



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 03:42 AM UTC

PDB ID : 7Z87 / pdb_00007z87
EMDB ID : EMD-14545
Title : DNA-PK in the active state
Authors : Liang, S.; Blundell, T.L.
Deposited on : 2022-03-16
Resolution : 2.91 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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

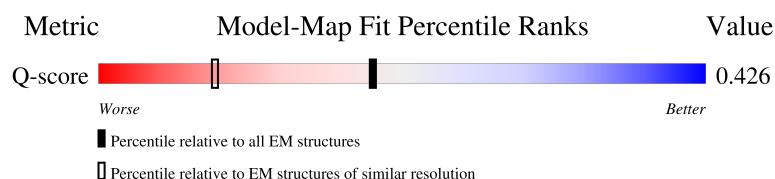
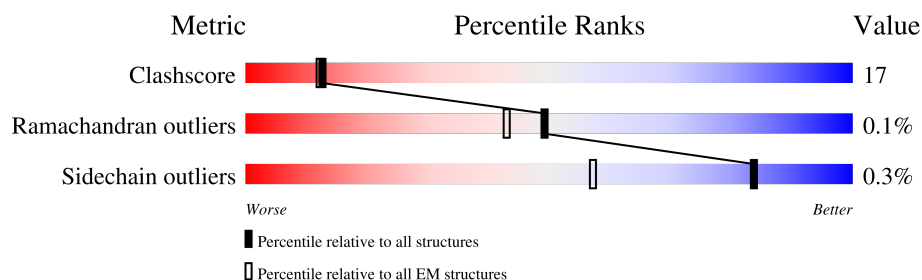
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.91 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	12972 (2.41 - 3.41)

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

Mol	Chain	Length	Quality of chain
1	A	4128	8% 60% 29% 11%
2	B	609	6% 49% 31% 20%
3	C	732	32% 49% 41% 10%
4	D	26	42% 58%

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Mol	Chain	Length	Quality of chain
5	E	26	 54% 46%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 39708 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3689	Total	C	N	O	S	1	0
			29194	18729	4950	5323	192		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	490	Total	C	N	O	S	2	0
			3953	2533	669	733	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	661	Total	C	N	O	S	0	0
			5267	3370	879	993	25		

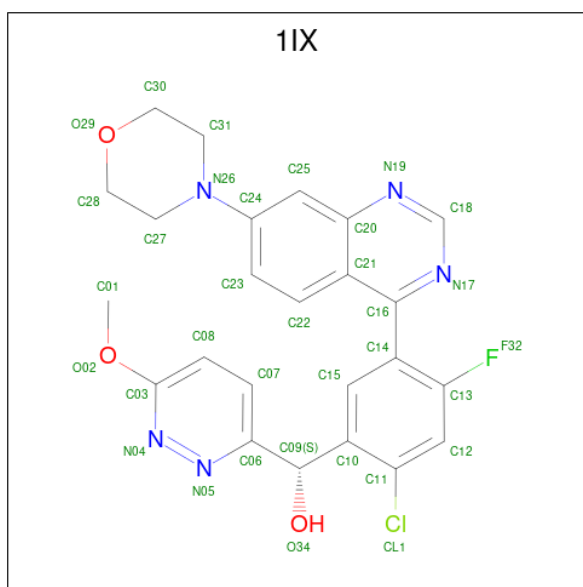
- Molecule 4 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	26	Total	C	N	O	P	0	0
			526	250	92	158	26		

- Molecule 5 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	26	Total	C	N	O	P	0	0
			540	254	106	154	26		

- Molecule 6 is ({S})-[2-chloranyl-4-fluoranyl-5-(7-morpholin-4-ylquinazolin-4-yl)phenyl]-(6-methoxypyridazin-3-yl)methanol (CCD ID: 1IX) (formula: C₂₄H₂₁ClFN₅O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	Cl	F	N	O	0
			34	24	1	1	5	3	

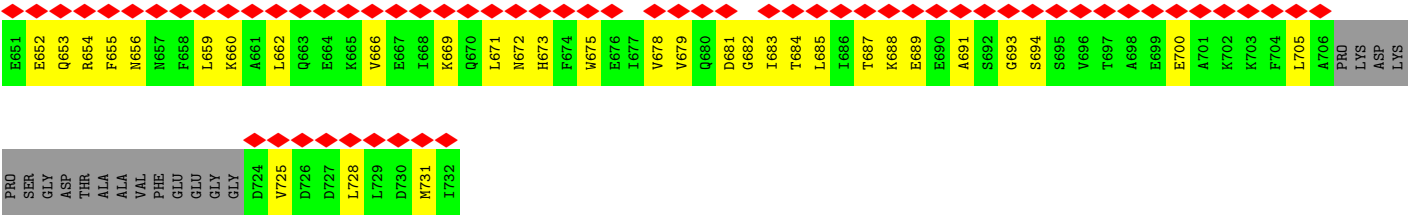
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	154	Total	O	0
			154	154	
7	B	25	Total	O	0
			25	25	
7	C	9	Total	O	0
			9	9	
7	D	4	Total	O	0
			4	4	
7	E	2	Total	O	0
			2	2	

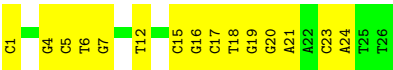
TYR	LEU	ALA	ASP	S2034	Q2050	SER	TYR	TYR	SER	TYR	TYR	SER	SER	GLN	ASP	PRO	ARG	PRO	ALA	ALA	THR	GLY	ARG	PHE	ARG	ARG	ARG	GLU	VAL	PRO	ARG	ASP	THR	PRO	ARG	VAL	LYS	LYS	TYR	ASP	VAL	LEU	LEU	E2082	L2083	M2085	D2086	E2087	N2089	R2090	H2091	C2092	C2093	N2094	A2095	P2096	L2097	L2100	M2104	S2107	R1883	L1884	F1885	K1886	D1887	L1888	V1889	H1890	A1891	K1892	E1893	S1894	K1895	I1896	N1897	K1898	V1899	F1900	S1903	C1904	I1905	T1906	E1907	G1908	T1912	K1913	T1914	L1915	I1916	K1917	L1918	C1919	Y1920	T1924	E1925	N1926	G1929	E1930	N1931	Q1932	L1933	R1937	A1944	Y1945	N1946	C1947	Y1951	V1955	F1956	K1960	R1806	K1807	D1808	L1809	P1810	R1811	L1812	Q1817	V1820	H1821	R1822	S1823	L1824	L1825	L1828	S1832	L1833	D1834	A1835	L1836	R1837	F1840	V1844	V1850	L1851	K1852	S1853	R1854	F1855	T1856	K1857	L1858	N1859	T1862	F1863	D1864	T1865	T1868	K1869	K1870	Y1873	Y1874	K1875	L1876	L1877	D1878	V1879	M1880	Y1881	S1882	E1708	R1711	R1712	L1717	A1720	H1721	F1722	P1723	R1727	E1728	F1729	P1730	P1731	P1734	R1735	F1736	N1737	N1738	K1744	L1750	L1754	M1757	L1758	V1773	M1774	E1775	E1776	L1777	F1778	S1781	F1782	T1785	R1788	G1789	S1790	T1793	Q1794	L1797	L1798	E1799	S1800	V1801	Y1802	F1803	R1806	Q1817	V1820	D1821	R1822	S1823	L1824	L1825	L1828	S1832	L1833	D1834	A1835	L1836	R1837	F1840	V1844	V1850	L1851	K1852	S1853	R1854	F1855	T1856	K1857	L1858	N1859	T1862	F1863	D1864	T1865	T1868	K1869	K1870	Y1873	Y1874	K1875	L1876	L1877	D1878	V1879	M1880	Y1881	S1882	E1498	C1499	L1514	L1515	C1525	L1538	S1539	T1540	A1541	SER	LEU	GLY	SER	GLN	SER	V1550	I1551	H1552	F1553	S1554	H1555	G1556	F1563	S1564	E1565	M1568	L1571	L1572	N1574	L1575	D1576	L1577	A1578	V1579	L1580	L1582	M1583	Q1584	M1592	V1593	S1594	A1595	V1596	L1597	N1598	L1601	ASP	G1494	ASP	V1373	Q1374	T1375	A1380	S1381	I1386	M1392	L1402	M1403	S1409	P1410	Y1411	I1414	H1418	L1419	R1420	E1421	K1422	I1423	T1424	A1425	Q1426	S1427	I1428	E1429	E1430	Y1434	G1438	D1444	R1445	S1446	R1447	C1455	L1458	M1466	I1467	L1468	S1472	T1473	L1483	V1487	G1494	ASP	A1302	M1303	HIS	ASP	I1E	I1E	ALA	ALA	GLU	LYS	CYS	PHE	GLY	THR	GLY	ALA	GLN	ASN	ARG	THR	S1323	E1328	R1329	Y1330	S1333	T1336	V1337	V1338	V1339	R1340	I1341	M1342	E1343	F1344	T1345	T1346	T1347	L1348	T1351	S1352	P1353	W1356	K1357	L1358	L1359	K1360	K1361	D1362	H1367	L1368	M1369	R1370	L1220	I1221	N1222	T1223	F1224	E1225	G1230	GLN	PRO	SER	GLY	ILE	LEU	ALA	GLN	PRO	L1241	L1242	Y1243	L1244	P1247	F1248	S1249	A1252	L1257	L1261	A1262	A1263	E1265	C1266	Y1267	M1268	R1274	T1275	V1276	L1279	L1282	G1283	T1284	E1285	A1286	Q1287	S1288	L1291	F1297	L1298	I1301	K1150	R1151	L1152	R1153	P1154	G1155	P1159	S1162	L1163	C1164	L1165	L1166	D1167	W1171	L1172	L1173	A1174	H1175	R1178	P1179	Q1180	H1184	R1185	L1186	S1187	I1188	E1189	L1190	F1191	Y1192	K1193	F1194	V1195	P1196	L1197	G1200	M1201	R1202	S1203	P1204	M1205	L1206	W1207	L1208	K1209	D1210	V1211	L1212	K1213	V1217	S1218	F1219	L1014	L1017	V1018	D1019	P1020	V1021	L1025	R1026	D1027	F1028	E1035	F1036	P1046	Q1047	Q1048	V1054	K1057	K1061	R1062	L1066	A1067	H1069	P1070	N1071	K1074	R1075	F1082	I1085	Y1086	E1088	R1089	L1090	E1093	V1096	E1097	E1102	V1105	I1106	Y1107	M1108	E1109	E1118	K1119	L1134	K1141	H1142	V1143	S1144	L1145	N1146	K1147	A1148	K1149	Q925	F926	R927	V928	H935	S936	H937	V938	H939	L942	T946	Q947	R948	P949	E950	C951	C952	Q953	G954	A955	P956	Y959	K963	L969	L970	R971	L972	D975	V976	P986	M989	Q990	L991	R997	F1001	L1014	T1017	V1018	D1019	P1020	V1021	L1025	R1026	D1027	F1028
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• Molecule 4: DNA (26-MER)



• Molecule 5: DNA (26-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	275300	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.22	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.034	Depositor
Minimum map value	-2.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	456.4, 456.4, 456.4	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.304, 1.304, 1.304	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/29781	0.51	12/40270 (0.0%)
2	B	0.31	0/4036	0.54	1/5438 (0.0%)
3	C	0.22	0/5368	0.46	1/7240 (0.0%)
4	D	0.37	0/587	0.45	0/902
5	E	0.33	0/607	0.38	0/936
All	All	0.28	0/40379	0.50	14/54786 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	THR	N-CA-C	-12.68	97.24	113.72
1	A	948	MET	CA-C-N	7.21	128.86	119.84
1	A	948	MET	C-N-CA	7.21	128.86	119.84
1	A	2137	ILE	N-CA-C	-6.50	107.53	113.71
1	A	165	LYS	N-CA-C	6.31	119.80	111.28
1	A	2547	SER	CA-C-N	5.76	127.04	119.84
1	A	2547	SER	C-N-CA	5.76	127.04	119.84
1	A	2576	MET	N-CA-C	-5.66	107.01	114.31
1	A	170	VAL	N-CA-C	-5.55	108.09	113.53
1	A	2093	CYS	N-CA-C	-5.53	107.78	114.75
1	A	3025	PRO	CA-N-CD	-5.41	104.43	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	PRO	CA-N-CD	-5.39	104.45	112.00
1	A	947	GLN	CA-C-O	5.37	121.06	117.94
3	C	612	ALA	N-CA-C	-5.02	108.19	114.56

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1020	PRO	Peptide
1	A	1960	LYS	Peptide
1	A	2122	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	29194	0	29449	903	0
2	B	3953	0	4031	171	0
3	C	5267	0	5261	246	0
4	D	526	0	293	24	0
5	E	540	0	291	9	0
6	A	34	0	0	1	0
7	A	154	0	0	17	0
7	B	25	0	0	4	0
7	C	9	0	0	0	0
7	D	4	0	0	1	0
7	E	2	0	0	0	0
All	All	39708	0	39325	1293	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 17.

