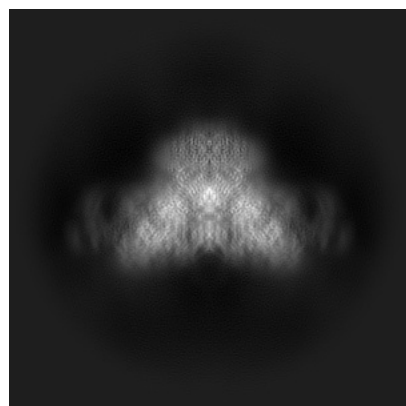
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27712. These allow visual inspection of the internal detail of the map and identification of artifacts.

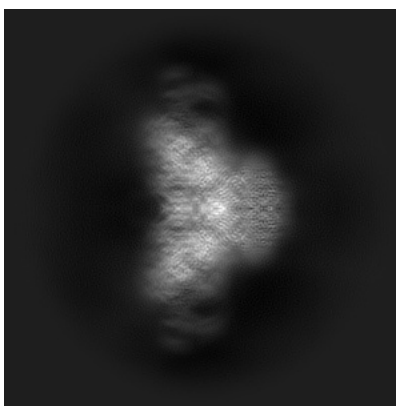
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

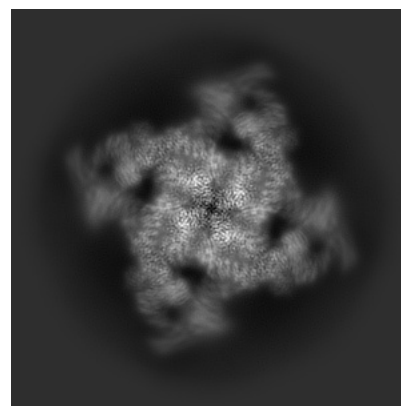
6.1.1 Primary map



X

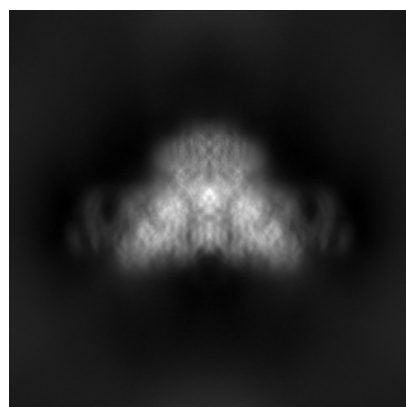


Y

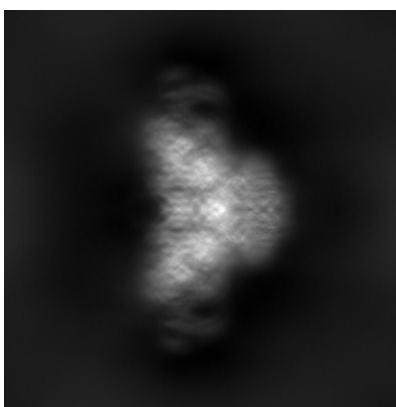


Z

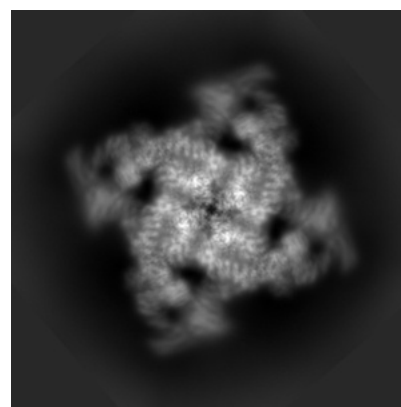
6.1.2 Raw map



X



Y

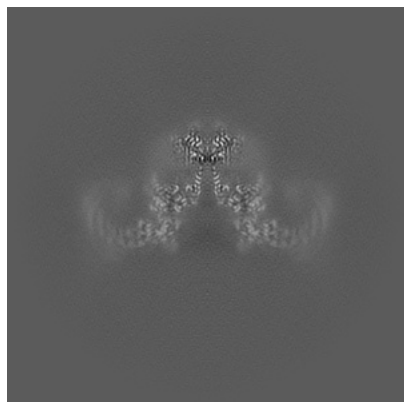


Z

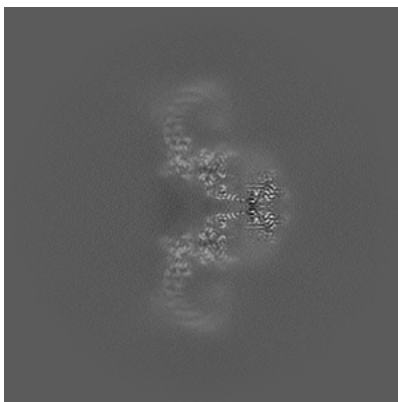
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

