



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:13 PM UTC

PDB ID : 9G9L / pdb_00009g9l
EMDB ID : EMD-51156
Title : DNA-PK + Polymerase lambda
Authors : Chaplin, A.K.; Amin, H.; Zahid, S.; Hardwick, S.W.
Deposited on : 2024-07-25
Resolution : 4.63 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

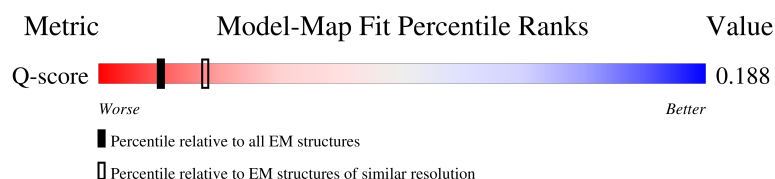
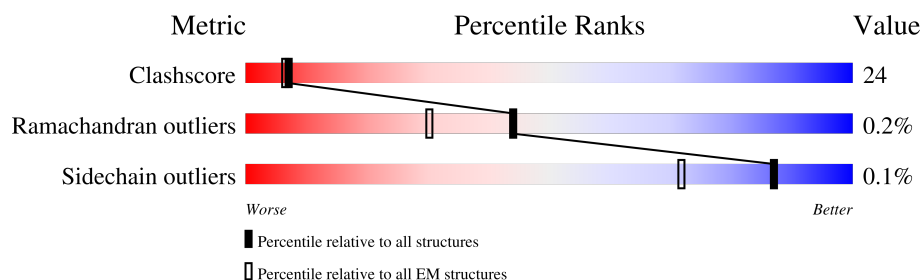
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.63 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	2068 (4.13 - 5.13)

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	4128	
2	B	609	
3	C	732	
4	F	575	

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Mol	Chain	Length	Quality of chain
5	M	204	<div><div></div><div>10%</div><div></div><div>89%</div></div>
6	D	24	<div><div></div><div>17%</div><div></div><div>83%</div></div>
7	E	23	<div><div></div><div>17%</div><div></div><div>83%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 39800 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 DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3688	Total	C	N	O	S	0	0
			29010	18609	4895	5318	188		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	488	Total	C	N	O	S	0	0
			3825	2453	645	709	18		

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	647	Total	C	N	O	S	0	0
			5093	3248	849	970	26		

- Molecule 4 is a protein called DNA polymerase lambda.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	98	Total	C	N	O	S	0	0
			755	482	141	129	3		

- Molecule 5 is a protein called Protein PAXX.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	23	Total	C	N	O	S	0	0
			155	99	25	30	1		

- Molecule 6 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	24	Total	C	N	O	P	0	0
			488	238	89	138	23		

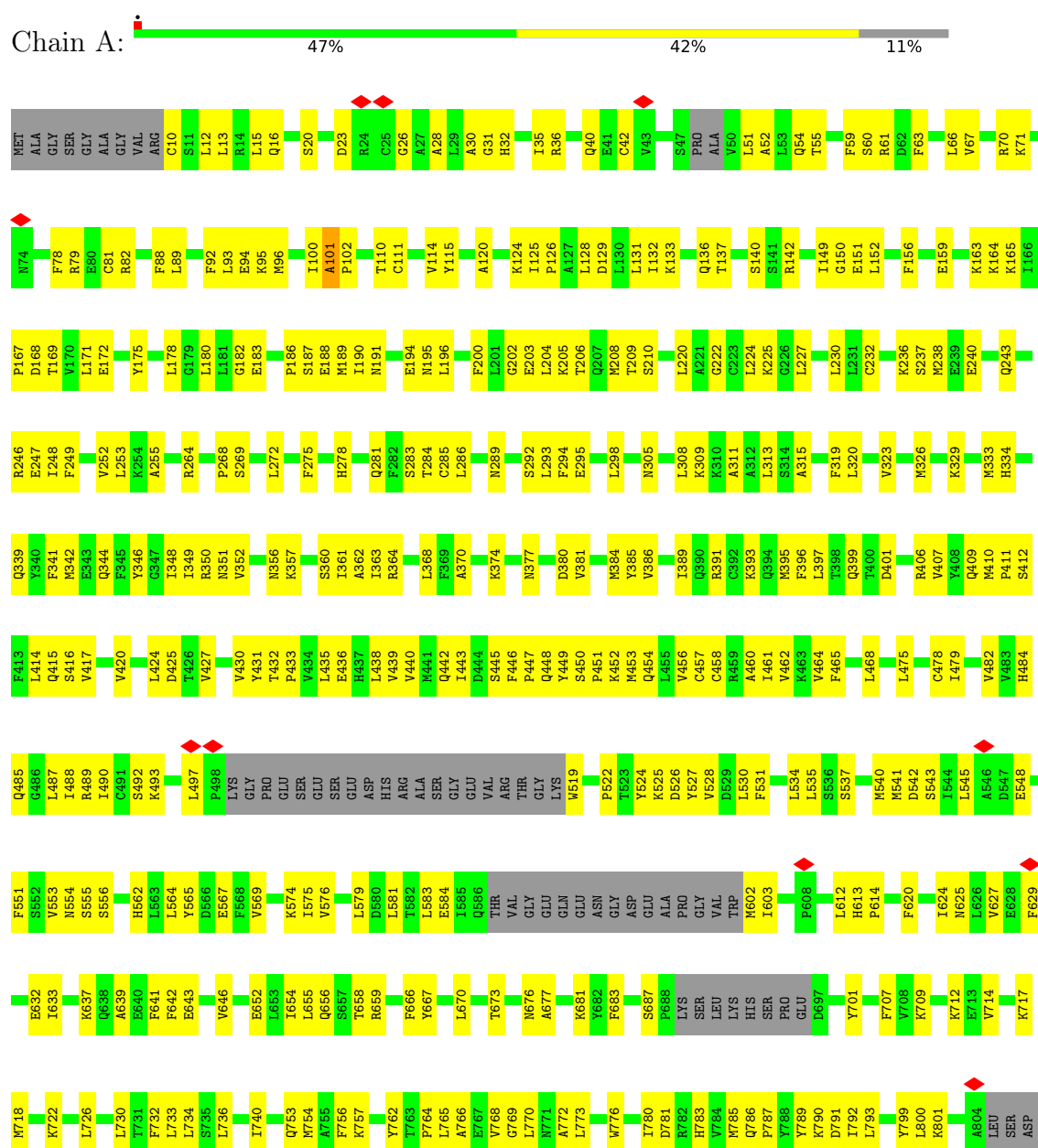
- Molecule 7 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	23	Total	C	N	O	P	0	0
			474	230	79	142	23		

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: DNA-dependent protein kinase catalytic subunit

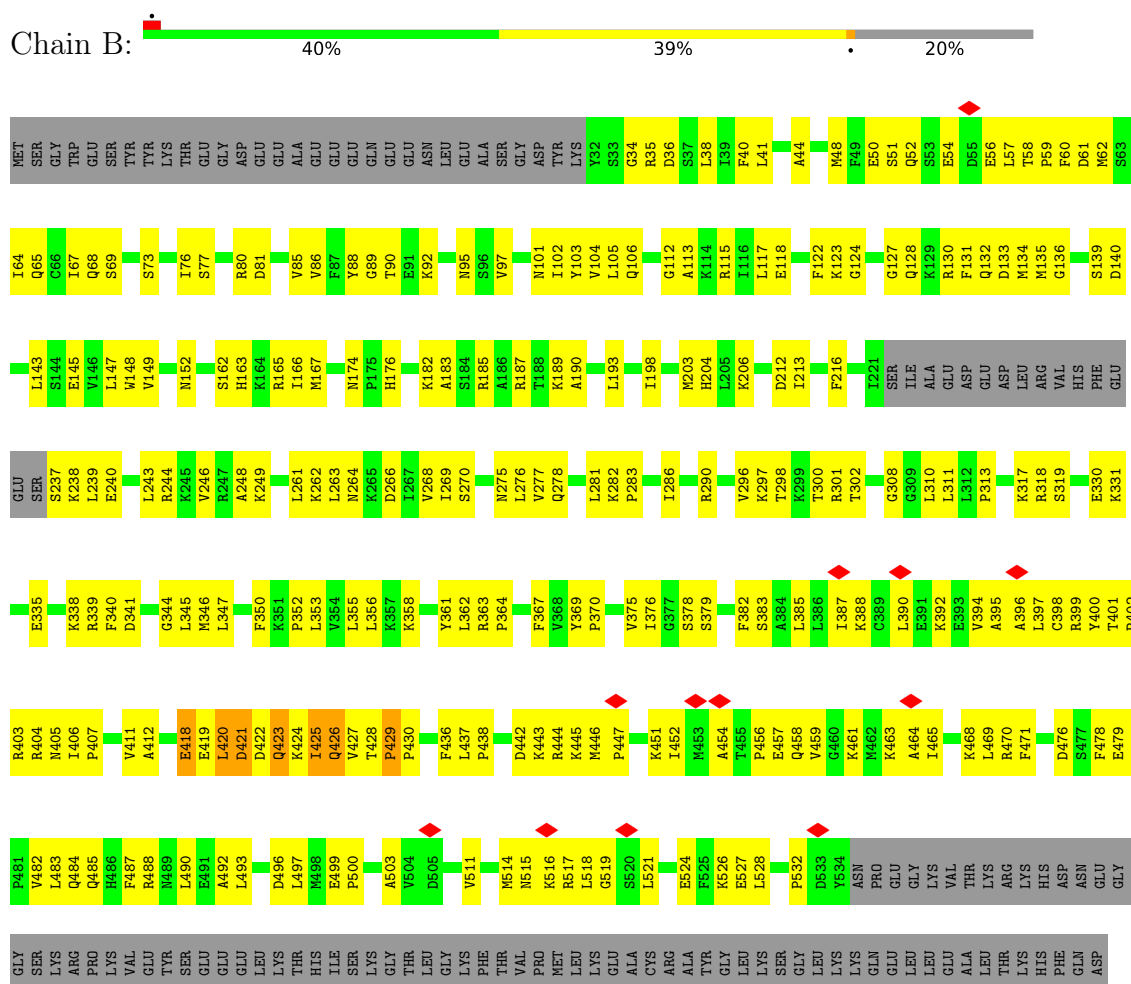


L1858	E1776	D1685	N1589	K1508	L1419	E1343	Y1267	T1181	E1102	V1018	N937	N869	GLU
N1859	L1777	L1686	M1592	G1513	R1420	F1344	F1270	R1184	V1105	D1019	V938	L870	THR
E1860	F1778	H1687	M1593	G1514	E1421	T1345	R1270	H1185	F1102	P1020	N940	L871	LYS
L1861	Q1779	L1688	V1593	E1516	K1422	L1348	R1275	H1186	M1108	F1021	F940	V1021	ASN
F1862	S1780	K1689	V1596	L1517	T1423	L1356	R1276	S1187	E1109	D1022	N941	S875	ASN
D1863	S1781	K1690	L1597	A1518	T1424	V1366	V1276	I1188	L1113	L1025	S876	S877	TRP
F1782	F1782	V1693	L1597	A1518	T1424	K1387	V1276	I1188	L1113	L1025	D877	D877	GLU
R1783	R1783	T1694	L1597	A1518	T1424	L1388	L1279	I1189	L1113	L1025	E878	E878	VAL
T1865	R1784	L1695	M1600	A1520	S1427	K1387	L1279	I1189	A1114	D1027	M879	M879	SER
L1866	L1785	L1696	L1601	F1521	I1428	L1388	L1279	I1189	H1115	F1028	M880	M880	ALA
T1867	L1786	L1697	F1521	F1521	E1429	L1359	F1191	F1191	H1115	C1029	K881	K881	LEU
L1868	A1786	G1522	G1522	G1522	E1430	K1360	L1282	K1193	K1119	G1030	S882	S882	SER
K1869	R1787	F1698	K1603	R1527	V1434	K1361	S1289	F1194	S1120	R1031	Y883	Y883	ARG
F1869	R1788	F1699	S1604	R1527	N1435	K1362	L1290	F1194	S1120	GLY	S884	S884	ALA
L1870	R1788	F1699	S1604	R1527	N1435	L1363	L1290	F1194	S1120	GLY	Y885	Y885	ALA
M1871	C1791	L1700	F1605	L1531	L1436	C1364	K1292	V1195	G1122	C1032	Y886	Y886	GLN
G1872	G1872	L1700	F1605	L1531	L1436	C1364	K1292	V1195	G1122	C1032	Y886	Y886	GLN
Y1873	T1793	V1713	R1608	V1537	Y1437	M1365	K1292	V1195	G1122	C1032	Y886	Y886	GLN
K1875	Q1794	L1714	Q1614	L1538	G1438	H1367	F1297	P1204	Q1126	F1036	P956	P956	LYS
L1876	Q1794	L1714	Q1614	L1538	G1438	H1367	F1297	P1204	Q1126	F1036	P956	P956	LYS
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D1878	L1797	Q1716	K1617	S1539	A1441	L1368	L1298	V1207	I1131	K1038	R888	R888	PHE
L1879	L1798	Q1717	L1618	T1540	A1441	L1368	L1298	V1207	I1131	K1038	R888	R888	PHE
V1801	V1801	I1718	L1618	T1540	A1441	L1368	L1298	V1207	I1131	K1038	R888	R888	PHE
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E1803	Y1802	I1718	L1618	T1540	A1441	L1368	L1298	V1207	I1131	K1038	R888	R888	PHE
M1804	Y1802	I1718	L1618	T1540	A1441	L1368	L1298	V1207	I1131	K1038	R888	R888	PHE
F1805	Y1802	I1718	L1618	T1540	A1441	L1368	L1298	V1207	I1131	K1038	R888	R888	PHE
R1806	Y1802	I1718	L1618	T1540	A1441	L1368	L1298	V1207	I1131	K1038	R888	R888	PHE
K1807	Y1802	I1718	L1618	T1540	A1441	L1368	L1298	V1207	I1131	K1038	R888	R888	PHE
Q1808	Y1802	I1718	L1618	T1540	A1441	L1368	L1298	V1207	I1131	K1038	R888	R888	PHE
S1809	Y1802	I1718	L1618	T1540	A1441	L1368	L1298	V1207	I1131	K1038	R888	R888	PHE
P1810	Y1802	I1718	L1618	T1540	A1441	L1368	L1298	V1207	I1131	K1038	R888	R888	PHE
K1895	Y1802	I1718	L1618	T1540	A1441	L1368	L1298	V1207	I1131	K1038	R888	R888	PHE
L1896	Y1802	I1718	L1618	T1540	A1441	L1368	L1298	V1207	I1131	K1038	R888	R888	PHE
N1897	Y1802	I1718	L1618	T1540	A1441	L1368	L1298	V1207	I1131	K1038	R888	R888	PHE
G1902	Y1802	I1718	L1618	T1540	A1441	L1368	L1298	V1207	I1131	K1038	R888	R888	PHE
S1903	Y1802	I1718	L1618	T1540	A1441	L1368	L1298	V1207	I1131	K1038	R888	R888	PHE
CYS	Y1802	I1718	L1618	T1540	A1441	L1368	L1298	V1207	I1131	K1038	R888	R888	PHE
ILE	Y1802	I1718	L1618	T1540	A1441	L1368	L1298	V1207	I1131	K1038	R888	R888	PHE
THR	Y1802	I1718	L1618	T1540	A1441	L1368	L1298	V1207	I1131	K1038	R888	R888	PHE
GLU	Y1802	I1718	L1618	T1540	A1441	L1368	L1298	V1207	I1131	K1038	R888	R888	PHE
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I846	I846	I846	I846	I846	I846	I846	I846	I846	I846	I846	I846	I846	I846
S847	S847	S847	S847	S847	S847	S847	S847	S847	S847	S847	S847	S847	S847
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I851	I851	I851	I851	I851	I851	I851	I851	I851	I851	I851	I851	I851	I851
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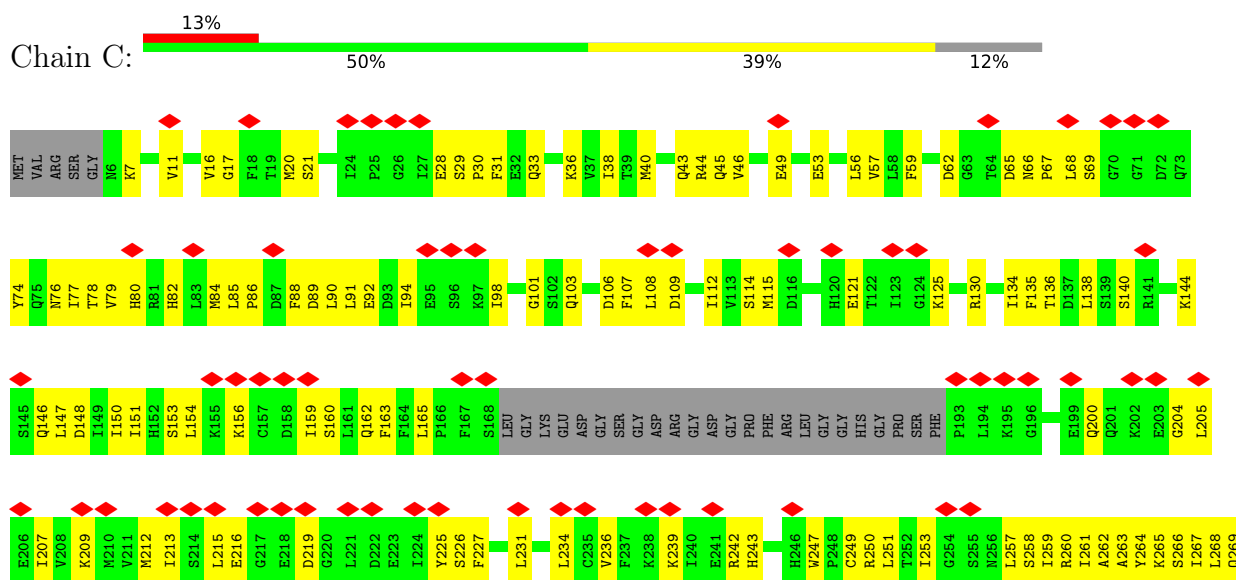
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F3035	E2935	L2869	K2786	ALA	LEU	SER	I2520	R2425	H2352	I2274	N2104	LEU	L1966
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Y3037	D2937			GLY	GLY	VAL	R2522	D2429	E2357	L2276	R2106	D2033	E1969
O3037	L2938	L2871	L2790	THR	SER	LEU	R2522	R2430	D2358		S2107	D2044	N1974
E3038	D2939	D2872	L2791	SER	SER	LEU	S2526	R2431	K2359	R2281	L2108	G2048	L1975
T3039	L2942	P2873	T2792	THR	THR	PRO	H2527	Q2432	F2360	A2282	GLY	V2049	L1976
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K3044	K2950	L2884	V2797	ARG	ASP	THR	L2531	I2438	L2364	C2292	GLY	TYR	L1982
L3045	T2953		L2798	ARG	THR	GLN	P2532	I2439	N2365	G2293	GLU	TYR	D1983
R3046			A2798	ALA	THR	ALA	H2534	Y2440	K2366	K2207	ASP	SER	L1984
L3049	L2957	F2887	Q2799	SER	THR	SER	T2535	K2441	V2367	D2208	SER	SER	K1985
K3050	F2957	I2803		PHE	THR	GLN	R2538	M2443	T2368	Q2295	VAL	GLN	R1986
L3051	D2964	A2804	L2803	ASP	SER	GLY	R2539	K2447	P2371	S2296	ASP	ASP	ARG
L3052	E2967	K2806	L2804	GLN	SER	THR	L2539		P2372	S2297	PRO	PRO	TYR
L3053		Q2807	A2805	GLY	ASP	LEU	L2542	L2451	L2374	E2298	ARG	ARG	ASN
A3057	Y2972	L2808	Q2807	LEU	SER	THR	N2543	R2452	A2375	F2300	ALA	ALA	PRO
O3058	L2976	F2809	F2809	LEU	LEU	THR	S2547	E2453	D2376	N2216	THR	THR	PRO
O3059	L2977	S2811	S2810	SER	PHE	THR		L2454	R2377	N2217	ALA	ALA	PRO
S3060	N2977	L2812	L2810	ALA	ALA	GLN	L2550	L2455	F2378	N2126	GLY	GLY	VAL
L3061	K2978	L2813	F2813	NET	HIS	GLY	E2551	K2456	M2379	K2127	VAL	VAL	GLU
L3062	K2978	L2888	S2814	TYR	LYS	GLY	V2552	P2457	V2382	F2128	ARG	ARG	VAL
T3063	Q2979	R2899	G2815	ARG	ARG	SER	H2553	C2469	L2385	N2220	PHE	PHE	GLU
F3064	D2980	L2892	L2816	LYS	GLY	LEU	F2554	R2470	L2386	K2221	GLU	GLU	VAL
L3065	W2981	L2893	L2817	GLY	ARG	ALA	L2555	E2471	L2387	H2222	ARG	ARG	VAL
D3066	V2982	P2902	L2818	VAL	LEU	TRP	S2556	Q2472	P2387	N2305	ARG	ARG	PRO
K3067	D2983	ALA	K2819	ALA	GLN	TRP	L2557	M2473	K2388	N2311	GLN	GLN	GLU
A3068	P2986	LEU	M2820	ARG	ARG	PRO	A2558	Y2474		V2310	ARG	ARG	ARG
M3069		PRO		LEU	ALA	VAL	T2559		K2394	V2312	ASP	ASP	LYS
E3072	K2991	ALA	K2824	GLN	PRO	ALA	N2560	M2478	T2395	V2315	THR	THR	LYS
K3075	W2994	LYS		LYS	PRO	ALA	F2561	W2479	L2396	Y2316	VAL	VAL	LYS
E3077	F2995	ARG	K2829	GLY	LEU	GLY	L2562	L2480	C2397	A2317	THR	THR	ILE
L3080	L2996	VAL	N2830	LYS	LYS	GLN	L2563	H2481	L2398	C2244	HIS	HIS	GLU
S2998	A2997	GLY	N2831	SER	SER	ILE	E2564		L2399	W2245	ASP	ASP	ILE
L2999	S2998	ARG	L2834	VAL	VAL	ARG	M2565	Y2484	E2399	F2145	VAL	VAL	ARG
S3083	D3000	GLY	K2835	GLY	GLY	ALA	R2565	R2485	V2400	T2153	LEU	LEU	LYS
L3086		LYS		PRO	PRO	THR	S2569		C2403	Y2252	ALA	ALA	ALA
L3089	H3004	ARG	Q2838	ASP	PHE	GLN	D2570	E2490	R2404	Y2253	GLU	GLU	ARG
A3006	L3005	LYS	D2839	GLY	GLY	GLN	Y2571	N2493	V2405	R2254	GLU	GLU	ARG
Y3102	F2918	MET	F2940	LYS	LYS	HIS	Y2572	D2494	E2406	F2157	ALA	ALA	ALA
	A3006	ARG		MET	ASP	ASP	F2573	S2495		R2158	ALA	ALA	ALA
	E3007	ARG	F2850	GLN	ARG	THR	N2574	Q2496	E2410	Y2160	ASN	ASN	GLY
							P2575		L2411	A2161	GLY	GLY	ASP
										F2260			
										V2330			

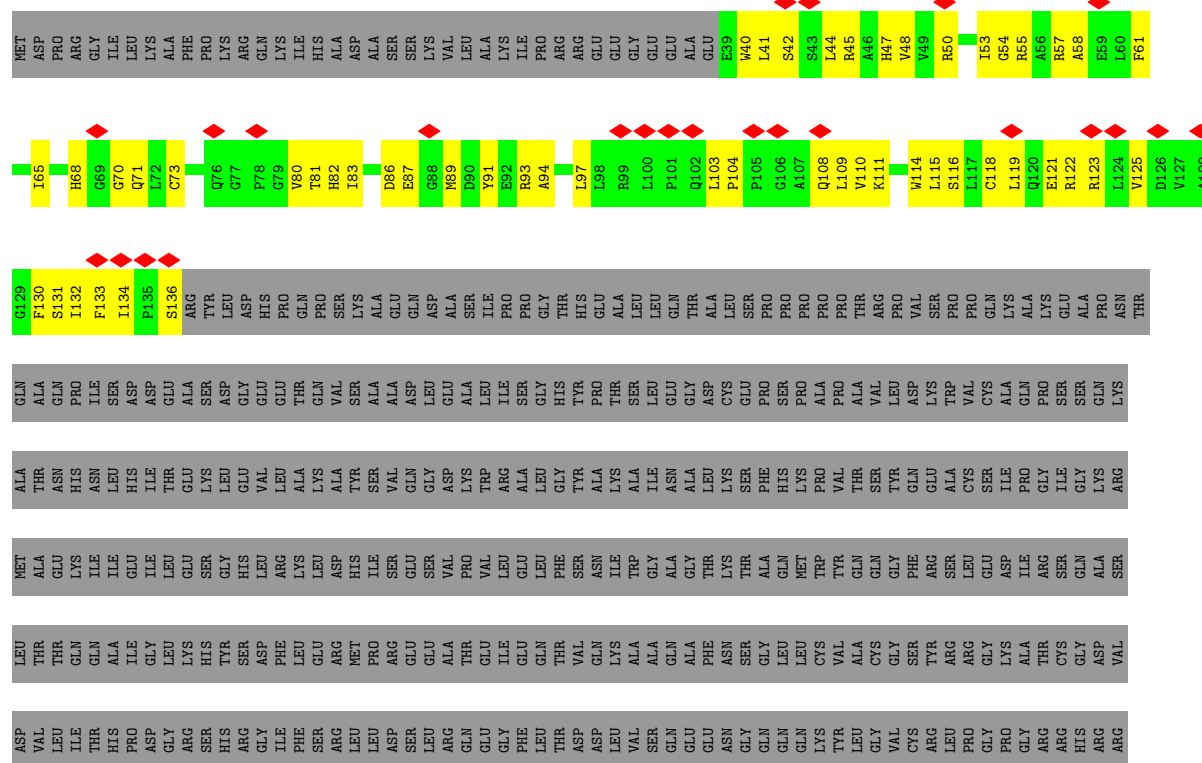


• Molecule 2: X-ray repair cross-complementing protein 6



• Molecule 3: X-ray repair cross-complementing protein 5



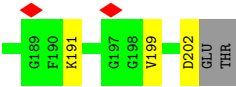


LEU	ASP	ILE	ILE	VAL	PRO	TYR	SER	GLU	PHE	ALA	CYS	ALA	LEU	LEU	TYR	THR	GLY	SER	ALA	HIS	PHE	ASN	ARG	SER	MET	ARG	ALA	LEU	ALA	LYS	THR	LYS	GLY	MET	SER	SER	LEU	SER	GLU	HIS	ALA	LEU	SER	THR	ALA	VAL	VAL	ARG	ASN	THR	HIS	GLY	CYS	LYS	VAL	GLY	PRO	GLY		
ARG	VAL	LEU	THR	PRO	PRO	GLU	LYS	ASP	VAL	PHE	ARG	LEU	LEU	GLY	LEU	PRO	TYR	ARG	GLU	PRO	ALA	ALA	GLU	ASP	TRP																																			

● Molecule 5: Protein PAXX



LEU	ARG	ALA	LEU	THR	GLY	LEU	ALA	LYS	THR	VAL	TRP	SER	SER	GLU	ARG	LEU	ALA	ALA	GLU	ALA	GLU	THR	ALA	VAL	VAL	SER	SER	PRO	PRO	ALA	GLY	PRO	GLN	PHE	LEU	THR	PRO	ASP	PRO	ASP	PRO	ASP	GLN	ARG	GLY	LYS	PRO	GLY	PRO	GLY	VAL	ARG	ARG	ARG	C180			
MET	ASP	PRO	LEU	SER	PRO	PRO	LEU	CYS	THR	GLU	LEU	PRO	PRO	GLY	PRO	ARG	PRO	PHE	VAL	CYS	TYR	CYS	GLU	GLY	GLU	GLU	SER	GLY	GLY	ASP	ARG	GLY	GLY	PHE	ASN	LEU	TYR	VAL	THR	THR	ASP	ASP	ALA	ALA	GLU	LEU	TRP	SER	THR	CYS	PHE	PRO	ASP	SER	LEU	ALA	ALA	LEU

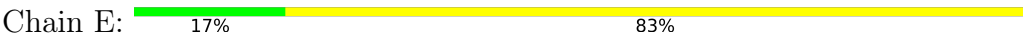


● Molecule 6: DNA



T20	A21	A24	A25	A26	C27	T28	A29	A30	A31	A32	A33	C34	T35	A36	T37	T38	A39	T40	T41	A42	T43
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● Molecule 7: DNA



A15	A16	T17	A18	A19	T20	A21	G22	T23	T24	T25	T26	T27	A28	G29	T30	T31	T32	A33	T34	T35	A36	G37
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12656	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.96	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.640	Depositor
Minimum map value	-0.137	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	417.28, 417.28, 417.28	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.304, 1.304, 1.304	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.18	0/29602	0.46	2/40074 (0.0%)
2	B	0.24	0/3900	0.49	2/5268 (0.0%)
3	C	0.15	0/5185	0.39	0/6998
4	F	0.27	0/771	0.50	0/1046
5	M	0.09	0/159	0.34	0/216
6	D	0.23	0/548	0.49	0/843
7	E	0.24	0/530	0.49	0/817
All	All	0.19	0/40695	0.46	4/55262 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	PRO	N-CA-CB	6.58	110.57	103.33
1	A	2297	SER	N-CA-C	-5.35	107.77	114.56
2	B	281	LEU	CA-C-N	5.24	130.90	120.94
2	B	281	LEU	C-N-CA	5.24	130.90	120.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	29010	0	28916	1364	0
2	B	3825	0	3813	248	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	5093	0	5039	247	0
4	F	755	0	767	54	0
5	M	155	0	135	3	0
6	D	488	0	275	39	0
7	E	474	0	266	29	0
All	All	39800	0	39211	1882	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 24.