All (1293) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:THR:HG23	4:D:12:DT:OP1	1.42	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:409:PHE:HB2	3:C:420:VAL:HG13	1.31	1.07
3:C:409:PHE:HB2	3:C:420:VAL:CG1	1.85	1.07
2:B:371:GLU:OE1	2:B:374:LEU:HD13	1.56	1.05
1:A:948:MET:HE2	1:A:948:MET:HA	1.41	1.03
3:C:136:THR:HG22	3:C:138:LEU:H	1.32	0.92
1:A:888:ARG:HH12	1:A:3889:ARG:HH11	1.22	0.87
1:A:1369:MET:HB2	1:A:1418:HIS:CD2	2.12	0.85
1:A:2165:LEU:HD21	1:A:2200:ALA:HB1	1.60	0.83
1:A:1874:TYR:CE2	1:A:1947:CYS:HB3	2.14	0.83
1:A:169:THR:CG2	4:D:12:DT:OP1	2.27	0.83
1:A:3484:THR:HG22	1:A:3513:ALA:HB2	1.60	0.82
1:A:948:MET:HA	1:A:948:MET:CE	2.07	0.82
2:B:263:LEU:HB2	2:B:267:ILE:HB	1.60	0.81
1:A:166:ILE:HG13	1:A:171:LEU:HG	1.60	0.81
1:A:236:LYS:H	1:A:281:GLN:HE21	1.26	0.81
1:A:948:MET:N	1:A:949:PRO:HD2	1.95	0.80
1:A:1483:LEU:HD11	1:A:1514:LEU:HD22	1.62	0.80
1:A:1551:ILE:HG13	1:A:1552:HIS:H	1.45	0.80
1:A:1102:GLU:HA	1:A:1154:PRO:HB3	1.63	0.80
1:A:3623:PRO:HG3	1:A:3633:ILE:HD13	1.66	0.78
1:A:899:ARG:HD3	1:A:2568:MET:HE2	1.64	0.78
1:A:1212:LEU:HD22	1:A:1217:VAL:HA	1.66	0.78
1:A:1874:TYR:CE2	1:A:1944:ALA:HA	2.20	0.77
1:A:495:VAL:HG22	1:A:523:THR:HB	1.67	0.77
2:B:468:LYS:HZ3	2:B:518:LEU:HB3	1.49	0.76
3:C:11:VAL:HB	3:C:132:ILE:HG22	1.68	0.76
3:C:409:PHE:CB	3:C:420:VAL:CG1	2.64	0.76
1:A:2953:THR:HB	1:A:2994:TRP:HE1	1.49	0.75
1:A:887:ASP:OD2	1:A:891:ARG:NH1	2.20	0.74
1:A:2439:ILE:O	1:A:2443:MET:HB2	1.86	0.74
2:B:130:ARG:HB3	2:B:134:MET:HE1	1.68	0.74
1:A:3728:VAL:HG22	1:A:3736:LYS:HG3	1.70	0.74
2:B:399:ARG:NH2	3:C:516:LEU:O	2.20	0.73
3:C:232:ARG:HA	3:C:515:MET:HE2	1.68	0.73
1:A:257:ARG:HH12	1:A:292:SER:HB2	1.53	0.73
1:A:910:PHE:HB2	1:A:937:MET:HE1	1.70	0.73
1:A:1946:ASN:HD22	1:A:2096:PRO:HG3	1.53	0.73
1:A:4064:LEU:HD21	1:A:4077:TYR:HB3	1.71	0.73
2:B:366:LEU:HB2	2:B:434:LEU:HD13	1.70	0.73
1:A:527:TYR:O	1:A:530:LEU:HB3	1.89	0.73
3:C:339:CYS:SG	3:C:394:ARG:NH1	2.62	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3544:ASP:HB2	1:A:3552:LYS:HZ3	1.54	0.73
1:A:51:LEU:HG	1:A:96:MET:HE1	1.71	0.72
1:A:1455:CYS:HA	1:A:1458:LEU:HD12	1.69	0.72
2:B:187:ARG:HG2	2:B:220:ILE:HD11	1.70	0.72
3:C:35:LYS:NZ	3:C:94:ILE:O	2.22	0.72
1:A:1684:LEU:HD21	1:A:1688:LEU:HB3	1.72	0.72
1:A:2837:LEU:HD11	1:A:2871:LEU:HA	1.71	0.72
1:A:3145:ILE:HD11	1:A:3196:LYS:HD2	1.71	0.72
3:C:492:GLN:HG2	3:C:509:GLN:HE22	1.55	0.72
1:A:2458:VAL:HG11	1:A:2476:ILE:HD11	1.71	0.71
1:A:1619:ALA:HB2	1:A:1655:ILE:HD11	1.72	0.71
2:B:528:LEU:HG	2:B:529:VAL:HG23	1.73	0.71
1:A:2424:MET:HE1	1:A:2439:ILE:HD11	1.73	0.71
1:A:793:LEU:HD12	1:A:869:ASN:HB2	1.71	0.71
1:A:1926:ASN:OD1	1:A:1974:ASN:ND2	2.24	0.71
2:B:92:LYS:N	7:B:702:HOH:O	2.24	0.71
3:C:115:MET:O	3:C:119:GLN:NE2	2.24	0.71
1:A:1809:ASP:OD1	3:C:627:ASN:ND2	2.24	0.71
2:B:329:LEU:HD12	2:B:333:GLU:HB3	1.71	0.71
3:C:20:MET:HG2	3:C:137:ASP:HB2	1.73	0.70
3:C:381:ILE:HD11	3:C:419:LEU:HB2	1.73	0.70
3:C:27:ILE:HG13	3:C:28:GLU:H	1.55	0.70
3:C:679:VAL:HG12	3:C:705:LEU:HD21	1.73	0.70
1:A:3864:ARG:NH2	1:A:3868:VAL:HG21	2.06	0.70
2:B:368:VAL:HB	2:B:432:PHE:HB2	1.74	0.70
1:A:665:GLY:HA2	1:A:668:LYS:HG3	1.74	0.69
1:A:1833:LEU:HB3	1:A:1836:LEU:HB2	1.74	0.69
2:B:305:THR:HG23	2:B:311:LEU:HD11	1.74	0.69
3:C:642:PHE:HB3	3:C:654:ARG:HH12	1.58	0.69
1:A:3912:CYS:SG	7:A:4397:HOH:O	2.49	0.69
3:C:409:PHE:O	3:C:419:LEU:HD12	1.91	0.69
1:A:3647:GLY:HA2	1:A:3651:LEU:HB2	1.74	0.69
3:C:684:THR:HG22	3:C:685:LEU:H	1.57	0.69
1:A:1173:LEU:HG	1:A:1191:PHE:HE2	1.56	0.69
2:B:261:LEU:HD23	2:B:269:ILE:HD11	1.74	0.69
3:C:65:ASP:H	3:C:78:THR:HG22	1.57	0.69
1:A:918:ALA:O	1:A:927:LYS:NZ	2.26	0.69
1:A:1487:VAL:HG11	1:A:1515:LEU:HD23	1.75	0.69
1:A:3820:MET:HB3	1:A:3824:GLU:HG3	1.75	0.69
2:B:469:LEU:HD21	2:B:514:MET:HG3	1.75	0.69
1:A:3922:ASP:O	1:A:3927:ASN:ND2	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2538:ARG:HE	1:A:2565:MET:HE2	1.58	0.68
1:A:2094:MET:HE1	1:A:2149:LEU:HA	1.74	0.68
1:A:1148:ALA:HB1	1:A:1162:SER:HB3	1.74	0.68
2:B:363:ARG:NH1	4:D:18:DT:OP1	2.27	0.68
1:A:227:LEU:HD21	1:A:248:ILE:HD12	1.75	0.68
1:A:2265:PRO:HB3	1:A:2309:PHE:CD1	2.28	0.68
2:B:443:LYS:NZ	3:C:480:THR:O	2.28	0.68
1:A:414:LEU:HG	1:A:464:VAL:HG21	1.77	0.67
1:A:121:ALA:HB2	1:A:167:PRO:HG2	1.76	0.67
1:A:1069:HIS:O	1:A:1075:ARG:NH1	2.26	0.67
1:A:1264:LEU:HD11	1:A:1341:ILE:HG13	1.77	0.67
3:C:184:ARG:HG2	3:C:185:LEU:H	1.59	0.67
2:B:419:GLU:HG2	2:B:428:THR:HG22	1.76	0.67
1:A:538:ASP:OD1	1:A:561:ASN:ND2	2.24	0.67
1:A:3631:LYS:HE2	1:A:3683:CYS:HA	1.76	0.67
2:B:215:LEU:HG	2:B:217:TYR:H	1.59	0.67
1:A:1261:LEU:HD13	1:A:1337:VAL:HG12	1.77	0.67
1:A:1896:ILE:HD12	1:A:1904:CYS:H	1.59	0.67
1:A:3445:LEU:HG	1:A:3449:LYS:HE2	1.76	0.67
1:A:3462:ARG:HH12	1:A:3708:ARG:HG3	1.58	0.67
2:B:262:LYS:HB3	2:B:268:VAL:HG12	1.76	0.67
3:C:267:ILE:HG22	3:C:361:VAL:HB	1.77	0.67
1:A:3082:TYR:O	1:A:3084:GLN:N	2.28	0.66
1:A:3958:LEU:O	1:A:4110:GLN:NE2	2.28	0.66
3:C:265:LYS:NZ	3:C:360:GLN:OE1	2.24	0.66
1:A:1261:LEU:HD11	1:A:1340:ARG:HG3	1.78	0.66
1:A:3842:TRP:HH2	1:A:3867:THR:HG22	1.61	0.66
2:B:90:THR:O	2:B:101:ASN:ND2	2.27	0.66
3:C:296:CYS:HA	3:C:304:GLU:HA	1.77	0.66
1:A:3651:LEU:HA	1:A:3654:MET:HB2	1.76	0.66
1:A:2154:GLU:OE1	1:A:2158:ARG:NH1	2.29	0.66
1:A:3858:MET:HE1	1:A:4119:ARG:HB2	1.78	0.66
3:C:413:LYS:HG2	3:C:416:TYR:CE1	2.31	0.66
1:A:2427:ARG:HH12	1:A:2464:HIS:CE1	2.13	0.66
2:B:168:LEU:HD23	2:B:202:LEU:HD13	1.76	0.66
1:A:1807:LYS:HG3	1:A:1809:ASP:HB2	1.77	0.66
