



Full wwPDB EM Validation Report ⓘ

May 18, 2026 – 05:13 pm BST

PDB ID : 9HYF / pdb_00009hyf
EMDB ID : EMD-52502
Title : Cryo-EM structure of the C. elegans UBR4/KCMF1 complex (composite map)
Authors : Grabarczyk, D.B.; Clausen, T.
Deposited on : 2025-01-09
Resolution : 3.00 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

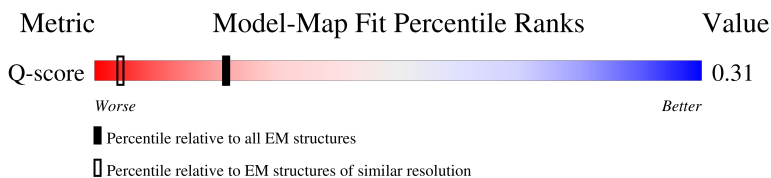
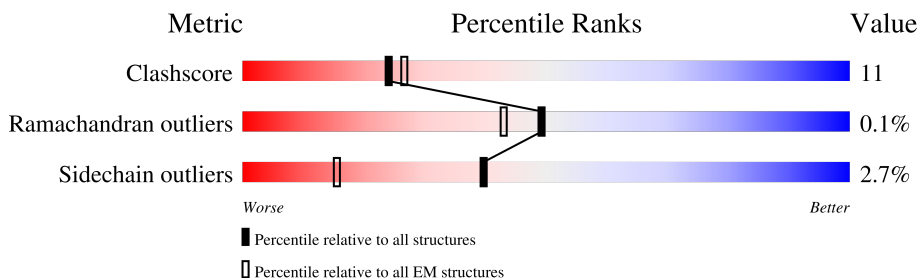
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	3861	
1	B	3861	
2	C	515	
2	D	515	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 64398 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 UBR-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3655	Total	C	N	O	S	0	0
			29401	18666	5003	5526	206		
1	B	3655	Total	C	N	O	S	0	0
			29401	18666	5003	5526	206		

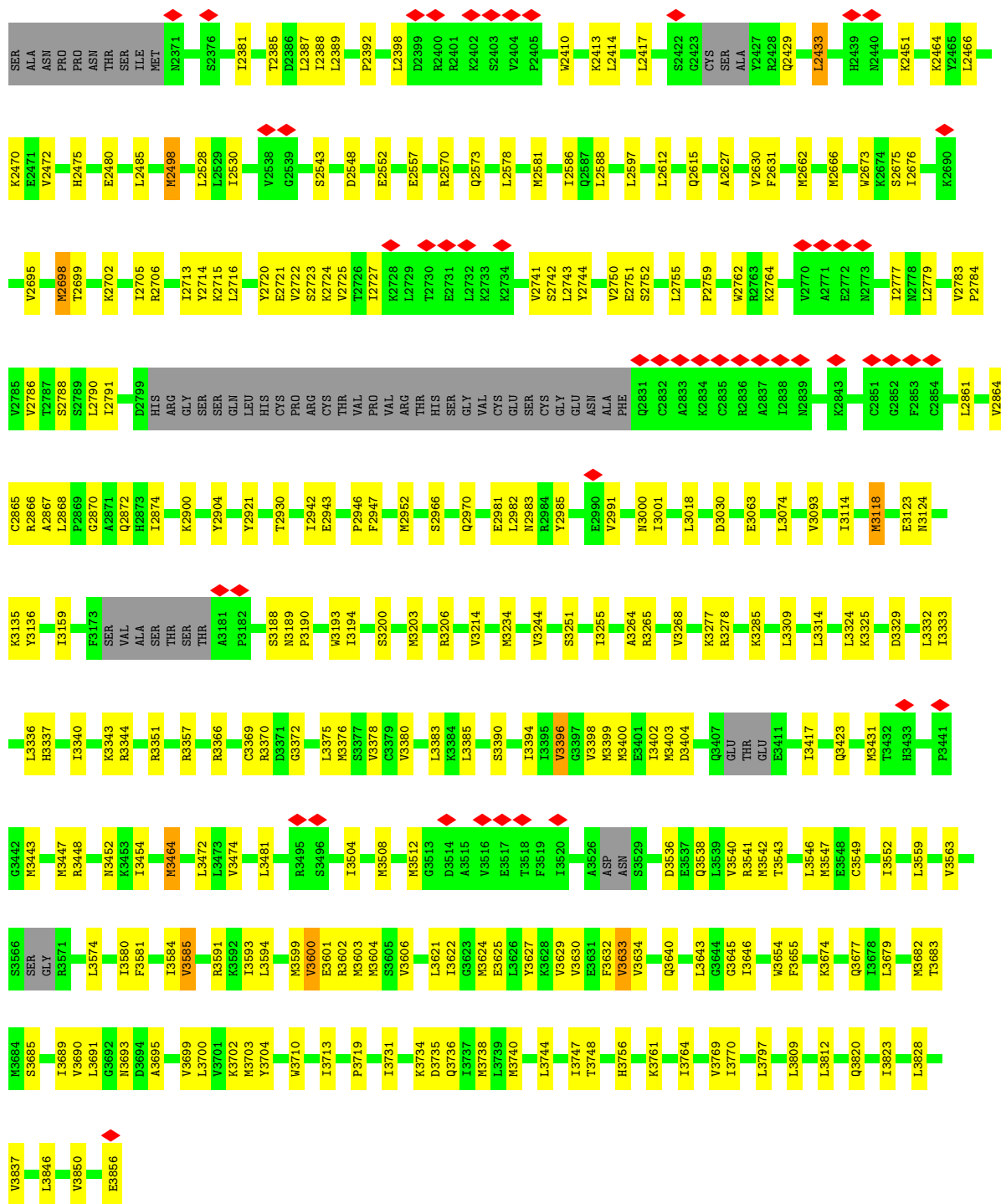
- Molecule 2 is a protein called E3 ubiquitin-protein ligase kcmf-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	353	Total	C	N	O	S	0	0
			2789	1751	470	547	21		
2	D	353	Total	C	N	O	S	0	0
			2789	1751	470	547	21		

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

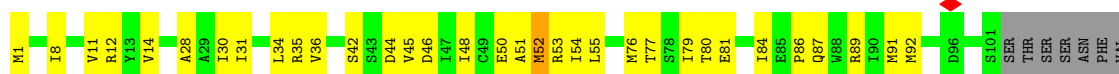
Mol	Chain	Residues	Atoms		AltConf
3	A	5	Total	Zn	0
			5	5	
3	C	4	Total	Zn	0
			4	4	
3	B	5	Total	Zn	0
			5	5	
3	D	4	Total	Zn	0
			4	4	

F2267	G2163	V2049	L1885	L1788	L1655	Q1488	T1398	C1275	L1185	L1041	F956	F2268	K2050	S2051	L2052	R1389	L1790	L1791	A1792	K1670	G1660	Q1495	R1495	R1399	T1398	C1275	L1185	L1041	F956	F2269	K2051	L2053	R1390	L1791	A1792	K1671	G1661	Q1496	R1496	R1399	T1399	C1276	L1186	L1042	F957	F2270	S2052	L2054	R1390	L1792	A1793	K1672	G1662	Q1497	R1497	R1399	T1400	C1277	L1187	L1043	F958	F2271	K2053	L2055	R1391	L1793	A1794	K1673	G1663	Q1498	R1498	R1399	T1401	C1278	L1188	L1044	F959	F2272	S2054	L2056	R1392	L1794	A1795	K1674	G1664	Q1499	R1499	R1399	T1402	C1279	L1189	L1045	F960	F2273	K2055	L2057	R1393	L1795	A1796	K1675	G1665	Q1500	R1500	R1393	T1403	C1280	L1190	L1046	F961	F2274	S2056	L2058	R1394	L1796	A1797	K1676	G1666	Q1501	R1501	R1393	T1404	C1281	L1191	L1047	F962	F2275	K2057	L2059	R1395	L1797	A1798	K1677	G1667	Q1502	R1502	R1393	T1405	C1282	L1192	L1048	F963	F2276	S2058	L2060	R1396	L1798	A1799	K1678	G1668	Q1503	R1503	R1393	T1406	C1283	L1193	L1049	F964	F2277	K2059	L2061	R1397	L1799	A1800	K1679	G1669	Q1504	R1504	R1393	T1407	C1284	L1194	L1050	F965	F2278	S2060	L2062	R1398	L1800	A1801	K1680	G1670	Q1505	R1505	R1393	T1408	C1285	L1195	L1051	F966	F2279	K2061	L2063	R1399	L1801	A1802	K1681	G1671	Q1506	R1506	R1393	T1409	C1286	L1196	L1052	F967	F2280	S2062	L2064	R1400	L1802	A1803	K1682	G1672	Q1507	R1507	R1393	T1410	C1287	L1197	L1053	F968	F2281	K2063	L2065	R1401	L1803	A1804	K1683	G1673	Q1508	R1508	R1393	T1411	C1288	L1198	L1054	F969	F2282	S2064	L2066	R1402	L1804	A1805	K1684	G1674	Q1509	R1509	R1393	T1412	C1289	L1199	L1055	F970	F2283	K2065	L2067	R1403	L1805	A1806	K1685	G1675	Q1510	R1510	R1393	T1413	C1290	L1200	L1056	F971	F2284	S2066	L2068	R1404	L1806	A1807	K1686	G1676	Q1511	R1511	R1393	T1414	C1291	L1201	L1057	F972	F2285	K2067	L2069	R1405	L1807	A1808	K1687	G1677	Q1512	R1512	R1393	T1415	C1292	L1202	L1058	F973	F2286	S2068	L2070	R1406	L1808	A1809	K1688	G1678	Q1513	R1513	R1393	T1416	C1293	L1203	L1059	F974	F2287	K2069	L2071	R1407	L1809	A1810	K1689	G1679	Q1514	R1514	R1393	T1417	C1294	L1204	L1060	F975	F2288	S2070	L2072	R1408	L1810	A1811	K1690	G1680	Q1515	R1515	R1393	T1418	C1295	L1205	L1061	F976	F2289	K2071	L2073	R1409	L1811	A1812	K1691	G1681	Q1516	R1516	R1393	T1419	C1296	L1206	L1062	F977	F2290	S2072	L2074	R1410	L1812	A1813	K1692	G1682	Q1517	R1517	R1393	T1420	C1297	L1207	L1063	F978	F2291	K2073	L2075	R1411	L1813	A1814	K1693	G1683	Q1518	R1518	R1393	T1421	C1298	L1208	L1064	F979	F2292	S2074	L2076	R1412	L1814	A1815	K1694	G1684	Q1519	R1519	R1393	T1422	C1299	L1209	L1065	F980	F2293	K2075	L2077	R1413	L1815	A1816	K1695	G1685	Q1520	R1520	R1393	T1423	C1300	L1210	L1066	F981	F2294	S2076	L2078	R1414	L1816	A1817	K1696	G1686	Q1521	R1521	R1393	T1424	C1301	L1211	L1067	F982	F2295	K2077	L2079	R1415	L1817	A1818	K1697	G1687	Q1522	R1522	R1393	T1425	C1302	L1212	L1068	F983	F2296	S2078	L2080	R1416	L1818	A1819	K1698	G1688	Q1523	R1523	R1393	T1426	C1303	L1213	L1069	F984	F2297	K2079	L2081	R1417	L1819	A1820	K1699	G1689	Q1524	R1524	R1393	T1427	C1304	L1214	L1070	F985	F2298	S2080	L2082	R1418	L1820	A1821	K1700	G1690	Q1525	R1525	R1393	T1428	C1305	L1215	L1071	F986	F2299	K2081	L2083	R1419	L1821	A1822	K1701	G1691	Q1526	R1526	R1393	T1429	C1306	L1216	L1072	F987	F2300	S2082	L2084	R1420	L1822	A1823	K1702	G1692	Q1527	R1527	R1393	T1430	C1307	L1217	L1073	F988	F2301	K2083	L2085	R1421	L1823	A1824	K1703	G1693	Q1528	R1528	R1393	T1431	C1308	L1218	L1074	F989	F2302	S2084	L2086	R1422	L1824	A1825	K1704	G1694	Q1529	R1529	R1393	T1432	C1309	L1219	L1075	F990	F2303	K2085	L2087	R1423	L1825	A1826	K1705	G1695	Q1530	R1530	R1393	T1433	C1310	L1220	L1076	F991	F2304	S2086	L2088	R1424	L1826	A1827	K1706	G1696	Q1531	R1531	R1393	T1434	C1311	L1221	L1077	F992	F2305	K2087	L2089	R1425	L1827	A1828	K1707	G1697	Q1532	R1532	R1393	T1435	C1312	L1222	L1078	F993	F2306	S2088	L2090	R1426	L1828	A1829	K1708	G1698	Q1533	R1533	R1393	T1436	C1313	L1223	L1079	F994	F2307	K2089	L2091	R1427	L1829	A1830	K1709	G1699	Q1534	R1534	R1393	T1437	C1314	L1224	L1080	F995	F2308	S2090	L2092	R1428	L1830	A1831	K1710	G1700	Q1535	R1535	R1393	T1438	C1315	L1225	L1081	F996	F2309	K2091	L2093	R1429	L1831	A1832	K1711	G1701	Q1536	R1536	R1393	T1439	C1316	L1226	L1082	F997	F2310	S2092	L2094	R1430	L1832	A1833	K1712	G1702	Q1537	R1537	R1393	T1440	C1317	L1227	L1083	F998	F2311	K2093	L2095	R1431	L1833	A1834	K1713	G1703	Q1538	R1538	R1393	T1441	C1318	L1228	L1084	F999	F2312	S2094	L2096	R1432	L1834	A1835	K1714	G1704	Q1539	R1539	R1393	T1442	C1319	L1229	L1085	F1000	F2313	K2095	L2097	R1433	L1835	A1836	K1715	G1705	Q1540	R1540	R1393	T1443	C1320	L1230	L1086	F1001	F2314	S2096	L2098	R1434	L1836	A1837	K1716	G1706	Q1541	R1541	R1393	T1444	C1321	L1231	L1087	F1002	F2315	K2097	L2099	R1435	L1837	A1838	K1717	G1707	Q1542	R1542	R1393	T1445	C1322	L1232	L1088	F1003	F2316	S2098	L2100	R1436	L1838	A1839	K1718	G1708	Q1543	R1543	R1393	T1446	C1323	L1233	L1089	F1004	F2317	K2099	L2101	R1437	L1839	A1840	K1719	G1709	Q1544	R1544	R1393	T1447	C1324	L1234	L1090	F1005	F2318	S2100	L2102	R1438	L1840	A1841	K1720	G1710	Q1545	R1545	R1393	T1448	C1325	L1235	L1091	F1006	F2319	K2101	L2103	R1439	L1841	A1842	K1721	G1711	Q1546	R1546	R1393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• Molecule 1: UBR-type domain-containing protein

Chain B:

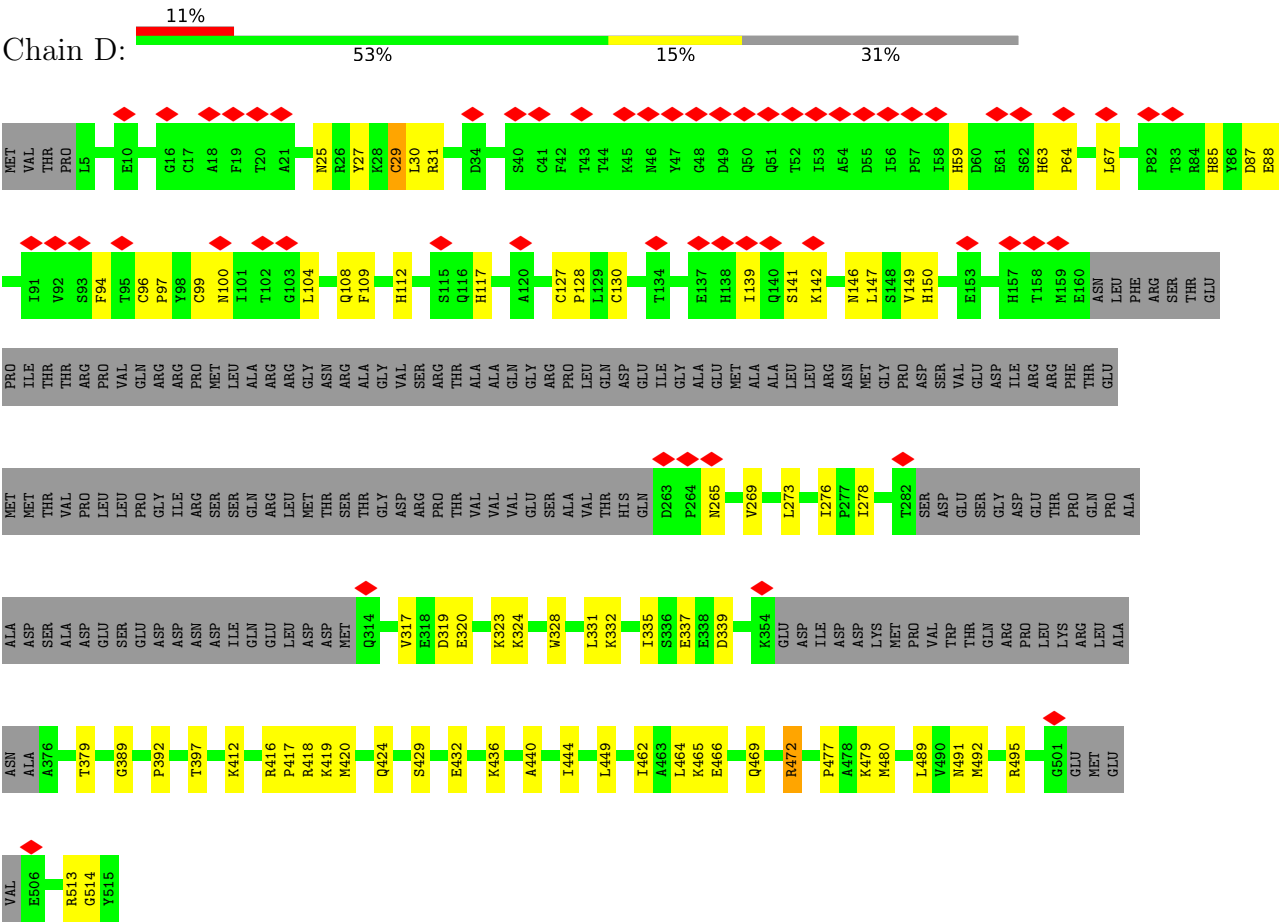








● Molecule 2: E3 ubiquitin-protein ligase kcmf-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	691759	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.054	Depositor
Minimum map value	0.000	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0104	Depositor
Map size (Å)	486.912, 486.912, 486.912	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.268, 1.268, 1.268	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/29920	0.37	0/40398
1	B	0.17	1/29920 (0.0%)	0.39	0/40398
2	C	0.16	0/2851	0.29	0/3868
2	D	0.17	0/2851	0.30	0/3868
All	All	0.17	1/65542 (0.0%)	0.37	0/88532

