



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 06:34 PM UTC

PDB ID : 9HXW / pdb_00009hwx
EMDB ID : EMD-52490
Title : Cryo-EM structure of the human UBR4/KCMF1/CALM1 complex (composite map)
Authors : Grabarczyk, D.B.; Clausen, T.
Deposited on : 2025-01-08
Resolution : 3.10 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:

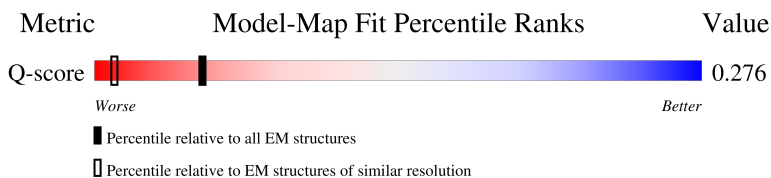
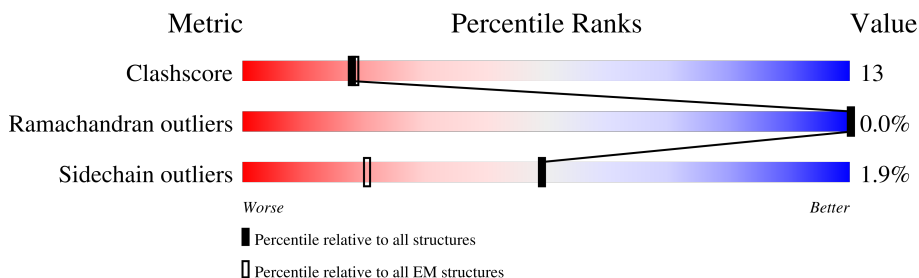
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.10 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	14724 (2.60 - 3.60)

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	C	331	
1	D	331	
2	E	158	
2	F	158	

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Mol	Chain	Length	Quality of chain
3	A	4781	<div><div>16%</div><div><div></div><div>60%</div><div>24%</div><div>•</div><div>15%</div></div></div>
3	B	4781	<div><div>16%</div><div><div></div><div>60%</div><div>24%</div><div>•</div><div>15%</div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 68636 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 E3 ubiquitin-protein ligase KCMF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	181	Total	C	N	O	S	0	0
			1423	875	247	285	16		
1	C	181	Total	C	N	O	S	0	0
			1423	875	247	285	16		

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	149	Total	C	N	O	S	0	0
			1174	719	189	256	10		
2	F	149	Total	C	N	O	S	0	0
			1174	719	189	256	10		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	MET	-	initiating methionine	UNP P0DP23
E	-7	ASP	-	expression tag	UNP P0DP23
E	-6	TYR	-	expression tag	UNP P0DP23
E	-5	LYS	-	expression tag	UNP P0DP23
E	-4	ASP	-	expression tag	UNP P0DP23
E	-3	ASP	-	expression tag	UNP P0DP23
E	-2	ASP	-	expression tag	UNP P0DP23
E	-1	ASP	-	expression tag	UNP P0DP23
E	0	LYS	-	expression tag	UNP P0DP23
F	-8	MET	-	initiating methionine	UNP P0DP23
F	-7	ASP	-	expression tag	UNP P0DP23
F	-6	TYR	-	expression tag	UNP P0DP23
F	-5	LYS	-	expression tag	UNP P0DP23
F	-4	ASP	-	expression tag	UNP P0DP23
F	-3	ASP	-	expression tag	UNP P0DP23
F	-2	ASP	-	expression tag	UNP P0DP23
F	-1	ASP	-	expression tag	UNP P0DP23

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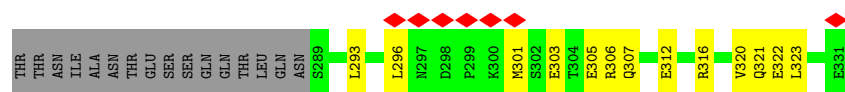
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	LYS	-	expression tag	UNP P0DP23

- Molecule 3 is a protein called E3 ubiquitin-protein ligase UBR4.

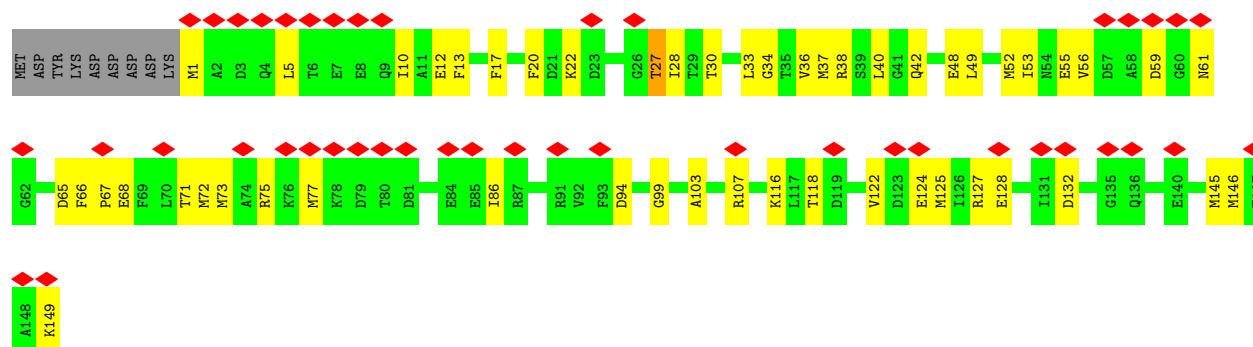
Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	4045	Total	C	N	O	S	0	0
			31711	20123	5410	5969	209		
3	B	4045	Total	C	N	O	S	0	0
			31711	20123	5410	5969	209		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

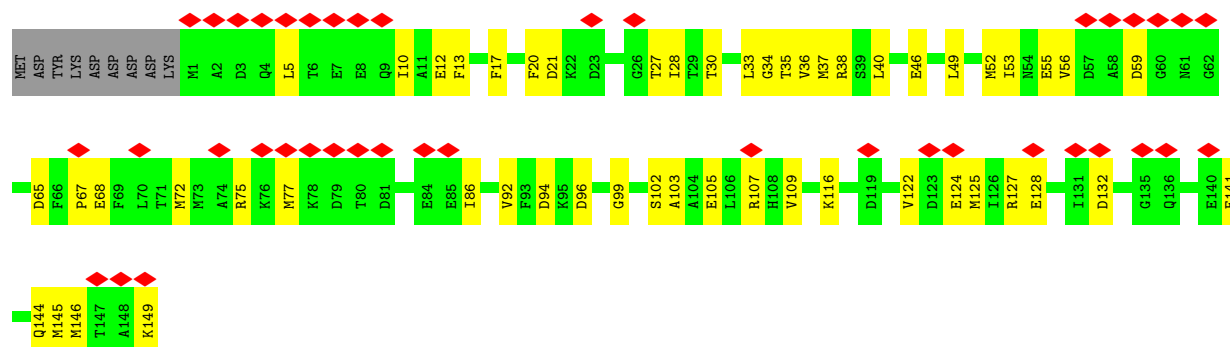
Mol	Chain	Residues	Atoms		AltConf
4	D	4	Total	Zn	0
			4	4	
4	A	6	Total	Zn	0
			6	6	
4	C	4	Total	Zn	0
			4	4	
4	B	6	Total	Zn	0
			6	6	



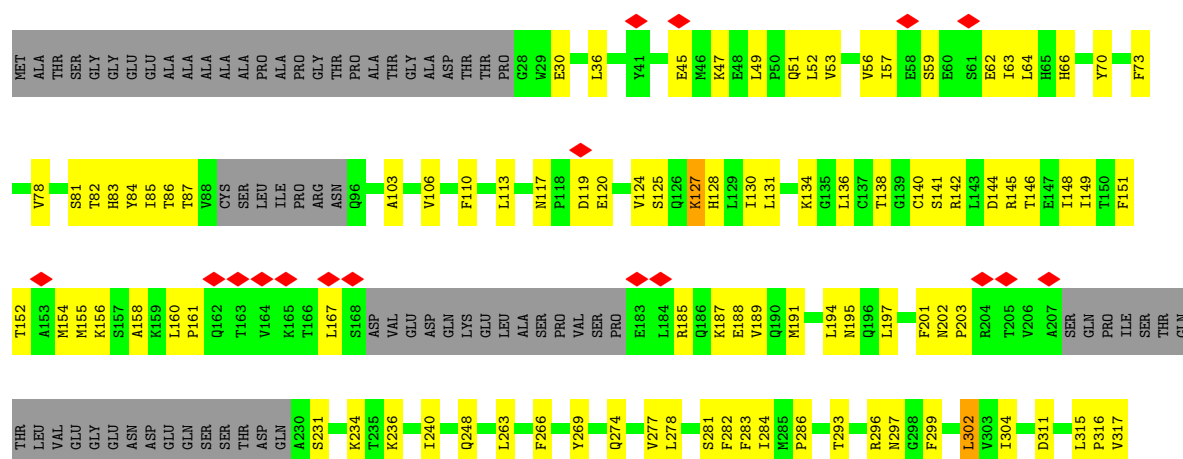
• Molecule 2: Calmodulin-1

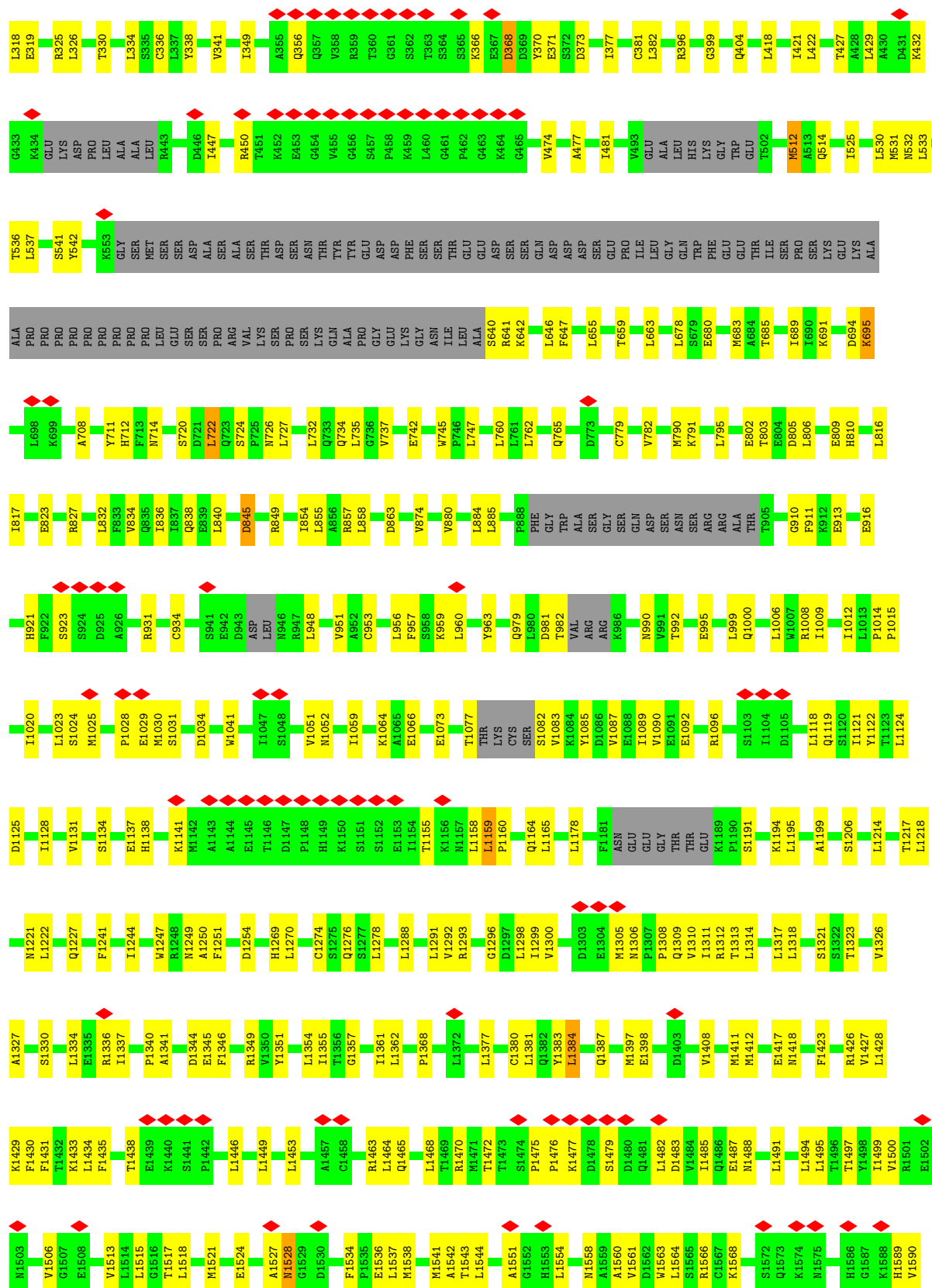


• Molecule 2: Calmodulin-1



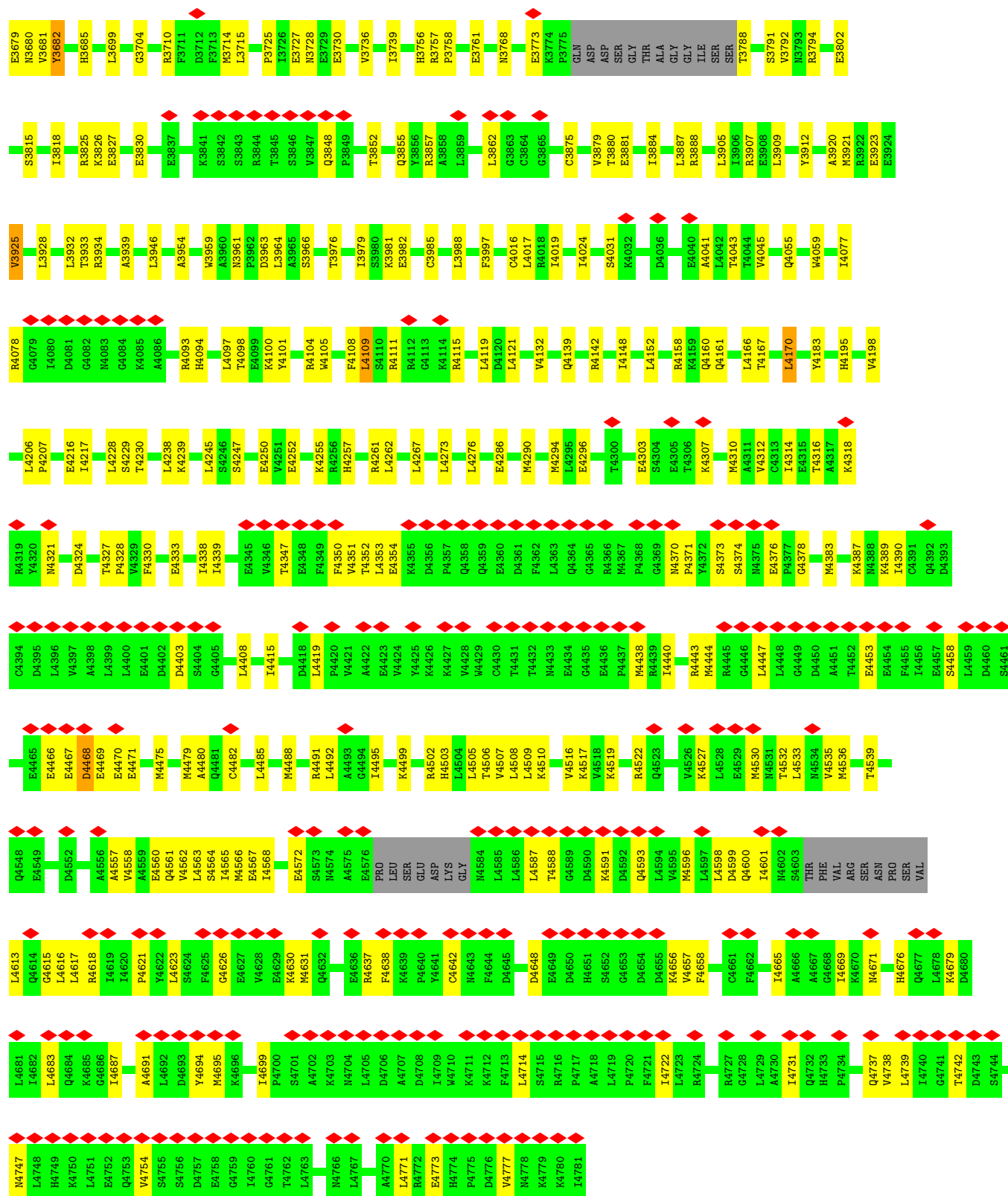
• Molecule 3: E3 ubiquitin-protein ligase UBR4







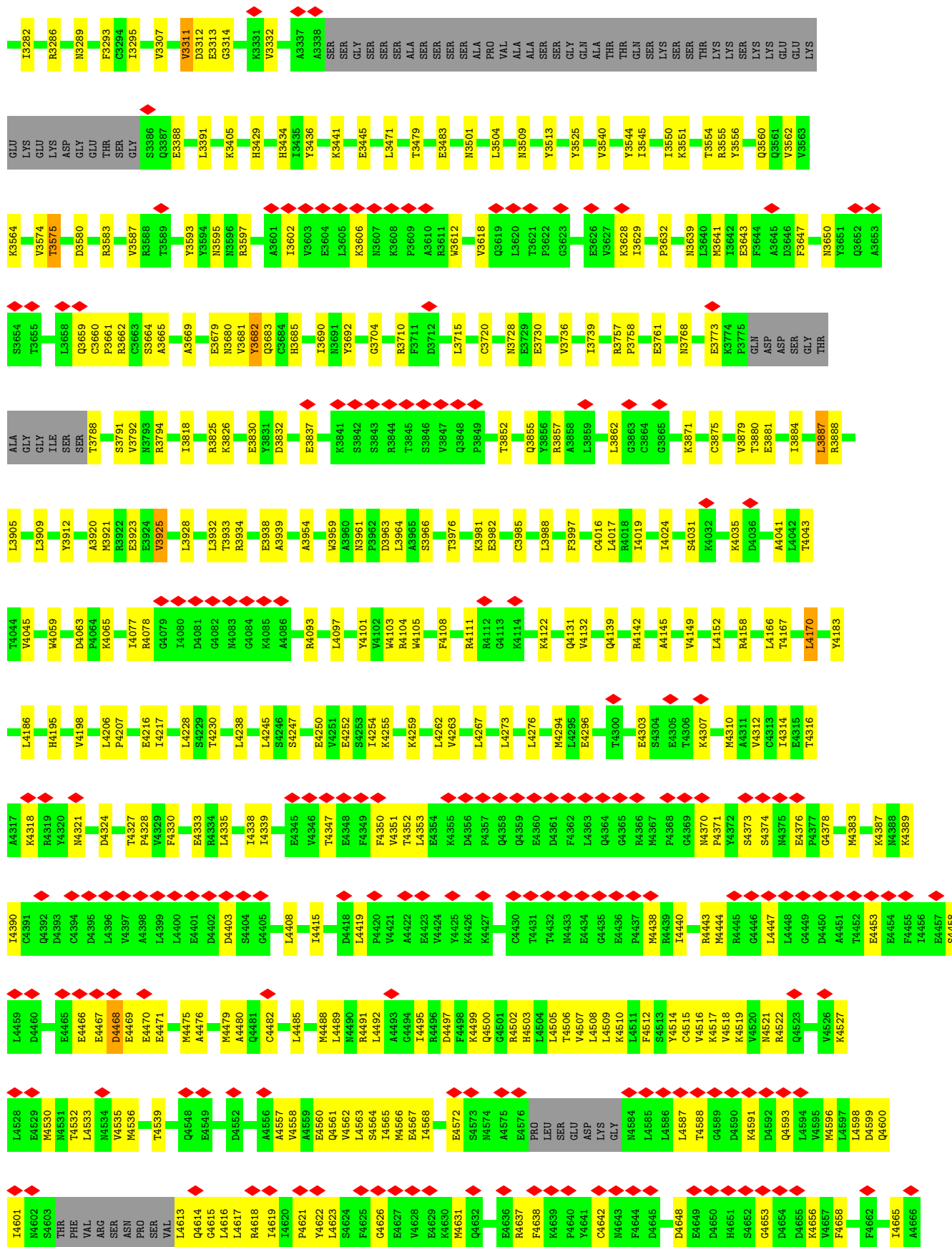


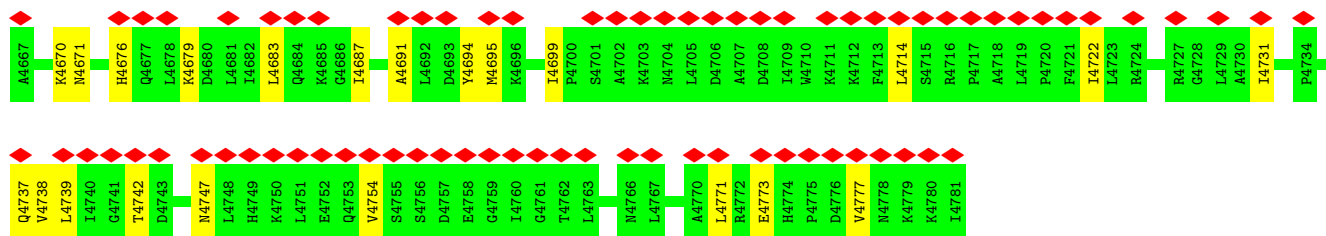




T1313	L1317	L1318	S1321	S1322	T1323	V1326	A1327	L1334	E1335	R1336	I1337	P1340	A1341	D1344	E1345	F1346	Y1351	L1354	I1355	T1356	G1357	C1358	Y1359	N1360	I1361	P1368	L1372	L1377	E1378	E1379	C1380	L1381	L1384	E1385	K1386	Q1387	L1388	M1471	E1389	S1390	S1391	R1394	E1398	D1403	S1404											
G1405	V1408	Q1409	ALA	GLU	M1411	M1412	E1417	N1418	F1423	R1426	V1427	L1428	K1429	F1430	F1431	K1433	E1345	F1435	T1438	E1439	K1440	S1441	P1442	C1443	L1446	L1449	L1453	A1457	C1458	V1459	E1460	R1463	L1464	Q1465	L1468	T1469	R1470	L1388	M1471	T1472	T1473	S1474	P1475	K1477	D1478	S1479	D1480	Q1481	L1482							
D1483	V1484	I1485	K1588	H1589	M1488	L1491	Y1498	R1501	E1502	M1503	E1508	V1513	L1514	L1515	G1516	T1517	L1518	M1521	A1527	M1528	G1529	D1530	F1534	L1537	M1538	M1541	A1542	T1543	L1544	A1551	L1554	M1558	A1559	A1560	V1561	D1562	W1563	L1564	S1565	R1566	C1567	K1568	K1574	N1575												
M1585	H1586	G1587	K1588	H1589	M1590	M1591	I1592	L1593	E1594	C1595	T1596	C1597	H1598	I1599	M1600	S1601	A1604	D1605	V1606	T1607	M1608	A1609	L1610	S1611	Q1612	S1613	N1614	GLY	GLN	GLY	PRO	SER	HIS	LEU	SER	VAL	ASP	GLY	GLU	GLU	ARG	ALA	ILE	GLU	VAL	GLU	GLU									
ASP	SER	GLN	ALA	ASP	ASP	ASP	ASP	GLU	D1655	S1656	L1657	C1658	M1659	K1660	L1661	C1662	T1663	F1664	T1665	I1666	T1667	Q1668	K1669	S1670	F1671	M1672	M1673	K1674	H1675	W1676	Y1677	H1678	T1681	C1682	K1683	M1684	V1685	D1686	V1690	C1691	T1692	K1696	V1697	C1698	H1699	K1700	D1701	H1702	E1703	I1704	S1705	Y1706	A1707	K1708	Y1709	G1710
S1711	C1716	K1719	E1720	D1721	G1722	S1723	C1724	L1725	A1726	L1727	V1728	K1729	R1730	T1731	P1732	S1733	SER	GLY	MET	SER	SER	THR	MET	LYS	GLU	SER	ALA	PHE	GLN	SER	PRO	ARG	ILE	SER	GLU	SER	LEU	VAL	ARG	HIS	ALA	SER	THR	SER	PRO	ALA	ASP	LYS	ALA	LYS	VAL	THR	ILE	SER	ASP	
GLY	LYS	VAL	ASP	GLU	GLU	GLY	LYS	PRO	LYS	SER	SER	LEU	CYS	ARG	THR	VAL	GLU	C1794	C1795	R1796	M1801	M1804	F1805	S1806	F1807	A1808	P1809	L1810	V1811	L1812	D1813	M1814	L1815	N1816	F1817	L1818	M1819	L1822	F1826	A1829	S1830	A1831	V1832	G1833	R1837	Q1840	L1845	H1846	K1850							
A1851	V1852	E1853	M1854	L1858	M1859	V1860	P1861	T1862	L1863	G1864	S1865	Q1866	E1867	F1870	E1871	M1872	V1873	R1874	M1875	I1876	Y1877	D1880	Q1881	T1884	I1885	R1886	Q1887	L1888	I1889	S1890	A1891	H1892	V1893	L1894	R1895	R1896	V1897	N1898	M1899	C1900	V1901	L1902	S1903	S1904	P1905	V1906	C1907	R1908	L1909	Q1910	L1911	L1912	A1913	V1914	S1915	
H1916	E1917	K1918	G1919	K1920	I1921	T1922	V1923	L1924	Q1925	L1926	S1927	A1928	L1929	L1930	K1931	Q1932	A1933	D1934	S1935	S1936	K1937	R1938	K1939	L1940	T1941	L1942	T1943	R1944	L1945	V1950	T1953	V1954	L1955	S1956	L1957	T1958	N1959	P1961	C1962	K1963	E1964	D1965	Y1966	L1967	A1968	V1969	C1970	G1971	L1972	C1975	H1976	V1977	L1978	T1979	F1980	
S1981	S1982	S1983	G1984	S1987	D1988	H1989	L1990	V1991	L1992	H1993	P1994	Q1995	L1996	A1997	T1998	M2000	F2001	I2002	I2003	K2004	A2005	V2006	W2007	G2010	E2014	L2015	A2016	I2017	V2018	T2019	A2020	V2023	K2024	I2025	Y2026	C2029	V2030	D2031	A2032	L2033	S2034	P2035	T2036	F2037	Y2038	F2039	L2040	L2041	P2042	S2043	I2046	R2047				
D2048	V2049	T2050	F2051	T2052	F2053	N2054	E2055	K2058	N2059	I2060	T2061	V2062	I2063	G2068	Y2069	T2070	Y2071	L2074	M2075	E2076	E2077	A2078	S2079	S2080	A2081	Q2082	Q2083	Q2084	P2085	F2086	Y2087	V2088	L2092	E2093	L2094	N2095	H2096	E2097	D2098	L2099	K2100	D2101	S2102	N2103	V2106	A2107	G2110	V2111	S2112	V2113	Y2114	Y2115	S2116			
H2117	V2118	L2119	Q2120	M2121	L2122	F2123	Y2126	K2130	S2131	T2135	I2136	S2137	T2138	R2139	T2139	L2140	L2141	E2142	L2144	Q2145	L2146	F2147	P2148	I2149	N2150	I2151	K2152	S2153	S2154	N2155	G2156	Q2157	S2158	K2159	T2160	S2161	P2162	A2163	L2164	C2165	Q2166	W2167	N2172	H2173	P2174	Q2181	Q2182	T2183	T2184	C2185	P2187	L2188	V2189			
V2192	K2193	Q2194	D2195	T2196	F2197	L2198	I2199	Q2200	E2201	I2202	K2203	T2204	L2205	P2206	A2207	K2208	A2209	K2210	I2211	Q2212	D2213	W2214	V2215	L2217	R2218	H2219	T2220	C2221	C2222	N2223	E2224	Q2225	Q2226	T2227	T2228	T2229	N2230	L2231	L2232	L2233	C2234	E2235	D2236	Q2237	S2238	L2239	R2240	L2241	Y2242	K2243	A2244	N2245	G2246	E2247	N2248	L2253







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1638723	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	0.055	Depositor
Minimum map value	0.000	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0089	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	C	0.10	0/1451	0.26	0/1962
1	D	0.12	0/1451	0.36	0/1962
2	E	0.14	0/1186	0.44	0/1590
2	F	0.14	0/1186	0.39	0/1590
3	A	0.13	0/32281	0.37	4/43722 (0.0%)
3	B	0.13	0/32281	0.38	3/43722 (0.0%)
All	All	0.13	0/69836	0.37	7/94548 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	2
3	B	0	2
All	All	0	4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1819	MET	CA-CB-CG	6.21	126.52	114.10
3	B	1599	ILE	CA-C-N	-5.46	111.02	121.94
3	B	1599	ILE	C-N-CA	-5.46	111.02	121.94
3	A	1599	ILE	CA-C-N	-5.34	111.26	121.94
3	A	1599	ILE	C-N-CA	-5.34	111.26	121.94
3	A	1600	MET	CA-CB-CG	5.18	124.47	114.10
3	A	1814	MET	CA-CB-CG	5.16	124.43	114.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	117	ASN	Peptide
3	A	4468	ASP	Peptide
3	B	117	ASN	Peptide
3	B	4468	ASP	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	C	1423	0	1335	38	0
1	D	1423	0	1335	52	0
2	E	1174	0	1105	46	0
2	F	1174	0	1105	39	0
3	A	31711	0	32086	859	0
3	B	31711	0	32086	860	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
All	All	68636	0	69052	1834	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 13.