2:B:48:MET:HE1	2:B:170:THR:HA	1.77	0.66
2:B:505:ASP:OD2	2:B:508:LEU:N	2.28	0.66
3:C:58:LEU:HD11	3:C:97:LYS:HD3	1.78	0.66
3:C:687:THR:HG22	3:C:700:GLU:HB2	1.76	0.66
2:B:388:LYS:HE2	3:C:451:LEU:HD12	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:640:ARG:HD2	3:C:643:ARG:HH21	1.59	0.66
1:A:1105:VAL:HG11	1:A:1154:PRO:HB2	1.78	0.66
1:A:1878:ASP:HB2	1:A:1947:CYS:HB2	1.77	0.66
1:A:1852:LYS:HZ1	1:A:1914:THR:HG23	1.62	0.65
2:B:31:LYS:HD2	2:B:160:LYS:HG2	1.78	0.65
3:C:312:GLN:NE2	3:C:328:GLU:OE2	2.30	0.65
1:A:1850:VAL:O	1:A:1870:LYS:NZ	2.30	0.65
3:C:148:ASP:O	3:C:152:HIS:ND1	2.29	0.65
1:A:377:ASN:ND2	1:A:380:ASP:OD2	2.29	0.65
1:A:358:GLU:HA	1:A:361:ILE:HG22	1.79	0.65
1:A:1853:SER:OG	1:A:1870:LYS:NZ	2.29	0.65
1:A:1639:LEU:HD21	1:A:1643:MET:HE3	1.78	0.65
1:A:3269:ARG:NH2	1:A:3271:ASP:OD2	2.27	0.65
1:A:3411:ASP:OD1	1:A:3412:ALA:N	2.30	0.65
1:A:1185:HIS:ND1	1:A:1189:GLU:OE2	2.29	0.65
1:A:3448:GLU:O	1:A:3452:LYS:HG2	1.96	0.65
1:A:1727:ARG:HD3	1:A:1773:VAL:HG22	1.79	0.64
1:A:1794:GLN:NE2	1:A:1832:SER:O	2.29	0.64
4:D:7:DG:H1	5:E:37:DC:H42	1.42	0.64
1:A:45:SER:O	1:A:95:LYS:NZ	2.27	0.64
1:A:1411:TYR:HD2	1:A:1414:ILE:HD11	1.62	0.64
1:A:3867:THR:HG21	1:A:4119:ARG:HH21	1.62	0.64
1:A:1178:ARG:O	1:A:1184:ARG:NH2	2.30	0.64
1:A:1153:LEU:HD11	1:A:1159:PRO:HA	1.78	0.64
1:A:3483:MET:SD	1:A:3513:ALA:HB1	2.38	0.64
2:B:362:LEU:HD12	2:B:363:ARG:HB2	1.80	0.64
1:A:1946:ASN:ND2	1:A:2096:PRO:HG3	2.12	0.64
1:A:391:ARG:HH12	1:A:395:MET:HB3	1.63	0.64
1:A:948:MET:HE2	1:A:948:MET:CA	2.24	0.64
1:A:1142:HIS:HE1	1:A:1165:LEU:HD22	1.63	0.64
1:A:2383:PHE:HE2	1:A:2408:MET:HE1	1.63	0.64
1:A:3416:LEU:HB3	1:A:3449:LYS:NZ	2.12	0.64
3:C:540:ILE:O	3:C:543:LYS:NZ	2.31	0.64
1:A:125:ILE:HD11	1:A:169:THR:HB	1.79	0.63
1:A:1803:GLU:OE1	1:A:1806:ARG:NH2	2.32	0.63
1:A:1820:VAL:HA	1:A:1824:LEU:HB3	1.80	0.63
3:C:678:VAL:O	3:C:682:GLY:N	2.29	0.63
1:A:3535:ILE:HG13	1:A:3797:THR:HA	1.79	0.63
3:C:140:SER:O	3:C:200:GLN:NE2	2.32	0.63
1:A:2342:CYS:SG	1:A:2377:ARG:NH1	2.72	0.63
3:C:66:ASN:ND2	3:C:68:LEU:O	2.21	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1403:MET:HE1	1:A:1458:LEU:HD23	1.80	0.63
1:A:1828:LEU:O	1:A:1883:ARG:NH2	2.32	0.63
1:A:3688:SER:O	1:A:3691:LYS:NZ	2.32	0.62
3:C:77:ILE:HD12	3:C:113:VAL:HG21	1.81	0.62
1:A:3739:ILE:HG22	1:A:3747:GLU:OE2	1.99	0.62
1:A:490:ILE:HA	1:A:493:LYS:HE2	1.80	0.62
1:A:997:ASN:O	1:A:1001:PHE:N	2.31	0.62
1:A:2251:ILE:HG13	1:A:2285:LEU:HD23	1.81	0.62
1:A:2122:LEU:HB3	1:A:2126:MET:HE2	1.80	0.62
1:A:3335:ARG:HG2	1:A:3339:ASN:ND2	2.15	0.62
1:A:538:ASP:O	1:A:542:ASP:N	2.24	0.62
1:A:1984:LEU:HD21	1:A:2142:ILE:HD12	1.81	0.62
1:A:3849:LYS:HB2	1:A:3854:ALA:HB2	1.80	0.62
1:A:520:LYS:NZ	1:A:526:ASP:OD2	2.33	0.62
1:A:2939:LEU:HD23	1:A:2942:ILE:HD12	1.80	0.62
1:A:3582:GLU:HB3	1:A:3586:LYS:NZ	2.14	0.62
2:B:368:VAL:HG23	2:B:434:LEU:HD11	1.80	0.62
3:C:486:ARG:NH2	4:D:20:DG:OP1	2.32	0.62
1:A:485:GLN:OE1	1:A:489:ARG:NH1	2.33	0.62
1:A:3868:VAL:HG22	1:A:4114:PRO:HB2	1.81	0.62
2:B:171:ASN:HB2	2:B:207:LYS:HG2	1.82	0.62
1:A:1017:ILE:HG13	1:A:1018:VAL:N	2.15	0.61
5:E:37:DC:H2"	5:E:38:DA:H5"	1.81	0.61
1:A:3447:VAL:HG11	1:A:3483:MET:HB2	1.82	0.61
1:A:1840:PHE:O	1:A:1844:VAL:HG23	2.00	0.61
1:A:3720:ALA:HB2	1:A:3743:HIS:HA	1.83	0.61
3:C:412:ILE:O	3:C:412:ILE:HG22	2.01	0.61
3:C:450:GLN:HB3	3:C:537:PHE:CZ	2.36	0.61
1:A:2311:ARG:NH2	1:A:2312:TYR:OH	2.33	0.61
3:C:533:ILE:HG23	3:C:537:PHE:CD2	2.35	0.61
1:A:3335:ARG:HG2	1:A:3339:ASN:HD21	1.66	0.61
1:A:774:GLU:HB2	1:A:858:MET:HE1	1.82	0.61
1:A:2744:ALA:HA	4:D:1:DC:C2	2.36	0.61
2:B:216:PHE:HA	2:B:218:ARG:NH1	2.16	0.61
3:C:550:ALA:HA	3:C:553:ILE:HG22	1.83	0.61
1:A:1551:ILE:HG13	1:A:1552:HIS:N	2.16	0.61
1:A:3378:TYR:OH	1:A:3426:LYS:NZ	2.33	0.61
3:C:613:SER:O	3:C:617:ILE:HG12	2.01	0.61
1:A:1268:ASN:ND2	1:A:1343:GLU:OE2	2.34	0.60
2:B:48:MET:HA	2:B:59:PRO:HG2	1.82	0.60
2:B:457:GLU:OE2	2:B:458:GLN:NE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1894:SER:HA	1:A:1897:ASN:HB2	1.84	0.60
1:A:3020:ASP:OD2	1:A:3029:LYS:NZ	2.34	0.60
1:A:3082:TYR:C	1:A:3084:GLN:H	2.09	0.60
3:C:660:LYS:HG3	3:C:685:LEU:HD11	1.82	0.60
1:A:396:PHE:HB3	1:A:410:MET:HE2	1.84	0.60
1:A:949:PRO:HB3	1:A:954:GLY:C	2.27	0.60
1:A:1734:PRO:O	1:A:1738:ASN:ND2	2.35	0.60
3:C:659:LEU:HD11	3:C:683:ILE:HG22	1.83	0.60
1:A:1852:LYS:NZ	1:A:1914:THR:HG23	2.17	0.60
1:A:2281:MET:HE3	1:A:2326:ILE:HG12	1.83	0.60
1:A:3593:ARG:NH2	1:A:3664:ASN:OD1	2.35	0.60
1:A:1874:TYR:CZ	1:A:1947:CYS:HB3	2.36	0.60
3:C:342:VAL:HG12	3:C:344:GLY:H	1.66	0.60
1:A:264:ARG:NH2	7:A:4332:HOH:O	2.34	0.60
1:A:3162:ASN:O	1:A:3166:ASN:ND2	2.30	0.60
2:B:215:LEU:O	2:B:218:ARG:NH1	2.34	0.60
2:B:40:PHE:HZ	2:B:70:VAL:HG11	1.67	0.59
1:A:269:SER:OG	1:A:273:ARG:NH2	2.35	0.59
1:A:3582:GLU:HB3	1:A:3586:LYS:HZ1	1.66	0.59
1:A:1914:THR:HA	1:A:1917:LYS:NZ	2.16	0.59
1:A:1744:LYS:HG2	1:A:1774:MET:HE1	1.84	0.59
1:A:3961:PHE:HE1	1:A:4107:LEU:HG	1.66	0.59
1:A:2743:TYR:HB3	4:D:1:DC:H42	1.67	0.59
1:A:3548:GLY:HA2	1:A:3551:ASN:HD22	1.66	0.59
1:A:1282:LEU:HD21	1:A:1291:LEU:HD11	1.83	0.59
2:B:49:PHE:HD2	2:B:128:GLN:HE21	1.50	0.59
2:B:95:ASN:OD1	2:B:98:ASN:N	2.35	0.59
1:A:532:ARG:NH2	1:A:632:GLU:O	2.36	0.59
1:A:1142:HIS:HA	1:A:1145:LEU:HG	1.85	0.59
2:B:84:ALA:HB2	2:B:108:LEU:HB3	1.85	0.59
1:A:1367:HIS:O	1:A:1370:ARG:HG3	2.02	0.59
1:A:3307:LEU:O	1:A:3326:GLN:NE2	2.35	0.59
1:A:1342:MET:HE1	1:A:1375:THR:HG21	1.83	0.59
1:A:2122:LEU:O	1:A:2127:LYS:NZ	2.35	0.59
1:A:385:TYR:HE2	1:A:428:PRO:HD2	1.68	0.58