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1450	ASP	CA-CB	5.83	1.61	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1705	THR	Peptide
1	B	1705	THR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	29401	0	29674	653	0
1	B	29401	0	29674	673	0
2	C	2789	0	2696	58	0
2	D	2789	0	2696	50	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
All	All	64398	0	64740	1397	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1397) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2321:CYS:HA	1:A:2388:ILE:HD11	1.47	0.93
1:B:2093:LEU:HD11	1:B:2104:ILE:HD11	1.54	0.90
1:B:2329:ILE:HD12	1:B:2413:LYS:HE2	1.55	0.89
1:B:2205:ILE:HG23	1:B:2236:LEU:HD11	1.57	0.87
2:C:29:CYS:SG	2:C:59:HIS:CE1	2.68	0.86
1:A:2093:LEU:HD11	1:A:2104:ILE:HD11	1.56	0.86
1:A:2205:ILE:HG23	1:A:2236:LEU:HD11	1.59	0.84
1:B:387:ARG:HG3	1:B:421:MET:HE1	1.61	0.83
1:B:1236:CYS:SG	1:B:1253:HIS:HE1	2.02	0.82
1:A:3000:ASN:HD21	2:D:489:LEU:HD22	1.43	0.81
1:B:3703:MET:HE1	1:B:3744:LEU:HD13	1.61	0.80
2:C:489:LEU:HD22	1:B:3000:ASN:HD21	1.47	0.80
1:B:298:ILE:O	1:B:302:MET:HB3	1.81	0.80
1:B:989:ASP:HB3	1:B:1028:VAL:HG23	1.64	0.79
1:A:1236:CYS:SG	1:A:1253:HIS:HE1	2.04	0.79
1:A:612:MET:HE3	1:A:612:MET:H	1.46	0.79
1:A:619:VAL:HG21	1:A:664:LEU:HD22	1.63	0.79
1:A:1552:ARG:HG2	1:A:1566:GLU:HG3	1.63	0.78
1:A:298:ILE:O	1:A:302:MET:HB3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2724:LYS:HB3	1:B:2864:VAL:HB	1.66	0.78
1:A:989:ASP:HB3	1:A:1028:VAL:HG23	1.66	0.78
1:A:3703:MET:HE1	1:A:3744:LEU:HD13	1.66	0.78
1:A:3447:MET:HE3	1:A:3472:LEU:HD12	1.64	0.78
1:A:2724:LYS:HB3	1:A:2864:VAL:HB	1.66	0.77
1:A:3581:PHE:O	1:A:3585:VAL:HB	1.83	0.77
1:B:3581:PHE:O	1:B:3585:VAL:HB	1.85	0.77
1:B:3447:MET:HE3	1:B:3472:LEU:HD12	1.67	0.76
1:A:420:GLU:HA	1:A:423:ARG:HE	1.50	0.75
1:A:2142:LYS:HA	1:A:2145:MET:HG2	1.67	0.75
1:B:302:MET:HG3	1:B:306:LEU:HG	1.69	0.75
1:A:302:MET:HG3	1:A:306:LEU:HG	1.69	0.74
1:B:1791:LEU:HD21	1:B:1851:ARG:HB3	1.69	0.73
1:B:11:VAL:HG21	1:B:48:ILE:HG22	1.70	0.73
1:A:2070:MET:HA	1:A:2081:MET:HE1	1.69	0.72
1:B:3634:VAL:HG21	1:B:3689:ILE:HG12	1.69	0.72
1:B:1835:THR:HB	1:B:1906:PRO:HG3	1.72	0.72
1:B:2318:ARG:HG2	1:B:2410:TRP:HZ2	1.54	0.72
1:B:473:ILE:HD12	1:B:516:ALA:HB2	1.70	0.72
1:B:1030:GLU:O	1:B:1034:LYS:HG2	1.88	0.72
1:A:1835:THR:HB	1:A:1906:PRO:HG3	1.72	0.71
1:B:741:PHE:HE1	1:B:898:ILE:HD13	1.55	0.71
1:A:473:ILE:HD12	1:A:516:ALA:HB2	1.71	0.71
1:B:612:MET:HE3	1:B:612:MET:H	1.54	0.71
1:A:1791:LEU:HD21	1:A:1851:ARG:HB3	1.72	0.71
1:B:898:ILE:O	1:B:902:LEU:HD12	1.91	0.71
1:B:880:LEU:HD13	1:B:944:PHE:HZ	1.55	0.70
1:B:2460:GLN:O	1:B:2464:LYS:HG3	1.91	0.70
1:A:261:LEU:HD21	1:A:298:ILE:HG22	1.73	0.70
1:A:387:ARG:HE	1:B:113:ILE:HD12	1.56	0.70
1:A:1247:VAL:HG22	1:A:1285:PRO:HG3	1.74	0.70
1:B:685:HIS:CD2	1:B:805:MET:HE2	2.27	0.70
1:B:2318:ARG:HG2	1:B:2410:TRP:CZ2	2.26	0.70
1:A:741:PHE:HE1	1:A:898:ILE:HD13	1.56	0.70
1:A:1012:LEU:HD23	1:A:1091:LEU:HD21	1.74	0.69
1:B:50:GLU:HA	1:B:53:ARG:HG2	1.73	0.69
1:A:1705:THR:HG22	1:A:1706:VAL:HG23	1.74	0.69
1:B:261:LEU:HD21	1:B:298:ILE:HG22	1.75	0.69
1:B:1247:VAL:HG22	1:B:1285:PRO:HG3	1.74	0.69
1:A:598:PRO:HB3	1:A:621:GLN:HG2	1.73	0.69
1:A:901:ASP:HA	1:A:904:GLN:HG2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3585:VAL:HG13	1:A:3633:VAL:HG23	1.74	0.69
1:A:3603:MET:HG2	1:A:3630:VAL:HG21	1.75	0.69
1:B:1705:THR:HG22	1:B:1706:VAL:HG23	1.73	0.68
1:B:3452:ASN:HA	1:B:3464:MET:HE1	1.75	0.68
1:A:3452:ASN:HA	1:A:3464:MET:HE1	1.76	0.68
1:B:900:LEU:O	1:B:904:GLN:HG2	1.93	0.68
1:B:1012:LEU:HD23	1:B:1091:LEU:HD21	1.75	0.68
1:B:2148:HIS:HE1	1:B:2153:LYS:HD2	1.57	0.68
1:B:276:LEU:O	1:B:280:ILE:HG12	1.93	0.68
1:A:291:LEU:HB2	1:A:293:ILE:HD11	1.75	0.67
1:A:633:LEU:HA	1:A:636:LYS:HG2	1.77	0.67
1:A:2148:HIS:HE1	1:A:2153:LYS:HD2	1.59	0.67
1:A:3734:LYS:HG3	1:A:3738:MET:HE3	1.77	0.67
1:B:3594:LEU:HB3	1:B:3599:MET:HE2	1.77	0.67
1:B:3063:GLU:HG2	1:B:3093:VAL:HG22	1.77	0.67
1:A:276:LEU:O	1:A:280:ILE:HG12	1.93	0.67
1:B:3699:VAL:HA	1:B:3702:LYS:HE3	1.75	0.67
1:A:3699:VAL:HA	1:A:3702:LYS:HE3	1.76	0.67
1:B:268:ILE:HD13	1:B:309:ILE:HD11	1.76	0.66
1:A:1426:LEU:HD12	1:A:1430:THR:HB	1.77	0.66
1:B:1947:LEU:O	1:B:1951:ILE:HG13	1.95	0.66
1:A:3683:THR:HG23	1:A:3747:ILE:HG13	1.78	0.66
1:A:3731:ILE:HG23	1:A:3735:ASP:HB2	1.78	0.66
1:B:1865:TYR:HB2	1:B:1905:ILE:HB	1.77	0.66
1:B:3713:ILE:HG13	1:B:3738:MET:SD	2.36	0.66
1:A:268:ILE:HD13	1:A:309:ILE:HD11	1.76	0.66
1:B:624:PHE:HZ	1:B:633:LEU:HD11	1.61	0.66
1:A:3324:LEU:HD22	1:A:3366:ARG:HH21	1.60	0.66
1:A:461:ASP:HB3	1:A:464:VAL:HG22	1.76	0.66
1:A:744:THR:HA	1:A:838:GLY:HA3	1.77	0.66
1:B:486:LYS:HD2	1:B:487:ARG:N	2.11	0.65
1:B:1447:HIS:HB3	1:B:1462:LEU:HD12	1.76	0.65
1:B:3324:LEU:HD22	1:B:3366:ARG:HH21	1.61	0.65
1:A:1865:TYR:HB2	1:A:1905:ILE:HB	1.77	0.65
1:A:3713:ILE:HG13	1:A:3738:MET:SD	2.36	0.65
1:B:1286:ASN:H	1:B:1790:LEU:HD13	1.61	0.65
1:B:2124:ARG:HD2	1:B:2234:ARG:HG2	1.79	0.65
2:D:273:LEU:HB2	2:D:392:PRO:HG2	1.77	0.65
1:A:1947:LEU:O	1:A:1951:ILE:HG13	1.95	0.65
1:B:387:ARG:HA	1:B:421:MET:SD	2.37	0.65
1:B:778:LYS:HZ3	1:B:781:ARG:HD2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:273:LEU:HB2	2:C:392:PRO:HG2	1.77	0.65
1:B:3443:MET:HE3	1:B:3443:MET:HA	1.79	0.65
2:D:127:CYS:HB3	2:D:130:CYS:SG	2.36	0.65
1:A:50:GLU:HA	1:A:53:ARG:HG2	1.78	0.65
1:B:3683:THR:HG23	1:B:3747:ILE:HG13	1.77	0.65
2:C:127:CYS:HB3	2:C:130:CYS:SG	2.36	0.65
1:B:685:HIS:HD2	1:B:805:MET:HE2	1.60	0.65
1:A:2079:GLN:HE21	1:A:2083:GLN:HE21	1.45	0.65
1:A:2698:MET:HE3	1:A:2699:THR:HG23	1.79	0.65
1:B:3734:LYS:HG3	1:B:3738:MET:HE3	1.79	0.64
1:B:3118:MET:SD	1:B:3190:PRO:HB2	2.37	0.64
1:B:3144:THR:HG22	1:B:3147:GLU:HG3	1.80	0.64
1:A:11:VAL:HG21	1:A:48:ILE:HG22	1.80	0.64
1:A:2045:TRP:CD1	1:A:2095:ASN:HD22	2.16	0.64
1:A:3063:GLU:HG2	1:A:3093:VAL:HG22	1.77	0.64
2:C:99:CYS:SG	2:C:112:HIS:HE1	2.15	0.64
1:B:619:VAL:HG21	1:B:664:LEU:HD22	1.78	0.64
1:B:3595:VAL:HG23	1:B:3599:MET:HE3	1.78	0.64
1:A:1286:ASN:H	1:A:1790:LEU:HD13	1.63	0.64
1:A:1795:CYS:HB3	1:A:1921:LEU:HB3	1.80	0.64
1:A:3736:GLN:O	1:A:3740:MET:HG2	1.97	0.64
1:A:3634:VAL:HG21	1:A:3689:ILE:HG12	1.80	0.64
1:B:2070:MET:HE1	1:B:2082:ALA:HB2	1.80	0.64
1:A:778:LYS:HZ3	1:A:781:ARG:HD2	1.61	0.63
1:B:3731:ILE:HG23	1:B:3735:ASP:HB2	1.78	0.63
1:B:2698:MET:HE3	1:B:2699:THR:HG23	1.81	0.63
1:A:276:LEU:HD23	1:A:279:ARG:HH12	1.64	0.63
1:A:1034:LYS:HG2	1:A:1103:TYR:HD2	1.64	0.63
1:B:598:PRO:HB3	1:B:621:GLN:HG2	1.80	0.63
1:A:399:MET:HE3	1:A:422:LEU:HD22	1.79	0.63
1:B:584:VAL:O	1:B:588:MET:HG2	1.98	0.63
1:B:3736:GLN:O	1:B:3740:MET:HG2	1.99	0.63
1:B:276:LEU:HD23	1:B:279:ARG:HH12	1.64	0.62
1:B:2142:LYS:O	1:B:2145:MET:HB2	1.99	0.62
1:B:3654:TRP:HE1	1:B:3682:MET:HG3	1.64	0.62
1:B:3704:TYR:HB3	1:B:3769:VAL:HG21	1.80	0.62
2:C:335:ILE:HD12	2:C:339:ASP:HB3	1.80	0.62
1:A:1:MET:HA	1:A:1:MET:HE2	1.81	0.62
1:A:2706:ARG:HG3	1:A:2752:SER:HB2	1.81	0.62
1:A:2464:LYS:HZ3	1:A:2480:GLU:HG3	1.64	0.62
1:B:3343:LYS:HG2	1:B:3357:ARG:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1400:ARG:HB3	1:B:1438:GLU:HB2	1.82	0.62
1:A:383:ILE:HD13	1:A:414:ILE:HG23	1.81	0.62
1:B:487:ARG:HA	1:B:490:TYR:CD1	2.34	0.62
1:B:516:ALA:O	1:B:520:PHE:HB2	2.00	0.62
1:B:383:ILE:HD13	1:B:414:ILE:HG23	1.82	0.62
1:B:1426:LEU:HD12	1:B:1430:THR:HB	1.81	0.62
1:B:2209:LEU:O	1:B:2213:THR:HG23	2.00	0.62
1:A:3343:LYS:HG2	1:A:3357:ARG:HD2	1.81	0.62
1:B:1795:CYS:HB3	1:B:1921:LEU:HB3	1.82	0.62
2:D:94:PHE:HD2	2:D:128:PRO:HB2	1.66	0.61
1:A:50:GLU:O	1:A:54:ILE:HG12	1.99	0.61
1:A:2104:ILE:HD12	1:A:2204:LEU:HD13	1.80	0.61
1:B:668:PHE:O	1:B:672:ILE:HG22	2.00	0.61
2:C:94:PHE:HD2	2:C:128:PRO:HB2	1.65	0.61
1:B:313:LEU:O	1:B:317:ILE:HG12	2.01	0.61
1:B:579:MET:HE2	1:B:579:MET:N	2.16	0.61
1:B:1462:LEU:H	1:B:1846:PHE:HZ	1.49	0.61
1:A:88:TRP:O	1:A:92:MET:HB3	2.00	0.61
1:A:758:VAL:HG23	1:A:894:LEU:HD11	1.82	0.61
1:A:3704:TYR:HB3	1:A:3769:VAL:HG21	1.80	0.61
1:A:2201:LEU:O	1:A:2205:ILE:HG12	2.01	0.61
1:B:2095:ASN:HD21	1:B:2163:GLY:H	1.47	0.61
1:A:1462:LEU:H	1:A:1846:PHE:HZ	1.49	0.61
1:A:2209:LEU:O	1:A:2213:THR:HG23	2.01	0.61
1:B:3508:MET:HE3	1:B:3508:MET:HA	1.83	0.61
1:A:2095:ASN:HD21	1:A:2163:GLY:H	1.49	0.60
1:B:1390:LEU:HD23	1:B:1748:ILE:HB	1.83	0.60
1:B:2706:ARG:HG3	1:B:2752:SER:HB2	1.82	0.60
1:A:206:ALA:HA	1:A:209:ARG:HE	1.66	0.60
1:A:440:VAL:O	1:A:444:ILE:HG12	2.01	0.60
1:A:3599:MET:HE1	1:A:3633:VAL:HG21	1.82	0.60
1:B:3585:VAL:HG13	1:B:3633:VAL:HG23	1.83	0.60
1:A:290:TRP:HA	1:B:123:GLN:NE2	2.16	0.60
1:A:3118:MET:SD	1:A:3190:PRO:HB2	2.42	0.60
1:A:2727:ILE:HB	1:A:2777:ILE:HB	1.84	0.60
1:B:584:VAL:HA	1:B:588:MET:HE3	1.83	0.60
1:B:905:ILE:HD13	1:B:908:LYS:HZ1	1.67	0.60
1:B:1324:ASP:HA	1:B:1327:LYS:HG3	1.83	0.60
1:B:2201:LEU:O	1:B:2205:ILE:HG12	2.01	0.60
1:B:2727:ILE:HB	1:B:2777:ILE:HB	1.84	0.60
2:D:335:ILE:HD12	2:D:339:ASP:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1400:ARG:HB3	1:A:1438:GLU:HB2	1.82	0.60
2:C:30:LEU:HB3	2:C:97:PRO:HB3	1.84	0.59
1:B:1952:LEU:O	1:B:1956:THR:HG23	2.02	0.59
2:C:513:ARG:HH11	2:C:514:GLY:H	1.49	0.59
1:B:484:ASP:HB3	1:B:487:ARG:HE	1.67	0.59
1:B:580:GLY:O	1:B:584:VAL:HG23	2.02	0.59
1:A:482:ASP:HB2	1:A:487:ARG:HH12	1.66	0.59
1:B:987:ILE:HG13	1:B:991:ILE:HD11	1.85	0.59
1:B:3543:THR:O	1:B:3547:MET:HG2	2.02	0.59
1:A:983:VAL:O	1:A:987:ILE:HG22	2.03	0.59
1:A:2548:ASP:O	1:A:2552:GLU:HG3	2.02	0.59
1:A:303:GLU:HA	1:A:306:LEU:HB2	1.82	0.59
1:B:584:VAL:HG22	1:B:617:TYR:HD2	1.67	0.59
1:A:2262:ASP:HB3	1:A:2265:LYS:HG2	1.85	0.59
1:B:1244:VAL:HG12	1:B:1270:CYS:HB2	1.85	0.59
2:D:99:CYS:SG	2:D:112:HIS:HE1	2.20	0.59
1:B:624:PHE:CZ	1:B:633:LEU:HD11	2.38	0.59
1:B:2329:ILE:HG12	1:B:2417:LEU:HD13	1.84	0.58
1:A:580:GLY:O	1:A:584:VAL:HG23	2.03	0.58
1:B:1120:LEU:HD13	1:B:1347:ILE:HG22	1.85	0.58
1:B:2043:THR:HB	1:B:2183:ILE:HD11	1.85	0.58
2:D:513:ARG:HH11	2:D:514:GLY:H	1.50	0.58
1:A:3600:VAL:O	1:A:3604:MET:HG2	2.03	0.58
1:B:2329:ILE:HD11	1:B:2417:LEU:HB2	1.84	0.58
1:A:1788:LEU:O	1:A:1791:LEU:HB3	2.03	0.58
1:A:162:TRP:CG	1:A:266:LYS:HZ1	2.20	0.58
1:A:2268:PRO:O	1:A:2269:MET:HE2	2.03	0.58
1:A:3332:LEU:HD22	1:A:3378:VAL:HG21	1.86	0.58
1:A:3417:ILE:HD13	1:A:3454:ILE:HD11	1.85	0.58
1:B:761:LYS:HD3	1:B:894:LEU:HB2	1.86	0.58
1:B:2548:ASP:O	1:B:2552:GLU:HG3	2.04	0.58
1:A:2108:LEU:HD11	1:A:2208:ILE:HG12	1.86	0.58
1:A:2722:VAL:HG21	1:A:2790:LEU:HD11	1.85	0.58
1:B:758:VAL:O	1:B:762:MET:HG2	2.04	0.58
1:A:486:LYS:HD2	1:A:487:ARG:N	2.18	0.58
1:A:758:VAL:O	1:A:762:MET:HG2	2.03	0.58
1:A:987:ILE:HG13	1:A:991:ILE:HD11	1.85	0.58
1:B:303:GLU:HA	1:B:306:LEU:HB2	1.85	0.58
1:B:576:TRP:HH2	1:B:602:ILE:H	1.51	0.58
1:A:1488:GLN:H	1:A:1488:GLN:CD	2.12	0.58
1:B:744:THR:HA	1:B:838:GLY:HA3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:ALA:O	1:A:520:PHE:HB2	2.04	0.57
1:A:1432:LEU:HD11	1:A:1446:LEU:HD12	1.85	0.57
1:B:930:LEU:HD21	1:B:945:ARG:HB3	1.86	0.57
1:A:369:VAL:O	1:A:372:TYR:HB3	2.04	0.57
1:B:2722:VAL:HG21	1:B:2790:LEU:HD11	1.85	0.57
1:B:3399:MET:HA	1:B:3402:ILE:HD12	1.86	0.57
1:B:1448:TYR:HB2	1:B:1463:ARG:HB2	1.86	0.57
1:A:3417:ILE:HD11	1:A:3443:MET:HE1	1.87	0.57
1:B:945:ARG:O	1:B:949:VAL:HG23	2.04	0.57
1:A:245:LEU:HD12	1:A:245:LEU:O	2.05	0.57
1:A:2070:MET:HG2	1:A:2119:LEU:HD13	1.86	0.57
2:C:265:ASN:HD22	1:B:2943:GLU:HG2	1.69	0.57
1:B:1:MET:HE2	1:B:1:MET:HA	1.86	0.57
1:B:1788:LEU:O	1:B:1791:LEU:HB3	2.04	0.57
1:A:400:ARG:HB2	1:A:439:ILE:HG22	1.87	0.57
1:A:3563:VAL:HA	1:A:3574:LEU:HD11	1.86	0.57
1:A:2318:ARG:HG2	1:A:2410:TRP:CZ2	2.39	0.57
1:A:3508:MET:HA	1:A:3508:MET:HE3	1.87	0.57
1:B:1120:LEU:HD12	1:B:1123:GLU:HB2	1.87	0.57
1:B:1895:LEU:HD21	1:B:1900:ILE:HG23	1.87	0.57
1:B:2046:PRO:O	1:B:2050:LYS:HE2	2.05	0.57
1:B:3372:GLY:HA3	1:B:3542:MET:HE1	1.85	0.57
1:A:2145:MET:HE3	1:A:2145:MET:HA	1.87	0.57
1:B:2262:ASP:HB3	1:B:2265:LYS:HG2	1.86	0.57
1:A:3114:ILE:HG22	1:A:3118:MET:HE2	1.87	0.57
1:B:704:THR:HA	1:B:707:LEU:HD12	1.87	0.57
1:B:1432:LEU:HD11	1:B:1446:LEU:HD12	1.87	0.57
1:B:1552:ARG:HG2	1:B:1566:GLU:HG3	1.85	0.57
1:A:1895:LEU:HD21	1:A:1900:ILE:HG23	1.87	0.56
1:A:2305:LEU:HD22	1:A:2398:LEU:HD11	1.87	0.56
1:A:3691:LEU:HB3	1:A:3756:HIS:HB3	1.86	0.56
1:B:983:VAL:O	1:B:987:ILE:HG22	2.05	0.56
1:A:286:ASP:O	1:A:290:TRP:HD1	1.88	0.56
1:A:379:LEU:HD23	1:A:414:ILE:HD13	1.87	0.56
1:A:584:VAL:HG22	1:A:617:TYR:HD2	1.69	0.56
2:C:278:ILE:HG13	2:C:389:GLY:HA2	1.87	0.56
1:B:960:LEU:HD13	1:B:977:ILE:HG21	1.86	0.56
1:B:1031:SER:O	1:B:1035:GLN:HG2	2.05	0.56
1:B:3563:VAL:HA	1:B:3574:LEU:HD11	1.86	0.56
2:D:30:LEU:HB3	2:D:97:PRO:HB3	1.86	0.56
1:A:2217:SER:HB3	1:A:2274:TYR:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3325:LYS:HZ3	1:B:3370:ARG:HE	1.52	0.56
1:A:420:GLU:HA	1:A:423:ARG:NE	2.19	0.56
1:B:579:MET:HA	1:B:582:ILE:HG12	1.88	0.56
1:B:652:MET:N	1:B:652:MET:HE2	2.20	0.56
1:B:2321:CYS:HA	1:B:2388:ILE:HD11	1.87	0.56
1:A:741:PHE:O	1:A:747:MET:HE3	2.06	0.56
1:A:1078:GLU:HG3	1:A:1079:PRO:HD3	1.87	0.56
1:A:1230:TRP:HZ2	1:A:1262:LYS:HE2	1.70	0.56
1:A:1287:SER:HB3	1:A:1793:GLU:HB2	1.87	0.56
1:B:51:ALA:O	1:B:55:LEU:HG	2.05	0.56
1:B:1424:ILE:HD12	1:B:1432:LEU:HD23	1.88	0.56
1:B:3398:VAL:O	1:B:3402:ILE:HG13	2.06	0.56
1:B:3417:ILE:HD13	1:B:3454:ILE:HD11	1.88	0.56
1:B:663:LYS:O	1:B:667:GLU:HG2	2.05	0.56
1:B:1287:SER:HB3	1:B:1793:GLU:HB2	1.87	0.56
1:B:3474:VAL:HG22	1:B:3504:ILE:HG12	1.88	0.56
1:A:286:ASP:O	1:A:290:TRP:CD1	2.59	0.56
1:A:3325:LYS:HZ3	1:A:3370:ARG:HH21	1.53	0.56
1:A:3543:THR:O	1:A:3547:MET:HG2	2.06	0.56
1:A:3563:VAL:HG21	1:A:3606:VAL:HG13	1.88	0.56
2:C:432:GLU:HG2	2:C:436:LYS:HE3	1.88	0.56
1:B:379:LEU:HD23	1:B:414:ILE:HD13	1.88	0.56
1:B:717:TRP:HH2	1:B:799:GLU:HB3	1.70	0.56
2:D:29:CYS:SG	2:D:59:HIS:HE1	2.18	0.56
1:A:717:TRP:HH2	1:A:799:GLU:HB3	1.71	0.56
1:A:741:PHE:CE1	1:A:898:ILE:HD13	2.37	0.56
1:B:440:VAL:O	1:B:444:ILE:HG12	2.06	0.56
1:A:264:PHE:CE1	1:A:268:ILE:HG13	2.41	0.56
1:A:383:ILE:HD12	1:A:417:ALA:HB3	1.88	0.56
1:B:805:MET:O	1:B:809:ILE:HG12	2.06	0.56
1:B:1380:ILE:HD13	1:B:1709:ILE:HB	1.87	0.56
1:B:1623:GLY:HA3	1:B:1626:MET:HE3	1.87	0.56
1:A:2713:ILE:HG12	1:A:2791:ILE:HG12	1.88	0.55
1:A:3474:VAL:HG22	1:A:3504:ILE:HG12	1.88	0.55
1:A:3600:VAL:HG12	1:A:3646:ILE:HG22	1.88	0.55
1:B:1230:TRP:HZ2	1:B:1262:LYS:HE2	1.70	0.55
1:A:209:ARG:HH22	1:A:238:TYR:HA	1.71	0.55
1:A:574:GLU:HG2	1:A:575:LYS:N	2.21	0.55
1:A:1469:ILE:HG13	1:A:1470:PRO:HD2	1.87	0.55
1:A:1475:SER:HB3	1:A:1486:CYS:HB2	1.88	0.55
1:A:2043:THR:HB	1:A:2183:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ARG:HH22	1:B:238:TYR:HA	1.71	0.55
1:B:1469:ILE:HG13	1:B:1470:PRO:HD2	1.88	0.55
1:A:584:VAL:HA	1:A:588:MET:HE3	1.89	0.55
1:A:1270:CYS:SG	1:A:1275:CYS:HB3	2.47	0.55
1:B:1498:PRO:HG2	1:B:1499:GLN:NE2	2.21	0.55
1:B:2268:PRO:O	1:B:2269:MET:HE2	2.07	0.55
1:A:1120:LEU:HD12	1:A:1123:GLU:HB3	1.87	0.55
1:A:2464:LYS:NZ	1:A:2480:GLU:HG3	2.21	0.55
1:B:2451:LYS:HA	1:B:2498:MET:HE1	1.87	0.55
1:A:667:GLU:HA	1:A:670:LYS:HE3	1.89	0.55
1:A:1952:LEU:O	1:A:1956:THR:HG23	2.06	0.55
1:A:3594:LEU:HB3	1:A:3599:MET:SD	2.47	0.55
1:A:241:LEU:O	1:A:245:LEU:HB3	2.06	0.55
1:A:408:PHE:HZ	1:A:447:PRO:HD2	1.71	0.55
1:A:1002:TYR:HD2	1:A:1049:LEU:HD13	1.72	0.55
1:B:539:ILE:O	1:B:543:ILE:HG23	2.07	0.55
1:B:634:HIS:HB3	1:B:638:TYR:CE1	2.42	0.55
1:A:1623:GLY:HA3	1:A:1626:MET:HE3	1.87	0.55
1:A:2252:PHE:CG	1:A:2308:ILE:HD11	2.42	0.55
1:B:238:TYR:O	1:B:242:ILE:HG22	2.06	0.55
1:B:408:PHE:HZ	1:B:447:PRO:HD2	1.72	0.55
1:B:2305:LEU:HD22	1:B:2398:LEU:HD11	1.88	0.55
1:B:1789:VAL:HA	1:B:1886:ARG:HE	1.72	0.55
1:B:3383:LEU:HD11	1:B:3399:MET:HE3	1.89	0.55
2:D:278:ILE:HG13	2:D:389:GLY:HA2	1.88	0.55
1:A:387:ARG:NH2	1:B:113:ILE:H	2.05	0.55
1:A:3546:LEU:HB3	1:A:3547:MET:HE2	1.89	0.55
1:A:3770:ILE:HG12	1:A:3812:LEU:HD13	1.89	0.55
1:B:369:VAL:O	1:B:372:TYR:HB3	2.06	0.55
1:B:843:LYS:HE3	1:B:843:LYS:HA	1.89	0.55
1:A:652:MET:HE2	1:A:652:MET:N	2.23	0.54
1:A:1244:VAL:HG12	1:A:1270:CYS:HB2	1.89	0.54
1:B:245:LEU:O	1:B:245:LEU:HD12	2.07	0.54
1:A:1495:ARG:HB3	1:A:1504:ASP:HB2	1.89	0.54
1:B:399:MET:HE3	1:B:422:LEU:HD22	1.89	0.54
1:B:619:VAL:HA	1:B:622:MET:HE1	1.88	0.54
1:B:894:LEU:O	1:B:898:ILE:HG22	2.07	0.54
1:B:3691:LEU:HB3	1:B:3756:HIS:HB3	1.89	0.54