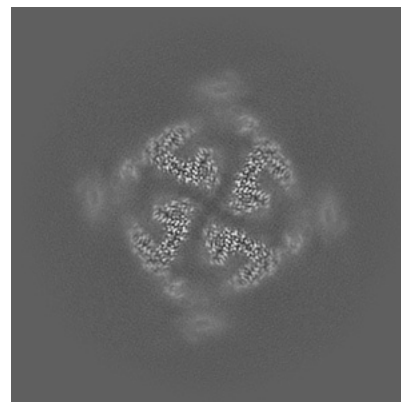
6.2.1 Primary map



X Index: 230

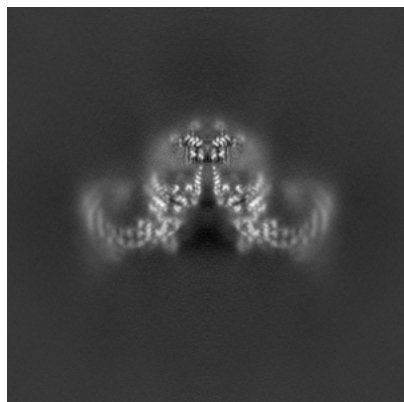


Y Index: 230

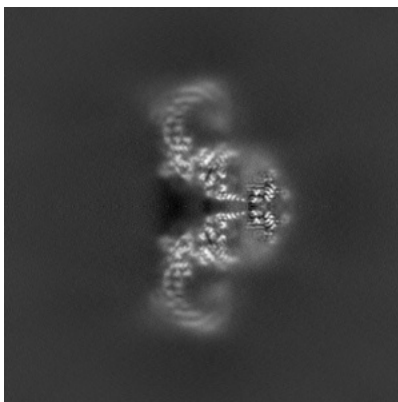


Z Index: 230

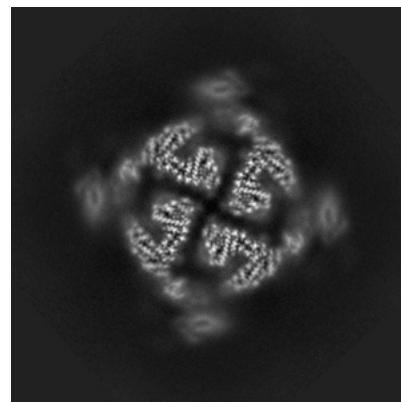
6.2.2 Raw map



X Index: 230



Y Index: 230

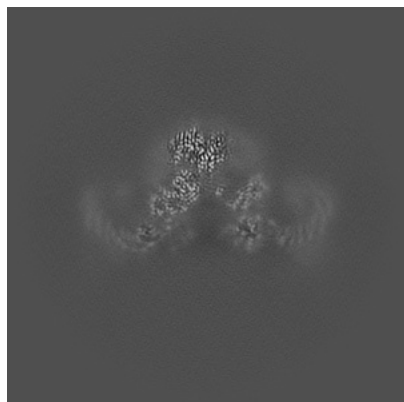


Z Index: 230

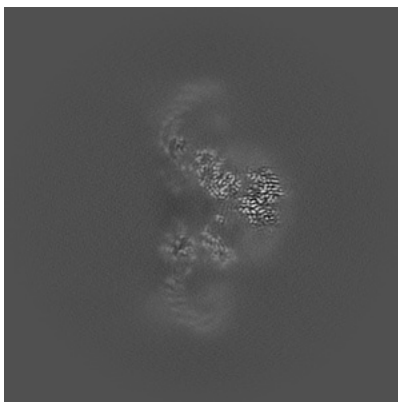
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