All (1834) 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)
3:B:1020:ILE:O	3:B:1024:SER:HB2	1.66	0.96
3:B:231:SER:HA	3:B:234:LYS:HE3	1.49	0.95
2:E:34:GLY:O	2:E:38:ARG:HB3	1.70	0.91
3:A:1020:ILE:O	3:A:1024:SER:HB2	1.71	0.90
3:B:3233:LEU:HD11	3:B:3282:ILE:HG21	1.57	0.87
3:B:1438:THR:HG23	3:B:1446:LEU:HB3	1.57	0.86
3:A:3233:LEU:HD11	3:A:3282:ILE:HG21	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1438:THR:HG23	3:A:1446:LEU:HB3	1.58	0.84
3:B:2559:SER:HG	3:B:2628:HIS:HE2	1.26	0.83
3:A:3010:LEU:HD23	3:A:3081:ILE:HG12	1.61	0.83
3:A:2309:LEU:HD22	1:C:87:GLY:HA3	1.62	0.82
3:B:4591:LYS:NZ	3:B:4631:MET:SD	2.53	0.81
3:A:4339:ILE:HD13	3:A:4475:MET:HB3	1.61	0.81
3:A:4467:GLU:HG2	3:A:4468:ASP:H	1.46	0.81
3:B:4467:GLU:HG2	3:B:4468:ASP:H	1.45	0.81
3:A:3270:ILE:HD11	3:A:3632:PRO:HG2	1.62	0.80
3:B:4339:ILE:HD13	3:B:4475:MET:HB3	1.62	0.80
3:A:4485:LEU:HA	3:A:4488:MET:HE3	1.64	0.80
3:B:3270:ILE:HD11	3:B:3632:PRO:HG2	1.63	0.80
3:A:2984:THR:HA	3:A:2987:GLN:HE21	1.47	0.79
3:B:1610:LEU:HD22	3:B:2492:VAL:HG22	1.65	0.79
1:D:330:ARG:HB3	3:B:4122:LYS:HZ2	1.47	0.79
3:B:1426:ARG:NH1	3:B:1426:ARG:O	2.16	0.78
3:A:2975:LEU:HB2	3:A:2976:MET:HE2	1.66	0.78
3:B:2214:MET:HE2	3:B:2230:MET:HE2	1.64	0.77
3:A:3593:TYR:HB2	3:A:3641:MET:HB3	1.67	0.77
3:B:3436:TYR:HH	3:B:3479:THR:HG1	1.33	0.77
3:A:2354:ILE:HG22	3:A:2420:VAL:HG22	1.66	0.76
3:B:2354:ILE:HG22	3:B:2420:VAL:HG22	1.67	0.76
3:B:3593:TYR:HB2	3:B:3641:MET:HB3	1.66	0.76
2:E:27:THR:HG23	2:E:65:ASP:HB3	1.66	0.76
2:E:37:MET:HG2	2:E:42:GLN:HE21	1.50	0.76
3:B:1391:SER:HA	3:B:1394:ARG:HE	1.50	0.76
3:B:4485:LEU:HA	3:B:4488:MET:HE3	1.68	0.76
3:B:62:GLU:O	3:B:66:HIS:NE2	2.18	0.75
3:B:1340:PRO:HD2	3:B:1344:ASP:HB2	1.66	0.75
3:A:1677:TYR:HA	3:A:1707:ALA:H	1.52	0.75
3:A:1340:PRO:HD2	3:A:1344:ASP:HB2	1.67	0.75
1:D:52:MET:HE2	1:D:52:MET:HA	1.69	0.75
3:A:3102:LEU:O	3:A:3197:TYR:OH	2.04	0.74
3:B:3102:LEU:O	3:B:3197:TYR:OH	2.05	0.74
3:B:1677:TYR:HA	3:B:1707:ALA:H	1.52	0.74
3:A:1859:MET:SD	3:A:2242:TYR:HB3	2.28	0.74
3:B:31:VAL:HA	3:B:34:ARG:HG3	1.69	0.74
3:B:1859:MET:SD	3:B:2242:TYR:HB3	2.28	0.73
3:A:3555:ARG:HD3	3:A:3606:LYS:HD3	1.71	0.73
3:B:73:PHE:HA	3:B:154:MET:HE1	1.69	0.73
3:B:4499:LYS:HA	3:B:4502:ARG:HH21	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:GLY:HA3	3:B:2309:LEU:HD22	1.70	0.72
3:B:1381:LEU:HD23	3:B:1384:LEU:HD11	1.69	0.72
3:B:1858:LEU:HD11	3:B:2198:LEU:HB3	1.70	0.72
3:A:2192:VAL:HG13	3:A:2197:PHE:HE1	1.55	0.72
3:A:4499:LYS:HA	3:A:4502:ARG:HH21	1.54	0.72
2:E:52:MET:HA	2:E:52:MET:HE3	1.70	0.72
1:D:113:CYS:HA	1:D:116:LEU:HB2	1.72	0.71
3:A:1858:LEU:HD11	3:A:2198:LEU:HB3	1.72	0.71
3:A:4591:LYS:HE3	3:A:4626:GLY:H	1.56	0.71
3:B:2975:LEU:HB2	3:B:2976:MET:HE2	1.72	0.71
2:F:52:MET:HA	2:F:52:MET:HE3	1.73	0.71
3:B:2025:ILE:HB	3:B:2037:PHE:HB2	1.73	0.71
3:B:2589:VAL:HG21	3:B:2670:CYS:HB2	1.73	0.71
3:B:2192:VAL:HG13	3:B:2197:PHE:HE1	1.56	0.70
3:B:3739:ILE:HD11	3:B:3825:ARG:HG2	1.71	0.70
3:A:2310:GLN:HE21	1:C:54:CYS:HB2	1.57	0.70
3:B:286:PRO:HB2	3:B:349:ILE:HD12	1.73	0.70
2:E:37:MET:HA	2:E:40:LEU:HG	1.74	0.70
3:A:1030:MET:SD	3:A:1096:ARG:NH1	2.64	0.70
3:B:816:LEU:HD22	3:B:880:VAL:HG11	1.73	0.70
3:A:3739:ILE:HD11	3:A:3825:ARG:HG2	1.72	0.69
3:B:1521:MET:HE3	3:B:1521:MET:H	1.54	0.69
3:B:2232:LEU:HB2	3:B:2240:ARG:HB2	1.74	0.69
3:B:802:GLU:OE1	3:B:802:GLU:N	2.20	0.69
3:B:1707:ALA:O	3:B:2353:ARG:NH2	2.25	0.69
3:B:4522:ARG:HH21	3:B:4568:ILE:HD11	1.57	0.69
3:A:64:LEU:HD12	3:A:113:LEU:HD21	1.74	0.69
3:B:2110:GLY:HA2	3:B:2126:TYR:HA	1.73	0.69
3:B:3229:ASP:OD2	3:B:3289:ASN:ND2	2.25	0.69
3:A:806:LEU:HD23	3:A:857:ARG:HD2	1.74	0.69
3:B:2972:MET:HB3	3:B:2976:MET:HE3	1.75	0.69
3:B:2969:ARG:O	3:B:2973:VAL:HG23	1.93	0.69
3:A:286:PRO:HB2	3:A:349:ILE:HD12	1.74	0.69
3:B:3555:ARG:HD3	3:B:3606:LYS:HD3	1.74	0.68
3:A:2589:VAL:HG21	3:A:2670:CYS:HB2	1.74	0.68
3:A:4558:VAL:O	3:A:4562:VAL:HG23	1.93	0.68
3:A:4596:MET:H	3:A:4596:MET:HE3	1.57	0.68
3:A:1707:ALA:O	3:A:2353:ARG:NH2	2.25	0.68
3:B:1244:ILE:HA	3:B:1293:ARG:HH22	1.59	0.68
3:B:4536:MET:SD	3:B:4566:MET:HE1	2.34	0.68
3:A:1244:ILE:HA	3:A:1293:ARG:HH22	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2025:ILE:HB	3:A:2037:PHE:HB2	1.76	0.68
3:A:913:GLU:OE1	3:A:913:GLU:N	2.25	0.67
3:A:2183:THR:HG23	3:A:2184:THR:HG23	1.76	0.67
3:A:4522:ARG:HH21	3:A:4568:ILE:HD11	1.59	0.67
3:B:806:LEU:HD23	3:B:857:ARG:HD2	1.75	0.67
3:B:4558:VAL:O	3:B:4562:VAL:HG23	1.94	0.67
3:A:4536:MET:SD	3:A:4566:MET:HE1	2.33	0.67
2:F:55:GLU:OE2	2:F:75:ARG:NH2	2.26	0.67
3:A:2530:ALA:O	3:A:2536:ARG:NH2	2.27	0.67
3:A:3909:LEU:HD12	3:A:3925:VAL:HG23	1.77	0.67
3:A:4536:MET:HG3	3:A:4565:ILE:HD11	1.77	0.67
3:A:326:LEU:O	3:A:330:THR:HG23	1.95	0.67
1:C:303:GLU:OE1	1:C:307:GLN:NE2	2.28	0.67
3:B:1900:CYS:SG	3:B:1959:GLY:N	2.66	0.67
3:A:1900:CYS:SG	3:A:1959:GLY:N	2.66	0.67
3:B:3909:LEU:HD12	3:B:3925:VAL:HG23	1.76	0.67
3:A:990:ASN:HD21	3:A:1276:GLN:HB2	1.59	0.67
3:B:2183:THR:HG23	3:B:2184:THR:HG23	1.77	0.67
3:B:3057:ARG:HH21	3:B:3139:PHE:HA	1.60	0.66
1:D:20:ARG:NH2	1:D:38:GLU:OE2	2.27	0.66
3:A:4695:MET:HE1	3:A:4722:ILE:HD13	1.77	0.66
3:A:2476:GLU:O	3:A:2480:VAL:HG23	1.96	0.66
3:B:4093:ARG:O	3:B:4097:LEU:HD12	1.95	0.66
3:A:2375:MET:SD	3:A:2375:MET:N	2.69	0.66
3:B:326:LEU:O	3:B:330:THR:HG23	1.95	0.66
3:B:2149:ILE:HG12	3:B:2197:PHE:HE2	1.60	0.66
3:A:236:LYS:O	3:A:240:ILE:HG13	1.96	0.66
3:A:802:GLU:OE1	3:A:802:GLU:N	2.21	0.66
3:A:816:LEU:HD22	3:A:880:VAL:HG11	1.77	0.66
3:A:2110:GLY:HA2	3:A:2126:TYR:HA	1.76	0.66
3:A:3229:ASP:OD2	3:A:3289:ASN:ND2	2.25	0.66
1:D:110:CYS:HB2	1:D:128:PHE:CE1	2.31	0.65
1:D:301:MET:HG2	1:D:305:GLU:HG3	1.77	0.65
3:A:1667:THR:HG22	3:A:1672:MET:HG2	1.77	0.65
1:D:330:ARG:HB3	3:B:4122:LYS:NZ	2.11	0.65
3:B:1667:THR:HG22	3:B:1672:MET:HG2	1.77	0.65
1:C:24:CYS:SG	1:C:46:HIS:HE1	2.19	0.65
3:B:708:ALA:O	3:B:712:HIS:ND1	2.30	0.65
2:E:124:GLU:HA	2:E:127:ARG:HE	1.61	0.65
3:A:127:LYS:HD2	3:A:304:ILE:HD11	1.79	0.65
3:B:1996:LEU:HD11	3:B:2002:ILE:HG13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4536:MET:HG3	3:B:4565:ILE:HD11	1.79	0.65
3:B:4588:THR:HB	3:B:4623:LEU:HD23	1.77	0.65
3:A:4093:ARG:O	3:A:4097:LEU:HD12	1.96	0.65
3:B:2375:MET:N	3:B:2375:MET:SD	2.70	0.65
3:B:1484:VAL:O	3:B:1488:ASN:ND2	2.30	0.65
2:E:34:GLY:O	2:E:38:ARG:CB	2.43	0.65
3:A:73:PHE:HA	3:A:154:MET:HE1	1.78	0.65
3:A:1178:LEU:HD11	3:A:1199:ALA:HB2	1.78	0.65
3:B:1125:ASP:OD2	3:B:1269:HIS:NE2	2.29	0.65
3:A:2978:LEU:HG	3:A:3006:LEU:HD12	1.78	0.65
3:A:1125:ASP:OD2	3:A:1269:HIS:NE2	2.28	0.64
3:A:2048:ASP:HB3	3:A:2113:VAL:HG12	1.79	0.64
3:A:2583:MET:SD	3:A:2584:ARG:NH1	2.70	0.64
3:A:3857:ARG:HH21	3:A:3862:LEU:HD13	1.60	0.64
1:C:27:CYS:SG	1:C:50:HIS:HE1	2.17	0.64
3:B:2010:GLY:O	3:B:2639:ASN:ND2	2.30	0.64
3:B:4591:LYS:HE3	3:B:4626:GLY:H	1.61	0.64
3:A:1446:LEU:HD23	3:A:1449:LEU:HD21	1.80	0.64
3:A:3007:THR:HB	3:A:3010:LEU:HD22	1.80	0.64
3:B:52:LEU:O	3:B:56:VAL:HG23	1.98	0.64
3:B:3662:ARG:HD2	3:B:3679:GLU:HG3	1.80	0.64
3:B:4353:LEU:HD22	3:B:4390:ILE:HD11	1.80	0.64
3:A:2214:MET:HE1	3:A:2232:LEU:HG	1.78	0.64
3:A:4353:LEU:HD22	3:A:4390:ILE:HD11	1.79	0.64
3:B:1389:GLU:O	3:B:1394:ARG:NH2	2.30	0.64
3:B:2368:ILE:HD12	3:B:2403:LEU:HD11	1.80	0.64
3:B:2530:ALA:O	3:B:2536:ARG:NH2	2.31	0.64
3:B:3556:TYR:HD2	3:B:3704:GLY:HA3	1.62	0.64
3:A:2484:GLU:HA	3:A:2487:GLU:HG2	1.78	0.64
3:B:3660:CYS:HB3	3:B:3665:ALA:H	1.63	0.64
3:B:53:VAL:O	3:B:57:ILE:HG13	1.98	0.64
3:B:3014:ASP:HB3	3:B:3017:ASP:HB3	1.79	0.64
3:A:4588:THR:HB	3:A:4623:LEU:HD23	1.80	0.64
3:B:236:LYS:O	3:B:240:ILE:HG13	1.98	0.64
3:A:691:LYS:NZ	3:A:734:GLN:O	2.28	0.64
3:A:3660:CYS:HB3	3:A:3665:ALA:H	1.64	0.63
3:B:514:GLN:OE1	3:B:514:GLN:N	2.31	0.63
3:B:1438:THR:HA	3:B:1446:LEU:HD13	1.80	0.63
3:A:3556:TYR:HD2	3:A:3704:GLY:HA3	1.62	0.63
2:E:38:ARG:HH22	3:A:4160:GLN:HB2	1.64	0.63
3:A:197:LEU:HD21	3:B:762:LEU:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:708:ALA:O	3:A:712:HIS:ND1	2.31	0.63
3:A:4350:PHE:HB3	3:A:4371:PRO:HB2	1.80	0.63
3:A:1030:MET:HE3	3:A:1030:MET:H	1.64	0.63
3:A:2232:LEU:HB2	3:A:2240:ARG:HB2	1.80	0.63
3:B:2987:GLN:OE1	3:B:2987:GLN:N	2.30	0.63
3:A:1351:TYR:O	3:A:1355:ILE:HG13	1.99	0.63
3:A:2149:ILE:HG12	3:A:2197:PHE:HE2	1.63	0.63
3:A:53:VAL:O	3:A:57:ILE:HG13	1.99	0.63
3:A:1384:LEU:HA	3:A:1387:GLN:HG3	1.81	0.63
3:A:3014:ASP:HB3	3:A:3017:ASP:HB3	1.81	0.63
1:C:20:ARG:NH2	1:C:38:GLU:OE2	2.32	0.63
3:A:2689:PRO:HB3	3:A:2995:ARG:HH12	1.63	0.63
3:B:1030:MET:SD	3:B:1096:ARG:NH1	2.71	0.63
3:B:4695:MET:HE1	3:B:4722:ILE:HD13	1.80	0.63
2:E:37:MET:HG2	2:E:42:GLN:NE2	2.14	0.63
2:F:124:GLU:HA	2:F:127:ARG:HE	1.62	0.63
3:A:1031:SER:H	3:A:1034:ASP:HB2	1.64	0.63
3:A:1438:THR:HA	3:A:1446:LEU:HD13	1.80	0.63
3:A:3158:GLN:OE1	3:A:3158:GLN:N	2.26	0.63
3:A:52:LEU:O	3:A:56:VAL:HG23	1.99	0.63
3:A:809:GLU:HB3	3:A:884:LEU:HD11	1.80	0.63
3:A:3662:ARG:HD2	3:A:3679:GLU:HG3	1.80	0.63
3:A:4488:MET:HB2	3:A:4508:LEU:HD11	1.80	0.63
3:B:84:TYR:O	3:B:87:THR:OG1	2.17	0.62
3:B:2689:PRO:HB3	3:B:2995:ARG:HH12	1.64	0.62
3:B:3034:MET:HE1	3:B:3097:TYR:HB2	1.80	0.62
3:B:3089:LEU:HD12	3:B:3094:ALA:HB2	1.81	0.62
3:B:4350:PHE:HB3	3:B:4371:PRO:HB2	1.80	0.62
3:A:2111:VAL:HG21	3:A:2163:ALA:HB1	1.81	0.62
3:A:3018:LYS:HA	3:A:3021:LEU:HD12	1.81	0.62
3:A:4255:LYS:HZ2	3:A:4255:LYS:HB3	1.64	0.62
3:B:2971:HIS:CE1	3:B:2975:LEU:HD21	2.33	0.62
3:B:2320:ARG:HE	3:B:2328:VAL:HG22	1.65	0.62
3:B:1317:LEU:HD12	3:B:1323:THR:HG21	1.79	0.62
2:E:30:THR:HG22	2:E:33:LEU:HD12	1.79	0.62
3:B:809:GLU:HB3	3:B:884:LEU:HD11	1.82	0.62
3:A:765:GLN:HE22	3:A:817:ILE:HG23	1.65	0.62
3:A:1222:LEU:O	3:A:1227:GLN:NE2	2.33	0.62
3:A:3501:ASN:HB3	3:A:3912:TYR:CD2	2.35	0.62
3:B:73:PHE:CE2	3:B:161:PRO:HD3	2.34	0.62
3:B:293:THR:HG23	3:B:296:ARG:HH21	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3267:ASP:N	3:B:3267:ASP:OD1	2.33	0.62
3:B:765:GLN:HE22	3:B:817:ILE:HG23	1.65	0.62
3:B:3509:ASN:OD1	3:B:3757:ARG:NH2	2.32	0.62
3:A:742:GLU:OE1	3:A:742:GLU:N	2.33	0.62
3:A:3136:MET:HB2	3:A:3145:VAL:HG21	1.82	0.62
3:A:4378:GLY:HA3	3:A:4389:LYS:HD3	1.81	0.62
3:B:1996:LEU:HD21	3:B:2019:THR:HG21	1.80	0.62
3:B:2111:VAL:HG21	3:B:2163:ALA:HB1	1.81	0.62
3:B:3025:LEU:HD11	3:B:3085:THR:HG22	1.80	0.62
3:A:1853:GLU:N	3:A:1853:GLU:OE1	2.33	0.62
3:A:4479:MET:HE3	3:A:4479:MET:H	1.63	0.62
3:B:1178:LEU:HD11	3:B:1199:ALA:HB2	1.82	0.62
3:B:2476:GLU:O	3:B:2480:VAL:HG23	2.00	0.62
3:B:3501:ASN:HB3	3:B:3912:TYR:CD2	2.34	0.62
3:A:845:ASP:N	3:A:845:ASP:OD1	2.30	0.61
3:A:2982:LEU:HB3	3:A:3027:GLN:HE22	1.65	0.61
3:A:3982:GLU:OE1	1:C:316:ARG:NH1	2.33	0.61
3:B:2048:ASP:HB3	3:B:2113:VAL:HG12	1.80	0.61
3:B:2063:ILE:HG23	3:B:2071:TYR:HB2	1.82	0.61
3:B:1446:LEU:HD23	3:B:1449:LEU:HD21	1.80	0.61
3:B:2970:LEU:O	3:B:2974:ARG:HG3	2.00	0.61
3:A:857:ARG:NH2	3:A:931:ARG:O	2.33	0.61
3:B:4378:GLY:HA3	3:B:4389:LYS:HD3	1.81	0.61
3:A:981:ASP:OD1	3:A:981:ASP:N	2.33	0.61
1:C:301:MET:HG2	1:C:305:GLU:HG3	1.82	0.61
3:B:82:THR:O	3:B:86:THR:HG23	2.00	0.61
3:A:82:THR:O	3:A:86:THR:HG23	2.00	0.61
3:A:1317:LEU:HD12	3:A:1323:THR:HG21	1.82	0.61
3:B:1306:ASN:OD1	3:B:1308:PRO:HD2	2.01	0.61
3:B:4510:LYS:O	3:B:4514:TYR:HD1	1.83	0.61
3:A:84:TYR:O	3:A:87:THR:OG1	2.19	0.61
3:A:399:GLY:HA3	3:B:399:GLY:HA3	1.83	0.61
3:A:3267:ASP:N	3:A:3267:ASP:OD1	2.32	0.61
3:B:691:LYS:NZ	3:B:734:GLN:O	2.29	0.61
3:A:1306:ASN:OD1	3:A:1308:PRO:HD2	2.01	0.61
3:A:3575:THR:HG22	3:A:3628:LYS:HD3	1.83	0.61
3:A:4387:LYS:NZ	3:A:4403:ASP:OD1	2.32	0.61
3:B:1832:VAL:O	3:B:1837:ARG:NH2	2.34	0.61
2:F:5:LEU:HB3	2:F:10:ILE:HD11	1.83	0.60
3:B:857:ARG:NH2	3:B:931:ARG:O	2.34	0.60
3:B:1853:GLU:OE1	3:B:1853:GLU:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2216:ALA:HB2	3:B:2230:MET:HE3	1.81	0.60
2:E:38:ARG:NH2	3:A:4160:GLN:HB2	2.16	0.60
3:A:2291:PHE:O	3:A:2295:ASN:ND2	2.33	0.60
3:A:2368:ILE:HD12	3:A:2403:LEU:HD11	1.82	0.60
3:B:1165:LEU:HG	3:B:1291:LEU:HD11	1.83	0.60
3:B:2014:GLU:OE1	3:B:2014:GLU:N	2.34	0.60
3:A:4031:SER:HB3	1:C:306:ARG:HG2	1.82	0.60
3:B:1308:PRO:HA	3:B:1311:ILE:HG12	1.82	0.60
3:A:2998:PRO:HA	3:A:3001:GLN:HB2	1.83	0.60
3:A:3509:ASN:OD1	3:A:3757:ARG:NH2	2.32	0.60
3:B:913:GLU:H	3:B:913:GLU:CD	2.09	0.60
3:B:1222:LEU:O	3:B:1227:GLN:NE2	2.34	0.60
3:B:1560:ALA:HA	3:B:1563:TRP:HB2	1.82	0.60
3:A:1165:LEU:HG	3:A:1291:LEU:HD11	1.82	0.60
3:B:2521:VAL:HG23	3:B:2522:GLN:OE1	2.01	0.60
1:D:82:TYR:OH	1:D:128:PHE:HB3	2.01	0.60
3:A:3888:ARG:HG3	3:A:3928:LEU:HB2	1.84	0.60
3:A:683:MET:HE3	3:A:727:LEU:HB3	1.84	0.60
3:A:1475:PRO:HG2	3:A:1482:LEU:HD23	1.83	0.60
3:A:3000:MET:HA	3:A:3003:ILE:HG13	1.82	0.60
3:A:4353:LEU:O	3:A:4370:ASN:ND2	2.29	0.60
3:A:1308:PRO:HA	3:A:1311:ILE:HG12	1.84	0.60
3:A:2063:ILE:HG23	3:A:2071:TYR:HB2	1.84	0.60
3:A:2308:LEU:HD23	3:A:2330:ASN:HD22	1.67	0.60
3:A:3583:ARG:NE	3:A:3583:ARG:O	2.34	0.60
3:B:2997:ILE:H	3:B:2997:ILE:HD12	1.66	0.60
3:B:3575:THR:HG22	3:B:3628:LYS:HD3	1.84	0.60
2:E:33:LEU:HD23	2:E:37:MET:HE1	1.84	0.60
3:B:1411:MET:HB3	3:B:1431:PHE:CZ	2.37	0.60
3:A:191:MET:HA	3:A:191:MET:HE3	1.83	0.59
3:A:1832:VAL:O	3:A:1837:ARG:NH2	2.35	0.59
3:A:1924:LEU:HD21	3:A:1942:LEU:HD13	1.83	0.59
3:B:845:ASP:OD1	3:B:845:ASP:N	2.33	0.59
3:B:4679:LYS:NZ	3:B:4731:ILE:O	2.35	0.59
2:E:5:LEU:HB3	2:E:10:ILE:HD11	1.84	0.59
3:A:2978:LEU:HD23	3:A:2981:LEU:HD21	1.84	0.59
3:B:4312:VAL:O	3:B:4316:THR:HG23	2.02	0.59
3:A:160:LEU:HD21	3:A:167:LEU:HG	1.85	0.59
3:A:293:THR:HG23	3:A:296:ARG:HH21	1.67	0.59
3:A:1427:VAL:O	3:A:1430:PHE:HB3	2.03	0.59
3:B:138:THR:OG1	3:B:142:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:981:ASP:N	3:B:981:ASP:OD1	2.34	0.59
3:A:2661:VAL:HG23	3:A:2682:TYR:HE1	1.68	0.59
3:B:284:ILE:HG22	3:B:286:PRO:HD3	1.84	0.59
3:B:3560:GLN:HE21	3:B:3643:GLU:HG3	1.68	0.59
3:B:2312:TYR:HB3	3:B:2320:ARG:HH12	1.67	0.59
3:B:3050:GLU:HG2	3:B:3153:PHE:CD2	2.38	0.59
3:B:3580:ASP:HB3	3:B:3710:ARG:HD3	1.84	0.59
1:D:38:GLU:HG2	3:B:2332:LYS:HE3	1.85	0.59
3:A:2487:GLU:OE1	3:A:2528:LEU:HB2	2.01	0.59
3:A:3580:ASP:HB3	3:A:3710:ARG:HD3	1.83	0.59
1:D:306:ARG:HG2	3:B:4031:SER:HB3	1.85	0.59
3:A:849:ARG:NH1	3:A:982:THR:OG1	2.36	0.59
3:B:3225:ARG:NH2	3:B:3229:ASP:OD1	2.36	0.59
3:B:4247:SER:HA	3:B:4250:GLU:OE2	2.02	0.59
1:D:316:ARG:NH1	3:B:3982:GLU:OE1	2.36	0.59
3:A:319:GLU:H	3:A:319:GLU:CD	2.11	0.59
3:A:1214:LEU:H	3:A:1214:LEU:HD12	1.67	0.59
3:A:1536:GLU:OE1	3:A:1536:GLU:N	2.34	0.59
3:A:2214:MET:HE3	3:A:2215:VAL:H	1.68	0.59
3:A:2997:ILE:H	3:A:2997:ILE:HD12	1.67	0.59
3:B:319:GLU:CD	3:B:319:GLU:H	2.11	0.59
3:A:284:ILE:HG22	3:A:286:PRO:HD3	1.85	0.59
3:A:4522:ARG:HB2	3:A:4572:GLU:HG2	1.85	0.59
3:B:1706:TYR:N	3:B:2386:ASP:OD2	2.28	0.59
3:B:3583:ARG:NE	3:B:3583:ARG:O	2.34	0.59
3:A:62:GLU:O	3:A:66:HIS:NE2	2.36	0.58
3:A:1590:VAL:HA	3:A:1593:LEU:HG	1.85	0.58
3:A:3089:LEU:HD12	3:A:3094:ALA:HB2	1.83	0.58
3:A:3959:TRP:NE1	3:B:3912:TYR:OH	2.28	0.58
3:A:4312:VAL:O	3:A:4316:THR:HG23	2.02	0.58
3:B:1485:ILE:HA	3:B:1488:ASN:HD22	1.69	0.58
3:B:3888:ARG:HG3	3:B:3928:LEU:HB2	1.85	0.58
3:B:4351:VAL:HA	3:B:4438:MET:HB3	1.84	0.58
3:B:1308:PRO:HB2	3:B:1312:ARG:NH1	2.18	0.58
3:B:2291:PHE:O	3:B:2295:ASN:ND2	2.34	0.58
3:B:4479:MET:HE3	3:B:4479:MET:H	1.68	0.58
3:A:134:LYS:HZ1	3:A:311:ASP:HA	1.68	0.58
3:A:2317:ILE:HG12	3:A:2320:ARG:HH21	1.69	0.58
3:A:1521:MET:SD	3:A:1521:MET:N	2.75	0.58
3:A:2307:ASP:HB3	3:A:2336:PHE:HB2	1.86	0.58
3:B:86:THR:OG1	3:B:140:CYS:SG	2.61	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1142:MET:HE3	3:B:1148:PRO:HA	1.86	0.58
3:B:2317:ILE:HG12	3:B:2320:ARG:HH22	1.68	0.58
3:B:2484:GLU:HA	3:B:2487:GLU:HG2	1.84	0.58
3:B:4255:LYS:HZ2	3:B:4255:LYS:HB3	1.69	0.58
3:A:73:PHE:CE2	3:A:161:PRO:HD3	2.39	0.58
3:A:762:LEU:HB3	3:B:197:LEU:HD21	1.85	0.58
3:A:4351:VAL:HA	3:A:4438:MET:HB3	1.84	0.58
3:B:4488:MET:O	3:B:4492:LEU:HD22	2.04	0.58
3:B:2308:LEU:HD23	3:B:2330:ASN:HD22	1.68	0.58
3:B:2583:MET:SD	3:B:2584:ARG:NH1	2.76	0.58
3:B:4206:LEU:HD13	3:B:4262:LEU:HD11	1.84	0.58
2:F:49:LEU:O	2:F:53:ILE:HG23	2.04	0.58
3:A:1996:LEU:HD11	3:A:2002:ILE:HG13	1.85	0.58
3:B:1118:LEU:HA	3:B:1121:ILE:HD12	1.86	0.58
3:B:1427:VAL:HG22	3:B:1431:PHE:CE2	2.38	0.58
3:B:1541:MET:HA	3:B:1544:LEU:HB2	1.85	0.58
3:B:4198:VAL:HG12	3:B:4254:ILE:HD11	1.84	0.58
3:A:1541:MET:HA	3:A:1544:LEU:HB2	1.86	0.57
3:A:3225:ARG:NH2	3:A:3229:ASP:OD1	2.37	0.57
3:B:542:TYR:HD2	3:B:689:ILE:HD12	1.69	0.57
3:B:959:LYS:NZ	3:B:960:LEU:H	2.02	0.57
3:A:3388:GLU:OE1	3:A:3388:GLU:N	2.34	0.57
3:A:3818:ILE:HD12	3:B:4230:THR:HG21	1.85	0.57
3:A:4321:ASN:O	3:A:4491:ARG:NH1	2.35	0.57
3:A:3560:GLN:HE21	3:A:3643:GLU:HG3	1.69	0.57
3:A:4247:SER:HA	3:A:4250:GLU:OE2	2.03	0.57
3:B:474:VAL:HG11	3:B:646:LEU:HG	1.87	0.57
3:B:4522:ARG:HB2	3:B:4572:GLU:HG2	1.87	0.57
3:A:3025:LEU:HD11	3:A:3085:THR:HG22	1.86	0.57
3:A:3560:GLN:HB3	3:A:3641:MET:HE1	1.85	0.57
3:A:4656:LYS:HD2	3:A:4657:VAL:N	2.18	0.57
3:A:4679:LYS:NZ	3:A:4731:ILE:O	2.38	0.57
3:B:2214:MET:SD	3:B:2232:LEU:HG	2.44	0.57
2:E:77:MET:SD	2:E:77:MET:N	2.76	0.57
3:A:1538:MET:HE3	3:A:1598:HIS:HB3	1.87	0.57
3:A:1600:MET:HE3	3:A:1600:MET:H	1.69	0.57
3:B:1475:PRO:HG2	3:B:1482:LEU:HD23	1.85	0.57
3:B:1214:LEU:H	3:B:1214:LEU:HD12	1.69	0.57
3:B:1858:LEU:HD23	3:B:2248:ASN:HB3	1.86	0.57
3:B:4699:ILE:HD13	3:B:4747:ASN:HB3	1.87	0.57
3:A:189:VAL:HG11	3:B:874:VAL:HG13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1118:LEU:HA	3:A:1121:ILE:HD12	1.87	0.57
3:A:4310:MET:O	3:A:4314:ILE:HG12	2.05	0.57
3:A:4408:LEU:HD13	3:A:4440:ILE:HG21	1.87	0.57
3:B:160:LEU:HD21	3:B:167:LEU:HG	1.85	0.57
3:B:2487:GLU:OE1	3:B:2528:LEU:HB2	2.04	0.57
3:B:4310:MET:SD	3:B:4310:MET:N	2.77	0.57
3:B:1590:VAL:HA	3:B:1593:LEU:HG	1.86	0.56
3:A:795:LEU:HD12	3:A:840:LEU:HD13	1.87	0.56
3:A:921:HIS:CE1	3:A:1274:CYS:HB2	2.40	0.56
3:A:1244:ILE:HG12	3:A:1293:ARG:HH12	1.70	0.56
3:A:1706:TYR:N	3:A:2386:ASP:OD2	2.28	0.56
3:B:64:LEU:HD12	3:B:113:LEU:HD21	1.85	0.56
3:B:1671:PHE:C	3:B:1672:MET:HE2	2.30	0.56
3:B:2544:ASP:OD2	3:B:2584:ARG:NH2	2.38	0.56
2:F:77:MET:SD	2:F:77:MET:N	2.70	0.56
3:A:514:GLN:OE1	3:A:514:GLN:N	2.38	0.56
3:A:1064:LYS:NZ	3:A:1066:GLU:HB2	2.19	0.56
3:A:1899:MET:HG2	3:A:1914:VAL:HG12	1.86	0.56
3:A:2970:LEU:O	3:A:2974:ARG:HG3	2.06	0.56
3:A:4310:MET:N	3:A:4310:MET:SD	2.78	0.56
3:A:4527:LYS:HB2	3:A:4530:MET:HE1	1.87	0.56
3:A:4598:LEU:HD13	3:A:4637:ARG:HH22	1.69	0.56
3:B:234:LYS:HD2	3:B:235:THR:N	2.20	0.56
3:B:2181:GLN:HB2	3:B:2185:GLY:H	1.71	0.56
3:B:3095:VAL:HB	3:B:3190:TRP:HZ2	1.70	0.56
3:B:3961:ASN:ND2	3:B:3963:ASP:OD2	2.38	0.56
3:A:2181:GLN:HB2	3:A:2185:GLY:H	1.71	0.56
2:E:122:VAL:HA	2:E:125:MET:HG2	1.88	0.56
3:A:474:VAL:HG11	3:A:646:LEU:HG	1.86	0.56
3:A:1292:VAL:HG21	3:A:1326:VAL:HG13	1.87	0.56
3:A:1807:PHE:HA	3:A:1810:LEU:HD23	1.88	0.56
3:B:3107:GLU:HA	3:B:3110:LYS:HG2	1.87	0.56
2:E:49:LEU:O	2:E:53:ILE:HG13	2.06	0.56
2:E:56:VAL:HG11	2:E:68:GLU:HG3	1.87	0.56
3:A:4338:ILE:HB	3:A:4475:MET:HE1	1.88	0.56
3:A:4699:ILE:HD13	3:A:4747:ASN:HB3	1.87	0.56
3:B:921:HIS:CE1	3:B:1274:CYS:HB2	2.40	0.56
3:B:1476:PRO:HG2	3:B:1479:SER:HB3	1.87	0.56
3:B:4466:GLU:HA	3:B:4469:GLU:HB3	1.88	0.56
2:F:122:VAL:HA	2:F:125:MET:HG2	1.87	0.56
3:A:1308:PRO:HB2	3:A:1312:ARG:NH1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2662:ASP:OD1	3:A:2663:ILE:N	2.39	0.56
3:B:1423:PHE:O	3:B:1427:VAL:HG12	2.06	0.56
3:B:4387:LYS:NZ	3:B:4403:ASP:OD1	2.32	0.56
3:A:2018:VAL:HG13	3:A:2023:VAL:HG22	1.86	0.56
3:B:429:LEU:HA	3:B:432:LYS:HG2	1.87	0.56
3:B:1819:MET:O	3:B:1819:MET:HE3	2.06	0.56
2:F:146:MET:HE3	3:B:4101:TYR:HD1	1.71	0.56
3:A:720:SER:O	3:A:722:LEU:HD22	2.05	0.56
3:A:1119:GLN:HA	3:A:1122:TYR:CZ	2.41	0.56
3:A:1428:LEU:HB3	3:A:1491:LEU:HD13	1.86	0.56
3:A:3107:GLU:HA	3:A:3110:LYS:HG2	1.88	0.56
3:B:720:SER:O	3:B:722:LEU:HD22	2.05	0.56
3:B:2698:LYS:O	3:B:2702:ILE:HG12	2.06	0.56
3:B:4518:VAL:HB	3:B:4521:ASN:HB3	1.87	0.56
3:A:1671:PHE:C	3:A:1672:MET:HE2	2.30	0.56
3:A:2676:ASN:OD1	3:A:2677:THR:N	2.39	0.56
3:A:4041:ALA:HA	3:A:4078:ARG:HH12	1.71	0.56
3:B:1119:GLN:HA	3:B:1122:TYR:CZ	2.41	0.55
3:B:4254:ILE:HD12	3:B:4254:ILE:H	1.72	0.55
3:B:4598:LEU:HD13	3:B:4637:ARG:HH22	1.70	0.55
2:E:55:GLU:OE2	2:E:75:ARG:NH2	2.37	0.55
3:A:992:THR:N	3:A:995:GLU:OE1	2.35	0.55
3:A:4466:GLU:HA	3:A:4469:GLU:HB3	1.87	0.55
3:A:4516:VAL:O	3:A:4522:ARG:NH2	2.39	0.55
3:A:4563:LEU:HD21	3:A:4615:GLY:HA3	1.87	0.55
3:A:4593:GLN:OE1	3:A:4593:GLN:N	2.23	0.55
3:B:3388:GLU:OE1	3:B:3388:GLU:N	2.35	0.55
2:E:65:ASP:OD2	2:E:67:PRO:HD2	2.06	0.55
2:E:132:ASP:OD1	2:E:132:ASP:N	2.39	0.55
3:A:533:LEU:O	3:A:537:LEU:HG	2.07	0.55
3:B:1915:SER:HB3	3:B:1957:LEU:HD11	1.88	0.55
3:A:1915:SER:HB3	3:A:1957:LEU:HD11	1.88	0.55
3:A:3095:VAL:HB	3:A:3190:TRP:HZ2	1.71	0.55
3:A:4596:MET:O	3:A:4600:GLN:HG2	2.06	0.55
3:B:2192:VAL:HG13	3:B:2197:PHE:CE1	2.41	0.55
3:B:1292:VAL:HG21	3:B:1326:VAL:HG13	1.89	0.55
3:B:2499:GLU:HA	3:B:2502:LYS:HD3	1.88	0.55
3:B:4216:GLU:OE2	3:B:4238:LEU:HD13	2.07	0.55
3:B:795:LEU:HD12	3:B:840:LEU:HD13	1.89	0.55
3:B:4353:LEU:O	3:B:4370:ASN:ND2	2.29	0.55
3:B:4596:MET:O	3:B:4600:GLN:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:542:TYR:HD2	3:A:689:ILE:HD12	1.72	0.55