2:C:25:ASN:HB3	2:C:67:LEU:HD11	1.90	0.54
1:B:279:ARG:O	1:B:283:LYS:HG2	2.07	0.54
1:A:1041:LEU:HD21	1:A:1107:MET:HE3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2874:ILE:HB	1:A:2985:TYR:CD2	2.42	0.54
1:A:3333:ILE:HB	1:A:3378:VAL:HB	1.89	0.54
1:B:2178:PRO:HA	1:B:2181:MET:HG2	1.88	0.54
1:A:243:LYS:HA	1:A:290:TRP:CZ3	2.42	0.54
1:A:713:SER:O	1:A:716:VAL:HG12	2.08	0.54
1:A:874:SER:O	1:A:878:LYS:HD2	2.07	0.54
1:A:1454:ASN:HD22	1:A:1457:GLN:HB2	1.73	0.54
1:A:2451:LYS:HA	1:A:2498:MET:HE1	1.88	0.54
1:B:1525:VAL:HG12	1:B:1526:ARG:HG2	1.90	0.54
1:A:938:ARG:HH21	1:A:997:PRO:HD3	1.73	0.54
1:A:3654:TRP:HE1	1:A:3682:MET:HG3	1.71	0.54
1:B:723:LEU:HD11	1:B:738:PHE:CE1	2.43	0.54
1:B:3770:ILE:HG12	1:B:3812:LEU:HD13	1.89	0.54
1:A:806:HIS:CE1	1:A:842:TYR:HE2	2.26	0.54
1:A:2943:GLU:HG2	2:D:265:ASN:HD22	1.72	0.54
1:A:3448:ARG:HB2	1:A:3481:LEU:HB3	1.89	0.54
1:B:1078:GLU:HG3	1:B:1079:PRO:HD3	1.88	0.54
1:B:2179:GLU:HA	1:B:2182:LEU:HD12	1.89	0.54
1:B:3337:HIS:HA	1:B:3340:ILE:HG12	1.90	0.54
1:B:3621:LEU:HA	1:B:3624:MET:SD	2.47	0.54
1:A:670:LYS:HD2	1:A:671:ILE:N	2.23	0.54
1:A:2389:LEU:HG	1:A:2433:LEU:HD12	1.90	0.54
1:B:1567:MET:HB3	1:B:1613:ILE:HG23	1.88	0.54
1:B:1691:LEU:HD21	1:B:1720:ILE:HD13	1.88	0.54
1:B:76:MET:HA	1:B:79:ILE:HG12	1.90	0.53
1:B:591:ARG:HH21	1:B:595:GLU:HB3	1.73	0.53
1:B:2725:VAL:HB	1:B:2779:LEU:HB2	1.90	0.53
2:D:25:ASN:HB3	2:D:67:LEU:HD11	1.89	0.53
1:A:286:ASP:HB3	1:A:290:TRP:HE1	1.73	0.53
1:A:584:VAL:O	1:A:588:MET:HG2	2.08	0.53
1:B:633:LEU:HA	1:B:636:LYS:HG2	1.91	0.53
1:A:539:ILE:O	1:A:543:ILE:HG23	2.07	0.53
1:B:1218:TYR:HD2	1:B:1278:MET:HE1	1.73	0.53
1:B:2217:SER:HB3	1:B:2274:TYR:HB3	1.90	0.53
1:B:2495:ARG:HH21	1:B:2497:ASP:CG	2.16	0.53
2:D:465:LYS:O	2:D:469:GLN:HB3	2.08	0.53
1:A:31:ILE:O	1:A:35:ARG:HG2	2.08	0.53
1:A:290:TRP:HA	1:B:123:GLN:HE22	1.73	0.53
1:A:896:MET:HA	1:A:896:MET:HE2	1.89	0.53
1:B:264:PHE:CE1	1:B:268:ILE:HG13	2.43	0.53
1:B:482:ASP:HB2	1:B:487:ARG:HH12	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1573:ASN:HB3	1:B:1594:SER:HB2	1.91	0.53
1:A:591:ARG:HH21	1:A:595:GLU:HB3	1.74	0.53
1:A:805:MET:O	1:A:809:ILE:HG12	2.09	0.53
1:B:31:ILE:O	1:B:35:ARG:HG2	2.08	0.53
1:B:938:ARG:HH21	1:B:997:PRO:HD3	1.73	0.53
1:B:2713:ILE:HG12	1:B:2791:ILE:HG12	1.89	0.53
1:B:3574:LEU:HB3	1:B:3622:ILE:HG21	1.90	0.53
1:A:207:LEU:HD13	1:A:263:ILE:HG21	1.89	0.53
1:A:484:ASP:HB3	1:A:487:ARG:HE	1.73	0.53
1:A:3574:LEU:HB3	1:A:3622:ILE:HG21	1.90	0.53
1:B:383:ILE:HD12	1:B:417:ALA:HB3	1.91	0.53
1:B:484:ASP:CB	1:B:487:ARG:HE	2.21	0.53
1:B:2104:ILE:HD12	1:B:2204:LEU:HD13	1.89	0.53
1:A:238:TYR:O	1:A:242:ILE:HG22	2.07	0.53
1:A:472:THR:HG22	1:A:476:MET:HE1	1.90	0.53
1:A:704:THR:HA	1:A:707:LEU:HD12	1.90	0.53
1:B:975:LEU:O	1:B:979:LYS:HG2	2.09	0.53
1:A:1120:LEU:HD13	1:A:1347:ILE:HG22	1.90	0.53
1:A:1563:PHE:CE2	1:A:1566:GLU:HB2	2.43	0.53
1:A:3621:LEU:HA	1:A:3624:MET:SD	2.48	0.53
1:B:1454:ASN:HD22	1:B:1457:GLN:HB2	1.73	0.53
1:A:1691:LEU:HD21	1:A:1720:ILE:HD13	1.91	0.53
1:A:3398:VAL:O	1:A:3402:ILE:HG13	2.08	0.53
2:C:424:GLN:HE21	2:C:429:SER:HA	1.73	0.53
1:B:638:TYR:HB3	1:B:641:LEU:HD12	1.91	0.53
1:B:3102:ALA:HB2	2:D:424:GLN:HE21	1.73	0.53
1:A:1525:VAL:HG12	1:A:1526:ARG:HG2	1.90	0.53
1:A:2326:GLU:HB3	1:A:2413:LYS:HE2	1.91	0.53
1:B:465:ARG:HD2	1:B:507:TYR:CD1	2.44	0.53
1:A:145:ILE:HG13	1:A:146:TRP:CD1	2.43	0.52
1:B:158:MET:HE2	1:B:158:MET:N	2.24	0.52
1:B:762:MET:HE2	1:B:762:MET:N	2.24	0.52
1:A:176:GLN:O	1:A:180:LEU:HG	2.08	0.52
1:A:754:MET:O	1:A:757:LYS:HG3	2.10	0.52
1:A:960:LEU:HD21	1:A:1017:HIS:CD2	2.45	0.52
1:A:2725:VAL:HB	1:A:2779:LEU:HB2	1.91	0.52
1:B:2041:VAL:HG11	1:B:2048:PHE:CD1	2.44	0.52
2:D:432:GLU:HG2	2:D:436:LYS:HE3	1.91	0.52
1:A:1789:VAL:HA	1:A:1886:ARG:HE	1.74	0.52
2:C:465:LYS:O	2:C:469:GLN:HB3	2.09	0.52
1:B:2874:ILE:HD12	1:B:2879:GLU:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3447:MET:HE2	1:B:3481:LEU:HA	1.91	0.52
1:A:313:LEU:O	1:A:317:ILE:HG12	2.10	0.52
1:A:1292:ARG:HA	1:A:1928:MET:HA	1.92	0.52
1:A:3351:ARG:HD3	1:B:2892:ILE:HD13	1.90	0.52
1:B:1292:ARG:HA	1:B:1928:MET:HA	1.91	0.52
1:A:314:VAL:HA	1:A:317:ILE:HG12	1.92	0.52
1:A:379:LEU:HA	1:A:382:ILE:HG22	1.92	0.52
1:A:1543:ILE:HG23	1:A:1554:TYR:HB2	1.91	0.52
1:A:2721:GLU:HG3	1:A:2786:VAL:HG22	1.92	0.52
1:B:1039:LYS:HA	1:B:1042:GLU:HG3	1.92	0.52
1:A:279:ARG:O	1:A:283:LYS:HG2	2.10	0.52
1:A:396:VAL:HG11	1:A:435:ASP:HB3	1.91	0.52
1:A:1380:ILE:HD11	1:A:1670:LYS:HE3	1.90	0.52
1:B:704:THR:O	1:B:707:LEU:HB2	2.09	0.52
1:B:705:GLU:O	1:B:708:VAL:HG22	2.10	0.52
1:B:713:SER:O	1:B:716:VAL:HG12	2.09	0.52
1:B:2045:TRP:CD1	1:B:2095:ASN:HD22	2.27	0.52
1:A:206:ALA:HA	1:A:209:ARG:NE	2.25	0.52
1:A:1323:CYS:O	1:A:1326:LEU:HB2	2.10	0.52
1:A:3337:HIS:HA	1:A:3340:ILE:HG12	1.92	0.52
1:B:672:ILE:HD11	1:B:714:ILE:HG13	1.92	0.52
1:B:2414:LEU:HD21	1:B:2433:LEU:HB3	1.91	0.52
1:B:2695:VAL:HG22	1:B:2864:VAL:HG22	1.92	0.52
1:A:1031:SER:HA	1:A:1034:LYS:HD2	1.92	0.52
1:A:132:ALA:HB1	1:A:137:LEU:HD22	1.93	0.51
1:A:2662:MET:HE3	1:A:2666:MET:HE3	1.91	0.51
1:A:3601:GLU:HG3	1:A:3602:ARG:N	2.24	0.51
1:A:292:LYS:HE3	1:B:42:SER:O	2.10	0.51
2:C:146:ASN:HB3	2:C:149:VAL:HG12	1.93	0.51
1:B:492:ASN:HB3	1:B:535:LEU:HD21	1.90	0.51
1:B:480:LEU:HD12	1:B:520:PHE:HE1	1.76	0.51
1:B:1173:ALA:HA	1:B:1178:LEU:HD12	1.92	0.51
1:B:2662:MET:HE3	1:B:2666:MET:HE3	1.91	0.51
1:B:3448:ARG:HB2	1:B:3481:LEU:HB3	1.91	0.51
1:B:3625:GLU:O	1:B:3629:VAL:HG23	2.10	0.51
1:A:1176:PHE:HB3	1:A:2044:ARG:HH21	1.75	0.51
1:B:76:MET:O	1:B:80:THR:HG23	2.11	0.51
1:B:464:VAL:HA	1:B:467:GLU:OE2	2.10	0.51
1:B:3713:ILE:HA	1:B:3738:MET:HE1	1.92	0.51
1:A:199:ALA:HB1	1:A:245:LEU:HD11	1.92	0.51
1:A:488:GLU:HA	1:A:491:VAL:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1244:VAL:HB	1:A:1248:CYS:HB2	1.93	0.51
1:A:1852:MET:HE2	1:A:1886:ARG:HG2	1.91	0.51
1:A:2270:SER:HB3	1:A:2273:SER:HB3	1.91	0.51
1:A:2699:THR:HA	1:A:2702:LYS:HD3	1.92	0.51
1:A:2727:ILE:HG12	1:A:2861:LEU:HD12	1.91	0.51
1:A:3685:SER:O	1:A:3689:ILE:HG13	2.11	0.51
1:B:495:HIS:CE1	1:B:539:ILE:HG12	2.46	0.51
1:A:52:MET:HA	1:A:55:LEU:HG	1.92	0.51
1:A:484:ASP:N	1:A:487:ARG:HH21	2.08	0.51
1:A:495:HIS:CE1	1:A:539:ILE:HG12	2.45	0.51
1:A:1046:GLN:O	1:A:1050:LEU:HG	2.10	0.51
1:B:2076:HIS:CD2	1:B:2077:ARG:HG2	2.46	0.51
1:B:3599:MET:SD	1:B:3633:VAL:HG11	2.50	0.51
1:A:3337:HIS:CD2	2:C:480:MET:HE1	2.45	0.51
1:A:3337:HIS:HD2	2:C:480:MET:HE1	1.76	0.51
1:B:397:GLN:O	1:B:401:VAL:HG22	2.10	0.51
1:B:574:GLU:HG2	1:B:575:LYS:N	2.25	0.51
1:A:465:ARG:HD2	1:A:507:TYR:CD1	2.46	0.51
1:A:934:ASP:HB2	1:A:937:LYS:HG2	1.93	0.51
1:A:1324:ASP:HA	1:A:1327:LYS:HG3	1.93	0.51
1:A:2179:GLU:HA	1:A:2182:LEU:HD12	1.92	0.51
1:A:3332:LEU:HD21	1:A:3375:LEU:HG	1.93	0.51
1:B:934:ASP:HB2	1:B:937:LYS:HG2	1.93	0.51
1:B:1291:LEU:HD13	1:B:1794:GLN:HB3	1.92	0.51
1:B:1495:ARG:HB3	1:B:1504:ASP:HB2	1.92	0.51
1:B:1495:ARG:HH21	1:B:2356:PRO:HD3	1.76	0.51
1:B:2705:ILE:HG23	1:B:2714:TYR:CE1	2.46	0.51
1:B:2721:GLU:HG3	1:B:2786:VAL:HG22	1.92	0.51
1:A:397:GLN:O	1:A:401:VAL:HG22	2.11	0.51
1:A:605:LEU:HA	1:A:651:PHE:CE2	2.45	0.51
1:A:1213:LEU:HB3	1:A:1285:PRO:HG2	1.92	0.51
1:A:2705:ILE:HG23	1:A:2714:TYR:CE1	2.46	0.51
1:A:3203:MET:HB3	1:A:3206:ARG:NH2	2.26	0.51
1:A:3447:MET:HE2	1:A:3481:LEU:HA	1.93	0.51
1:A:3448:ARG:HA	1:A:3481:LEU:HD22	1.93	0.51
1:B:1598:LEU:HB3	1:B:1619:VAL:HG22	1.92	0.51
1:B:2073:MET:HG3	1:B:2074:PRO:HD2	1.93	0.51
1:B:2237:ALA:HB1	1:B:2289:VAL:HG21	1.93	0.51
1:B:2252:PHE:CG	1:B:2308:ILE:HD11	2.46	0.51
1:B:2727:ILE:HG12	1:B:2861:LEU:HD12	1.92	0.51
1:B:3599:MET:O	1:B:3603:MET:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:THR:O	1:A:707:LEU:HB2	2.11	0.51
1:A:1390:LEU:HD23	1:A:1748:ILE:HB	1.93	0.51
1:A:2744:TYR:HB2	1:A:2791:ILE:HB	1.93	0.51
1:B:1011:PRO:O	1:B:1015:ILE:HG13	2.11	0.51
1:B:2699:THR:HA	1:B:2702:LYS:HD3	1.93	0.51
1:A:761:LYS:HD3	1:A:894:LEU:HD12	1.93	0.50
1:A:1102:LEU:O	1:A:1106:LYS:HG3	2.11	0.50
1:A:3399:MET:HA	1:A:3402:ILE:HD12	1.94	0.50
1:A:3625:GLU:O	1:A:3629:VAL:HG23	2.11	0.50
1:A:3734:LYS:O	1:A:3738:MET:HE2	2.12	0.50
1:B:379:LEU:HA	1:B:382:ILE:HG22	1.93	0.50
1:B:396:VAL:HG11	1:B:435:ASP:HB3	1.92	0.50
1:B:605:LEU:HA	1:B:651:PHE:CE2	2.46	0.50
1:B:738:PHE:O	1:B:741:PHE:HB3	2.11	0.50
1:B:1543:ILE:HG23	1:B:1554:TYR:HB2	1.92	0.50
1:B:3336:LEU:HD21	1:B:3398:VAL:HG11	1.93	0.50
1:B:3538:GLN:O	1:B:3542:MET:HG2	2.12	0.50
2:D:146:ASN:HB3	2:D:149:VAL:HG12	1.93	0.50
1:A:492:ASN:HB3	1:A:535:LEU:HD21	1.92	0.50
1:A:712:PHE:O	1:A:715:GLU:HB3	2.10	0.50
1:B:2270:SER:HB3	1:B:2273:SER:HB3	1.93	0.50
1:B:2866:ARG:HD3	1:B:2867:ALA:N	2.26	0.50
1:A:252:LYS:HE3	1:A:253:ASP:OD2	2.11	0.50
1:B:2107:PHE:HA	1:B:2110:ILE:HD12	1.92	0.50
1:A:541:LEU:HD22	1:A:597:LEU:HD23	1.93	0.50
1:A:930:LEU:HD21	1:A:945:ARG:HB3	1.94	0.50
1:A:975:LEU:O	1:A:979:LYS:HG2	2.11	0.50
1:B:214:SER:HA	1:B:231:TYR:OH	2.10	0.50
1:B:1690:CYS:SG	1:B:1700:ASN:HB2	2.51	0.50
1:B:1767:GLU:OE2	1:B:1769:TYR:HB2	2.12	0.50
1:B:30:ILE:O	1:B:34:LEU:HG	2.11	0.50
1:B:1176:PHE:HB3	1:B:2044:ARG:HH21	1.75	0.50
1:B:1213:LEU:HB3	1:B:1285:PRO:HG2	1.92	0.50
1:B:3251:SER:O	1:B:3255:ILE:HG12	2.11	0.50
1:A:158:MET:N	1:A:158:MET:HE2	2.27	0.50
1:A:3251:SER:O	1:A:3255:ILE:HG12	2.11	0.50
1:B:2744:TYR:HB2	1:B:2791:ILE:HB	1.92	0.50
1:A:214:SER:HA	1:A:231:TYR:OH	2.12	0.50
1:A:1424:ILE:HD12	1:A:1432:LEU:HD23	1.94	0.50
1:A:1573:ASN:HB3	1:A:1594:SER:HB2	1.93	0.50
1:B:3538:GLN:HG3	1:B:3541:ARG:HE	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3820:GLN:HE22	1:B:3856:GLU:HB2	1.77	0.50
1:A:482:ASP:HB2	1:A:487:ARG:HH22	1.76	0.50
1:A:1259:ALA:HB1	1:A:1882:THR:HB	1.93	0.50
1:B:400:ARG:HE	1:B:401:VAL:HG13	1.77	0.50
1:B:1323:CYS:O	1:B:1326:LEU:HB2	2.12	0.50
1:B:1475:SER:HB3	1:B:1486:CYS:HB2	1.93	0.50
1:B:2067:ARG:HG3	1:B:2110:ILE:HG12	1.94	0.50
1:B:3601:GLU:HG3	1:B:3602:ARG:N	2.25	0.50
1:A:3820:GLN:HE22	1:A:3856:GLU:HB2	1.77	0.50
1:B:2389:LEU:HD21	1:B:2429:GLN:HB3	1.92	0.50
1:B:3385:LEU:HD22	2:D:479:LYS:HE3	1.94	0.50
1:A:189:PHE:HD1	1:A:192:MET:HE1	1.77	0.49
1:A:1034:LYS:HG2	1:A:1103:TYR:CD2	2.45	0.49
1:A:2318:ARG:HG2	1:A:2410:TRP:HZ2	1.77	0.49
1:B:482:ASP:CB	1:B:487:ARG:HH22	2.24	0.49
1:B:2874:ILE:HG12	1:B:2981:GLU:OE2	2.12	0.49
1:A:400:ARG:HE	1:A:401:VAL:HG13	1.76	0.49
1:A:2325:LEU:HD11	1:A:2417:LEU:HD22	1.94	0.49
1:B:647:ILE:HA	1:B:650:LYS:HG2	1.94	0.49
1:B:1737:VAL:HG22	1:B:1748:ILE:HG23	1.94	0.49
1:A:123:GLN:NE2	1:B:290:TRP:HA	2.28	0.49
1:A:436:PHE:CZ	1:A:459:ILE:HG12	2.47	0.49
1:A:1031:SER:O	1:A:1035:GLN:HG3	2.12	0.49
1:B:132:ALA:HB1	1:B:137:LEU:HD22	1.93	0.49
1:A:2543:SER:HB3	1:A:2588:LEU:HD21	1.94	0.49
1:A:3719:PRO:HD3	1:A:3734:LYS:HE2	1.94	0.49
2:C:492:MET:HE1	1:B:2991:VAL:HG11	1.94	0.49
1:B:1244:VAL:HB	1:B:1248:CYS:HB2	1.94	0.49
1:B:1705:THR:HG22	1:B:1706:VAL:H	1.77	0.49
1:B:3809:LEU:HD22	1:B:3823:ILE:HD13	1.95	0.49
1:A:133:LEU:HD12	1:A:192:MET:HG3	1.95	0.49
1:A:520:PHE:HA	1:A:523:VAL:HG12	1.95	0.49
1:A:3559:LEU:O	1:A:3563:VAL:HG23	2.13	0.49
1:B:2145:MET:HE1	1:B:2192:ILE:HG12	1.95	0.49
1:A:199:ALA:HB1	1:A:245:LEU:CD1	2.43	0.49
1:A:520:PHE:CZ	1:A:536:ALA:HA	2.47	0.49
1:A:576:TRP:HZ3	1:A:602:ILE:HG22	1.77	0.49
1:A:612:MET:HA	1:A:615:LEU:HD12	1.95	0.49
1:A:1434:VAL:HG12	1:A:1446:LEU:HD13	1.94	0.49
1:A:2702:LYS:HD2	1:A:2705:ILE:HD11	1.94	0.49
1:A:3214:VAL:HA	1:A:3255:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3417:ILE:HD12	1:A:3431:MET:HE1	1.94	0.49
1:A:3423:GLN:HE21	1:A:3512:MET:HE1	1.77	0.49
2:D:130:CYS:HB3	2:D:142:LYS:HG2	1.95	0.49
1:A:1705:THR:HG22	1:A:1706:VAL:H	1.76	0.49
1:A:2107:PHE:HA	1:A:2110:ILE:HD12	1.94	0.49
1:A:3679:LEU:HA	1:A:3682:MET:HB2	1.94	0.49
1:A:3731:ILE:HG22	1:A:3736:GLN:HG2	1.95	0.49
1:B:630:GLY:O	1:B:633:LEU:HD12	2.13	0.49
1:B:1259:ALA:HB1	1:B:1882:THR:HB	1.94	0.49
1:A:318:LEU:HD21	1:A:405:GLU:HG3	1.95	0.49
1:A:956:PHE:CD2	1:A:977:ILE:HD13	2.48	0.49
1:A:2866:ARG:HD3	1:A:2867:ALA:N	2.26	0.49
2:C:29:CYS:HB2	2:C:35:TYR:HB3	1.95	0.49
1:B:1037:PHE:HB2	1:B:1092:PHE:HE2	1.77	0.49
1:B:3203:MET:HB3	1:B:3206:ARG:NH2	2.27	0.49
1:A:264:PHE:CE2	1:A:284:PHE:HB2	2.47	0.49
1:A:1718:ARG:HH21	1:A:1740:TYR:HD2	1.61	0.49
1:A:2318:ARG:HA	1:A:2321:CYS:HB2	1.95	0.49
1:A:2723:SER:HB3	1:A:2784:PRO:HB3	1.95	0.49
2:C:440:ALA:O	2:C:444:ILE:HG13	2.12	0.49
1:B:149:ASP:HB3	1:B:152:GLU:HG2	1.94	0.49
1:B:918:LYS:O	1:B:922:ARG:HG2	2.11	0.49
1:B:1234:TYR:CD2	1:B:1239:MET:HE3	2.48	0.49
1:B:2244:ASP:OD1	1:B:2246:VAL:HG22	2.12	0.49
1:A:576:TRP:HH2	1:A:602:ILE:H	1.57	0.49
1:A:647:ILE:HA	1:A:650:LYS:HG2	1.95	0.49
1:A:1846:PHE:HD1	1:A:1925:ARG:HH12	1.61	0.49
1:A:2414:LEU:HD21	1:A:2433:LEU:HB3	1.94	0.49
2:C:112:HIS:O	2:C:117:HIS:HB3	2.13	0.49
1:B:2318:ARG:HB2	1:B:2318:ARG:NH1	2.28	0.49
2:D:440:ALA:O	2:D:444:ILE:HG13	2.12	0.49
1:A:418:ALA:O	1:A:421:MET:HG2	2.13	0.48
1:A:579:MET:HE2	1:A:579:MET:N	2.27	0.48
1:A:3690:VAL:HG21	1:A:3700:LEU:HD22	1.95	0.48
1:B:959:LEU:HD21	1:B:973:ALA:HB1	1.94	0.48
1:B:3719:PRO:HD3	1:B:3734:LYS:HE2	1.95	0.48
1:A:30:ILE:O	1:A:34:LEU:HG	2.13	0.48
1:A:663:LYS:O	1:A:667:GLU:HG2	2.13	0.48
1:A:1026:ARG:O	1:A:1030:GLU:HG3	2.13	0.48
1:A:1291:LEU:HD13	1:A:1794:GLN:HB3	1.94	0.48
1:A:1690:CYS:SG	1:A:1700:ASN:HB2	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2046:PRO:O	1:A:2050:LYS:HG3	2.13	0.48
1:B:487:ARG:HA	1:B:490:TYR:HD1	1.78	0.48
1:B:531:ARG:NH1	1:B:531:ARG:HB2	2.29	0.48
1:B:3417:ILE:HD12	1:B:3431:MET:HE1	1.94	0.48
1:A:738:PHE:O	1:A:741:PHE:HB3	2.14	0.48
1:A:742:TRP:HA	1:A:742:TRP:CE3	2.48	0.48
1:A:2385:THR:HA	1:A:2388:ILE:HG22	1.94	0.48
1:B:3448:ARG:HA	1:B:3481:LEU:HD22	1.95	0.48
1:B:3559:LEU:O	1:B:3563:VAL:HG23	2.13	0.48
1:A:139:ARG:NH2	1:A:151:GLU:H	2.12	0.48
1:A:741:PHE:CD1	1:A:895:PHE:HE1	2.31	0.48
1:A:1173:ALA:HA	1:A:1178:LEU:HD12	1.94	0.48
1:A:3761:LYS:HA	1:A:3764:ILE:HD12	1.96	0.48
1:B:46:ASP:O	1:B:50:GLU:HG2	2.13	0.48
1:B:436:PHE:CE1	1:B:459:ILE:HG12	2.48	0.48
1:B:544:LEU:HD12	1:B:563:ASN:H	1.78	0.48
1:B:2705:ILE:HG23	1:B:2714:TYR:HE1	1.78	0.48
1:B:3679:LEU:HA	1:B:3682:MET:HB2	1.94	0.48
1:B:3734:LYS:O	1:B:3738:MET:HE2	2.12	0.48
1:A:1721:MET:HB3	1:A:1739:ILE:O	2.14	0.48
1:A:3713:ILE:HA	1:A:3738:MET:HE1	1.95	0.48
1:B:264:PHE:CE2	1:B:284:PHE:HB2	2.48	0.48
1:B:3547:MET:HE1	1:B:3552:ILE:HD11	1.96	0.48
1:A:835:VAL:HG23	1:A:842:TYR:HD1	1.77	0.48
1:B:133:LEU:HD12	1:B:192:MET:HG3	1.95	0.48
1:B:241:LEU:O	1:B:245:LEU:HB3	2.13	0.48
1:B:591:ARG:HE	1:B:595:GLU:HB3	1.78	0.48
1:B:619:VAL:HG11	1:B:664:LEU:HD22	1.95	0.48
1:B:754:MET:O	1:B:757:LYS:HG3	2.13	0.48
1:B:1750:GLU:HG3	1:B:1751:THR:O	2.13	0.48
1:B:3214:VAL:HA	1:B:3255:ILE:HD11	1.95	0.48
1:B:3563:VAL:HG21	1:B:3606:VAL:HG13	1.95	0.48
2:D:85:HIS:CE1	2:D:87:ASP:HB2	2.49	0.48
2:D:419:LYS:H	2:D:419:LYS:HG2	1.39	0.48
1:A:686:GLU:HA	1:A:805:MET:HB3	1.96	0.48
1:A:1245:CYS:HB3	1:A:1268:CYS:HB2	1.96	0.48
1:A:2067:ARG:HG3	1:A:2110:ILE:HG12	1.94	0.48
1:B:318:LEU:HD21	1:B:405:GLU:HG3	1.96	0.48
1:B:1101:HIS:NE2	1:B:1318:LEU:HD21	2.29	0.48
1:B:1270:CYS:SG	1:B:1275:CYS:HB3	2.54	0.48
1:B:3396:VAL:O	1:B:3580:ILE:HD11	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:LEU:H	1:A:679:LEU:HD22	1.78	0.48
1:A:3538:GLN:HG3	1:A:3541:ARG:HE	1.79	0.48
2:C:85:HIS:HB3	2:C:88:GLU:HB3	1.95	0.48
1:B:654:LYS:HZ3	1:B:657:LYS:HD2	1.78	0.48
1:B:3594:LEU:CB	1:B:3599:MET:HE2	2.43	0.48
2:D:328:TRP:NE1	2:D:332:LYS:HE2	2.29	0.48
1:A:704:THR:HG21	1:A:815:LYS:HE2	1.96	0.48
1:A:1966:MET:HE2	1:A:1966:MET:HA	1.96	0.48
1:A:3603:MET:HE1	1:A:3627:TYR:HA	1.95	0.48
1:A:487:ARG:HA	1:A:490:TYR:CD1	2.49	0.48
1:A:632:GLU:HG3	1:A:636:LYS:HE3	1.95	0.48
1:A:876:ILE:HD11	1:A:895:PHE:CD1	2.49	0.48
1:A:1863:PRO:HG2	1:A:1875:ILE:HD11	1.96	0.48
1:B:579:MET:O	1:B:583:LEU:HG	2.14	0.48
1:B:1722:THR:HG22	1:B:1739:ILE:HB	1.96	0.48
1:B:1990:LYS:HB2	1:B:1990:LYS:HE2	1.67	0.48
1:B:3332:LEU:HB3	1:B:3378:VAL:HG21	1.94	0.48
2:D:130:CYS:SG	2:D:150:HIS:CE1	3.07	0.48
2:D:472:ARG:HD2	2:D:472:ARG:HA	1.59	0.48
1:A:172:ASP:O	1:A:176:GLN:HG2	2.14	0.47
1:A:3547:MET:HE1	1:A:3552:ILE:HD11	1.95	0.47
1:B:465:ARG:HH11	1:B:465:ARG:HG2	1.78	0.47
1:B:520:PHE:HA	1:B:523:VAL:HG12	1.96	0.47
1:B:3344:ARG:HH21	1:B:3394:ILE:HD11	1.78	0.47