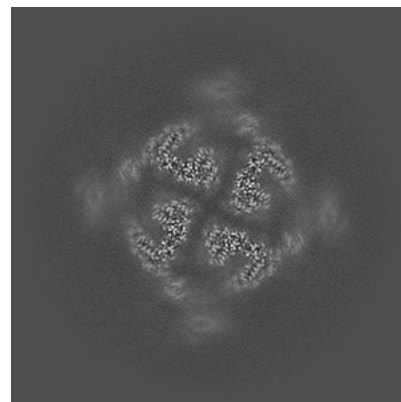
6.3.1 Primary map



X Index: 236

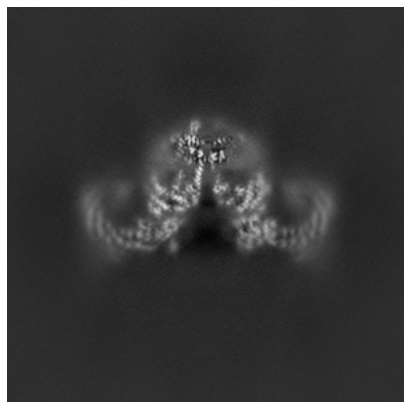


Y Index: 236

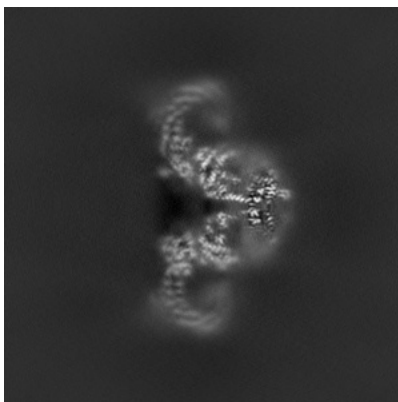


Z Index: 229

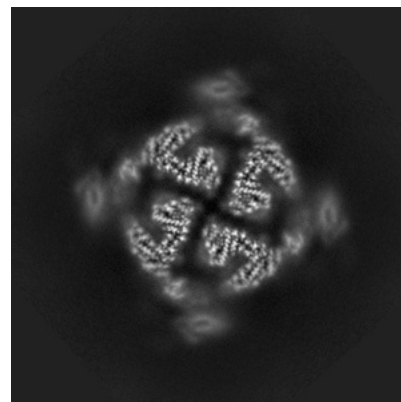
6.3.2 Raw map



X Index: 232



Y Index: 232

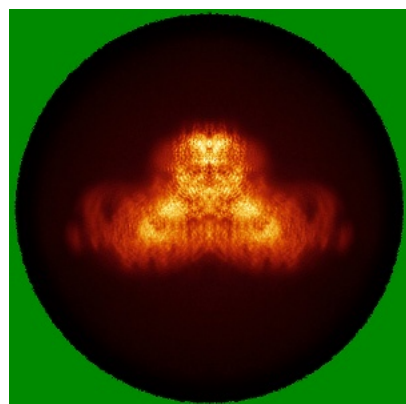


Z Index: 230

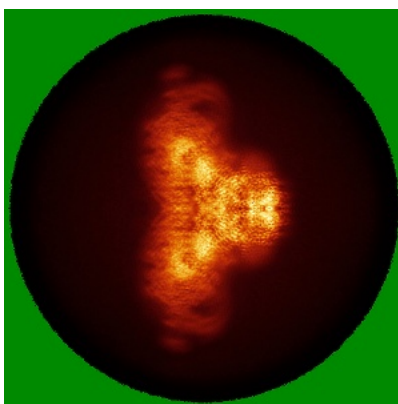
The images above show the largest variance slices of the map in three orthogonal directions.