All (1882) 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)
2:B:420:LEU:HA	2:B:426:GLN:CA	1.78	1.12
2:B:420:LEU:CA	2:B:426:GLN:HA	1.79	1.11
1:A:3226:ASP:N	1:A:3229:SER:HG	1.69	0.89
1:A:3868:VAL:HG12	1:A:3872:ARG:HE	1.38	0.88
2:B:407:PRO:HG2	3:C:486:ARG:HD2	1.54	0.88
1:A:2806:LYS:HG2	1:A:2857:CYS:HB3	1.54	0.87
3:C:362:LEU:H	3:C:421:TYR:HB3	1.39	0.87
1:A:924:ARG:HH12	1:A:2769:VAL:HG12	1.40	0.87
1:A:865:GLN:HB3	1:A:3170:ASP:HB2	1.56	0.87
1:A:252:VAL:HA	3:C:553:ILE:HD11	1.54	0.86
2:B:35:ARG:H	2:B:162:SER:H	1.23	0.84
2:B:457:GLU:HG3	2:B:458:GLN:HE21	1.44	0.83
1:A:1766:LEU:HD13	1:A:1778:PHE:HD2	1.43	0.82
3:C:690:GLU:H	3:C:695:SER:HB3	1.43	0.82
6:D:42:DA:H2'	7:E:16:DA:N3	1.95	0.82
1:A:1359:LEU:H	1:A:1361:LYS:HZ3	1.23	0.81
1:A:3999:THR:HA	1:A:4002:MET:HE2	1.62	0.81
1:A:3503:VAL:O	1:A:3506:LEU:HB2	1.81	0.80
1:A:3466:PRO:HB2	1:A:4004:VAL:HG11	1.64	0.80
1:A:3729:MET:HE1	1:A:3737:ARG:HG2	1.65	0.79
2:B:379:SER:HA	2:B:382:PHE:HB2	1.65	0.79
1:A:1179:PRO:HA	1:A:1262:ALA:HB2	1.65	0.79
1:A:60:SER:HA	1:A:63:PHE:HB3	1.66	0.78
1:A:2873:PRO:HB2	1:A:2925:GLU:HG3	1.66	0.78
1:A:3593:ARG:HD2	1:A:3660:ASN:HB2	1.66	0.78
2:B:345:LEU:HB3	2:B:400:TYR:HD1	1.50	0.77
3:C:361:VAL:HG13	3:C:421:TYR:H	1.49	0.77
2:B:261:LEU:HB3	2:B:269:ILE:HG22	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:406:GLY:HA2	3:C:424:LEU:HD23	1.67	0.77
1:A:447:PRO:HG3	1:A:522:PRO:HB3	1.67	0.77
1:A:2455:LEU:HD21	1:A:2501:LEU:HD23	1.67	0.77
1:A:1328:GLU:HG2	1:A:1329:ARG:HE	1.50	0.76
2:B:318:ARG:HD2	3:C:276:TRP:HB3	1.68	0.76
1:A:3503:VAL:HA	1:A:3506:LEU:HD23	1.66	0.76
4:F:45:ARG:HB2	4:F:81:THR:H	1.49	0.76
4:F:110:VAL:HA	4:F:131:SER:HA	1.69	0.75
2:B:51:SER:HA	2:B:58:THR:HG22	1.65	0.75
2:B:261:LEU:O	2:B:268:VAL:HA	1.86	0.75
1:A:1452:VAL:HA	1:A:1517:LEU:HD11	1.67	0.74
1:A:3235:LYS:HA	1:A:3238:MET:HE2	1.68	0.74
1:A:255:ALA:HB3	3:C:553:ILE:HD12	1.67	0.74
1:A:3130:GLN:HB3	1:A:3178:ILE:HG12	1.70	0.74
1:A:2405:VAL:HG21	1:A:2441:LYS:HG3	1.70	0.74
1:A:2538:ARG:NH1	1:A:2565:MET:SD	2.61	0.74
1:A:264:ARG:HB3	1:A:305:ASN:HB2	1.70	0.74
1:A:1976:LEU:HD13	1:A:2145:PHE:HD2	1.52	0.74
1:A:2891:ARG:HH22	1:A:3898:LEU:HB3	1.50	0.74
1:A:3240:MET:HE3	1:A:3262:LEU:HD22	1.69	0.74
1:A:1890:HIS:H	1:A:1894:SER:HB2	1.52	0.73
3:C:59:PHE:HB3	3:C:77:ILE:HD13	1.70	0.73
1:A:93:LEU:O	1:A:136:GLN:NE2	2.20	0.73
1:A:1070:PRO:HD3	1:A:3741:ARG:HH11	1.52	0.73
1:A:1384:PHE:HB2	1:A:1386:ILE:HG23	1.68	0.73
1:A:2411:LEU:HD21	1:A:2442:MET:HB2	1.70	0.73
1:A:551:PHE:HA	1:A:554:ASN:HB3	1.71	0.73
1:A:4082:ARG:HH12	1:A:4091:ALA:HA	1.54	0.73
3:C:493:CYS:HA	3:C:506:PRO:HD2	1.71	0.73
6:D:28:DT:O2	7:E:29:DG:N2	2.20	0.73
1:A:3104:GLN:O	1:A:3108:GLN:NE2	2.21	0.73
2:B:64:ILE:HG22	2:B:68:GLN:HE22	1.53	0.73
2:B:521:LEU:HA	2:B:524:GLU:HG2	1.70	0.73
1:A:714:VAL:HG13	1:A:733:LEU:HD11	1.69	0.73
1:A:3518:VAL:HA	1:A:3521:ILE:HG22	1.69	0.73
1:A:734:LEU:HD21	1:A:769:GLY:HA2	1.71	0.73
2:B:296:VAL:HA	3:C:298:ASN:H	1.54	0.73
1:A:1082:PHE:HA	1:A:1085:ILE:HG12	1.70	0.72
1:A:1872:GLY:HA2	1:A:1875:LYS:HE2	1.70	0.72
1:A:881:LYS:HG2	1:A:883:TYR:H	1.55	0.72
1:A:1222:ASN:O	1:A:1231:GLN:NE2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:470:ARG:H	5:M:202:ASP:H	1.36	0.72
2:B:61:ASP:O	2:B:65:GLN:NE2	2.22	0.72
1:A:222:GLY:HA2	1:A:225:LYS:HD2	1.71	0.72
1:A:2411:LEU:HA	1:A:2414:GLN:NE2	2.05	0.72
1:A:2589:TYR:HB2	1:A:2777:HIS:HB2	1.70	0.72
3:C:602:VAL:O	3:C:606:LYS:N	2.21	0.72
3:C:251:LEU:HA	3:C:340:PHE:HB2	1.72	0.71
1:A:1981:LEU:HB3	1:A:1984:LEU:HD21	1.71	0.71
1:A:3380:ARG:O	1:A:3384:HIS:ND1	2.21	0.71
1:A:2547:SER:HB3	1:A:2550:ILE:HG12	1.73	0.71
1:A:2504:ASP:O	1:A:2508:GLN:NE2	2.24	0.71
1:A:3707:GLY:O	1:A:3708:ARG:NH1	2.23	0.71
1:A:1436:LEU:O	1:A:1445:ARG:NH2	2.23	0.71
1:A:2271:SER:HB3	1:A:2315:VAL:HG12	1.72	0.71
3:C:640:ARG:HG3	3:C:685:LEU:HD12	1.71	0.71
1:A:2432:GLN:NE2	1:A:2469:CYS:SG	2.64	0.70
1:A:2219:LEU:O	1:A:2223:VAL:N	2.24	0.70
1:A:4006:VAL:HG22	1:A:4040:PRO:HB3	1.72	0.70
1:A:2330:VAL:C	1:A:2332:GLU:H	1.99	0.70
1:A:3183:ILE:HG13	1:A:3242:MET:HE3	1.73	0.70
2:B:528:LEU:HB3	3:C:372:ALA:HB1	1.72	0.70
1:A:3502:MET:O	1:A:3505:LEU:HB3	1.91	0.70
1:A:1927:MET:HE1	1:A:1974:ASN:HB2	1.73	0.70
1:A:2896:ALA:O	1:A:2900:LEU:HB2	1.92	0.70
1:A:3028:ASN:OD1	1:A:3029:LYS:N	2.22	0.70
1:A:2869:LEU:HD23	1:A:2892:LEU:HD12	1.74	0.70
1:A:2895:GLU:HA	1:A:2898:LEU:HG	1.74	0.70
1:A:1239:PRO:HB2	1:A:1292:LYS:HD2	1.73	0.69
2:B:73:SER:HB3	2:B:244:ARG:HH22	1.57	0.69
1:A:4035:GLU:OE1	1:A:4038:TRP:N	2.22	0.69
1:A:4113:ASP:HB3	1:A:4116:ILE:HD13	1.74	0.69
1:A:1982:ILE:HG23	1:A:2090:ARG:HD3	1.74	0.69
1:A:2254:ARG:HH21	1:A:2293:GLY:H	1.38	0.69
1:A:1764:GLU:HA	1:A:1819:PHE:HE1	1.57	0.69
1:A:3817:LEU:HD22	1:A:3825:LYS:HG3	1.74	0.69
1:A:433:PRO:O	1:A:436:GLU:HG3	1.93	0.69
1:A:895:ALA:HB1	1:A:902:LYS:HB3	1.73	0.69
1:A:1022:ASP:HB3	1:A:1025:LEU:HB3	1.74	0.69
1:A:1101:PHE:HB3	1:A:1154:PRO:HG3	1.75	0.69
1:A:1441:ALA:O	1:A:1445:ARG:NH1	2.25	0.69
3:C:407:VAL:HG12	3:C:424:LEU:HD21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:PHE:HZ	1:A:707:PHE:HD2	1.37	0.68
1:A:1765:VAL:HA	1:A:1768:ARG:HH21	1.59	0.68
2:B:86:VAL:HG23	2:B:104:VAL:HG12	1.74	0.68
1:A:2893:LEU:HD21	1:A:2922:ARG:HB3	1.74	0.68
1:A:2840:PHE:HB2	1:A:2871:LEU:HD11	1.74	0.68
1:A:4090:ARG:N	1:A:4109:ASP:OD2	2.26	0.68
1:A:528:VAL:HA	1:A:633:ILE:HD11	1.75	0.68
1:A:1313:PHE:O	1:A:1319:GLY:N	2.26	0.68
2:B:383:SER:HB2	3:C:446:PRO:HD3	1.75	0.68
1:A:180:LEU:HA	1:A:230:LEU:HG	1.75	0.68
1:A:2820:MET:HE1	1:A:2829:LYS:HG2	1.76	0.68
3:C:20:MET:HE2	3:C:30:PRO:HG2	1.75	0.68
1:A:1178:ARG:HG2	1:A:1180:GLN:H	1.59	0.68
1:A:3716:HIS:O	1:A:3718:ARG:NH1	2.26	0.68
1:A:1102:GLU:HG3	1:A:1154:PRO:HA	1.76	0.67
1:A:3924:HIS:HE1	1:A:3926:ASN:HB2	1.59	0.67
1:A:913:ARG:HE	1:A:2803:ILE:HD11	1.59	0.67
1:A:3443:PRO:HA	1:A:3446:VAL:HG12	1.75	0.67
1:A:3183:ILE:HG23	1:A:3238:MET:HG3	1.77	0.67
1:A:4082:ARG:NH1	1:A:4091:ALA:HA	2.08	0.67
1:A:3751:LEU:HB3	1:A:3803:ILE:HG23	1.77	0.67
1:A:205:LYS:O	1:A:209:THR:N	2.26	0.67
1:A:1368:LEU:HG	1:A:1372:LEU:HD23	1.76	0.67
6:D:42:DA:N3	7:E:16:DA:H2'	2.10	0.67
1:A:3588:TRP:CD1	1:A:3613:MET:HE3	2.30	0.67
1:A:3680:LEU:HD12	1:A:3682:GLU:HG2	1.76	0.67
1:A:3796:MET:HE1	1:A:3802:LEU:HD23	1.75	0.67
1:A:1766:LEU:HD13	1:A:1778:PHE:CD2	2.29	0.67
6:D:35:DT:H2'	6:D:36:DA:C8	2.30	0.67
1:A:2803:ILE:HG22	1:A:2806:LYS:HD3	1.77	0.66
2:B:76:ILE:HD12	2:B:248:ALA:H	1.58	0.66
1:A:1772:HIS:HD2	1:A:1822:ARG:HH22	1.41	0.66
1:A:3924:HIS:HB3	1:A:4125:GLU:OE2	1.94	0.66
1:A:2216:LEU:HD22	1:A:2249:LEU:HD23	1.77	0.66
2:B:421:ASP:HB3	2:B:425:ILE:O	1.95	0.66
1:A:753:GLN:NE2	1:A:791:ASP:O	2.29	0.66
1:A:1572:LEU:HD11	1:A:1603:GLN:HG2	1.78	0.66
1:A:4054:ALA:HA	1:A:4096:SER:HA	1.78	0.66
1:A:16:GLN:O	1:A:20:SER:N	2.24	0.66
1:A:1775:GLU:OE2	1:A:1822:ARG:NH2	2.29	0.66
2:B:456:PRO:HA	2:B:459:VAL:HG22	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:ILE:HG23	1:A:1036:PHE:HD1	1.61	0.66
1:A:1784:ARG:HB3	1:A:1788:ARG:HH21	1.60	0.66
1:A:1985:LYS:HZ3	1:A:2180:GLU:HG2	1.61	0.66
2:B:490:LEU:HB3	3:C:316:TYR:HE2	1.61	0.66
3:C:66:ASN:ND2	3:C:68:LEU:O	2.29	0.66
3:C:483:PRO:HG2	3:C:488:GLN:HE22	1.62	0.65
1:A:1373:VAL:HG11	1:A:1422:LYS:HE2	1.78	0.65
1:A:3583:LEU:HD13	1:A:3733:ARG:HD3	1.78	0.65
2:B:290:ARG:NH1	3:C:308:GLU:O	2.27	0.65
2:B:427:VAL:O	2:B:428:THR:C	2.40	0.65
7:E:31:DT:C6	7:E:32:DT:H72	2.30	0.65
3:C:279:VAL:HG12	3:C:286:LYS:HD3	1.79	0.65
1:A:3168:TYR:CZ	1:A:3241:LYS:HE2	2.32	0.65
1:A:2252:PRO:O	1:A:2291:GLN:NE2	2.30	0.65
4:F:87:GLU:HA	4:F:132:ILE:HD12	1.78	0.65
1:A:2260:PHE:O	1:A:2306:ASN:ND2	2.30	0.65
1:A:2410:GLU:OE2	1:A:2413:PHE:N	2.28	0.65
3:C:728:LEU:HA	3:C:732:ILE:HA	1.79	0.65
1:A:1933:LEU:HG	1:A:1937:ARG:HB2	1.78	0.65
2:B:77:SER:HB3	2:B:249:LYS:HG3	1.79	0.65
4:F:48:VAL:HG21	4:F:61:PHE:HB3	1.78	0.65
7:E:30:DT:H2'	7:E:31:DT:C6	2.32	0.65
1:A:3518:VAL:HG22	1:A:3522:THR:HB	1.77	0.64
1:A:3624:GLY:HA2	1:A:3686:TRP:H	1.62	0.64
2:B:263:LEU:HA	2:B:347:LEU:HB3	1.78	0.64
1:A:1371:VAL:O	1:A:1374:GLN:HG3	1.97	0.64
1:A:2404:ARG:HH21	1:A:2406:GLU:HB2	1.63	0.64
2:B:458:GLN:HA	2:B:461:LYS:HE3	1.79	0.64
1:A:989:MET:HG3	1:A:993:HIS:CE1	2.31	0.64
2:B:278:GLN:HG2	3:C:431:ARG:HH12	1.63	0.64
1:A:3879:PRO:O	1:A:3966:GLN:NE2	2.29	0.64
1:A:3922:ASP:O	1:A:3927:ASN:ND2	2.30	0.64
2:B:445:LYS:N	3:C:242:ARG:O	2.30	0.64
1:A:3492:CYS:SG	1:A:3524:ASN:ND2	2.70	0.64
1:A:4037:ASN:HD22	1:A:4066:LEU:HD22	1.62	0.64
4:F:45:ARG:NE	4:F:81:THR:OG1	2.28	0.64
1:A:238:MET:SD	1:A:284:THR:OG1	2.56	0.64
1:A:722:LYS:O	1:A:726:LEU:N	2.26	0.64
1:A:3700:GLU:HA	1:A:3718:ARG:HA	1.78	0.64
1:A:92:PHE:HD1	1:A:96:MET:HE3	1.63	0.64
2:B:290:ARG:HH21	3:C:311:ILE:HD13	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3891:SER:HB2	1:A:3900:LEU:HD21	1.78	0.64
1:A:4014:LYS:HZ2	1:A:4033:VAL:HG12	1.63	0.64
3:C:378:SER:O	3:C:382:HIS:ND1	2.30	0.63
2:B:350:PHE:HB2	3:C:461:MET:HG3	1.81	0.63
2:B:468:LYS:HE3	2:B:521:LEU:HD21	1.80	0.63
1:A:1767:CYS:HA	1:A:1822:ARG:HH11	1.63	0.63
1:A:2205:VAL:HG12	1:A:2207:LYS:H	1.63	0.63
1:A:2365:ASN:OD1	1:A:2366:LYS:NZ	2.29	0.63
2:B:35:ARG:HG3	2:B:80:ARG:HE	1.63	0.63
1:A:2437:ASP:O	1:A:2441:LYS:HG2	1.99	0.63
4:F:40:TRP:HZ2	4:F:119:LEU:HA	1.63	0.63
1:A:2978:LYS:HE2	1:A:2981:TRP:HA	1.81	0.63
1:A:1115:HIS:CD2	1:A:1181:THR:H	2.17	0.63
1:A:2161:ALA:HA	1:A:2164:TRP:HB2	1.80	0.63
1:A:2543:ASN:ND2	1:A:2839:ASP:OD2	2.31	0.63
1:A:3183:ILE:HD12	1:A:3238:MET:HB2	1.81	0.63
1:A:1860:GLU:HG2	1:A:1862:THR:H	1.63	0.63
1:A:2357:GLU:O	1:A:2361:ILE:N	2.32	0.63
1:A:286:LEU:HD12	1:A:319:PHE:HD1	1.64	0.63
1:A:1147:LYS:HZ2	1:A:1149:LYS:HG2	1.64	0.63
4:F:54:GLY:H	4:F:57:ARG:HE	1.45	0.63
4:F:83:ILE:HD11	4:F:104:PRO:HG2	1.81	0.63
1:A:187:SER:O	1:A:191:ASN:ND2	2.33	0.62
1:A:1519:PHE:HE2	1:A:1566:THR:HB	1.65	0.62
2:B:444:ARG:N	3:C:266:SER:O	2.31	0.62
1:A:524:TYR:HB2	1:A:629:PHE:HD1	1.65	0.62
2:B:128:GLN:HG2	2:B:132:GLN:HE21	1.64	0.62
1:A:3924:HIS:CE1	1:A:3926:ASN:HB2	2.33	0.62
1:A:1027:ASP:O	1:A:1031:ARG:HG2	2.00	0.62
1:A:1300:SER:HA	1:A:1304:HIS:HB2	1.82	0.62
1:A:1583:MET:HE1	1:A:1628:LYS:HB2	1.81	0.62
1:A:2140:LEU:HA	1:A:2143:ARG:HD3	1.82	0.62
2:B:301:ARG:NH2	2:B:311:LEU:O	2.33	0.62
1:A:2474:TYR:O	1:A:2478:MET:HG2	2.00	0.62
1:A:2586:PHE:CZ	1:A:2782:ASP:HB3	2.35	0.62
2:B:454:ALA:HB3	3:C:379:SER:HB2	1.81	0.62
1:A:3568:ILE:HD11	1:A:3697:ASN:HD21	1.65	0.62
1:A:3769:GLN:HA	1:A:3772:ASN:HD22	1.64	0.62
2:B:346:MET:N	2:B:399:ARG:O	2.32	0.62
1:A:488:ILE:HD11	1:A:575:ILE:HG12	1.82	0.62
1:A:2902:PRO:HG2	1:A:2919:ASP:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3499:ILE:HG12	1:A:3529:ILE:HG22	1.82	0.62
2:B:419:GLU:O	2:B:420:LEU:C	2.43	0.62
2:B:526:LYS:HE2	2:B:528:LEU:HD12	1.80	0.62
1:A:658:THR:HG21	1:A:1388:ASP:HB2	1.82	0.61
3:C:381:ILE:HB	3:C:410:PRO:HG3	1.82	0.61
6:D:37:DT:H2'	6:D:38:DT:C2	2.35	0.61
1:A:2411:LEU:HA	1:A:2414:GLN:HE21	1.64	0.61
1:A:3834:ALA:O	1:A:3838:GLU:N	2.23	0.61
3:C:21:SER:HA	3:C:31:PHE:HB3	1.80	0.61
3:C:595:ALA:HA	3:C:598:PHE:CE2	2.35	0.61
1:A:2571:ASP:O	1:A:2787:HIS:ND1	2.30	0.61
1:A:3796:MET:N	1:A:3796:MET:SD	2.73	0.61
4:F:89:MET:HB2	4:F:93:ARG:HG2	1.82	0.61
1:A:1868:THR:HA	1:A:1871:MET:HG3	1.83	0.61
1:A:3037:GLN:HA	1:A:3040:TYR:CD2	2.36	0.61
3:C:160:SER:HB2	3:C:239:LYS:HG2	1.82	0.61
1:A:2580:PRO:HA	1:A:2783:ILE:HG12	1.83	0.61
2:B:286:ILE:HD12	3:C:315:ARG:HB2	1.81	0.61
1:A:111:CYS:HA	1:A:114:VAL:HG22	1.82	0.61
1:A:1356:TRP:NE1	1:A:1358:LEU:O	2.34	0.61
1:A:3679:ASN:OD1	1:A:3726:VAL:N	2.27	0.61
1:A:602:MET:SD	1:A:1087:ARG:NH1	2.74	0.61
1:A:3758:LEU:HD21	1:A:3793:VAL:HB	1.81	0.61
1:A:939:MET:HE3	1:A:2783:ILE:HA	1.82	0.61
1:A:1363:LEU:HB3	1:A:1367:HIS:HE1	1.65	0.61
1:A:2551:GLU:OE2	1:A:2850:PHE:N	2.34	0.61
2:B:352:PRO:HA	2:B:394:VAL:HG22	1.83	0.61
2:B:421:ASP:H	2:B:427:VAL:H	1.47	0.61
3:C:450:GLN:NE2	3:C:536:LEU:O	2.30	0.61
1:A:564:LEU:O	1:A:567:GLU:HG2	2.01	0.60
1:A:790:LYS:HA	1:A:869:ASN:HB3	1.82	0.60
1:A:1686:LEU:HD12	1:A:1721:HIS:HB3	1.83	0.60
1:A:2550:ILE:HB	1:A:2553:HIS:CE1	2.36	0.60
1:A:3030:ILE:O	1:A:3037:GLN:NE2	2.34	0.60
7:E:23:DT:H2'	7:E:24:DT:H71	1.83	0.60
1:A:717:LYS:NZ	1:A:1120:SER:OG	2.31	0.60
1:A:3592:VAL:HA	1:A:3595:GLU:HG2	1.83	0.60
2:B:425:ILE:HG23	5:M:191:LYS:HE3	1.83	0.60
3:C:656:ASN:HB3	3:C:688:LYS:HB2	1.82	0.60
1:A:1476:HIS:ND1	1:A:1522:GLY:O	2.25	0.60
1:A:2253:TYR:HB2	1:A:2291:GLN:HE22	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ASP:OD2	7:E:22:DG:H8	1.83	0.60
1:A:1101:PHE:HE2	1:A:1163:LEU:HB3	1.65	0.60
1:A:1108:MET:HE1	1:A:1178:ARG:HH22	1.67	0.60
3:C:108:LEU:HD13	3:C:150:ILE:HG21	1.81	0.60
1:A:2551:GLU:HA	1:A:2554:PHE:CD2	2.37	0.60
1:A:3500:SER:O	1:A:3504:ALA:N	2.30	0.60
3:C:280:ASP:OD1	3:C:281:ALA:N	2.34	0.60
1:A:79:ARG:O	1:A:82:ARG:HG2	2.02	0.60
1:A:399:GLN:HG3	1:A:401:ASP:H	1.66	0.60
1:A:439:VAL:HA	1:A:442:GLN:HG3	1.84	0.60
2:B:422:ASP:C	2:B:424:LYS:H	2.10	0.60
1:A:320:LEU:HG	1:A:368:LEU:HD22	1.81	0.60
1:A:1933:LEU:HB2	1:A:1936:ARG:HB2	1.83	0.60
1:A:2239:LYS:HZ3	1:A:2282:ALA:HB3	1.65	0.60
6:D:21:DA:H1'	7:E:36:DA:C2	2.35	0.60
1:A:542:ASP:OD1	1:A:543:SER:N	2.35	0.60
1:A:958:MET:HB3	1:A:961:LEU:HB3	1.84	0.60
1:A:1039:TRP:HA	1:A:1042:LYS:HG2	1.83	0.60
1:A:2820:MET:HE2	1:A:2824:LYS:HG3	1.82	0.60
1:A:3886:ALA:HA	1:A:3889:ARG:HD3	1.82	0.60
1:A:4062:ASP:HA	1:A:4065:LEU:HD12	1.84	0.60
1:A:718:MET:HE2	1:A:733:LEU:HD12	1.84	0.60
1:A:773:LEU:HA	1:A:776:TRP:NE1	2.17	0.60
1:A:3590:ASN:HB2	1:A:4022:LYS:HE3	1.84	0.60
2:B:458:GLN:NE2	2:B:527:GLU:OE1	2.34	0.60
3:C:328:GLU:O	3:C:332:LYS:N	2.34	0.60
1:A:3526:PRO:O	1:A:3527:GLN:HG3	2.01	0.59
2:B:485:GLN:HA	2:B:488:ARG:HE	1.65	0.59
2:B:353:LEU:HD13	2:B:395:ALA:HB2	1.83	0.59
1:A:584:GLU:N	1:A:613:HIS:O	2.32	0.59
1:A:1684:LEU:HA	1:A:1688:LEU:HD12	1.85	0.59
1:A:2529:THR:OG1	1:A:2530:ARG:NH1	2.35	0.59
1:A:3446:VAL:HA	1:A:3449:LYS:HG2	1.83	0.59
1:A:3883:LEU:HB2	1:A:3970:LEU:HD21	1.83	0.59
3:C:646:ALA:HA	3:C:651:GLU:HB3	1.85	0.59
1:A:3789:ARG:NH1	1:A:3790:THR:O	2.35	0.59
2:B:369:TYR:OH	3:C:436:SER:O	2.20	0.59
1:A:687:SER:HB3	1:A:701:TYR:HB2	1.83	0.59
1:A:3522:THR:HG23	1:A:3561:LYS:HE2	1.85	0.59
3:C:344:GLY:HA3	5:M:199:VAL:HG21	1.84	0.59
1:A:3642:LYS:O	1:A:3646:LYS:NZ	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3846:MET:HG2	1:A:3858:MET:SD	2.43	0.59
2:B:40:PHE:HD1	2:B:167:MET:HG2	1.67	0.59
2:B:73:SER:HB2	2:B:249:LYS:HD2	1.85	0.59
2:B:244:ARG:NH2	2:B:246:VAL:O	2.35	0.59
1:A:414:LEU:HB2	1:A:460:ALA:HB1	1.84	0.59
1:A:1359:LEU:H	1:A:1361:LYS:NZ	2.00	0.59
1:A:1651:LYS:O	1:A:1654:GLN:HG3	2.02	0.59
1:A:3496:ILE:HD12	1:A:3707:GLY:HA2	1.84	0.59
1:A:3856:MET:O	1:A:3860:LYS:NZ	2.36	0.59
3:C:66:ASN:HD21	3:C:69:SER:HA	1.67	0.59
1:A:28:ALA:O	1:A:32:HIS:ND1	2.36	0.59
1:A:531:PHE:O	1:A:535:LEU:N	2.31	0.59
1:A:652:GLU:O	1:A:655:LEU:HB2	2.02	0.59
1:A:2214:ARG:NH1	1:A:2214:ARG:O	2.36	0.59
1:A:2857:CYS:O	1:A:2861:ILE:HG12	2.03	0.59
1:A:247:GLU:HG2	1:A:285:CYS:HB3	1.85	0.58
1:A:1985:LYS:NZ	1:A:2180:GLU:O	2.36	0.58
1:A:3252:PHE:HB3	1:A:3256:MET:HE1	1.84	0.58
1:A:3509:ASP:CG	1:A:3548:GLY:H	2.11	0.58
1:A:204:LEU:O	1:A:208:MET:HB2	2.03	0.58
1:A:531:PHE:CD1	1:A:534:LEU:HD12	2.37	0.58
1:A:1793:THR:O	1:A:1797:LEU:HG	2.02	0.58
1:A:2813:PHE:HE2	1:A:2868:LEU:HD11	1.68	0.58
1:A:2815:GLY:O	1:A:2818:LYS:HG3	2.03	0.58
2:B:430:PRO:HD2	3:C:435:PHE:HB2	1.84	0.58
1:A:781:ASP:OD2	1:A:783:HIS:ND1	2.37	0.58
1:A:1876:ILE:HA	1:A:1879:VAL:HG12	1.84	0.58
1:A:2364:LEU:HA	1:A:2367:VAL:HG22	1.85	0.58
1:A:100:ILE:O	1:A:101:ALA:C	2.45	0.58
1:A:2181:GLY:HA3	1:A:2222:HIS:CD2	2.39	0.58
1:A:1505:LEU:HA	1:A:1508:LYS:HD2	1.86	0.58
1:A:3506:LEU:HD11	1:A:3554:PHE:HD2	1.69	0.58
1:A:323:VAL:HA	1:A:326:MET:HG2	1.86	0.58
1:A:2539:LEU:HA	1:A:2542:LEU:HD23	1.85	0.58
4:F:91:TYR:HE1	4:F:103:LEU:HD22	1.68	0.58
1:A:3468:LEU:HA	1:A:3471:ILE:HB	1.85	0.58
1:A:186:PRO:HG2	1:A:189:MET:HE1	1.85	0.58
1:A:934:LEU:HA	1:A:937:MET:HG3	1.85	0.58
1:A:998:ASN:OD1	1:A:999:LYS:N	2.37	0.58
1:A:3814:ASP:O	1:A:3818:ASN:ND2	2.36	0.58
1:A:449:TYR:HB3	1:A:453:MET:SD	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:LYS:HB3	1:A:1061:LYS:NZ	2.19	0.58
1:A:1274:ARG:NH2	1:A:1276:VAL:O	2.37	0.58
1:A:1409:SER:O	1:A:1412:LYS:NZ	2.33	0.58
1:A:3259:LEU:HG	1:A:3276:TRP:NE1	2.19	0.58
1:A:200:PHE:CE2	1:A:227:LEU:HD21	2.39	0.58
1:A:142:ARG:HE	1:A:182:GLY:HA3	1.69	0.57
1:A:4098:LEU:HB3	1:A:4102:THR:HG23	1.84	0.57
3:C:106:ASP:OD2	3:C:146:GLN:NE2	2.37	0.57
1:A:59:PHE:O	1:A:63:PHE:N	2.37	0.57
1:A:3029:LYS:O	1:A:3033:GLU:N	2.37	0.57
1:A:3008:TRP:O	1:A:3011:LEU:N	2.37	0.57
2:B:174:ASN:OD1	2:B:176:HIS:NE2	2.37	0.57
1:A:129:ASP:O	1:A:133:LYS:HG2	2.04	0.57
1:A:530:LEU:O	1:A:534:LEU:N	2.37	0.57
1:A:789:TYR:HA	1:A:792:ILE:HB	1.85	0.57
1:A:1727:ARG:HH22	1:A:1774:MET:H	1.53	0.57
2:B:471:PHE:HB3	3:C:346:CYS:HB3	1.86	0.57
1:A:395:MET:HG3	1:A:396:PHE:HD1	1.70	0.57
1:A:913:ARG:NE	1:A:2803:ILE:HD11	2.19	0.57
3:C:323:PHE:HE1	3:C:328:GLU:HG2	1.69	0.57