3:A:1357:GLY:O	3:A:1361:ILE:HG22	2.06	0.55
3:A:2499:GLU:HA	3:A:2502:LYS:HD3	1.89	0.55
3:A:4468:ASP:HB3	3:A:4471:GLU:HB3	1.89	0.55
3:A:2543:LYS:HE2	3:A:2547:LEU:HD12	1.89	0.55
3:B:2018:VAL:HG13	3:B:2023:VAL:HG22	1.87	0.55
3:B:2998:PRO:HA	3:B:3001:GLN:HB2	1.89	0.55
1:D:56:LEU:HD11	3:B:2311:VAL:HG13	1.88	0.55
3:B:655:LEU:O	3:B:659:THR:HG23	2.07	0.55
3:B:2676:ASN:OD1	3:B:2677:THR:N	2.40	0.55
3:B:3163:MET:HE1	3:B:3166:ARG:HH12	1.72	0.55
3:A:429:LEU:HA	3:A:432:LYS:HG2	1.87	0.55
3:A:655:LEU:O	3:A:659:THR:HG23	2.07	0.55
3:A:1896:ARG:NH1	3:A:2213:ASP:OD2	2.40	0.55
3:A:2521:VAL:HG23	3:A:2522:GLN:OE1	2.07	0.55
3:A:3144:TYR:O	3:A:3148:HIS:ND1	2.36	0.55
3:A:3556:TYR:CD2	3:A:3704:GLY:HA3	2.42	0.55
3:B:418:LEU:HD11	3:B:477:ALA:HA	1.89	0.55
3:B:4563:LEU:HD21	3:B:4615:GLY:HA3	1.89	0.55
3:B:1357:GLY:O	3:B:1361:ILE:HG23	2.07	0.54
3:B:1807:PHE:HA	3:B:1810:LEU:HD23	1.89	0.54
3:B:3560:GLN:HB3	3:B:3641:MET:HE1	1.89	0.54
3:B:4338:ILE:HB	3:B:4475:MET:HE1	1.89	0.54
3:A:2990:ASN:OD1	3:A:2990:ASN:N	2.40	0.54
3:B:533:LEU:O	3:B:537:LEU:HG	2.07	0.54
3:B:2662:ASP:OD1	3:B:2663:ILE:N	2.40	0.54
3:B:4195:HIS:HA	3:B:4198:VAL:HG22	1.90	0.54
3:B:4273:LEU:HA	3:B:4276:LEU:HD23	1.88	0.54
3:B:4527:LYS:HB2	3:B:4530:MET:HE1	1.88	0.54
3:A:2027:ASP:OD2	3:A:2027:ASP:N	2.39	0.54
3:A:3669:ALA:O	3:A:3682:TYR:OH	2.24	0.54
3:B:2978:LEU:HG	3:B:3006:LEU:HD12	1.88	0.54
3:B:3000:MET:HB2	3:B:3058:LEU:HD13	1.87	0.54
3:A:3023:ASN:O	3:A:3027:GLN:HG3	2.07	0.54
1:C:312:GLU:HG3	1:C:316:ARG:HD2	1.90	0.54
3:B:1521:MET:H	3:B:1521:MET:CE	2.21	0.54
3:B:2976:MET:O	3:B:2980:ARG:HG2	2.06	0.54
3:B:3313:GLU:OE1	3:B:3313:GLU:N	2.21	0.54
3:B:4593:GLN:OE1	3:B:4593:GLN:N	2.28	0.54
3:A:1973:LYS:HD3	3:A:1996:LEU:HD13	1.89	0.54
3:A:4239:LYS:NZ	3:A:4290:MET:SD	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1558:ASN:O	3:B:1561:VAL:HB	2.08	0.54
1:D:63:LEU:HD11	3:B:2414:VAL:HG11	1.89	0.54
3:A:1678:HIS:N	3:A:1705:SER:O	2.36	0.54
3:A:2637:PRO:HD3	3:A:2648:PRO:HG2	1.90	0.54
3:A:3050:GLU:HG2	3:A:3153:PHE:CD2	2.42	0.54
3:B:1408:VAL:O	3:B:1411:MET:HG3	2.08	0.54
3:B:1678:HIS:N	3:B:1705:SER:O	2.36	0.54
3:B:2474:VAL:HG23	3:B:2475:LEU:HD12	1.89	0.54
3:B:4509:LEU:HD13	3:B:4561:GLN:OE1	2.07	0.54
3:A:1495:LEU:O	3:A:1499:ILE:HG12	2.08	0.54
3:A:3905:LEU:HD23	3:A:3932:LEU:HD11	1.90	0.54
3:A:4352:THR:N	3:A:4438:MET:O	2.35	0.54
3:B:1859:MET:HB3	3:B:2200:GLN:NE2	2.22	0.54
3:B:2135:THR:O	3:B:2144:LEU:N	2.40	0.54
3:B:4408:LEU:HD13	3:B:4440:ILE:HG21	1.90	0.54
3:B:4532:THR:HG22	3:B:4536:MET:HE3	1.90	0.54
2:F:33:LEU:HD13	2:F:53:ILE:HG22	1.90	0.54
3:A:1476:PRO:HG2	3:A:1479:SER:HB3	1.89	0.54
3:A:4273:LEU:HA	3:A:4276:LEU:HD23	1.89	0.54
3:B:659:THR:HA	3:B:663:LEU:HD12	1.90	0.54
3:B:1244:ILE:HG12	3:B:1293:ARG:HH12	1.73	0.54
3:B:3669:ALA:O	3:B:3682:TYR:OH	2.23	0.54
3:A:1924:LEU:HD12	3:A:1925:GLN:N	2.23	0.54
3:B:1899:MET:HG2	3:B:1914:VAL:HG12	1.88	0.54
3:B:3556:TYR:CD2	3:B:3704:GLY:HA3	2.42	0.54
3:A:145:ARG:O	3:A:149:ILE:HG12	2.07	0.53
3:A:2972:MET:O	3:A:2976:MET:HG2	2.07	0.53
3:A:4024:ILE:HD13	1:C:320:VAL:HG13	1.91	0.53
3:B:373:ASP:O	3:B:377:ILE:HG22	2.07	0.53
3:B:3680:ASN:OD1	3:B:3681:VAL:N	2.41	0.53
3:B:3905:LEU:HD23	3:B:3932:LEU:HD11	1.91	0.53
1:D:17:PHE:CE1	1:D:33:CYS:HB2	2.43	0.53
1:D:57:THR:O	1:D:61:PHE:N	2.40	0.53
3:A:1858:LEU:HD23	3:A:2248:ASN:HB3	1.90	0.53
3:B:3045:ARG:HG3	3:B:3050:GLU:OE2	2.08	0.53
3:B:4517:LYS:HA	3:B:4522:ARG:HH22	1.73	0.53
3:A:1384:LEU:HD11	3:A:1430:PHE:CE2	2.43	0.53
3:A:2131:SER:HB2	3:A:2149:ILE:HB	1.91	0.53
3:A:2135:THR:O	3:A:2144:LEU:N	2.40	0.53
3:A:3680:ASN:OD1	3:A:3681:VAL:N	2.41	0.53
3:A:4324:ASP:OD1	3:A:4324:ASP:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4468:ASP:O	3:A:4470:GLU:N	2.42	0.53
3:B:2307:ASP:HB3	3:B:2336:PHE:HB2	1.88	0.53
3:A:1487:GLU:O	3:A:1491:LEU:HG	2.08	0.53
3:B:992:THR:N	3:B:995:GLU:OE1	2.36	0.53
3:B:1351:TYR:O	3:B:1355:ILE:HG13	2.08	0.53
3:B:1564:LEU:HD21	3:B:1807:PHE:HE2	1.72	0.53
3:B:3007:THR:HG22	3:B:3010:LEU:HD22	1.90	0.53
3:A:1160:PRO:O	3:A:1164:GLN:HG2	2.09	0.53
3:A:3597:ARG:O	3:A:3639:ASN:ND2	2.41	0.53
3:A:3961:ASN:ND2	3:A:3963:ASP:OD2	2.41	0.53
3:A:4737:GLN:NE2	3:A:4773:GLU:OE1	2.41	0.53
3:B:134:LYS:HZ1	3:B:311:ASP:HA	1.72	0.53
3:B:1538:MET:O	3:B:1542:ALA:HB3	2.09	0.53
3:B:1877:TYR:O	3:B:1886:ARG:NH2	2.42	0.53
3:A:4100:LYS:HZ3	3:A:4104:ARG:NH2	2.06	0.53
3:A:4596:MET:HA	3:A:4599:ASP:OD1	2.09	0.53
3:B:145:ARG:O	3:B:149:ILE:HG12	2.09	0.53
3:B:2070:ILE:HB	3:B:2092:LEU:HB2	1.90	0.53
3:B:2290:ASP:OD2	3:B:2294:HIS:NE2	2.41	0.53
3:B:2511:LEU:O	3:B:2515:LEU:HD12	2.09	0.53
3:A:3005:MET:HA	3:A:3008:THR:HG23	1.89	0.53
3:B:2335:GLY:CA	3:B:2405:ILE:O	2.57	0.53
1:D:137:ARG:NH1	1:D:138:ALA:H	2.07	0.53
3:A:2529:LEU:HG	3:A:2539:TYR:CD1	2.43	0.53
3:A:2580:ILE:HG22	3:A:2588:LEU:HB2	1.91	0.53
3:B:1874:ARG:HA	3:B:2212:GLN:HE22	1.73	0.53
3:B:2121:MET:SD	3:B:2122:LEU:N	2.82	0.53
3:A:2070:ILE:HB	3:A:2092:LEU:HB2	1.90	0.53
1:D:322:GLU:OE2	3:B:4158:ARG:NH2	2.32	0.53
3:A:1387:GLN:HE22	3:A:1397:MET:HG2	1.74	0.53
3:A:4638:PHE:HA	3:A:4658:PHE:CZ	2.43	0.53
3:B:1859:MET:HE2	3:B:1859:MET:HA	1.91	0.53
3:B:4041:ALA:HA	3:B:4078:ARG:HH12	1.73	0.53
3:B:4468:ASP:HB3	3:B:4471:GLU:HB3	1.90	0.53
1:D:25:LEU:O	1:D:109:ILE:N	2.29	0.52
3:A:1874:ARG:HA	3:A:2212:GLN:HE22	1.73	0.52
3:A:2313:ASN:O	3:A:2317:ILE:HG13	2.09	0.52
3:A:2538:ALA:O	3:A:2542:HIS:ND1	2.42	0.52
3:A:3101:VAL:HG11	3:A:3164:VAL:HG21	1.91	0.52
3:A:4216:GLU:OE2	3:A:4238:LEU:HD13	2.08	0.52
3:B:2131:SER:HB2	3:B:2149:ILE:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3050:GLU:HG2	3:B:3153:PHE:HD2	1.73	0.52
3:B:3921:MET:O	3:B:3925:VAL:HG12	2.09	0.52
3:B:4252:GLU:N	3:B:4252:GLU:OE1	2.41	0.52
3:A:1345:GLU:OE2	3:A:1349:ARG:NH1	2.42	0.52
3:B:4468:ASP:O	3:B:4470:GLU:N	2.42	0.52
1:D:94:GLN:HA	1:D:132:LEU:HD13	1.91	0.52
3:A:281:SER:OG	3:A:282:PHE:N	2.42	0.52
3:A:418:LEU:HD11	3:A:477:ALA:HA	1.91	0.52
3:A:1861:PRO:HB3	3:A:2242:TYR:CZ	2.45	0.52
3:A:2511:LEU:O	3:A:2515:LEU:HD12	2.09	0.52
3:B:4691:ALA:O	3:B:4695:MET:HG2	2.09	0.52
3:A:2976:MET:O	3:A:2980:ARG:HG2	2.10	0.52
3:B:913:GLU:OE1	3:B:913:GLU:N	2.31	0.52
3:B:1318:LEU:HA	3:B:1327:ALA:HB1	1.90	0.52
3:B:1600:MET:SD	3:B:2481:SER:HB2	2.49	0.52
3:B:4737:GLN:NE2	3:B:4773:GLU:OE1	2.42	0.52
3:A:1158:LEU:HB3	3:A:1298:LEU:HD21	1.91	0.52
3:A:1610:LEU:HD21	3:A:2492:VAL:HG13	1.91	0.52
3:A:1859:MET:HB3	3:A:2200:GLN:NE2	2.24	0.52
3:A:3921:MET:O	3:A:3925:VAL:HG12	2.09	0.52
3:B:1309:GLN:H	3:B:1309:GLN:CD	2.17	0.52
3:B:2637:PRO:HD3	3:B:2648:PRO:HG2	1.91	0.52
2:F:5:LEU:HD21	2:F:13:PHE:HE2	1.74	0.52
2:F:17:PHE:HE1	2:F:28:ILE:HG12	1.74	0.52
3:A:1124:LEU:O	3:A:1128:ILE:HG12	2.09	0.52
3:A:1318:LEU:HA	3:A:1327:ALA:HB1	1.91	0.52
3:A:1538:MET:O	3:A:1542:ALA:HB3	2.09	0.52
3:A:1564:LEU:HD21	3:A:1807:PHE:HE2	1.75	0.52
3:A:1859:MET:HA	3:A:1859:MET:HE2	1.91	0.52
3:A:2335:GLY:CA	3:A:2405:ILE:O	2.58	0.52
3:A:4166:LEU:O	3:A:4183:TYR:OH	2.27	0.52
3:B:532:ASN:O	3:B:536:THR:OG1	2.27	0.52
3:B:2980:ARG:HA	3:B:2980:ARG:NH1	2.24	0.52
3:A:51:GLN:OE1	3:A:51:GLN:N	2.38	0.52
3:A:1015:PRO:HG3	3:A:1041:TRP:HE1	1.74	0.52
3:A:1408:VAL:O	3:A:1411:MET:HG3	2.09	0.52
3:A:1446:LEU:HA	3:A:1449:LEU:HG	1.91	0.52
3:A:1888:LEU:HD12	3:A:1893:VAL:HB	1.92	0.52
3:A:2327:TYR:OH	1:C:63:LEU:O	2.26	0.52
3:A:3000:MET:HB2	3:A:3058:LEU:HD13	1.91	0.52
3:B:2181:GLN:NE2	3:B:2186:VAL:O	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4516:VAL:O	3:B:4522:ARG:NH2	2.42	0.52
2:E:59:ASP:OD1	2:E:59:ASP:N	2.41	0.52
3:A:2317:ILE:HA	3:A:2320:ARG:HH21	1.75	0.52
3:A:2356:ILE:HG22	3:A:2417:ILE:HA	1.92	0.52
3:A:4230:THR:HG21	3:B:3818:ILE:HD12	1.91	0.52
3:B:281:SER:OG	3:B:282:PHE:N	2.42	0.52
3:B:4613:LEU:HD12	3:B:4614:GLN:N	2.25	0.52
3:A:1381:LEU:HD13	3:A:1426:ARG:HG3	1.91	0.52
3:A:1877:TYR:O	3:A:1886:ARG:NH2	2.42	0.52
3:A:2117:HIS:O	3:A:2120:GLN:NE2	2.43	0.52
3:A:2544:ASP:OD2	3:A:2584:ARG:NH2	2.43	0.52
1:C:120:ASP:HB3	1:C:123:HIS:HB2	1.92	0.52
3:B:2979:GLU:HA	3:B:2982:LEU:HD12	1.92	0.52
3:B:3593:TYR:OH	3:B:3643:GLU:OE1	2.27	0.52
3:B:4314:ILE:O	3:B:4318:LYS:HG2	2.10	0.52
3:B:4321:ASN:O	3:B:4491:ARG:NH1	2.39	0.52
2:E:12:GLU:OE1	2:E:40:LEU:HD22	2.10	0.52
3:A:2192:VAL:HG13	3:A:2197:PHE:CE1	2.39	0.52
3:A:2243:MET:HE3	3:A:2243:MET:C	2.35	0.52
3:A:2290:ASP:OD2	3:A:2294:HIS:NE2	2.41	0.52
3:A:3021:LEU:O	3:A:3025:LEU:HD23	2.09	0.52
3:A:3048:LEU:O	3:A:3051:VAL:HG22	2.10	0.52
3:B:959:LYS:HZ2	3:B:960:LEU:H	1.57	0.52
3:B:1015:PRO:HG3	3:B:1041:TRP:HE1	1.74	0.52
3:B:1446:LEU:HA	3:B:1449:LEU:HG	1.92	0.52
3:B:3021:LEU:O	3:B:3025:LEU:HD23	2.09	0.52
3:B:4324:ASP:N	3:B:4324:ASP:OD1	2.40	0.52
2:E:38:ARG:HH12	3:A:4160:GLN:HG3	1.75	0.51
3:A:1494:LEU:O	3:A:1497:THR:OG1	2.25	0.51
3:A:3074:ILE:HG22	3:A:3076:GLU:H	1.76	0.51
3:B:3597:ARG:O	3:B:3639:ASN:ND2	2.43	0.51
1:D:88:TYR:HD1	1:D:92:SER:HB3	1.75	0.51
3:A:1663:THR:O	3:A:1667:THR:HG23	2.11	0.51
3:A:2216:ALA:C	3:A:2217:ILE:HD13	2.35	0.51
3:A:3190:TRP:O	3:A:3194:LEU:HB3	2.11	0.51
3:A:4444:MET:HE1	3:A:4447:LEU:HB2	1.91	0.51
3:B:73:PHE:HB2	3:B:158:ALA:HB1	1.91	0.51
3:B:322:ASN:OD1	3:B:323:PRO:HD2	2.09	0.51
3:B:3934:ARG:HH21	3:B:3981:LYS:HD2	1.75	0.51
2:E:34:GLY:HA2	2:E:49:LEU:HD21	1.93	0.51
3:A:659:THR:HA	3:A:663:LEU:HD12	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1077:THR:O	3:A:1082:SER:N	2.43	0.51
3:A:3278:ALA:O	3:A:3282:ILE:HG22	2.10	0.51
3:A:4267:LEU:HD11	3:A:4316:THR:HG21	1.92	0.51
3:B:2352:MET:HE1	3:B:2403:LEU:HD13	1.92	0.51
3:B:3938:GLU:OE1	3:B:3938:GLU:N	2.34	0.51
3:B:4488:MET:HB2	3:B:4508:LEU:HD11	1.92	0.51
1:D:320:VAL:HG13	3:B:4024:ILE:HD13	1.93	0.51
3:A:2368:ILE:HG23	3:A:2377:LEU:HD11	1.92	0.51
3:A:3048:LEU:O	3:A:3052:HIS:ND1	2.43	0.51
3:A:3593:TYR:OH	3:A:3643:GLU:OE1	2.27	0.51
3:A:4195:HIS:HA	3:A:4198:VAL:HG22	1.93	0.51
3:A:4642:CYS:HB2	3:A:4687:ILE:HD11	1.90	0.51
3:B:202:ASN:HB2	3:B:203:PRO:HA	1.92	0.51
3:A:1028:PRO:HB2	3:A:1029:GLU:OE1	2.11	0.51
3:A:1134:SER:O	3:A:1137:GLU:HG3	2.10	0.51
3:A:4415:ILE:HG23	3:A:4419:LEU:HD12	1.92	0.51
3:A:1218:LEU:HA	3:A:1221:ASN:HD21	1.76	0.51
3:A:4314:ILE:O	3:A:4318:LYS:HG2	2.11	0.51
3:A:4532:THR:HG22	3:A:4536:MET:HE3	1.93	0.51
3:B:60:GLU:OE2	3:B:106:VAL:HG22	2.11	0.51
3:B:1124:LEU:O	3:B:1128:ILE:HG12	2.10	0.51
3:B:1385:GLU:HG2	3:B:1430:PHE:HD2	1.75	0.51
3:B:1391:SER:HA	3:B:1394:ARG:NE	2.22	0.51
3:A:802:GLU:HG2	3:A:803:THR:HG23	1.91	0.51
3:A:1605:ASP:HA	3:A:1608:ASN:HD21	1.76	0.51
3:A:2356:ILE:HD12	3:A:2379:LEU:HD11	1.93	0.51
3:A:4509:LEU:HD13	3:A:4561:GLN:OE1	2.10	0.51
3:B:3278:ALA:O	3:B:3282:ILE:HG22	2.11	0.51
2:E:30:THR:HA	2:E:33:LEU:HB2	1.93	0.51
3:A:138:THR:OG1	3:A:142:ARG:NH2	2.44	0.51
3:A:790:MET:HB3	3:A:858:LEU:HD21	1.92	0.51
3:A:1558:ASN:O	3:A:1561:VAL:HB	2.11	0.51
3:A:1924:LEU:HD12	3:A:1925:GLN:H	1.76	0.51
3:A:4517:LYS:HA	3:A:4522:ARG:HH22	1.74	0.51
3:B:1134:SER:O	3:B:1137:GLU:HG3	2.11	0.51
3:B:1158:LEU:HB3	3:B:1298:LEU:HD21	1.93	0.51
3:B:1538:MET:HE3	3:B:1598:HIS:HB3	1.91	0.51
3:A:2352:MET:HE1	3:A:2403:LEU:HD13	1.93	0.51
3:A:2496:ILE:O	3:A:2500:ARG:HG2	2.11	0.51
3:A:3007:THR:HA	3:A:3010:LEU:HD13	1.93	0.51
3:A:4353:LEU:HD23	3:A:4440:ILE:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1247:TRP:HA	3:B:1251:PHE:HB2	1.93	0.51
3:B:1592:ILE:O	3:B:1596:THR:HG23	2.11	0.51
3:B:4476:ALA:HA	3:B:4479:MET:HE1	1.93	0.51
3:B:4642:CYS:HB2	3:B:4687:ILE:HD11	1.92	0.51
3:B:4683:LEU:HD11	3:B:4739:LEU:HD22	1.93	0.51
3:A:1608:ASN:OD1	3:A:1609:ALA:N	2.44	0.51
3:B:1218:LEU:HA	3:B:1221:ASN:HD21	1.75	0.51
3:B:1663:THR:O	3:B:1667:THR:HG23	2.11	0.51
3:B:1861:PRO:HB3	3:B:2242:TYR:CZ	2.45	0.51
3:B:3190:TRP:O	3:B:3194:LEU:HB3	2.10	0.51
2:F:59:ASP:N	2:F:59:ASP:OD1	2.40	0.50
3:B:103:ALA:O	3:B:107:LEU:HG	2.11	0.50
3:B:1896:ARG:NH1	3:B:2213:ASP:OD2	2.43	0.50
3:B:3162:GLU:OE1	3:B:3163:MET:HE2	2.11	0.50
3:B:4415:ILE:HG23	3:B:4419:LEU:HD12	1.91	0.50
3:A:3332:VAL:HG11	3:A:3434:HIS:NE2	2.26	0.50
3:A:3934:ARG:HH21	3:A:3981:LYS:HD2	1.75	0.50
3:A:4158:ARG:NH2	1:C:322:GLU:OE2	2.38	0.50
3:B:49:LEU:O	3:B:53:VAL:HG23	2.12	0.50
3:B:2496:ILE:O	3:B:2500:ARG:HG2	2.11	0.50
3:B:3773:GLU:OE1	3:B:3794:ARG:NH2	2.44	0.50
2:E:17:PHE:HE1	2:E:28:ILE:HG12	1.76	0.50
2:F:116:LYS:HZ2	3:B:4077:ILE:HG12	1.76	0.50
3:A:2698:LYS:O	3:A:2702:ILE:HG12	2.11	0.50
3:A:4683:LEU:HD11	3:A:4739:LEU:HD22	1.93	0.50
3:B:30:GLU:CD	3:B:30:GLU:H	2.20	0.50
3:B:1888:LEU:HD12	3:B:1893:VAL:HB	1.91	0.50
3:B:3101:VAL:HG11	3:B:3164:VAL:HG21	1.92	0.50
3:B:4383:MET:HE3	3:B:4408:LEU:HD12	1.94	0.50
1:D:85:LYS:HB3	1:D:88:TYR:HE2	1.73	0.50
3:A:525:ILE:HD13	3:A:530:LEU:HD13	1.94	0.50
3:A:3788:THR:O	3:A:3791:SER:OG	2.23	0.50
3:B:1384:LEU:O	3:B:1387:GLN:NE2	2.35	0.50
3:B:2245:ASN:ND2	3:B:2248:ASN:OD1	2.45	0.50
3:B:2316:GLN:O	3:B:2320:ARG:HG3	2.11	0.50
3:B:2320:ARG:HH21	3:B:2328:VAL:HG22	1.75	0.50
2:E:116:LYS:HZ2	3:A:4077:ILE:HG23	1.76	0.50
3:A:317:VAL:O	3:A:325:ARG:NH2	2.25	0.50
3:A:1411:MET:HB3	3:A:1431:PHE:CZ	2.46	0.50
3:A:2621:PHE:O	3:A:2625:LEU:HG	2.12	0.50
3:B:2990:ASN:OD1	3:B:2990:ASN:N	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:131:LEU:HB2	3:A:142:ARG:HG2	1.94	0.50
3:A:2118:VAL:HG21	3:A:2174:PRO:HB3	1.93	0.50
3:A:3230:LEU:HD23	3:A:3296:LYS:NZ	2.26	0.50
3:A:4383:MET:HE3	3:A:4408:LEU:HD12	1.94	0.50
3:B:1428:LEU:HB3	3:B:1491:LEU:HD13	1.94	0.50
3:B:1534:PHE:HA	3:B:1537:LEU:HG	1.94	0.50
3:B:2540:HIS:HA	3:B:2543:LYS:HZ2	1.77	0.50
3:B:3136:MET:HA	3:B:3136:MET:HE3	1.93	0.50
3:B:4593:GLN:HA	3:B:4596:MET:SD	2.52	0.50
3:A:202:ASN:HB2	3:A:203:PRO:HA	1.93	0.50
3:A:1090:VAL:HG21	3:A:1131:VAL:HG23	1.93	0.50
3:A:1191:SER:H	3:A:1194:LYS:HE2	1.77	0.50
3:A:1247:TRP:HA	3:A:1251:PHE:HB2	1.93	0.50
3:A:3032:LEU:HD23	3:A:3052:HIS:HD2	1.77	0.50
1:C:46:HIS:HA	1:C:50:HIS:CE1	2.46	0.50
3:B:62:GLU:OE1	3:B:66:HIS:NE2	2.44	0.50
3:B:2529:LEU:HG	3:B:2539:TYR:CD1	2.47	0.50
3:B:2580:ILE:HG22	3:B:2588:LEU:HB2	1.94	0.50
3:B:2621:PHE:O	3:B:2625:LEU:HG	2.11	0.50
3:B:4353:LEU:HD23	3:B:4440:ILE:HB	1.93	0.50
2:F:34:GLY:HA3	2:F:49:LEU:HD11	1.94	0.50
2:F:124:GLU:HG3	2:F:128:GLU:OE2	2.12	0.50
3:A:404:GLN:HG2	3:B:396:ARG:HH21	1.76	0.50
3:A:2414:VAL:HG11	1:C:63:LEU:HD11	1.94	0.50
3:B:78:VAL:HG11	3:B:110:PHE:HE1	1.77	0.50
3:B:283:PHE:O	3:B:338:TYR:OH	2.17	0.50
3:B:1160:PRO:O	3:B:1164:GLN:HG2	2.12	0.50
3:B:1924:LEU:HD12	3:B:1925:GLN:N	2.26	0.50
3:B:4267:LEU:HD11	3:B:4316:THR:HG21	1.92	0.50
3:B:4352:THR:N	3:B:4438:MET:O	2.35	0.50
3:A:2982:LEU:HB3	3:A:3027:GLN:NE2	2.27	0.50
3:B:1090:VAL:HG21	3:B:1131:VAL:HG23	1.93	0.50
3:B:1359:TYR:CE2	3:B:1405:GLY:HA2	2.47	0.50
3:B:1487:GLU:O	3:B:1491:LEU:HG	2.12	0.50
3:B:1604:ALA:HA	3:B:1607:THR:HG22	1.94	0.50
3:B:2313:ASN:O	3:B:2317:ILE:HG13	2.12	0.50
3:B:2368:ILE:HG23	3:B:2377:LEU:HD11	1.92	0.50
3:A:1309:GLN:HG3	3:A:1312:ARG:HH21	1.77	0.49
3:A:4533:LEU:HD23	3:A:4587:LEU:HD11	1.94	0.49
3:B:1924:LEU:HD21	3:B:1942:LEU:HD13	1.93	0.49
3:B:3332:VAL:HG11	3:B:3434:HIS:NE2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:102:SER:N	2:F:105:GLU:OE1	2.45	0.49
3:A:3003:ILE:HA	3:A:3006:LEU:HB2	1.94	0.49
3:B:802:GLU:HG2	3:B:803:THR:HG23	1.93	0.49
3:B:1368:PRO:HG3	3:B:1418:ASN:HB3	1.93	0.49
2:E:5:LEU:HD21	2:E:13:PHE:HE2	1.76	0.49
2:E:103:ALA:O	2:E:107:ARG:HG2	2.12	0.49
2:F:46:GLU:OE1	2:F:46:GLU:HA	2.13	0.49
3:A:863:ASP:OD1	3:A:1008:ARG:NH2	2.45	0.49
3:B:1850:LYS:NZ	3:B:2194:PRO:O	2.45	0.49
3:B:1902:LEU:HD21	3:B:1967:LEU:HB2	1.93	0.49
3:B:3144:TYR:O	3:B:3148:HIS:ND1	2.37	0.49
3:B:3513:TYR:CZ	3:B:3525:TYR:HB3	2.47	0.49
1:D:312:GLU:HG3	1:D:316:ARG:HD2	1.93	0.49
2:F:35:THR:HA	2:F:38:ARG:HB3	1.94	0.49
3:A:3976:THR:HA	3:A:4019:ILE:HD11	1.94	0.49
3:B:1077:THR:O	3:B:1082:SER:N	2.45	0.49
3:B:1201:VAL:HG12	3:B:1202:LEU:HD22	1.93	0.49
2:E:38:ARG:HH12	3:A:4160:GLN:CG	2.25	0.49
3:A:532:ASN:O	3:A:536:THR:OG1	2.27	0.49
3:A:3773:GLU:OE1	3:A:3794:ARG:NH2	2.45	0.49
3:B:37:LEU:O	3:B:40:SER:OG	2.25	0.49
3:A:1902:LEU:HD21	3:A:1967:LEU:HB2	1.94	0.49
3:A:3225:ARG:HH21	3:A:3286:ARG:CZ	2.24	0.49
3:B:2702:ILE:HA	3:B:3005:MET:SD	2.53	0.49
3:B:4245:LEU:HB3	3:B:4294:MET:HE1	1.94	0.49
3:A:152:THR:O	3:A:156:LYS:HG2	2.13	0.49
3:A:953:CYS:HA	3:A:956:LEU:HB2	1.95	0.49
3:A:1537:LEU:HB3	3:A:1541:MET:HE1	1.95	0.49
3:A:1604:ALA:HA	3:A:1607:THR:HG22	1.95	0.49
3:A:2098:ASP:O	3:A:2130:LYS:NZ	2.46	0.49
3:A:2974:ARG:HB3	3:A:3006:LEU:HD13	1.93	0.49
3:B:678:LEU:HD12	3:B:683:MET:HE2	1.93	0.49
3:B:882:HIS:ND1	3:B:907:LEU:HD22	2.28	0.49
3:B:1309:GLN:HG3	3:B:1312:ARG:NH2	2.28	0.49
3:B:3188:HIS:HA	3:B:3191:PHE:CD2	2.48	0.49
3:B:3225:ARG:HH21	3:B:3286:ARG:NE	2.11	0.49
3:A:1564:LEU:O	3:A:1568:LYS:N	2.41	0.49
3:A:1592:ILE:O	3:A:1596:THR:HG23	2.12	0.49
3:A:2474:VAL:HG23	3:A:2475:LEU:HD12	1.94	0.49
3:A:2991:VAL:O	3:A:2995:ARG:HD3	2.12	0.49
3:A:3095:VAL:HB	3:A:3190:TRP:CZ2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4492:LEU:HD12	3:A:4539:THR:HG21	1.95	0.49
1:C:85:LYS:HB3	1:C:88:TYR:HE2	1.77	0.49
3:B:1308:PRO:HG2	3:B:1309:GLN:NE2	2.28	0.49
3:B:1310:VAL:HA	3:B:1313:THR:HG22	1.94	0.49
3:B:2540:HIS:HA	3:B:2543:LYS:HG2	1.95	0.49
3:B:2969:ARG:HG2	3:B:2970:LEU:N	2.27	0.49
3:B:3074:ILE:HG22	3:B:3076:GLU:H	1.76	0.49
3:B:4466:GLU:HG2	3:B:4469:GLU:HG2	1.95	0.49
2:E:145:MET:HE3	3:A:4105:TRP:CD1	2.48	0.49
3:A:541:SER:OG	3:A:647:PHE:O	2.31	0.49
3:A:2245:ASN:HB3	3:A:2248:ASN:HB2	1.95	0.49
3:A:3136:MET:HA	3:A:3136:MET:HE3	1.94	0.49
3:A:3513:TYR:CZ	3:A:3525:TYR:HB3	2.48	0.49
3:A:4618:ARG:O	3:A:4621:PRO:HD2	2.13	0.49
3:B:78:VAL:HG11	3:B:110:PHE:CE1	2.47	0.49
3:B:1484:VAL:HG12	3:B:1488:ASN:HD21	1.78	0.49
3:B:2626:VAL:HG21	3:B:2681:ILE:HD12	1.95	0.49
2:E:59:ASP:OD2	2:E:61:ASN:ND2	2.46	0.49
2:F:30:THR:HG22	2:F:33:LEU:HD12	1.95	0.49
2:F:145:MET:HE3	3:B:4105:TRP:CD1	2.48	0.49
3:A:2971:HIS:O	3:A:2975:LEU:HG	2.13	0.49
3:A:3023:ASN:O	3:A:3026:SER:OG	2.25	0.49
3:A:4466:GLU:HG2	3:A:4469:GLU:HG2	1.94	0.49
3:A:4691:ALA:O	3:A:4695:MET:HG2	2.12	0.49
3:B:56:VAL:HG12	3:B:106:VAL:HG11	1.94	0.49
3:B:640:SER:OG	3:B:641:ARG:N	2.46	0.49
3:B:1138:HIS:HA	3:B:1141:LYS:HE3	1.95	0.49
3:B:2245:ASN:HB3	3:B:2248:ASN:HB2	1.95	0.49
3:B:4653:GLY:O	3:B:4656:LYS:HG3	2.13	0.49
3:A:640:SER:OG	3:A:641:ARG:N	2.46	0.48
3:A:1309:GLN:CD	3:A:1309:GLN:H	2.20	0.48
3:A:1518:LEU:HD23	3:A:1541:MET:HB3	1.94	0.48
3:A:2014:GLU:OE1	3:A:2014:GLU:N	2.45	0.48
3:A:3041:LYS:HD3	3:A:3041:LYS:N	2.28	0.48
3:A:3243:LEU:HD11	3:A:3271:SER:HB2	1.95	0.48
3:A:3429:HIS:HA	3:A:3471:LEU:HD11	1.95	0.48
3:A:874:VAL:HG13	3:B:189:VAL:HG11	1.96	0.48
3:A:1398:GLU:HA	3:A:1398:GLU:OE2	2.12	0.48
3:A:2483:LEU:HB2	3:A:2524:GLN:NE2	2.28	0.48
3:B:144:ASP:OD2	3:B:146:THR:OG1	2.28	0.48
3:B:4492:LEU:HA	3:B:4495:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:30:GLU:CD	3:A:30:GLU:H	2.21	0.48
3:A:283:PHE:O	3:A:338:TYR:OH	2.18	0.48
3:A:959:LYS:NZ	3:A:960:LEU:H	2.10	0.48
3:A:1310:VAL:HA	3:A:1313:THR:HG22	1.96	0.48
3:A:1426:ARG:O	3:A:1426:ARG:HD3	2.12	0.48
3:A:1551:ALA:HA	3:A:1554:LEU:HD23	1.94	0.48
3:A:2111:VAL:HG12	3:A:2165:CYS:HB3	1.95	0.48
3:A:2332:LYS:HE3	1:C:38:GLU:HG2	1.94	0.48
3:B:127:LYS:O	3:B:130:ILE:HG22	2.13	0.48
3:B:685:THR:O	3:B:689:ILE:HG12	2.13	0.48
3:B:1859:MET:HG3	3:B:2242:TYR:HD2	1.78	0.48
3:B:4444:MET:HE1	3:B:4447:LEU:HB2	1.94	0.48
3:A:732:LEU:HD21	3:A:760:LEU:HD13	1.94	0.48
3:A:1859:MET:HG3	3:A:2242:TYR:HD2	1.77	0.48
3:A:2310:GLN:NE2	1:C:54:CYS:HB2	2.26	0.48
3:B:1804:ASN:HA	3:B:2494:PRO:HD3	1.95	0.48
3:B:2316:GLN:HB3	3:B:2320:ARG:NH1	2.28	0.48
3:B:3095:VAL:HB	3:B:3190:TRP:CZ2	2.47	0.48
3:B:4618:ARG:O	3:B:4621:PRO:HD2	2.13	0.48
3:A:2622:ILE:HD13	3:A:2622:ILE:N	2.29	0.48
3:A:2660:LEU:O	3:A:2664:ILE:HG12	2.14	0.48
3:B:525:ILE:HD13	3:B:530:LEU:HD13	1.94	0.48
3:B:2243:MET:HE3	3:B:2243:MET:C	2.37	0.48
3:B:3052:HIS:O	3:B:3055:VAL:HG12	2.14	0.48
3:B:3976:THR:HA	3:B:4019:ILE:HD11	1.95	0.48
3:A:70:TYR:CE1	3:A:161:PRO:HA	2.48	0.48
3:A:948:LEU:HD12	3:A:1012:ILE:HG22	1.95	0.48
3:A:4094:HIS:O	3:A:4098:THR:OG1	2.26	0.48
3:B:1398:GLU:OE2	3:B:1398:GLU:HA	2.14	0.48
3:B:2025:ILE:O	3:B:2036:THR:N	2.46	0.48
3:B:3225:ARG:HH21	3:B:3286:ARG:CZ	2.26	0.48
3:B:4139:GLN:HG3	3:B:4142:ARG:HH21	1.78	0.48
3:B:4509:LEU:HD12	3:B:4510:LYS:N	2.28	0.48
3:A:1811:VAL:HA	3:A:1814:MET:SD	2.54	0.48
3:A:3595:ASN:OD1	3:A:3639:ASN:HB2	2.13	0.48
1:C:114:ALA:HA	1:C:121:PRO:HA	1.96	0.48
3:B:269:TYR:HE2	3:B:302:LEU:HD11	1.79	0.48
3:B:868:GLN:OE1	3:B:871:LYS:NZ	2.47	0.48
3:B:1161:ALA:HA	3:B:1164:GLN:HE21	1.79	0.48
3:B:1853:GLU:OE2	3:B:2196:THR:HB	2.14	0.48
3:B:4564:SER:HA	3:B:4567:GLU:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:ARG:NE	3:B:4122:LYS:HZ2	2.11	0.48
3:A:2550:LYS:HD3	3:A:2551:ALA:N	2.29	0.48
3:A:4694:TYR:HB3	3:A:4695:MET:HE2	1.96	0.48
3:B:519:GLN:HA	3:B:522:GLN:HG2	1.96	0.48
3:B:3429:HIS:HA	3:B:3471:LEU:HD11	1.96	0.48
3:B:4166:LEU:O	3:B:4183:TYR:OH	2.27	0.48
3:A:299:PHE:HB3	3:A:373:ASP:OD1	2.14	0.48
3:A:396:ARG:HH21	3:B:404:GLN:HG2	1.77	0.48
3:A:3188:HIS:HA	3:A:3191:PHE:CD2	2.49	0.48
3:A:3225:ARG:HH21	3:A:3286:ARG:NE	2.11	0.48
3:B:154:MET:SD	3:B:158:ALA:HB2	2.54	0.48