1:A:1147:LYS:HE2	1:A:1149:LYS:HZ2	1.67	0.58
1:A:1564:SER:O	1:A:1568:ASN:ND2	2.36	0.58
1:A:1844:VAL:HG11	1:A:1898:GLN:HE22	1.67	0.58
1:A:1774:MET:HE3	1:A:1777:LEU:HD12	1.86	0.58
1:A:2395:THR:O	1:A:2399:GLU:HG3	2.04	0.58
1:A:3543:LYS:HB2	1:A:3545:THR:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3872:ARG:NH1	1:A:3875:GLU:OE2	2.32	0.58
3:C:27:ILE:HG13	3:C:28:GLU:N	2.18	0.58
1:A:2254:ARG:NH2	1:A:2292:CYS:O	2.36	0.58
3:C:265:LYS:NZ	5:E:21:DG:OP1	2.35	0.58
2:B:351:LYS:HB3	2:B:355:LEU:HD21	1.84	0.58
1:A:631:ARG:NH2	1:A:668:LYS:HD3	2.18	0.58
1:A:1096:VAL:HG21	1:A:1141:LYS:HE3	1.85	0.58
1:A:1857:LYS:NZ	1:A:1932:GLN:HG3	2.18	0.58
1:A:2091:HIS:O	1:A:2091:HIS:ND1	2.37	0.58
3:C:609:PHE:HZ	3:C:654:ARG:HE	1.51	0.58
1:A:487:LEU:HD23	1:A:490:ILE:HD11	1.86	0.58
1:A:2432:GLN:OE1	1:A:2461:PHE:CE2	2.57	0.58
3:C:448:GLU:O	3:C:452:ASN:ND2	2.37	0.58
1:A:1572:LEU:HB3	1:A:1614:GLN:NE2	2.19	0.58
1:A:2464:HIS:ND1	1:A:2465:PRO:O	2.26	0.58
1:A:3170:ASP:N	1:A:3174:ASP:OD2	2.35	0.58
1:A:3416:LEU:HB3	1:A:3449:LYS:HZ1	1.68	0.58
1:A:1337:VAL:O	1:A:1341:ILE:HD12	2.04	0.58
1:A:1594:SER:O	1:A:1598:ASN:ND2	2.30	0.58
1:A:1972:GLU:OE2	1:A:1973:LYS:NZ	2.31	0.58
3:C:57:VAL:HG12	3:C:79:VAL:HA	1.86	0.58
3:C:688:LYS:HB3	3:C:694:SER:HB2	1.85	0.58
1:A:1708:GLU:OE1	1:A:1712:ARG:NH2	2.37	0.57
1:A:3051:LEU:O	1:A:3056:GLU:HG3	2.04	0.57
1:A:3137:GLU:OE2	1:A:3186:ARG:NH2	2.29	0.57
1:A:3949:ALA:HA	1:A:3953:LEU:HD13	1.86	0.57
1:A:491:CYS:O	1:A:625:ASN:ND2	2.37	0.57
1:A:1664:SER:HA	1:A:1668:PHE:HB3	1.86	0.57
2:B:151:ALA:HB2	2:B:193:LEU:HD21	1.85	0.57
1:A:1178:ARG:NE	1:A:1180:GLN:OE1	2.34	0.57
2:B:352:PRO:HA	2:B:394:VAL:HA	1.87	0.57
1:A:1881:TYR:HE1	1:A:1889:VAL:HG11	1.69	0.57
1:A:3544:ASP:HA	1:A:3548:GLY:HA3	1.86	0.57
1:A:572:VAL:HG22	1:A:626:LEU:HD11	1.85	0.57
3:C:12:LEU:HD23	3:C:133:GLU:HB2	1.85	0.57
1:A:852:ARG:HB3	1:A:3111:MET:HE1	1.86	0.57
1:A:3485:LYS:O	1:A:3488:SER:OG	2.23	0.57
2:B:132:GLN:OE1	2:B:137:HIS:ND1	2.36	0.57
2:B:438:PRO:HG2	3:C:267:ILE:HD11	1.86	0.57
3:C:184:ARG:HG2	3:C:185:LEU:N	2.19	0.57
3:C:689:GLU:HG3	3:C:691:ALA:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2452:ARG:HG2	1:A:2498:ILE:HG23	1.87	0.57
1:A:3522:THR:HA	1:A:3529:ILE:HG21	1.85	0.57
1:A:1775:GLU:OE2	1:A:1822:ARG:NH2	2.38	0.57
1:A:3028:ASN:HA	1:A:3031:TRP:HD1	1.68	0.57
1:A:2166:SER:O	1:A:2170:GLN:CB	2.53	0.56
1:A:2573:PRO:HD2	1:A:2575:PRO:HG3	1.87	0.56
1:A:2085:MET:HB2	1:A:2090:ARG:HD2	1.87	0.56
1:A:2931:ARG:NH2	1:A:3000:ASP:OD1	2.38	0.56
1:A:4049:ARG:NH2	1:A:4062:ASP:OD2	2.29	0.56
3:C:61:THR:OG1	3:C:63:GLY:O	2.22	0.56
3:C:391:ALA:HB3	3:C:408:ALA:HB3	1.87	0.56
1:A:1886:LYS:HD3	1:A:1956:PHE:HA	1.88	0.56
1:A:3763:ARG:HA	1:A:3766:GLN:HG2	1.86	0.56
3:C:431:ARG:NH2	4:D:17:DC:OP2	2.38	0.56
1:A:699:GLU:O	1:A:702:SER:OG	2.22	0.56
3:C:137:ASP:OD1	3:C:201:GLN:NE2	2.39	0.56
3:C:666:VAL:HA	3:C:671:LEU:HD21	1.87	0.56
1:A:1017:ILE:HG13	1:A:1018:VAL:HG13	1.88	0.56
1:A:2265:PRO:HB3	1:A:2309:PHE:HD1	1.69	0.56
1:A:3267:LYS:HA	1:A:3273:LEU:HD12	1.87	0.56
1:A:3283:LEU:O	1:A:3287:ARG:HG2	2.05	0.56
3:C:64:THR:OG1	3:C:76:ASN:N	2.36	0.56
1:A:164:LYS:HG3	1:A:165:LYS:HE3	1.88	0.56
1:A:1082:PHE:HZ	1:A:1134:LEU:HD13	1.71	0.56
1:A:1711:ARG:HH21	1:A:1757:MET:HG2	1.71	0.56
1:A:1833:LEU:HG	1:A:1835:ALA:H	1.71	0.56
1:A:1881:TYR:CD2	1:A:1951:VAL:HG22	2.41	0.56
1:A:2281:MET:HE1	1:A:2287:PRO:HD3	1.88	0.56
3:C:112:ILE:HA	3:C:115:MET:HE2	1.88	0.56
1:A:153:PHE:HE1	1:A:196:LEU:HD22	1.71	0.56
1:A:1840:PHE:CD1	1:A:1880:MET:HE1	2.40	0.56
1:A:1964:GLY:O	1:A:1968:SER:OG	2.20	0.56
1:A:428:PRO:O	1:A:429:GLU:HG2	2.06	0.56
1:A:2551:GLU:OE1	1:A:2847:THR:OG1	2.23	0.56
1:A:3981:TYR:HB2	1:A:4108:MET:HE1	1.88	0.56
1:A:72:SER:O	1:A:82:ARG:NH1	2.38	0.56
1:A:1852:LYS:NZ	1:A:1914:THR:CG2	2.69	0.56
3:C:406:GLY:HA2	3:C:424:LEU:HB2	1.88	0.56
1:A:3354:ASP:O	1:A:3357:ARG:NE	2.39	0.56
1:A:101:ALA:HB1	1:A:143:LEU:HD11	1.87	0.55
1:A:971:ARG:HA	1:A:1025:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1723:PRO:HG3	1:A:1729:PHE:CZ	2.41	0.55
1:A:3075:LYS:NZ	7:A:4326:HOH:O	2.38	0.55
1:A:3731:SER:OG	6:A:4201:1IX:CL1	2.61	0.55
1:A:1027:ASP:OD1	1:A:1028:PHE:N	2.39	0.55
3:C:45:GLN:OE1	3:C:50:ASN:ND2	2.37	0.55
3:C:409:PHE:HB2	3:C:420:VAL:HG12	1.84	0.55
1:A:43:VAL:O	1:A:95:LYS:NZ	2.35	0.55
1:A:1420:ARG:HE	1:A:1467:ILE:HA	1.71	0.55
1:A:1572:LEU:HB3	1:A:1614:GLN:HE21	1.71	0.55
1:A:2471:GLU:O	1:A:2475:ASN:ND2	2.36	0.55
2:B:42:VAL:HG12	2:B:169:PHE:HB2	1.88	0.55
3:C:600:VAL:HA	3:C:603:LYS:HE2	1.89	0.55
1:A:919:LEU:HD23	1:A:972:LEU:HD13	1.87	0.55
1:A:2166:SER:O	1:A:2170:GLN:HB2	2.07	0.55
3:C:188:HIS:H	3:C:232:ARG:NH1	2.05	0.55
1:A:418:ALA:HB2	1:A:464:VAL:HG22	1.88	0.55
1:A:1876:ILE:O	1:A:1880:MET:HG2	2.06	0.55
1:A:2182:ILE:HD11	1:A:2185:MET:HB2	1.87	0.55
1:A:648:SER:O	1:A:652:GLU:HG2	2.06	0.55
1:A:2440:TYR:HD1	1:A:2476:ILE:HG22	1.71	0.55
2:B:252:ARG:NH2	7:B:708:HOH:O	2.40	0.55
3:C:476:LEU:HD21	3:C:519:PRO:HG2	1.87	0.55
1:A:1641:THR:O	1:A:1645:VAL:HG23	2.07	0.55
1:A:3418:ASP:OD1	1:A:3419:PHE:N	2.40	0.55
3:C:43:GLN:HG2	3:C:491:PHE:HB3	1.87	0.55
1:A:1874:TYR:HE2	1:A:1944:ALA:HA	1.72	0.55
1:A:2921:LEU:O	1:A:2925:GLU:HG2	2.07	0.55
1:A:3519:GLU:O	1:A:3522:THR:OG1	2.24	0.55
3:C:351:VAL:HG21	3:C:390:VAL:HG21	1.88	0.55
3:C:642:PHE:HB3	3:C:654:ARG:NH1	2.20	0.55
4:D:16:DG:H4'	4:D:17:DC:OP1	2.06	0.55
1:A:948:MET:N	1:A:949:PRO:CD	2.69	0.55
1:A:1338:VAL:O	1:A:1342:MET:HG3	2.07	0.55
1:A:2089:ASN:HA	1:A:2094:MET:HG2	1.88	0.55