1:A:450:SER:O	1:A:454:GLN:N	2.36	0.57
1:A:1367:HIS:HA	1:A:1370:ARG:HG2	1.85	0.57
1:A:2157:PHE:O	1:A:2161:ALA:N	2.37	0.57
3:C:20:MET:O	3:C:29:SER:OG	2.20	0.57
1:A:3598:LYS:HG3	1:A:3599:THR:HG22	1.87	0.57
1:A:655:LEU:HD13	1:A:1388:ASP:HB3	1.86	0.57
1:A:2208:ASP:OD1	1:A:2209:GLU:N	2.37	0.57
1:A:2405:VAL:HG11	1:A:2441:LYS:HD3	1.86	0.57
1:A:3692:VAL:HG21	1:A:3720:ALA:HA	1.85	0.57
2:B:425:ILE:O	2:B:427:VAL:N	2.37	0.57
1:A:2866:ALA:HA	1:A:2869:LEU:HD12	1.87	0.57
1:A:3843:LEU:O	1:A:3847:SER:OG	2.22	0.57
2:B:362:LEU:HD21	2:B:438:PRO:HA	1.85	0.57
1:A:440:VAL:HG11	1:A:485:GLN:HB3	1.87	0.57
1:A:3450:MET:HE2	1:A:3468:LEU:HD21	1.86	0.57
1:A:3463:LEU:O	1:A:4000:ASN:ND2	2.38	0.57
2:B:296:VAL:HG12	3:C:297:LEU:HD12	1.87	0.57
1:A:754:MET:HA	1:A:757:LYS:HG2	1.87	0.56
1:A:801:LYS:NZ	1:A:3114:TYR:O	2.34	0.56
1:A:2921:LEU:O	1:A:2925:GLU:HG2	2.06	0.56
1:A:3483:MET:O	1:A:3487:ILE:HB	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:28:DT:H2'	6:D:29:DA:C8	2.40	0.56
6:D:33:DA:H2''	6:D:34:DC:C4	2.40	0.56
1:A:435:LEU:O	1:A:438:LEU:HB2	2.05	0.56
1:A:865:GLN:OE1	1:A:865:GLN:N	2.37	0.56
1:A:2528:GLU:HA	1:A:2532:PRO:HA	1.87	0.56
1:A:462:VAL:HG11	1:A:540:MET:SD	2.45	0.56
1:A:677:ALA:O	1:A:681:LYS:N	2.37	0.56
1:A:870:LEU:HD23	1:A:870:LEU:H	1.70	0.56
1:A:2386:LEU:O	1:A:2394:LYS:NZ	2.34	0.56
1:A:3361:GLU:HG3	1:A:3373:VAL:HG21	1.87	0.56
3:C:65:ASP:H	3:C:78:THR:HG22	1.70	0.56
6:D:39:DA:C2	7:E:19:DA:C6	2.94	0.56
1:A:849:GLU:O	1:A:853:ILE:HG23	2.05	0.56
1:A:1070:PRO:HD3	1:A:3741:ARG:NH1	2.21	0.56
1:A:3897:PHE:CZ	1:A:3901:ARG:HD2	2.41	0.56
2:B:60:PHE:O	2:B:64:ILE:HG12	2.05	0.56
2:B:101:ASN:ND2	2:B:140:ASP:OD1	2.38	0.56
1:A:734:LEU:HD21	1:A:769:GLY:CA	2.35	0.56
3:C:253:ILE:HB	3:C:257:LEU:HD12	1.86	0.56
3:C:394:ARG:NE	3:C:403:PRO:HB3	2.20	0.56
6:D:20:DT:H1'	7:E:36:DA:C8	2.41	0.56
1:A:208:MET:HE3	1:A:208:MET:O	2.06	0.56
1:A:1364:CYS:SG	1:A:1365:ASN:N	2.79	0.56
1:A:2257:PHE:HA	1:A:2260:PHE:CE1	2.40	0.56
1:A:3572:ILE:HA	1:A:3575:LEU:HD12	1.86	0.56
1:A:3868:VAL:O	1:A:3872:ARG:HG3	2.05	0.56
1:A:397:LEU:HD21	1:A:438:LEU:HD23	1.87	0.56
1:A:892:LEU:HB2	1:A:907:LEU:H	1.71	0.56
2:B:64:ILE:O	2:B:68:GLN:NE2	2.39	0.56
1:A:89:LEU:O	1:A:133:LYS:NZ	2.27	0.56
1:A:1154:PRO:HD3	1:A:1163:LEU:HD11	1.88	0.56
1:A:1202:ARG:NH2	1:A:1210:ASP:OD1	2.39	0.56
3:C:271:ARG:O	3:C:273:LYS:NZ	2.38	0.56
6:D:27:DC:H2''	6:D:28:DT:C5	2.41	0.56
1:A:172:GLU:HG3	1:A:220:LEU:HA	1.87	0.56
1:A:3831:ASP:O	1:A:3833:ARG:N	2.39	0.56
2:B:145:GLU:O	2:B:148:TRP:HB3	2.06	0.56
2:B:147:LEU:HD13	2:B:189:LYS:HB3	1.88	0.56
2:B:344:GLY:N	2:B:401:THR:O	2.39	0.56
3:C:216:GLU:HB3	3:C:219:ASP:HB2	1.86	0.56
3:C:323:PHE:CE1	3:C:328:GLU:HG2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLU:HG2	1:A:96:MET:HG3	1.88	0.55
1:A:1946:ASN:HA	1:A:1949:ILE:HD12	1.88	0.55
1:A:3170:ASP:HB3	1:A:3173:MET:HB3	1.87	0.55
1:A:3931:ALA:O	1:A:3935:GLY:N	2.38	0.55
1:A:583:LEU:HD13	1:A:612:LEU:HD13	1.87	0.55
1:A:639:ALA:HB2	1:A:676:ASN:HB3	1.87	0.55
1:A:2320:ALA:HB1	1:A:2366:LYS:HB2	1.88	0.55
1:A:2365:ASN:ND2	1:A:2399:GLU:OE2	2.36	0.55
2:B:403:ARG:HB3	2:B:406:ILE:HG13	1.86	0.55
3:C:33:GLN:HE22	3:C:231:LEU:HD22	1.70	0.55
1:A:1190:LEU:HA	1:A:1193:LYS:HD3	1.88	0.55
1:A:1758:LEU:HD23	1:A:1761:LEU:HD12	1.88	0.55
1:A:1870:LYS:HA	1:A:1873:TYR:HD2	1.71	0.55
1:A:2501:LEU:HD12	1:A:2504:ASP:HB2	1.88	0.55
4:F:109:LEU:HG	4:F:132:ILE:HB	1.87	0.55
1:A:1575:LEU:HD21	1:A:1617:LYS:HD2	1.89	0.55
1:A:2891:ARG:NH2	1:A:3894:PRO:O	2.40	0.55
1:A:309:LYS:O	1:A:313:LEU:HG	2.07	0.55
1:A:2319:ALA:HA	1:A:2322:VAL:HG22	1.89	0.55
1:A:2410:GLU:O	1:A:2414:GLN:NE2	2.33	0.55
1:A:3352:GLU:HG3	1:A:3356:ALA:H	1.72	0.55
1:A:3686:TRP:O	1:A:3690:PHE:N	2.40	0.55
2:B:308:GLY:O	4:F:57:ARG:HD3	2.07	0.55
2:B:363:ARG:HB2	2:B:436:PHE:HD2	1.70	0.55
2:B:80:ARG:NH2	2:B:81:ASP:OD1	2.40	0.55
3:C:378:SER:O	3:C:381:ILE:HG12	2.07	0.55
3:C:613:SER:OG	3:C:654:ARG:NH2	2.39	0.55
4:F:121:GLU:HG3	4:F:123:ARG:HB2	1.88	0.55
1:A:292:SER:HA	1:A:295:GLU:CD	2.32	0.55
1:A:3506:LEU:HD11	1:A:3554:PHE:CD2	2.41	0.55
1:A:855:VAL:HA	1:A:858:MET:HG3	1.88	0.55
1:A:862:LEU:HD12	1:A:866:ILE:HG21	1.87	0.55
1:A:1202:ARG:NE	1:A:1210:ASP:OD2	2.40	0.55
3:C:165:LEU:H	3:C:226:SER:HA	1.70	0.55
4:F:116:SER:HA	4:F:119:LEU:HD12	1.88	0.55
1:A:2373:PRO:O	1:A:2377:ARG:NH1	2.40	0.55
1:A:2944:THR:HG22	1:A:2957:LEU:HD13	1.89	0.55
1:A:3233:SER:HA	1:A:3272:TRP:HZ2	1.71	0.55
1:A:3739:ILE:HG22	1:A:3747:GLU:OE2	2.07	0.55
1:A:3748:HIS:HB2	1:A:3750:PHE:HE1	1.71	0.55
2:B:59:PRO:HA	2:B:62:MET:HG2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:GLN:HG2	3:C:431:ARG:NH1	2.22	0.55
2:B:492:ALA:HB2	2:B:500:PRO:HD3	1.88	0.55
1:A:2835:LYS:HD2	1:A:2838:GLN:HE21	1.72	0.55
1:A:3065:ILE:HA	1:A:3068:ALA:HB3	1.89	0.55
2:B:362:LEU:HD11	2:B:438:PRO:HB3	1.89	0.55
1:A:1537:VAL:HA	1:A:1554:SER:HA	1.89	0.54
2:B:41:LEU:HB3	2:B:88:TYR:HE1	1.72	0.54
4:F:111:LYS:HB2	4:F:130:PHE:HB3	1.89	0.54
1:A:489:ARG:O	1:A:492:SER:OG	2.23	0.54
1:A:1328:GLU:OE1	1:A:1328:GLU:N	2.41	0.54
1:A:3974:MET:HE2	1:A:3977:THR:C	2.33	0.54
2:B:446:MET:HG3	3:C:363:LYS:HG3	1.89	0.54
1:A:1760:GLU:HA	1:A:1763:THR:HG22	1.89	0.54
1:A:3123:GLN:O	1:A:3127:THR:HG23	2.06	0.54
1:A:3509:ASP:O	1:A:3551:ASN:ND2	2.41	0.54
1:A:2120:ARG:HD2	1:A:2163:HIS:NE2	2.22	0.54
1:A:2919:ASP:O	1:A:2923:TRP:N	2.39	0.54
1:A:3664:ASN:O	1:A:3667:LEU:HB3	2.07	0.54
3:C:144:LYS:HB3	3:C:207:ILE:HG21	1.89	0.54
3:C:363:LYS:HD2	3:C:418:CYS:HB2	1.88	0.54
1:A:1096:VAL:HA	1:A:1100:VAL:HG13	1.89	0.54
1:A:1400:VAL:HG23	1:A:1457:GLN:HE21	1.72	0.54
1:A:3274:VAL:HA	1:A:3277:VAL:HG22	1.90	0.54
3:C:112:ILE:HA	3:C:115:MET:HE2	1.90	0.54
1:A:272:LEU:HB2	1:A:311:ALA:HB1	1.89	0.54
1:A:1877:LEU:HA	1:A:1880:MET:SD	2.48	0.54
1:A:3041:LEU:HA	1:A:3044:MET:HE2	1.88	0.54
1:A:3122:HIS:HA	1:A:3125:ARG:HE	1.73	0.54
3:C:271:ARG:HH12	7:E:29:DG:H2'	1.72	0.54
1:A:1098:GLN:OE1	1:A:1152:ARG:N	2.40	0.54
1:A:1178:ARG:NH2	1:A:1229:CYS:SG	2.80	0.54
1:A:1391:VAL:HA	1:A:1394:HIS:CE1	2.43	0.54
1:A:3165:THR:HA	1:A:3168:TYR:CZ	2.42	0.54
1:A:3518:VAL:O	1:A:3522:THR:N	2.28	0.54
2:B:319:SER:N	3:C:277:THR:O	2.37	0.54
3:C:527:GLN:HA	3:C:530:LEU:HB2	1.89	0.54
1:A:381:VAL:HG23	1:A:424:LEU:HD13	1.89	0.54
1:A:396:PHE:CE1	1:A:406:ARG:HB2	2.43	0.54
1:A:2385:LEU:HD13	1:A:2388:LYS:HD2	1.90	0.54
1:A:3226:ASP:N	1:A:3229:SER:OG	2.38	0.54
2:B:89:GLY:O	2:B:139:SER:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4065:LEU:HD23	1:A:4074:PHE:CZ	2.42	0.54
2:B:296:VAL:HA	3:C:297:LEU:HA	1.89	0.54
1:A:417:VAL:HA	1:A:420:VAL:HG22	1.90	0.53
1:A:864:GLY:H	1:A:3169:PRO:HA	1.73	0.53
4:F:41:LEU:HD21	4:F:115:LEU:HD11	1.89	0.53
1:A:232:CYS:HB2	1:A:278:HIS:CE1	2.44	0.53
1:A:1019:ASP:O	1:A:1026:ARG:NH1	2.41	0.53
1:A:2254:ARG:HH12	1:A:2288:TYR:HE1	1.56	0.53
1:A:3724:GLU:HG3	1:A:3725:ARG:HH21	1.72	0.53
1:A:4002:MET:HE1	1:A:4048:LYS:HE3	1.88	0.53
2:B:276:LEU:HG	2:B:277:VAL:HG13	1.90	0.53
1:A:527:TYR:HB2	1:A:629:PHE:HE1	1.73	0.53
1:A:553:VAL:HB	1:A:1550:VAL:HG12	1.91	0.53
1:A:1184:ARG:HE	1:A:1265:GLU:HB2	1.73	0.53
1:A:2312:TYR:O	1:A:2315:VAL:HG22	2.09	0.53
1:A:2330:VAL:C	1:A:2332:GLU:N	2.66	0.53
1:A:3108:GLN:HA	1:A:3111:MET:HG2	1.89	0.53
1:A:4065:LEU:HD23	1:A:4074:PHE:HZ	1.74	0.53
3:C:162:GLN:NE2	3:C:163:PHE:O	2.41	0.53
3:C:215:LEU:HG	3:C:216:GLU:HG2	1.91	0.53
4:F:50:ARG:O	4:F:55:ARG:NH1	2.41	0.53
1:A:370:ALA:O	1:A:374:LYS:N	2.35	0.53
1:A:1149:LYS:H	1:A:1151:ARG:HH21	1.56	0.53
1:A:2519:LEU:O	1:A:2522:ARG:HG3	2.09	0.53
1:A:4065:LEU:O	1:A:4069:GLU:HG2	2.07	0.53
2:B:269:ILE:HA	2:B:375:VAL:HG11	1.90	0.53
1:A:465:PHE:HE2	1:A:564:LEU:HD21	1.74	0.53
1:A:1811:ARG:HD3	1:A:1819:PHE:CE2	2.44	0.53
1:A:2352:HIS:HB2	1:A:2356:MET:HG3	1.91	0.53
1:A:2429:ASP:OD1	1:A:2430:GLU:N	2.42	0.53
1:A:3580:ASN:HD21	1:A:3582:GLU:HB2	1.74	0.53
2:B:418:GLU:C	2:B:420:LEU:H	2.16	0.53
1:A:203:GLU:HG3	1:A:224:LEU:HD11	1.91	0.53
1:A:770:LEU:HD11	1:A:858:MET:HG2	1.91	0.53
1:A:776:TRP:CZ3	1:A:785:MET:HG2	2.44	0.53
1:A:1717:LEU:O	1:A:1721:HIS:ND1	2.40	0.53
1:A:3179:TRP:HB3	1:A:3242:MET:HE1	1.91	0.53
2:B:204:HIS:ND1	2:B:212:ASP:OD1	2.37	0.53
3:C:66:ASN:HB3	3:C:77:ILE:HG22	1.90	0.53
1:A:3864:ARG:HG3	1:A:4115:ASN:HB2	1.90	0.53
1:A:4009:PRO:O	1:A:4015:ASN:ND2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:151:ILE:HD12	3:C:154:LEU:HD21	1.89	0.53
3:C:644:GLU:HA	3:C:647:ILE:HD12	1.91	0.53
1:A:389:ILE:HG22	1:A:393:LYS:NZ	2.24	0.53
1:A:962:TYR:HD2	1:A:1007:VAL:HG11	1.73	0.53
1:A:1291:LEU:HG	1:A:1363:LEU:HD11	1.90	0.53
1:A:1345:THR:HA	1:A:1348:LEU:HD12	1.90	0.53
1:A:2323:LEU:HA	1:A:2326:ILE:HG22	1.91	0.53
1:A:3744:ASP:O	1:A:3746:ARG:NH1	2.42	0.53
2:B:57:LEU:HD23	2:B:65:GLN:HE21	1.72	0.53
1:A:26:GLY:HA2	1:A:30:ALA:HB3	1.90	0.53
1:A:3154:GLN:HG2	1:A:3157:LEU:HD12	1.90	0.53
1:A:3443:PRO:O	1:A:3447:VAL:HG12	2.09	0.53
1:A:3595:GLU:HA	1:A:3598:LYS:HG2	1.91	0.53
1:A:3886:ALA:HA	1:A:3889:ARG:HH11	1.74	0.53
1:A:3966:GLN:O	1:A:3970:LEU:N	2.39	0.53
3:C:651:GLU:HG3	3:C:654:ARG:HD3	1.91	0.53
1:A:391:ARG:HH21	1:A:395:MET:HB3	1.73	0.53
1:A:667:TYR:HB3	1:A:732:PHE:HB2	1.90	0.53
1:A:855:VAL:HA	1:A:858:MET:CG	2.39	0.53
1:A:1115:HIS:HD2	1:A:1181:THR:HG22	1.74	0.53
1:A:1565:GLU:HA	1:A:1568:ASN:ND2	2.24	0.53
1:A:1760:GLU:OE1	1:A:1801:VAL:HA	2.09	0.53
1:A:3700:GLU:HG2	1:A:3718:ARG:HG3	1.89	0.53
1:A:3887:PHE:HA	1:A:3890:MET:SD	2.49	0.53
2:B:302:THR:HG23	2:B:311:LEU:HB2	1.91	0.53
2:B:341:ASP:OD2	2:B:346:MET:HE3	2.09	0.53
2:B:421:ASP:N	2:B:427:VAL:H	2.07	0.53
4:F:108:GLN:HE22	4:F:110:VAL:HB	1.74	0.53
1:A:391:ARG:HG3	1:A:395:MET:HE3	1.91	0.52
1:A:443:ILE:O	1:A:527:TYR:OH	2.20	0.52
1:A:959:TYR:CE1	1:A:1007:VAL:HB	2.44	0.52
1:A:1235:ILE:HG23	1:A:1259:LEU:HD11	1.91	0.52
1:A:4122:GLU:HG3	1:A:4127:TRP:HZ3	1.73	0.52
2:B:297:LYS:N	3:C:296:CYS:O	2.42	0.52
3:C:368:ARG:HE	3:C:369:ASP:H	1.56	0.52
1:A:128:LEU:O	1:A:132:ILE:HD12	2.09	0.52
1:A:407:VAL:HA	1:A:410:MET:HG2	1.91	0.52
1:A:938:VAL:HA	1:A:941:MET:HG3	1.91	0.52
1:A:4011:PHE:O	1:A:4038:TRP:NE1	2.32	0.52
2:B:122:PHE:HB3	2:B:131:PHE:HB2	1.92	0.52
3:C:624:LEU:HA	3:C:671:LEU:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ARG:NH2	1:A:102:PRO:HB2	2.24	0.52
1:A:1298:LEU:HG	1:A:1367:HIS:HB3	1.91	0.52
1:A:1719:VAL:HB	3:C:631:TYR:HB2	1.92	0.52
1:A:2560:ASN:OD1	1:A:2561:PHE:N	2.43	0.52
1:A:3659:PHE:HA	1:A:3662:ILE:HD13	1.92	0.52
1:A:3934:THR:HG23	1:A:3936:GLY:H	1.73	0.52
1:A:4053:GLY:O	1:A:4098:LEU:N	2.38	0.52
2:B:443:LYS:HE3	2:B:445:LYS:HA	1.90	0.52
1:A:1976:LEU:HB3	1:A:2145:PHE:HE2	1.75	0.52
2:B:424:LYS:O	2:B:426:GLN:N	2.43	0.52
4:F:118:CYS:HB3	4:F:123:ARG:O	2.08	0.52
1:A:163:LYS:HD3	1:A:164:LYS:HB2	1.92	0.52
1:A:764:PRO:HG3	1:A:846:ILE:HG21	1.90	0.52
1:A:801:LYS:HA	1:A:3115:SER:HA	1.92	0.52
1:A:2866:ALA:O	1:A:2899:ARG:NH2	2.43	0.52
1:A:3332:THR:HA	1:A:3335:ARG:HG2	1.91	0.52
1:A:3588:TRP:CE2	1:A:3609:MET:HE3	2.45	0.52
1:A:3750:PHE:HA	1:A:3805:TRP:H	1.75	0.52
2:B:204:HIS:HA	2:B:213:ILE:HG13	1.91	0.52
4:F:41:LEU:HB2	4:F:68:HIS:HB2	1.92	0.52
1:A:1242:LEU:O	1:A:1311:LYS:NZ	2.42	0.52
6:D:30:DA:H2"	6:D:31:DA:N7	2.24	0.52
1:A:1576:ASP:OD1	1:A:1577:LEU:N	2.42	0.52
1:A:1871:MET:HE2	1:A:1940:TYR:HB2	1.92	0.52
1:A:2422:GLN:HA	1:A:2425:ARG:HE	1.75	0.52
2:B:166:ILE:HG12	2:B:198:ILE:HD11	1.92	0.52
2:B:298:THR:OG1	2:B:300:THR:OG1	2.20	0.52
2:B:300:THR:HA	3:C:293:THR:HB	1.92	0.52
2:B:463:LYS:HG3	3:C:383:ALA:HB1	1.91	0.52
1:A:475:LEU:O	1:A:479:ILE:HD12	2.10	0.52
1:A:2556:SER:HB2	1:A:2799:GLN:HA	1.92	0.52
1:A:2891:ARG:HH22	1:A:3898:LEU:HD23	1.74	0.52
1:A:4068:HIS:HB3	1:A:4071:ALA:HB3	1.92	0.52
2:B:511:VAL:HA	2:B:514:MET:HB3	1.92	0.52
1:A:63:PHE:HA	1:A:66:LEU:HD12	1.91	0.52
1:A:992:ILE:O	1:A:996:THR:HG22	2.10	0.52
1:A:1173:LEU:HA	1:A:1176:CYS:SG	2.50	0.52
1:A:1210:ASP:O	1:A:1213:LYS:NZ	2.37	0.52
1:A:1805:PHE:O	1:A:1816:ARG:NH1	2.43	0.52
1:A:2220:MET:HA	1:A:2223:VAL:HG12	1.91	0.52
1:A:3881:ASP:OD1	1:A:3884:LYS:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:493:CYS:O	3:C:505:LEU:HD22	2.10	0.52
3:C:602:VAL:HG21	3:C:642:PHE:HE1	1.75	0.52
4:F:42:SER:HA	4:F:70:GLY:HA2	1.91	0.52
1:A:412:SER:O	1:A:415:GLN:HG3	2.10	0.52
1:A:1863:PHE:HA	1:A:1866:GLN:HG2	1.91	0.52
1:A:2793:PRO:HA	1:A:2796:ALA:HB3	1.92	0.52
2:B:385:LEU:HA	2:B:392:LYS:HD3	1.92	0.52
1:A:16:GLN:HG2	1:A:59:PHE:HE1	1.75	0.51
1:A:1949:ILE:HG21	1:A:2096:PRO:HB3	1.92	0.51
1:A:2088:LEU:HA	1:A:2094:MET:HE2	1.93	0.51
1:A:2437:ASP:OD1	1:A:2472:GLN:HG2	2.09	0.51
1:A:2930:TYR:HB2	1:A:2939:LEU:HD22	1.91	0.51
1:A:2936:TYR:HA	1:A:2939:LEU:HB3	1.92	0.51
1:A:3000:ASP:O	1:A:3004:HIS:ND1	2.43	0.51
3:C:40:MET:O	3:C:43:GLN:HG3	2.09	0.51
3:C:262:ALA:N	3:C:365:PHE:O	2.38	0.51
3:C:596:GLU:HA	3:C:599:ARG:HE	1.75	0.51
1:A:1716:GLN:HA	1:A:1719:VAL:HG22	1.92	0.51
1:A:2143:ARG:NH2	1:A:2170:GLN:OE1	2.43	0.51
1:A:2991:LYS:HA	1:A:2994:TRP:CE3	2.44	0.51
1:A:3385:LEU:HB3	1:A:3416:LEU:HD21	1.92	0.51
1:A:3608:LYS:O	1:A:3612:ARG:HG2	2.11	0.51
4:F:50:ARG:NH2	4:F:55:ARG:O	2.43	0.51
1:A:167:PRO:HD2	1:A:171:LEU:HD13	1.92	0.51
1:A:1279:LEU:HD13	1:A:1282:LEU:HD11	1.93	0.51
1:A:1368:LEU:HA	1:A:1371:VAL:HG22	1.91	0.51
1:A:3061:LEU:O	1:A:3065:ILE:HG12	2.10	0.51
1:A:3259:LEU:HG	1:A:3276:TRP:CE2	2.45	0.51
2:B:92:LYS:NZ	2:B:133:ASP:O	2.40	0.51
3:C:140:SER:O	3:C:200:GLN:HG2	2.11	0.51
4:F:89:MET:HE1	4:F:94:ALA:HA	1.91	0.51
1:A:110:THR:O	1:A:114:VAL:HG13	2.10	0.51
1:A:446:PHE:HA	1:A:449:TYR:CD2	2.45	0.51
1:A:2413:PHE:HA	1:A:2416:LYS:HG2	1.92	0.51
1:A:3660:ASN:O	1:A:3663:THR:HB	2.10	0.51
1:A:3967:PHE:HA	1:A:3970:LEU:HG	1.92	0.51
2:B:469:LEU:HD22	3:C:345:PHE:H	1.75	0.51
1:A:537:SER:O	1:A:541:MET:HE3	2.11	0.51
1:A:1059:LEU:HD23	1:A:1062:ARG:HH21	1.74	0.51
1:A:2891:ARG:NH2	1:A:3898:LEU:HB3	2.22	0.51
1:A:2937:ASP:HB3	1:A:3979:LEU:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3986:HIS:O	1:A:3989:ARG:HD3	2.11	0.51
1:A:971:ARG:NH1	1:A:1022:ASP:OD2	2.44	0.51
1:A:1257:LEU:HD23	1:A:1260:LEU:HD12	1.92	0.51
1:A:2376:ASP:HB2	1:A:2377:ARG:HH11	1.75	0.51
1:A:3809:THR:HG22	1:A:3931:ALA:HA	1.93	0.51
1:A:3908:HIS:HA	1:A:3911:ILE:HG12	1.93	0.51
3:C:616:LEU:O	3:C:620:ILE:HG12	2.11	0.51
1:A:445:SER:OG	1:A:448:GLN:NE2	2.36	0.51
1:A:786:GLN:HA	1:A:789:TYR:CG	2.46	0.51
1:A:3955:VAL:HG21	1:A:4121:TRP:CD2	2.45	0.51
3:C:531:SER:HA	3:C:534:LYS:HG2	1.92	0.51
4:F:87:GLU:OE1	4:F:87:GLU:N	2.44	0.51
1:A:1807:LYS:NZ	1:A:1808:ASP:OD1	2.39	0.51
1:A:3064:PHE:O	1:A:3068:ALA:N	2.44	0.51
1:A:3659:PHE:O	1:A:3663:THR:N	2.36	0.51
3:C:74:TYR:HB3	3:C:77:ILE:HG13	1.92	0.51
1:A:448:GLN:HB3	1:A:519:TRP:CD1	2.46	0.51
1:A:1689:LYS:O	1:A:1693:VAL:HG13	2.11	0.51
1:A:2327:LEU:O	1:A:2328:ARG:C	2.54	0.51
1:A:3904:PHE:O	1:A:3908:HIS:HB2	2.10	0.51
1:A:850:GLU:O	1:A:853:ILE:HG12	2.11	0.51
1:A:1047:GLN:O	1:A:1051:LYS:HG2	2.11	0.51
1:A:1070:PRO:O	1:A:1075:ARG:NH1	2.44	0.51
1:A:1694:THR:HG23	1:A:1695:LEU:HD22	1.92	0.51
1:A:1764:GLU:O	1:A:1768:ARG:NH2	2.44	0.51
1:A:3626:GLY:O	1:A:3630:ARG:HG2	2.11	0.51
1:A:3978:GLY:N	1:A:3980:MET:SD	2.83	0.51
1:A:4089:ILE:N	1:A:4109:ASP:OD2	2.44	0.51
3:C:134:ILE:HB	3:C:163:PHE:HA	1.93	0.51
3:C:247:TRP:HE3	3:C:263:ALA:HB3	1.76	0.51
3:C:529:PRO:HA	3:C:532:LYS:HG2	1.93	0.51
1:A:1310:GLU:O	1:A:1311:LYS:HG2	2.12	0.50
1:A:1379:PRO:HB2	1:A:1383:GLY:O	2.10	0.50
1:A:1396:PRO:HA	1:A:1457:GLN:HE22	1.74	0.50
1:A:2887:PRO:HG2	1:A:3895:GLU:HB3	1.93	0.50
2:B:425:ILE:O	2:B:426:GLN:C	2.55	0.50
1:A:736:LEU:HD12	1:A:740:ILE:HB	1.92	0.50
1:A:1195:VAL:HG11	1:A:1204:PRO:HA	1.94	0.50
1:A:2876:VAL:HG21	1:A:2892:LEU:HD23	1.91	0.50
2:B:76:ILE:HD12	2:B:248:ALA:N	2.26	0.50
2:B:412:ALA:HB2	2:B:437:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:SER:HA	1:A:190:ILE:HB	1.91	0.50
1:A:346:TYR:HA	1:A:349:ILE:HG12	1.92	0.50
1:A:709:LYS:HA	1:A:712:LYS:HG2	1.94	0.50
1:A:1154:PRO:HD2	1:A:1157:PHE:HB2	1.92	0.50
1:A:1339:VAL:HG12	1:A:1395:LEU:HD21	1.94	0.50
1:A:2129:LEU:HA	1:A:2132:LYS:HB3	1.93	0.50
1:A:2838:GLN:NE2	1:A:2839:ASP:OD1	2.44	0.50
2:B:276:LEU:HD21	3:C:354:ARG:NH1	2.26	0.50
1:A:1257:LEU:HA	1:A:1260:LEU:HD12	1.93	0.50
1:A:3759:ARG:N	1:A:3795:PRO:HG3	2.26	0.50
1:A:3955:VAL:HG21	1:A:4121:TRP:CG	2.46	0.50
3:C:165:LEU:N	3:C:226:SER:HA	2.26	0.50
3:C:633:MET:HA	3:C:636:ILE:HG12	1.92	0.50
1:A:2217:ASN:HA	1:A:2220:MET:HG2	1.92	0.50
1:A:2835:LYS:O	1:A:2838:GLN:HG3	2.11	0.50
1:A:3464:LYS:HE3	1:A:3997:LEU:HD23	1.93	0.50
1:A:3485:LYS:O	1:A:3488:SER:OG	2.20	0.50
2:B:40:PHE:CD1	2:B:167:MET:HG2	2.47	0.50
2:B:183:ALA:HB1	2:B:187:ARG:HH12	1.76	0.50
2:B:276:LEU:HD22	2:B:367:PHE:HB2	1.93	0.50
3:C:332:LYS:HG2	3:C:334:LYS:HZ3	1.76	0.50
1:A:800:LEU:O	1:A:3115:SER:OG	2.26	0.50
1:A:1208:LEU:HA	1:A:1211:VAL:HG22	1.94	0.50
1:A:1519:PHE:HB3	1:A:1573:LYS:HE3	1.94	0.50
1:A:2120:ARG:NH1	1:A:2159:PRO:O	2.45	0.50
1:A:2581:LEU:HD12	1:A:2781:PRO:HD2	1.94	0.50
1:A:3337:ILE:HG23	1:A:3377:LEU:HD21	1.94	0.50
1:A:3924:HIS:HB3	1:A:4125:GLU:CD	2.37	0.50
2:B:145:GLU:O	2:B:149:VAL:HG13	2.12	0.50
2:B:492:ALA:HA	2:B:497:LEU:HB2	1.94	0.50