3:B:910:GLY:HA2	3:B:934:CYS:H	1.78	0.48
3:B:1460:GLU:HG2	3:B:1463:ARG:HG2	1.95	0.48
3:B:4383:MET:HE3	3:B:4383:MET:HB2	1.79	0.48
1:D:51:PRO:HG2	1:D:81:PRO:O	2.14	0.48
3:A:2151:ILE:HG23	3:A:2199:ILE:HD12	1.94	0.48
3:A:3880:THR:O	3:A:3884:ILE:HG12	2.14	0.48
3:A:3966:SER:OG	3:B:3768:ASN:ND2	2.47	0.48
3:B:1191:SER:H	3:B:1194:LYS:HE2	1.79	0.48
3:B:1384:LEU:HA	3:B:1387:GLN:HG3	1.95	0.48
3:B:1428:LEU:HA	3:B:1431:PHE:HD2	1.79	0.48
3:B:3243:LEU:HD11	3:B:3271:SER:HB2	1.96	0.48
3:B:4617:LEU:HD13	3:B:4665:ILE:HG13	1.95	0.48
3:A:512:MET:HE3	3:A:512:MET:HB3	1.77	0.47
3:A:1218:LEU:HA	3:A:1221:ASN:ND2	2.28	0.47
3:A:2979:GLU:HA	3:A:2982:LEU:HD12	1.96	0.47
3:A:4139:GLN:HG3	3:A:4142:ARG:HH21	1.78	0.47
3:A:4467:GLU:HG2	3:A:4468:ASP:N	2.23	0.47
3:B:299:PHE:HB3	3:B:373:ASP:OD1	2.14	0.47
3:B:541:SER:OG	3:B:647:PHE:O	2.32	0.47
3:B:1159:LEU:HD21	3:B:1299:ILE:HD12	1.95	0.47
3:B:1411:MET:HB3	3:B:1431:PHE:HZ	1.76	0.47
3:B:2151:ILE:HG23	3:B:2199:ILE:HD12	1.95	0.47
3:B:3587:VAL:HG22	3:B:3647:PHE:HE1	1.79	0.47
3:B:3661:PRO:HB3	3:B:3685:HIS:CE1	2.49	0.47
3:B:4467:GLU:HG2	3:B:4468:ASP:N	2.22	0.47
3:A:685:THR:O	3:A:689:ILE:HG12	2.14	0.47
3:A:1309:GLN:HG3	3:A:1312:ARG:NH2	2.28	0.47
3:A:2010:GLY:O	3:A:2639:ASN:ND2	2.47	0.47
3:A:2321:LEU:HD22	3:A:2420:VAL:HG23	1.96	0.47
3:A:4059:TRP:CE3	1:C:323:LEU:HD21	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:152:THR:O	3:B:156:LYS:HG2	2.13	0.47
3:B:995:GLU:O	3:B:999:LEU:HD23	2.15	0.47
3:B:2356:ILE:HG22	3:B:2417:ILE:HA	1.95	0.47
3:B:3595:ASN:OD1	3:B:3639:ASN:HB2	2.13	0.47
2:E:124:GLU:HG3	2:E:128:GLU:OE2	2.14	0.47
2:E:146:MET:HE3	3:A:4101:TYR:HD1	1.79	0.47
3:A:154:MET:SD	3:A:158:ALA:HB2	2.55	0.47
3:A:849:ARG:NH1	3:A:979:GLN:O	2.47	0.47
3:A:1368:PRO:HG3	3:A:1418:ASN:HB3	1.96	0.47
3:A:2245:ASN:ND2	3:A:2248:ASN:OD1	2.47	0.47
3:B:1031:SER:H	3:B:1034:ASP:HB2	1.79	0.47
3:B:1064:LYS:HE3	3:B:1067:HIS:CE1	2.49	0.47
3:B:1218:LEU:HA	3:B:1221:ASN:ND2	2.29	0.47
3:B:2111:VAL:HG12	3:B:2165:CYS:HB3	1.97	0.47
3:B:2117:HIS:O	3:B:2120:GLN:NE2	2.48	0.47
3:B:2136:ILE:HA	3:B:2143:VAL:HA	1.97	0.47
3:B:2356:ILE:HD12	3:B:2379:LEU:HD11	1.95	0.47
1:D:64:TYR:CD1	3:B:2311:VAL:HG11	2.50	0.47
3:A:3933:THR:HG22	3:A:3939:ALA:HB1	1.96	0.47
3:B:4561:GLN:O	3:B:4565:ILE:HG23	2.14	0.47
3:B:1244:ILE:HA	3:B:1293:ARG:NH2	2.28	0.47
3:B:3003:ILE:HA	3:B:3006:LEU:HB2	1.96	0.47
3:B:4515:CYS:SG	3:B:4521:ASN:ND2	2.87	0.47
1:D:86:MET:SD	3:B:2310:GLN:HG3	2.54	0.47
3:A:680:GLU:OE1	3:A:680:GLU:N	2.30	0.47
3:A:2245:ASN:O	3:A:2249:THR:N	2.47	0.47
3:A:2678:ALA:O	3:A:2681:ILE:HG12	2.14	0.47
3:A:3912:TYR:OH	3:B:3959:TRP:NE1	2.33	0.47
3:B:356:GLN:HG2	3:B:427:THR:HG22	1.97	0.47
3:B:1919:GLY:O	3:B:1950:VAL:N	2.47	0.47
3:B:3063:MET:HE2	3:B:3063:MET:HA	1.97	0.47
3:B:3880:THR:O	3:B:3884:ILE:HG12	2.14	0.47
2:F:149:LYS:OXT	3:B:4111:ARG:NH2	2.46	0.47
3:A:78:VAL:HG11	3:A:110:PHE:CD2	2.49	0.47
3:A:125:SER:H	3:A:128:HIS:HD2	1.62	0.47
3:A:366:LYS:HG3	3:A:370:TYR:CE2	2.50	0.47
3:A:1676:TRP:HZ2	3:A:1708:LYS:HE2	1.80	0.47
3:A:1804:ASN:HA	3:A:2494:PRO:HD3	1.96	0.47
3:A:2136:ILE:HA	3:A:2143:VAL:HA	1.96	0.47
3:B:64:LEU:HD12	3:B:113:LEU:HD11	1.96	0.47
3:B:1020:ILE:O	3:B:1024:SER:CB	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1412:MET:HE2	3:B:1463:ARG:HD2	1.96	0.47
3:B:1604:ALA:HB2	3:B:2484:GLU:OE1	2.15	0.47
3:B:2622:ILE:HD13	3:B:2622:ILE:N	2.28	0.47
3:B:2660:LEU:O	3:B:2664:ILE:HG12	2.14	0.47
3:B:2971:HIS:HA	3:B:2974:ARG:HD3	1.96	0.47
3:B:4035:LYS:HD2	3:B:4035:LYS:HA	1.62	0.47
3:A:1464:LEU:HD12	3:A:1465:GLN:N	2.29	0.47
3:A:1930:LEU:HB3	3:A:2219:HIS:CE1	2.50	0.47
3:A:2627:ASN:O	3:A:2631:LYS:HG2	2.14	0.47
3:A:2993:GLY:HA3	3:A:3153:PHE:HE2	1.80	0.47
3:A:4695:MET:HE2	3:A:4695:MET:N	2.30	0.47
1:C:27:CYS:HB3	1:C:30:TYR:CE1	2.49	0.47
3:B:953:CYS:HA	3:B:956:LEU:HB2	1.97	0.47
3:B:3933:THR:HG22	3:B:3939:ALA:HB1	1.96	0.47
3:B:4017:LEU:HD11	3:B:4132:VAL:HG11	1.97	0.47
2:F:12:GLU:OE1	2:F:40:LEU:HD22	2.15	0.47
3:A:274:GLN:OE1	3:A:274:GLN:HA	2.15	0.47
3:A:1901:VAL:HG21	3:A:2217:ILE:HD11	1.96	0.47
3:B:1085:TYR:O	3:B:1089:ILE:HG22	2.14	0.47
3:B:1924:LEU:HD12	3:B:1925:GLN:H	1.78	0.47
3:B:2118:VAL:HG21	3:B:2174:PRO:HB3	1.95	0.47
3:B:4638:PHE:HA	3:B:4658:PHE:CZ	2.50	0.47
3:A:1138:HIS:HA	3:A:1141:LYS:HE3	1.97	0.47
3:A:1850:LYS:NZ	3:A:2194:PRO:O	2.48	0.47
3:A:4771:LEU:HB3	3:A:4777:VAL:HG11	1.96	0.47
3:B:4771:LEU:HB3	3:B:4777:VAL:HG11	1.96	0.47
3:A:3768:ASN:ND2	3:B:3966:SER:OG	2.47	0.46
3:A:4492:LEU:HA	3:A:4495:ILE:HD12	1.97	0.46
3:B:1464:LEU:HD12	3:B:1465:GLN:N	2.31	0.46
3:B:3562:VAL:HG22	3:B:3641:MET:SD	2.55	0.46
1:D:37:TYR:CE1	1:D:52:MET:HG2	2.50	0.46
2:E:38:ARG:HD2	2:E:38:ARG:O	2.15	0.46
3:A:724:SER:OG	3:A:726:ASN:OD1	2.21	0.46
3:A:1023:LEU:HD21	3:A:1041:TRP:CZ3	2.50	0.46
3:A:1384:LEU:HD11	3:A:1430:PHE:HE2	1.80	0.46
3:A:2559:SER:OG	3:A:2628:HIS:NE2	2.35	0.46
3:A:4443:ARG:NH2	3:A:4453:GLU:OE1	2.46	0.46
3:A:4561:GLN:O	3:A:4565:ILE:HG23	2.14	0.46
3:B:83:HIS:O	3:B:87:THR:HG23	2.15	0.46
3:B:145:ARG:HH21	3:B:148:ILE:HD12	1.80	0.46
3:B:1608:ASN:OD1	3:B:1609:ALA:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:269:TYR:HE2	3:A:302:LEU:HD11	1.80	0.46
3:A:1000:GLN:HA	3:A:1270:LEU:HD13	1.97	0.46
3:A:1408:VAL:O	3:A:1412:MET:HG2	2.15	0.46
3:A:1423:PHE:O	3:A:1427:VAL:HG12	2.16	0.46
3:A:1468:LEU:O	3:A:1472:THR:OG1	2.20	0.46
3:A:1853:GLU:OE2	3:A:2196:THR:HB	2.15	0.46
3:A:3224:TYR:O	3:A:3228:ARG:HG3	2.14	0.46
3:B:680:GLU:OE1	3:B:680:GLU:N	2.24	0.46
3:B:823:GLU:O	3:B:827:ARG:HG2	2.15	0.46
3:B:866:LEU:HD13	3:B:1013:LEU:HD21	1.97	0.46
3:B:1377:LEU:HA	3:B:1380:CYS:SG	2.56	0.46
3:B:1498:TYR:HD1	3:B:1501:ARG:HH12	1.62	0.46
3:B:4503:HIS:O	3:B:4507:VAL:HG13	2.15	0.46
3:A:86:THR:HG22	3:A:136:LEU:HD13	1.97	0.46
3:A:1308:PRO:HG2	3:A:1309:GLN:NE2	2.31	0.46
3:A:1600:MET:SD	3:A:2481:SER:HB2	2.55	0.46
3:A:1610:LEU:HD12	3:A:1610:LEU:O	2.14	0.46
3:A:2298:LEU:HD13	3:A:2347:MET:HE2	1.97	0.46
3:A:2320:ARG:NH1	3:A:2328:VAL:HG22	2.30	0.46
3:A:2480:VAL:HG13	3:A:2524:GLN:OE1	2.15	0.46
3:A:4535:VAL:O	3:A:4539:THR:HG23	2.15	0.46
3:B:1318:LEU:H	3:B:1318:LEU:HD12	1.81	0.46
3:B:4310:MET:HE3	3:B:4310:MET:HA	1.97	0.46
3:A:1241:PHE:HE2	3:A:1269:HIS:CD2	2.34	0.46
3:A:1318:LEU:HD12	3:A:1318:LEU:H	1.81	0.46
3:A:1604:ALA:HB2	3:A:2484:GLU:OE1	2.15	0.46
3:A:3017:ASP:O	3:A:3021:LEU:HG	2.16	0.46
3:A:4738:VAL:O	3:A:4742:THR:OG1	2.34	0.46
3:B:70:TYR:CE1	3:B:161:PRO:HA	2.50	0.46
3:B:366:LYS:HG3	3:B:370:TYR:CE2	2.51	0.46
3:B:948:LEU:HD12	3:B:1012:ILE:HG22	1.97	0.46
3:B:1119:GLN:HA	3:B:1122:TYR:CE2	2.50	0.46
3:B:4512:PHE:HA	3:B:4515:CYS:SG	2.56	0.46
1:D:316:ARG:O	1:D:320:VAL:HG12	2.15	0.46
3:A:201:PHE:CE2	3:A:203:PRO:HB3	2.50	0.46
3:A:356:GLN:HG2	3:A:427:THR:HG22	1.98	0.46
3:A:995:GLU:O	3:A:999:LEU:HD23	2.15	0.46
3:A:3587:VAL:HG22	3:A:3647:PHE:HE1	1.80	0.46
3:A:3661:PRO:HB3	3:A:3685:HIS:CE1	2.50	0.46
3:A:4245:LEU:HB3	3:A:4294:MET:HE1	1.97	0.46
3:B:1460:GLU:OE1	3:B:1463:ARG:NE	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1518:LEU:HD23	3:B:1541:MET:HB3	1.97	0.46
3:B:1554:LEU:HD21	3:B:1795:CYS:HB2	1.98	0.46
3:B:1605:ASP:HA	3:B:1608:ASN:HD21	1.80	0.46
3:B:2698:LYS:HE3	3:B:2698:LYS:HB3	1.74	0.46
3:B:2981:LEU:O	3:B:2985:LEU:HD23	2.15	0.46
3:B:3000:MET:HA	3:B:3003:ILE:HG13	1.97	0.46
1:D:56:LEU:HD21	3:B:2311:VAL:HG22	1.97	0.46
3:A:1296:GLY:O	3:A:1299:ILE:HG22	2.15	0.46
3:A:1412:MET:HG3	3:A:1463:ARG:NH2	2.31	0.46
3:A:1499:ILE:HG23	3:A:1506:VAL:HG21	1.97	0.46
3:A:3063:MET:HA	3:A:3063:MET:HE2	1.97	0.46
3:A:3213:LEU:O	3:A:3217:ILE:HG22	2.16	0.46
3:A:4017:LEU:HD11	3:A:4132:VAL:HG11	1.98	0.46
3:B:1000:GLN:HA	3:B:1270:LEU:HD13	1.96	0.46
3:B:1069:SER:O	3:B:1073:GLU:HG2	2.16	0.46
3:B:1513:VAL:O	3:B:1517:THR:HG23	2.16	0.46
3:B:1818:LEU:O	3:B:1822:ILE:HG12	2.15	0.46
3:B:2098:ASP:O	3:B:2130:LYS:NZ	2.47	0.46
2:E:17:PHE:CD2	2:E:66:PHE:HD2	2.34	0.46
2:F:103:ALA:O	2:F:107:ARG:HG2	2.16	0.46
3:A:127:LYS:O	3:A:130:ILE:HG22	2.16	0.46
3:A:145:ARG:HH21	3:A:148:ILE:HD12	1.81	0.46
3:A:1527:ALA:HB2	3:A:1566:ARG:HH12	1.81	0.46
3:A:1660:LYS:O	3:A:1730:ARG:NH2	2.49	0.46
3:A:2054:ASN:HB3	3:A:2060:ILE:HD11	1.98	0.46
1:C:293:LEU:HA	1:C:296:LEU:HD23	1.98	0.46
3:B:75:SER:O	3:B:78:VAL:HG12	2.16	0.46
3:B:2321:LEU:HD13	3:B:2420:VAL:HB	1.97	0.46
3:B:2321:LEU:HD22	3:B:2420:VAL:HG23	1.97	0.46
3:B:4535:VAL:O	3:B:4539:THR:HG23	2.15	0.46
1:D:131:HIS:O	1:D:136:HIS:HB2	2.16	0.46
2:E:73:MET:SD	2:E:73:MET:N	2.88	0.46
2:F:20:PHE:CE2	2:F:36:VAL:HA	2.51	0.46
3:A:1434:LEU:O	3:A:1438:THR:OG1	2.27	0.46
3:A:2521:VAL:HA	3:A:2524:GLN:HG2	1.98	0.46
3:A:3052:HIS:O	3:A:3055:VAL:HG12	2.16	0.46
3:B:274:GLN:OE1	3:B:274:GLN:HA	2.15	0.46
3:B:2379:LEU:HD21	3:B:2385:PHE:HE1	1.81	0.46
3:B:2395:LEU:HD23	3:B:2432:TRP:CZ3	2.51	0.46
3:B:2542:HIS:HA	3:B:2545:GLN:OE1	2.16	0.46
3:B:2982:LEU:HB3	3:B:3027:GLN:NE2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:149:LYS:OXT	3:A:4111:ARG:NH2	2.47	0.46
3:A:296:ARG:HG2	3:A:297:ASN:H	1.81	0.46
3:A:765:GLN:NE2	3:A:817:ILE:HG23	2.31	0.46
3:A:1119:GLN:HA	3:A:1122:TYR:CE2	2.51	0.46
3:A:1677:TYR:OH	3:A:2293:GLU:OE2	2.22	0.46
3:A:1819:MET:HA	3:A:1822:ILE:HB	1.98	0.46
3:A:2626:VAL:HG21	3:A:2681:ILE:HD12	1.97	0.46
3:B:1538:MET:O	3:B:1542:ALA:CB	2.65	0.46
3:B:2483:LEU:HB2	3:B:2524:GLN:NE2	2.31	0.46
3:B:2521:VAL:HA	3:B:2524:GLN:HG2	1.97	0.46
3:B:3213:LEU:O	3:B:3217:ILE:HG22	2.16	0.46
3:B:3261:GLY:N	3:B:3837:GLU:OE2	2.42	0.46
3:B:3985:CYS:HB3	3:B:3988:LEU:HD12	1.98	0.46
1:D:64:TYR:HA	3:B:2329:ALA:HB3	1.98	0.45
2:E:56:VAL:HG21	2:E:72:MET:HE2	1.98	0.45
3:A:86:THR:OG1	3:A:140:CYS:SG	2.65	0.45
3:A:144:ASP:OD2	3:A:146:THR:OG1	2.31	0.45
3:A:1513:VAL:O	3:A:1517:THR:HG23	2.16	0.45
3:A:2379:LEU:HD21	3:A:2385:PHE:HE1	1.81	0.45
3:B:447:ILE:O	3:B:450:ARG:HG3	2.16	0.45
3:B:1676:TRP:HZ2	3:B:1708:LYS:HE2	1.80	0.45
3:B:2972:MET:O	3:B:2976:MET:HG2	2.15	0.45
3:B:2974:ARG:HB3	3:B:3006:LEU:HD13	1.98	0.45
2:E:107:ARG:HD3	2:E:122:VAL:HG21	1.98	0.45
2:F:34:GLY:O	2:F:38:ARG:CB	2.65	0.45
3:A:2115:TYR:HB2	3:A:2122:LEU:HD13	1.97	0.45
3:A:3544:TYR:O	3:A:3545:ILE:HD13	2.16	0.45
3:A:4617:LEU:HD13	3:A:4665:ILE:HG13	1.97	0.45
3:B:115:LEU:HD23	3:B:129:LEU:HD12	1.98	0.45
3:B:317:VAL:O	3:B:325:ARG:NH2	2.25	0.45
3:B:1660:LYS:O	3:B:1730:ARG:NH2	2.49	0.45
3:B:4506:THR:HG22	3:B:4510:LYS:HZ1	1.81	0.45
3:B:4557:ALA:O	3:B:4560:GLU:HG3	2.16	0.45
3:A:447:ILE:O	3:A:450:ARG:HG3	2.16	0.45
3:A:1919:GLY:O	3:A:1950:VAL:N	2.47	0.45
3:A:1960:ASN:HD22	3:A:2007:TRP:CG	2.33	0.45
3:A:2210:LYS:N	3:A:2235:GLU:OE1	2.49	0.45
3:A:2320:ARG:CZ	3:A:2328:VAL:HG22	2.47	0.45
3:A:2395:LEU:HD23	3:A:2432:TRP:CZ3	2.51	0.45
3:A:3727:GLU:OE1	3:A:3727:GLU:N	2.50	0.45
3:A:4564:SER:HA	3:A:4567:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:THR:HG21	1:C:131:HIS:HB2	1.99	0.45
3:B:3021:LEU:O	3:B:3024:LEU:HG	2.16	0.45
3:B:3224:TYR:O	3:B:3228:ARG:HG3	2.16	0.45
3:B:3312:ASP:OD1	3:B:3314:GLY:N	2.48	0.45
3:A:45:GLU:HG3	3:A:47:LYS:H	1.81	0.45
3:A:83:HIS:O	3:A:87:THR:HG23	2.17	0.45
3:A:1596:THR:O	3:A:1597:CYS:C	2.59	0.45
3:A:2219:HIS:NE2	3:A:2229:THR:OG1	2.48	0.45
3:A:3307:VAL:O	3:A:3311:VAL:HG23	2.16	0.45
3:A:3618:VAL:HG21	3:A:3629:ILE:HG12	1.98	0.45
3:A:4591:LYS:HZ3	3:A:4631:MET:HG2	1.81	0.45
3:A:4648:ASP:OD2	3:A:4694:TYR:OH	2.34	0.45
3:B:1214:LEU:HD13	3:B:1354:LEU:HD12	1.98	0.45
3:B:3618:VAL:HG21	3:B:3629:ILE:HG12	1.98	0.45
1:D:112:ILE:HB	1:D:136:HIS:CE1	2.52	0.45
1:D:114:ALA:HA	1:D:121:PRO:HA	1.99	0.45
3:A:124:VAL:HG12	3:A:128:HIS:HB2	1.97	0.45
3:A:694:ASP:OD1	3:A:695:LYS:N	2.49	0.45
3:A:2320:ARG:HA	3:A:2326:MET:SD	2.57	0.45
3:A:3273:MET:HE3	3:A:3633:LEU:HG	1.99	0.45
3:A:3728:ASN:ND2	3:A:3730:GLU:OE2	2.49	0.45
3:B:125:SER:N	3:B:128:HIS:HD2	2.15	0.45
3:B:293:THR:O	3:B:297:ASN:ND2	2.49	0.45
3:B:296:ARG:HG2	3:B:297:ASN:H	1.81	0.45
3:B:1960:ASN:HD22	3:B:2007:TRP:CG	2.34	0.45
3:B:2538:ALA:O	3:B:2542:HIS:ND1	2.50	0.45
3:B:2550:LYS:O	3:B:2553:GLN:HG3	2.16	0.45
1:D:324:LEU:HD11	3:B:4152:LEU:HD11	1.98	0.45
3:A:293:THR:O	3:A:297:ASN:ND2	2.49	0.45
3:A:680:GLU:H	3:A:680:GLU:CD	2.21	0.45
3:A:2550:LYS:O	3:A:2553:GLN:HG3	2.16	0.45
3:A:2636:LYS:HB2	3:A:2649:GLY:HA3	1.99	0.45
3:A:4108:PHE:CD1	3:A:4108:PHE:C	2.94	0.45
3:B:125:SER:H	3:B:128:HIS:HD2	1.65	0.45
3:B:201:PHE:CE2	3:B:203:PRO:HB3	2.52	0.45
3:B:201:PHE:CZ	3:B:203:PRO:HB3	2.51	0.45
3:B:336:CYS:SG	3:B:381:CYS:HA	2.57	0.45
3:B:3728:ASN:ND2	3:B:3730:GLU:OE2	2.49	0.45
3:B:4063:ASP:OD1	3:B:4065:LYS:NZ	2.49	0.45
3:B:4695:MET:HE2	3:B:4695:MET:N	2.32	0.45
3:A:185:ARG:O	3:A:188:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2228:THR:HB	3:A:2244:ALA:HB3	1.99	0.45
3:A:2317:ILE:HG12	3:A:2320:ARG:NH2	2.30	0.45
3:A:3018:LYS:HA	3:A:3021:LEU:CD1	2.47	0.45
1:C:316:ARG:O	1:C:320:VAL:HG12	2.17	0.45
3:B:3210:VAL:HA	3:B:3213:LEU:HG	1.99	0.45
3:B:3736:VAL:O	3:B:3739:ILE:HG22	2.17	0.45
3:B:4103:TRP:HZ3	3:B:4104:ARG:HH21	1.64	0.45
3:B:4443:ARG:NH2	3:B:4453:GLU:OE1	2.46	0.45
3:A:2037:PHE:CE2	3:A:2075:MET:HB2	2.52	0.45
3:A:3312:ASP:OD1	3:A:3314:GLY:N	2.45	0.45
3:A:3881:GLU:HG2	3:A:3921:MET:SD	2.57	0.45
3:B:1241:PHE:HE2	3:B:1269:HIS:CD2	2.34	0.45
3:B:1441:SER:O	3:B:1441:SER:OG	2.31	0.45
3:B:1596:THR:O	3:B:1597:CYS:C	2.59	0.45
3:B:1685:VAL:HG21	3:B:2381:ARG:HD2	1.98	0.45
3:B:1814:MET:HA	3:B:1817:PHE:CE1	2.51	0.45
3:B:1845:LEU:HD21	3:B:2119:LEU:HD22	1.98	0.45
3:B:2054:ASN:HB3	3:B:2060:ILE:HD11	1.98	0.45
3:B:2187:PRO:HG2	3:B:2202:ILE:HB	1.98	0.45
3:B:2210:LYS:N	3:B:2235:GLU:OE1	2.50	0.45
3:B:2589:VAL:HG22	3:B:2667:TYR:CD1	2.51	0.45
3:B:3293:PHE:C	3:B:3293:PHE:CD1	2.95	0.45
3:B:4259:LYS:O	3:B:4263:VAL:HG13	2.17	0.45
3:A:1254:ASP:C	3:A:1254:ASP:OD1	2.60	0.45
3:A:2543:LYS:C	3:A:2543:LYS:HD3	2.42	0.45
3:B:131:LEU:HB2	3:B:142:ARG:HG2	1.99	0.45
3:B:765:GLN:NE2	3:B:817:ILE:HG23	2.31	0.45
3:B:1023:LEU:HD21	3:B:1041:TRP:CZ3	2.50	0.45
3:B:1334:LEU:HA	3:B:1334:LEU:HD23	1.80	0.45
3:B:1677:TYR:OH	3:B:2293:GLU:OE2	2.22	0.45
3:B:1692:THR:OG1	3:B:2293:GLU:OE2	2.24	0.45
3:B:3050:GLU:O	3:B:3054:VAL:HG22	2.17	0.45
3:B:3233:LEU:HB3	3:B:3293:PHE:CE2	2.52	0.45
3:B:4327:THR:OG1	3:B:4328:PRO:HD3	2.16	0.45
3:B:4648:ASP:OD2	3:B:4694:TYR:OH	2.34	0.45
3:A:849:ARG:NH2	3:A:982:THR:O	2.47	0.45
3:A:1059:ILE:HD13	3:A:1059:ILE:HA	1.88	0.45
3:A:1538:MET:HA	3:A:1541:MET:SD	2.57	0.45
3:B:683:MET:HE3	3:B:727:LEU:HD12	1.99	0.45
3:B:1381:LEU:O	3:B:1384:LEU:HD12	2.16	0.45
3:B:2529:LEU:HG	3:B:2539:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2678:ALA:O	3:B:2681:ILE:HG12	2.16	0.45
3:B:3544:TYR:O	3:B:3545:ILE:HD13	2.17	0.45
3:A:125:SER:N	3:A:128:HIS:HD2	2.15	0.44
3:A:128:HIS:O	3:A:131:LEU:HD12	2.17	0.44
3:A:910:GLY:HA2	3:A:934:CYS:H	1.82	0.44
3:A:1336:ARG:HE	3:A:1337:ILE:HD11	1.82	0.44
3:A:1924:LEU:HD11	3:A:1942:LEU:HB3	1.99	0.44
3:A:2692:ALA:O	3:A:2696:SER:OG	2.26	0.44
3:B:2115:TYR:HA	3:B:2122:LEU:HA	1.99	0.44
3:A:336:CYS:SG	3:A:381:CYS:HA	2.57	0.44
3:A:4479:MET:SD	3:A:4480:ALA:N	2.90	0.44
3:A:4563:LEU:HA	3:A:4566:MET:HG2	1.98	0.44
1:C:132:LEU:HA	1:C:136:HIS:HB2	1.98	0.44
3:B:1930:LEU:HB3	3:B:2219:HIS:CE1	2.52	0.44
3:B:2706:ARG:NH2	3:B:2707:PRO:O	2.50	0.44
3:B:3035:ASP:OD1	3:B:3035:ASP:N	2.44	0.44
3:B:3871:LYS:HD3	3:B:3871:LYS:N	2.32	0.44
2:E:1:MET:HE1	2:E:71:THR:HA	1.99	0.44
2:F:56:VAL:HG11	2:F:72:MET:HE2	1.99	0.44
3:A:1685:VAL:HG21	3:A:2381:ARG:HD2	1.98	0.44
3:A:2060:ILE:HG21	3:A:2141:LEU:HD21	2.00	0.44
3:A:2589:VAL:HG22	3:A:2667:TYR:CD1	2.53	0.44
3:A:3756:HIS:ND1	3:A:3802:GLU:OE2	2.48	0.44
3:A:4591:LYS:HE2	3:A:4631:MET:HE3	1.99	0.44
3:B:1408:VAL:O	3:B:1412:MET:HG2	2.18	0.44
3:B:1672:MET:HE2	3:B:1672:MET:N	2.32	0.44
3:B:3887:LEU:HD13	3:B:3887:LEU:HA	1.85	0.44
3:B:4216:GLU:OE2	3:B:4217:ILE:HG13	2.18	0.44
3:B:4714:LEU:HD11	3:B:4754:VAL:HG11	1.99	0.44
3:A:957:PHE:HZ	3:A:1014:PRO:HG2	1.82	0.44
3:A:1672:MET:HE2	3:A:1672:MET:N	2.32	0.44
3:A:2978:LEU:O	3:A:2981:LEU:HG	2.18	0.44
3:A:3007:THR:CB	3:A:3010:LEU:HD22	2.47	0.44
3:A:3210:VAL:HA	3:A:3213:LEU:HG	1.99	0.44
3:A:3852:THR:HG23	3:A:3855:GLN:H	1.83	0.44
3:B:2654:GLU:O	3:B:2658:ASN:ND2	2.30	0.44
3:B:3023:ASN:C	3:B:3023:ASN:OD1	2.61	0.44
3:B:3192:TYR:C	3:B:3192:TYR:CD1	2.94	0.44
3:B:4108:PHE:CD1	3:B:4108:PHE:C	2.95	0.44
3:B:4167:THR:O	3:B:4170:LEU:HB2	2.18	0.44
1:D:120:ASP:HB3	1:D:123:HIS:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:73:MET:HA	2:E:73:MET:HE3	2.00	0.44
3:A:338:TYR:O	3:A:338:TYR:HD1	2.00	0.44
3:A:418:LEU:HA	3:A:421:ILE:HG22	2.00	0.44
3:A:1030:MET:H	3:A:1030:MET:CE	2.29	0.44
3:A:1206:SER:H	3:A:1321:SER:HB2	1.82	0.44
3:A:2968:ASN:O	3:A:2971:HIS:N	2.50	0.44
3:B:418:LEU:HA	3:B:421:ILE:HG22	1.99	0.44
3:B:1816:ASN:O	3:B:1819:MET:HB3	2.18	0.44
3:B:3583:ARG:HG3	3:B:3650:ASN:HD22	1.83	0.44
1:D:293:LEU:HA	1:D:296:LEU:HD23	1.99	0.44
2:F:65:ASP:OD1	2:F:67:PRO:HD2	2.18	0.44
3:A:201:PHE:CZ	3:A:203:PRO:HB3	2.52	0.44
3:A:832:LEU:O	3:A:836:ILE:HG12	2.18	0.44
3:A:834:VAL:O	3:A:838:GLN:HG3	2.18	0.44
3:A:1909:ARG:HH12	3:A:1980:PHE:HB2	1.82	0.44
3:A:2971:HIS:HA	3:A:2974:ARG:HD3	1.99	0.44
3:A:4152:LEU:HD23	1:C:321:GLN:HG2	2.00	0.44
3:A:4479:MET:HA	3:A:4482:CYS:SG	2.58	0.44
3:A:4509:LEU:HD12	3:A:4510:LYS:N	2.33	0.44
3:A:4557:ALA:O	3:A:4560:GLU:HG3	2.18	0.44
1:C:125:THR:HG22	1:C:127:ASP:H	1.83	0.44
3:B:779:CYS:O	3:B:782:VAL:HG12	2.18	0.44
3:B:1227:GLN:CD	3:B:1227:GLN:N	2.76	0.44
3:B:2151:ILE:HD11	3:B:2164:LEU:HD11	2.00	0.44
3:B:3881:GLU:HG2	3:B:3921:MET:SD	2.57	0.44
3:B:4479:MET:SD	3:B:4480:ALA:N	2.91	0.44
3:B:4521:ASN:C	3:B:4521:ASN:OD1	2.61	0.44
3:A:1428:LEU:HB3	3:A:1491:LEU:CD1	2.48	0.44
3:A:3233:LEU:HB3	3:A:3293:PHE:CE2	2.53	0.44
3:A:4167:THR:HA	3:A:4170:LEU:HD23	2.00	0.44
3:B:119:ASP:OD1	3:B:120:GLU:N	2.49	0.44
3:B:1159:LEU:HD12	3:B:1159:LEU:HA	1.88	0.44
3:B:1811:VAL:HA	3:B:1814:MET:SD	2.58	0.44
3:B:2037:PHE:CE2	3:B:2075:MET:HB2	2.52	0.44
3:B:4314:ILE:HD11	3:B:4335:LEU:HD11	1.99	0.44
2:F:116:LYS:HE2	2:F:116:LYS:HB2	1.56	0.44
2:F:132:ASP:OD1	2:F:132:ASP:N	2.38	0.44
3:A:124:VAL:HG22	3:A:151:PHE:CE1	2.52	0.44
3:A:1025:MET:SD	3:A:1025:MET:N	2.82	0.44
3:A:1299:ILE:HD11	3:A:1305:MET:SD	2.58	0.44
3:A:1810:LEU:O	3:A:1814:MET:SD	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1845:LEU:HD21	3:A:2119:LEU:HD22	2.00	0.44
3:A:3312:ASP:OD1	3:A:3312:ASP:C	2.61	0.44
3:A:4519:LYS:HA	3:A:4519:LYS:HD3	1.87	0.44
3:B:86:THR:HG22	3:B:136:LEU:HD13	1.99	0.44
3:B:127:LYS:HE2	3:B:127:LYS:HB2	1.86	0.44
3:B:680:GLU:H	3:B:680:GLU:CD	2.17	0.44
3:B:2971:HIS:O	3:B:2975:LEU:HG	2.18	0.44
3:B:4495:ILE:HD13	3:B:4505:LEU:HG	1.99	0.44
3:B:4596:MET:SD	3:B:4596:MET:N	2.89	0.44
3:A:678:LEU:HD12	3:A:683:MET:HE2	2.00	0.44
3:A:779:CYS:O	3:A:782:VAL:HG12	2.17	0.44
3:A:1020:ILE:O	3:A:1024:SER:CB	2.56	0.44
3:A:1538:MET:N	3:A:1538:MET:SD	2.90	0.44
3:A:1854:MET:HG3	3:A:2199:ILE:HD11	2.00	0.44
3:A:2323:SER:HB3	3:A:2326:MET:HE1	1.99	0.44
3:A:3295:ILE:HD11	3:A:3391:LEU:HD22	2.00	0.44
3:A:4167:THR:O	3:A:4170:LEU:HB2	2.18	0.44
3:A:4216:GLU:OE1	3:A:4238:LEU:HB2	2.18	0.44
3:A:4310:MET:HA	3:A:4310:MET:HE3	2.00	0.44
3:A:4503:HIS:O	3:A:4507:VAL:HG13	2.17	0.44
3:A:4671:ASN:OD1	3:A:4676:HIS:NE2	2.51	0.44
3:B:2335:GLY:HA3	3:B:2405:ILE:O	2.18	0.44
3:B:3039:VAL:O	3:B:3042:LYS:HG2	2.18	0.44
3:B:4519:LYS:HA	3:B:4519:LYS:HD3	1.85	0.44
3:A:302:LEU:HB3	3:A:377:ILE:HD12	1.99	0.43
3:A:747:LEU:HB2	3:A:805:ASP:HA	1.99	0.43
3:A:1085:TYR:O	3:A:1089:ILE:HG22	2.18	0.43
3:A:3293:PHE:CD1	3:A:3293:PHE:C	2.96	0.43
3:A:3575:THR:OG1	3:A:3714:MET:HB3	2.18	0.43
3:A:3583:ARG:HG3	3:A:3650:ASN:HD22	1.83	0.43
3:A:4206:LEU:HD13	3:A:4262:LEU:HD11	1.99	0.43
3:A:4383:MET:HE3	3:A:4383:MET:HB2	1.82	0.43
3:A:4562:VAL:O	3:A:4565:ILE:HG12	2.18	0.43
1:C:24:CYS:HB2	1:C:46:HIS:HE1	1.83	0.43
3:B:1138:HIS:O	3:B:1142:MET:HB2	2.19	0.43
3:B:1278:LEU:HD23	3:B:1278:LEU:HA	1.89	0.43
3:B:1538:MET:SD	3:B:1538:MET:N	2.91	0.43
3:B:2115:TYR:HB2	3:B:2122:LEU:HD13	2.00	0.43
3:B:4419:LEU:HD21	3:B:4458:SER:HA	2.00	0.43
1:D:323:LEU:HD21	3:B:4059:TRP:CE3	2.53	0.43
3:A:1341:ALA:HA	3:A:1346:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1377:LEU:HA	3:A:1380:CYS:SG	2.57	0.43
3:A:1429:LYS:HD3	3:A:1433:LYS:HG3	2.00	0.43
3:A:1485:ILE:HA	3:A:1488:ASN:HD22	1.84	0.43
3:A:2151:ILE:HD11	3:A:2164:LEU:HD11	1.99	0.43
3:A:2356:ILE:HD11	3:A:2385:PHE:CD1	2.53	0.43
3:A:2578:ARG:NE	3:A:2662:ASP:OD2	2.46	0.43
3:A:3234:ASP:O	3:A:3238:ARG:HG3	2.18	0.43
3:A:3875:CYS:O	3:A:3879:VAL:HG23	2.17	0.43
3:B:858:LEU:HD23	3:B:858:LEU:HA	1.87	0.43
3:B:1270:LEU:HD23	3:B:1270:LEU:HA	1.87	0.43
3:B:2636:LYS:HB2	3:B:2649:GLY:HA3	2.00	0.43
3:B:4479:MET:HA	3:B:4482:CYS:SG	2.57	0.43
2:F:34:GLY:HA2	2:F:49:LEU:HD21	2.00	0.43
3:A:1159:LEU:HD21	3:A:1299:ILE:HD12	2.00	0.43
3:A:1244:ILE:HA	3:A:1293:ARG:NH2	2.28	0.43
3:A:1483:ASP:OD1	3:A:1483:ASP:N	2.50	0.43
3:A:1538:MET:O	3:A:1542:ALA:CB	2.66	0.43
3:A:1589:HIS:O	3:A:1592:ILE:HG22	2.18	0.43
3:A:1593:LEU:HD12	3:A:1594:GLU:N	2.34	0.43
3:A:2187:PRO:HG2	3:A:2202:ILE:HB	2.00	0.43
3:A:2335:GLY:HA3	3:A:2405:ILE:O	2.18	0.43
3:B:185:ARG:O	3:B:188:GLU:HG3	2.18	0.43
3:B:368:ASP:O	3:B:371:GLU:HG3	2.18	0.43