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

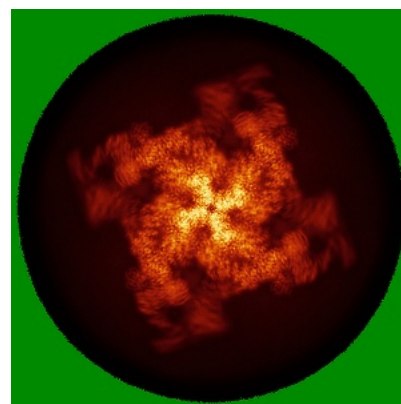
6.4.1 Primary map



X



Y

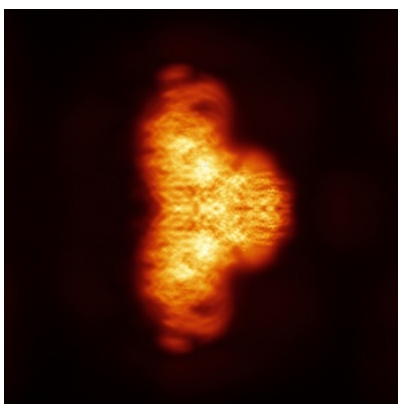


Z

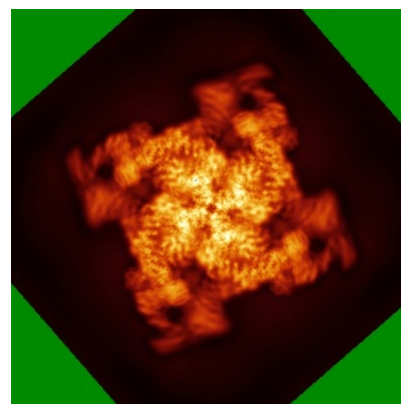
6.4.2 Raw map



X



Y

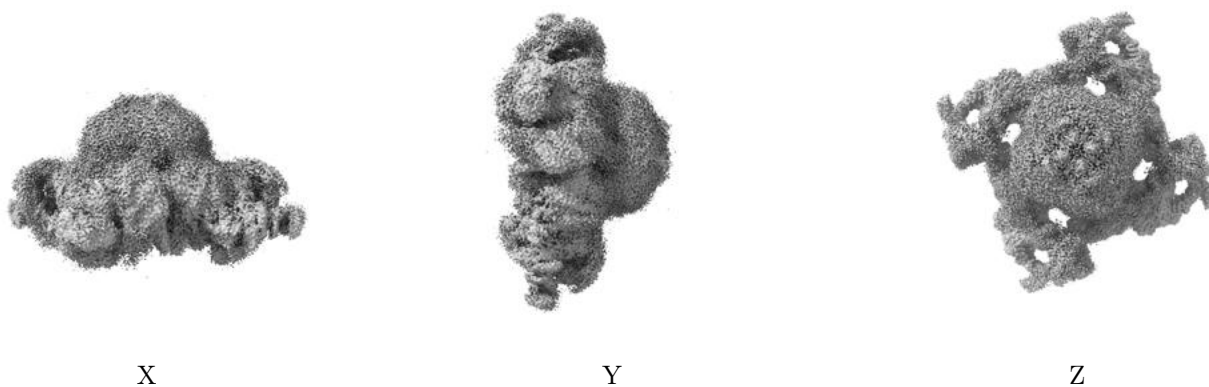


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

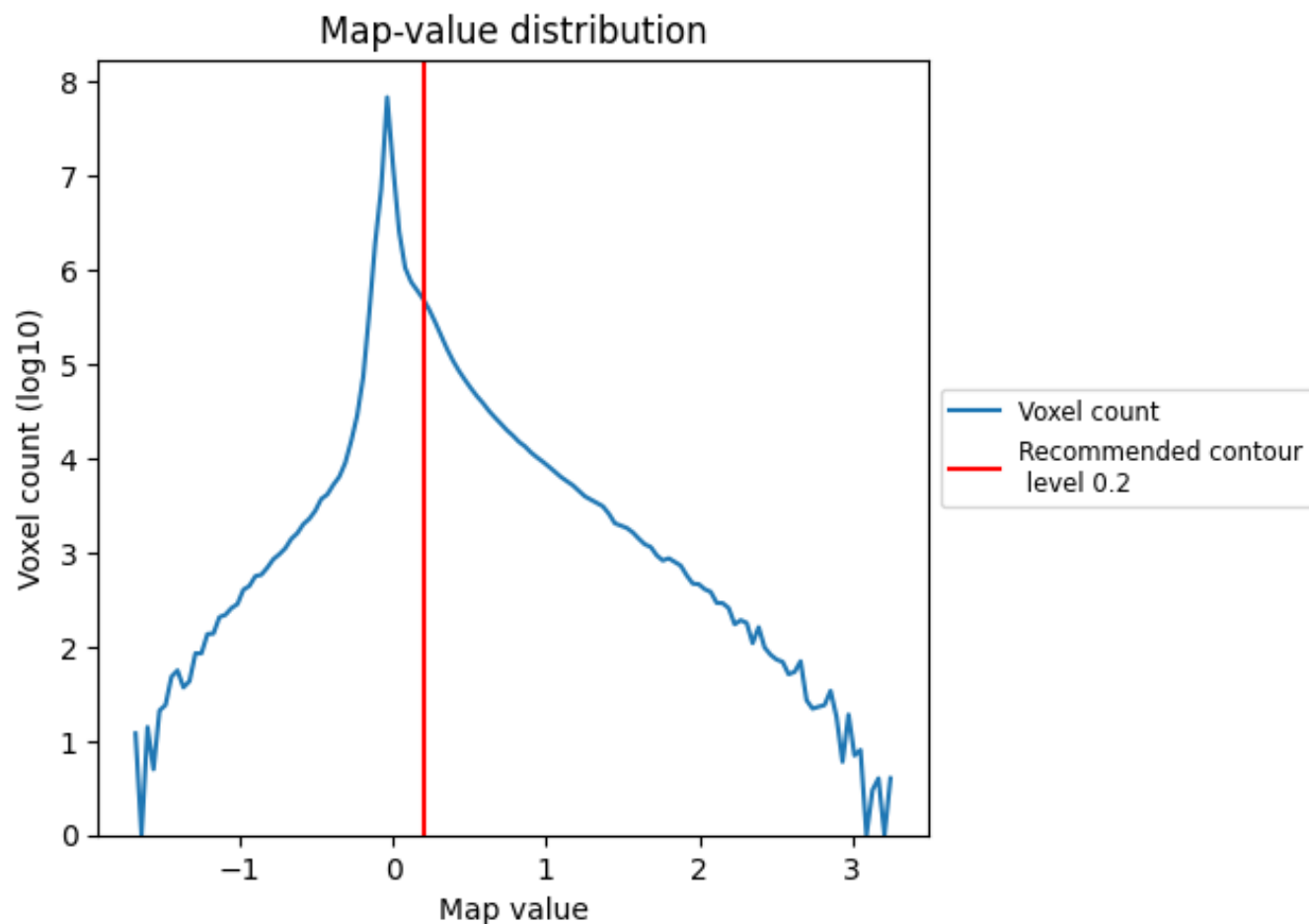
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