3:C:251:LEU:HD23	3:C:261:ILE:HD13	1.93	0.50
4:F:82:HIS:HA	4:F:108:GLN:H	1.77	0.50
1:A:348:ILE:HG13	1:A:362:ALA:HB2	1.92	0.50
1:A:1597:LEU:HD21	1:A:1648:LEU:HD22	1.92	0.50
1:A:1605:PHE:O	1:A:1608:ARG:NH1	2.38	0.50
1:A:1767:CYS:SG	1:A:1819:PHE:HA	2.51	0.50
1:A:2470:ARG:HA	1:A:2473:MET:HE2	1.94	0.50
1:A:3301:LEU:O	1:A:3305:SER:HB3	2.12	0.50
2:B:64:ILE:O	2:B:67:ILE:HG22	2.12	0.50
2:B:276:LEU:HD23	2:B:276:LEU:H	1.76	0.50
2:B:402:PRO:HD2	2:B:406:ILE:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:404:ARG:NH1	6:D:32:DA:OP2	2.45	0.50
2:B:468:LYS:HB2	2:B:518:LEU:HG	1.93	0.50
1:A:554:ASN:ND2	1:A:556:SER:O	2.45	0.50
1:A:683:PHE:HZ	1:A:707:PHE:CD2	2.25	0.50
1:A:4007:LYS:NZ	1:A:4040:PRO:HB2	2.26	0.50
2:B:282:LYS:NZ	2:B:283:PRO:O	2.38	0.50
2:B:310:LEU:HD11	3:C:292:GLU:HB3	1.93	0.50
4:F:111:LYS:HA	4:F:132:ILE:HD11	1.94	0.50
1:A:801:LYS:HD3	1:A:3115:SER:HA	1.94	0.50
1:A:3009:LYS:HA	1:A:3012:GLU:OE2	2.12	0.50
1:A:3049:LEU:HA	1:A:3052:LEU:HD12	1.94	0.50
1:A:3671:ASN:OD1	1:A:3672:LYS:N	2.43	0.50
1:A:965:THR:O	1:A:968:VAL:HG12	2.12	0.49
1:A:1448:LEU:O	1:A:1452:VAL:HG13	2.12	0.49
1:A:1956:PHE:HE2	1:A:1961:PHE:HA	1.76	0.49
1:A:3117:ILE:HD11	1:A:3124:SER:HB2	1.94	0.49
1:A:3714:GLU:O	1:A:3718:ARG:NH2	2.42	0.49
2:B:345:LEU:HB3	2:B:400:TYR:CD1	2.39	0.49
3:C:165:LEU:O	3:C:227:PHE:N	2.38	0.49
3:C:357:MET:HG2	3:C:425:PRO:HB3	1.93	0.49
3:C:457:LEU:HD23	3:C:529:PRO:HB2	1.92	0.49
6:D:43:DT:H3	7:E:15:DA:H4'	1.76	0.49
1:A:240:GLU:OE2	1:A:246:ARG:NH1	2.44	0.49
1:A:381:VAL:HA	1:A:384:MET:HG3	1.93	0.49
1:A:3262:LEU:HD23	1:A:3276:TRP:HD1	1.76	0.49
2:B:397:LEU:HD21	3:C:477:PHE:HD2	1.76	0.49
3:C:17:GLY:O	3:C:101:GLY:N	2.45	0.49
1:A:210:SER:O	3:C:549:THR:N	2.31	0.49
1:A:430:VAL:O	1:A:433:PRO:HD2	2.11	0.49
1:A:1391:VAL:HG23	1:A:1392:MET:SD	2.52	0.49
1:A:1476:HIS:HB3	1:A:1479:VAL:HG12	1.94	0.49
1:A:2494:ASP:O	1:A:2497:GLU:HG2	2.12	0.49
2:B:69:SER:O	2:B:244:ARG:NH1	2.46	0.49
2:B:290:ARG:NH2	3:C:311:ILE:HD13	2.25	0.49
2:B:311:LEU:HD21	3:C:288:ASP:O	2.13	0.49
3:C:45:GLN:O	3:C:49:GLU:N	2.45	0.49
3:C:679:VAL:HG13	3:C:683:ILE:HD11	1.94	0.49
1:A:175:TYR:O	1:A:227:LEU:HD13	2.13	0.49
1:A:545:LEU:HA	1:A:548:GLU:HG2	1.93	0.49
1:A:620:PHE:O	1:A:624:ILE:HG12	2.12	0.49
1:A:1225:GLU:HB3	1:A:1231:GLN:HE22	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1645:VAL:HA	1:A:1648:LEU:HG	1.93	0.49
1:A:1725:GLN:OE1	1:A:1726:SER:N	2.45	0.49
1:A:2357:GLU:HG3	1:A:2358:ASP:H	1.77	0.49
1:A:3114:TYR:O	1:A:3117:ILE:HG22	2.12	0.49
1:A:396:PHE:HE1	1:A:406:ARG:HB2	1.76	0.49
1:A:1335:CYS:O	1:A:1339:VAL:HG13	2.12	0.49
1:A:1714:LEU:O	1:A:1718:ILE:HG12	2.13	0.49
1:A:3033:GLU:HB2	1:A:3034:PRO:HD3	1.92	0.49
1:A:3775:LEU:HD13	1:A:3786:LEU:HB3	1.92	0.49
1:A:4047:ALA:O	1:A:4050:LYS:HG2	2.12	0.49
1:A:385:TYR:CE2	1:A:427:VAL:HG23	2.47	0.49
1:A:876:SER:HB2	1:A:879:MET:HB2	1.95	0.49
1:A:1166:LEU:HB3	1:A:1170:LYS:NZ	2.27	0.49
1:A:1458:LEU:O	1:A:1462:GLY:N	2.42	0.49
1:A:2270:ASN:HD22	1:A:2309:PHE:HE2	1.61	0.49
1:A:4012:ASP:H	1:A:4015:ASN:HB2	1.78	0.49
2:B:355:LEU:HB2	3:C:473:LEU:HD13	1.95	0.49
3:C:136:THR:HG22	3:C:138:LEU:H	1.77	0.49
3:C:622:GLN:NE2	3:C:623:PHE:HB2	2.28	0.49
4:F:86:ASP:HB2	4:F:89:MET:HG2	1.95	0.49
1:A:966:PHE:HB2	1:A:1011:GLU:CD	2.38	0.49
1:A:1115:HIS:CD2	1:A:1181:THR:HG22	2.46	0.49
1:A:1817:GLN:HA	1:A:1820:VAL:HG22	1.93	0.49
1:A:1949:ILE:HG12	1:A:2100:LEU:HD11	1.95	0.49
1:A:2429:ASP:O	1:A:2432:GLN:HG2	2.13	0.49
1:A:4020:MET:SD	1:A:4027:TRP:HB3	2.52	0.49
3:C:394:ARG:HE	3:C:403:PRO:HB3	1.78	0.49
1:A:487:LEU:O	1:A:490:ILE:HG22	2.12	0.49
1:A:603:ILE:HD11	1:A:1031:ARG:HD2	1.95	0.49
1:A:683:PHE:HE2	1:A:740:ILE:HD11	1.77	0.49
1:A:974:CYS:SG	1:A:1025:LEU:HB2	2.52	0.49
1:A:1582:LEU:HD11	1:A:1593:VAL:HG22	1.94	0.49
1:A:2266:ASN:HA	1:A:2311:ARG:HG2	1.94	0.49
1:A:2573:PRO:HA	1:A:2786:LYS:HD3	1.94	0.49
1:A:2976:LEU:O	1:A:2979:GLN:NE2	2.45	0.49
1:A:4088:ASN:HD21	1:A:4113:ASP:HB2	1.77	0.49
2:B:90:THR:HG21	2:B:103:TYR:HB2	1.95	0.49
3:C:265:LYS:HB3	3:C:268:LEU:HD11	1.94	0.49
4:F:121:GLU:O	4:F:123:ARG:NH1	2.46	0.49
6:D:36:DA:H2'	6:D:37:DT:H1'	1.94	0.49
6:D:43:DT:C4	7:E:16:DA:C5	3.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ASN:O	1:A:409:GLN:NE2	2.45	0.49
1:A:914:VAL:HA	1:A:917:LEU:HG	1.93	0.49
1:A:1493:PRO:HB3	1:A:1500:LEU:H	1.78	0.49
1:A:2254:ARG:HH21	1:A:2293:GLY:N	2.09	0.49
2:B:369:TYR:CD1	2:B:370:PRO:HD2	2.48	0.49
4:F:54:GLY:H	4:F:57:ARG:NE	2.10	0.49
1:A:31:GLY:O	1:A:35:ILE:HG12	2.13	0.49
1:A:150:GLY:HA2	1:A:188:GLU:OE2	2.13	0.49
1:A:2135:ASN:O	1:A:2138:VAL:HG22	2.13	0.49
1:A:2135:ASN:O	1:A:2143:ARG:NH1	2.45	0.49
1:A:2559:THR:OG1	1:A:2795:GLN:NE2	2.46	0.49
1:A:3144:PHE:HA	1:A:3150:ASN:HD22	1.77	0.49
1:A:3588:TRP:NE1	1:A:3613:MET:HE3	2.28	0.49
1:A:756:PHE:O	1:A:799:TYR:OH	2.26	0.48
1:A:1887:ASP:OD1	1:A:1888:ASP:N	2.44	0.48
1:A:2157:PHE:HB3	1:A:2164:TRP:CD1	2.48	0.48
1:A:2318:ALA:O	1:A:2322:VAL:HG13	2.13	0.48
1:A:2376:ASP:OD1	1:A:2404:ARG:HD3	2.13	0.48
2:B:297:LYS:HE3	3:C:296:CYS:SG	2.53	0.48
3:C:280:ASP:OD2	3:C:282:LYS:NZ	2.46	0.48
3:C:649:PHE:CE2	3:C:651:GLU:HB2	2.48	0.48
4:F:91:TYR:HB2	4:F:134:ILE:HA	1.95	0.48
1:A:111:CYS:O	1:A:114:VAL:HG22	2.13	0.48
1:A:200:PHE:CZ	1:A:227:LEU:HD21	2.48	0.48
1:A:205:LYS:HA	1:A:208:MET:HB3	1.95	0.48
1:A:210:SER:OG	2:B:339:ARG:NH1	2.28	0.48
1:A:1057:LYS:HB3	1:A:1061:LYS:HZ1	1.78	0.48
2:B:446:MET:HE2	3:C:363:LYS:HB2	1.94	0.48
6:D:36:DA:H2'	6:D:37:DT:C1'	2.43	0.48
1:A:360:SER:HA	1:A:363:ILE:HG12	1.95	0.48
1:A:734:LEU:HD22	1:A:768:VAL:HG13	1.95	0.48
1:A:2269:ASP:N	1:A:2269:ASP:OD1	2.46	0.48
1:A:4114:PRO:HA	1:A:4117:LEU:HD12	1.94	0.48
7:E:26:DT:H2'	7:E:27:DT:H73	1.96	0.48
1:A:171:LEU:HD23	1:A:171:LEU:H	1.79	0.48
1:A:1986:ARG:HD2	1:A:2184:TYR:HA	1.94	0.48
1:A:2338:GLU:OE2	1:A:2340:SER:OG	2.32	0.48
1:A:3424:LEU:O	1:A:3428:GLU:N	2.36	0.48
1:A:1093:GLU:OE1	1:A:1093:GLU:N	2.46	0.48
1:A:1333:SER:O	1:A:1337:VAL:HG13	2.13	0.48
1:A:2397:CYS:HA	1:A:2400:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2421:VAL:O	1:A:2425:ARG:HG3	2.14	0.48
1:A:3809:THR:OG1	1:A:3929:MET:SD	2.64	0.48
1:A:4064:LEU:HD13	1:A:4077:TYR:HB3	1.96	0.48
2:B:490:LEU:HB3	3:C:316:TYR:CE2	2.44	0.48
3:C:94:ILE:HG23	3:C:98:ILE:HG13	1.95	0.48
4:F:44:LEU:HG	4:F:82:HIS:CD2	2.48	0.48
1:A:12:LEU:HD23	1:A:15:LEU:HD12	1.95	0.48
1:A:208:MET:HG2	1:A:249:PHE:HD1	1.77	0.48
1:A:898:PHE:CD1	1:A:2535:THR:HG21	2.49	0.48
1:A:1575:LEU:HD12	1:A:1576:ASP:N	2.28	0.48
1:A:1816:ARG:HA	1:A:1819:PHE:HD2	1.78	0.48
1:A:1966:LEU:H	1:A:1969:GLU:CD	2.20	0.48
1:A:2158:ARG:NH2	1:A:2195:SER:O	2.46	0.48
1:A:2205:VAL:HG12	1:A:2207:LYS:N	2.29	0.48
1:A:2262:GLY:HA3	1:A:2270:ASN:ND2	2.27	0.48
1:A:2420:PHE:CE1	1:A:2424:MET:HB3	2.49	0.48
1:A:3261:GLU:OE1	1:A:3261:GLU:N	2.32	0.48
1:A:3702:PRO:HB2	1:A:3794:VAL:HG11	1.96	0.48
2:B:130:ARG:HA	2:B:133:ASP:OD2	2.14	0.48
3:C:526:SER:O	3:C:530:LEU:N	2.39	0.48
3:C:610:GLU:OE2	3:C:654:ARG:NE	2.36	0.48
1:A:461:ILE:HA	1:A:464:VAL:HG22	1.95	0.48
1:A:1244:LEU:HD11	1:A:1310:GLU:HB2	1.96	0.48
1:A:1740:VAL:HA	1:A:1743:MET:HG2	1.95	0.48
1:A:1791:CYS:SG	1:A:1792:VAL:N	2.87	0.48
1:A:1894:SER:HB3	1:A:1910:GLU:N	2.29	0.48
1:A:2365:ASN:HB2	1:A:2396:LEU:HD23	1.94	0.48
1:A:2891:ARG:HA	1:A:2894:GLU:HG2	1.96	0.48
2:B:112:GLY:H	2:B:115:ARG:HG3	1.77	0.48
4:F:71:GLN:HE22	4:F:73:CYS:HB3	1.78	0.48
6:D:31:DA:H2"	6:D:32:DA:C8	2.48	0.48
1:A:151:GLU:HA	4:F:133:PHE:CE2	2.49	0.48
1:A:451:PRO:HA	1:A:454:GLN:HB2	1.96	0.48
1:A:734:LEU:HD23	1:A:734:LEU:O	2.13	0.48
1:A:1037:LEU:O	1:A:1040:SER:OG	2.29	0.48
1:A:1399:CYS:SG	1:A:1403:MET:HE1	2.54	0.48
1:A:1804:MET:O	1:A:1811:ARG:NH2	2.47	0.48
1:A:2561:PHE:HB3	1:A:2565:MET:HE1	1.96	0.48
1:A:3086:LEU:HD23	1:A:3089:LEU:HD21	1.96	0.48
1:A:3511:ALA:O	1:A:3515:GLN:N	2.42	0.48
2:B:103:TYR:CD1	2:B:135:MET:HG2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:411:VAL:HG12	2:B:436:PHE:HD1	1.79	0.48
2:B:492:ALA:HB2	2:B:499:GLU:HA	1.96	0.48
3:C:11:VAL:HG21	3:C:114:SER:HB2	1.95	0.48
1:A:562:HIS:HB2	1:A:641:PHE:CE1	2.48	0.48
1:A:1565:GLU:H	1:A:1565:GLU:CD	2.21	0.48
1:A:2104:MET:O	1:A:2108:LEU:HG	2.13	0.48
1:A:2122:LEU:HB3	1:A:2127:LYS:HD3	1.95	0.48
1:A:2345:VAL:HA	1:A:2348:GLN:HG3	1.95	0.48
1:A:2358:ASP:N	1:A:2358:ASP:OD1	2.45	0.48
1:A:3467:ARG:O	1:A:3470:GLN:HG2	2.14	0.48
1:A:3911:ILE:HD12	1:A:3928:PHE:CE1	2.49	0.48
3:C:377:LEU:O	3:C:381:ILE:HG23	2.14	0.48
1:A:910:PHE:CE1	1:A:2807:GLN:HG3	2.49	0.48
1:A:1527:ARG:O	1:A:1531:LEU:HG	2.14	0.48
1:A:2044:ASP:O	1:A:2048:GLY:N	2.47	0.48
1:A:2576:MET:SD	1:A:2576:MET:N	2.87	0.48
1:A:3493:TRP:HA	1:A:3521:ILE:HD11	1.96	0.48
1:A:3531:TYR:HB3	1:A:3796:MET:HA	1.95	0.48
2:B:41:LEU:HD13	2:B:86:VAL:HG13	1.96	0.48
2:B:375:VAL:HG13	2:B:378:SER:OG	2.13	0.48
3:C:263:ALA:HB1	3:C:362:LEU:HD11	1.95	0.48
3:C:457:LEU:CD1	3:C:533:ILE:HG13	2.44	0.48
2:B:143:LEU:H	2:B:182:LYS:HD3	1.79	0.47
2:B:388:LYS:HB3	2:B:390:LEU:HD23	1.95	0.47
1:A:1718:ILE:HA	1:A:1722:PHE:HD1	1.79	0.47
1:A:1762:MET:HE1	1:A:1782:PHE:HE1	1.78	0.47
1:A:1809:ASP:O	1:A:1811:ARG:N	2.44	0.47
1:A:2576:MET:HE1	1:A:2785:ILE:HG13	1.96	0.47
1:A:3008:TRP:CE2	1:A:3050:LYS:HG3	2.49	0.47
1:A:3577:GLN:OE1	1:A:3629:ARG:NE	2.43	0.47
1:A:3750:PHE:HA	1:A:3804:GLU:HA	1.96	0.47
1:A:3772:ASN:OD1	1:A:3787:GLN:HB2	2.14	0.47
1:A:3806:LEU:O	1:A:3807:GLU:HG3	2.14	0.47
1:A:4057:ALA:HB2	1:A:4090:ARG:HD2	1.96	0.47
2:B:341:ASP:CG	2:B:346:MET:HE3	2.39	0.47
4:F:40:TRP:HZ2	4:F:119:LEU:CA	2.25	0.47
6:D:43:DT:N3	7:E:15:DA:H4'	2.29	0.47
1:A:897:PRO:HB2	1:A:2569:SER:OG	2.14	0.47
1:A:3083:SER:O	1:A:3102:TYR:HB3	2.14	0.47
1:A:3923:ARG:HD3	1:A:3928:PHE:CZ	2.48	0.47
2:B:375:VAL:HA	3:C:540:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:20:DT:O2	7:E:36:DA:H5"	2.14	0.47
1:A:531:PHE:HD1	1:A:534:LEU:HD12	1.76	0.47
1:A:1468:LEU:HD13	1:A:1521:PHE:HE2	1.80	0.47
1:A:2519:LEU:HD11	1:A:2522:ARG:HH21	1.79	0.47
1:A:3549:HIS:HA	1:A:3552:LYS:HB2	1.94	0.47
1:A:3718:ARG:H	1:A:3743:HIS:CE1	2.31	0.47
1:A:3828:TYR:HH	1:A:4127:TRP:CD1	2.33	0.47
2:B:345:LEU:HB2	2:B:398:CYS:SG	2.54	0.47
2:B:355:LEU:HD13	3:C:473:LEU:HB2	1.95	0.47
2:B:442:ASP:OD1	3:C:269:GLN:HG2	2.15	0.47
3:C:33:GLN:HA	3:C:36:LYS:HG2	1.97	0.47
3:C:148:ASP:O	3:C:151:ILE:HG22	2.14	0.47
1:A:237:SER:HB2	1:A:283:SER:OG	2.14	0.47
1:A:1175:HIS:CG	1:A:1229:CYS:HA	2.49	0.47
1:A:1395:LEU:O	1:A:1399:CYS:HB2	2.15	0.47
1:A:1825:LEU:HD12	1:A:1826:THR:N	2.30	0.47
1:A:1828:LEU:HD11	1:A:1879:VAL:HG13	1.96	0.47
1:A:3050:LYS:HD3	1:A:3053:LEU:HD21	1.95	0.47
1:A:3168:TYR:CE1	1:A:3241:LYS:HE2	2.50	0.47
1:A:3190:LEU:HD22	1:A:3231:ILE:HG12	1.96	0.47
1:A:3479:THR:O	1:A:3480:LEU:HD22	2.14	0.47
1:A:3839:TYR:HE2	1:A:4122:GLU:HB2	1.80	0.47
1:A:3951:GLN:HE21	1:A:4063:GLU:HB3	1.78	0.47
1:A:4013:TRP:CD1	1:A:4035:GLU:HB3	2.49	0.47
2:B:203:MET:HG2	2:B:239:LEU:HB3	1.96	0.47
3:C:106:ASP:OD1	3:C:107:PHE:N	2.46	0.47
1:A:320:LEU:HA	1:A:323:VAL:HG22	1.95	0.47
1:A:1029:CYS:HA	1:A:1032:CYS:SG	2.53	0.47
1:A:1178:ARG:HD3	1:A:1180:GLN:HB2	1.95	0.47
1:A:2415:LEU:HB3	1:A:2420:PHE:HB2	1.95	0.47
1:A:2555:LEU:HD12	1:A:2555:LEU:HA	1.76	0.47
2:B:488:ARG:NH1	2:B:503:ALA:O	2.48	0.47
1:A:848:LEU:O	1:A:851:ILE:HB	2.14	0.47
1:A:921:ALA:HB3	1:A:927:LYS:HG3	1.96	0.47
1:A:1076:LEU:HD23	1:A:1121:LEU:HD21	1.97	0.47
1:A:1235:ILE:HG22	1:A:1256:TRP:NE1	2.30	0.47
1:A:1513:GLY:O	1:A:1516:GLU:HG3	2.14	0.47
1:A:3759:ARG:O	1:A:3762:GLN:HG3	2.15	0.47
1:A:3820:MET:HB3	1:A:3882:LEU:HD11	1.96	0.47
2:B:105:LEU:HD21	2:B:131:PHE:HE1	1.79	0.47
2:B:275:ASN:O	3:C:431:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:532:PRO:HG2	3:C:259:ILE:HD12	1.97	0.47
3:C:7:LYS:NZ	3:C:121:GLU:O	2.46	0.47
3:C:413:LYS:HG3	3:C:415:ASN:H	1.80	0.47
3:C:496:HIS:O	3:C:500:HIS:N	2.29	0.47
1:A:286:LEU:HD12	1:A:319:PHE:CD1	2.47	0.47
1:A:1948:ALA:HA	1:A:1951:VAL:HG12	1.96	0.47
1:A:2964:ASP:O	1:A:2967:GLU:N	2.48	0.47
1:A:3567:VAL:O	1:A:3571:PHE:HB2	2.14	0.47
3:C:457:LEU:HD11	3:C:533:ILE:HG13	1.96	0.47
1:A:349:ILE:HG13	1:A:350:ARG:N	2.29	0.47
1:A:374:LYS:NZ	1:A:425:ASP:OD1	2.47	0.47
1:A:632:GLU:OE1	1:A:632:GLU:N	2.48	0.47
1:A:1031:ARG:NH1	1:A:1084:ASN:OD1	2.48	0.47
1:A:1601:LEU:HG	1:A:1655:ILE:HD12	1.96	0.47
1:A:1959:LEU:HG	1:A:1960:LYS:H	1.80	0.47
1:A:2576:MET:HG3	1:A:2787:HIS:CD2	2.49	0.47
1:A:3466:PRO:HA	1:A:3469:LEU:HB3	1.97	0.47
1:A:3571:PHE:CE2	1:A:3575:LEU:HD11	2.50	0.47
1:A:3965:ARG:HA	1:A:3968:ILE:HG12	1.97	0.47
2:B:276:LEU:O	3:C:431:ARG:N	2.44	0.47
2:B:344:GLY:O	2:B:401:THR:N	2.39	0.47
2:B:370:PRO:HB3	2:B:382:PHE:HB3	1.97	0.47
2:B:458:GLN:HB2	3:C:379:SER:OG	2.15	0.47
1:A:248:ILE:O	1:A:252:VAL:HG23	2.15	0.47
1:A:1105:VAL:O	1:A:1108:MET:HG3	2.15	0.47
1:A:2517:LEU:O	1:A:2521:ILE:HG12	2.14	0.47
1:A:3052:LEU:HD23	1:A:3057:ALA:HA	1.96	0.47
1:A:3072:GLU:OE2	1:A:3075:LYS:NZ	2.47	0.47
1:A:3868:VAL:HG13	1:A:4114:PRO:HB2	1.97	0.47
1:A:128:LEU:O	1:A:131:LEU:HG	2.15	0.46
1:A:1714:LEU:HD11	1:A:1761:LEU:HD22	1.97	0.46
1:A:2365:ASN:HD22	1:A:2399:GLU:CD	2.23	0.46
1:A:2854:PHE:CE2	1:A:2858:ILE:HD11	2.49	0.46
1:A:3981:TYR:HA	1:A:3984:MET:HE2	1.97	0.46
2:B:345:LEU:HA	2:B:400:TYR:HA	1.97	0.46
2:B:468:LYS:O	2:B:517:ARG:NH1	2.44	0.46
3:C:250:ARG:HG2	3:C:260:ARG:HA	1.97	0.46
3:C:389:MET:HE2	3:C:389:MET:HA	1.97	0.46
3:C:598:PHE:CZ	3:C:616:LEU:HB3	2.50	0.46
4:F:54:GLY:N	4:F:57:ARG:HE	2.12	0.46
6:D:24:DA:H1'	6:D:25:DA:H5'	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:ALA:HB1	1:A:642:PHE:HB3	1.96	0.46
1:A:1761:LEU:HD23	1:A:1764:GLU:OE2	2.15	0.46
1:A:2133:LEU:O	1:A:2143:ARG:NH2	2.49	0.46
1:A:2891:ARG:HG3	1:A:3894:PRO:HB3	1.97	0.46
1:A:3692:VAL:HA	1:A:3696:ARG:HH21	1.80	0.46
1:A:3842:TRP:HA	1:A:3845:LYS:HG2	1.98	0.46
1:A:3988:LEU:HD23	1:A:4100:GLU:HB2	1.97	0.46
2:B:203:MET:HE2	2:B:237:SER:HB2	1.97	0.46
2:B:206:LYS:HB3	2:B:212:ASP:OD2	2.15	0.46
3:C:261:ILE:HG22	3:C:366:ALA:HA	1.96	0.46
1:A:36:ARG:HE	1:A:40:GLN:HG2	1.80	0.46
1:A:527:TYR:HB2	1:A:629:PHE:CE1	2.51	0.46
1:A:1856:THR:OG1	1:A:1857:LYS:N	2.48	0.46
1:A:2782:ASP:O	1:A:2785:ILE:HG23	2.15	0.46
4:F:111:LYS:N	4:F:130:PHE:O	2.43	0.46
1:A:447:PRO:HB3	1:A:526:ASP:HB3	1.97	0.46
1:A:762:TYR:HD2	1:A:765:LEU:HG	1.81	0.46
1:A:786:GLN:N	1:A:787:PRO:HD2	2.30	0.46
1:A:1339:VAL:HA	1:A:1342:MET:HG3	1.96	0.46
1:A:1400:VAL:HG23	1:A:1457:GLN:NE2	2.30	0.46
1:A:2265:PRO:HB3	1:A:2309:PHE:HA	1.96	0.46
1:A:2320:ALA:HB2	1:A:2363:CYS:HA	1.98	0.46
1:A:2372:PRO:HB2	1:A:2404:ARG:NH1	2.31	0.46
1:A:2413:PHE:CB	2:B:148:TRP:HH2	2.28	0.46
1:A:2978:LYS:O	1:A:2981:TRP:NE1	2.48	0.46
1:A:3236:PHE:CD2	1:A:3262:LEU:HD11	2.49	0.46
1:A:3266:SER:OG	1:A:3273:LEU:HA	2.16	0.46
1:A:3646:LYS:HB3	1:A:3651:LEU:HD23	1.98	0.46
2:B:352:PRO:HD2	3:C:464:ALA:H	1.81	0.46
3:C:249:CYS:SG	3:C:250:ARG:N	2.88	0.46
3:C:368:ARG:HG3	3:C:369:ASP:H	1.79	0.46
1:A:989:MET:O	1:A:993:HIS:ND1	2.49	0.46
1:A:1122:GLY:O	1:A:1126:GLN:HG2	2.16	0.46
1:A:1161:ALA:O	1:A:1163:LEU:HD22	2.16	0.46
1:A:1640:GLU:HA	1:A:1643:MET:HE2	1.97	0.46
1:A:3029:LYS:HB3	1:A:3033:GLU:HG3	1.98	0.46
1:A:3256:MET:HE3	1:A:3287:ARG:NH1	2.31	0.46
1:A:3460:GLU:O	1:A:3464:LYS:HG2	2.16	0.46
1:A:3666:LEU:HD23	1:A:3669:LYS:HD3	1.98	0.46
1:A:3736:LYS:O	1:A:3751:LEU:HD12	2.15	0.46
3:C:89:ASP:O	3:C:92:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:MET:HA	3:C:130:ARG:HH12	1.80	0.46
6:D:20:DT:C5	7:E:35:DT:H72	2.51	0.46
1:A:876:SER:O	1:A:880:MET:HE3	2.16	0.46
1:A:1015:ASP:OD1	1:A:1016:GLY:N	2.49	0.46
1:A:2234:ASN:HA	1:A:2237:ILE:HG12	1.97	0.46
1:A:2386:LEU:HB2	1:A:2387:PRO:HD3	1.98	0.46
1:A:2533:SER:HA	1:A:2538:ARG:HH21	1.81	0.46
1:A:2554:PHE:O	1:A:2557:LEU:HG	2.16	0.46
1:A:2803:ILE:HA	1:A:2806:LYS:HD3	1.97	0.46
1:A:3384:HIS:O	1:A:3387:GLU:HG2	2.16	0.46
2:B:362:LEU:HD23	2:B:363:ARG:NH1	2.31	0.46
2:B:387:ILE:HG13	2:B:388:LYS:HG3	1.97	0.46
3:C:265:LYS:NZ	3:C:360:GLN:HG3	2.30	0.46
1:A:1952:ILE:HD11	1:A:1956:PHE:HD2	1.80	0.46
1:A:2364:LEU:CD1	1:A:2400:VAL:HG11	2.45	0.46
1:A:2439:ILE:HA	1:A:2442:MET:HG3	1.98	0.46
1:A:3356:ALA:HB1	1:A:3360:LEU:HB2	1.97	0.46
1:A:3413:TYR:HB2	1:A:3453:ALA:HB2	1.98	0.46
1:A:4046:TYR:CZ	1:A:4066:LEU:HD11	2.51	0.46
2:B:452:ILE:HG12	3:C:375:VAL:HG12	1.97	0.46
3:C:512:ILE:HA	3:C:515:MET:HE2	1.97	0.46
1:A:1428:ILE:H	1:A:1428:ILE:HD12	1.81	0.46
1:A:1569:THR:HA	1:A:1572:LEU:HD12	1.97	0.46
1:A:1649:LEU:HA	1:A:1652:ILE:HG22	1.98	0.46
1:A:2122:LEU:HD21	1:A:2163:HIS:CD2	2.51	0.46
1:A:2422:GLN:HB2	1:A:2425:ARG:HH21	1.81	0.46
1:A:2776:ARG:NH2	1:A:2782:ASP:OD2	2.49	0.46
1:A:3133:GLN:O	1:A:3137:GLU:HG3	2.16	0.46
1:A:3179:TRP:CE3	1:A:3242:MET:HE1	2.51	0.46
1:A:3294:SER:HA	1:A:3297:VAL:HG22	1.97	0.46
1:A:3881:ASP:O	1:A:3885:ARG:HG3	2.16	0.46
1:A:4089:ILE:H	1:A:4089:ILE:HD12	1.81	0.46
2:B:36:ASP:HA	2:B:163:HIS:O	2.16	0.46
2:B:38:LEU:HD12	2:B:167:MET:CE	2.46	0.46
1:A:656:GLN:HG3	1:A:666:PHE:CZ	2.51	0.46
1:A:931:CYS:HA	1:A:934:LEU:HG	1.98	0.46
1:A:1756:PRO:O	1:A:1760:GLU:HG2	2.16	0.46
1:A:1762:MET:HA	1:A:1765:VAL:HG22	1.98	0.46