1:A:2237:ALA:HB1	1:A:2289:VAL:HG21	1.96	0.47
1:A:2759:PRO:HA	1:A:2762:TRP:CE2	2.49	0.47
2:C:130:CYS:HB3	2:C:142:LYS:HG2	1.96	0.47
1:B:482:ASP:HB2	1:B:487:ARG:HH22	1.79	0.47
1:B:3277:LYS:HG3	2:D:477:PRO:HB3	1.95	0.47
2:D:328:TRP:CD1	2:D:332:LYS:HE2	2.48	0.47
1:B:14:VAL:CG1	1:B:54:ILE:HD11	2.44	0.47
1:B:991:ILE:HD12	1:B:991:ILE:H	1.78	0.47
1:B:1721:MET:HB3	1:B:1739:ILE:O	2.15	0.47
1:B:3731:ILE:HG22	1:B:3736:GLN:HG2	1.96	0.47
2:D:139:ILE:HG22	2:D:141:SER:H	1.78	0.47
1:A:991:ILE:H	1:A:991:ILE:HD12	1.79	0.47
1:A:2466:LEU:O	1:A:2470:LYS:HG2	2.14	0.47
1:B:1125:ILE:HG13	1:B:1130:VAL:HG23	1.95	0.47
1:B:3332:LEU:HD22	1:B:3378:VAL:HG21	1.94	0.47
1:B:3603:MET:SD	1:B:3630:VAL:HG21	2.55	0.47
1:A:429:HIS:CE1	1:A:431:ILE:HG13	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1448:TYR:HB2	1:A:1463:ARG:HB2	1.97	0.47
1:A:2695:VAL:HG22	1:A:2864:VAL:HG22	1.94	0.47
1:B:659:GLU:HA	1:B:662:MET:HE3	1.96	0.47
1:B:1059:LYS:HE2	1:B:1131:CYS:SG	2.54	0.47
1:B:3547:MET:SD	1:B:3593:ILE:HG21	2.55	0.47
2:D:85:HIS:HB3	2:D:88:GLU:HB3	1.95	0.47
1:A:51:ALA:O	1:A:55:LEU:HG	2.14	0.47
1:A:3396:VAL:O	1:A:3580:ILE:HD11	2.14	0.47
1:A:3809:LEU:HD22	1:A:3823:ILE:HD13	1.95	0.47
2:C:139:ILE:HG22	2:C:141:SER:H	1.80	0.47
1:B:28:ALA:HB1	1:B:92:MET:HE1	1.97	0.47
1:B:189:PHE:HD1	1:B:192:MET:HE1	1.79	0.47
1:B:2720:TYR:CE1	1:B:2867:ALA:HA	2.49	0.47
1:A:31:ILE:O	1:A:34:LEU:HD12	2.15	0.47
1:A:609:ASP:HA	1:A:663:LYS:NZ	2.30	0.47
1:A:894:LEU:O	1:A:898:ILE:HG22	2.15	0.47
1:A:2991:VAL:HG11	2:D:492:MET:HE1	1.96	0.47
1:B:87:GLN:O	1:B:91:MET:HG2	2.14	0.47
1:B:199:ALA:HB1	1:B:245:LEU:CD1	2.45	0.47
1:B:429:HIS:CE1	1:B:431:ILE:HG13	2.49	0.47
1:B:679:LEU:HD22	1:B:679:LEU:H	1.80	0.47
1:B:1346:GLN:OE1	1:B:1346:GLN:HA	2.15	0.47
1:B:1863:PRO:HG2	1:B:1875:ILE:HD11	1.97	0.47
1:B:3369:CYS:HB3	1:B:3370:ARG:NH1	2.29	0.47
1:A:482:ASP:CB	1:A:487:ARG:HH22	2.28	0.47
1:A:520:PHE:CE2	1:A:539:ILE:HB	2.49	0.47
1:A:2705:ILE:HG23	1:A:2714:TYR:HE1	1.79	0.47
1:B:36:VAL:HG12	1:B:84:ILE:HD13	1.96	0.47
1:B:52:MET:HA	1:B:55:LEU:HG	1.96	0.47
1:B:412:THR:HG23	1:B:413:LEU:HD22	1.96	0.47
1:B:1103:TYR:CD2	1:B:1107:MET:HE1	2.50	0.47
1:B:1390:LEU:HD13	1:B:1750:GLU:OE1	2.15	0.47
1:B:2985:TYR:CD1	1:B:2985:TYR:C	2.93	0.47
1:B:3193:TRP:CE2	1:B:3194:ILE:HG13	2.50	0.47
1:A:473:ILE:HA	1:A:476:MET:SD	2.54	0.47
1:A:1990:LYS:HB2	1:A:1990:LYS:HE2	1.68	0.47
1:A:3538:GLN:O	1:A:3541:ARG:HG2	2.14	0.47
2:C:476:LYS:HE3	2:C:476:LYS:HB2	1.76	0.47
1:B:240:GLU:O	1:B:244:LYS:HG2	2.13	0.47
1:B:256:VAL:O	1:B:260:THR:HG23	2.15	0.47
1:B:287:SER:HA	1:B:290:TRP:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:LEU:CD1	1:B:587:ASN:HD21	2.27	0.47
1:B:714:ILE:HG23	1:B:806:HIS:CE1	2.50	0.47
1:B:2466:LEU:O	1:B:2470:LYS:HG2	2.14	0.47
1:A:1567:MET:HB3	1:A:1613:ILE:HG23	1.97	0.47
1:A:2868:LEU:HG	1:A:2870:GLY:N	2.30	0.47
1:A:3375:LEU:HD13	1:A:3402:ILE:HG23	1.97	0.47
2:C:27:TYR:CZ	2:C:67:LEU:HD13	2.50	0.47
1:B:286:ASP:HA	1:B:289:GLU:OE1	2.15	0.47
1:B:520:PHE:CZ	1:B:536:ALA:HA	2.50	0.47
1:B:3600:VAL:HG12	1:B:3646:ILE:HG22	1.97	0.47
1:A:2244:ASP:O	1:A:2248:ILE:HG13	2.14	0.46
1:A:3536:ASP:O	1:A:3540:VAL:HG23	2.15	0.46
2:C:85:HIS:CE1	2:C:87:ASP:HB2	2.50	0.46
1:B:2759:PRO:HA	1:B:2762:TRP:CE2	2.49	0.46
1:A:651:PHE:C	1:A:652:MET:HE2	2.39	0.46
1:A:705:GLU:O	1:A:708:VAL:HG22	2.15	0.46
1:A:1039:LYS:HA	1:A:1042:GLU:HG3	1.98	0.46
2:C:328:TRP:NE1	2:C:332:LYS:HE2	2.31	0.46
1:B:379:LEU:O	1:B:383:ILE:HG12	2.15	0.46
1:B:576:TRP:HZ3	1:B:602:ILE:HG22	1.80	0.46
1:B:2946:PRO:HA	1:B:2947:PHE:HA	1.59	0.46
1:A:698:LEU:HG	1:A:812:HIS:CE1	2.51	0.46
1:A:2742:SER:HB3	1:A:2764:LYS:HE3	1.97	0.46
1:B:3761:LYS:HA	1:B:3764:ILE:HD12	1.96	0.46
1:A:186:PHE:HB3	1:A:189:PHE:CZ	2.51	0.46
1:A:877:LEU:HD23	1:A:877:LEU:HA	1.81	0.46
1:A:2142:LYS:O	1:A:2145:MET:HB2	2.14	0.46
1:A:2281:ARG:NH2	1:A:2387:LEU:HB2	2.31	0.46
2:C:424:GLN:NE2	2:C:429:SER:HA	2.30	0.46
1:A:1722:THR:HG22	1:A:1739:ILE:HB	1.96	0.46
1:A:2321:CYS:SG	1:A:2392:PRO:HG3	2.56	0.46
1:B:186:PHE:HB3	1:B:189:PHE:CZ	2.50	0.46
1:A:256:VAL:O	1:A:260:THR:HG23	2.14	0.46
1:A:317:ILE:HG23	1:A:376:ARG:CZ	2.46	0.46
1:A:584:VAL:HG22	1:A:617:TYR:CD2	2.48	0.46
1:A:630:GLY:O	1:A:633:LEU:HD12	2.16	0.46
1:A:2475:HIS:HA	1:A:2783:VAL:HB	1.98	0.46
1:A:2720:TYR:CE1	1:A:2867:ALA:HA	2.51	0.46
1:B:545:LYS:HE2	1:B:597:LEU:HD13	1.96	0.46
1:B:704:THR:HG21	1:B:815:LYS:HE2	1.96	0.46
1:B:1037:PHE:HB2	1:B:1092:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1846:PHE:HD1	1:B:1925:ARG:HH12	1.64	0.46
1:B:2742:SER:HB3	1:B:2764:LYS:HE3	1.97	0.46
1:B:2868:LEU:HG	1:B:2870:GLY:N	2.30	0.46
1:B:3690:VAL:HG21	1:B:3700:LEU:HD22	1.97	0.46
2:D:112:HIS:O	2:D:117:HIS:HB3	2.15	0.46
1:A:762:MET:HA	1:A:765:ILE:HG12	1.98	0.46
1:A:931:MET:HB3	1:A:990:LYS:HE3	1.96	0.46
1:A:1452:ARG:HG3	1:A:1768:ARG:HD3	1.98	0.46
1:B:669:ALA:HB2	1:B:710:ILE:HD13	1.98	0.46
1:B:2543:SER:HB3	1:B:2588:LEU:HD21	1.98	0.46
1:B:3154:THR:HB	1:B:3158:ASN:HD22	1.80	0.46
1:B:3695:ALA:O	1:B:3699:VAL:HG23	2.16	0.46
1:A:2329:ILE:HG12	1:A:2417:LEU:HD13	1.98	0.46
1:A:3203:MET:HB2	1:B:2921:TYR:CE1	2.51	0.46
1:B:2075:LEU:HD23	1:B:2075:LEU:H	1.79	0.46
1:B:2133:ARG:HH22	1:B:2169:GLY:HA3	1.81	0.46
1:B:2715:LYS:HD2	1:B:2751:GLU:HA	1.97	0.46
2:D:269:VAL:HB	2:D:397:THR:HG22	1.98	0.46
1:A:486:LYS:HD2	1:A:487:ARG:HG3	1.98	0.46
1:A:960:LEU:HD12	1:A:977:ILE:HG21	1.97	0.46
1:A:1750:GLU:HG3	1:A:1751:THR:O	2.15	0.46
1:B:1101:HIS:HD2	1:B:1318:LEU:HD11	1.81	0.46
1:B:1992:HIS:HB2	1:B:1999:LEU:HD12	1.98	0.46
1:B:2200:TRP:CD1	1:B:2200:TRP:H	2.34	0.46
1:B:2266:ILE:O	1:B:2273:SER:HB2	2.15	0.46
1:B:2702:LYS:HD2	1:B:2705:ILE:HD11	1.97	0.46
1:A:2185:LYS:HD2	1:A:2185:LYS:O	2.15	0.46
1:B:2249:ARG:NH2	1:B:2250:ASN:HB2	2.31	0.46
1:B:2389:LEU:HG	1:B:2433:LEU:HD12	1.98	0.46
1:B:3423:GLN:O	1:B:3427:LEU:HG	2.16	0.46
2:D:64:PRO:HG3	2:D:100:ASN:HB2	1.98	0.46
1:A:149:ASP:HB3	1:A:152:GLU:HG2	1.96	0.45
1:A:419:ILE:O	1:A:423:ARG:HG3	2.16	0.45
1:A:591:ARG:HE	1:A:595:GLU:HB3	1.80	0.45
1:A:1678:VAL:HG23	1:A:1691:LEU:C	2.41	0.45
1:A:2081:MET:HB3	1:A:2081:MET:HE2	1.58	0.45
1:A:3344:ARG:HH21	1:A:3394:ILE:HD11	1.81	0.45
1:B:1169:HIS:CD2	1:B:1990:LYS:HA	2.50	0.45
1:B:1245:CYS:HB3	1:B:1268:CYS:HB2	1.97	0.45
1:B:1952:LEU:HD23	1:B:1952:LEU:HA	1.75	0.45
1:B:3547:MET:N	1:B:3547:MET:HE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:27:TYR:CZ	2:D:67:LEU:HD13	2.51	0.45
1:A:452:ILE:O	1:A:456:ILE:HG12	2.16	0.45
1:A:3376:MET:O	1:A:3380:VAL:HG23	2.17	0.45
1:A:3710:TRP:HE3	1:A:3713:ILE:HG21	1.82	0.45
1:B:86:PRO:HA	1:B:89:ARG:HH12	1.81	0.45
1:B:320:LEU:HD11	1:B:372:TYR:HB2	1.97	0.45
1:B:875:SER:HA	1:B:878:LYS:HD2	1.98	0.45
1:B:948:ILE:HD13	1:B:948:ILE:HA	1.64	0.45
1:A:36:VAL:HG12	1:A:84:ILE:HD13	1.97	0.45
1:A:465:ARG:HH22	1:A:466:LYS:NZ	2.14	0.45
1:A:1691:LEU:HD13	1:A:1723:TYR:CE1	2.52	0.45
1:B:419:ILE:O	1:B:423:ARG:HG3	2.16	0.45
1:B:1174:LYS:HE2	1:B:1174:LYS:HB2	1.74	0.45
1:B:1229:HIS:CE1	1:B:1263:LYS:HD2	2.52	0.45
1:B:1718:ARG:HH21	1:B:1740:TYR:HD2	1.63	0.45
1:B:3390:SER:O	1:B:3394:ILE:HG13	2.16	0.45
1:A:1229:HIS:CE1	1:A:1263:LYS:HD2	2.51	0.45
1:A:2052:LEU:HD21	1:A:2059:VAL:HA	1.98	0.45
1:A:2145:MET:HE1	1:A:2192:ILE:HG12	1.98	0.45
1:A:3277:LYS:HG3	2:C:477:PRO:HB3	1.99	0.45
1:B:139:ARG:NH2	1:B:151:GLU:H	2.14	0.45
1:B:832:LEU:HA	1:B:835:VAL:HG12	1.98	0.45
1:B:2188:GLU:OE2	1:B:2188:GLU:HA	2.17	0.45
1:B:3332:LEU:HD21	1:B:3375:LEU:HG	1.98	0.45
2:D:97:PRO:HD2	2:D:147:LEU:HD22	1.98	0.45
1:A:412:THR:HG23	1:A:413:LEU:HD22	1.98	0.45
1:A:631:MET:O	1:A:635:ARG:HG2	2.17	0.45
1:A:737:MET:HE3	1:A:895:PHE:CD2	2.51	0.45
1:A:2200:TRP:H	1:A:2200:TRP:CD1	2.34	0.45
1:A:3630:VAL:O	1:A:3634:VAL:HG23	2.17	0.45
2:C:416:ARG:HE	2:C:418:ARG:HD3	1.80	0.45
1:B:979:LYS:O	1:B:982:GLU:HG3	2.16	0.45
1:B:3337:HIS:ND1	2:D:480:MET:HE1	2.31	0.45
1:B:3581:PHE:HA	1:B:3584:ILE:HG22	1.99	0.45
1:A:87:GLN:O	1:A:91:MET:HG2	2.17	0.45
1:A:2266:ILE:O	1:A:2273:SER:HB2	2.17	0.45
1:A:2946:PRO:HA	1:A:2947:PHE:HA	1.58	0.45
1:A:3193:TRP:CE2	1:A:3194:ILE:HG13	2.50	0.45
1:B:598:PRO:HG2	1:B:624:PHE:CD2	2.52	0.45
1:B:612:MET:HA	1:B:615:LEU:HD12	1.99	0.45
1:B:651:PHE:C	1:B:652:MET:HE2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:688:ILE:HG13	1:B:691:TRP:CE3	2.52	0.45
1:B:1399:ARG:HH21	1:B:1743:VAL:HG23	1.82	0.45
1:B:1691:LEU:HD13	1:B:1723:TYR:CE1	2.51	0.45
1:B:3200:SER:O	1:B:3206:ARG:HD3	2.16	0.45
1:A:379:LEU:O	1:A:383:ILE:HG12	2.17	0.45
1:A:711:CYS:SG	1:A:809:ILE:HG21	2.57	0.45
1:A:1106:LYS:HB3	1:A:1106:LYS:HE3	1.70	0.45
1:A:1390:LEU:HD13	1:A:1750:GLU:OE1	2.17	0.45
1:A:3390:SER:O	1:A:3394:ILE:HG13	2.16	0.45
1:B:1504:ASP:HB3	1:B:2351:TRP:CE2	2.51	0.45
1:B:3674:LYS:O	1:B:3677:GLN:HG3	2.17	0.45
1:A:464:VAL:O	1:A:467:GLU:HG3	2.16	0.45
1:A:1564:VAL:HG12	1:A:1565:GLU:OE1	2.17	0.45
1:A:1857:VAL:HB	1:A:1862:GLY:HA3	1.99	0.45
2:C:130:CYS:SG	2:C:150:HIS:CE1	3.09	0.45
1:B:45:VAL:HA	1:B:48:ILE:HD11	1.99	0.45
1:B:465:ARG:HH22	1:B:466:LYS:NZ	2.14	0.45
1:B:629:GLU:O	1:B:633:LEU:HG	2.17	0.45
1:A:512:ILE:HA	1:A:515:LYS:HZ2	1.82	0.45
1:A:1125:ILE:HG13	1:A:1130:VAL:HG23	1.98	0.45
1:A:2715:LYS:HD2	1:A:2751:GLU:HA	1.98	0.45
1:A:2868:LEU:HG	1:A:2870:GLY:H	1.81	0.45
1:A:3372:GLY:H	1:A:3541:ARG:NH2	2.14	0.45
1:A:3674:LYS:O	1:A:3677:GLN:HG3	2.17	0.45
2:C:64:PRO:HG3	2:C:100:ASN:HB2	1.99	0.45
1:B:488:GLU:HA	1:B:491:VAL:HG22	1.98	0.45
1:B:1692:SER:HB2	1:B:1698:GLN:HE21	1.81	0.45
1:B:3018:LEU:HD12	1:B:3018:LEU:HA	1.84	0.45
1:B:3325:LYS:HZ3	1:B:3370:ARG:NE	2.15	0.45
1:A:670:LYS:O	1:A:674:ILE:HG13	2.17	0.45
1:A:918:LYS:O	1:A:922:ARG:HG2	2.16	0.45
1:A:998:LYS:HE3	1:A:998:LYS:O	2.17	0.45
1:A:3400:MET:HA	1:A:3403:MET:HG3	1.99	0.45
1:A:3695:ALA:O	1:A:3699:VAL:HG23	2.17	0.45
2:C:97:PRO:HD2	2:C:147:LEU:HD22	1.99	0.45
1:B:172:ASP:O	1:B:176:GLN:HG2	2.17	0.45
1:B:1250:ILE:HD13	1:B:1790:LEU:HG	1.99	0.45
1:A:286:ASP:HA	1:A:289:GLU:OE1	2.17	0.44
1:A:1441:GLN:HB3	1:A:1472:ASN:HB2	1.99	0.44
1:A:2074:PRO:HG2	1:A:2077:ARG:HG3	1.99	0.44
1:A:2985:TYR:CD1	1:A:2985:TYR:C	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3383:LEU:HD11	1:A:3399:MET:HE3	1.98	0.44
1:A:3547:MET:HE2	1:A:3547:MET:N	2.32	0.44
1:B:475:ARG:HH21	1:B:479:ASP:N	2.15	0.44
1:B:1010:GLU:HB2	1:B:1011:PRO:HD3	1.99	0.44
1:B:1432:LEU:HD13	1:B:1448:TYR:CE2	2.52	0.44
1:B:2261:TYR:HD1	1:B:2320:LEU:HD22	1.82	0.44
1:B:2982:LEU:HD23	1:B:2982:LEU:HA	1.81	0.44
1:A:1334:GLN:O	1:A:1337:PHE:HB3	2.17	0.44
1:A:2475:HIS:HD1	1:A:2475:HIS:C	2.25	0.44
1:A:3585:VAL:HG12	1:A:3632:PHE:CE2	2.52	0.44
1:B:520:PHE:CE2	1:B:539:ILE:HB	2.52	0.44
1:B:762:MET:HA	1:B:765:ILE:HG12	1.99	0.44
1:B:1034:LYS:HB3	1:B:1103:TYR:CE2	2.52	0.44
1:B:3600:VAL:O	1:B:3604:MET:HG2	2.17	0.44
1:B:3710:TRP:HE3	1:B:3713:ILE:HG21	1.81	0.44
1:A:42:SER:O	1:B:292:LYS:HE3	2.17	0.44
1:A:736:GLN:O	1:A:740:ARG:HG2	2.17	0.44
1:A:742:TRP:HZ3	1:A:743:LYS:HZ3	1.64	0.44
1:A:1394:HIS:CE1	1:A:1398:THR:HG22	2.52	0.44
1:A:1504:ASP:HB3	1:A:2351:TRP:CE2	2.52	0.44
1:B:1291:LEU:HA	1:B:1791:LEU:HD13	2.00	0.44
1:B:1394:HIS:CE1	1:B:1398:THR:HG22	2.52	0.44
1:B:1845:ASN:HA	1:B:1847:ARG:NH1	2.32	0.44
1:B:3380:VAL:HA	1:B:3383:LEU:HB2	1.99	0.44
1:A:948:ILE:HD13	1:A:948:ILE:HA	1.71	0.44
1:A:1122:HIS:O	1:A:1125:ILE:HG22	2.17	0.44
1:A:3336:LEU:HD21	1:A:3398:VAL:HG11	1.98	0.44
1:A:3369:CYS:HB3	1:A:3370:ARG:NH1	2.32	0.44
1:A:3538:GLN:HA	1:A:3541:ARG:HG2	2.00	0.44
1:B:44:ASP:O	1:B:48:ILE:HG12	2.18	0.44
1:B:956:PHE:CD1	1:B:977:ILE:HD13	2.53	0.44
1:A:32:TYR:HB3	1:A:92:MET:HE3	2.00	0.44
1:A:258:LYS:O	1:A:262:ILE:HG22	2.18	0.44
1:A:475:ARG:O	1:A:475:ARG:HD3	2.17	0.44
1:A:3332:LEU:HB3	1:A:3378:VAL:HG21	1.99	0.44
1:A:3547:MET:SD	1:A:3593:ILE:HG21	2.57	0.44
1:B:1046:GLN:O	1:B:1050:LEU:HG	2.17	0.44
1:B:1808:ILE:HG22	1:B:1834:GLN:HG2	2.00	0.44
1:B:3265:ARG:HB3	2:D:464:LEU:HD23	2.00	0.44
1:B:3380:VAL:HG11	1:B:3549:CYS:HB2	1.99	0.44
1:A:3734:LYS:O	1:A:3738:MET:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:LEU:HA	1:B:444:ILE:HG12	2.00	0.44
1:B:1002:TYR:CD2	1:B:1049:LEU:HD22	2.53	0.44
1:B:1455:LEU:HD22	1:B:1735:TYR:CE2	2.53	0.44
1:B:3630:VAL:O	1:B:3634:VAL:HG23	2.17	0.44
2:D:320:GLU:HB3	2:D:324:LYS:NZ	2.33	0.44
2:D:412:LYS:HB2	2:D:412:LYS:HE2	1.58	0.44
1:A:633:LEU:O	1:A:637:PHE:HB3	2.17	0.44
1:A:880:LEU:HA	1:A:880:LEU:HD23	1.76	0.44
1:A:2322:LEU:HD23	1:A:2322:LEU:HA	1.78	0.44
1:A:3136:TYR:CE1	2:C:436:LYS:HD3	2.52	0.44
1:A:3581:PHE:HA	1:A:3584:ILE:HG22	1.99	0.44
1:B:400:ARG:HB2	1:B:439:ILE:HG22	1.99	0.44
1:B:436:PHE:CZ	1:B:459:ILE:HG12	2.52	0.44
1:B:2035:LEU:HD11	1:B:2081:MET:HB2	2.00	0.44
1:B:2177:THR:H	1:B:2180:SER:HB2	1.83	0.44
1:B:2868:LEU:HG	1:B:2870:GLY:H	1.83	0.44
1:B:3585:VAL:HG12	1:B:3632:PHE:CE2	2.52	0.44
1:A:695:ILE:HD12	1:A:695:ILE:H	1.82	0.44
1:A:1805:CYS:HB2	1:A:1839:LEU:HD23	2.00	0.44
1:A:3265:ARG:HB3	2:C:464:LEU:HD23	1.99	0.44
1:A:3447:MET:HE2	1:A:3481:LEU:HD23	1.99	0.44
1:A:2528:LEU:HD23	1:A:2528:LEU:HA	1.87	0.44
1:A:3385:LEU:HD22	2:C:479:LYS:HE3	1.99	0.44
1:B:1244:VAL:HG11	1:B:1253:HIS:CD2	2.53	0.44
1:A:236:HIS:O	1:A:240:GLU:HG2	2.19	0.43
1:A:260:THR:O	1:A:263:ILE:HG22	2.18	0.43
1:A:1678:VAL:HA	1:A:1692:SER:HA	2.00	0.43
1:A:1808:ILE:HG22	1:A:1834:GLN:HG2	1.99	0.43
1:A:2249:ARG:HH12	1:A:2250:ASN:HA	1.83	0.43
1:A:3591:ARG:HG2	1:A:3633:VAL:HG22	2.00	0.43
2:C:472:ARG:HD2	2:C:472:ARG:HA	1.64	0.43
1:B:469:VAL:HG11	1:B:508:ALA:HB2	1.99	0.43
1:B:470:GLU:O	1:B:473:ILE:HG12	2.18	0.43
1:B:670:LYS:O	1:B:674:ILE:HG13	2.17	0.43
1:B:959:LEU:HD22	1:B:977:ILE:HD11	2.00	0.43
1:B:1461:ALA:HA	1:B:1846:PHE:CZ	2.53	0.43
1:A:416:HIS:O	1:A:420:GLU:HG3	2.18	0.43
1:A:619:VAL:O	1:A:622:MET:HE2	2.18	0.43
1:A:933:VAL:HG12	1:A:993:PHE:CD1	2.53	0.43
1:A:2047:TYR:CE2	1:A:2186:ILE:HD12	2.52	0.43
1:A:2698:MET:HE2	1:A:2698:MET:HB3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:698:LEU:HG	1:B:812:HIS:CE1	2.52	0.43
1:B:736:GLN:O	1:B:740:ARG:HG2	2.18	0.43
1:B:1122:HIS:O	1:B:1125:ILE:HG22	2.18	0.43
1:B:2066:MET:HE2	1:B:2066:MET:HB3	1.95	0.43
1:B:2557:GLU:HA	1:B:2557:GLU:OE1	2.18	0.43
1:B:3734:LYS:O	1:B:3738:MET:HG2	2.18	0.43
1:B:3748:THR:HG21	1:B:3812:LEU:HG	2.00	0.43
1:A:283:LYS:O	1:A:286:ASP:HB2	2.18	0.43
1:A:1250:ILE:HD13	1:A:1790:LEU:HG	2.00	0.43
1:A:1635:TYR:CE1	1:A:1655:LEU:HD22	2.53	0.43
1:A:2741:VAL:HG21	1:A:2777:ILE:HD13	2.00	0.43
1:A:3380:VAL:HG11	1:A:3549:CYS:HB2	2.01	0.43
1:B:162:TRP:CD2	1:B:266:LYS:NZ	2.86	0.43
1:B:417:ALA:O	1:B:421:MET:HG2	2.19	0.43
1:B:463:LYS:HB3	1:B:463:LYS:HE3	1.82	0.43
1:B:762:MET:HE1	1:B:894:LEU:HD22	2.01	0.43
1:B:1450:ASP:OD1	1:B:1450:ASP:O	2.35	0.43
1:B:2997:LYS:HD2	1:B:2998:PRO:O	2.17	0.43
1:A:263:ILE:O	1:A:266:LYS:HG3	2.18	0.43
1:A:648:PHE:O	1:A:652:MET:HG2	2.18	0.43
1:A:989:ASP:OD1	1:A:989:ASP:C	2.62	0.43
1:A:1000:HIS:HD1	1:A:1000:HIS:H	1.66	0.43
1:A:2673:TRP:O	1:A:2676:ILE:HG12	2.19	0.43
1:B:612:MET:HA	1:B:615:LEU:HB2	2.01	0.43
1:B:1293:GLY:HA3	1:B:1889:ARG:HG2	2.00	0.43
1:B:3574:LEU:HB2	1:B:3622:ILE:HD13	2.00	0.43
2:D:319:ASP:O	2:D:323:LYS:HG3	2.19	0.43
1:A:408:PHE:CZ	1:A:447:PRO:HD2	2.52	0.43
1:A:560:VAL:HG21	1:A:629:GLU:HG3	2.00	0.43
1:A:853:ILE:HD12	1:A:853:ILE:HA	1.91	0.43
1:A:1363:GLU:OE1	1:A:1363:GLU:HA	2.18	0.43
2:C:515:TYR:HA	1:B:2448:MET:HE1	2.00	0.43
1:B:127:ILE:HG23	1:B:131:PHE:CZ	2.53	0.43
1:B:520:PHE:CZ	1:B:539:ILE:HB	2.54	0.43
1:B:741:PHE:CE1	1:B:898:ILE:HD13	2.43	0.43
1:B:1857:VAL:HB	1:B:1862:GLY:HA3	2.00	0.43
1:B:2586:ILE:HD13	1:B:2597:LEU:HD23	2.01	0.43
1:B:2673:TRP:O	1:B:2676:ILE:HG12	2.18	0.43
1:A:608:ILE:HG13	1:A:663:LYS:HE2	2.00	0.43
1:A:1244:VAL:HG11	1:A:1253:HIS:CD2	2.53	0.43
1:A:1820:ARG:HA	1:A:1827:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:PRO:HD2	1:B:248:HIS:CE1	2.53	0.43
1:B:320:LEU:HD22	1:B:376:ARG:NH1	2.34	0.43
1:B:452:ILE:O	1:B:456:ILE:HG12	2.18	0.43
1:B:1387:ILE:HG22	1:B:1749:TRP:HE3	1.84	0.43
1:B:1805:CYS:HB2	1:B:1839:LEU:HD23	2.00	0.43
1:B:3376:MET:O	1:B:3380:VAL:HG23	2.18	0.43
2:D:104:LEU:HB3	2:D:108:GLN:HG3	2.01	0.43
1:A:1488:GLN:CD	1:A:1488:GLN:N	2.77	0.43
1:A:1866:LEU:HD12	1:A:1885:LEU:HD11	2.01	0.43
1:A:2188:GLU:OE1	1:A:2188:GLU:HA	2.18	0.43
1:A:2991:VAL:HG12	2:D:495:ARG:NH1	2.33	0.43
1:A:3580:ILE:O	1:A:3584:ILE:HG22	2.19	0.43