1:A:2247:ASP:OD2	1:A:2248:CYS:N	2.40	0.55
1:A:2306:ASN:HA	1:A:2309:PHE:CD2	2.42	0.55
1:A:3544:ASP:HB2	1:A:3552:LYS:NZ	2.20	0.55
2:B:68:GLN:HG3	2:B:123:LYS:HE3	1.90	0.55
2:B:126:GLN:O	2:B:129:LYS:HG3	2.06	0.55
2:B:340:PHE:HB2	2:B:408:PRO:HD3	1.89	0.55
2:B:371:GLU:OE1	2:B:374:LEU:CD1	2.44	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:ASP:OD1	3:C:17:GLY:N	2.39	0.55
3:C:184:ARG:H	3:C:184:ARG:HD3	1.72	0.54
4:D:19:DG:H2''	4:D:20:DG:C8	2.42	0.54
5:E:35:DG:H2''	5:E:36:DG:C8	2.42	0.54
1:A:125:ILE:HD11	1:A:169:THR:CB	2.37	0.54
3:C:59:PHE:HB3	3:C:110:ALA:HB2	1.90	0.54
3:C:728:LEU:HA	3:C:731:MET:HE2	1.89	0.54
1:A:2973:ASP:OD1	1:A:2974:GLU:N	2.40	0.54
1:A:3940:ILE:HG22	1:A:3941:ASP:HB2	1.90	0.54
1:A:3172:LYS:O	1:A:3173:MET:HE2	2.08	0.54
1:A:3462:ARG:NH1	1:A:3708:ARG:HG3	2.23	0.54
1:A:274:LEU:HD12	1:A:278:HIS:HD2	1.72	0.54
1:A:1148:ALA:HA	1:A:1164:CYS:HB3	1.90	0.54
1:A:1720:ALA:HB1	3:C:596:GLU:HB2	1.88	0.54
3:C:361:VAL:HG22	3:C:422:VAL:HG22	1.88	0.54
1:A:1686:LEU:HD11	1:A:1721:HIS:HB3	1.89	0.54
1:A:4125:GLU:OE2	1:A:4127:TRP:NE1	2.41	0.54
1:A:718:MET:HE1	1:A:751:ALA:HA	1.90	0.54
2:B:446:MET:HE3	3:C:264:TYR:HB2	1.90	0.54
3:C:151:ILE:HD11	3:C:211:VAL:HG13	1.89	0.54
1:A:303:HIS:O	1:A:303:HIS:ND1	2.40	0.54
1:A:2533:SER:HA	1:A:2565:MET:HE1	1.90	0.54
1:A:3481:SER:HA	1:A:3484:THR:HG23	1.89	0.54
3:C:447:THR:HG22	3:C:449:ALA:H	1.72	0.54
4:D:6:DT:H1'	4:D:7:DG:C8	2.42	0.54
1:A:877:ASP:OD2	1:A:881:LYS:NZ	2.41	0.54
1:A:2427:ARG:NH1	1:A:2432:GLN:NE2	2.55	0.54
1:A:3312:VAL:O	1:A:3314:SER:N	2.41	0.54
3:C:357:MET:HE2	3:C:429:ASP:HB3	1.89	0.54
3:C:423:GLN:HG2	3:C:424:LEU:H	1.72	0.54
1:A:621:SER:O	1:A:625:ASN:ND2	2.41	0.54
1:A:96:MET:HG3	1:A:100:ILE:HD11	1.88	0.53
1:A:628:GLU:O	1:A:632:GLU:HG2	2.08	0.53
1:A:1890:HIS:HA	1:A:1908:GLY:HA3	1.89	0.53
1:A:2402:LEU:HA	1:A:2405:VAL:HG23	1.90	0.53
2:B:41:LEU:HB3	2:B:168:LEU:HD12	1.91	0.53
1:A:231:LEU:HD12	1:A:274:LEU:HD11	1.89	0.53
1:A:1203:SER:O	1:A:1207:TRP:HD1	1.91	0.53
1:A:2452:ARG:HD2	1:A:2494:ASP:HA	1.89	0.53
1:A:3341:LEU:HD23	1:A:3348:LEU:HD12	1.90	0.53
1:A:1173:LEU:HG	1:A:1191:PHE:CE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:LEU:HD11	2:B:167:MET:HG3	1.90	0.53
2:B:368:VAL:HG23	2:B:434:LEU:CD1	2.38	0.53
1:A:1651:LYS:O	1:A:1655:ILE:HG23	2.08	0.53
1:A:3633:ILE:HA	1:A:3636:PHE:HB2	1.91	0.53
2:B:58:THR:HG22	2:B:61:ASP:HB2	1.90	0.53
1:A:15:LEU:O	1:A:18:THR:HG22	2.08	0.53
1:A:4090:ARG:NH2	1:A:4113:ASP:OD2	2.36	0.53
2:B:303:PHE:HA	2:B:311:LEU:HD13	1.89	0.53
1:A:9:ARG:NH1	7:A:4343:HOH:O	2.42	0.53
1:A:2264:ASP:O	1:A:2266:ASN:N	2.36	0.53
1:A:3547:THR:O	1:A:3551:ASN:ND2	2.42	0.53
3:C:131:HIS:ND1	3:C:160:SER:O	2.32	0.53
3:C:185:LEU:HD13	3:C:511:HIS:HB3	1.90	0.53
1:A:1164:CYS:SG	1:A:1165:LEU:N	2.82	0.53
1:A:2547:SER:O	1:A:2549:LYS:N	2.42	0.53
1:A:3021:SER:OG	1:A:3022:GLU:OE1	2.26	0.53
1:A:3472:ILE:HG13	1:A:3483:MET:HE3	1.91	0.53
2:B:371:GLU:O	2:B:371:GLU:HG2	2.09	0.53
2:B:375:VAL:HA	3:C:542:ALA:HB3	1.90	0.53
1:A:228:SER:HA	1:A:274:LEU:HD13	1.91	0.53
1:A:235:THR:HA	1:A:281:GLN:NE2	2.23	0.53
1:A:1610:ASN:OD1	1:A:1611:GLN:N	2.42	0.53
3:C:449:ALA:HA	3:C:452:ASN:HD21	1.74	0.53
1:A:759:GLY:C	1:A:761:SER:H	2.17	0.53
1:A:1062:ARG:NH2	1:A:3746:ARG:HH12	2.07	0.53
1:A:3628:PHE:CE2	1:A:3686:TRP:HD1	2.27	0.53
1:A:4054:ALA:HA	1:A:4096:SER:HA	1.90	0.53
3:C:640:ARG:HH21	3:C:681:ASP:HB3	1.74	0.53
1:A:3979:LEU:N	7:A:4334:HOH:O	2.34	0.53
3:C:265:LYS:HD3	3:C:268:LEU:HD22	1.90	0.53
1:A:737:PRO:C	1:A:739:ASN:H	2.17	0.52
1:A:1036:PHE:HE1	1:A:1054:VAL:HG23	1.74	0.52
1:A:1539:SER:HA	1:A:1551:ILE:HA	1.90	0.52
1:A:2083:LEU:HD21	1:A:2089:ASN:HB3	1.91	0.52
1:A:3798:SER:O	1:A:3799:ARG:HG2	2.09	0.52
1:A:116:THR:HG23	1:A:117:LYS:HG3	1.91	0.52
1:A:1014:LEU:O	1:A:1018:VAL:HG22	2.10	0.52
1:A:1984:LEU:HD23	1:A:2141:ASN:HB2	1.91	0.52
1:A:3628:PHE:HE2	1:A:3686:TRP:HD1	1.56	0.52
2:B:35:ARG:NH2	2:B:80:ARG:O	2.41	0.52
3:C:30:PRO:HB3	3:C:166:PRO:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:616:LEU:HD22	3:C:642:PHE:CZ	2.44	0.52
1:A:1539:SER:HB3	1:A:1551:ILE:HG22	1.91	0.52
1:A:2743:TYR:HB3	4:D:1:DC:N4	2.24	0.52
1:A:2851:PHE:CE2	1:A:2853:PRO:HG2	2.45	0.52
1:A:3428:GLU:OE1	1:A:3474:ARG:NE	2.43	0.52
2:B:458:GLN:HG3	2:B:528:LEU:HD11	1.91	0.52
3:C:371:GLU:OE1	3:C:374:ALA:HB3	2.10	0.52
1:A:3136:THR:O	1:A:3140:GLU:HG3	2.09	0.52
1:A:462:VAL:HG11	1:A:541:MET:HE3	1.92	0.52
1:A:1221:ILE:O	1:A:1225:GLU:N	2.43	0.52
1:A:1623:LEU:HD21	1:A:1652:ILE:HG21	1.92	0.52
1:A:3531:TYR:O	1:A:3535:ILE:HD12	2.09	0.52
2:B:277:VAL:HG23	3:C:430:LEU:HA	1.90	0.52
2:B:499:GLU:HB2	2:B:500:PRO:HD3	1.91	0.52
1:A:719:LYS:O	1:A:1026:ARG:NH2	2.43	0.52
1:A:894:PHE:HB3	1:A:907:LEU:HD23	1.91	0.52
1:A:2519:LEU:HG	1:A:2523:ASN:HD21	1.75	0.52
1:A:3530:VAL:O	1:A:3534:ILE:HG13	2.10	0.52
1:A:2288:TYR:OH	1:A:2294:ILE:O	2.23	0.52
1:A:168:ASP:HA	1:A:171:LEU:HB2	1.91	0.52
3:C:628:GLU:HB2	3:C:631:TYR:HD2	1.75	0.52
1:A:256:ILE:O	1:A:300:TRP:NE1	2.37	0.52
1:A:1297:PHE:O	1:A:1301:ILE:HG23	2.10	0.52
1:A:2086:ASP:OD1	1:A:2086:ASP:N	2.43	0.52
1:A:3125:ARG:NH2	7:A:4342:HOH:O	2.42	0.52
3:C:69:SER:HA	3:C:74:TYR:HB2	1.91	0.52
3:C:266:SER:OG	3:C:267:ILE:N	2.38	0.52
1:A:1970:LYS:HB2	1:A:1975:LEU:HD22	1.91	0.51
1:A:2122:LEU:HG	1:A:2123:PRO:HD2	1.92	0.51
1:A:2133:LEU:HG	1:A:2167:PRO:HB2	1.91	0.51
3:C:10:VAL:HG12	3:C:131:HIS:HB3	1.92	0.51
1:A:117:LYS:HD2	3:C:300:ASP:HA	1.91	0.51
1:A:238:MET:HE2	1:A:285:CYS:SG	2.49	0.51