1:A:2410:GLU:OE2	1:A:2412:TYR:N	2.49	0.46
1:A:2817:LEU:HD12	1:A:2865:HIS:CE1	2.51	0.46
1:A:3012:GLU:OE2	1:A:3051:LEU:HD11	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3493:TRP:CZ3	1:A:3525:TYR:HB2	2.50	0.46
2:B:338:LYS:NZ	2:B:405:ASN:O	2.48	0.46
2:B:447:PRO:HD3	3:C:243:HIS:CE1	2.50	0.46
3:C:53:GLU:HG2	3:C:85:LEU:HD22	1.98	0.46
3:C:356:PHE:O	3:C:357:MET:HE2	2.16	0.46
4:F:41:LEU:H	4:F:68:HIS:HB3	1.81	0.46
1:A:525:LYS:O	1:A:528:VAL:HG22	2.16	0.46
1:A:1758:LEU:HA	1:A:1761:LEU:HD12	1.97	0.46
1:A:1976:LEU:HB3	1:A:2145:PHE:CE2	2.51	0.46
1:A:2128:PHE:O	1:A:2132:LYS:N	2.28	0.46
1:A:3515:GLN:O	1:A:3518:VAL:HG12	2.16	0.46
2:B:493:LEU:HD22	3:C:323:PHE:HD2	1.81	0.46
4:F:114:TRP:HB2	4:F:130:PHE:CG	2.50	0.46
7:E:32:DT:H2''	7:E:33:DA:N7	2.31	0.46
1:A:435:LEU:HA	1:A:438:LEU:HD12	1.97	0.45
1:A:903:PRO:HB3	1:A:2815:GLY:C	2.41	0.45
1:A:922:SER:C	1:A:924:ARG:H	2.23	0.45
1:A:996:THR:HB	1:A:1036:PHE:CE1	2.51	0.45
1:A:1487:VAL:HB	1:A:1559:PHE:CE1	2.51	0.45
1:A:2300:PHE:HA	1:A:2303:LEU:HD12	1.97	0.45
1:A:2371:PHE:HD2	1:A:2374:LEU:HG	1.81	0.45
1:A:2470:ARG:HA	1:A:2473:MET:HG2	1.98	0.45
1:A:3291:GLN:OE1	1:A:3343:SER:OG	2.32	0.45
1:A:3567:VAL:O	1:A:3571:PHE:CB	2.64	0.45
3:C:62:ASP:OD1	3:C:62:ASP:N	2.45	0.45
7:E:27:DT:H2''	7:E:28:DA:H5'	1.99	0.45
1:A:196:LEU:HB3	1:A:200:PHE:CZ	2.51	0.45
1:A:497:LEU:HD23	1:A:497:LEU:H	1.80	0.45
1:A:1308:ALA:H	1:A:1319:GLY:N	2.15	0.45
1:A:1369:MET:HE2	1:A:1418:HIS:ND1	2.31	0.45
1:A:1696:LEU:HG	1:A:1749:ALA:HB1	1.97	0.45
1:A:3164:TRP:HA	1:A:3167:ARG:HG2	1.97	0.45
2:B:350:PHE:HA	2:B:396:ALA:HA	1.97	0.45
2:B:452:ILE:HG23	3:C:378:SER:HB3	1.97	0.45
6:D:21:DA:H1'	7:E:36:DA:C4	2.51	0.45
1:A:194:GLU:HG2	1:A:195:ASN:N	2.31	0.45
1:A:283:SER:C	1:A:285:CYS:H	2.25	0.45
1:A:895:ALA:HA	1:A:903:PRO:O	2.15	0.45
1:A:913:ARG:O	1:A:917:LEU:HG	2.15	0.45
1:A:1135:CYS:O	1:A:1138:ILE:N	2.49	0.45
1:A:1157:PHE:HZ	1:A:1167:ASP:O	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:CYS:HA	1:A:1368:LEU:HB3	1.98	0.45
1:A:1653:LEU:HG	1:A:1698:PHE:HD2	1.82	0.45
1:A:1664:SER:HA	1:A:1668:PHE:CD2	2.51	0.45
1:A:2526:SER:O	1:A:2538:ARG:NH2	2.48	0.45
1:A:3493:TRP:HB2	1:A:3524:ASN:ND2	2.31	0.45
2:B:41:LEU:HD12	2:B:88:TYR:HD1	1.81	0.45
2:B:480:ASN:HB2	3:C:428:GLU:OE2	2.16	0.45
1:A:71:LYS:HG2	1:A:78:PHE:CG	2.51	0.45
1:A:111:CYS:O	1:A:115:TYR:HD1	1.98	0.45
1:A:236:LYS:N	1:A:281:GLN:OE1	2.36	0.45
1:A:238:MET:SD	1:A:243:GLN:NE2	2.89	0.45
1:A:1493:PRO:HB3	1:A:1500:LEU:HD22	1.99	0.45
1:A:1579:VAL:O	1:A:1583:MET:HG3	2.16	0.45
1:A:2218:PHE:HA	1:A:2221:LYS:NZ	2.32	0.45
1:A:3961:PHE:CE2	1:A:3963:LEU:HB2	2.52	0.45
2:B:515:ASN:OD1	2:B:516:LYS:N	2.49	0.45
3:C:147:LEU:HA	3:C:150:ILE:HG12	1.98	0.45
4:F:47:HIS:HB2	4:F:73:CYS:O	2.16	0.45
1:A:61:ARG:HH22	1:A:102:PRO:HB2	1.81	0.45
1:A:152:LEU:HB3	1:A:156:PHE:HE2	1.81	0.45
1:A:654:ILE:HD11	1:A:707:PHE:HE1	1.82	0.45
1:A:801:LYS:HE3	1:A:3119:VAL:HG12	1.98	0.45
1:A:878:GLU:HA	1:A:881:LYS:HE2	1.97	0.45
1:A:1538:LEU:HD11	1:A:1555:HIS:CG	2.52	0.45
1:A:1803:GLU:O	1:A:1806:ARG:NH1	2.49	0.45
1:A:2273:GLY:O	1:A:2276:LEU:HG	2.17	0.45
1:A:2330:VAL:O	1:A:2332:GLU:N	2.46	0.45
1:A:2382:VAL:HB	1:A:2397:CYS:SG	2.56	0.45
1:A:2888:VAL:HB	1:A:3894:PRO:HG2	1.98	0.45
1:A:3178:ILE:H	1:A:3178:ILE:HD12	1.81	0.45
1:A:3411:ASP:HA	1:A:3414:MET:HG2	1.99	0.45
1:A:3549:HIS:HA	1:A:3552:LYS:HD3	1.98	0.45
1:A:3749:PRO:O	1:A:3805:TRP:N	2.50	0.45
1:A:3813:LYS:N	1:A:3925:LEU:HB3	2.32	0.45
2:B:444:ARG:HD3	3:C:265:LYS:O	2.16	0.45
2:B:458:GLN:HE22	2:B:527:GLU:HB2	1.81	0.45
3:C:138:LEU:HD22	3:C:204:GLY:HA3	1.98	0.45
3:C:225:TYR:CD2	3:C:236:VAL:HG12	2.52	0.45
3:C:336:GLU:O	3:C:399:LYS:HD3	2.17	0.45
1:A:78:PHE:O	1:A:81:CYS:HB2	2.17	0.45
1:A:124:LYS:HA	1:A:169:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:VAL:HA	1:A:579:LEU:HG	1.98	0.45
1:A:863:GLY:H	1:A:866:ILE:HD12	1.80	0.45
1:A:886:TRP:HE1	1:A:912:PRO:HG3	1.81	0.45
1:A:1135:CYS:SG	1:A:1136:ARG:N	2.90	0.45
1:A:1202:ARG:HB2	1:A:1207:TRP:HB2	1.99	0.45
1:A:2257:PHE:HA	1:A:2260:PHE:HE1	1.80	0.45
1:A:3107:ILE:HD11	1:A:3139:GLN:NE2	2.31	0.45
1:A:3864:ARG:O	1:A:3868:VAL:HG23	2.17	0.45
6:D:33:DA:H2''	6:D:34:DC:C5	2.52	0.45
1:A:903:PRO:HB2	1:A:905:ILE:HD11	1.97	0.45
1:A:1313:PHE:CZ	1:A:1321:ARG:HD2	2.52	0.45
1:A:1672:PHE:O	1:A:1676:ILE:HG12	2.17	0.45
1:A:2364:LEU:O	1:A:2368:THR:HG22	2.17	0.45
1:A:2422:GLN:HA	1:A:2425:ARG:NE	2.32	0.45
1:A:3240:MET:HE3	1:A:3262:LEU:CD2	2.44	0.45
1:A:4080:VAL:HG13	1:A:4116:ILE:HG13	1.98	0.45
3:C:28:GLU:OE1	3:C:36:LYS:NZ	2.49	0.45
1:A:289:ASN:OD1	1:A:292:SER:HB3	2.17	0.45
1:A:776:TRP:O	1:A:780:ILE:N	2.45	0.45
1:A:890:LYS:HB3	1:A:906:PHE:CG	2.51	0.45
1:A:1416:GLU:HG3	1:A:1420:ARG:HH22	1.81	0.45
1:A:1583:MET:CE	1:A:1628:LYS:HB2	2.44	0.45
1:A:2122:LEU:HD13	1:A:2127:LYS:HD3	1.98	0.45
1:A:2265:PRO:HA	1:A:2309:PHE:CG	2.52	0.45
1:A:2880:CYS:SG	1:A:2889:GLY:HA3	2.57	0.45
1:A:2884:LEU:HD13	1:A:3117:ILE:HA	1.97	0.45
1:A:3113:ASN:HB3	1:A:3128:LYS:NZ	2.32	0.45
1:A:3372:LYS:HA	1:A:3375:ALA:HB3	1.98	0.45
2:B:390:LEU:HD23	2:B:390:LEU:H	1.82	0.45
3:C:43:GLN:HA	3:C:46:VAL:HG22	1.98	0.45
1:A:493:LYS:O	1:A:625:ASN:ND2	2.50	0.45
1:A:913:ARG:HD2	1:A:916:GLU:OE2	2.17	0.45
3:C:88:PHE:HA	3:C:91:LEU:HG	1.99	0.45
3:C:600:VAL:HA	3:C:603:LYS:HG2	1.99	0.45
1:A:92:PHE:O	1:A:133:LYS:NZ	2.50	0.45
1:A:885:ALA:HB3	1:A:888:ARG:HA	1.99	0.45
1:A:2193:ILE:HA	1:A:2196:TRP:NE1	2.32	0.45
1:A:3419:PHE:O	1:A:3422:GLN:HG2	2.18	0.45
1:A:3622:ALA:O	1:A:3625:LEU:HD22	2.17	0.45
1:A:3638:LYS:O	1:A:3642:LYS:N	2.44	0.45
1:A:3976:GLU:CD	1:A:3977:THR:HG23	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4104:VAL:HA	1:A:4107:LEU:HD12	1.98	0.45
2:B:282:LYS:HD2	2:B:283:PRO:HD2	1.99	0.45
2:B:526:LYS:C	2:B:528:LEU:H	2.25	0.45
3:C:306:LEU:HG	3:C:308:GLU:H	1.81	0.45
1:A:289:ASN:HD21	1:A:292:SER:HB3	1.81	0.44
1:A:450:SER:OG	1:A:453:MET:HG3	2.17	0.44
1:A:969:LEU:HB3	1:A:984:TYR:OH	2.17	0.44
1:A:1070:PRO:HD2	1:A:3741:ARG:HD2	1.99	0.44
1:A:3335:ARG:HH22	1:A:3418:ASP:HB3	1.82	0.44
2:B:44:ALA:HB3	2:B:89:GLY:O	2.17	0.44
2:B:193:LEU:HB2	2:B:198:ILE:CG2	2.48	0.44
1:A:851:ILE:O	1:A:855:VAL:HG23	2.17	0.44
1:A:1021:VAL:O	1:A:1026:ARG:NH1	2.50	0.44
1:A:1216:GLY:HA2	1:A:1219:PHE:HB3	1.97	0.44
1:A:1492:ALA:HB2	1:A:1555:HIS:HE1	1.81	0.44
1:A:1714:LEU:HA	1:A:1717:LEU:HD12	1.99	0.44
1:A:1776:GLU:HA	1:A:1779:GLN:HG2	1.99	0.44
1:A:2214:ARG:HH22	1:A:2221:LYS:HZ3	1.65	0.44
1:A:3479:THR:C	1:A:3480:LEU:HD22	2.41	0.44
1:A:3530:VAL:HA	1:A:3533:PHE:HB3	2.00	0.44
1:A:3819:THR:HG21	1:A:3886:ALA:HB2	2.00	0.44
2:B:54:GLU:HB3	2:B:56:GLU:HG2	1.99	0.44
3:C:413:LYS:HG3	3:C:415:ASN:N	2.32	0.44
1:A:264:ARG:HD3	1:A:305:ASN:HB2	2.00	0.44
1:A:493:LYS:HA	1:A:493:LYS:HD3	1.78	0.44
1:A:535:LEU:HD13	1:A:637:LYS:HB2	1.99	0.44
1:A:1248:PHE:HB3	1:A:1319:GLY:HA2	1.98	0.44
1:A:1496:GLU:HG3	1:A:1498:GLN:HB2	1.99	0.44
1:A:2493:ASN:OD1	1:A:2494:ASP:N	2.51	0.44
1:A:3526:PRO:C	1:A:3528:ALA:H	2.24	0.44
2:B:464:ALA:O	2:B:468:LYS:HG3	2.17	0.44
4:F:114:TRP:HE1	4:F:125:VAL:C	2.26	0.44
1:A:850:GLU:HA	1:A:853:ILE:HG12	1.99	0.44
1:A:2430:GLU:N	1:A:2430:GLU:OE1	2.48	0.44
1:A:3296:GLN:O	1:A:3300:VAL:HG23	2.18	0.44
1:A:3350:GLU:OE1	1:A:3350:GLU:N	2.43	0.44
1:A:3730:ALA:HA	1:A:3734:ARG:HA	1.98	0.44
2:B:364:PRO:HG3	3:C:357:MET:HA	1.99	0.44
4:F:53:ILE:N	4:F:86:ASP:OD1	2.51	0.44
1:A:432:THR:O	1:A:435:LEU:HG	2.17	0.44
1:A:1661:PHE:HA	1:A:1665:HIS:HE1	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1777:LEU:O	1:A:1780:SER:OG	2.29	0.44
1:A:1786:ALA:HB1	1:A:1831:CYS:HA	1.99	0.44
1:A:1811:ARG:HG3	1:A:1816:ARG:HH21	1.82	0.44
1:A:2220:MET:SD	1:A:2252:PRO:HG3	2.58	0.44
1:A:2559:THR:HG22	1:A:2808:LEU:HD11	2.00	0.44
1:A:2563:LEU:HD13	1:A:2795:GLN:CB	2.47	0.44
1:A:3839:TYR:OH	1:A:4120:THR:O	2.30	0.44
3:C:44:ARG:NH2	3:C:234:LEU:HD13	2.32	0.44
3:C:86:PRO:HA	3:C:90:LEU:HD21	1.99	0.44
3:C:363:LYS:NZ	3:C:418:CYS:SG	2.75	0.44
3:C:665:LYS:HD2	3:C:665:LYS:HA	1.85	0.44
4:F:45:ARG:H	4:F:81:THR:HB	1.83	0.44
6:D:27:DC:H1'	6:D:28:DT:C2	2.53	0.44
6:D:30:DA:C4	6:D:31:DA:C6	3.06	0.44
6:D:39:DA:C2	7:E:19:DA:C5	3.05	0.44
1:A:1017:ILE:HA	1:A:1026:ARG:HG2	1.98	0.44
1:A:1097:GLU:O	1:A:1151:ARG:HD3	2.17	0.44
1:A:1185:HIS:HA	1:A:1188:ILE:HG12	1.99	0.44
1:A:1267:TYR:HA	1:A:1270:PHE:HB2	1.99	0.44
1:A:1306:ILE:O	1:A:1320:ASN:HB2	2.17	0.44
1:A:1375:THR:HA	1:A:1379:PRO:HA	1.99	0.44
1:A:1945:TYR:HE2	1:A:2097:LEU:HD11	1.82	0.44
1:A:3478:GLU:HG2	1:A:3483:MET:HE3	2.00	0.44
1:A:3660:ASN:O	1:A:3664:ASN:N	2.45	0.44
1:A:3856:MET:HG2	1:A:4077:TYR:OH	2.17	0.44
2:B:376:ILE:HG12	3:C:540:ILE:HG12	2.00	0.44
1:A:63:PHE:O	1:A:67:VAL:HG23	2.18	0.44
1:A:208:MET:SD	1:A:253:LEU:HG	2.58	0.44
1:A:210:SER:HB2	3:C:548:VAL:HG23	2.00	0.44
1:A:865:GLN:HA	1:A:868:LYS:HG2	2.00	0.44
1:A:1413:ASP:O	1:A:1417:THR:HG23	2.18	0.44
1:A:1424:THR:HG1	1:A:1427:SER:H	1.65	0.44
1:A:2326:ILE:C	1:A:2328:ARG:H	2.25	0.44
1:A:2899:ARG:HD2	1:A:2900:LEU:N	2.33	0.44
1:A:3079:GLU:HG2	1:A:3080:LEU:N	2.33	0.44
1:A:3320:ILE:HG21	1:A:3394:GLU:OE1	2.18	0.44
2:B:50:GLU:HG3	2:B:52:GLN:H	1.81	0.44
2:B:131:PHE:HA	2:B:134:MET:HG3	1.99	0.44
1:A:101:ALA:HB3	1:A:102:PRO:CD	2.48	0.44
1:A:364:ARG:HA	1:A:415:GLN:HE22	1.83	0.44
1:A:535:LEU:HD23	1:A:535:LEU:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:ARG:HH22	1:A:1389:VAL:HA	1.83	0.44
1:A:1326:GLU:O	1:A:1330:TYR:N	2.49	0.44
1:A:2490:GLU:O	1:A:2495:SER:OG	2.31	0.44
1:A:3059:GLN:HE22	1:A:3062:LEU:HD23	1.82	0.44
1:A:3555:VAL:HA	1:A:3558:ILE:HG22	1.99	0.44
1:A:3726:VAL:HG23	1:A:3738:ILE:HG13	2.00	0.44
1:A:3809:THR:HG21	1:A:3938:ILE:HD13	2.00	0.44
2:B:174:ASN:CB	2:B:216:PHE:HB3	2.48	0.44
2:B:190:ALA:HA	2:B:193:LEU:HG	1.99	0.44
2:B:317:LYS:HD3	2:B:330:GLU:OE1	2.18	0.44
2:B:335:GLU:OE2	2:B:405:ASN:ND2	2.50	0.44
2:B:422:ASP:C	2:B:424:LYS:N	2.75	0.44
2:B:478:PHE:C	3:C:427:MET:HE1	2.43	0.44
3:C:67:PRO:HD3	3:C:79:VAL:HG11	2.00	0.44
7:E:19:DA:H2'	7:E:20:DT:O4'	2.17	0.44
1:A:484:HIS:CE1	1:A:574:LYS:HG3	2.53	0.44
1:A:793:LEU:HD21	1:A:867:ASN:HA	1.99	0.44
1:A:989:MET:HG3	1:A:993:HIS:HE1	1.80	0.44
1:A:1712:ARG:HE	1:A:1712:ARG:HB2	1.56	0.44
1:A:1713:VAL:O	1:A:1716:GLN:HG3	2.18	0.44
1:A:1718:ILE:HA	1:A:1722:PHE:CD1	2.53	0.44
1:A:2872:ASP:OD1	1:A:2872:ASP:N	2.51	0.44
1:A:3631:LYS:O	1:A:3635:THR:HG22	2.17	0.44
2:B:353:LEU:H	2:B:394:VAL:HA	1.82	0.44
1:A:411:PRO:HB3	1:A:456:VAL:HG12	2.00	0.43
1:A:1073:PHE:O	1:A:1076:LEU:HG	2.17	0.43
1:A:2095:ALA:HB3	1:A:2096:PRO:HD3	2.00	0.43
1:A:3413:TYR:CD1	1:A:3449:LYS:HB2	2.53	0.43
1:A:3735:PRO:HB3	1:A:3751:LEU:HD11	1.98	0.43
1:A:3847:SER:HA	1:A:3858:MET:HE1	2.00	0.43
1:A:3986:HIS:O	1:A:3989:ARG:NH1	2.51	0.43
2:B:97:VAL:HG11	2:B:149:VAL:HG12	2.00	0.43
2:B:358:LYS:HA	3:C:353:ARG:HH22	1.82	0.43
2:B:480:ASN:HB3	2:B:483:LEU:HB2	1.99	0.43
3:C:115:MET:SD	3:C:130:ARG:NH2	2.91	0.43
3:C:130:ARG:HG2	3:C:159:ILE:HG23	2.00	0.43
3:C:599:ARG:HH11	3:C:641:ALA:HB3	1.83	0.43
4:F:119:LEU:O	4:F:122:ARG:HD2	2.18	0.43
1:A:478:CYS:O	1:A:482:VAL:HG13	2.19	0.43
1:A:1941:HIS:HB2	1:A:1974:ASN:O	2.19	0.43
1:A:2099:ALA:HA	1:A:2102:LYS:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2574:ASN:O	1:A:2787:HIS:ND1	2.52	0.43
1:A:2938:VAL:O	1:A:2942:ILE:HG12	2.18	0.43
1:A:3321:LEU:O	1:A:3324:ARG:HG2	2.18	0.43
1:A:3765:GLU:OE2	1:A:3791:TYR:N	2.34	0.43
1:A:3815:LEU:HA	1:A:3818:ASN:HD21	1.83	0.43
2:B:34:GLY:HA3	2:B:162:SER:HB3	2.01	0.43
2:B:85:VAL:HB	2:B:106:GLN:HB2	1.99	0.43
2:B:246:VAL:O	2:B:249:LYS:NZ	2.49	0.43
2:B:484:GLN:HA	2:B:487:PHE:HD2	1.82	0.43
3:C:250:ARG:HE	3:C:260:ARG:HG2	1.83	0.43
1:A:159:GLU:O	1:A:165:LYS:HG3	2.18	0.43
1:A:172:GLU:O	1:A:175:TYR:HB2	2.18	0.43
1:A:583:LEU:HD22	1:A:612:LEU:HB3	2.00	0.43
1:A:889:GLU:HG3	1:A:891:ARG:HG2	1.99	0.43
1:A:943:GLY:HA3	1:A:2577:PHE:CE2	2.54	0.43
1:A:1344:PHE:CE2	1:A:1348:LEU:HD11	2.53	0.43
1:A:1363:LEU:HB3	1:A:1367:HIS:CE1	2.47	0.43
1:A:1400:VAL:O	1:A:1404:LYS:HG2	2.19	0.43
1:A:1740:VAL:HA	1:A:1743:MET:HE3	2.01	0.43
1:A:1780:SER:HA	1:A:1783:ARG:HG2	2.00	0.43
1:A:1857:LYS:O	1:A:1858:LEU:HD22	2.19	0.43
1:A:2098:THR:HG22	1:A:2153:THR:HG23	2.01	0.43
1:A:2418:LYS:NZ	2:B:152:ASN:HA	2.33	0.43
1:A:2809:PHE:HA	1:A:2812:LEU:HG	2.01	0.43
1:A:2972:TYR:HB2	1:A:2998:SER:HB2	2.00	0.43
1:A:2986:PRO:HG3	1:A:2994:TRP:CH2	2.53	0.43
1:A:3113:ASN:HB3	1:A:3128:LYS:HZ1	1.83	0.43
1:A:3681:LYS:HE3	1:A:3723:ASP:O	2.17	0.43
1:A:3806:LEU:HG	1:A:3938:ILE:HG21	1.99	0.43
1:A:3833:ARG:CZ	1:A:3877:LYS:HZ1	2.30	0.43
1:A:4058:VAL:HG21	1:A:4095:GLU:HB3	2.00	0.43
3:C:135:PHE:HD1	3:C:227:PHE:HE1	1.67	0.43
1:A:133:LYS:O	1:A:137:THR:HG23	2.18	0.43
1:A:415:GLN:NE2	1:A:416:SER:OG	2.51	0.43
1:A:531:PHE:HA	1:A:534:LEU:HB2	2.00	0.43
1:A:643:GLU:HA	1:A:646:VAL:HG13	1.98	0.43
1:A:898:PHE:H	1:A:902:LYS:HE3	1.83	0.43
1:A:1186:LYS:O	1:A:1190:LEU:HB2	2.19	0.43
1:A:2424:MET:SD	1:A:2457:PRO:HB2	2.58	0.43
1:A:2519:LEU:HD12	1:A:2522:ARG:HE	1.84	0.43
1:A:2933:ILE:HG23	1:A:3121:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3410:ILE:HG22	1:A:3453:ALA:HA	1.99	0.43
1:A:3531:TYR:HB2	1:A:3532:PRO:HD3	1.99	0.43
1:A:3737:ARG:HD2	1:A:3805:TRP:CG	2.53	0.43
2:B:318:ARG:HH21	2:B:331:LYS:HD2	1.84	0.43
2:B:442:ASP:HB3	3:C:267:ILE:HG23	2.00	0.43
2:B:496:ASP:OD1	2:B:497:LEU:HD22	2.18	0.43
1:A:624:ILE:O	1:A:627:VAL:HG22	2.18	0.43
1:A:860:GLY:HA2	1:A:3132:VAL:HG13	2.00	0.43
1:A:885:ALA:HB3	1:A:888:ARG:HE	1.82	0.43
1:A:930:ALA:O	1:A:933:LEU:HG	2.18	0.43
1:A:1050:GLU:OE2	1:A:1057:LYS:NZ	2.49	0.43
1:A:1696:LEU:O	1:A:1700:THR:HG23	2.18	0.43
1:A:1813:SER:HB3	1:A:1936:ARG:HH21	1.82	0.43
1:A:3727:THR:O	1:A:3736:LYS:HA	2.19	0.43
1:A:4020:MET:HE2	1:A:4027:TRP:HD1	1.84	0.43
2:B:41:LEU:HD12	2:B:88:TYR:CD1	2.53	0.43
2:B:451:LYS:HE3	2:B:451:LYS:HB2	1.81	0.43
2:B:479:GLU:HA	3:C:427:MET:SD	2.58	0.43
3:C:74:TYR:CD1	3:C:109:ASP:HB3	2.54	0.43
3:C:394:ARG:HA	3:C:405:VAL:HG12	1.99	0.43
3:C:512:ILE:O	3:C:516:LEU:HG	2.18	0.43
3:C:594:PRO:HB2	3:C:619:HIS:CE1	2.53	0.43
4:F:73:CYS:SG	4:F:80:VAL:HG22	2.59	0.43
6:D:20:DT:H6	6:D:20:DT:H2'	1.71	0.43
6:D:35:DT:C2	7:E:22:DG:N2	2.86	0.43
1:A:374:LYS:HD3	1:A:381:VAL:HG21	2.01	0.43
1:A:870:LEU:HD21	1:A:3129:LEU:HD11	2.00	0.43
1:A:1423:ILE:HD11	1:A:1428:ILE:HD11	2.00	0.43
1:A:1657:SER:O	1:A:1660:SER:OG	2.34	0.43
1:A:2126:MET:CE	1:A:2130:HIS:HE1	2.30	0.43
1:A:2239:LYS:NZ	1:A:2282:ALA:HB3	2.32	0.43
1:A:2305:ASN:O	1:A:2308:SER:OG	2.23	0.43
1:A:2382:VAL:O	1:A:2386:LEU:HG	2.18	0.43
1:A:2447:LYS:O	1:A:2451:LEU:HG	2.19	0.43
1:A:2515:PRO:HA	1:A:2518:GLN:HE21	1.84	0.43
1:A:3046:ARG:O	1:A:3050:LYS:HG2	2.19	0.43
1:A:3320:ILE:HG22	1:A:3324:ARG:HH21	1.83	0.43
1:A:3568:ILE:H	1:A:3568:ILE:HD12	1.84	0.43
1:A:3762:GLN:NE2	1:A:3763:ARG:HD2	2.34	0.43
1:A:4090:ARG:NH1	1:A:4110:GLN:HA	2.34	0.43
3:C:677:ILE:O	3:C:680:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:967:PRO:HA	1:A:970:LEU:HG	2.00	0.43
1:A:1322:THR:HG22	1:A:1324:PRO:HD2	2.01	0.43
1:A:1618:LEU:O	1:A:1622:ILE:HG12	2.19	0.43
1:A:2143:ARG:HH21	1:A:2171:LEU:HB3	1.83	0.43
1:A:2349:LEU:HB3	1:A:2360:PHE:CE1	2.53	0.43
1:A:2563:LEU:HD11	1:A:2792:THR:HA	2.00	0.43
1:A:3179:TRP:O	1:A:3183:ILE:HG12	2.18	0.43
2:B:240:GLU:HA	2:B:243:LEU:HD12	2.01	0.43
2:B:264:ASN:HD21	2:B:266:ASP:HB2	1.84	0.43
2:B:376:ILE:HG23	3:C:540:ILE:HG12	2.01	0.43
3:C:7:LYS:HB2	3:C:125:LYS:HG3	1.99	0.43
3:C:261:ILE:HA	3:C:366:ALA:HA	2.00	0.43
1:A:922:SER:OG	1:A:923:ASP:N	2.49	0.43
1:A:2403:CYS:SG	1:A:2404:ARG:N	2.92	0.43
1:A:3500:SER:HB3	1:A:3532:PRO:HB3	1.99	0.43
1:A:3663:THR:O	1:A:3667:LEU:N	2.41	0.43
1:A:3759:ARG:O	1:A:3763:ARG:HD3	2.18	0.43
1:A:3828:TYR:O	1:A:3834:ALA:HB1	2.18	0.43
1:A:3913:ILE:O	1:A:3917:ILE:HG12	2.19	0.43
2:B:182:LYS:HA	2:B:185:ARG:HG2	2.01	0.43
1:A:52:ALA:O	1:A:55:THR:OG1	2.35	0.43
1:A:293:LEU:HD12	1:A:294:PHE:N	2.34	0.43
1:A:452:LYS:HG3	1:A:453:MET:H	1.83	0.43
1:A:479:ILE:HG21	1:A:567:GLU:OE1	2.17	0.43
1:A:624:ILE:O	1:A:625:ASN:C	2.61	0.43
1:A:1471:GLN:HA	1:A:1477:HIS:NE2	2.34	0.43
1:A:1986:ARG:HB2	1:A:2183:HIS:C	2.43	0.43
1:A:2824:LYS:HB3	1:A:2824:LYS:HE2	1.76	0.43
1:A:3974:MET:HG2	1:A:3978:GLY:HA3	2.01	0.43
1:A:3980:MET:SD	1:A:3980:MET:N	2.90	0.43
2:B:187:ARG:HH11	2:B:187:ARG:HG3	1.84	0.43
3:C:209:LYS:HA	3:C:212:MET:HE2	2.00	0.43
3:C:596:GLU:HB3	3:C:599:ARG:HH21	1.84	0.43
1:A:351:ASN:OD1	1:A:352:VAL:N	2.51	0.43
1:A:1299:GLU:HG3	1:A:1304:HIS:CD2	2.54	0.43
1:A:1558:TYR:O	1:A:1562:LEU:HG	2.19	0.43
1:A:1592:MET:SD	1:A:1592:MET:N	2.92	0.43
1:A:1632:TRP:CD1	1:A:1645:VAL:HB	2.53	0.43
1:A:2950:LYS:HE3	1:A:2986:PRO:HB3	2.01	0.43
1:A:3266:SER:OG	1:A:3273:LEU:HD12	2.19	0.43
1:A:3737:ARG:NH1	1:A:3751:LEU:HD13	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:TYR:CE1	3:C:435:PHE:HB3	2.54	0.43
2:B:476:ASP:HA	3:C:427:MET:HE3	2.01	0.43
1:A:151:GLU:HG3	1:A:152:LEU:HD22	2.00	0.42
1:A:326:MET:HA	1:A:329:LYS:HE2	1.99	0.42
1:A:339:GLN:HA	1:A:342:MET:HE3	2.00	0.42
1:A:1248:PHE:CE1	1:A:1321:ARG:HD3	2.54	0.42
1:A:1298:LEU:HA	1:A:1367:HIS:CG	2.54	0.42