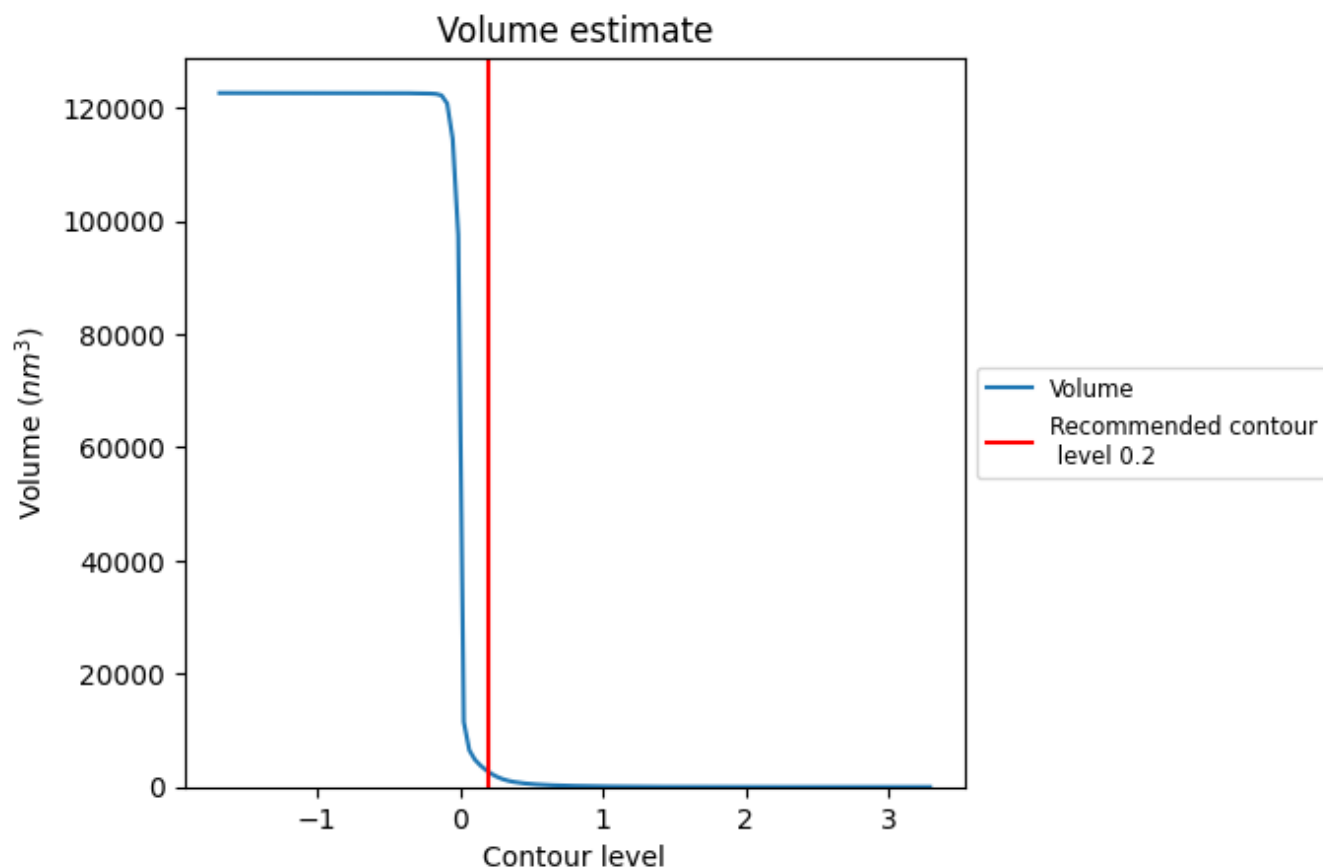
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

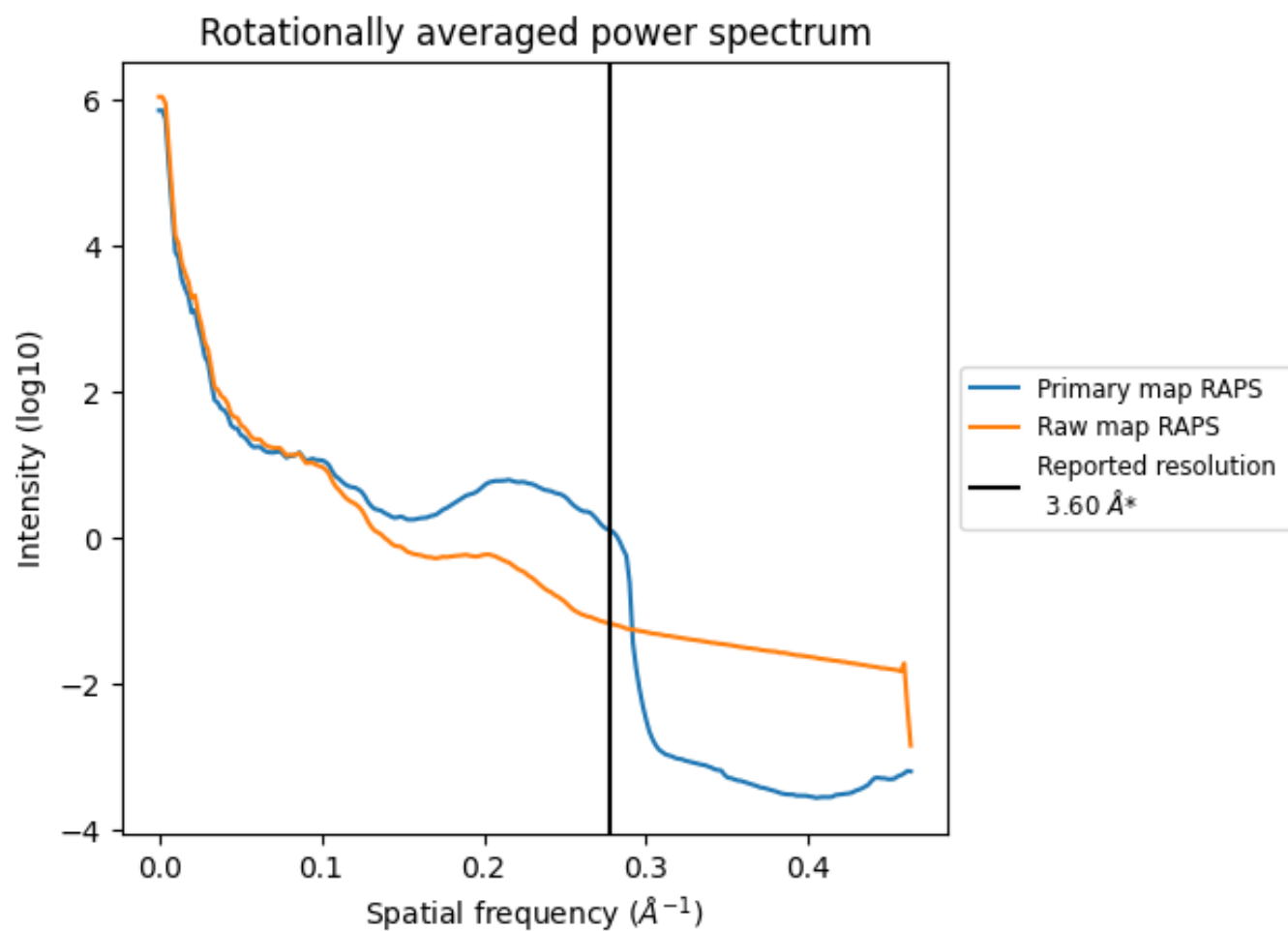
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2673 nm^3 ; this corresponds to an approximate mass of 2415 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 ⓘ