3:B:1527:ALA:HB2	3:B:1566:ARG:HH12	1.83	0.43
3:B:1585:MET:N	3:B:1585:MET:HE2	2.33	0.43
3:B:1607:THR:HG21	3:B:2488:SER:OG	2.18	0.43
3:B:1690:VAL:HG12	3:B:1716:CYS:HB2	2.00	0.43
3:B:1837:ARG:O	3:B:1840:GLN:HG2	2.18	0.43
3:B:3099:LEU:HD22	3:B:3103:LYS:HZ1	1.83	0.43
3:B:3136:MET:HB2	3:B:3145:VAL:HG21	1.99	0.43
3:B:4347:THR:O	3:B:4374:SER:OG	2.36	0.43
1:D:22:TYR:HD1	1:D:52:MET:SD	2.41	0.43
1:D:25:LEU:HD11	1:D:79:THR:HB	2.00	0.43
3:A:81:SER:O	3:A:85:ILE:HG13	2.18	0.43
3:A:231:SER:HA	3:A:234:LYS:HE2	2.01	0.43
3:A:745:TRP:HE1	3:A:810:HIS:CE1	2.37	0.43
3:A:3047:ALA:O	3:A:3051:VAL:HG13	2.18	0.43
3:A:3099:LEU:HD22	3:A:3103:LYS:HZ1	1.83	0.43
3:A:3192:TYR:C	3:A:3192:TYR:CD2	2.96	0.43
3:A:4495:ILE:HD13	3:A:4505:LEU:HG	2.00	0.43
3:B:1023:LEU:HD21	3:B:1041:TRP:CE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2978:LEU:HD23	3:B:2981:LEU:HD21	2.00	0.43
3:B:4216:GLU:OE1	3:B:4238:LEU:HB2	2.19	0.43
3:A:855:LEU:HA	3:A:855:LEU:HD12	1.77	0.43
3:A:4327:THR:OG1	3:A:4328:PRO:HD3	2.17	0.43
3:B:1206:SER:H	3:B:1321:SER:HB2	1.84	0.43
3:B:2228:THR:HB	3:B:2244:ALA:HB3	2.00	0.43
3:B:3140:PHE:CZ	3:B:3153:PHE:HE1	2.37	0.43
3:B:3293:PHE:C	3:B:3293:PHE:HD1	2.26	0.43
3:B:3307:VAL:O	3:B:3311:VAL:HG23	2.19	0.43
3:B:3920:ALA:O	3:B:3923:GLU:HG3	2.19	0.43
3:B:4518:VAL:O	3:B:4522:ARG:HG2	2.19	0.43
2:E:20:PHE:CE2	2:E:36:VAL:HA	2.53	0.43
3:A:1023:LEU:HD21	3:A:1041:TRP:CE3	2.54	0.43
3:A:2025:ILE:O	3:A:2036:THR:N	2.51	0.43
3:A:4216:GLU:OE2	3:A:4217:ILE:HG13	2.18	0.43
3:A:4695:MET:CE	3:A:4722:ILE:HG21	2.48	0.43
3:A:4714:LEU:HD11	3:A:4754:VAL:HG11	2.00	0.43
3:B:75:SER:HB2	3:B:123:ALA:HB3	2.00	0.43
3:B:263:LEU:HD12	3:B:266:PHE:CD2	2.54	0.43
3:B:745:TRP:HE1	3:B:810:HIS:CE1	2.37	0.43
3:B:1811:VAL:HG11	3:B:2486:LEU:HG	1.99	0.43
3:B:2060:ILE:HG21	3:B:2141:LEU:HD21	2.01	0.43
3:B:2991:VAL:O	3:B:2995:ARG:HD3	2.18	0.43
3:B:3852:THR:HG23	3:B:3855:GLN:H	1.83	0.43
2:E:118:THR:O	2:E:122:VAL:HG22	2.19	0.43
3:A:248:GLN:NE2	3:A:316:PRO:O	2.51	0.43
3:A:711:TYR:OH	3:A:885:LEU:O	2.37	0.43
3:A:1278:LEU:HD23	3:A:1278:LEU:HA	1.89	0.43
3:A:2706:ARG:NH2	3:A:2707:PRO:O	2.52	0.43
3:A:3039:VAL:O	3:A:3042:LYS:HG2	2.18	0.43
3:A:4419:LEU:HD21	3:A:4458:SER:HA	1.99	0.43
3:B:59:SER:O	3:B:63:ILE:HG13	2.19	0.43
3:B:338:TYR:O	3:B:338:TYR:HD1	2.01	0.43
3:B:965:GLU:H	3:B:965:GLU:CD	2.26	0.43
3:B:1538:MET:HA	3:B:1541:MET:SD	2.59	0.43
3:B:1904:SER:N	3:B:1964:GLU:OE1	2.51	0.43
3:B:1909:ARG:HH12	3:B:1980:PHE:HB2	1.83	0.43
3:B:3192:TYR:C	3:B:3192:TYR:HD1	2.27	0.43
3:B:3312:ASP:OD1	3:B:3312:ASP:C	2.61	0.43
3:B:3875:CYS:O	3:B:3879:VAL:HG23	2.19	0.43
3:B:4593:GLN:H	3:B:4593:GLN:CD	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:78:VAL:HG11	3:A:110:PHE:HD2	1.84	0.43
3:A:187:LYS:O	3:A:191:MET:HG2	2.19	0.43
3:A:1214:LEU:HD13	3:A:1354:LEU:HD12	2.01	0.43
3:A:1930:LEU:HD22	3:A:2219:HIS:CD2	2.54	0.43
3:A:1961:PRO:HB2	3:A:2641:PHE:CZ	2.54	0.43
3:A:2115:TYR:HA	3:A:2122:LEU:HA	2.01	0.43
3:A:2218:ARG:NH2	3:A:2253:LEU:HD13	2.33	0.43
3:A:3045:ARG:HG3	3:A:3050:GLU:OE2	2.19	0.43
3:B:36:LEU:HD22	3:B:84:TYR:HD2	1.84	0.43
3:B:81:SER:O	3:B:85:ILE:HG13	2.19	0.43
3:B:834:VAL:O	3:B:838:GLN:HG3	2.18	0.43
3:B:1593:LEU:O	3:B:1596:THR:OG1	2.30	0.43
3:B:1807:PHE:CD1	3:B:1810:LEU:HD23	2.54	0.43
3:B:1909:ARG:HD3	3:B:1911:HIS:CD2	2.53	0.43
3:B:3271:SER:HA	3:B:3274:GLU:OE1	2.19	0.43
3:B:3295:ILE:HD11	3:B:3391:LEU:HD22	2.00	0.43
2:F:34:GLY:O	2:F:38:ARG:HB3	2.18	0.43
3:A:1214:LEU:HD11	3:A:1383:TYR:CE2	2.54	0.43
3:A:1227:GLN:N	3:A:1227:GLN:CD	2.77	0.43
3:A:1427:VAL:HG22	3:A:1431:PHE:CE2	2.53	0.43
3:A:1477:LYS:HA	3:A:1477:LYS:HD3	1.86	0.43
3:A:2139:THR:HG23	3:A:2140:THR:HG23	2.01	0.43
3:A:2153:SER:OG	3:A:2155:ASN:O	2.36	0.43
3:A:3042:LYS:N	3:A:3042:LYS:HD2	2.34	0.43
3:A:4593:GLN:HA	3:A:4596:MET:HE1	2.00	0.43
3:B:66:HIS:CD2	3:B:74:TYR:CE2	3.07	0.43
3:B:1300:VAL:HG22	3:B:1336:ARG:CZ	2.48	0.43
3:B:1568:LYS:HE2	3:B:1814:MET:HB3	2.00	0.43
3:B:3161:THR:O	3:B:3165:LEU:HD23	2.19	0.43
3:A:195:ASN:C	3:A:195:ASN:OD1	2.62	0.43
3:A:1814:MET:HB2	3:A:1818:LEU:HD23	2.01	0.43
3:A:1837:ARG:O	3:A:1840:GLN:HG2	2.19	0.43
3:A:1909:ARG:HD3	3:A:1911:HIS:CD2	2.53	0.43
3:A:3387:GLN:O	3:A:3391:LEU:HG	2.18	0.43
3:A:4109:LEU:HD13	3:A:4115:ARG:HD3	2.01	0.43
3:A:4347:THR:O	3:A:4374:SER:OG	2.37	0.43
3:B:48:GLU:HA	3:B:51:GLN:NE2	2.33	0.43
3:B:700:GLY:H	3:B:703:ASP:HB3	1.83	0.43
3:B:2038:TYR:CD2	3:B:2085:PRO:HB3	2.54	0.43
3:B:2218:ARG:NH2	3:B:2253:LEU:HD13	2.34	0.43
3:B:2320:ARG:HA	3:B:2326:MET:SD	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3564:LYS:HB3	3:B:3602:ILE:HD11	2.01	0.43
3:A:73:PHE:HB2	3:A:158:ALA:HB1	2.01	0.42
3:A:823:GLU:O	3:A:827:ARG:HG2	2.19	0.42
3:A:2212:GLN:H	3:A:2234:CYS:HA	1.84	0.42
3:A:2214:MET:CE	3:A:2232:LEU:HG	2.48	0.42
3:A:2355:GLN:HB2	3:A:2384:TRP:CE2	2.54	0.42
3:A:2969:ARG:HG2	3:A:2970:LEU:N	2.34	0.42
3:A:3564:LYS:HB3	3:A:3602:ILE:HD11	1.99	0.42
3:A:4252:GLU:OE1	3:A:4252:GLU:N	2.52	0.42
3:A:4598:LEU:HA	3:A:4601:ILE:HD12	2.00	0.42
3:B:73:PHE:CD1	3:B:155:MET:HE1	2.54	0.42
3:B:135:GLY:HA2	3:B:142:ARG:HH21	1.84	0.42
3:B:823:GLU:OE1	3:B:826:ARG:NH2	2.38	0.42
3:B:1593:LEU:HD12	3:B:1594:GLU:N	2.34	0.42
3:B:4533:LEU:HD23	3:B:4587:LEU:HD11	2.00	0.42
3:B:4562:VAL:O	3:B:4565:ILE:HG12	2.19	0.42
3:B:4566:MET:HB3	3:B:4619:ILE:HD11	2.00	0.42
3:A:59:SER:O	3:A:63:ILE:HG13	2.19	0.42
3:A:368:ASP:O	3:A:371:GLU:HG3	2.18	0.42
3:A:1677:TYR:HA	3:A:1707:ALA:N	2.28	0.42
3:A:2038:TYR:CD2	3:A:2085:PRO:HB3	2.54	0.42
3:A:3574:VAL:HG22	3:A:3715:LEU:HD23	2.00	0.42
3:B:855:LEU:HA	3:B:855:LEU:HD12	1.78	0.42
3:B:964:ASP:OD1	3:B:1016:SER:OG	2.37	0.42
3:B:1305:MET:HE1	3:B:1307:PRO:HA	2.01	0.42
3:B:1589:HIS:O	3:B:1592:ILE:HG22	2.19	0.42
3:B:2627:ASN:O	3:B:2631:LYS:HG2	2.19	0.42
3:B:3207:ARG:O	3:B:3210:VAL:HG12	2.19	0.42
3:B:3501:ASN:HB3	3:B:3912:TYR:CE2	2.54	0.42
3:B:4506:THR:O	3:B:4509:LEU:HG	2.19	0.42
3:B:4695:MET:CE	3:B:4722:ILE:HG21	2.49	0.42
3:A:1431:PHE:O	3:A:1434:LEU:HD12	2.19	0.42
3:A:1904:SER:N	3:A:1964:GLU:OE1	2.52	0.42
3:A:3010:LEU:HG	3:A:3021:LEU:HD21	2.01	0.42
3:A:3050:GLU:O	3:A:3054:VAL:HG22	2.19	0.42
3:A:4330:PHE:HA	3:A:4333:GLU:HG3	2.01	0.42
3:B:82:THR:HG22	3:B:107:LEU:HD13	2.01	0.42
3:B:1336:ARG:HE	3:B:1337:ILE:HD11	1.83	0.42
3:B:4489:LEU:HD23	3:B:4489:LEU:HA	1.85	0.42
1:D:86:MET:HB3	3:B:2309:LEU:HB3	2.02	0.42
2:F:21:ASP:HA	2:F:28:ILE:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:49:LEU:O	3:A:53:VAL:HG23	2.19	0.42
3:A:1300:VAL:HG22	3:A:1336:ARG:CZ	2.49	0.42
3:A:1607:THR:HG21	3:A:2488:SER:OG	2.18	0.42
3:A:2329:ALA:HB3	1:C:64:TYR:HA	2.02	0.42
3:A:2529:LEU:HA	3:A:2532:LEU:HD12	2.01	0.42
3:B:1155:THR:HB	3:B:1298:LEU:HD11	2.02	0.42
3:B:1429:LYS:HD3	3:B:1433:LYS:HG3	2.02	0.42
3:B:1589:HIS:CE1	3:B:1590:VAL:HG23	2.54	0.42
3:B:1909:ARG:NH2	3:B:1980:PHE:O	2.44	0.42
3:B:1930:LEU:HD22	3:B:2219:HIS:CD2	2.53	0.42
3:B:2968:ASN:O	3:B:2971:HIS:HB3	2.19	0.42
3:A:1515:LEU:HD23	3:A:1541:MET:HB2	2.01	0.42
3:A:1560:ALA:HA	3:A:1563:TRP:HB2	2.01	0.42
3:A:2542:HIS:HA	3:A:2545:GLN:OE1	2.20	0.42
3:A:3161:THR:O	3:A:3165:LEU:HD23	2.20	0.42
3:A:3547:LEU:HD21	3:A:3563:VAL:HG11	2.00	0.42
3:B:694:ASP:OD1	3:B:695:LYS:N	2.52	0.42
3:B:1125:ASP:O	3:B:1128:ILE:HG13	2.19	0.42
3:B:1249:ASN:OD1	3:B:1250:ALA:N	2.49	0.42
3:B:1515:LEU:HD23	3:B:1541:MET:HB2	2.00	0.42
3:B:1810:LEU:H	3:B:1810:LEU:HD22	1.85	0.42
3:B:3758:PRO:O	3:B:3761:GLU:HG2	2.19	0.42
2:F:37:MET:HA	2:F:40:LEU:HG	2.00	0.42
3:A:318:LEU:HA	3:A:325:ARG:NH2	2.34	0.42
3:A:642:LYS:HE2	3:A:642:LYS:HB2	1.88	0.42
3:A:1138:HIS:O	3:A:1141:LYS:HG2	2.19	0.42
3:A:2181:GLN:NE2	3:A:2186:VAL:O	2.34	0.42
3:A:2211:ILE:HA	3:A:2234:CYS:HA	2.01	0.42
3:A:4121:LEU:HG	3:A:4161:GLN:HG3	2.01	0.42
3:B:301:SER:O	3:B:304:ILE:HG22	2.20	0.42
3:B:1341:ALA:HA	3:B:1346:PHE:CD2	2.54	0.42
3:B:1596:THR:O	3:B:1599:ILE:HG12	2.19	0.42
3:B:3154:GLU:H	3:B:3154:GLU:HG2	1.71	0.42
3:A:790:MET:SD	3:A:854:ILE:HG23	2.60	0.42
3:A:1125:ASP:O	3:A:1128:ILE:HG13	2.20	0.42
3:A:1589:HIS:CE1	3:A:1590:VAL:HG23	2.54	0.42
3:A:3032:LEU:HD23	3:A:3032:LEU:HA	1.87	0.42
3:A:3633:LEU:HD23	3:A:3633:LEU:HA	1.92	0.42
3:A:3736:VAL:O	3:A:3739:ILE:HG22	2.19	0.42
3:B:34:ARG:HG3	3:B:34:ARG:HH11	1.85	0.42
3:B:128:HIS:O	3:B:131:LEU:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1483:ASP:N	3:B:1483:ASP:OD1	2.49	0.42
3:B:3788:THR:O	3:B:3791:SER:OG	2.27	0.42
3:B:4303:GLU:HB3	3:B:4307:LYS:NZ	2.35	0.42
1:D:26:ILE:HG12	1:D:108:VAL:HG12	2.01	0.42
3:A:141:SER:H	3:A:142:ARG:NH2	2.18	0.42
3:A:913:GLU:H	3:A:913:GLU:CD	2.17	0.42
3:A:1155:THR:HB	3:A:1298:LEU:HD11	2.01	0.42
3:A:1314:LEU:HD12	3:A:1330:SER:HB2	2.02	0.42
3:A:2002:ILE:HA	3:A:2019:THR:HG22	2.01	0.42
3:A:2316:GLN:O	3:A:2320:ARG:HG3	2.20	0.42
3:A:3207:ARG:O	3:A:3210:VAL:HG12	2.19	0.42
3:A:3293:PHE:C	3:A:3293:PHE:HD1	2.28	0.42
3:A:4303:GLU:HB3	3:A:4307:LYS:NZ	2.35	0.42
3:B:115:LEU:HD21	3:B:129:LEU:HB2	2.02	0.42
3:B:833:PHE:CZ	3:B:858:LEU:HD22	2.55	0.42
3:B:1090:VAL:HG11	3:B:1131:VAL:HG21	2.01	0.42
3:B:1163:LEU:HD13	3:B:1313:THR:HG21	2.01	0.42
3:B:3042:LYS:N	3:B:3042:LYS:HD2	2.35	0.42
3:B:4492:LEU:HD13	3:B:4508:LEU:HD23	2.01	0.42
3:B:4566:MET:N	3:B:4566:MET:SD	2.93	0.42
1:D:4:HIS:NE2	1:D:19:GLY:O	2.48	0.42
3:A:131:LEU:HB2	3:A:142:ARG:CG	2.49	0.42
3:A:963:TYR:OH	3:A:1014:PRO:O	2.32	0.42
3:B:747:LEU:HB2	3:B:805:ASP:HA	2.02	0.42
3:B:1254:ASP:C	3:B:1254:ASP:OD1	2.63	0.42
3:B:1976:HIS:CD2	3:B:1991:VAL:HG13	2.55	0.42
3:B:2662:ASP:OD1	3:B:2662:ASP:C	2.63	0.42
3:B:2700:ALA:O	3:B:2703:ARG:HG3	2.20	0.42
3:B:3141:LEU:O	3:B:3145:VAL:HG23	2.19	0.42
3:B:4438:MET:HE3	3:B:4440:ILE:HG13	2.02	0.42
3:B:4622:TYR:OH	3:B:4670:LYS:NZ	2.53	0.42
3:A:1994:PRO:HG3	3:A:2002:ILE:HD11	2.01	0.42
3:A:2121:MET:HE1	3:A:2123:PHE:CE2	2.55	0.42
3:A:4438:MET:HE3	3:A:4440:ILE:HG13	2.02	0.42
3:B:1564:LEU:O	3:B:1568:LYS:N	2.43	0.42
3:B:2016:ALA:HB2	3:B:2025:ILE:HG12	2.02	0.42
3:B:2356:ILE:HD11	3:B:2385:PHE:CD1	2.55	0.42
3:B:4596:MET:CE	3:B:4596:MET:H	2.33	0.42
3:B:4694:TYR:HB3	3:B:4695:MET:HE2	2.02	0.42
3:A:36:LEU:HD22	3:A:84:TYR:HD2	1.84	0.41
3:A:1908:ARG:NH1	3:A:1910:GLN:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2661:VAL:HG23	3:A:2682:TYR:CE1	2.50	0.41
3:B:1083:VAL:O	3:B:1087:VAL:HG22	2.20	0.41
3:B:1296:GLY:O	3:B:1299:ILE:HG22	2.20	0.41
3:B:1899:MET:HE2	3:B:1899:MET:HB2	1.92	0.41
3:B:2355:GLN:HB2	3:B:2384:TRP:CE2	2.54	0.41
2:E:22:LYS:HD3	2:E:22:LYS:N	2.35	0.41
3:A:1600:MET:HE3	3:A:1600:MET:N	2.34	0.41
3:A:3021:LEU:O	3:A:3024:LEU:HG	2.21	0.41
3:A:3051:VAL:HA	3:A:3054:VAL:HG22	2.02	0.41
3:A:3979:ILE:HG21	3:A:4019:ILE:HG23	2.02	0.41
3:A:4286:GLU:OE1	3:A:4286:GLU:HA	2.19	0.41
1:C:61:PHE:CE2	1:C:72:VAL:HG23	2.55	0.41
3:B:1116:PRO:HD3	3:B:1172:PHE:CE1	2.55	0.41
3:B:2335:GLY:HA2	3:B:2405:ILE:O	2.20	0.41
3:B:3158:GLN:OE1	3:B:3158:GLN:N	2.44	0.41
2:F:116:LYS:HZ2	3:B:4077:ILE:H	1.68	0.41
3:A:418:LEU:HA	3:A:418:LEU:HD23	1.95	0.41
3:A:695:LYS:HE3	3:A:695:LYS:HB3	1.87	0.41
3:A:2311:VAL:HG11	1:C:64:TYR:CD1	2.55	0.41
3:A:3218:CYS:O	3:A:3220:SER:N	2.52	0.41
3:A:3259:SER:HB2	3:A:3848:GLN:HG2	2.02	0.41
3:A:4043:THR:HG22	3:A:4045:VAL:H	1.85	0.41
3:A:4637:ARG:HH21	3:A:4638:PHE:HE1	1.68	0.41
1:C:24:CYS:CB	1:C:46:HIS:HE1	2.34	0.41
3:B:124:VAL:HG12	3:B:128:HIS:HB2	2.02	0.41
3:B:1563:TRP:O	3:B:1566:ARG:HB2	2.20	0.41
3:B:2153:SER:OG	3:B:2155:ASN:O	2.37	0.41
3:B:2211:ILE:HA	3:B:2234:CYS:HA	2.02	0.41
3:B:2993:GLY:HA3	3:B:3050:GLU:HB3	2.01	0.41
1:D:22:TYR:HB3	1:D:52:MET:SD	2.60	0.41
1:D:65:TYR:OH	3:B:2311:VAL:O	2.29	0.41
3:A:263:LEU:HD12	3:A:266:PHE:CD2	2.55	0.41
3:A:1334:LEU:HD23	3:A:1334:LEU:HA	1.79	0.41
3:A:1814:MET:HA	3:A:1817:PHE:CE1	2.55	0.41
3:A:2564:ASP:OD1	3:A:2564:ASP:C	2.63	0.41
3:A:2700:ALA:O	3:A:2703:ARG:HG3	2.20	0.41
3:A:3015:GLU:HA	3:A:3018:LYS:HG2	2.02	0.41
3:A:3557:THR:O	3:A:3699:LEU:HB2	2.21	0.41
3:A:3725:PRO:HA	3:A:3827:GLU:OE2	2.20	0.41
3:A:3997:PHE:HB2	3:A:4016:CYS:HB3	2.02	0.41
3:A:4257:HIS:HE1	3:A:4261:ARG:NH2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4506:THR:O	3:A:4509:LEU:HG	2.19	0.41
3:B:108:ILE:HD13	3:B:108:ILE:HA	1.82	0.41
3:B:152:THR:O	3:B:155:MET:HB3	2.20	0.41
3:B:879:GLN:HA	3:B:907:LEU:HD21	2.02	0.41
3:B:1537:LEU:HB3	3:B:1541:MET:HE1	2.02	0.41
3:B:2540:HIS:CG	3:B:2543:LYS:HZ2	2.38	0.41
3:B:2988:LEU:HD23	3:B:2996:ALA:HB1	2.01	0.41
3:B:3167:LEU:O	3:B:3171:ILE:HG12	2.20	0.41
3:B:3690:ILE:HB	3:B:3692:TYR:CE1	2.55	0.41
1:D:20:ARG:HD3	1:D:64:TYR:OH	2.20	0.41
3:A:911:PHE:HD1	3:A:911:PHE:HA	1.76	0.41
3:A:1191:SER:H	3:A:1194:LYS:CE	2.34	0.41
3:A:1412:MET:HG3	3:A:1463:ARG:HH21	1.86	0.41
3:A:1563:TRP:O	3:A:1566:ARG:HB2	2.20	0.41
3:A:1960:ASN:HA	3:A:2007:TRP:CD1	2.55	0.41
3:A:2113:VAL:HG22	3:A:2122:LEU:HD11	2.03	0.41
3:A:2486:LEU:HD23	3:A:2486:LEU:HA	1.93	0.41
3:A:3920:ALA:O	3:A:3923:GLU:HG3	2.20	0.41
3:A:4206:LEU:HB2	3:A:4207:PRO:HD3	2.02	0.41
1:C:91:THR:O	1:C:94:GLN:HG2	2.21	0.41
3:B:318:LEU:HA	3:B:325:ARG:NH2	2.35	0.41
3:B:2139:THR:HG23	3:B:2140:THR:HG23	2.02	0.41
3:B:2486:LEU:HD23	3:B:2486:LEU:HA	1.92	0.41
3:B:3659:GLN:HG2	3:B:3664:SER:HA	2.03	0.41
3:B:3857:ARG:HH21	3:B:3862:LEU:HD23	1.84	0.41
3:B:4145:ALA:O	3:B:4149:VAL:HG22	2.21	0.41
3:B:4167:THR:HA	3:B:4170:LEU:HD23	2.02	0.41
3:B:4330:PHE:HA	3:B:4333:GLU:HG3	2.01	0.41
3:A:119:ASP:OD1	3:A:120:GLU:N	2.49	0.41
3:A:1064:LYS:HZ3	3:A:1066:GLU:HB2	1.86	0.41
3:A:1178:LEU:HD23	3:A:1178:LEU:HA	1.84	0.41
3:A:1249:ASN:OD1	3:A:1250:ALA:N	2.50	0.41
3:A:1362:LEU:HD23	3:A:1362:LEU:HA	1.89	0.41
3:A:1690:VAL:HG12	3:A:1716:CYS:HB2	2.01	0.41
3:A:2483:LEU:HB2	3:A:2524:GLN:HE21	1.86	0.41
3:A:2662:ASP:OD1	3:A:2662:ASP:C	2.63	0.41
3:A:4148:ILE:HD13	3:A:4148:ILE:HA	1.89	0.41
3:A:4566:MET:N	3:A:4566:MET:SD	2.93	0.41
1:C:26:ILE:HG12	1:C:108:VAL:HG12	2.02	0.41
3:B:1960:ASN:HA	3:B:2007:TRP:CD1	2.56	0.41
3:B:3000:MET:H	3:B:3000:MET:HG2	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3612:TRP:CH2	3:B:3641:MET:HB2	2.55	0.41
3:B:4043:THR:HG22	3:B:4045:VAL:H	1.86	0.41
1:D:25:LEU:HD21	1:D:53:GLN:HB2	2.02	0.41
3:A:141:SER:OG	3:A:142:ARG:NH1	2.54	0.41
3:A:655:LEU:HD12	3:A:655:LEU:HA	1.88	0.41
3:A:1006:LEU:HA	3:A:1009:ILE:HG22	2.02	0.41
3:A:2181:GLN:HE22	3:A:2188:LEU:HD12	1.86	0.41
3:A:2480:VAL:HA	3:A:2524:GLN:HE22	1.84	0.41
3:A:2699:GLN:HA	3:A:2702:ILE:HG12	2.02	0.41
3:A:2982:LEU:O	3:A:2985:LEU:HG	2.20	0.41
3:A:4669:ILE:HG21	3:A:4679:LYS:HG3	2.02	0.41
3:B:105:LYS:HE2	3:B:250:LEU:HD21	2.03	0.41
3:B:125:SER:O	3:B:129:LEU:HG	2.21	0.41
3:B:957:PHE:HZ	3:B:1014:PRO:HG2	1.85	0.41
3:B:1468:LEU:O	3:B:1472:THR:OG1	2.23	0.41
3:B:1846:HIS:NE2	3:B:2144:LEU:HD23	2.35	0.41
3:B:2517:ALA:HB3	3:B:2522:GLN:OE1	2.20	0.41
3:B:2999:TYR:O	3:B:3003:ILE:HG13	2.21	0.41
3:B:3574:VAL:HG22	3:B:3715:LEU:HD23	2.01	0.41
3:B:3954:ALA:HA	3:B:3964:LEU:HD22	2.03	0.41
3:B:4497:ASP:OD1	3:B:4500:GLN:N	2.35	0.41
2:F:65:ASP:OD1	2:F:65:ASP:C	2.64	0.41
3:A:53:VAL:HG13	3:A:103:ALA:HB2	2.03	0.41
3:A:1596:THR:O	3:A:1599:ILE:HG12	2.21	0.41
3:A:2219:HIS:ND1	3:A:2220:THR:O	2.51	0.41
3:A:2499:GLU:O	3:A:2502:LYS:NZ	2.40	0.41
3:A:3501:ASN:HB3	3:A:3912:TYR:CE2	2.56	0.41
3:B:1280:LEU:HD23	3:B:1280:LEU:HA	1.81	0.41
3:B:3057:ARG:O	3:B:3061:VAL:HG23	2.20	0.41
3:B:3218:CYS:O	3:B:3220:SER:N	2.53	0.41
3:B:4637:ARG:HH21	3:B:4638:PHE:HE1	1.67	0.41
1:D:301:MET:HE2	1:D:301:MET:HB3	1.95	0.41
3:A:56:VAL:HG12	3:A:106:VAL:HG11	2.03	0.41
3:A:735:LEU:HB3	3:A:737:VAL:HG22	2.03	0.41
3:A:1023:LEU:HD11	3:A:1041:TRP:HZ3	1.86	0.41
3:A:1083:VAL:O	3:A:1087:VAL:HG22	2.21	0.41
3:A:1090:VAL:HG11	3:A:1131:VAL:HG21	2.03	0.41
3:A:1214:LEU:O	3:A:1217:THR:OG1	2.39	0.41
3:A:1417:GLU:HA	3:A:1470:ARG:NH1	2.36	0.41
3:A:1521:MET:H	3:A:1521:MET:CE	2.34	0.41
3:A:1534:PHE:HA	3:A:1537:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2517:ALA:HB3	3:A:2522:GLN:OE1	2.21	0.41
3:A:3536:ASN:HB3	3:A:3815:SER:OG	2.20	0.41
3:A:3818:ILE:HD13	3:A:3818:ILE:HA	1.89	0.41
3:A:3985:CYS:HB3	3:A:3988:LEU:HD12	2.02	0.41
3:A:4352:THR:HG22	3:A:4354:GLU:HG3	2.03	0.41
3:A:4694:TYR:HB3	3:A:4695:MET:CE	2.51	0.41
3:B:833:PHE:HZ	3:B:858:LEU:O	2.04	0.41
3:B:1005:ILE:O	3:B:1009:ILE:HG22	2.20	0.41
3:B:1822:ILE:HG22	3:B:2475:LEU:HB3	2.02	0.41
3:B:1908:ARG:NH1	3:B:1910:GLN:OE1	2.54	0.41
3:B:2212:GLN:H	3:B:2234:CYS:HA	1.85	0.41
3:B:3997:PHE:HB2	3:B:4016:CYS:HB3	2.02	0.41
3:B:4596:MET:HA	3:B:4599:ASP:OD1	2.21	0.41
3:B:4598:LEU:HD23	3:B:4601:ILE:HD12	2.02	0.41
3:B:4631:MET:H	3:B:4631:MET:HG2	1.67	0.41
3:A:302:LEU:HD12	3:A:377:ILE:HD11	2.02	0.41
3:A:1387:GLN:HE22	3:A:1397:MET:CG	2.34	0.41
3:A:1524:GLU:O	3:A:1528:ASN:ND2	2.45	0.41
3:A:1859:MET:HB3	3:A:2200:GLN:HE22	1.86	0.41
3:A:1899:MET:SD	3:A:2213:ASP:HB2	2.61	0.41
3:A:2061:ILE:HG23	3:A:2073:GLN:HB3	2.03	0.41
3:A:4228:LEU:HD23	3:A:4228:LEU:O	2.21	0.41
3:B:1809:PRO:O	3:B:1812:LEU:HD12	2.21	0.41
3:B:1961:PRO:HB2	3:B:2641:PHE:CZ	2.55	0.41
3:B:2653:ILE:H	3:B:2653:ILE:HG12	1.65	0.41
3:B:3106:LEU:HD13	3:B:3193:PHE:CE1	2.56	0.41
1:D:79:THR:O	1:D:111:PRO:HG3	2.22	0.40
2:F:68:GLU:O	2:F:72:MET:HG3	2.20	0.40
3:A:1092:GLU:O	3:A:1096:ARG:HG3	2.21	0.40
3:A:1846:HIS:NE2	3:A:2144:LEU:HD23	2.36	0.40
3:A:3586:MET:SD	3:A:3648:TYR:HB3	2.61	0.40
3:B:1426:ARG:HD2	3:B:1426:ARG:HA	1.80	0.40
3:B:1514:LEU:HD23	3:B:1544:LEU:HD11	2.03	0.40
3:B:3090:LEU:HD13	3:B:3090:LEU:HA	1.97	0.40
3:B:3551:LYS:HE2	3:B:3554:THR:HB	2.03	0.40
3:B:4671:ASN:OD1	3:B:4676:HIS:NE2	2.54	0.40
3:A:152:THR:O	3:A:155:MET:HB3	2.21	0.40
3:A:1020:ILE:HD13	3:A:1041:TRP:CH2	2.56	0.40
3:A:1270:LEU:HD23	3:A:1270:LEU:HA	1.87	0.40
3:A:2067:ALA:O	3:A:2105:GLN:HA	2.22	0.40
3:A:2666:GLY:O	3:A:2669:THR:OG1	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2702:ILE:HA	3:A:3005:MET:SD	2.61	0.40
3:A:3233:LEU:HB3	3:A:3293:PHE:CD2	2.56	0.40
3:A:4055:GLN:HG2	3:A:4119:LEU:HD23	2.03	0.40
1:C:25:LEU:HD21	1:C:53:GLN:HB2	2.03	0.40
1:C:301:MET:HE2	1:C:301:MET:HB3	1.95	0.40
3:B:699:LYS:HA	3:B:699:LYS:HD3	1.74	0.40
3:B:742:GLU:OE1	3:B:742:GLU:N	2.40	0.40
3:B:1020:ILE:HD13	3:B:1041:TRP:CH2	2.56	0.40
3:B:1191:SER:H	3:B:1194:LYS:NZ	2.19	0.40
3:B:1378:GLU:OE1	3:B:1378:GLU:HA	2.21	0.40
3:B:1854:MET:HG3	3:B:2199:ILE:HD11	2.02	0.40
3:B:2151:ILE:O	3:B:2161:SER:OG	2.31	0.40
3:B:2342:ASN:ND2	3:B:2347:MET:SD	2.94	0.40
3:B:2550:LYS:HD3	3:B:2551:ALA:N	2.36	0.40
3:B:3053:LEU:O	3:B:3056:MET:HG2	2.21	0.40
3:B:3220:SER:OG	3:B:3222:GLU:OE2	2.40	0.40
3:B:3683:GLN:HB3	3:B:3690:ILE:HG12	2.02	0.40
3:B:4206:LEU:HB2	3:B:4207:PRO:HD3	2.02	0.40
2:E:94:ASP:OD1	2:E:99:GLY:N	2.42	0.40
2:F:94:ASP:OD1	2:F:99:GLY:N	2.40	0.40
2:F:96:ASP:OD1	2:F:96:ASP:N	2.54	0.40
2:F:141:GLU:O	2:F:144:GLN:HG3	2.21	0.40
3:A:1596:THR:HA	3:A:1599:ILE:HG12	2.04	0.40
3:A:1692:THR:OG1	3:A:2293:GLU:OE2	2.24	0.40
3:A:3167:LEU:N	3:A:3168:PRO:HD2	2.37	0.40
3:A:4373:SER:HB3	3:A:4376:GLU:HG3	2.04	0.40
3:B:531:MET:HE3	3:B:531:MET:HB3	1.95	0.40
3:B:807:ASN:OD1	3:B:807:ASN:N	2.54	0.40
3:B:1135:LEU:HD23	3:B:1135:LEU:HA	1.86	0.40
3:B:1417:GLU:HA	3:B:1470:ARG:NH1	2.37	0.40
3:B:1551:ALA:O	3:B:1554:LEU:HB2	2.21	0.40
3:B:2503:ASN:O	3:B:2506:GLN:HG2	2.22	0.40
3:B:2566:ASP:HB2	3:B:2569:VAL:HG12	2.04	0.40
3:B:2700:ALA:HA	3:B:2703:ARG:HG2	2.03	0.40
3:B:3441:LYS:O	3:B:3445:GLU:HG3	2.21	0.40
1:D:85:LYS:HD2	1:D:85:LYS:HA	1.92	0.40
1:D:321:GLN:HG2	3:B:4152:LEU:HD23	2.03	0.40
3:A:1064:LYS:HZ2	3:A:1066:GLU:HB2	1.87	0.40
3:A:1195:LEU:HD23	3:A:1195:LEU:HA	1.83	0.40
3:A:1497:THR:HA	3:A:1500:VAL:HG22	2.02	0.40
3:A:1976:HIS:CD2	3:A:1991:VAL:HG13	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2131:SER:HB3	3:A:2149:ILE:HD12	2.03	0.40
3:A:3090:LEU:HD13	3:A:3090:LEU:HA	1.93	0.40
3:A:3659:GLN:HG2	3:A:3664:SER:HA	2.03	0.40
3:A:3758:PRO:O	3:A:3761:GLU:HG2	2.20	0.40
3:A:3954:ALA:HA	3:A:3964:LEU:HD22	2.03	0.40
1:C:88:TYR:HD1	1:C:92:SER:HB3	1.85	0.40
3:B:195:ASN:OD1	3:B:195:ASN:C	2.64	0.40
3:B:1471:MET:N	3:B:1471:MET:SD	2.94	0.40
3:B:2018:VAL:HG21	3:B:2049:VAL:HB	2.04	0.40
3:B:4019:ILE:HD13	3:B:4019:ILE:HA	1.91	0.40
3:B:4738:VAL:O	3:B:4742:THR:OG1	2.34	0.40
3:A:531:MET:HE3	3:A:531:MET:HB3	1.92	0.40
3:A:791:LYS:HD3	3:A:836:ILE:HD12	2.04	0.40
3:A:2121:MET:SD	3:A:2133:ALA:HB1	2.62	0.40
3:A:3170:GLN:O	3:A:3173:LYS:HG3	2.22	0.40
3:A:3907:ARG:NH1	3:A:3946:LEU:HD21	2.36	0.40
3:A:4591:LYS:HB2	3:A:4630:LYS:HD2	2.04	0.40
3:A:4593:GLN:H	3:A:4593:GLN:CD	2.21	0.40
3:B:1191:SER:H	3:B:1194:LYS:CE	2.35	0.40
3:B:3170:GLN:O	3:B:3173:LYS:HG3	2.22	0.40
3:B:3818:ILE:HD13	3:B:3818:ILE:HA	1.89	0.40
3:B:4373:SER:HB3	3:B:4376:GLU:HG3	2.03	0.40
3:B:4616:LEU:HD12	3:B:4617:LEU:N	2.36	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	C	177/331 (54%)	173 (98%)	4 (2%)	0	100	100
1	D	177/331 (54%)	174 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	147/158 (93%)	144 (98%)	3 (2%)	0	100	100
2	F	147/158 (93%)	144 (98%)	3 (2%)	0	100	100
3	A	3999/4781 (84%)	3856 (96%)	142 (4%)	1 (0%)	100	100
3	B	3999/4781 (84%)	3862 (97%)	136 (3%)	1 (0%)	100	100
All	All	8646/10540 (82%)	8353 (97%)	291 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	923	SER
3	B	923	SER