1:A:1339:VAL:O	1:A:1342:MET:HG3	2.19	0.42
1:A:1372:LEU:HA	1:A:1375:THR:HG22	2.00	0.42
1:A:1438:GLY:O	1:A:1445:ARG:NH2	2.51	0.42
1:A:1444:ASP:N	1:A:1444:ASP:OD1	2.51	0.42
1:A:1491:ILE:HD12	1:A:1558:TYR:HD2	1.84	0.42
1:A:1629:CYS:HB3	1:A:1633:TRP:HE1	1.84	0.42
1:A:2950:LYS:NZ	1:A:2983:ASP:O	2.47	0.42
1:A:3810:VAL:HG12	1:A:3932:MET:HE3	2.00	0.42
3:C:265:LYS:HD2	3:C:362:LEU:HD13	2.01	0.42
6:D:40:DT:C4	7:E:17:DT:O4	2.72	0.42
6:D:43:DT:C4	7:E:16:DA:C6	3.07	0.42
1:A:275:PHE:HD2	1:A:315:ALA:HB1	1.83	0.42
1:A:465:PHE:CE2	1:A:564:LEU:HD21	2.52	0.42
1:A:1098:GLN:O	1:A:1152:ARG:HB2	2.19	0.42
1:A:1157:PHE:HE2	1:A:1168:LEU:HD13	1.84	0.42
1:A:1571:LEU:HD23	1:A:1600:MET:HE3	2.00	0.42
1:A:1614:GLN:O	1:A:1618:LEU:HG	2.19	0.42
1:A:2295:GLN:OE1	1:A:2298:GLU:N	2.50	0.42
1:A:2440:TYR:O	1:A:2443:MET:HG3	2.19	0.42
1:A:2931:ARG:HG2	1:A:2936:TYR:CE1	2.54	0.42
1:A:3189:PHE:O	1:A:3193:ILE:HG12	2.19	0.42
1:A:4064:LEU:HD23	1:A:4068:HIS:CE1	2.54	0.42
3:C:205:LEU:O	3:C:209:LYS:HB2	2.19	0.42
4:F:50:ARG:HH21	4:F:55:ARG:HA	1.85	0.42
6:D:34:DC:C6	6:D:35:DT:C4	3.07	0.42
1:A:465:PHE:HA	1:A:468:LEU:HG	2.02	0.42
1:A:1175:HIS:HB3	1:A:1178:ARG:NH1	2.34	0.42
1:A:2093:CYS:C	1:A:2096:PRO:HD2	2.45	0.42
1:A:2563:LEU:HD13	1:A:2795:GLN:HB3	2.02	0.42
1:A:2804:ILE:HG22	1:A:2808:LEU:HD23	2.01	0.42
1:A:3175:PRO:HA	1:A:3249:GLN:HE22	1.84	0.42
1:A:3862:ALA:O	1:A:4119:ARG:NH2	2.38	0.42
2:B:48:MET:N	2:B:48:MET:SD	2.91	0.42
2:B:420:LEU:HA	2:B:426:GLN:HA	0.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:292:GLU:HG3	4:F:54:GLY:HA3	2.01	0.42
1:A:896:VAL:HG12	1:A:903:PRO:HG2	2.02	0.42
1:A:933:LEU:HD12	1:A:934:LEU:N	2.34	0.42
1:A:1149:LYS:N	1:A:1163:LEU:O	2.52	0.42
1:A:1565:GLU:OE1	1:A:1565:GLU:N	2.40	0.42
1:A:3067:LYS:HB2	1:A:3067:LYS:HE2	1.80	0.42
1:A:3442:TYR:N	1:A:3443:PRO:HD2	2.34	0.42
1:A:3581:PRO:HD3	1:A:3629:ARG:HH11	1.85	0.42
1:A:3696:ARG:NH1	1:A:3698:GLU:HA	2.34	0.42
1:A:3924:HIS:H	1:A:3927:ASN:HD22	1.67	0.42
2:B:361:TYR:C	2:B:362:LEU:HD12	2.44	0.42
3:C:33:GLN:NE2	3:C:231:LEU:HD22	2.34	0.42
1:A:656:GLN:HG3	1:A:666:PHE:HZ	1.84	0.42
1:A:901:MET:HA	1:A:2819:GLU:HG2	2.01	0.42
1:A:1264:LEU:HD11	1:A:1341:ILE:HB	2.02	0.42
1:A:1632:TRP:HB3	1:A:1645:VAL:HG11	2.01	0.42
1:A:2200:ALA:O	1:A:2245:TRP:NE1	2.48	0.42
1:A:2852:PRO:HB2	1:A:2853:PRO:HD3	2.01	0.42
1:A:3063:THR:HA	1:A:3066:ASP:OD2	2.19	0.42
1:A:3066:ASP:HA	1:A:3069:MET:HE1	2.01	0.42
1:A:3171:ALA:HA	1:A:3179:TRP:HE1	1.84	0.42
1:A:3755:GLY:HA2	1:A:3800:LEU:HA	2.00	0.42
1:A:3950:THR:HG22	1:A:3957:GLU:O	2.19	0.42
3:C:593:ASN:HB2	3:C:594:PRO:HD3	2.01	0.42
1:A:172:GLU:HG3	1:A:220:LEU:CA	2.50	0.42
1:A:1066:LEU:O	1:A:1074:LYS:HB3	2.19	0.42
1:A:1897:ASN:O	1:A:1902:GLY:N	2.41	0.42
1:A:1952:ILE:HD12	1:A:1956:PHE:HB3	2.01	0.42
1:A:2092:GLU:OE1	1:A:2092:GLU:N	2.53	0.42
1:A:3816:LEU:O	1:A:3820:MET:HG3	2.19	0.42
1:A:3953:LEU:HD22	1:A:4026:SER:HB3	2.01	0.42
1:A:4014:LYS:NZ	1:A:4032:ASN:O	2.52	0.42
2:B:124:GLY:O	2:B:128:GLN:HB2	2.20	0.42
6:D:43:DT:H3	7:E:15:DA:C4'	2.32	0.42
1:A:289:ASN:ND2	1:A:292:SER:HB3	2.34	0.42
1:A:1794:GLN:O	1:A:1798:LEU:HG	2.20	0.42
1:A:2316:TYR:CZ	1:A:2359:LYS:HG2	2.55	0.42
1:A:2320:ALA:CB	1:A:2363:CYS:HA	2.49	0.42
1:A:3006:ALA:HB3	1:A:3257:LYS:HD2	2.02	0.42
1:A:3959:MET:HE2	1:A:4124:TRP:CE3	2.54	0.42
1:A:3964:THR:HG22	1:A:4128:MET:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:ASN:OD1	2:B:95:ASN:N	2.53	0.42
2:B:301:ARG:HH22	2:B:313:PRO:HD3	1.85	0.42
2:B:401:THR:HG23	2:B:406:ILE:HB	2.02	0.42
3:C:434:MET:SD	3:C:435:PHE:N	2.93	0.42
3:C:635:SER:O	3:C:639:ILE:HG12	2.19	0.42
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.89	0.42
1:A:269:SER:HB2	1:A:308:LEU:HD23	2.02	0.42
1:A:357:LYS:O	1:A:361:ILE:HG12	2.18	0.42
1:A:905:ILE:HG23	1:A:2811:SER:HB2	2.01	0.42
1:A:1154:PRO:HG2	1:A:1157:PHE:HD2	1.84	0.42
1:A:1164:CYS:SG	1:A:1165:LEU:N	2.92	0.42
1:A:1715:GLU:O	1:A:1719:VAL:HG13	2.20	0.42
1:A:2304:VAL:HA	1:A:2307:MET:HG3	2.02	0.42
1:A:2481:HIS:O	1:A:2485:ARG:HB3	2.20	0.42
1:A:2918:PRO:HA	1:A:2921:LEU:HB3	2.01	0.42
1:A:3154:GLN:HA	1:A:3157:LEU:HD12	2.02	0.42
1:A:3669:LYS:HE2	1:A:3669:LYS:HB3	1.77	0.42
1:A:3875:GLU:CB	1:A:3965:ARG:HD2	2.49	0.42
1:A:4042:GLN:OE1	1:A:4042:GLN:N	2.53	0.42
3:C:57:VAL:HA	3:C:79:VAL:HA	2.02	0.42
3:C:346:CYS:SG	3:C:390:VAL:HG23	2.59	0.42
3:C:510:GLN:HA	3:C:513:TRP:HD1	1.84	0.42
3:C:644:GLU:O	3:C:648:LYS:HG3	2.19	0.42
6:D:37:DT:H2'	6:D:38:DT:N1	2.33	0.42
1:A:89:LEU:HB3	1:A:133:LYS:HE2	2.02	0.42
1:A:386:VAL:HG12	1:A:431:TYR:HE2	1.83	0.42
1:A:414:LEU:HA	1:A:417:VAL:HG12	2.00	0.42
1:A:764:PRO:O	1:A:768:VAL:HG12	2.20	0.42
1:A:1326:GLU:HA	1:A:1329:ARG:HB2	2.02	0.42
1:A:1565:GLU:HG2	1:A:1566:THR:H	1.85	0.42
1:A:2394:LYS:O	1:A:2398:LEU:HG	2.20	0.42
1:A:3820:MET:HE1	1:A:3824:GLU:C	2.45	0.42
1:A:3843:LEU:HD13	1:A:3855:TYR:CE1	2.55	0.42
2:B:95:ASN:ND2	2:B:102:ILE:HB	2.34	0.42
3:C:66:ASN:OD1	3:C:66:ASN:N	2.53	0.42
4:F:93:ARG:HE	4:F:97:LEU:HG	1.85	0.42
1:A:565:TYR:O	1:A:569:VAL:HG23	2.20	0.42
1:A:1769:GLU:HB3	1:A:1772:HIS:CG	2.55	0.42
1:A:2126:MET:O	1:A:2130:HIS:ND1	2.49	0.42
1:A:2240:THR:O	1:A:2243:GLU:HG3	2.20	0.42
1:A:2891:ARG:O	1:A:2892:LEU:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3169:PRO:HD2	1:A:3179:TRP:CZ3	2.55	0.42
1:A:3409:VAL:HG22	1:A:3413:TYR:CE2	2.54	0.42
1:A:3574:ALA:HB1	1:A:3686:TRP:HB3	2.01	0.42
1:A:3971:MET:HE2	1:A:3980:MET:HE2	2.02	0.42
1:A:4055:ASN:HB2	1:A:4095:GLU:HA	2.02	0.42
3:C:16:VAL:HG12	3:C:59:PHE:O	2.20	0.42
1:A:323:VAL:HA	1:A:326:MET:CG	2.49	0.41
1:A:722:LYS:HD3	1:A:722:LYS:HA	1.78	0.41
1:A:907:LEU:HA	1:A:910:PHE:CE2	2.55	0.41
1:A:1477:HIS:O	1:A:1481:THR:OG1	2.24	0.41
1:A:1803:GLU:OE2	1:A:1804:MET:HE3	2.20	0.41
1:A:1945:TYR:CE2	1:A:1949:ILE:HD11	2.54	0.41
1:A:3537:SER:HA	1:A:3540:TYR:CG	2.55	0.41
1:A:3574:ALA:HB3	1:A:3687:MET:HE3	2.02	0.41
1:A:3959:MET:HG3	1:A:4124:TRP:CH2	2.55	0.41
1:A:4089:ILE:O	1:A:4093:GLU:N	2.53	0.41
1:A:4115:ASN:OD1	1:A:4119:ARG:NH2	2.53	0.41
2:B:89:GLY:HA2	2:B:140:ASP:O	2.20	0.41
3:C:209:LYS:O	3:C:213:ILE:HG23	2.20	0.41
1:A:136:GLN:O	1:A:140:SER:N	2.53	0.41
1:A:156:PHE:HA	1:A:159:GLU:OE1	2.20	0.41
1:A:202:GLY:O	1:A:206:THR:HG23	2.20	0.41
1:A:389:ILE:HG22	1:A:393:LYS:HZ1	1.83	0.41
1:A:411:PRO:HG3	1:A:457:CYS:SG	2.60	0.41
1:A:1188:ILE:HG13	1:A:1189:GLU:N	2.35	0.41
1:A:1407:LYS:HA	1:A:1412:LYS:HD3	2.01	0.41
1:A:1436:LEU:HG	1:A:1437:TYR:H	1.84	0.41
1:A:2260:PHE:HA	1:A:2273:GLY:HA3	2.01	0.41
1:A:2274:ILE:HG23	1:A:2306:ASN:ND2	2.36	0.41
1:A:2281:MET:HE2	1:A:2326:ILE:CD1	2.50	0.41
1:A:2813:PHE:CE2	1:A:2868:LEU:HD11	2.51	0.41
1:A:2927:ALA:HB1	1:A:2931:ARG:HH12	1.84	0.41
1:A:3631:LYS:HB3	1:A:3631:LYS:HE3	1.87	0.41
1:A:3704:GLN:CD	1:A:3716:HIS:HB3	2.45	0.41
1:A:3806:LEU:C	1:A:3807:GLU:HG3	2.45	0.41
1:A:3967:PHE:O	1:A:3970:LEU:N	2.54	0.41
1:A:4114:PRO:HA	1:A:4117:LEU:HB2	2.01	0.41
2:B:64:ILE:HG21	2:B:123:LYS:HB3	2.02	0.41
2:B:86:VAL:HA	2:B:104:VAL:HA	2.00	0.41
3:C:632:PHE:O	3:C:636:ILE:HG23	2.20	0.41
4:F:50:ARG:NH2	4:F:58:ALA:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:VAL:O	1:A:120:ALA:HA	2.20	0.41
1:A:333:MET:HG3	1:A:334:HIS:N	2.35	0.41
1:A:1297:PHE:HA	1:A:1300:SER:OG	2.20	0.41
1:A:2244:CYS:SG	1:A:2245:TRP:N	2.93	0.41
1:A:2551:GLU:HA	1:A:2554:PHE:HD2	1.83	0.41
1:A:2953:THR:OG1	1:A:2994:TRP:NE1	2.47	0.41
1:A:2978:LYS:HG2	1:A:2981:TRP:CE2	2.55	0.41
1:A:3840:LYS:HD2	1:A:3840:LYS:HA	1.92	0.41
2:B:113:ALA:O	2:B:117:LEU:HG	2.19	0.41
2:B:262:LYS:HA	2:B:268:VAL:HG12	2.01	0.41
2:B:347:LEU:HA	2:B:398:CYS:SG	2.60	0.41
2:B:356:LEU:HG	2:B:358:LYS:NZ	2.35	0.41
2:B:404:ARG:CZ	6:D:31:DA:H3'	2.50	0.41
2:B:484:GLN:HG2	2:B:488:ARG:CZ	2.50	0.41
3:C:338:LYS:HG3	3:C:398:ASP:HA	2.02	0.41
3:C:609:PHE:O	3:C:612:ALA:N	2.42	0.41
1:A:416:SER:O	1:A:420:VAL:HG13	2.20	0.41
1:A:3147:LYS:NZ	1:A:3149:GLY:H	2.19	0.41
1:A:3192:LYS:HA	1:A:3192:LYS:HD2	1.87	0.41
1:A:3570:ASP:N	1:A:3570:ASP:OD1	2.53	0.41
2:B:482:VAL:HG22	3:C:333:TYR:CD2	2.55	0.41
2:B:515:ASN:O	2:B:519:GLY:N	2.54	0.41
3:C:56:LEU:HD23	3:C:80:HIS:ND1	2.35	0.41
3:C:342:VAL:HG22	3:C:393:VAL:HG22	2.02	0.41
3:C:528:ILE:HB	3:C:529:PRO:HD3	2.03	0.41
4:F:80:VAL:HG11	4:F:83:ILE:HG13	2.02	0.41
1:A:42:CYS:HB2	1:A:88:PHE:CG	2.55	0.41
1:A:51:LEU:O	1:A:54:GLN:NE2	2.48	0.41
1:A:70:ARG:HB2	1:A:78:PHE:HD2	1.86	0.41
1:A:294:PHE:CE2	1:A:298:LEU:HD11	2.55	0.41
1:A:581:LEU:HD22	1:A:620:PHE:HD1	1.85	0.41
1:A:766:ALA:HB3	1:A:851:ILE:HD12	2.02	0.41
1:A:876:SER:C	1:A:880:MET:HE3	2.46	0.41
1:A:1983:ASP:H	1:A:2090:ARG:CZ	2.34	0.41
1:A:2218:PHE:HA	1:A:2221:LYS:HZ3	1.86	0.41
1:A:2411:LEU:O	1:A:2415:LEU:HG	2.21	0.41
1:A:2436:LEU:HD12	1:A:2469:CYS:HB2	2.03	0.41
1:A:3036:TYR:O	1:A:3039:THR:OG1	2.32	0.41
1:A:3298:LEU:HD23	1:A:3337:ILE:HB	2.03	0.41
1:A:3388:ALA:O	1:A:3392:ALA:N	2.45	0.41
1:A:3681:LYS:C	1:A:3688:SER:HB3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3749:PRO:HB3	1:A:3805:TRP:HD1	1.86	0.41
2:B:65:GLN:HA	2:B:68:GLN:NE2	2.36	0.41
2:B:90:THR:OG1	2:B:136:GLY:HA3	2.20	0.41
2:B:290:ARG:HG2	3:C:309:ASP:C	2.45	0.41
6:D:39:DA:H2'	6:D:40:DT:C5	2.55	0.41
7:E:33:DA:C4	7:E:34:DT:C4	3.09	0.41
1:A:1724:MET:HG2	1:A:1768:ARG:HD3	2.03	0.41
1:A:1864:ASP:HA	1:A:1867:ILE:HG22	2.01	0.41
1:A:3028:ASN:O	1:A:3029:LYS:HD2	2.20	0.41
1:A:3340:ALA:O	1:A:3343:SER:OG	2.38	0.41
1:A:3705:TYR:OH	1:A:3714:GLU:OE1	2.38	0.41
1:A:3762:GLN:HB3	1:A:3793:VAL:HG23	2.02	0.41
1:A:3821:SER:OG	1:A:3823:GLU:OE1	2.31	0.41
1:A:3875:GLU:HB3	1:A:3965:ARG:HD2	2.02	0.41
1:A:4056:PRO:HA	1:A:4059:ILE:HG12	2.02	0.41
2:B:340:PHE:HE2	3:C:485:PRO:HB2	1.86	0.41
3:C:251:LEU:O	3:C:258:SER:HA	2.20	0.41
3:C:546:ASP:OD1	3:C:547:GLN:N	2.54	0.41
1:A:95:LYS:NZ	1:A:140:SER:OG	2.28	0.41
1:A:268:PRO:HG2	1:A:308:LEU:HD21	2.03	0.41
1:A:985:GLU:N	1:A:986:PRO:HD2	2.36	0.41
1:A:1483:LEU:HD11	1:A:1518:ALA:HB1	2.01	0.41
1:A:1653:LEU:HD23	1:A:1695:LEU:HD12	2.02	0.41
1:A:1791:CYS:HB2	1:A:1835:ALA:HB2	2.02	0.41
1:A:2927:ALA:HB1	1:A:2931:ARG:NH1	2.36	0.41
1:A:3667:LEU:HA	1:A:3670:MET:HG3	2.02	0.41
1:A:4040:PRO:HA	1:A:4043:LYS:HD2	2.02	0.41
1:A:4048:LYS:HE2	1:A:4048:LYS:HA	2.01	0.41
1:A:4101:GLU:O	1:A:4105:LYS:HG2	2.20	0.41
2:B:446:MET:HE1	3:C:264:TYR:CG	2.56	0.41
3:C:11:VAL:HG21	3:C:114:SER:CB	2.51	0.41
4:F:111:LYS:HG3	4:F:132:ILE:HD13	2.03	0.41
1:A:20:SER:HA	1:A:23:ASP:CB	2.51	0.41
1:A:196:LEU:HB3	1:A:200:PHE:CE2	2.56	0.41
1:A:581:LEU:HD22	1:A:620:PHE:CD1	2.55	0.41
1:A:583:LEU:HA	1:A:614:PRO:HA	2.03	0.41
1:A:726:LEU:O	1:A:730:LEU:HG	2.21	0.41
1:A:871:LEU:HD21	1:A:3122:HIS:HB2	2.03	0.41
1:A:1235:ILE:HD12	1:A:1289:SER:HB2	2.03	0.41
1:A:2452:ARG:HD3	1:A:2494:ASP:HA	2.02	0.41
1:A:3164:TRP:HB3	1:A:3186:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4073:ALA:O	1:A:4077:TYR:N	2.42	0.41
2:B:38:LEU:HD13	2:B:165:ARG:O	2.21	0.41
2:B:269:ILE:HG13	2:B:270:SER:H	1.85	0.41
2:B:429:PRO:HB3	3:C:435:PHE:CD2	2.56	0.41
3:C:301:ASP:OD1	3:C:301:ASP:N	2.52	0.41
3:C:643:ARG:HH21	3:C:647:ILE:HG13	1.86	0.41
6:D:29:DA:N1	7:E:28:DA:C2	2.89	0.41
1:A:10:CYS:N	1:A:13:LEU:HD12	2.36	0.41
1:A:149:ILE:HG21	1:A:183:GLU:HB2	2.02	0.41
1:A:165:LYS:HA	1:A:165:LYS:HD3	1.82	0.41
1:A:734:LEU:HD21	1:A:769:GLY:N	2.36	0.41
1:A:925:GLN:HA	1:A:928:VAL:HG22	2.03	0.41
1:A:960:GLN:CD	1:A:960:GLN:H	2.28	0.41
1:A:1070:PRO:HA	1:A:1075:ARG:NH2	2.36	0.41
1:A:1076:LEU:HD22	1:A:1121:LEU:HD11	2.03	0.41
1:A:1081:ALA:O	1:A:1085:ILE:HG23	2.21	0.41
1:A:1191:PHE:O	1:A:1195:VAL:HG23	2.21	0.41
1:A:1430:GLU:O	1:A:1434:VAL:HG13	2.21	0.41
1:A:1748:ASP:OD1	1:A:1749:ALA:N	2.54	0.41
1:A:1836:LEU:HB3	1:A:1840:PHE:CZ	2.56	0.41
1:A:1888:ASP:HB2	1:A:1896:ILE:HG12	2.02	0.41
1:A:1986:ARG:H	1:A:2183:HIS:HA	1.86	0.41
1:A:2126:MET:HB2	1:A:2164:TRP:CZ2	2.56	0.41
1:A:2281:MET:SD	1:A:2287:PRO:HA	2.61	0.41
1:A:2379:MET:HA	1:A:2382:VAL:HG22	2.03	0.41
1:A:2571:ASP:HA	1:A:2574:ASN:HB2	2.03	0.41
1:A:2795:GLN:HA	1:A:2798:ALA:HB3	2.03	0.41
1:A:2831:ASN:HD22	1:A:2834:GLN:NE2	2.18	0.41
1:A:2891:ARG:HH21	1:A:3897:PHE:HD2	1.69	0.41
1:A:3315:TYR:HD1	1:A:3318:LYS:HE3	1.86	0.41
1:A:3320:ILE:CG2	1:A:3324:ARG:HH21	2.34	0.41
1:A:3763:ARG:O	1:A:3766:GLN:HG3	2.20	0.41
1:A:3840:LYS:O	1:A:3844:THR:HG23	2.20	0.41
1:A:3972:LEU:N	1:A:3973:PRO:HD2	2.36	0.41
1:A:4021:LEU:HA	1:A:4028:ILE:HG22	2.02	0.41
2:B:302:THR:HA	3:C:291:LYS:HA	2.03	0.41
2:B:465:ILE:O	2:B:518:LEU:HD11	2.21	0.41
3:C:65:ASP:N	3:C:78:THR:HG22	2.35	0.41
3:C:82:HIS:CE1	3:C:84:MET:HG2	2.56	0.41
3:C:368:ARG:HG3	3:C:369:ASP:N	2.36	0.41
3:C:622:GLN:NE2	3:C:631:TYR:HD2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:65:ILE:HG23	4:F:70:GLY:HA3	2.02	0.41
6:D:20:DT:H2"	6:D:21:DA:OP2	2.21	0.41
7:E:19:DA:C6	7:E:20:DT:C2	3.09	0.41
1:A:178:LEU:HB2	1:A:227:LEU:HD13	2.03	0.41
1:A:458:CYS:HA	1:A:461:ILE:HG12	2.02	0.41
1:A:1336:THR:O	1:A:1339:VAL:HG22	2.21	0.41
1:A:2102:LYS:O	1:A:2106:ARG:HD3	2.21	0.41
1:A:2414:GLN:O	1:A:2418:LYS:HG2	2.21	0.41
1:A:2421:VAL:HG23	1:A:2457:PRO:HG3	2.03	0.41
1:A:3410:ILE:HG21	1:A:3456:LEU:HB2	2.02	0.41
1:A:3493:TRP:H	1:A:3521:ILE:HD11	1.85	0.41
1:A:3771:MET:HE1	1:A:3998:LEU:HD21	2.02	0.41
1:A:3821:SER:O	1:A:3825:LYS:N	2.48	0.41
1:A:3839:TYR:CE2	1:A:4122:GLU:HB2	2.56	0.41
2:B:127:GLY:HA2	2:B:130:ARG:HG2	2.03	0.41
3:C:153:SER:HA	3:C:156:LYS:HE2	2.03	0.41
3:C:553:ILE:HD13	3:C:553:ILE:HA	1.90	0.41
1:A:453:MET:HA	1:A:456:VAL:HB	2.03	0.40
1:A:554:ASN:OD1	1:A:555:SER:N	2.54	0.40
1:A:1109:GLU:O	1:A:1113:LEU:HG	2.21	0.40
1:A:1133:HIS:O	1:A:1136:ARG:HG2	2.21	0.40
1:A:1140:LYS:HB3	1:A:1140:LYS:HE2	1.89	0.40
1:A:1554:SER:OG	1:A:1555:HIS:N	2.54	0.40
1:A:1935:GLU:OE1	1:A:1935:GLU:N	2.51	0.40
1:A:2298:GLU:HA	1:A:2301:GLN:HB3	2.02	0.40
1:A:2454:LEU:C	1:A:2457:PRO:HD2	2.47	0.40
1:A:3280:TYR:CE1	1:A:3304:VAL:HG21	2.56	0.40
2:B:203:MET:SD	2:B:238:LYS:HB2	2.61	0.40
3:C:59:PHE:HA	3:C:76:ASN:O	2.20	0.40
4:F:109:LEU:CG	4:F:132:ILE:HB	2.51	0.40
1:A:670:LEU:HA	1:A:673:THR:HB	2.03	0.40
1:A:772:ALA:O	1:A:776:TRP:CD1	2.75	0.40
1:A:1244:LEU:HD21	1:A:1310:GLU:HB2	2.02	0.40
1:A:1537:VAL:CG2	1:A:1552:HIS:HB3	2.51	0.40
1:A:1596:VAL:O	1:A:1600:MET:HG2	2.21	0.40
1:A:1916:ILE:HD12	1:A:1916:ILE:H	1.85	0.40
1:A:2091:HIS:CG	1:A:2092:GLU:H	2.39	0.40
1:A:2364:LEU:HD13	1:A:2400:VAL:HG11	2.03	0.40
1:A:2930:TYR:O	1:A:2934:GLY:N	2.54	0.40
1:A:3273:LEU:HD21	1:A:3307:LEU:HD21	2.03	0.40
1:A:3822:GLN:HA	1:A:3825:LYS:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:ARG:O	2:B:118:GLU:HG2	2.21	0.40
3:C:326:VAL:O	3:C:329:GLU:HG2	2.22	0.40
3:C:427:MET:SD	3:C:427:MET:N	2.92	0.40
4:F:111:LYS:HG3	4:F:132:ILE:CD1	2.51	0.40
1:A:333:MET:HG3	1:A:334:HIS:H	1.86	0.40
1:A:452:LYS:HG3	1:A:453:MET:N	2.35	0.40
1:A:1009:LEU:O	1:A:1013:ILE:HG12	2.22	0.40
1:A:1127:CYS:O	1:A:1131:ILE:HG12	2.21	0.40
1:A:2187:VAL:HA	1:A:2190:VAL:HG22	2.02	0.40
1:A:2787:HIS:O	1:A:2790:LEU:HG	2.21	0.40
1:A:2806:LYS:HD2	1:A:2853:PRO:O	2.22	0.40
1:A:3685:PRO:O	1:A:3688:SER:OG	2.31	0.40
1:A:3840:LYS:HG2	1:A:4122:GLU:OE2	2.21	0.40
1:A:4040:PRO:HD2	1:A:4041:ARG:NH1	2.36	0.40
1:A:4093:GLU:HG3	1:A:4098:LEU:HD22	2.04	0.40
2:B:148:TRP:O	2:B:152:ASN:ND2	2.55	0.40
2:B:276:LEU:HD11	3:C:354:ARG:HD3	2.03	0.40
2:B:331:LYS:N	2:B:331:LYS:HD3	2.35	0.40
2:B:446:MET:HE2	3:C:363:LYS:CB	2.52	0.40
3:C:356:PHE:CG	3:C:422:VAL:HG21	2.56	0.40
4:F:91:TYR:CD2	4:F:136:SER:HB2	2.56	0.40
1:A:209:THR:O	1:A:210:SER:C	2.64	0.40
1:A:439:VAL:HG23	1:A:440:VAL:HG13	2.03	0.40
1:A:762:TYR:CZ	1:A:764:PRO:HG2	2.57	0.40
1:A:1184:ARG:O	1:A:1188:ILE:HG12	2.21	0.40
1:A:1279:LEU:HA	1:A:1282:LEU:HG	2.03	0.40
1:A:1392:MET:HA	1:A:1395:LEU:HD12	2.04	0.40
1:A:2480:ILE:HG23	1:A:2484:TYR:HD2	1.87	0.40
1:A:2996:LEU:HA	1:A:2999:LEU:HD12	2.02	0.40
1:A:3417:ALA:HA	1:A:3446:VAL:HG21	2.03	0.40
1:A:3558:ILE:HD12	1:A:3558:ILE:HA	1.93	0.40
1:A:3682:GLU:HA	1:A:3685:PRO:HA	2.04	0.40
1:A:3827:ALA:HA	1:A:3831:ASP:HB2	2.03	0.40
1:A:4121:TRP:O	1:A:4126:PRO:HD3	2.22	0.40
2:B:58:THR:OG1	2:B:61:ASP:N	2.43	0.40
3:C:38:ILE:HD12	3:C:38:ILE:HA	1.96	0.40
3:C:62:ASP:HA	3:C:103:GLN:HE22	1.86	0.40
3:C:398:ASP:H	3:C:401:ALA:HB3	1.85	0.40
1:A:283:SER:O	1:A:284:THR:OG1	2.39	0.40
1:A:341:PHE:HD1	1:A:344:GLN:NE2	2.20	0.40
1:A:377:ASN:HB3	1:A:380:ASP:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ARG:NH1	1:A:1734:PRO:HA	2.36	0.40
1:A:670:LEU:HB3	1:A:732:PHE:HE1	1.87	0.40
1:A:1589:ASN:OD1	1:A:1592:MET:HE1	2.22	0.40
1:A:1876:ILE:O	1:A:1879:VAL:HG12	2.22	0.40
1:A:2254:ARG:HE	1:A:2292:CYS:HG	1.66	0.40
1:A:2376:ASP:HB2	1:A:2377:ARG:HD3	2.04	0.40
1:A:3443:PRO:HA	1:A:3446:VAL:CG1	2.49	0.40
1:A:4002:MET:O	1:A:4006:VAL:HG12	2.22	0.40
6:D:33:DA:C8	6:D:34:DC:N3	2.89	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	3652/4128 (88%)	3389 (93%)	258 (7%)	5 (0%)	48	83
2	B	484/609 (80%)	434 (90%)	44 (9%)	6 (1%)	10	42
3	C	639/732 (87%)	586 (92%)	52 (8%)	1 (0%)	43	77
4	F	96/575 (17%)	91 (95%)	5 (5%)	0	100	100
5	M	21/204 (10%)	21 (100%)	0	0	100	100
All	All	4892/6248 (78%)	4521 (92%)	359 (7%)	12 (0%)	44	77