1:A:2491:THR:HB	1:A:2495:SER:HB3	1.92	0.51
1:A:2919:ASP:OD2	1:A:2922:ARG:NH1	2.39	0.51
1:A:3176:MET:HE2	1:A:3246:ALA:HB2	1.92	0.51
3:C:146:GLN:HB2	3:C:149:ILE:HG22	1.92	0.51
3:C:281:ALA:O	3:C:282:LYS:HG2	2.11	0.51
3:C:302:GLU:CD	3:C:302:GLU:H	2.16	0.51
3:C:364:VAL:CG2	3:C:419:LEU:HB3	2.41	0.51
3:C:662:LEU:O	3:C:666:VAL:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ARG:HB3	1:A:57:LEU:HD13	1.92	0.51
1:A:2764:LYS:O	1:A:2768:GLN:HB2	2.11	0.51
2:B:123:LYS:NZ	7:B:709:HOH:O	2.43	0.51
2:B:266:ASP:N	7:B:707:HOH:O	2.36	0.51
1:A:659:ARG:HG3	1:A:660:LEU:HG	1.92	0.51
1:A:859:LEU:HD11	1:A:870:LEU:HD21	1.92	0.51
1:A:1684:LEU:HD11	1:A:1688:LEU:HD13	1.92	0.51
1:A:3809:THR:HG22	1:A:3931:ALA:HA	1.92	0.51
2:B:351:LYS:HG2	3:C:463:LEU:HB2	1.91	0.51
1:A:243:GLN:O	1:A:247:GLU:HG3	2.10	0.51
1:A:4126:PRO:HD2	1:A:4127:TRP:CZ3	2.46	0.51
5:E:20:DT:H2''	5:E:21:DG:C8	2.46	0.51
1:A:975:ASP:CG	1:A:976:VAL:H	2.19	0.51
1:A:2251:ILE:HG21	1:A:2280:VAL:HG21	1.92	0.51
1:A:3256:MET:O	1:A:3260:LYS:HG2	2.11	0.51
4:D:15:DC:H2'	4:D:16:DG:C8	2.45	0.51
1:A:539:GLN:O	1:A:543:SER:OG	2.26	0.51
1:A:901:MET:HE2	1:A:2535:THR:HB	1.93	0.51
1:A:949:PRO:HB3	1:A:954:GLY:O	2.11	0.51
1:A:2517:LEU:HA	1:A:2520:ILE:HD12	1.92	0.51
2:B:409:TYR:HE2	2:B:436:PHE:HB3	1.75	0.51
2:B:463:LYS:HA	2:B:466:VAL:HG12	1.93	0.51
2:B:466:VAL:HG21	3:C:389:MET:HG2	1.91	0.51
3:C:11:VAL:HG22	3:C:55:ALA:HB3	1.91	0.51
1:A:2820:MET:HE1	1:A:2829:LYS:HB2	1.93	0.51
2:B:45:SER:O	2:B:137:HIS:HD2	1.92	0.51
2:B:258:ARG:NH2	5:E:31:DA:OP2	2.44	0.51
1:A:67:VAL:HG12	1:A:71:LYS:HE2	1.92	0.51
1:A:1420:ARG:NH1	1:A:1466:ASN:O	2.40	0.51
1:A:2205:VAL:HG12	1:A:2208:ASP:H	1.75	0.51
2:B:277:VAL:HG22	3:C:357:MET:CE	2.41	0.51
1:A:1069:HIS:CD2	1:A:1074:LYS:HG3	2.46	0.51
1:A:1859:ASN:HB3	1:A:1862:THR:HG22	1.92	0.51
1:A:3008:TRP:HB2	1:A:3051:LEU:HD13	1.93	0.51
3:C:636:ILE:HA	3:C:639:ILE:HG22	1.93	0.51
1:A:169:THR:HG23	4:D:12:DT:P	2.45	0.50
1:A:451:PRO:C	1:A:453:MET:H	2.18	0.50
1:A:3176:MET:HE1	1:A:3242:MET:HG2	1.93	0.50
2:B:252:ARG:HD2	3:C:431:ARG:CZ	2.42	0.50
2:B:256:LEU:HD13	2:B:275:ASN:HB2	1.92	0.50
2:B:256:LEU:CD1	2:B:275:ASN:HD22	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:SER:OG	2:B:375:VAL:HG12	2.10	0.50
1:A:1217:VAL:HG11	1:A:1285:GLU:HB3	1.92	0.50
1:A:2572:TYR:HE2	1:A:2788:SER:HB2	1.76	0.50
2:B:126:GLN:HE22	2:B:130:ARG:HD2	1.76	0.50
2:B:370:PRO:HD3	2:B:382:PHE:CE1	2.46	0.50
1:A:56:SER:HB3	1:A:3097:ASP:HB2	1.94	0.50
1:A:3838:GLU:OE1	1:A:3874:ARG:NH1	2.43	0.50
2:B:40:PHE:CE2	2:B:83:LEU:HD12	2.45	0.50
1:A:116:THR:HB	1:A:155:LYS:HZ1	1.76	0.50
1:A:1190:LEU:O	1:A:1194:PHE:HB2	2.12	0.50
3:C:608:SER:OG	3:C:611:GLU:OE1	2.30	0.50
1:A:1175:HIS:CE1	1:A:1178:ARG:HB3	2.45	0.50
1:A:1266:CYS:SG	1:A:1267:TYR:N	2.84	0.50
1:A:4042:GLN:OE1	1:A:4043:LYS:NZ	2.44	0.50
2:B:38:LEU:HB3	2:B:83:LEU:HD13	1.94	0.50
3:C:629:THR:HA	3:C:632:PHE:HD2	1.76	0.50
1:A:1825:LEU:HD22	1:A:1879:VAL:HG21	1.93	0.50
3:C:138:LEU:HD12	3:C:205:LEU:HD12	1.93	0.50
3:C:409:PHE:CB	3:C:420:VAL:HG12	2.39	0.50
3:C:633:MET:O	3:C:636:ILE:HG22	2.11	0.50
3:C:652:GLU:O	3:C:656:ASN:ND2	2.44	0.50
1:A:2162:LYS:HG2	1:A:2200:ALA:HA	1.93	0.50
1:A:3310:ASN:C	1:A:3312:VAL:H	2.20	0.50
1:A:3353:GLU:HG2	1:A:3354:ASP:H	1.77	0.50
2:B:265:LYS:HD2	2:B:266:ASP:HB2	1.94	0.50
3:C:475:ASP:OD1	3:C:475:ASP:N	2.45	0.50
1:A:1424:THR:HA	1:A:1468:LEU:HD21	1.93	0.50
3:C:147:LEU:O	3:C:151:ILE:HG12	2.11	0.50
1:A:364:ARG:NH2	1:A:415:GLN:OE1	2.44	0.50
1:A:925:GLN:HA	1:A:2769:VAL:HG12	1.93	0.50
1:A:1852:LYS:HZ2	1:A:1918:LEU:HD23	1.76	0.50
1:A:2572:TYR:N	1:A:2573:PRO:HD3	2.27	0.50
2:B:132:GLN:CD	2:B:137:HIS:HD1	2.20	0.50
1:A:201:LEU:HD11	1:A:244:THR:HG23	1.92	0.49
1:A:852:ARG:HB3	1:A:3111:MET:CE	2.42	0.49
1:A:2255:LEU:O	1:A:2259:LYS:HG2	2.11	0.49
1:A:2383:PHE:CE2	1:A:2408:MET:HE1	2.45	0.49
1:A:3701:ILE:HG22	1:A:3717:VAL:O	2.11	0.49
3:C:161:LEU:HD23	3:C:161:LEU:H	1.77	0.49
3:C:238:LYS:O	3:C:239:LYS:HG3	2.13	0.49
1:A:3051:LEU:HG	1:A:3056:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4084:SER:OG	1:A:4086:ASP:OD1	2.30	0.49
2:B:479:GLU:HG3	2:B:484:GLN:HG3	1.94	0.49
3:C:20:MET:HE1	3:C:31:PHE:HD1	1.77	0.49
1:A:408:TYR:CE1	1:A:453:MET:HE3	2.47	0.49
1:A:1356:TRP:O	1:A:1360:LYS:N	2.45	0.49
3:C:496:HIS:CG	3:C:506:PRO:HG3	2.47	0.49
1:A:447:PRO:HB3	1:A:526:ASP:CB	2.41	0.49
1:A:763:THR:HG23	1:A:851:ILE:HG13	1.94	0.49
1:A:1987:ARG:HH21	1:A:2179:GLY:HA3	1.78	0.49
1:A:2216:LEU:HG	1:A:2220:MET:HE2	1.95	0.49
1:A:2380:ASN:ND2	2:B:192:ASP:OD2	2.46	0.49
1:A:2459:VAL:HB	1:A:2505:VAL:HG21	1.94	0.49
1:A:3960:PRO:O	7:A:4301:HOH:O	2.20	0.49
2:B:195:ASP:OD1	2:B:196:THR:N	2.46	0.49
2:B:263:LEU:HD13	2:B:347:LEU:HD13	1.93	0.49
2:B:526:LYS:HZ3	3:C:256:ASN:HB3	1.77	0.49
5:E:42:DG:H2"	5:E:43:DG:C8	2.48	0.49
1:A:2527:HIS:HB3	1:A:2530:ARG:HH11	1.77	0.49
1:A:1345:THR:HA	1:A:1348:LEU:HD12	1.94	0.49
1:A:1932:GLN:HG2	1:A:1933:LEU:N	2.27	0.49
1:A:2097:LEU:HD23	1:A:2100:LEU:HD21	1.92	0.49
1:A:2190:VAL:HA	1:A:2193:ILE:HG22	1.94	0.49
1:A:2476:ILE:HG21	7:A:4322:HOH:O	2.11	0.49
2:B:257:SER:HB2	2:B:273:ILE:HB	1.95	0.49
3:C:212:MET:HG3	3:C:220:GLY:HA3	1.93	0.49
1:A:167:PRO:O	4:D:12:DT:OP1	2.30	0.49
1:A:2135:ASN:OD1	1:A:2137:ILE:HG12	2.13	0.49
1:A:2225:HIS:O	1:A:2227:LYS:N	2.46	0.49
1:A:3767:LEU:HD13	1:A:3918:LEU:HD22	1.95	0.49
1:A:1990:PHE:HE2	1:A:2144:LEU:HD23	1.76	0.49
1:A:2100:LEU:O	1:A:2104:MET:HG2	2.12	0.49
1:A:2283:ASN:HB2	1:A:2285:LEU:HD13	1.94	0.49
1:A:3536:SER:HB3	1:A:3540:TYR:HE1	1.78	0.49