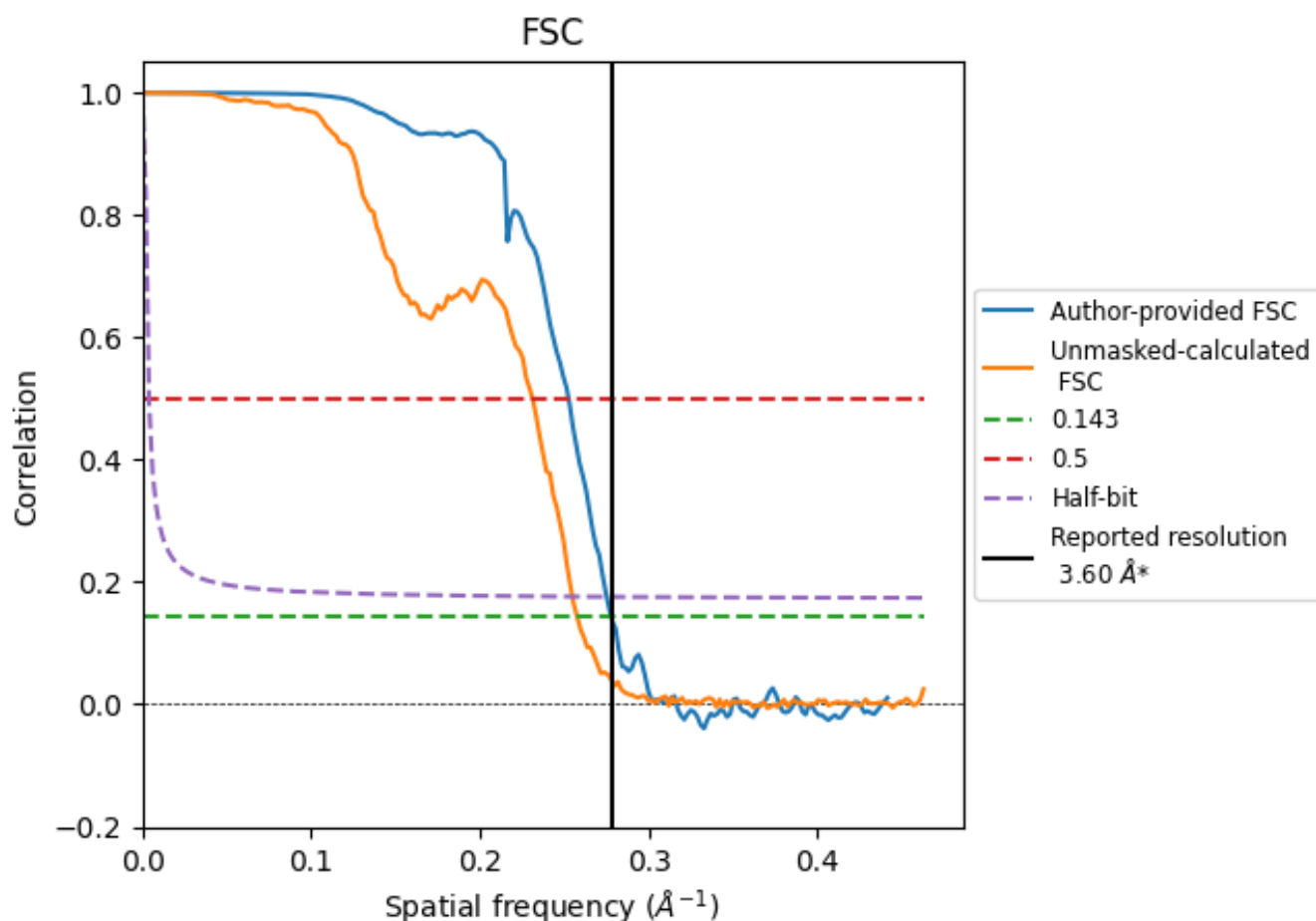


*Reported resolution corresponds to spatial frequency of $0.278 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