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	C	160/287 (56%)	160 (100%)	0	100	100
1	D	160/287 (56%)	156 (98%)	4 (2%)	42	69
2	E	127/136 (93%)	124 (98%)	3 (2%)	43	69
2	F	127/136 (93%)	123 (97%)	4 (3%)	35	64
3	A	3569/4176 (86%)	3505 (98%)	64 (2%)	51	73
3	B	3569/4176 (86%)	3500 (98%)	69 (2%)	50	73
All	All	7712/9198 (84%)	7568 (98%)	144 (2%)	49	73

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	27	CYS
1	D	82	TYR
1	D	83	CYS
1	D	110	CYS
2	E	27	THR

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Mol	Chain	Res	Type
2	E	48	GLU
2	E	86	ILE
2	F	27	THR
2	F	86	ILE
2	F	92	VAL
2	F	109	VAL
3	A	127	LYS
3	A	194	LEU
3	A	277	VAL
3	A	278	LEU
3	A	302	LEU
3	A	315	LEU
3	A	334	LEU
3	A	341	VAL
3	A	368	ASP
3	A	382	LEU
3	A	422	LEU
3	A	481	ILE
3	A	512	MET
3	A	695	LYS
3	A	714	ASN
3	A	722	LEU
3	A	845	ASP
3	A	916	GLU
3	A	951	VAL
3	A	1051	VAL
3	A	1052	ASN
3	A	1073	GLU
3	A	1159	LEU
3	A	1288	LEU
3	A	1384	LEU
3	A	1435	PHE
3	A	1453	LEU
3	A	1528	ASN
3	A	1543	THR
3	A	1899	MET
3	A	1977	VAL
3	A	1990	LEU
3	A	2063	ILE
3	A	2143	VAL
3	A	2515	LEU
3	A	2672	LEU