1:A:3891:SER:O	1:A:3892:THR:HG22	2.13	0.49
1:A:1987:ARG:NH1	1:A:1989:ASN:HA	2.28	0.49
1:A:3052:LEU:HD21	1:A:3058:ASP:O	2.12	0.49
1:A:3680:LEU:HD12	1:A:3682:GLU:H	1.78	0.49
1:A:3754:GLY:HA2	1:A:3800:LEU:HA	1.94	0.49
2:B:368:VAL:HG12	2:B:382:PHE:HE2	1.78	0.49
3:C:653:GLN:HA	3:C:656:ASN:HD21	1.78	0.49
1:A:1105:VAL:HG23	1:A:1171:TRP:CH2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1832:SER:H	1:A:1883:ARG:HH12	1.61	0.49
3:C:296:CYS:O	3:C:297:LEU:HG	2.13	0.49
3:C:447:THR:N	3:C:450:GLN:OE1	2.39	0.49
1:A:384:MET:C	1:A:386:VAL:H	2.19	0.48
1:A:3274:VAL:HG11	1:A:3315:TYR:CE1	2.48	0.48
2:B:290:ARG:HE	3:C:311:ILE:HG23	1.78	0.48
3:C:24:ILE:HG12	3:C:26:GLY:H	1.78	0.48
1:A:1578:ALA:O	1:A:1582:LEU:HB2	2.14	0.48
1:A:1652:ILE:O	1:A:1655:ILE:HG12	2.13	0.48
1:A:1782:PHE:HA	1:A:1785:ILE:HD12	1.94	0.48
1:A:2743:TYR:CD1	1:A:2746:LYS:HD3	2.48	0.48
2:B:183:ALA:HB1	2:B:187:ARG:HH12	1.78	0.48
3:C:312:GLN:HG2	3:C:324:SER:HB2	1.95	0.48
3:C:378:SER:O	3:C:382:HIS:ND1	2.44	0.48
1:A:166:ILE:H	1:A:166:ILE:HG12	1.36	0.48
1:A:639:ALA:O	1:A:641:PHE:N	2.46	0.48
1:A:3150:ASN:C	1:A:3151:LEU:HD23	2.39	0.48
1:A:3676:PRO:HG2	1:A:3677:PRO:HD3	1.95	0.48
2:B:118:GLU:O	2:B:121:GLN:HG2	2.12	0.48
2:B:462:MET:HE3	2:B:525:PHE:CG	2.47	0.48
3:C:151:ILE:HG23	3:C:215:LEU:HD12	1.95	0.48
3:C:519:PRO:HB2	3:C:521:GLU:OE1	2.14	0.48
3:C:601:LEU:O	3:C:604:GLN:HG3	2.14	0.48
1:A:528:VAL:HG13	1:A:529:ASP:N	2.28	0.48
1:A:2202:PRO:HG3	1:A:2245:TRP:CE2	2.48	0.48
1:A:2398:LEU:HA	1:A:2401:VAL:HG12	1.96	0.48
1:A:2538:ARG:NE	1:A:2565:MET:HE2	2.27	0.48
1:A:3123:GLN:HA	1:A:3126:LEU:HB2	1.96	0.48
1:A:3508:LYS:NZ	1:A:3510:GLN:HE21	2.12	0.48
2:B:265:LYS:HD2	2:B:266:ASP:N	2.28	0.48
5:E:18:DA:H1'	5:E:19:DA:OP2	2.13	0.48
1:A:201:LEU:HD21	1:A:248:ILE:HD13	1.95	0.48
1:A:1656:ASP:OD1	1:A:1656:ASP:N	2.44	0.48
1:A:1754:GLN:NE2	1:A:1788:ARG:HD2	2.28	0.48
1:A:1896:ILE:HD13	1:A:1906:THR:O	2.14	0.48
1:A:2183:HIS:HA	1:A:2186:VAL:HG22	1.96	0.48
1:A:2484:TYR:CE2	1:A:2498:ILE:HD11	2.48	0.48
3:C:72:ASP:OD1	3:C:73:GLN:N	2.47	0.48
1:A:275:PHE:HZ	1:A:286:LEU:HD11	1.79	0.48
1:A:639:ALA:HA	1:A:680:ILE:HD11	1.94	0.48
1:A:2872:ASP:HB3	1:A:2875:ALA:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3421:ASP:OD1	1:A:3425:ARG:NE	2.46	0.48
2:B:58:THR:CG2	2:B:61:ASP:H	2.26	0.48
3:C:44:ARG:HD2	3:C:491:PHE:HE2	1.79	0.48
3:C:81:ARG:HG2	3:C:90:LEU:HD11	1.96	0.48
3:C:523:THR:HG22	3:C:527:GLN:NE2	2.29	0.48
3:C:610:GLU:OE1	3:C:613:SER:OG	2.32	0.48
1:A:1298:LEU:HD23	1:A:1367:HIS:HD1	1.77	0.48
1:A:2277:LEU:HA	1:A:2280:VAL:HG12	1.95	0.48
1:A:2336:ILE:HG13	1:A:2336:ILE:O	2.13	0.48
1:A:473:PRO:HG2	1:A:1553:PHE:HZ	1.78	0.48
1:A:1297:PHE:HD2	1:A:1298:LEU:HD12	1.78	0.48
1:A:2197:THR:HG21	1:A:2244:CYS:SG	2.53	0.48
1:A:3351:ILE:HG13	1:A:3351:ILE:O	2.14	0.48
2:B:141:TYR:OH	2:B:172:GLU:OE1	2.30	0.48
2:B:356:LEU:O	2:B:356:LEU:HD12	2.13	0.48
1:A:674:VAL:HG11	1:A:736:LEU:HA	1.96	0.48
1:A:1422:LYS:HG3	1:A:1423:ILE:HG23	1.96	0.48
1:A:1658:SER:O	1:A:1661:PHE:HB3	2.14	0.48
1:A:1836:LEU:HB3	1:A:1840:PHE:CZ	2.49	0.48
1:A:2394:LYS:HD3	1:A:2423:VAL:HG21	1.96	0.48
2:B:443:LYS:HA	3:C:267:ILE:HG13	1.95	0.48
3:C:28:GLU:HB2	3:C:33:GLN:HE21	1.79	0.48
3:C:238:LYS:O	3:C:240:ILE:HG13	2.14	0.48
3:C:265:LYS:HA	3:C:362:LEU:HD23	1.95	0.48
3:C:489:ARG:O	3:C:492:GLN:HG3	2.14	0.48
1:A:1105:VAL:O	1:A:1109:GLU:HG2	2.14	0.48
1:A:1750:LEU:HG	1:A:1785:ILE:HD11	1.95	0.48
1:A:1920:TYR:OH	1:A:1968:SER:O	2.29	0.48
1:A:3335:ARG:O	1:A:3339:ASN:ND2	2.47	0.48
3:C:136:THR:HG22	3:C:138:LEU:N	2.16	0.48
3:C:232:ARG:O	3:C:483:PRO:HD3	2.14	0.48
2:B:278:GLN:HG2	4:D:17:DC:OP2	2.14	0.47
2:B:466:VAL:HG23	3:C:345:PHE:CG	2.49	0.47
1:A:44:LEU:HD21	1:A:819:SER:HA	1.96	0.47
1:A:1208:LEU:HD11	1:A:1220:LEU:HD21	1.95	0.47
1:A:1672:PHE:O	1:A:1676:ILE:HG12	2.14	0.47
1:A:2432:GLN:OE1	1:A:2461:PHE:HE2	1.96	0.47
1:A:2957:LEU:HD23	1:A:2957:LEU:HA	1.78	0.47
1:A:3451:LEU:HD12	1:A:3490:VAL:HG21	1.94	0.47
2:B:361:TYR:OH	3:C:358:GLY:N	2.47	0.47
3:C:381:ILE:HG21	3:C:417:GLU:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:655:PHE:O	3:C:659:LEU:HD23	2.14	0.47
4:D:23:DC:H2'	4:D:24:DA:C8	2.48	0.47
1:A:1857:LYS:HZ1	1:A:1932:GLN:HG3	1.77	0.47
1:A:1914:THR:HA	1:A:1917:LYS:HZ2	1.78	0.47
1:A:2256:ILE:HG22	1:A:2260:PHE:HE1	1.78	0.47
1:A:2938:VAL:O	7:A:4302:HOH:O	2.20	0.47
1:A:2980:ASP:N	1:A:2980:ASP:OD1	2.45	0.47
1:A:3357:ARG:HD2	1:A:3358:ARG:N	2.29	0.47
1:A:4069:GLU:O	1:A:4070:LYS:HG3	2.14	0.47
2:B:277:VAL:HG22	3:C:357:MET:HE1	1.95	0.47
2:B:369:TYR:CG	2:B:370:PRO:HD2	2.50	0.47
1:A:2288:TYR:CE1	1:A:2290:PRO:HA	2.50	0.47
2:B:410:PHE:HE2	3:C:482:ILE:HD11	1.79	0.47
3:C:104:GLN:HG2	3:C:140:SER:HB3	1.97	0.47
3:C:345:PHE:HB3	3:C:389:MET:SD	2.55	0.47
1:A:294:PHE:HE1	1:A:320:LEU:HD21	1.80	0.47
1:A:733:LEU:HA	1:A:736:LEU:HD13	1.96	0.47
3:C:660:LYS:HE2	3:C:685:LEU:HD21	1.96	0.47
1:A:8:VAL:O	1:A:9:ARG:HG2	2.15	0.47
1:A:1297:PHE:CD2	1:A:1298:LEU:HD12	2.48	0.47
1:A:1757:MET:HB3	7:A:4360:HOH:O	2.13	0.47
1:A:3591:ASP:O	1:A:3595:GLU:HG2	2.15	0.47
1:A:3864:ARG:HH21	1:A:3868:VAL:HG21	1.77	0.47
3:C:542:ALA:C	3:C:543:LYS:HD3	2.39	0.47
1:A:164:LYS:HE2	1:A:164:LYS:HB2	1.42	0.47
1:A:529:ASP:N	1:A:529:ASP:OD1	2.44	0.47
1:A:1018:VAL:HB	1:A:1074:LYS:HD3	1.97	0.47
1:A:1221:ILE:HG12	1:A:1288:SER:HB3	1.97	0.47
1:A:1279:LEU:HA	1:A:1358:LEU:HD13	1.97	0.47
1:A:1370:ARG:HA	1:A:1373:VAL:HG12	1.96	0.47
1:A:1912:THR:OG1	1:A:1913:LYS:N	2.47	0.47
1:A:2388:LYS:NZ	2:B:161:MET:HE1	2.30	0.47