1:A:3797:LEU:HD22	1:A:3837:VAL:HG11	2.01	0.43
2:C:104:LEU:HB3	2:C:108:GLN:HG3	1.99	0.43
1:B:127:ILE:HD13	1:B:127:ILE:HA	1.89	0.43
1:B:160:GLN:HB3	1:B:162:TRP:CH2	2.54	0.43
1:B:877:LEU:HD23	1:B:877:LEU:HA	1.81	0.43
1:B:1678:VAL:HG23	1:B:1691:LEU:C	2.44	0.43
1:A:707:LEU:O	1:A:710:ILE:HB	2.17	0.43
1:A:1399:ARG:HH21	1:A:1743:VAL:HG23	1.84	0.43
1:A:1841:ALA:HB3	1:A:1900:ILE:HB	2.01	0.43
1:A:1925:ARG:HA	1:A:1928:MET:SD	2.59	0.43
1:A:2530:ILE:HD11	1:A:2581:MET:HB2	2.01	0.43
1:A:2557:GLU:OE1	1:A:2557:GLU:HA	2.18	0.43
1:A:3285:LYS:HB3	1:A:3285:LYS:HE2	1.74	0.43
1:B:1363:GLU:HA	1:B:1363:GLU:OE1	2.18	0.43
1:B:1925:ARG:HA	1:B:1928:MET:SD	2.58	0.43
1:A:76:MET:HA	1:A:79:ILE:HG12	1.99	0.43
1:A:240:GLU:O	1:A:244:LYS:HG2	2.19	0.43
1:A:395:ILE:HD11	1:A:421:MET:HG3	2.01	0.43
1:A:856:ARG:HA	1:A:856:ARG:HD2	1.67	0.43
1:A:2079:GLN:O	1:A:2083:GLN:HG3	2.19	0.43
1:A:2921:TYR:CE1	1:B:3203:MET:HB2	2.53	0.43
1:A:3574:LEU:HB2	1:A:3622:ILE:HD13	2.01	0.43
1:A:3748:THR:HG21	1:A:3812:LEU:HG	2.01	0.43
1:B:35:ARG:CZ	1:B:35:ARG:HA	2.48	0.43
1:B:723:LEU:HD21	1:B:738:PHE:HE1	1.84	0.43
1:B:852:LYS:O	1:B:852:LYS:HD3	2.19	0.43
1:B:1388:GLU:OE2	1:B:1752:SER:HA	2.18	0.43
1:B:1622:PRO:HG2	1:B:1646:LEU:HD11	2.01	0.43
1:A:959:LEU:HD21	1:A:973:ALA:HB1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2180:SER:O	1:A:2183:ILE:HG22	2.18	0.43
1:B:31:ILE:O	1:B:34:LEU:HD12	2.19	0.43
1:B:145:ILE:HG13	1:B:146:TRP:CD1	2.54	0.43
1:B:177:ALA:O	1:B:181:ILE:HG12	2.18	0.43
1:B:406:LEU:HD21	1:B:414:ILE:HG22	2.01	0.43
1:B:463:LYS:O	1:B:467:GLU:HG3	2.19	0.43
1:A:486:LYS:HD3	1:A:490:TYR:CE1	2.54	0.42
1:A:1293:GLY:HA3	1:A:1889:ARG:HG2	2.01	0.42
1:A:2083:GLN:O	1:A:2087:LYS:HG3	2.18	0.42
1:A:2983:ASN:ND2	2:D:491:ASN:HB2	2.33	0.42
1:B:275:VAL:O	1:B:278:GLN:HG3	2.19	0.42
1:B:608:ILE:HG13	1:B:663:LYS:HE2	2.01	0.42
1:B:907:SER:HA	1:B:910:TRP:CE2	2.54	0.42
1:B:1234:TYR:CZ	1:B:1881:LYS:HA	2.53	0.42
1:B:3276:ILE:HD12	1:B:3276:ILE:HA	1.91	0.42
1:B:3797:LEU:HD22	1:B:3837:VAL:HG11	2.01	0.42
1:A:35:ARG:CZ	1:A:35:ARG:HA	2.49	0.42
1:A:1680:ALA:O	1:A:1690:CYS:HA	2.19	0.42
1:A:1998:GLU:OE1	1:A:1998:GLU:HA	2.19	0.42
1:A:2035:LEU:HD11	1:A:2081:MET:HB2	2.01	0.42
1:A:2872:GLN:O	1:A:2874:ILE:HD13	2.19	0.42
1:A:3538:GLN:HG2	1:A:3542:MET:CE	2.49	0.42
2:C:495:ARG:NH1	1:B:2991:VAL:HG12	2.33	0.42
1:B:139:ARG:HG2	1:B:150:LEU:HD12	2.00	0.42
1:B:512:ILE:HA	1:B:515:LYS:HZ2	1.84	0.42
1:B:874:SER:HB2	1:B:878:LYS:HE3	2.01	0.42
1:B:3333:ILE:HB	1:B:3378:VAL:HB	2.00	0.42
1:A:1169:HIS:CD2	1:A:1990:LYS:HA	2.54	0.42
1:A:2157:LEU:HD11	1:A:2176:LYS:HG3	2.01	0.42
2:C:385:GLU:OE1	2:C:385:GLU:HA	2.18	0.42
1:B:246:TRP:CG	1:B:247:PRO:HD3	2.54	0.42
1:B:609:ASP:HA	1:B:663:LYS:NZ	2.33	0.42
1:B:1791:LEU:HG	1:B:1852:MET:HE3	2.00	0.42
1:B:1841:ALA:HB3	1:B:1900:ILE:HB	2.00	0.42
1:B:2698:MET:SD	1:B:2861:LEU:HD23	2.60	0.42
1:B:3546:LEU:HB3	1:B:3547:MET:HE2	2.01	0.42
1:A:671:ILE:HD12	1:A:671:ILE:HA	1.83	0.42
1:A:1109:LYS:HB2	1:A:1333:VAL:HG22	2.01	0.42
1:A:1845:ASN:HA	1:A:1847:ARG:NH1	2.33	0.42
1:A:2102:GLN:OE1	1:A:2102:GLN:N	2.51	0.42
2:C:465:LYS:HE3	2:C:465:LYS:HB3	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:THR:O	1:B:156:LYS:HG2	2.19	0.42
1:B:560:VAL:HG21	1:B:629:GLU:HG3	2.01	0.42
1:B:575:LYS:HA	1:B:575:LYS:HD2	1.83	0.42
1:B:1441:GLN:HB3	1:B:1472:ASN:HB2	2.01	0.42
1:A:153:THR:O	1:A:156:LYS:HG2	2.19	0.42
1:A:153:THR:HA	1:A:156:LYS:HG2	2.02	0.42
1:A:462:GLU:HG3	1:A:465:ARG:NH2	2.34	0.42
1:A:1346:GLN:OE1	1:A:1346:GLN:HA	2.20	0.42
1:A:2017:TRP:HB3	1:A:2027:ARG:HH11	1.85	0.42
1:A:3599:MET:H	1:A:3599:MET:HG2	1.62	0.42
1:A:3710:TRP:O	1:A:3713:ILE:HG22	2.20	0.42
2:C:112:HIS:HA	2:C:116:GLN:OE1	2.19	0.42
2:C:412:LYS:HE2	2:C:412:LYS:HB2	1.59	0.42
1:B:2281:ARG:HA	1:B:2281:ARG:HD3	1.87	0.42
1:B:2389:LEU:CD2	1:B:2429:GLN:HB3	2.49	0.42
1:B:2741:VAL:HG21	1:B:2777:ILE:HD13	2.01	0.42
2:D:465:LYS:HB3	2:D:465:LYS:HE3	1.71	0.42
1:A:275:VAL:O	1:A:278:GLN:HG3	2.19	0.42
1:A:832:LEU:HA	1:A:835:VAL:HG12	2.01	0.42
1:A:1002:TYR:CD2	1:A:1049:LEU:HD13	2.52	0.42
1:A:1971:LEU:HD23	1:A:1971:LEU:HA	1.88	0.42
2:C:320:GLU:HB3	2:C:324:LYS:NZ	2.34	0.42
1:B:258:LYS:O	1:B:262:ILE:HG22	2.20	0.42
1:B:2332:TRP:HE1	1:B:2381:ILE:HG22	1.84	0.42
1:A:737:MET:HE3	1:A:895:PHE:CE2	2.54	0.42
1:A:1697:HIS:HB3	1:A:1716:VAL:O	2.20	0.42
1:A:3655:PHE:CD2	1:A:3699:VAL:HG12	2.55	0.42
2:C:424:GLN:HE21	2:C:429:SER:CA	2.32	0.42
1:B:131:PHE:HB3	1:B:135:PHE:CE2	2.54	0.42
1:B:131:PHE:N	1:B:131:PHE:CD1	2.86	0.42
1:B:657:LYS:O	1:B:660:LEU:HB2	2.20	0.42
1:B:1866:LEU:HD12	1:B:1885:LEU:HD11	2.02	0.42
1:B:2322:LEU:HG	1:B:2410:TRP:NE1	2.34	0.42
1:B:3419:LYS:HE2	1:B:3427:LEU:HB2	2.02	0.42
1:A:286:ASP:O	1:A:289:GLU:HB2	2.19	0.42
1:A:506:LYS:HD3	1:A:507:TYR:CD2	2.55	0.42
1:A:1056:ILE:HD12	1:A:1057:ILE:H	1.85	0.42
1:B:470:GLU:HA	1:B:473:ILE:HG12	2.02	0.42
1:B:738:PHE:HA	1:B:741:PHE:HB3	2.02	0.42
1:B:1559:HIS:CE1	1:B:1562:ASN:HD22	2.37	0.42
1:A:25:GLU:HG3	1:A:95:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ASP:H	1:A:487:ARG:HH21	1.68	0.42
1:A:3188:SER:O	1:A:3189:ASN:C	2.63	0.42
1:A:3621:LEU:HD12	1:A:3622:ILE:HG13	2.02	0.42
1:A:3645:GLY:HA3	1:A:3693:ASN:HB2	2.01	0.42
1:B:291:LEU:HB2	1:B:293:ILE:HD11	2.01	0.42
1:B:989:ASP:OD1	1:B:989:ASP:C	2.63	0.42
1:B:3655:PHE:CD2	1:B:3699:VAL:HG12	2.54	0.42
2:C:515:TYR:HB2	1:B:2408:ASP:OD1	2.20	0.42
1:B:614:ASP:HA	1:B:617:TYR:HB2	2.02	0.42
1:B:1635:TYR:CE1	1:B:1655:LEU:HD22	2.55	0.42
1:B:1680:ALA:O	1:B:1690:CYS:HA	2.20	0.42
1:B:1852:MET:HE2	1:B:1886:ARG:HG2	2.02	0.42
1:A:439:ILE:O	1:A:443:VAL:HG23	2.20	0.41
1:A:1463:ARG:HG2	1:A:1847:ARG:CZ	2.48	0.41
1:A:1495:ARG:HH21	1:A:2356:PRO:HD3	1.84	0.41
1:B:188:LEU:HD23	1:B:191:GLU:CD	2.45	0.41
1:B:233:SER:O	1:B:237:ILE:HG12	2.19	0.41
1:B:1339:GLU:H	1:B:1339:GLU:HG2	1.74	0.41
1:B:1691:LEU:HD12	1:B:1699:VAL:HG13	2.02	0.41
1:B:2454:MET:HE2	1:B:2498:MET:HE2	2.02	0.41
1:B:3621:LEU:HD12	1:B:3622:ILE:HG13	2.01	0.41
2:D:424:GLN:OE1	2:D:429:SER:HA	2.19	0.41
1:A:131:PHE:HB3	1:A:135:PHE:CE2	2.55	0.41
1:A:188:LEU:HD11	1:B:187:ASP:O	2.19	0.41
1:A:931:MET:HA	1:A:990:LYS:HD2	2.02	0.41
1:A:992:THR:O	1:A:995:PRO:HD2	2.20	0.41
1:A:1676:ASN:HB3	1:A:1694:ASN:HD21	1.85	0.41
1:A:3200:SER:O	1:A:3206:ARG:HD3	2.19	0.41
2:C:326:GLU:HA	2:C:329:LYS:HD2	2.02	0.41
1:B:53:ARG:HB3	1:B:131:PHE:CD2	2.56	0.41
1:B:200:ASN:HB3	1:B:204:TYR:CE2	2.55	0.41
1:B:206:ALA:HA	1:B:209:ARG:NE	2.35	0.41
1:B:1359:LEU:HD22	1:B:2023:PHE:HE2	1.85	0.41
1:B:1632:SER:OG	1:B:1645:SER:HB3	2.20	0.41
1:B:1820:ARG:HA	1:B:1827:LEU:HB2	2.02	0.41
1:B:3123:GLU:HG2	1:B:3124:ASN:N	2.35	0.41
1:B:3603:MET:HA	1:B:3606:VAL:HB	2.02	0.41
1:A:32:TYR:CB	1:A:92:MET:HE3	2.50	0.41
1:A:658:ILE:C	1:A:662:MET:HE3	2.45	0.41
1:A:843:LYS:HE3	1:A:843:LYS:HA	2.02	0.41
1:A:1324:ASP:OD1	1:A:1324:ASP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2389:LEU:HD22	1:A:2429:GLN:HB3	2.02	0.41
1:A:2389:LEU:O	1:A:2392:PRO:HD2	2.19	0.41
1:A:2966:SER:O	1:A:2970:GLN:HG2	2.19	0.41
1:A:3640:GLN:HA	1:A:3643:LEU:HD12	2.02	0.41
1:A:3704:TYR:CE2	1:A:3744:LEU:HD11	2.55	0.41
2:C:419:LYS:H	2:C:419:LYS:HG2	1.40	0.41
1:B:110:MET:HE3	1:B:110:MET:HB3	1.93	0.41
1:B:288:CYS:HA	1:B:293:ILE:HD12	2.01	0.41
1:B:667:GLU:HA	1:B:670:LYS:HG3	2.01	0.41
1:B:1418:ARG:HH11	1:B:1691:LEU:HD23	1.85	0.41
1:B:2086:VAL:O	1:B:2089:VAL:HG12	2.20	0.41
1:A:188:LEU:HD23	1:A:191:GLU:CD	2.46	0.41
1:A:1291:LEU:HD22	1:A:1794:GLN:HB3	2.02	0.41
1:A:1344:LEU:O	1:A:1347:ILE:HG12	2.20	0.41
1:A:1540:ARG:HB3	1:A:1542:LEU:HG	2.03	0.41
1:A:2570:ARG:HD2	1:A:2615:GLN:HE22	1.85	0.41
1:A:2586:ILE:HD13	1:A:2597:LEU:HD23	2.02	0.41
1:A:2722:VAL:HA	1:A:2865:CYS:SG	2.60	0.41
1:A:2874:ILE:HG12	1:A:2981:GLU:OE2	2.20	0.41
1:A:3018:LEU:HD12	1:A:3018:LEU:HA	1.86	0.41
1:A:3828:LEU:HD23	1:A:3828:LEU:HA	1.95	0.41
2:C:515:TYR:HD1	1:B:2448:MET:SD	2.43	0.41
1:B:199:ALA:HB1	1:B:245:LEU:HD11	2.01	0.41
1:B:880:LEU:HD13	1:B:944:PHE:CZ	2.44	0.41
1:B:907:SER:HB2	1:B:976:LYS:HD3	2.02	0.41
1:B:1697:HIS:HB3	1:B:1716:VAL:O	2.20	0.41
1:B:1977:HIS:CG	1:B:1978:PRO:HD2	2.55	0.41
1:B:3072:ASP:HB3	1:B:3104:PRO:HD2	2.03	0.41
2:D:96:CYS:HA	2:D:109:PHE:HE1	1.85	0.41
1:A:2017:TRP:HB3	1:A:2027:ARG:NH1	2.36	0.41
1:A:2198:PHE:CD1	1:A:2201:LEU:HD12	2.56	0.41
1:A:2982:LEU:HD23	1:A:2982:LEU:HA	1.82	0.41
1:A:3264:ALA:O	1:A:3268:VAL:HG23	2.21	0.41
1:A:3538:GLN:O	1:A:3542:MET:HG2	2.20	0.41
2:C:462:ILE:O	2:C:466:GLU:HG3	2.20	0.41
1:B:541:LEU:HD13	1:B:587:ASN:HD21	1.86	0.41
1:B:634:HIS:HB3	1:B:638:TYR:CZ	2.55	0.41
1:B:844:LYS:HD2	1:B:844:LYS:HA	1.68	0.41
1:B:1122:HIS:HB3	1:B:1125:ILE:HG22	2.03	0.41
1:B:1510:LEU:HD12	1:B:1510:LEU:HA	1.86	0.41
1:B:2209:LEU:HD23	1:B:2209:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2570:ARG:NH2	1:B:2684:LEU:HB3	2.35	0.41
2:D:416:ARG:HE	2:D:418:ARG:HD3	1.85	0.41
1:A:654:LYS:HZ3	1:A:657:LYS:HD2	1.86	0.41
1:A:668:PHE:CZ	1:A:805:MET:HE1	2.56	0.41
1:A:688:ILE:HG13	1:A:691:TRP:CE3	2.55	0.41
1:A:1055:LEU:HD23	1:A:1138:LYS:HD3	2.02	0.41
1:A:1238:MET:O	1:A:1239:MET:HE2	2.21	0.41
1:A:1387:ILE:HG22	1:A:1749:TRP:HE3	1.85	0.41
1:A:2089:VAL:HG13	1:A:2103:LEU:HD21	2.03	0.41
1:A:2177:THR:H	1:A:2180:SER:HB2	1.85	0.41
1:A:3278:ARG:HA	1:A:3278:ARG:HD2	1.87	0.41
1:B:77:THR:HG23	1:B:81:GLU:OE1	2.21	0.41
1:B:938:ARG:HB2	1:B:993:PHE:CZ	2.55	0.41
1:B:2530:ILE:HD11	1:B:2581:MET:HB2	2.02	0.41
1:B:3188:SER:O	1:B:3189:ASN:C	2.63	0.41
2:D:417:PRO:HA	2:D:420:MET:HE3	2.03	0.41
1:A:691:TRP:O	1:A:695:ILE:HD12	2.21	0.41
2:C:96:CYS:HA	2:C:109:PHE:HE1	1.85	0.41
2:C:489:LEU:HD22	1:B:3000:ASN:ND2	2.25	0.41
1:B:236:HIS:O	1:B:240:GLU:HG2	2.21	0.41
1:B:489:GLY:HA2	1:B:492:ASN:ND2	2.35	0.41
1:B:1940:ILE:HD13	1:B:1940:ILE:HA	1.98	0.41
1:B:1951:ILE:HG13	1:B:1951:ILE:H	1.69	0.41
1:B:2627:ALA:O	1:B:2631:PHE:HB2	2.21	0.41
1:B:3136:TYR:CE1	2:D:436:LYS:HD3	2.56	0.41
1:B:3710:TRP:O	1:B:3713:ILE:HG22	2.19	0.41
2:D:462:ILE:O	2:D:466:GLU:HG3	2.21	0.41
1:A:453:ILE:H	1:A:453:ILE:HG12	1.67	0.41
1:A:677:LYS:HA	1:A:677:LYS:HD2	1.82	0.41
1:A:810:ALA:HA	1:A:813:LEU:HB2	2.03	0.41
1:A:2075:LEU:H	1:A:2075:LEU:HD23	1.84	0.41
1:A:2240:LEU:HD13	1:A:2240:LEU:HA	1.95	0.41
1:B:260:THR:O	1:B:263:ILE:HG22	2.20	0.41
1:B:462:GLU:HG3	1:B:465:ARG:NH2	2.35	0.41
1:B:1064:LEU:HB3	1:B:1131:CYS:SG	2.60	0.41
1:B:1344:LEU:O	1:B:1347:ILE:HG12	2.20	0.41
1:B:1435:LEU:HG	1:B:1445:GLN:HB2	2.03	0.41
1:B:1461:ALA:HA	1:B:1846:PHE:HZ	1.86	0.41
1:B:1672:LEU:HD22	1:B:1702:PHE:HE2	1.85	0.41
1:B:1676:ASN:HB3	1:B:1694:ASN:HD21	1.85	0.41
1:B:2443:ASN:O	1:B:2446:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2457:LEU:HD22	1:B:2491:LEU:HD21	2.03	0.41
1:B:2719:ASN:HD21	1:B:2786:VAL:HG12	1.85	0.41
1:B:2743:LEU:HD13	1:B:2779:LEU:HD13	2.03	0.41
1:B:2750:VAL:HG23	1:B:2755:LEU:HG	2.03	0.41
1:B:3640:GLN:HA	1:B:3643:LEU:HD12	2.02	0.41
1:B:3645:GLY:HA3	1:B:3693:ASN:HB2	2.01	0.41
1:A:288:CYS:SG	1:A:298:ILE:HG21	2.61	0.41
1:A:1234:TYR:CZ	1:A:1881:LYS:HA	2.55	0.41
1:A:2048:PHE:CD2	1:A:2048:PHE:C	2.99	0.41
1:A:2210:GLU:OE1	1:A:2214:ARG:HD2	2.21	0.41
1:A:2698:MET:SD	1:A:2861:LEU:HD23	2.61	0.41
1:A:2750:VAL:HG23	1:A:2755:LEU:HG	2.03	0.41
1:A:3846:LEU:O	1:A:3850:VAL:HG23	2.21	0.41
1:B:153:THR:HA	1:B:156:LYS:HG2	2.02	0.41
1:B:408:PHE:CZ	1:B:447:PRO:HD2	2.54	0.41
1:B:853:ILE:HD12	1:B:853:ILE:HA	1.92	0.41
1:B:1008:PHE:O	1:B:1011:PRO:HD2	2.20	0.41
1:B:1864:GLU:HG3	1:B:1907:ARG:HG3	2.03	0.41
1:B:2312:LEU:HD23	1:B:2312:LEU:HA	1.77	0.41
1:B:2570:ARG:HD2	1:B:2615:GLN:HE22	1.85	0.41
1:B:3475:ASN:HD22	1:B:3492:LEU:HG	1.86	0.41
1:B:3552:ILE:HD13	1:B:3552:ILE:N	2.36	0.41
1:B:3580:ILE:O	1:B:3584:ILE:HG22	2.20	0.41
1:B:3704:TYR:CE2	1:B:3744:LEU:HD11	2.55	0.41
1:A:127:ILE:HD13	1:A:127:ILE:HA	1.89	0.41
1:A:467:GLU:O	1:A:470:GLU:HG2	2.21	0.41
1:A:938:ARG:HB2	1:A:993:PHE:CE2	2.56	0.41
1:A:1292:ARG:HG2	1:A:1928:MET:HA	2.03	0.41
1:A:2236:LEU:HD12	1:A:2236:LEU:HA	1.84	0.41
1:A:2627:ALA:O	1:A:2631:PHE:HB2	2.21	0.41
1:A:3314:LEU:HD13	1:A:3324:LEU:HD13	2.03	0.41
1:B:467:GLU:HA	1:B:470:GLU:HG2	2.02	0.41
1:B:480:LEU:HD23	1:B:480:LEU:HA	1.91	0.41
1:B:891:LEU:HG	1:B:895:PHE:CE2	2.56	0.41
1:B:1055:LEU:HD23	1:B:1138:LYS:HD3	2.03	0.41
1:B:3264:ALA:O	1:B:3268:VAL:HG23	2.21	0.41
1:A:815:LYS:HD2	1:A:815:LYS:HA	1.82	0.40
1:A:1011:PRO:O	1:A:1015:ILE:HG13	2.22	0.40
1:A:1691:LEU:HD12	1:A:1699:VAL:HG13	2.02	0.40
1:A:2080:MET:HE2	1:A:2080:MET:N	2.37	0.40
1:A:2332:TRP:HE1	1:A:2381:ILE:HG22	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2900:LYS:HG2	1:A:2930:THR:HG23	2.03	0.40
1:A:3159:ILE:HD12	1:A:3159:ILE:HA	1.83	0.40
1:B:180:LEU:HA	1:B:183:LYS:NZ	2.37	0.40
1:B:668:PHE:HA	1:B:671:ILE:HG22	2.03	0.40
1:B:2745:TYR:HB2	1:B:2787:THR:HG21	2.03	0.40
1:B:3206:ARG:HD2	1:B:3244:VAL:O	2.22	0.40
1:B:3343:LYS:HB3	1:B:3343:LYS:HE3	1.89	0.40
2:D:31:ARG:HD2	2:D:63:HIS:CD2	2.56	0.40
1:A:246:TRP:CG	1:A:247:PRO:HD3	2.56	0.40
1:A:530:ILE:HG13	1:A:531:ARG:N	2.35	0.40
1:A:643:GLY:O	1:A:647:ILE:HG12	2.21	0.40
1:A:902:LEU:HA	1:A:905:ILE:HG22	2.03	0.40
1:A:1000:HIS:ND1	1:A:1000:HIS:N	2.69	0.40
1:A:1798:ILE:HD11	1:A:1922:GLY:HA3	2.03	0.40
1:A:1977:HIS:CG	1:A:1978:PRO:HD2	2.56	0.40
1:A:2294:ARG:HA	1:A:2294:ARG:HD2	1.85	0.40
1:A:2743:LEU:HD13	1:A:2779:LEU:HD13	2.03	0.40
2:C:110:GLY:HA3	2:C:151:TRP:CZ2	2.56	0.40
1:B:76:MET:SD	1:B:76:MET:C	3.05	0.40
1:B:973:ALA:O	1:B:977:ILE:HG12	2.21	0.40
1:B:1103:TYR:CG	1:B:1107:MET:HE1	2.56	0.40
1:B:1229:HIS:HA	1:B:1263:LYS:HA	2.04	0.40
1:B:1343:ASP:O	1:B:1347:ILE:HG23	2.22	0.40
1:B:1463:ARG:HG2	1:B:1847:ARG:CZ	2.51	0.40
1:B:2183:ILE:HA	1:B:2183:ILE:HD12	1.77	0.40
1:A:178:ALA:HB2	1:A:237:ILE:HG22	2.03	0.40
1:A:187:ASP:O	1:B:188:LEU:HD11	2.21	0.40
1:A:470:GLU:HA	1:A:473:ILE:HG12	2.02	0.40
1:A:1418:ARG:HH11	1:A:1691:LEU:HD23	1.86	0.40
1:A:1632:SER:OG	1:A:1645:SER:HB3	2.21	0.40
1:A:1864:GLU:HG3	1:A:1907:ARG:HG3	2.03	0.40
1:A:2160:LYS:HE2	1:A:2160:LYS:HB2	1.92	0.40
1:B:725:LEU:HD11	1:B:769:GLN:HG2	2.03	0.40
1:B:1120:LEU:HD12	1:B:1120:LEU:HA	1.85	0.40
1:B:2379:SER:HA	1:B:2382:ILE:HG22	2.03	0.40
1:B:2723:SER:C	1:B:2781:LEU:HB2	2.47	0.40
1:B:2759:PRO:HA	1:B:2762:TRP:CD2	2.57	0.40
1:A:160:GLN:HB3	1:A:162:TRP:CZ2	2.57	0.40
1:A:873:VAL:HA	1:A:876:ILE:HG22	2.03	0.40
1:A:1376:ASP:C	1:A:1376:ASP:OD1	2.64	0.40
1:A:3309:LEU:HD23	1:A:3309:LEU:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:PHE:HE1	1:B:280:ILE:HD12	1.86	0.40
1:B:467:GLU:O	1:B:470:GLU:HG2	2.21	0.40
1:B:578:LYS:HB3	1:B:579:MET:HE2	2.03	0.40
1:B:668:PHE:HD2	1:B:710:ILE:HD12	1.86	0.40
1:B:810:ALA:HA	1:B:813:LEU:HB2	2.04	0.40
1:B:1106:LYS:O	1:B:1110:LYS:HD2	2.22	0.40
1:B:2089:VAL:HG22	1:B:2103:LEU:HD21	2.03	0.40
1:B:2198:PHE:CD1	1:B:2201:LEU:HD12	2.57	0.40
1:B:2716:LEU:HD12	1:B:2788:SER:HA	2.03	0.40
1:B:2878:ALA:O	1:B:2882:GLN:HG3	2.22	0.40
1:B:2892:ILE:H	1:B:2892:ILE:HG12	1.46	0.40
1:A:8:ILE:HG23	1:A:12:ARG:NH1	2.36	0.40
1:A:67:PHE:HB2	1:A:72:TRP:NE1	2.37	0.40
1:A:629:GLU:O	1:A:633:LEU:HG	2.21	0.40
1:A:2716:LEU:HD12	1:A:2788:SER:HA	2.03	0.40
1:A:3123:GLU:HG2	1:A:3124:ASN:N	2.37	0.40
1:A:3285:LYS:O	1:A:3285:LYS:HG2	2.21	0.40
2:C:29:CYS:SG	2:C:59:HIS:HE1	2.31	0.40
2:C:496:ASP:HB3	2:C:499:THR:HG23	2.03	0.40
1:B:8:ILE:HG23	1:B:12:ARG:NH1	2.36	0.40
1:B:420:GLU:HG3	1:B:423:ARG:HE	1.87	0.40
1:B:677:LYS:NZ	1:B:681:PHE:HB2	2.36	0.40
1:B:1434:VAL:HG12	1:B:1446:LEU:HD13	2.03	0.40
1:B:3538:GLN:HG2	1:B:3542:MET:HE2	2.04	0.40
1:B:3738:MET:SD	1:B:3738:MET:N	2.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3617/3861 (94%)	3494 (97%)	120 (3%)	3 (0%)	48	80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	3617/3861 (94%)	3489 (96%)	126 (4%)	2 (0%)	48	80
2	C	343/515 (67%)	328 (96%)	15 (4%)	0	100	100
2	D	343/515 (67%)	329 (96%)	14 (4%)	0	100	100
All	All	7920/8752 (90%)	7640 (96%)	275 (4%)	5 (0%)	49	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	743	LYS
1	A	2268	PRO
1	B	2268	PRO
1	A	1706	VAL
1	B	1706	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3338/3522 (95%)	3251 (97%)	87 (3%)	40	72
1	B	3338/3522 (95%)	3241 (97%)	97 (3%)	37	70
2	C	314/455 (69%)	311 (99%)	3 (1%)	68	84
2	D	314/455 (69%)	306 (98%)	8 (2%)	42	72
All	All	7304/7954 (92%)	7109 (97%)	195 (3%)	40	71