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	426	GLN
2	B	418	GLU
2	B	420	LEU
2	B	425	ILE
2	B	429	PRO

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Mol	Chain	Res	Type
1	A	101	ALA
1	A	125	ILE
1	A	2330	VAL
1	A	2331	MET
2	B	423	GLN
3	C	509	GLN
1	A	3832	PRO

5.3.2 Protein sidechains [i](#)

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	3158/3671 (86%)	3157 (100%)	1 (0%)	100	100
2	B	414/548 (76%)	412 (100%)	2 (0%)	81	81
3	C	559/649 (86%)	559 (100%)	0	100	100
4	F	78/480 (16%)	78 (100%)	0	100	100
5	M	15/160 (9%)	15 (100%)	0	100	100
All	All	4224/5508 (77%)	4221 (100%)	3 (0%)	87	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	855	VAL
2	B	421	ASP
2	B	423	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	ASN
1	A	250	ASN
1	A	278	HIS
1	A	322	GLN

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Mol	Chain	Res	Type
1	A	330	ASN
1	A	415	GLN
1	A	448	GLN
1	A	738	HIS
1	A	739	ASN
1	A	753	GLN
1	A	990	GLN
1	A	1048	GLN
1	A	1125	GLN
1	A	1238	GLN
1	A	1304	HIS
1	A	1320	ASN
1	A	1367	HIS
1	A	1390	GLN
1	A	1457	GLN
1	A	1603	GLN
1	A	1610	ASN
1	A	1687	HIS
1	A	1738	ASN
1	A	1771	GLN
1	A	1941	HIS
1	A	1957	ASN
1	A	2176	ASN
1	A	2213	ASN
1	A	2270	ASN
1	A	2306	ASN
1	A	2351	GLN
1	A	2352	HIS
1	A	2432	GLN
1	A	2475	ASN
1	A	2496	GLN
1	A	2518	GLN
1	A	2768	GLN
1	A	2807	GLN
1	A	2830	ASN
1	A	2831	ASN
1	A	2838	GLN
1	A	2977	ASN
1	A	3108	GLN
1	A	3150	ASN
1	A	3250	ASN
1	A	3311	ASN

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Mol	Chain	Res	Type
1	A	3524	ASN
1	A	3580	ASN
1	A	3643	HIS
1	A	3660	ASN
1	A	3697	ASN
1	A	3772	ASN
1	A	3818	ASN
1	A	3927	ASN
1	A	3951	GLN
1	A	4037	ASN
2	B	65	GLN
2	B	68	GLN
2	B	132	GLN
2	B	458	GLN
2	B	485	GLN
2	B	489	ASN
3	C	50	ASN
3	C	131	HIS
3	C	352	GLN
3	C	359	ASN
3	C	411	HIS
3	C	547	GLN
3	C	622	GLN
4	F	108	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

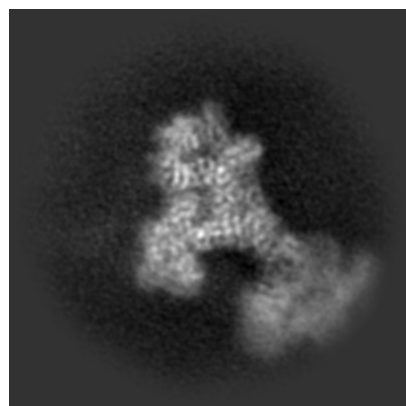
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51156. These allow visual inspection of the internal detail of the map and identification of artifacts.

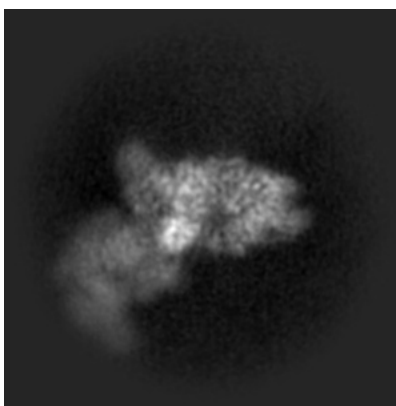
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

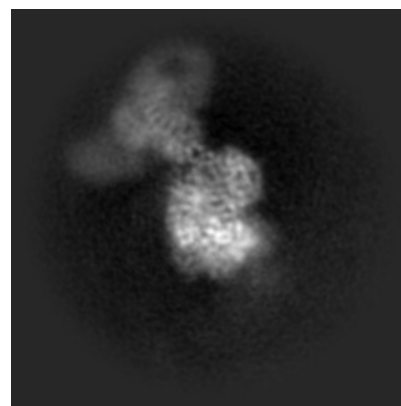
6.1.1 Primary map



X

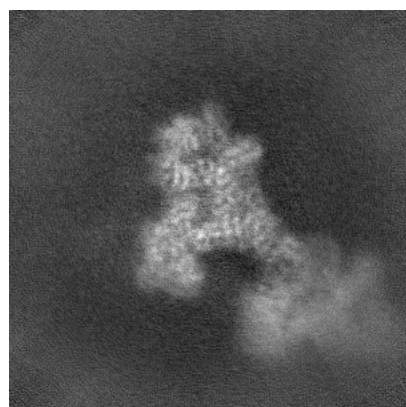


Y

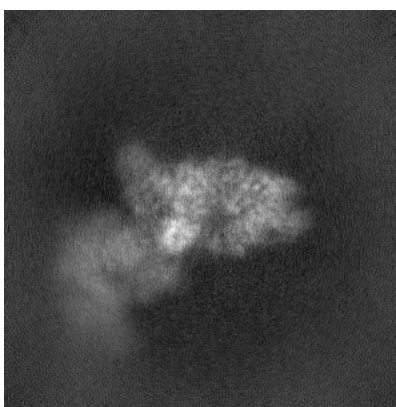


Z

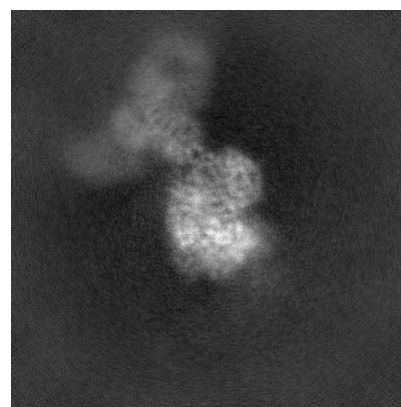
6.1.2 Raw map



X



Y

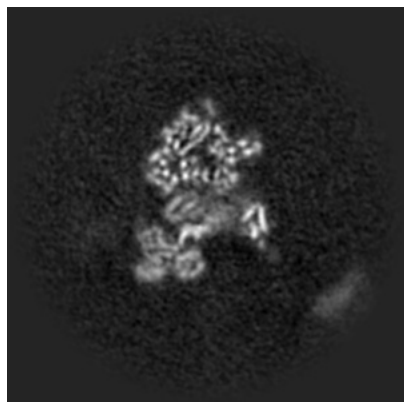


Z

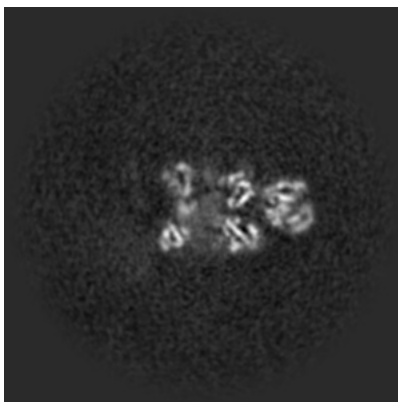
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

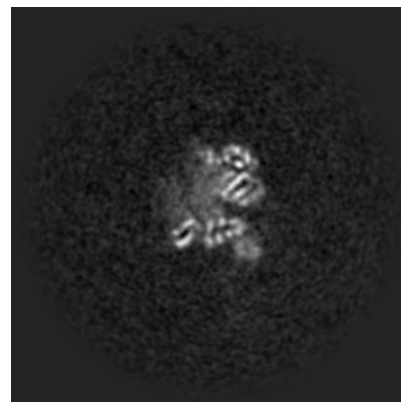
6.2.1 Primary map



X Index: 160

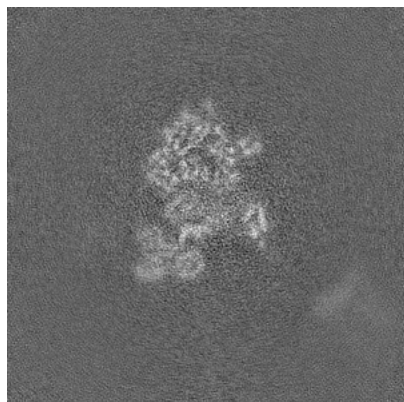


Y Index: 160

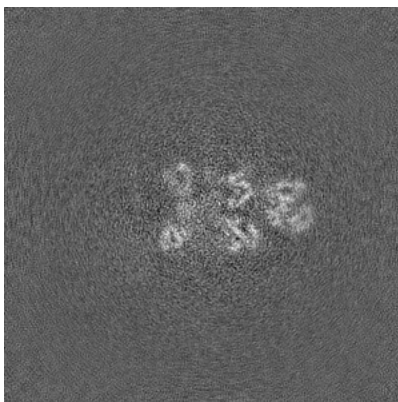


Z Index: 160

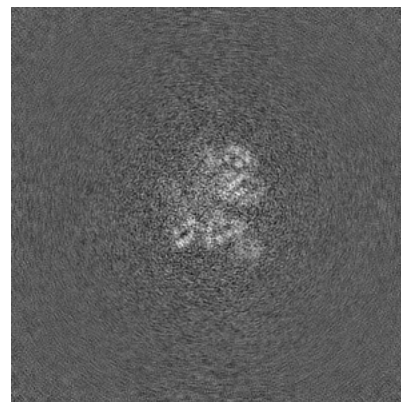
6.2.2 Raw map



X Index: 160



Y Index: 160

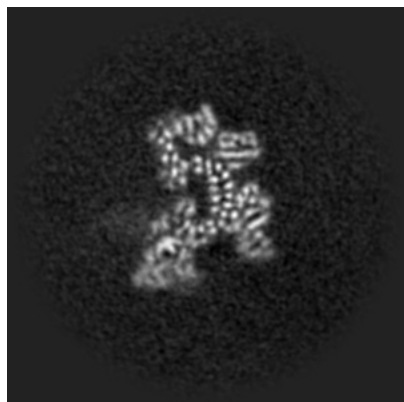


Z Index: 160

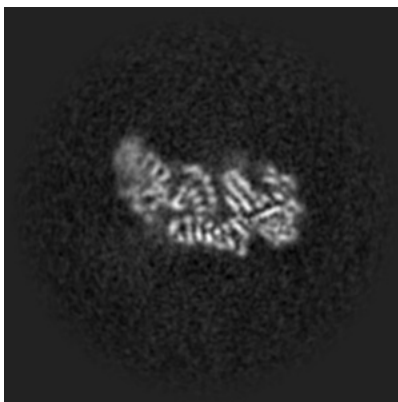
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