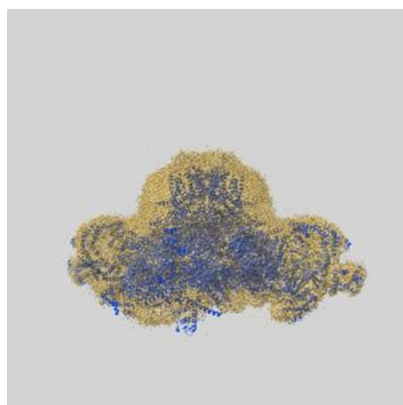
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	3.96	3.64
Unmasked-calculated*	3.88	4.32	3.92

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

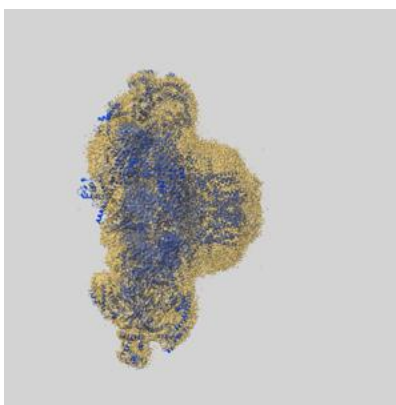
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27712 and PDB model 8DTZ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

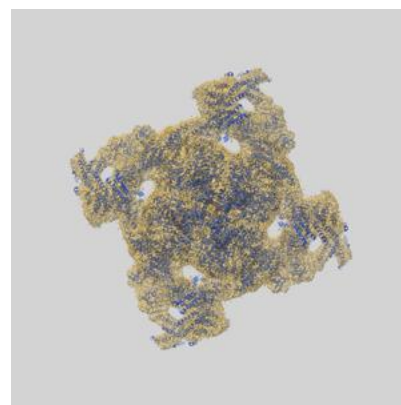
9.1 Map-model overlay [i](#)