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	MET
1	A	110	MET
1	A	165	VAL
1	A	189	PHE
1	A	198	PHE
1	A	238	TYR

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Mol	Chain	Res	Type
1	A	265	GLU
1	A	276	LEU
1	A	388	THR
1	A	416	HIS
1	A	455	VAL
1	A	588	MET
1	A	623	LYS
1	A	708	VAL
1	A	799	GLU
1	A	863	LYS
1	A	919	LEU
1	A	923	LEU
1	A	933	VAL
1	A	946	ILE
1	A	948	ILE
1	A	961	GLU
1	A	984	LEU
1	A	1005	ILE
1	A	1026	ARG
1	A	1028	VAL
1	A	1036	LEU
1	A	1039	LYS
1	A	1060	THR
1	A	1063	TYR
1	A	1085	VAL
1	A	1155	SER
1	A	1161	VAL
1	A	1289	TYR
1	A	1324	ASP
1	A	1362	THR
1	A	1385	LYS
1	A	1449	MET
1	A	1453	THR
1	A	1463	ARG
1	A	1567	MET
1	A	1568	VAL
1	A	1576	ASP
1	A	1589	ILE
1	A	1692	SER
1	A	1693	THR
1	A	1706	VAL
1	A	1748	ILE

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Mol	Chain	Res	Type
1	A	1957	LEU
1	A	1995	VAL
1	A	2025	GLU
1	A	2080	MET
1	A	2089	VAL
1	A	2116	THR
1	A	2129	GLU
1	A	2143	LYS
1	A	2240	LEU
1	A	2282	SER
1	A	2291	LEU
1	A	2318	ARG
1	A	2433	LEU
1	A	2472	VAL
1	A	2485	LEU
1	A	2498	MET
1	A	2573	GLN
1	A	2578	LEU
1	A	2612	LEU
1	A	2630	VAL
1	A	2675	SER
1	A	2698	MET
1	A	2904	TYR
1	A	2942	ILE
1	A	2952	MET
1	A	3001	ILE
1	A	3030	ASP
1	A	3074	LEU
1	A	3118	MET
1	A	3135	LYS
1	A	3234	MET
1	A	3244	VAL
1	A	3329	ASP
1	A	3396	VAL
1	A	3404	ASP
1	A	3464	MET
1	A	3585	VAL
1	A	3600	VAL
1	A	3633	VAL
2	C	267	GLN
2	C	276	ILE
2	C	379	THR