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Mol	Chain	Res	Type
3	A	2972	MET
3	A	3000	MET
3	A	3005	MET
3	A	3163	MET
3	A	3166	ARG
3	A	3214	LEU
3	A	3224	TYR
3	A	3233	LEU
3	A	3244	LEU
3	A	3267	ASP
3	A	3271	SER
3	A	3311	VAL
3	A	3483	GLU
3	A	3504	LEU
3	A	3540	VAL
3	A	3550	ILE
3	A	3682	TYR
3	A	3792	VAL
3	A	3826	LYS
3	A	3830	GLU
3	A	3887	LEU
3	A	3925	VAL
3	A	4109	LEU
3	A	4170	LEU
3	A	4229	SER
3	A	4296	GLU
3	A	4613	LEU
3	A	4616	LEU
3	B	80	LEU
3	B	194	LEU
3	B	277	VAL
3	B	278	LEU
3	B	302	LEU
3	B	315	LEU
3	B	334	LEU
3	B	341	VAL
3	B	368	ASP
3	B	382	LEU
3	B	422	LEU
3	B	481	ILE
3	B	714	ASN
3	B	722	LEU

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Mol	Chain	Res	Type
3	B	845	ASP
3	B	916	GLU
3	B	951	VAL
3	B	970	LEU
3	B	1051	VAL
3	B	1052	ASN
3	B	1092	GLU
3	B	1131	VAL
3	B	1159	LEU
3	B	1167	ASP
3	B	1288	LEU
3	B	1299	ILE
3	B	1410	ILE
3	B	1434	LEU
3	B	1435	PHE
3	B	1453	LEU
3	B	1528	ASN
3	B	1543	THR
3	B	1899	MET
3	B	1977	VAL
3	B	1990	LEU
3	B	2063	ILE
3	B	2143	VAL
3	B	2672	LEU
3	B	3000	MET
3	B	3163	MET
3	B	3166	ARG
3	B	3201	GLN
3	B	3214	LEU
3	B	3224	TYR
3	B	3233	LEU
3	B	3242	LYS
3	B	3244	LEU
3	B	3249	ILE
3	B	3267	ASP
3	B	3311	VAL
3	B	3405	LYS
3	B	3483	GLU
3	B	3504	LEU
3	B	3540	VAL
3	B	3550	ILE
3	B	3575	THR