X



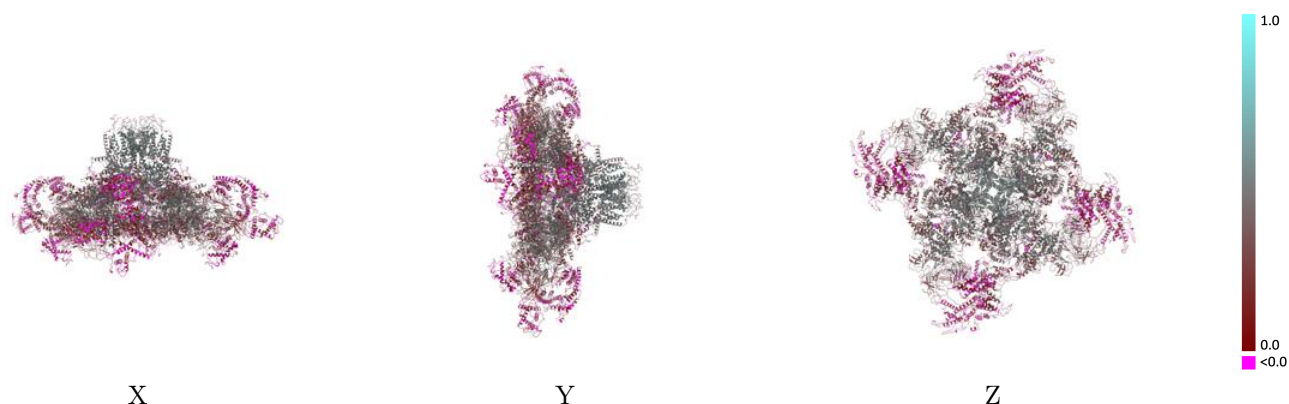
Y



Z

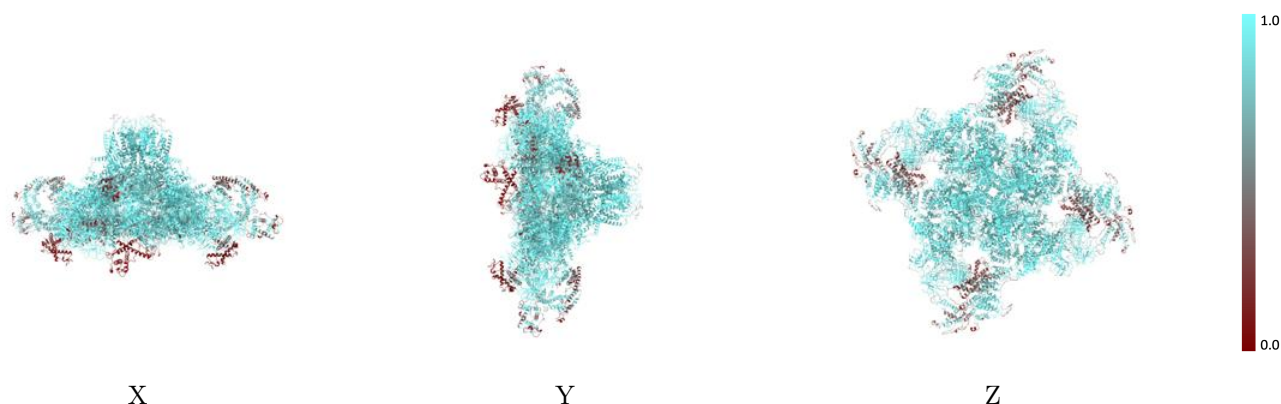
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



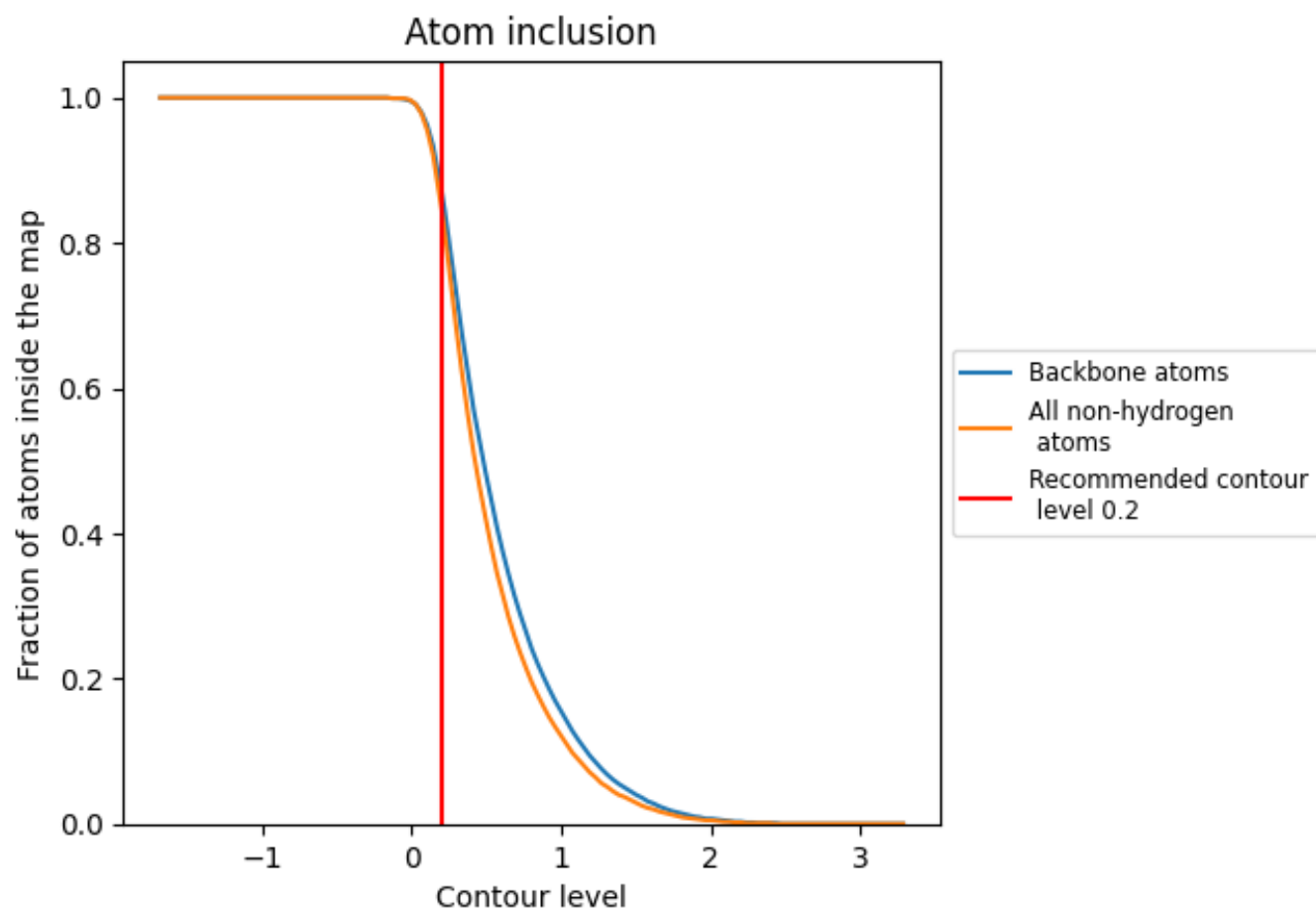
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 85% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8470	0.3020
A	0.8450	0.3010
B	0.8450	0.3000
C	0.8460	0.3000
D	0.8450	0.3010
E	0.9380	0.3560
F	0.9370	0.3550
G	0.9340	0.3570
H	0.9370	0.3580