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Mol	Chain	Res	Type
1	B	52	MET
1	B	110	MET
1	B	127	ILE
1	B	165	VAL
1	B	189	PHE
1	B	198	PHE
1	B	238	TYR
1	B	265	GLU
1	B	276	LEU
1	B	388	THR
1	B	416	HIS
1	B	651	PHE
1	B	711	CYS
1	B	799	GLU
1	B	876	ILE
1	B	878	LYS
1	B	919	LEU
1	B	933	VAL
1	B	946	ILE
1	B	947	TYR
1	B	948	ILE
1	B	961	GLU
1	B	984	LEU
1	B	1000	HIS
1	B	1005	ILE
1	B	1012	LEU
1	B	1026	ARG
1	B	1028	VAL
1	B	1036	LEU
1	B	1039	LYS
1	B	1059	LYS
1	B	1060	THR
1	B	1063	TYR
1	B	1085	VAL
1	B	1123	GLU
1	B	1161	VAL
1	B	1211	MET
1	B	1289	TYR
1	B	1362	THR
1	B	1390	LEU
1	B	1453	THR
1	B	1463	ARG

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Mol	Chain	Res	Type
1	B	1543	ILE
1	B	1565	GLU
1	B	1567	MET
1	B	1568	VAL
1	B	1576	ASP
1	B	1581	ASN
1	B	1589	ILE
1	B	1693	THR
1	B	1706	VAL
1	B	1714	THR
1	B	1726	MET
1	B	1748	ILE
1	B	1940	ILE
1	B	1995	VAL
1	B	2012	LYS
1	B	2025	GLU
1	B	2028	LEU
1	B	2089	VAL
1	B	2113	ASP
1	B	2116	THR
1	B	2129	GLU
1	B	2183	ILE
1	B	2192	ILE
1	B	2240	LEU
1	B	2255	LEU
1	B	2287	LEU
1	B	2384	CYS
1	B	2388	ILE
1	B	2390	LEU
1	B	2395	LEU
1	B	2433	LEU
1	B	2472	VAL
1	B	2485	LEU
1	B	2494	ILE
1	B	2498	MET
1	B	2578	LEU
1	B	2630	VAL
1	B	2675	SER
1	B	2698	MET
1	B	2886	GLU
1	B	2892	ILE
1	B	2904	TYR

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Mol	Chain	Res	Type
1	B	2942	ILE
1	B	2952	MET
1	B	2999	GLN
1	B	3001	ILE
1	B	3167	GLU
1	B	3203	MET
1	B	3244	VAL
1	B	3396	VAL
1	B	3404	ASP
1	B	3464	MET
1	B	3585	VAL
1	B	3600	VAL
1	B	3633	VAL
2	D	29	CYS
2	D	276	ILE
2	D	317	VAL
2	D	331	LEU
2	D	337	GLU
2	D	379	THR
2	D	449	LEU
2	D	472	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	478	ASN
1	A	577	ASN
1	A	675	ASN
1	A	812	HIS
1	A	1025	ASN
1	A	1113	GLN
1	A	1122	HIS
1	A	1488	GLN
1	A	1522	ASN
1	A	1549	GLN
1	A	1634	HIS
1	A	1661	ASN
1	A	1814	HIS
1	A	2083	GLN
1	A	2095	ASN
1	A	2148	HIS
1	A	2301	ASN

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Mol	Chain	Res	Type
1	A	2439	HIS
1	A	2506	HIS
1	A	2937	ASN
1	A	2965	HIS
1	A	3000	ASN
1	A	3053	GLN
1	A	3192	GLN
1	A	3247	GLN
1	A	3292	ASN
1	A	3297	ASN
1	A	3468	ASN
1	B	478	ASN
1	B	581	ASN
1	B	685	HIS
1	B	1017	HIS
1	B	1025	ASN
1	B	1441	GLN
1	B	1499	GLN
1	B	1522	ASN
1	B	1559	HIS
1	B	1582	GLN
1	B	1634	HIS
1	B	1698	GLN
1	B	1754	ASN
1	B	1814	HIS
1	B	2076	HIS
1	B	2301	ASN
1	B	2506	HIS
1	B	2615	GLN
1	B	2937	ASN
1	B	2965	HIS
1	B	3000	ASN
1	B	3053	GLN
1	B	3247	GLN
1	B	3297	ASN
1	B	3468	ASN
2	D	133	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

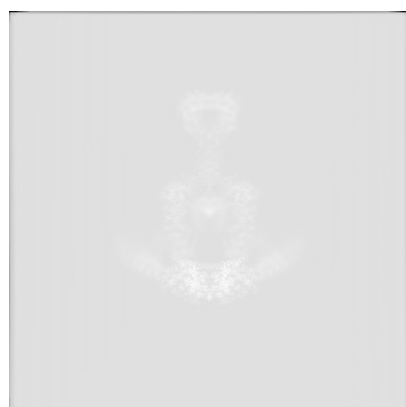
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52502. These allow visual inspection of the internal detail of the map and identification of artifacts.

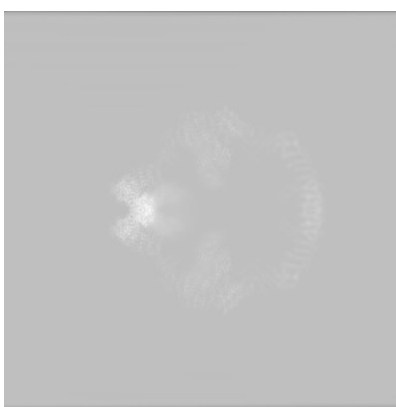
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

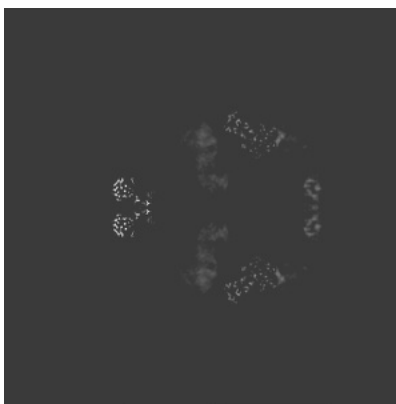
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

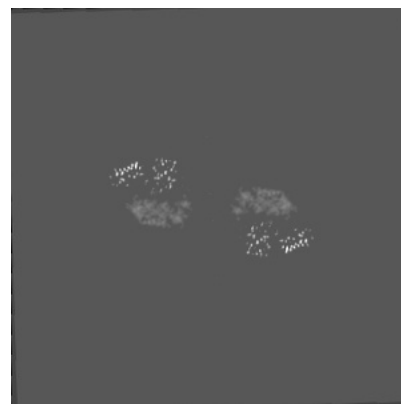
6.2.1 Primary map



X Index: 192



Y Index: 192

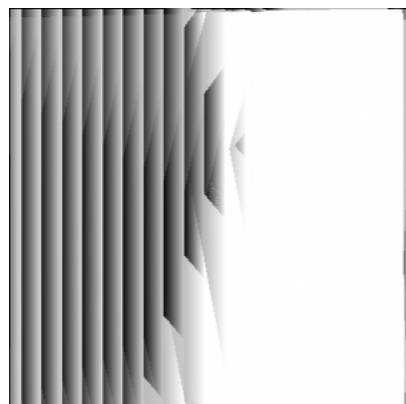


Z Index: 192

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

6.3 Largest variance slices [i](#)

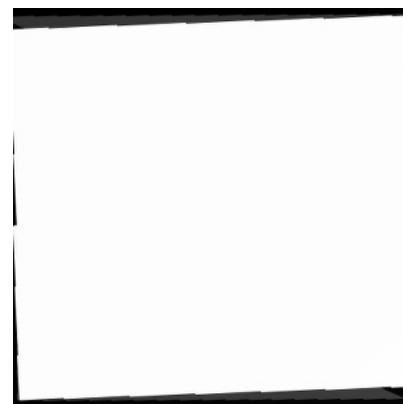
6.3.1 Primary map



X Index: 0



Y Index: 0

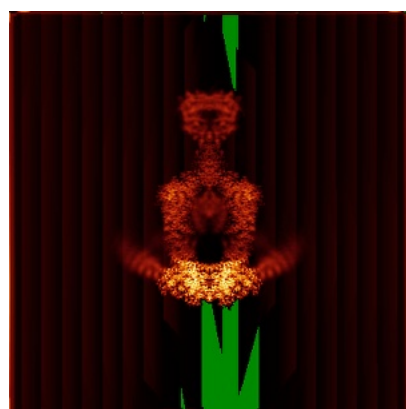


Z Index: 383

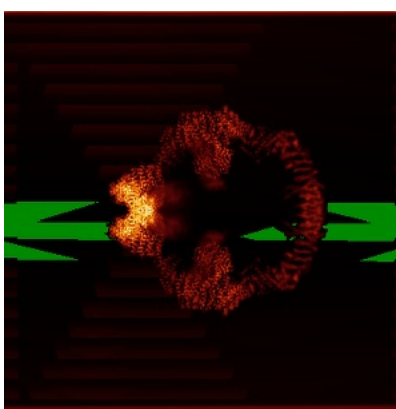
The images above show the largest variance slices of the map in three orthogonal directions.