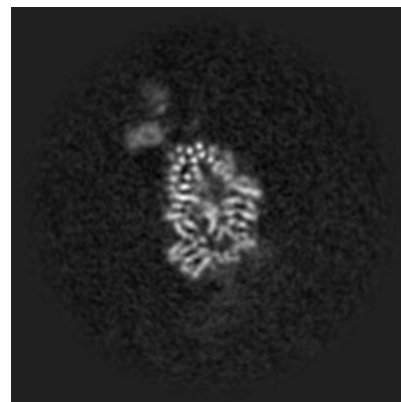
6.3.1 Primary map



X Index: 176

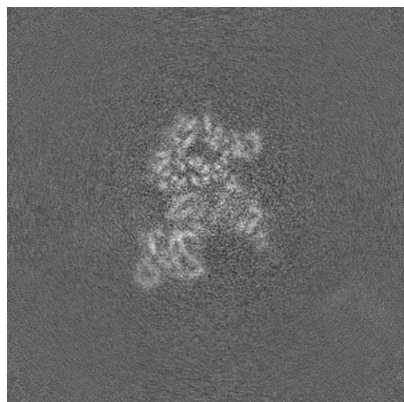


Y Index: 141

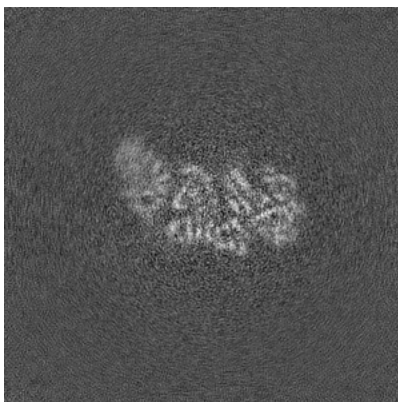


Z Index: 141

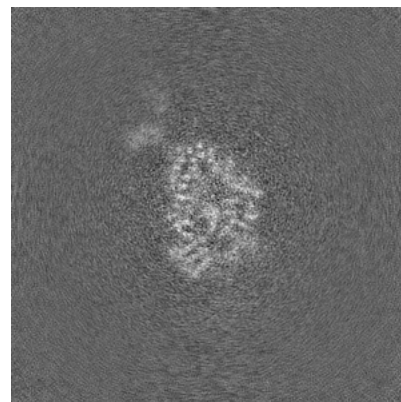
6.3.2 Raw map



X Index: 165



Y Index: 142

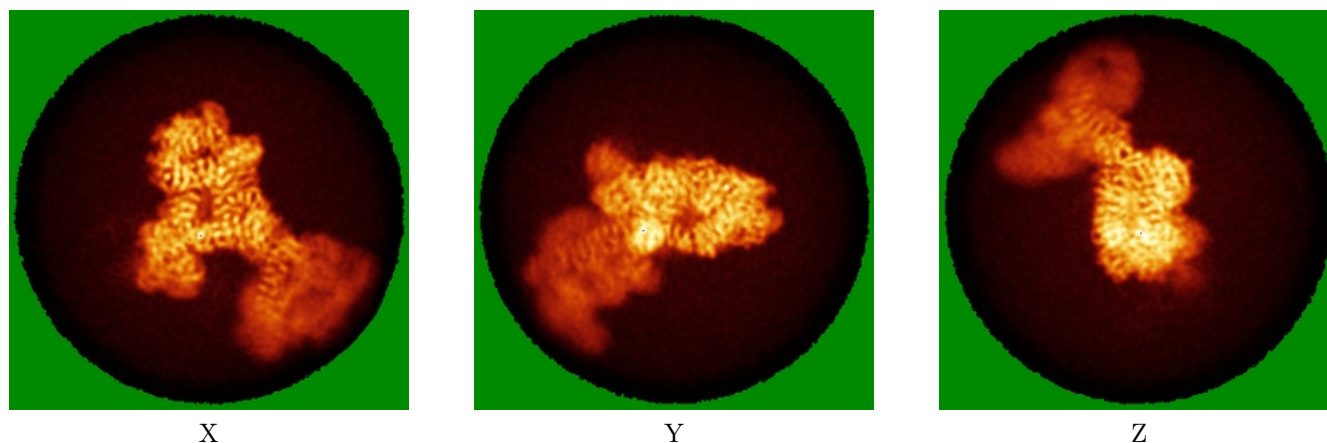


Z Index: 142

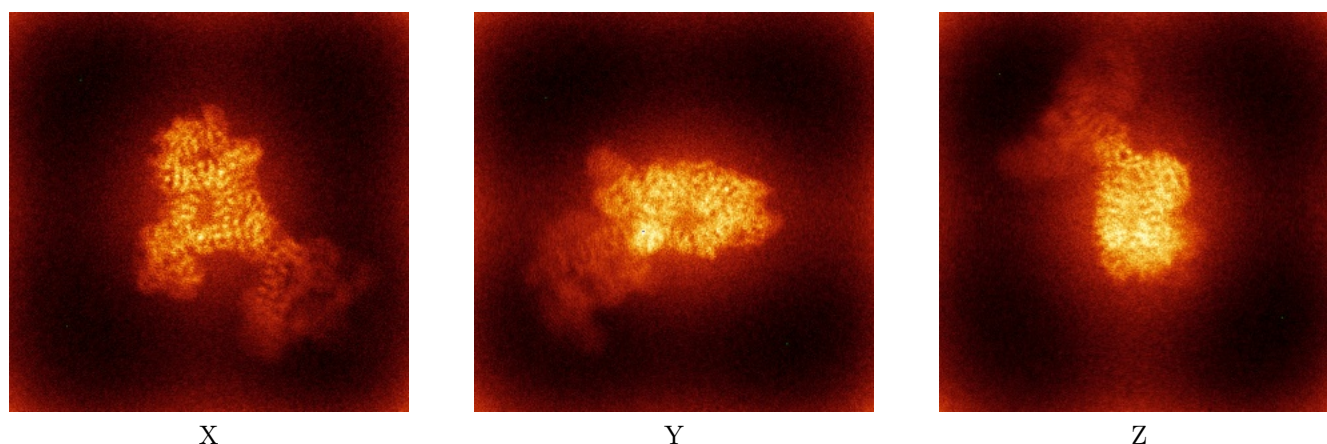
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

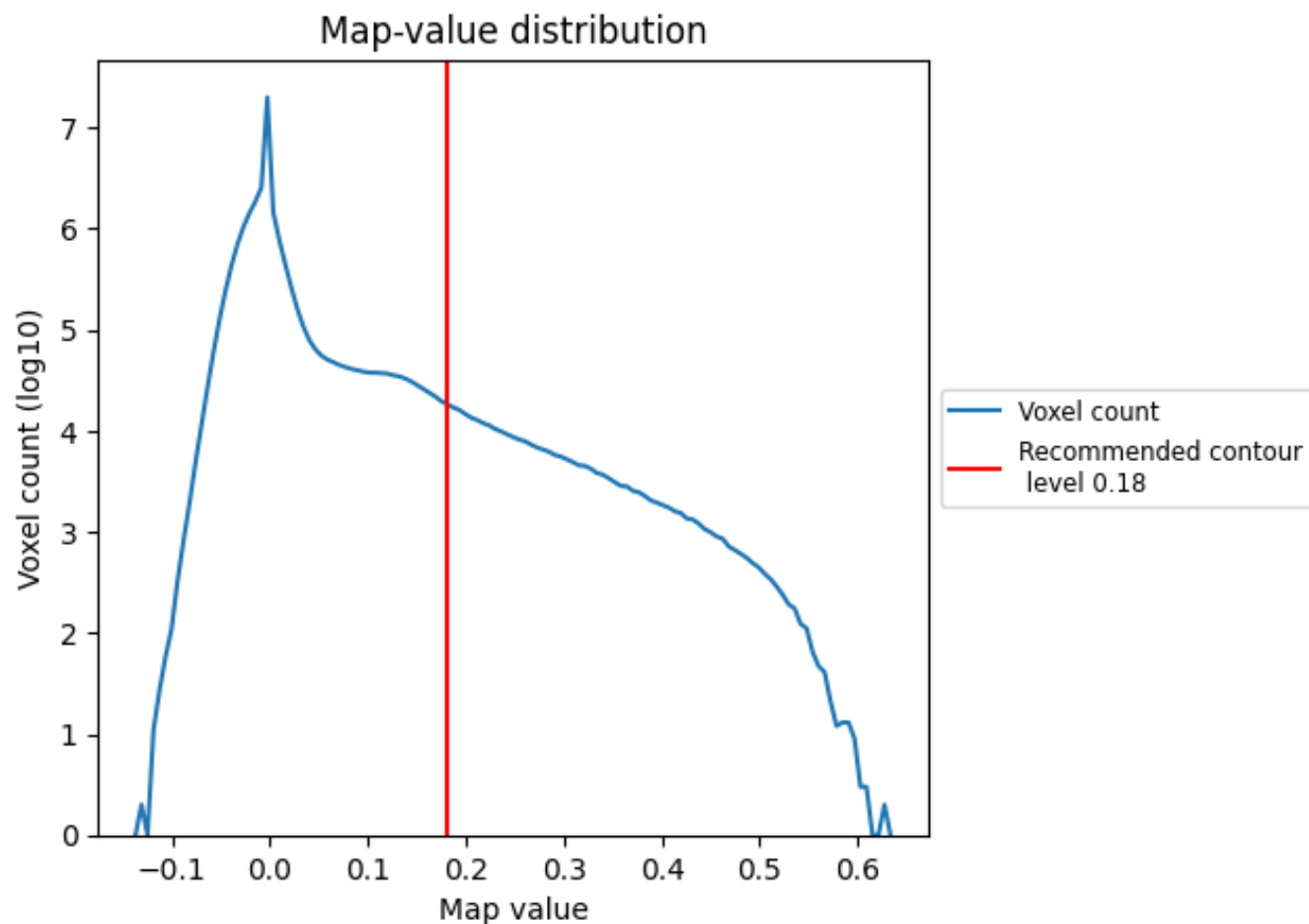
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

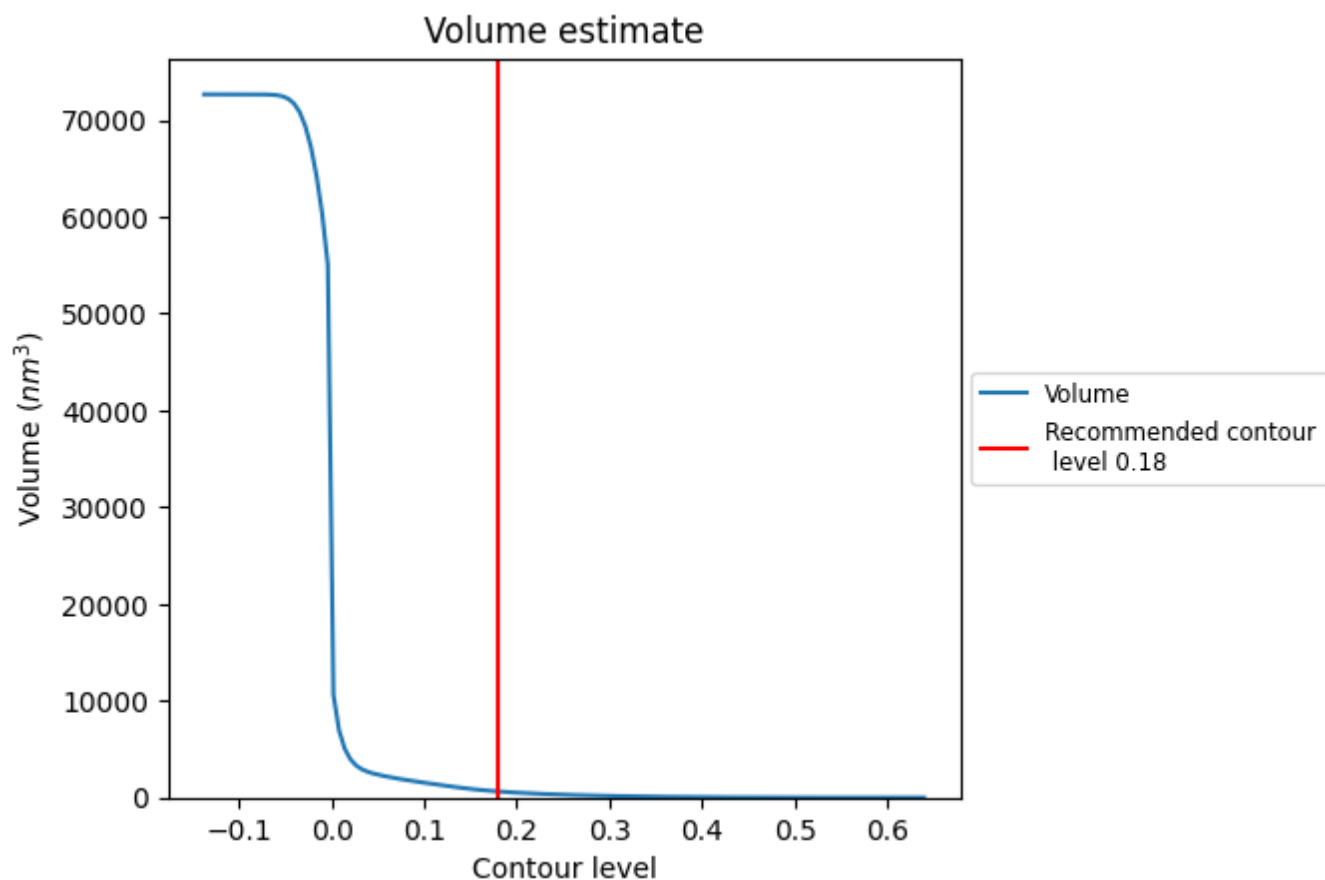
This section contains the results of statistical analysis of the map.

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.

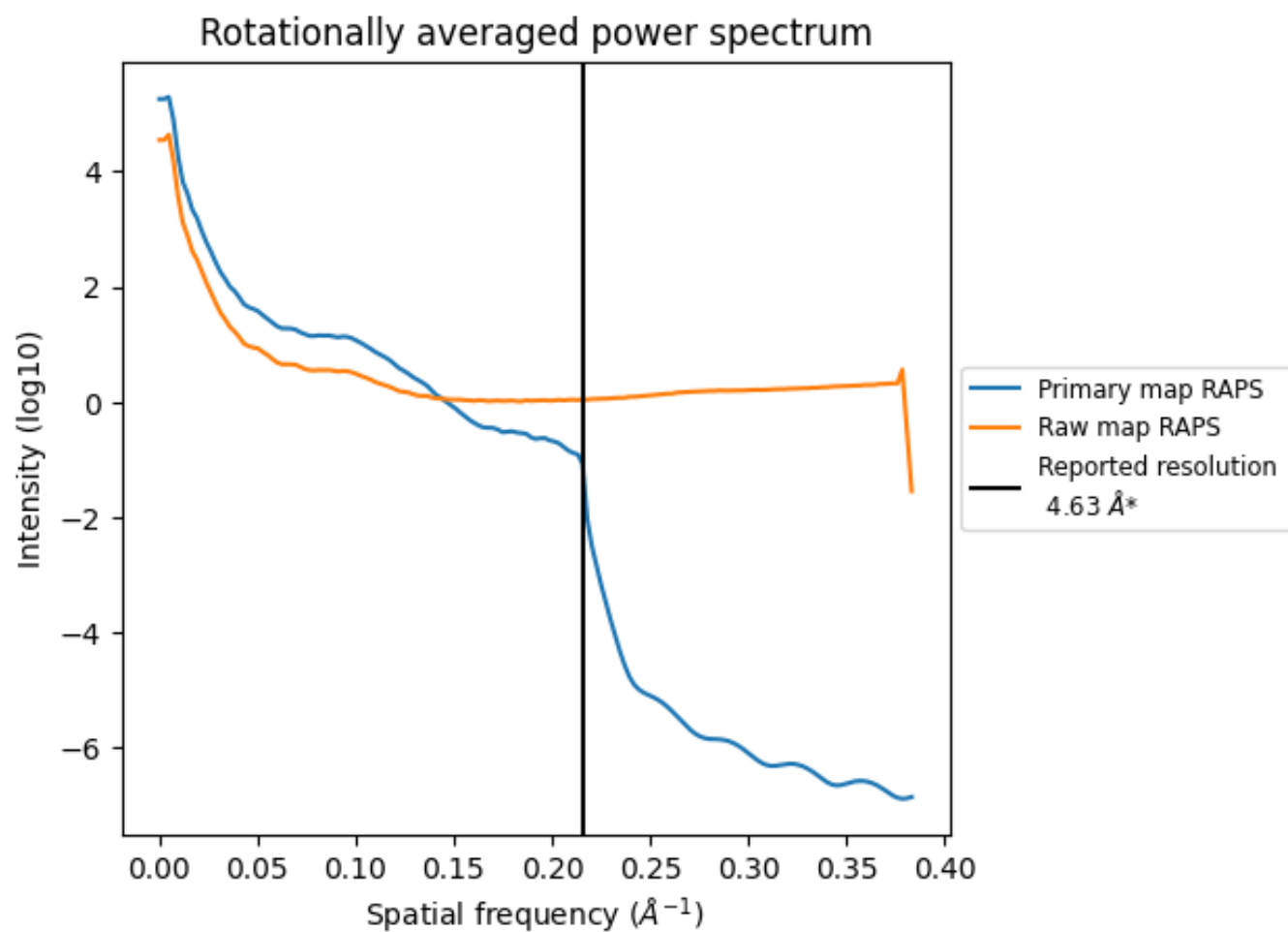
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 632 nm³; this corresponds to an approximate mass of 570 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 ⓘ

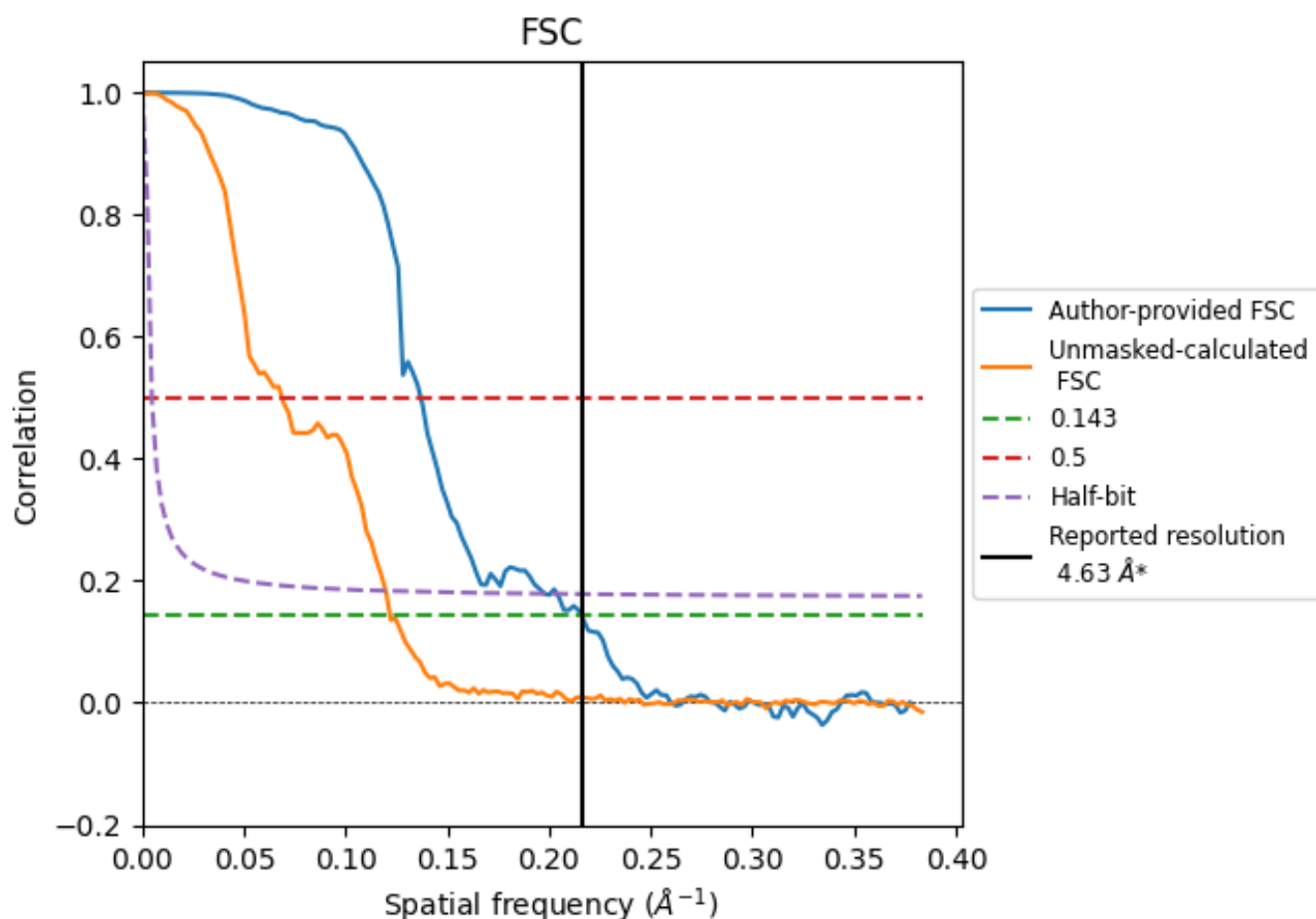


*Reported resolution corresponds to spatial frequency of 0.216 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.216 Å⁻¹

8.2 Resolution estimates [i](#)

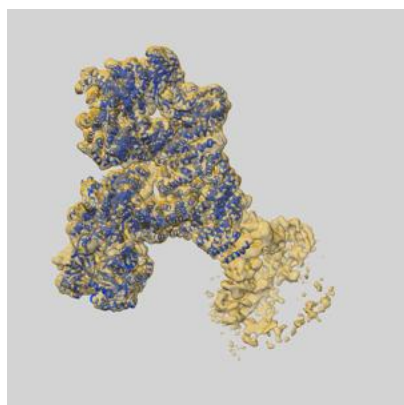
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.63	-	-
Author-provided FSC curve	4.63	7.30	5.05
Unmasked-calculated*	8.20	14.56	8.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.20 differs from the reported value 4.63 by more than 10 %

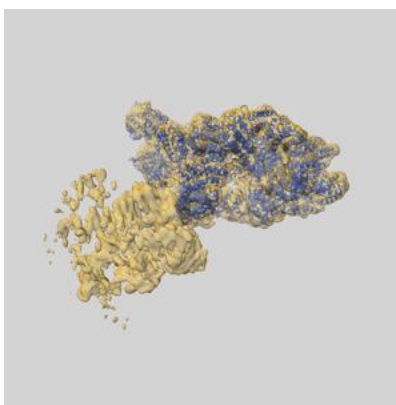
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51156 and PDB model 9G9L. Per-residue inclusion information can be found in section [3](#) on page [6](#).

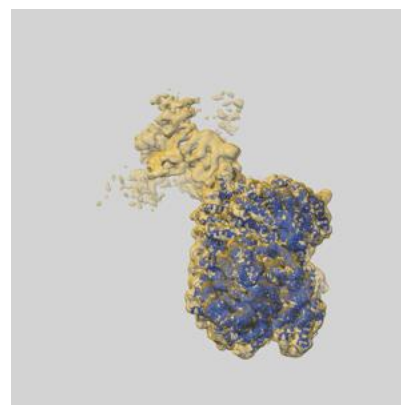
9.1 Map-model overlay [i](#)



X



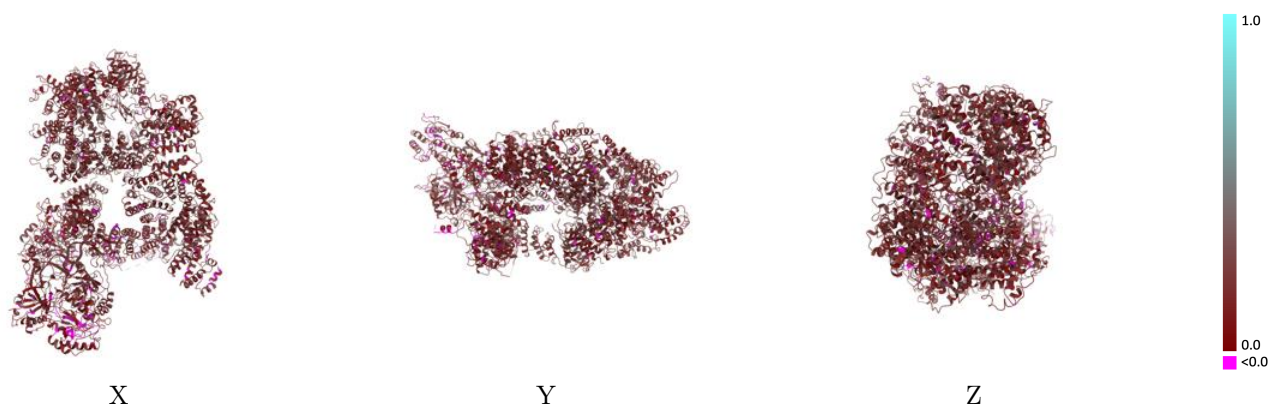
Y



Z

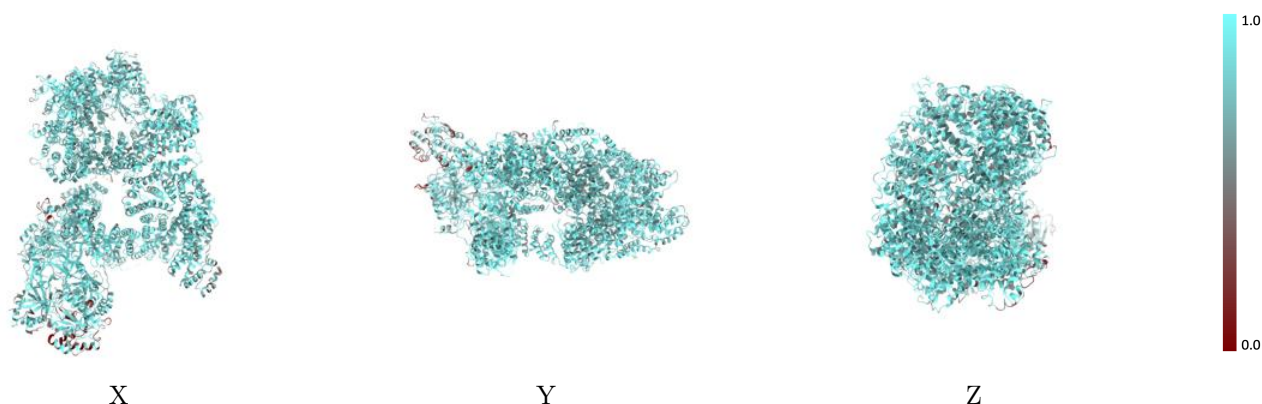
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



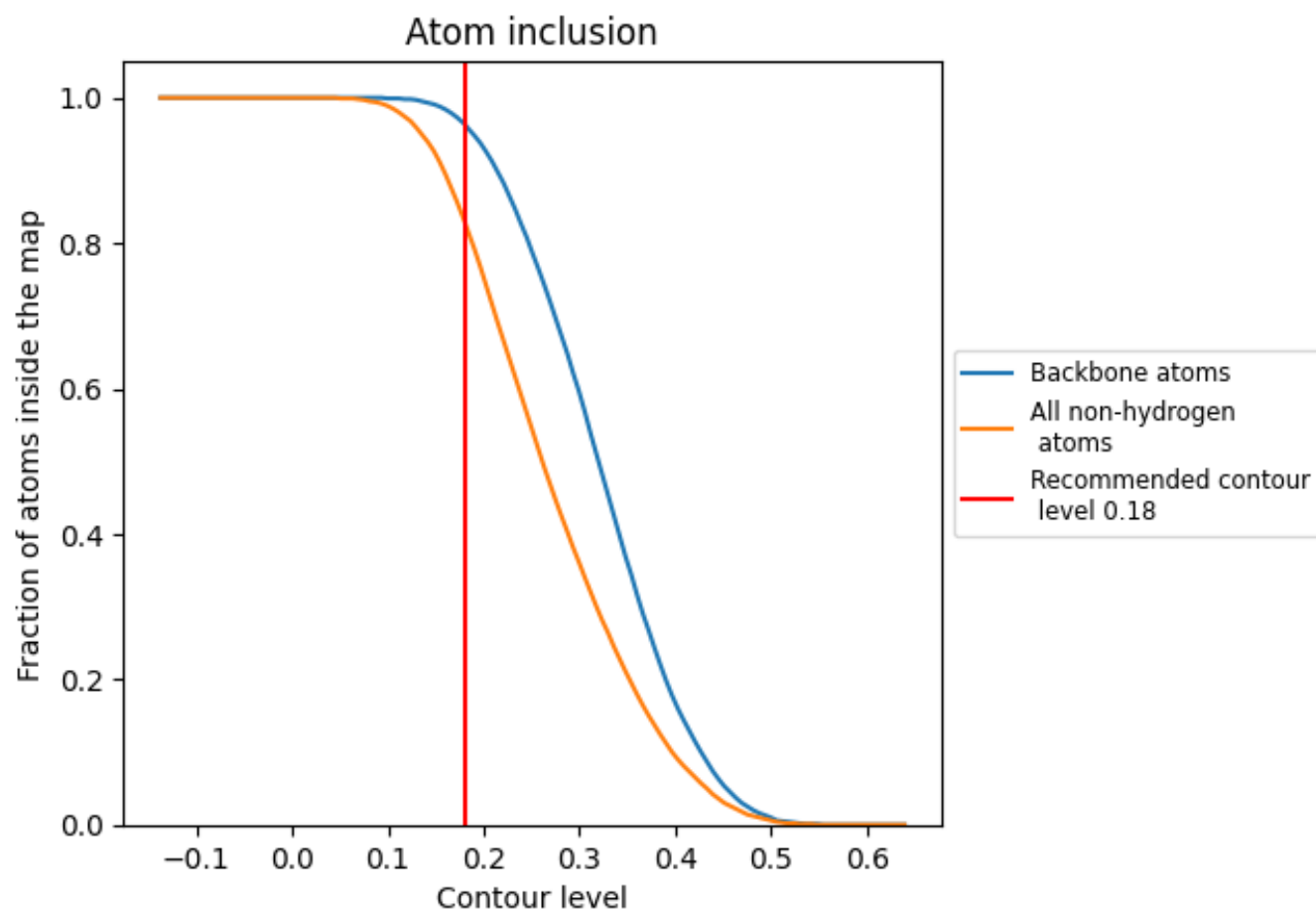
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 83% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8300</div>	<div><div></div>0.1880</div>
A	<div><div></div>0.8470</div>	<div><div></div>0.1930</div>
B	<div><div></div>0.8470</div>	<div><div></div>0.1870</div>
C	<div><div></div>0.7270</div>	<div><div></div>0.1580</div>
D	<div><div></div>0.9570</div>	<div><div></div>0.2320</div>
E	<div><div></div>0.9410</div>	<div><div></div>0.2140</div>
F	<div><div></div>0.6190</div>	<div><div></div>0.1540</div>
M	<div><div></div>0.8520</div>	<div><div></div>0.2220</div>

1.0

0.0

<0.0