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Mol	Chain	Res	Type
3	B	3682	TYR
3	B	3720	CYS
3	B	3792	VAL
3	B	3826	LYS
3	B	3830	GLU
3	B	3832	ASP
3	B	3887	LEU
3	B	3925	VAL
3	B	4131	GLN
3	B	4170	LEU
3	B	4186	LEU
3	B	4228	LEU
3	B	4296	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	122	ASN
1	D	131	HIS
2	E	9	GLN
2	F	9	GLN
2	F	42	GLN
3	A	128	HIS
3	A	196	GLN
3	A	202	ASN
3	A	237	ASN
3	A	404	GLN
3	A	479	HIS
3	A	882	HIS
3	A	1179	GLN
3	A	1266	GLN
3	A	1387	GLN
3	A	1409	GLN
3	A	1488	ASN
3	A	1876	ASN
3	A	1976	HIS
3	A	2166	GLN
3	A	2245	ASN
3	A	2248	ASN
3	A	2310	GLN
3	A	2319	HIS
3	A	2987	GLN

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Mol	Chain	Res	Type
3	A	3201	GLN
3	A	3231	HIS
3	A	3306	GLN
3	A	3400	ASN
3	A	3500	GLN
3	A	3506	ASN
3	A	3591	ASN
3	A	3927	GLN
3	A	4651	HIS
1	C	46	HIS
1	C	122	ASN
3	B	202	ASN
3	B	479	HIS
3	B	881	GLN
3	B	1179	GLN
3	B	1266	GLN
3	B	1488	ASN
3	B	1823	GLN
3	B	1876	ASN
3	B	2166	GLN
3	B	2245	ASN
3	B	2248	ASN
3	B	2319	HIS
3	B	2501	ASN
3	B	3113	GLN
3	B	3306	GLN
3	B	3400	ASN
3	B	3506	ASN
3	B	3569	HIS
3	B	3759	GLN
3	B	3762	ASN
3	B	3927	GLN
3	B	4602	ASN
3	B	4690	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 20 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-52490. 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](#)

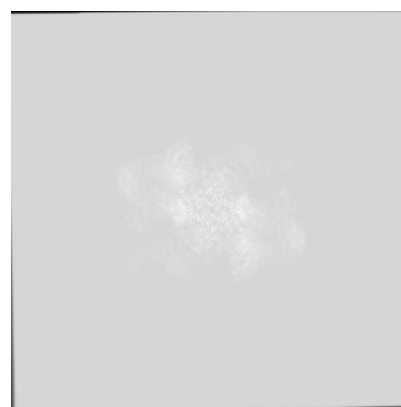
6.1.1 Primary map



X



Y

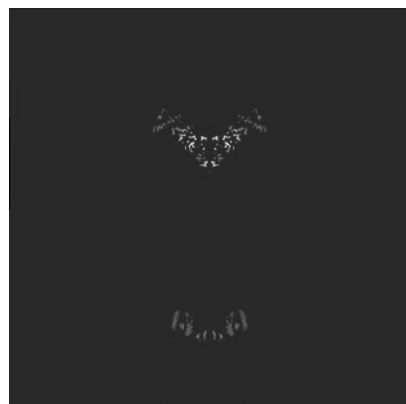


Z

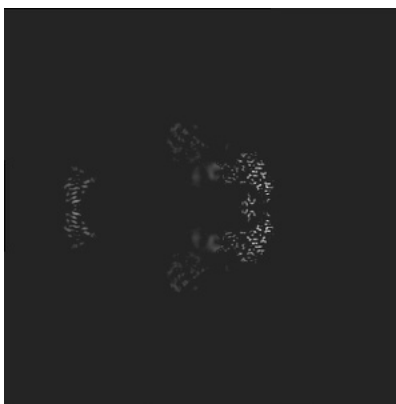
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

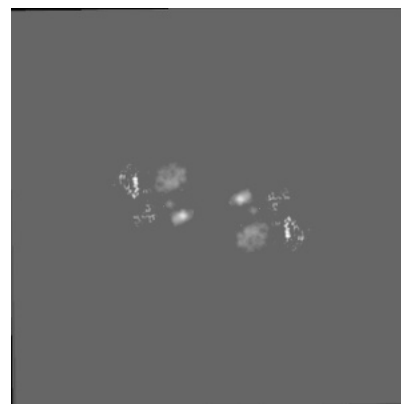
6.2.1 Primary map



X Index: 192



Y Index: 192

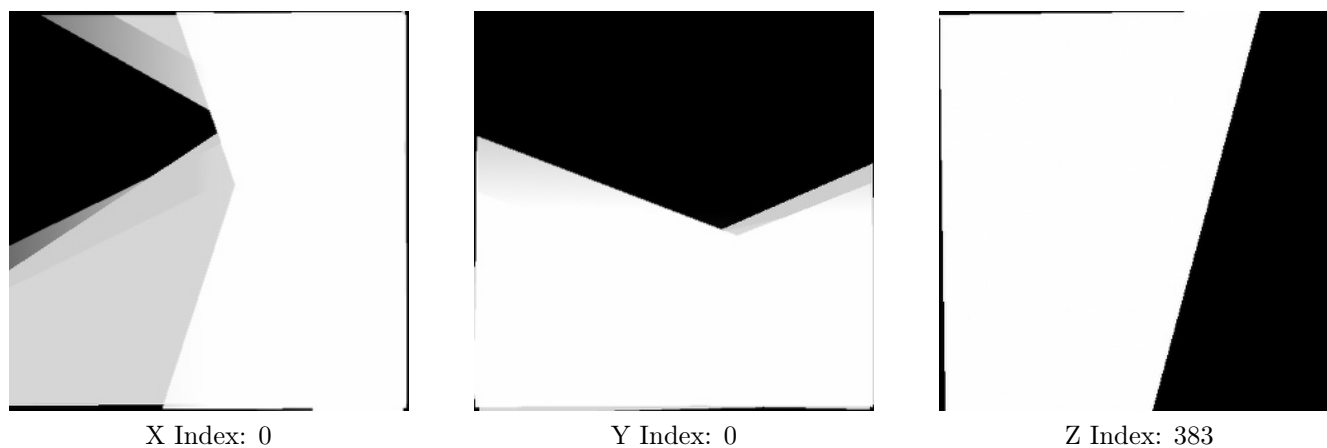


Z Index: 192

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

6.3 Largest variance slices [i](#)

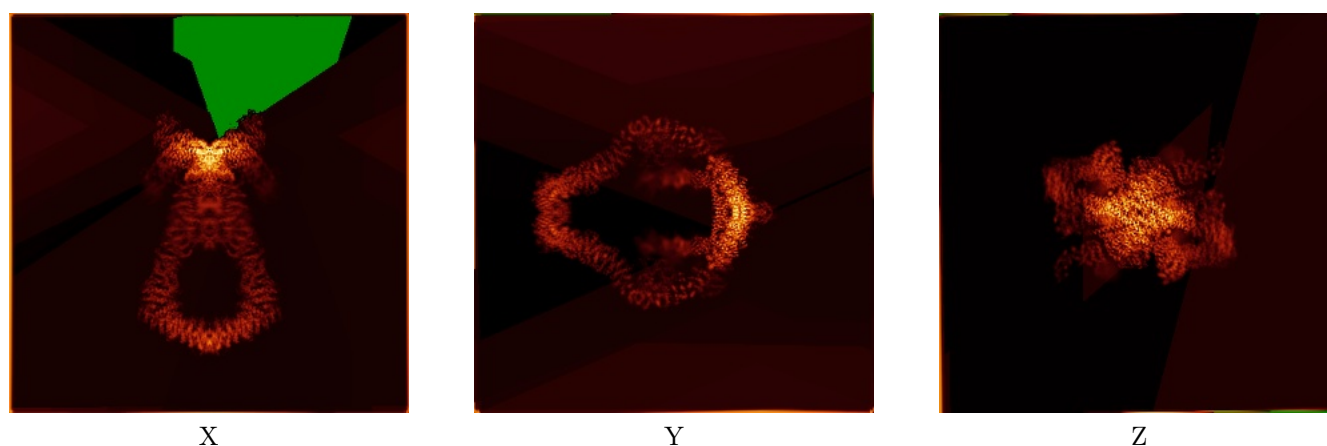
6.3.1 Primary map



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



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0089. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

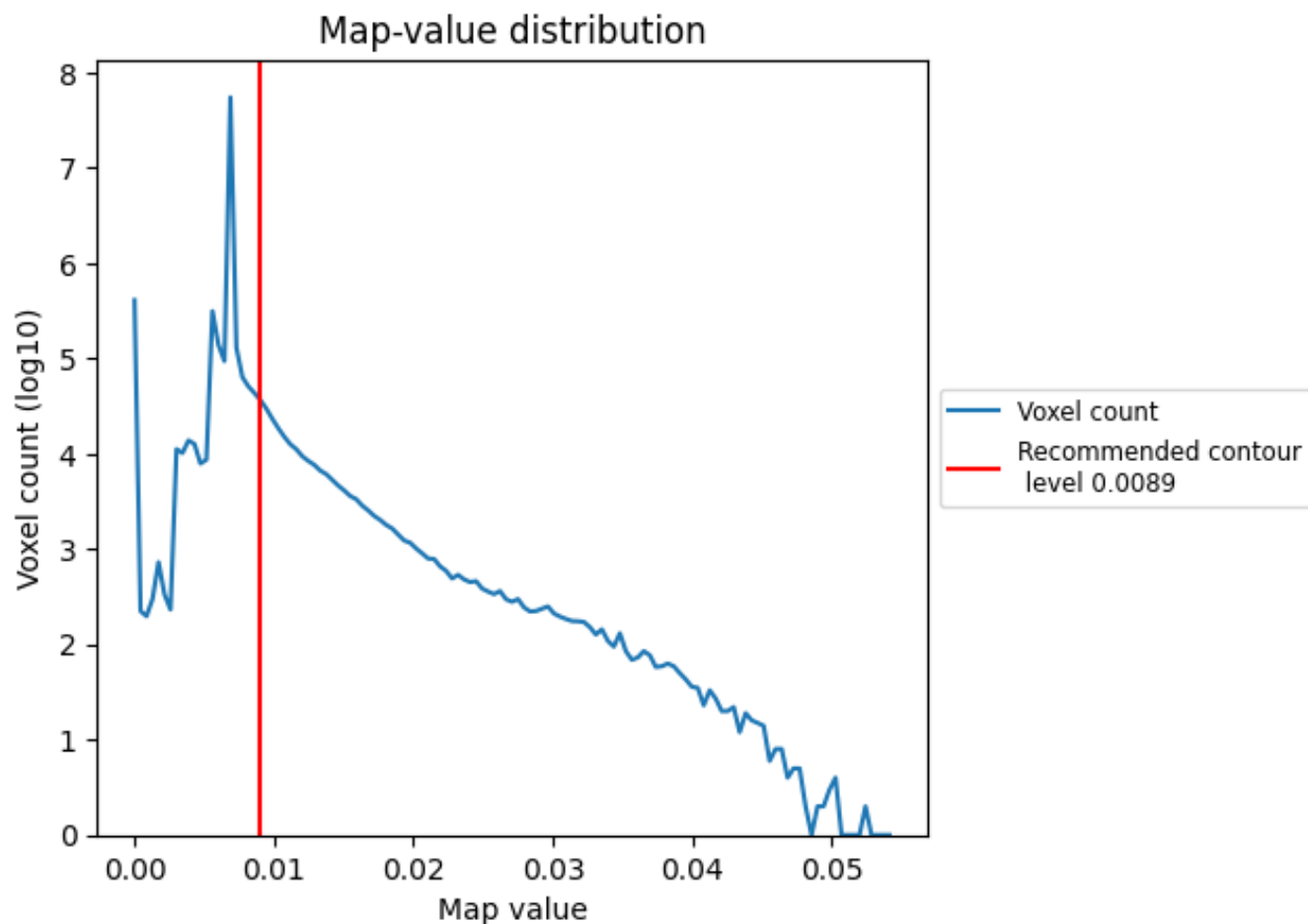
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

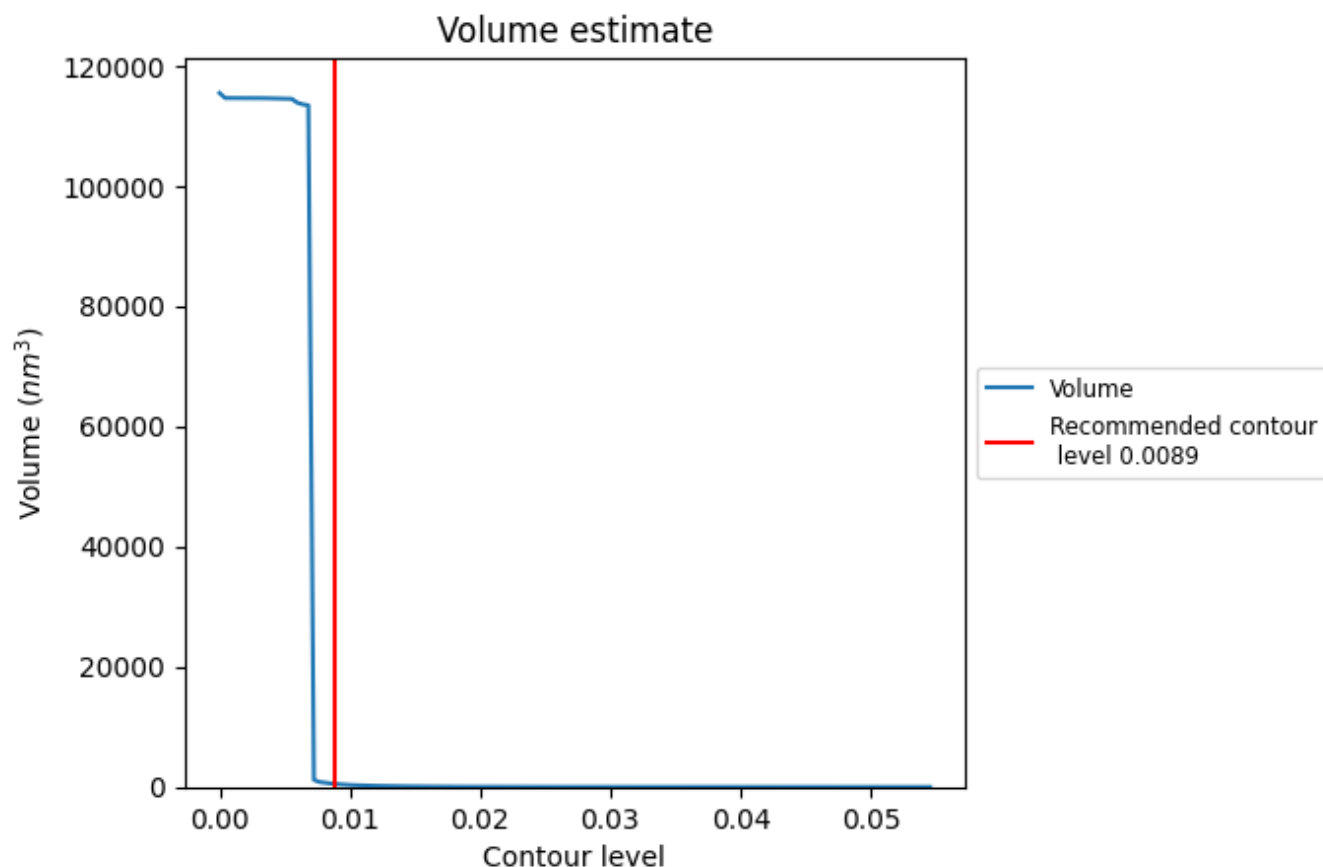
This section contains the results of statistical analysis of the map.

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.

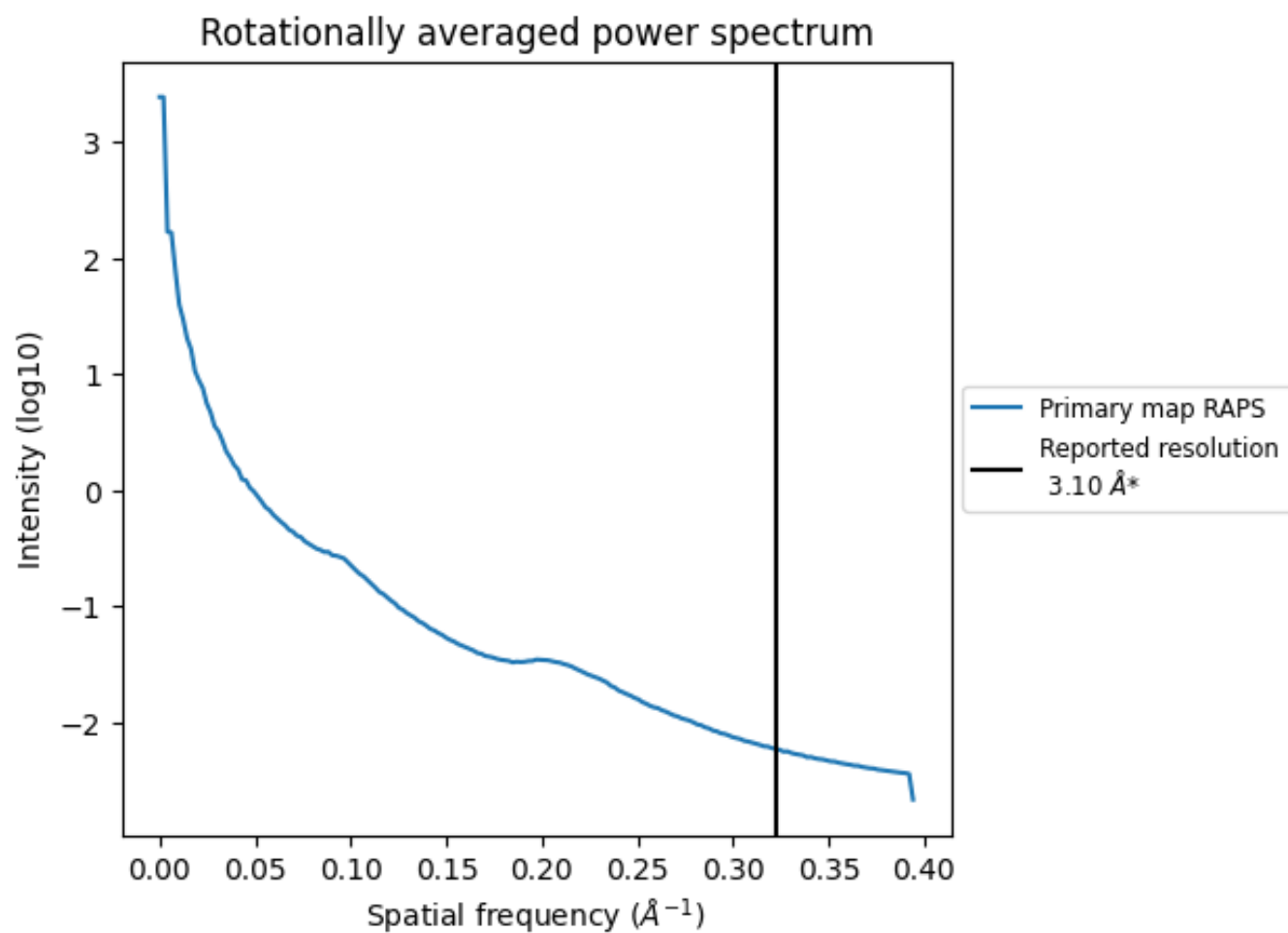
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 507 nm³; this corresponds to an approximate mass of 458 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 0.323 Å⁻¹

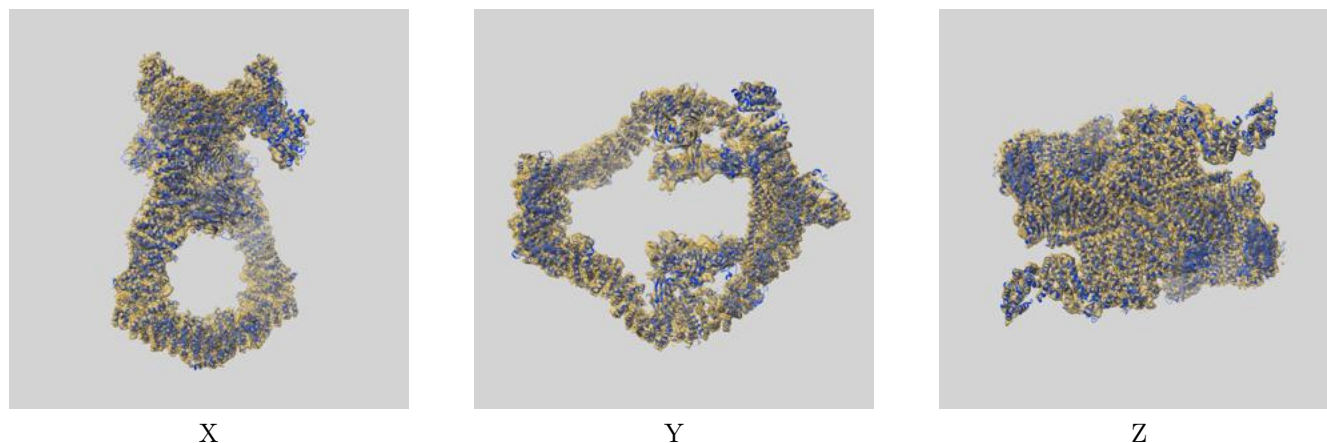
8 Fourier-Shell correlation

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-52490 and PDB model 9HXW. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



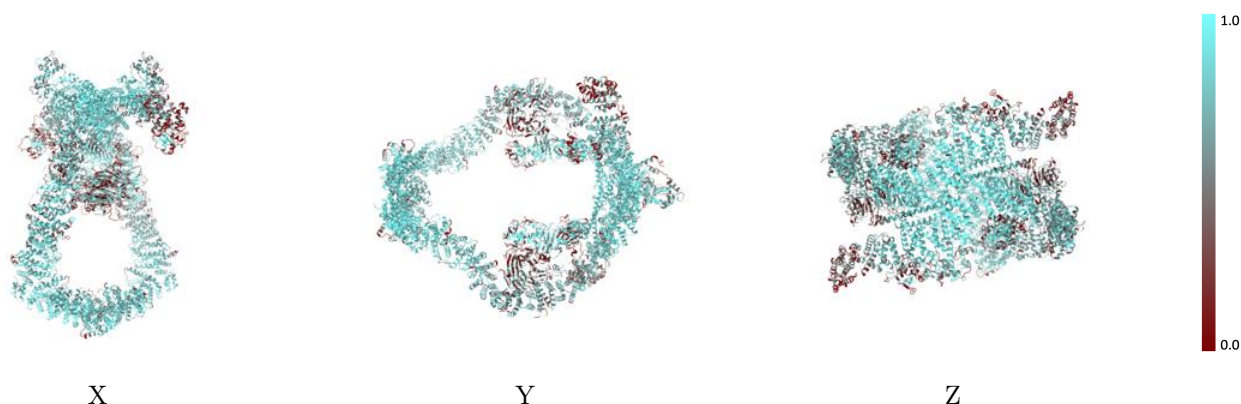
The images above show the 3D surface view of the map at the recommended contour level 0.0089 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



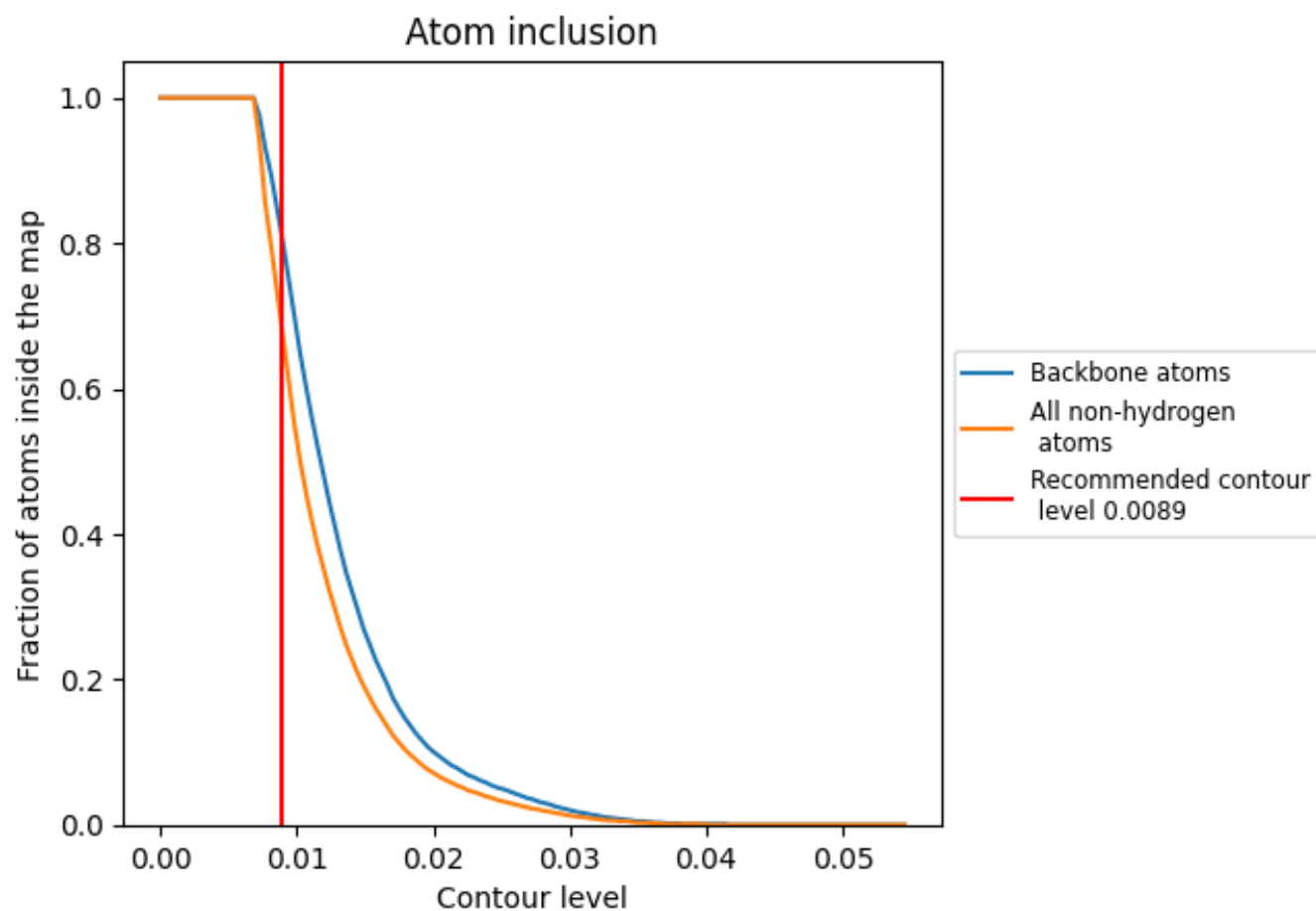
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0089).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 68% 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 (0.0089) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.6810</div>	<div><div></div>0.2760</div>
A	<div><div></div>0.6890</div>	<div><div></div>0.2820</div>
B	<div><div></div>0.6910</div>	<div><div></div>0.2820</div>
C	<div><div></div>0.6150</div>	<div><div></div>0.1550</div>
D	<div><div></div>0.5610</div>	<div><div></div>0.1460</div>
E	<div><div></div>0.5590</div>	<div><div></div>0.2670</div>
F	<div><div></div>0.5710</div>	<div><div></div>0.2760</div>

1.0

0.0

<0.0