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

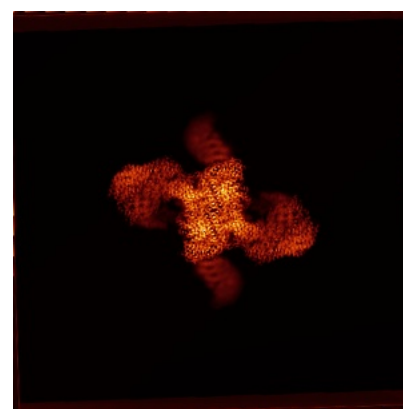
6.4.1 Primary map



X



Y

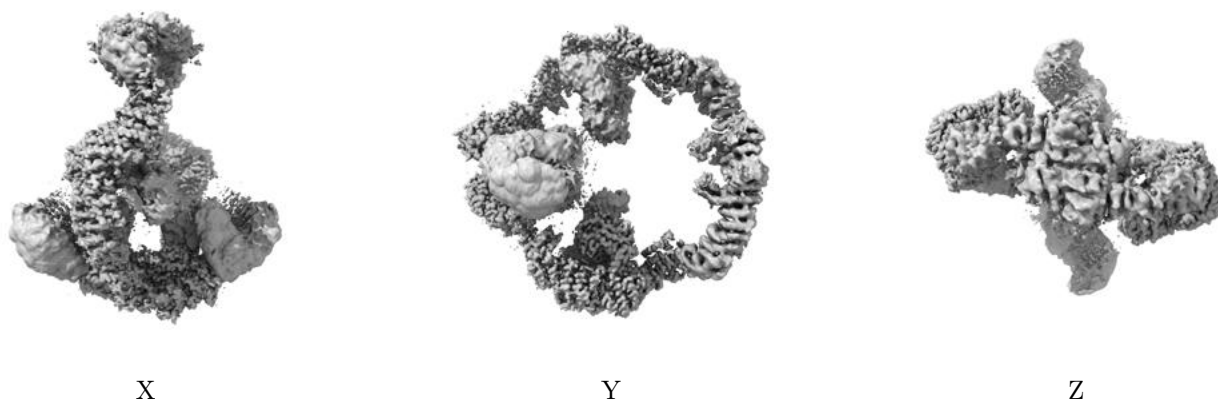


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0104. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

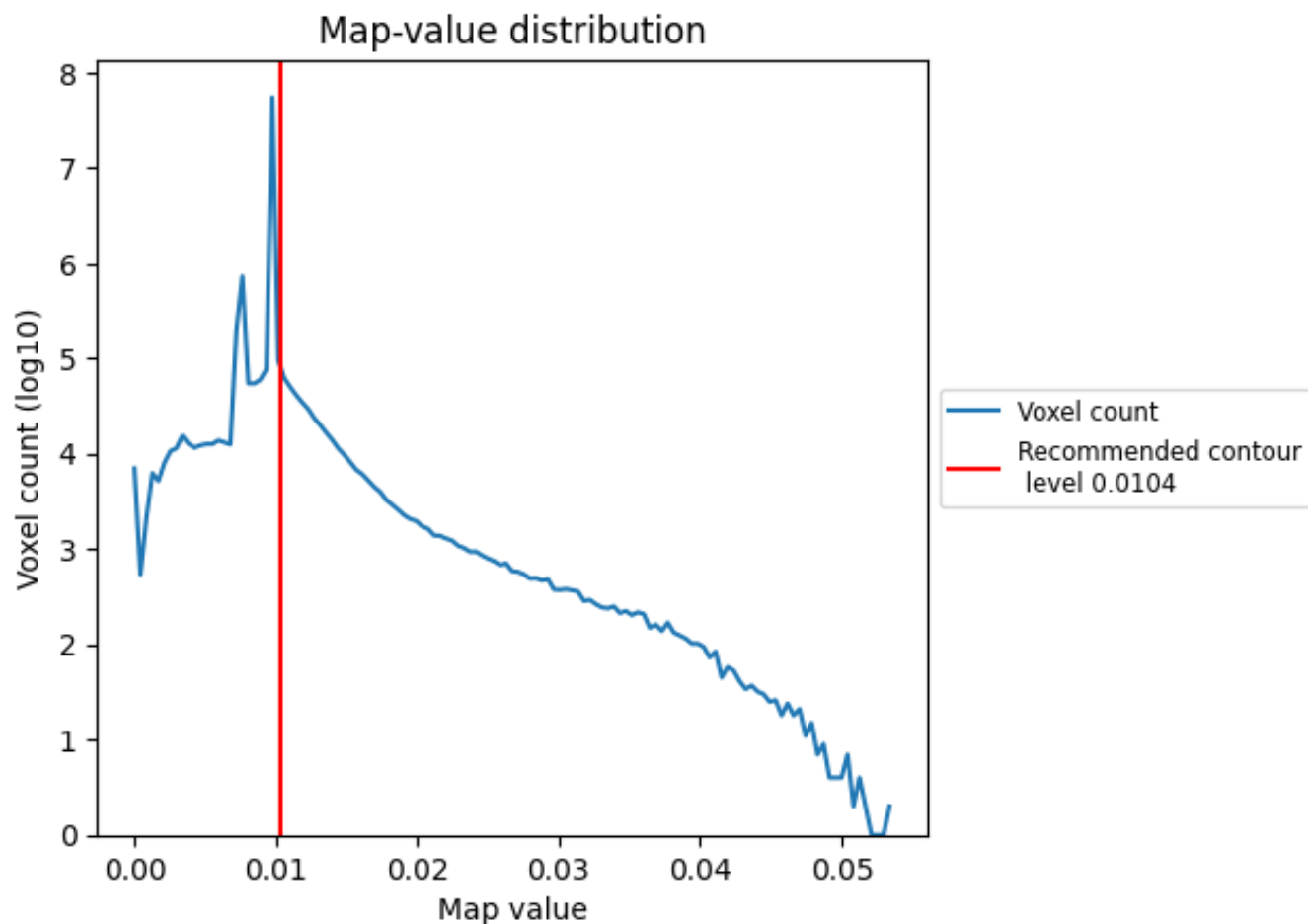
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

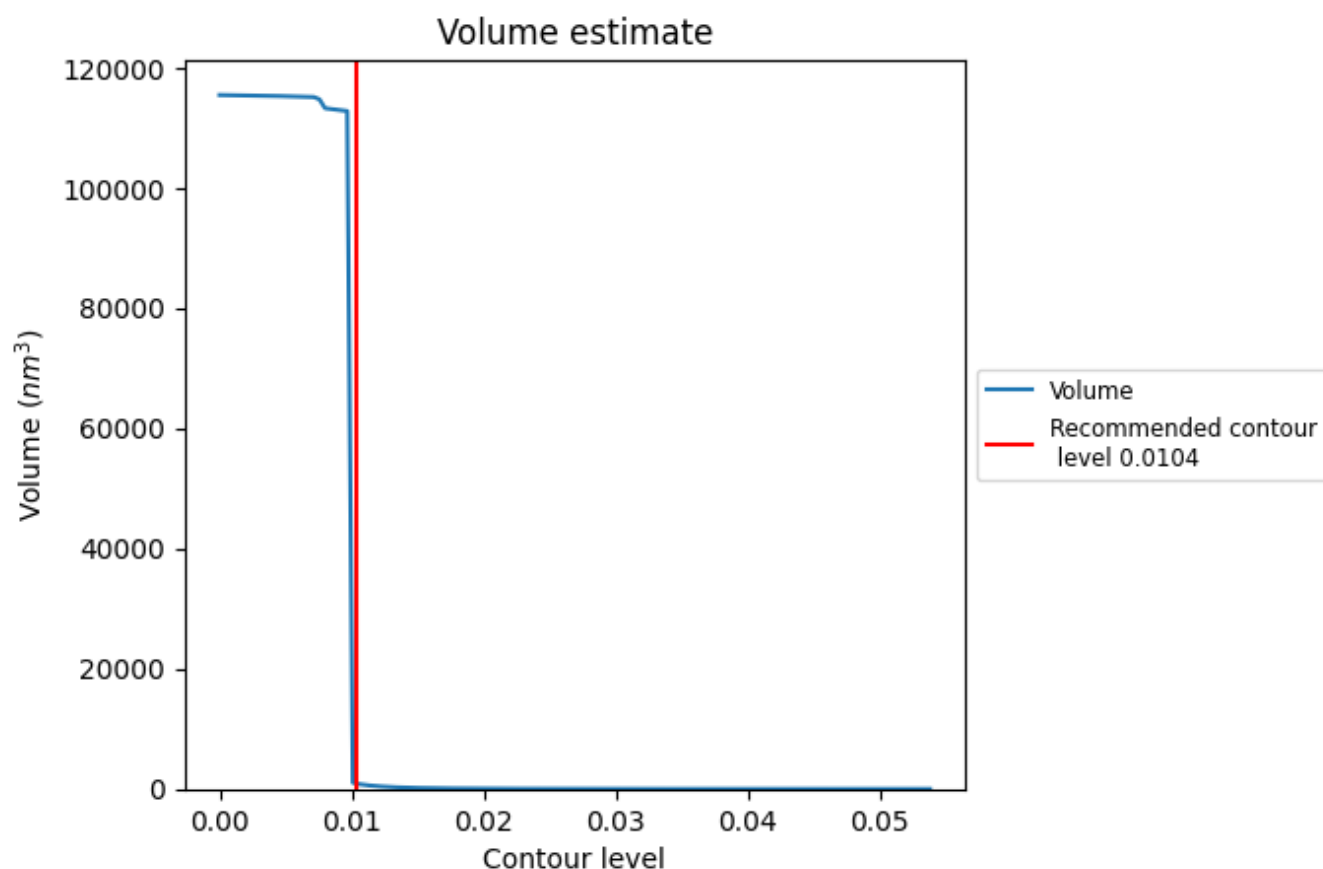
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

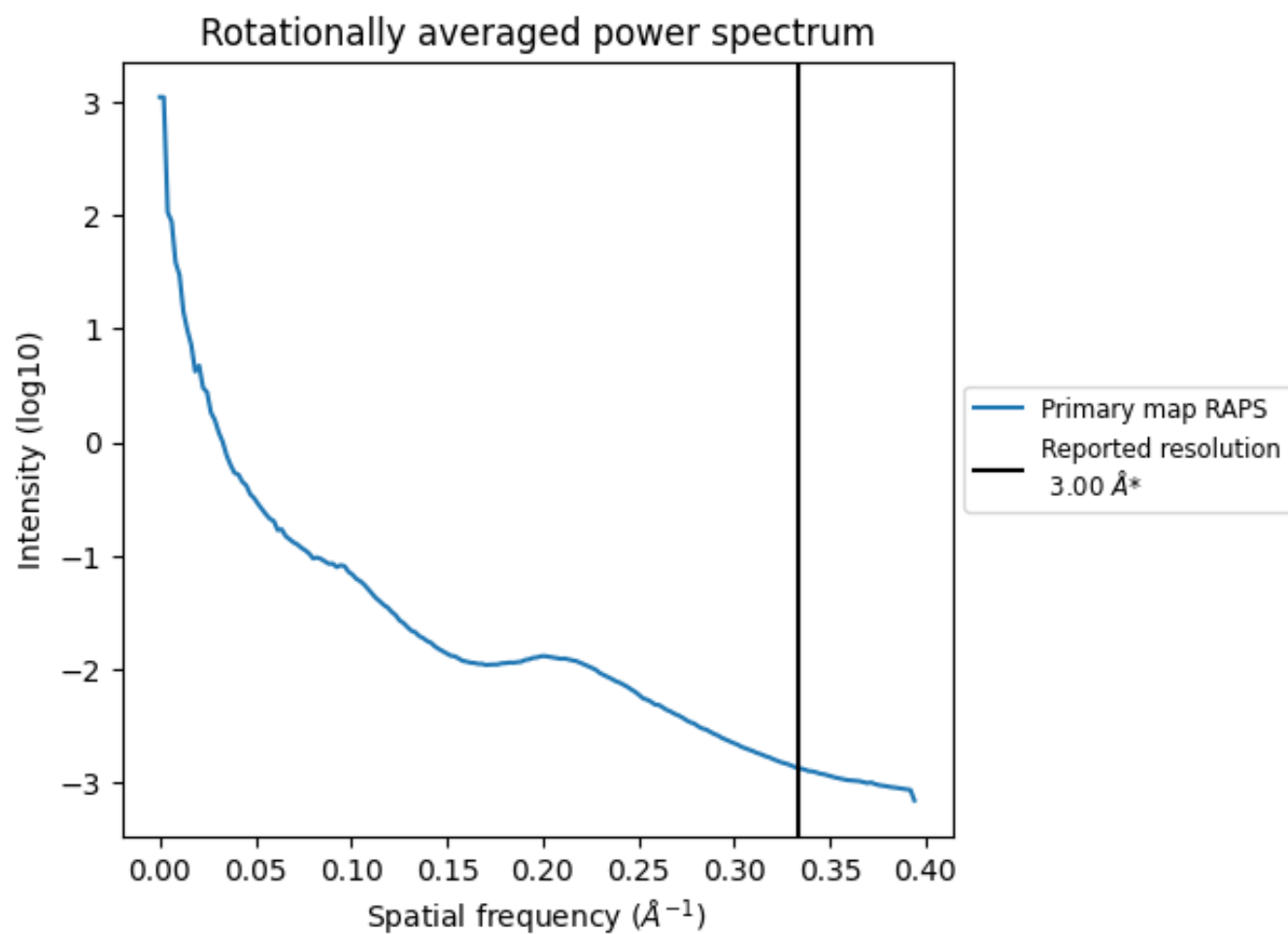
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 878 nm^3 ; this corresponds to an approximate mass of 793 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 0.333 Å⁻¹

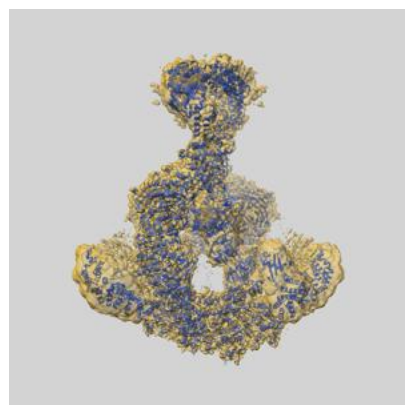
8 Fourier-Shell correlation

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

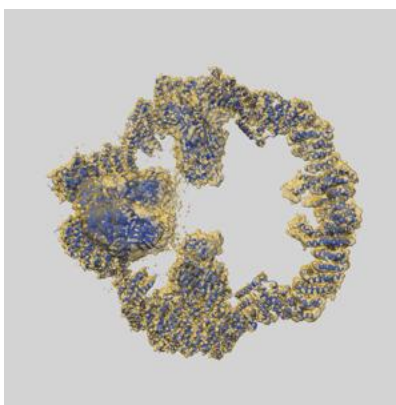
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52502 and PDB model 9HYF. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

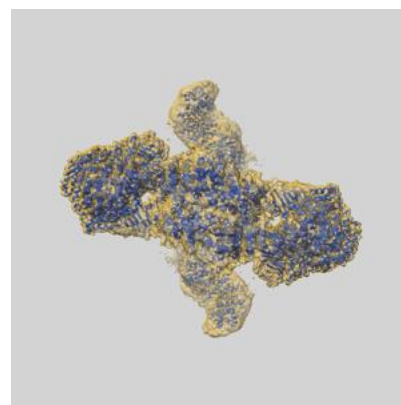
9.1 Map-model overlay [i](#)



X



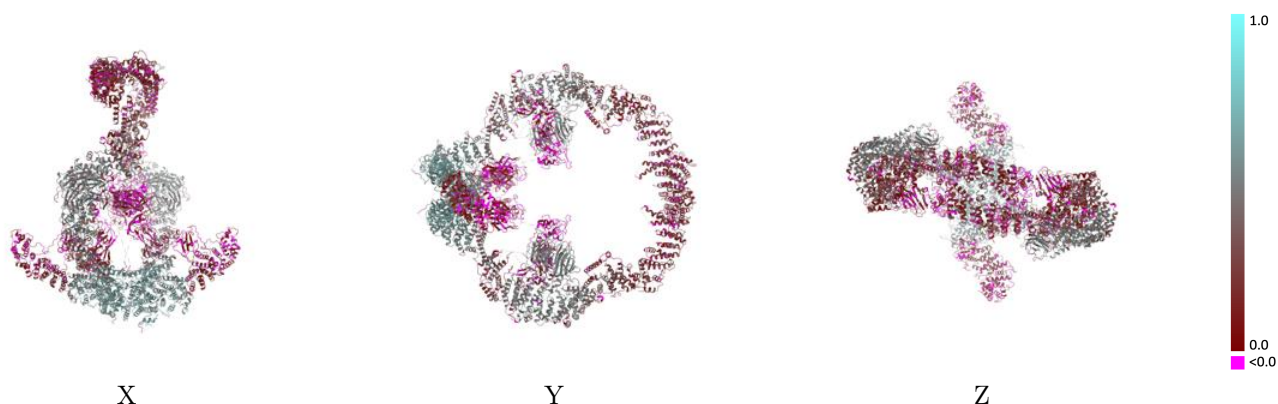
Y



Z

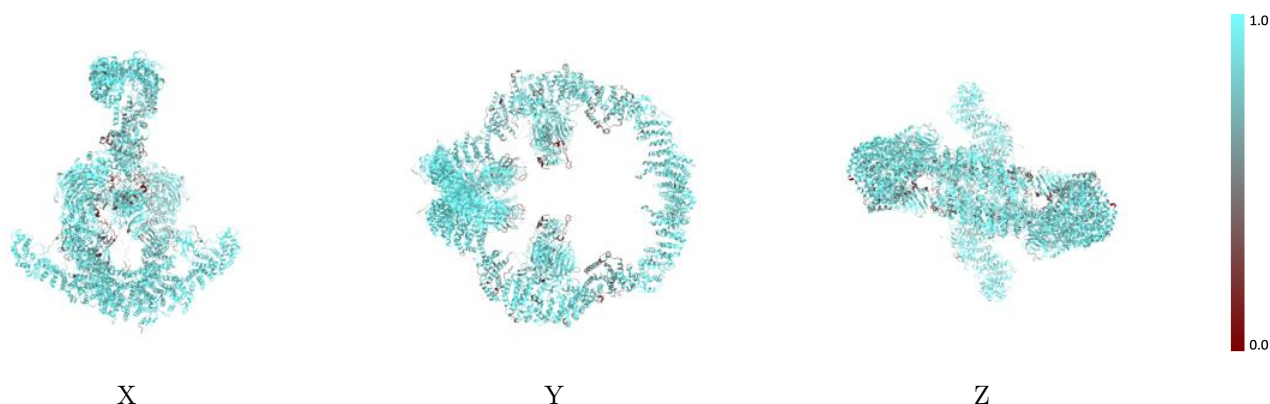
The images above show the 3D surface view of the map at the recommended contour level 0.0104 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



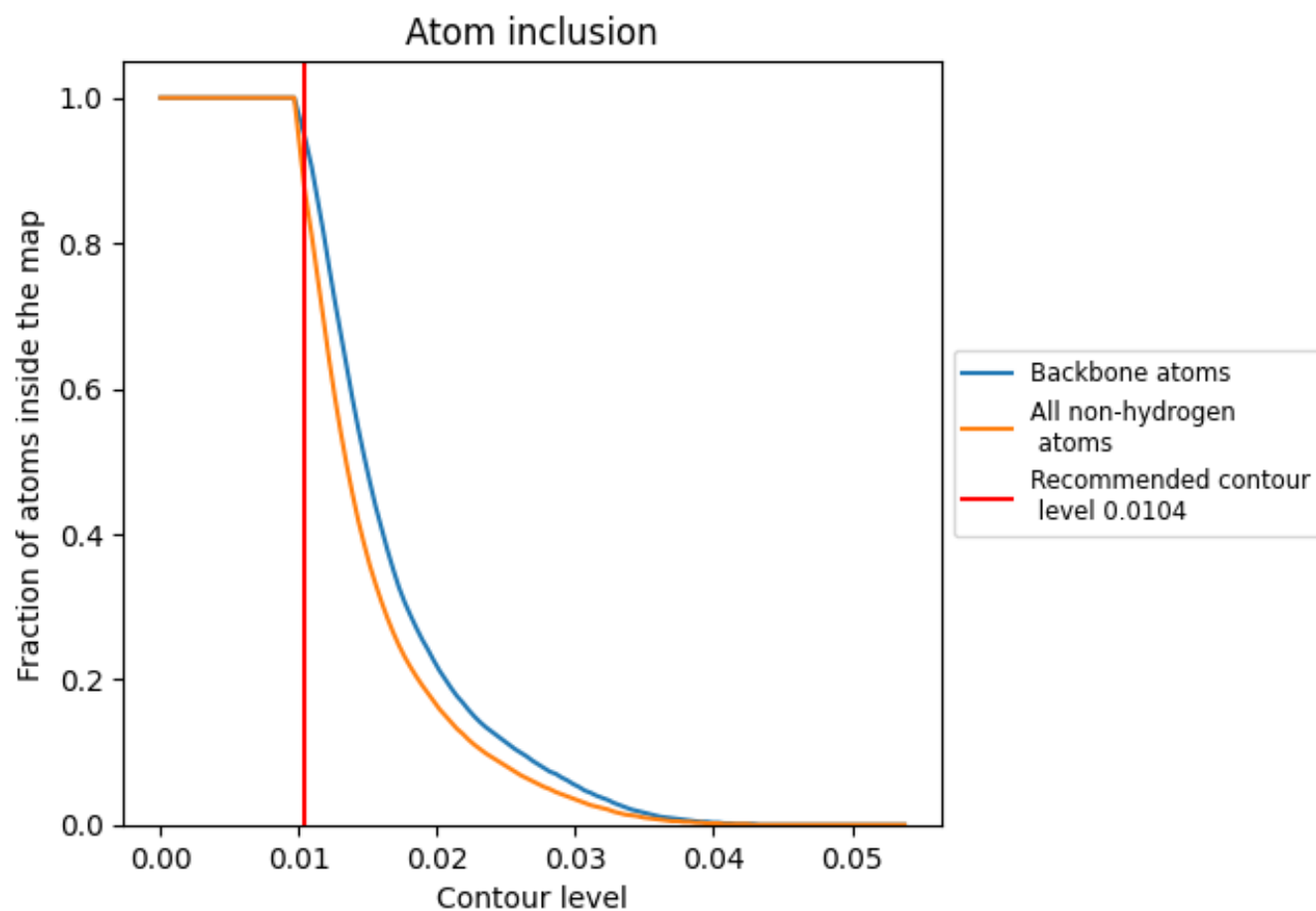
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0104).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 88% 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 (0.0104) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8760	<div></div> 0.3100
A	<div></div> 0.8840	<div></div> 0.3120
B	<div></div> 0.8840	<div></div> 0.3120
C	<div></div> 0.7950	<div></div> 0.2870
D	<div></div> 0.7950	<div></div> 0.2890