1:A:3536:SER:HB3	1:A:3540:TYR:CE1	2.49	0.47
1:A:3918:LEU:HD12	1:A:3918:LEU:O	2.15	0.47
2:B:447:PRO:HD3	3:C:243:HIS:HB3	1.97	0.47
3:C:251:LEU:O	3:C:258:SER:HA	2.15	0.47
1:A:262:LEU:HD21	3:C:553:ILE:HD11	1.96	0.47
1:A:1688:LEU:HG	1:A:1691:GLN:HE21	1.80	0.47
1:A:3278:GLN:O	1:A:3282:ARG:HG2	2.14	0.47
1:A:3598:LYS:HD2	1:A:3599:THR:N	2.29	0.47
1:A:1257:LEU:HD11	1:A:1330:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:THR:O	1:A:1351:THR:HG23	2.15	0.47
1:A:2327:LEU:HA	1:A:2330:VAL:HG22	1.97	0.47
1:A:3727:THR:HG23	1:A:3737:ARG:HG3	1.96	0.47
2:B:143:LEU:HD22	2:B:175:PRO:HG2	1.97	0.47
2:B:271:VAL:HG21	2:B:368:VAL:HG13	1.97	0.47
1:A:165:LYS:HA	1:A:165:LYS:HD3	1.56	0.47
1:A:607:ASP:HB3	1:A:608:PRO:HD3	1.97	0.47
1:A:1684:LEU:HD21	1:A:1688:LEU:HD22	1.96	0.47
1:A:2410:GLU:C	1:A:2412:TYR:H	2.23	0.47
1:A:3291:GLN:HE22	1:A:3299:THR:HG21	1.78	0.47
1:A:3300:VAL:HG11	1:A:3336:ILE:HG21	1.96	0.47
1:A:3421:ASP:OD2	1:A:3467:ARG:NE	2.46	0.47
1:A:268:PRO:O	1:A:272:LEU:HG	2.15	0.46
1:A:1069:HIS:HD2	1:A:1071:ASN:HB3	1.80	0.46
1:A:1781:SER:O	1:A:1785:ILE:HG13	2.14	0.46
1:A:3660:ASN:O	1:A:3663:THR:OG1	2.29	0.46
1:A:1302:ALA:HB2	1:A:1370:ARG:NH1	2.31	0.46
1:A:1984:LEU:HD21	1:A:2142:ILE:CD1	2.45	0.46
1:A:3175:PRO:HB2	1:A:3177:ASN:OD1	2.14	0.46
1:A:3586:LYS:HG3	1:A:3667:LEU:HD23	1.97	0.46
2:B:37:SER:HB3	2:B:154:PHE:HE1	1.79	0.46
1:A:1386:ILE:HA	1:A:1392:MET:SD	2.55	0.46
1:A:3293:CYS:C	1:A:3295:GLU:H	2.22	0.46
2:B:296:VAL:HG21	3:C:310:ILE:HD11	1.96	0.46
2:B:473:TYR:HB3	3:C:350:GLN:HB3	1.97	0.46
1:A:180:LEU:O	1:A:184:VAL:HG22	2.16	0.46
1:A:1852:LYS:HZ1	1:A:1914:THR:CG2	2.26	0.46
1:A:2220:MET:HE1	1:A:2252:PRO:HD2	1.96	0.46
1:A:2536:LEU:HD21	1:A:2832:ILE:HD13	1.98	0.46
1:A:3980:MET:O	1:A:3984:MET:HG3	2.15	0.46
3:C:50:ASN:ND2	3:C:52:ASP:OD2	2.48	0.46
3:C:147:LEU:HD13	3:C:150:ILE:HD11	1.96	0.46
1:A:116:THR:HB	1:A:155:LYS:NZ	2.30	0.46
1:A:809:THR:HB	1:A:2765:GLN:HG3	1.98	0.46
1:A:885:ALA:HB2	1:A:3892:THR:HB	1.97	0.46
1:A:896:VAL:O	1:A:902:LYS:HA	2.15	0.46
1:A:1275:THR:OG1	1:A:1276:VAL:N	2.49	0.46
1:A:3496:ILE:HG21	1:A:3705:TYR:HB3	1.98	0.46
2:B:83:LEU:O	2:B:115:ARG:NH2	2.49	0.46
3:C:219:ASP:OD1	3:C:219:ASP:N	2.48	0.46
1:A:395:MET:HE2	1:A:396:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1351:THR:HB	1:A:1353:PRO:HD2	1.96	0.46
1:A:1579:VAL:O	1:A:1583:MET:HG3	2.16	0.46
1:A:1649:LEU:O	1:A:1653:LEU:HG	2.16	0.46
1:A:2940:ARG:NH1	1:A:2940:ARG:HB3	2.30	0.46
1:A:3445:LEU:HG	1:A:3449:LYS:CE	2.44	0.46
2:B:94:LYS:O	2:B:104:VAL:HG22	2.15	0.46
2:B:388:LYS:HA	2:B:388:LYS:HD3	1.66	0.46
2:B:468:LYS:NZ	2:B:518:LEU:HB3	2.25	0.46
1:A:528:VAL:HB	1:A:632:GLU:OE2	2.14	0.46
1:A:1086:TYR:OH	1:A:1087:ARG:NH1	2.25	0.46
1:A:1668:PHE:HZ	1:A:1702:LEU:HD22	1.79	0.46
1:A:3786:LEU:HB3	1:A:3910:LEU:HD22	1.96	0.46
1:A:3962:ARG:HD2	1:A:4124:TRP:CH2	2.51	0.46
1:A:3999:THR:HG22	1:A:4048:LYS:HG2	1.98	0.46
2:B:176:HIS:HB2	2:B:179:ASP:O	2.16	0.46
2:B:241:ASP:OD1	2:B:242:LEU:N	2.49	0.46
1:A:145:ASP:OD1	1:A:185:HIS:NE2	2.39	0.46
1:A:663:ILE:HG21	1:A:666:PHE:CD2	2.50	0.46
1:A:883:TYR:CD1	1:A:3120:LEU:HD12	2.51	0.46
1:A:1018:VAL:HG11	1:A:1066:LEU:HD22	1.98	0.46
1:A:1575:LEU:HD21	1:A:1618:LEU:HA	1.97	0.46
1:A:2424:MET:HB2	1:A:2424:MET:HE3	1.80	0.46
1:A:1297:PHE:CE1	1:A:1301:ILE:HG21	2.50	0.46
1:A:1854:ARG:NH1	1:A:1856:THR:HA	2.31	0.46
1:A:2962:ARG:O	1:A:2964:ASP:N	2.49	0.46
1:A:3508:LYS:HZ3	1:A:3510:GLN:HG3	1.81	0.46
1:A:3976:GLU:OE1	1:A:3976:GLU:N	2.38	0.46
1:A:1167:ASP:OD1	1:A:1167:ASP:N	2.49	0.45
1:A:2743:TYR:HA	1:A:2746:LYS:HB3	1.99	0.45
2:B:488:ARG:HD2	2:B:503:ALA:HB2	1.97	0.45
3:C:533:ILE:HG23	3:C:537:PHE:HD2	1.77	0.45
3:C:616:LEU:HD22	3:C:642:PHE:CE2	2.51	0.45
1:A:525:LYS:O	1:A:528:VAL:HG12	2.16	0.45
1:A:643:GLU:O	1:A:646:VAL:HG22	2.16	0.45
1:A:859:LEU:HD22	1:A:870:LEU:HD11	1.98	0.45
1:A:871:LEU:HD11	1:A:3125:ARG:HD3	1.99	0.45
1:A:1799:GLU:O	1:A:1803:GLU:HG2	2.16	0.45
1:A:3294:SER:HB2	1:A:3351:ILE:HD11	1.97	0.45
1:A:3929:MET:HG2	1:A:3940:ILE:HG13	1.98	0.45
2:B:85:VAL:HG21	2:B:119:LEU:HD21	1.99	0.45
3:C:133:GLU:OE1	3:C:162:GLN:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:328:GLU:O	3:C:332:LYS:HB3	2.17	0.45
1:A:670:LEU:HB3	1:A:732:PHE:CD1	2.51	0.45
1:A:2122:LEU:CB	1:A:2126:MET:HE2	2.45	0.45
1:A:2428:ASP:O	1:A:2432:GLN:HG3	2.17	0.45
1:A:2929:LEU:O	1:A:2932:SER:OG	2.33	0.45
1:A:3294:SER:HB3	1:A:3348:LEU:HD22	1.98	0.45
1:A:3296:GLN:O	1:A:3300:VAL:HG22	2.16	0.45
1:A:4039:TYR:HB3	1:A:4040:PRO:HD3	1.98	0.45
1:A:4090:ARG:NH1	1:A:4109:ASP:OD2	2.47	0.45
1:A:290:TYR:CZ	1:A:337:LYS:HG2	2.51	0.45
1:A:447:PRO:HB3	1:A:526:ASP:HB3	1.99	0.45
1:A:1082:PHE:HA	1:A:1085:ILE:HG12	1.98	0.45
1:A:1984:LEU:HD23	1:A:1984:LEU:HA	1.72	0.45
2:B:58:THR:HG23	2:B:61:ASP:H	1.82	0.45
3:C:327:ASP:O	3:C:331:MET:HG2	2.16	0.45
3:C:398:ASP:OD1	3:C:401:ALA:N	2.45	0.45
4:D:4:DG:H2"	4:D:5:DC:C6	2.51	0.45
1:A:1369:MET:CB	1:A:1418:HIS:CD2	2.94	0.45
1:A:2800:ARG:HD2	1:A:2800:ARG:HA	1.85	0.45
2:B:262:LYS:HD2	2:B:346:MET:HG2	1.99	0.45
3:C:167:PHE:HD2	3:C:192:PHE:HA	1.81	0.45
1:A:306:VAL:HG13	1:A:307:GLU:HG2	1.99	0.45
1:A:1118:GLU:CD	1:A:1119:LYS:H	2.24	0.45
1:A:1149:LYS:NZ	1:A:1151:ARG:HH21	2.14	0.45
1:A:1563:PHE:O	1:A:1565:GLU:N	2.49	0.45
1:A:2540:LEU:HD21	1:A:2832:ILE:HG23	1.98	0.45
1:A:3310:ASN:O	1:A:3312:VAL:HG23	2.17	0.45
2:B:289:TYR:CE2	2:B:291:GLU:HB2	2.52	0.45
3:C:36:LYS:O	3:C:39:THR:HG22	2.17	0.45
3:C:313:GLY:HA2	3:C:321:VAL:O	2.17	0.45
1:A:646:VAL:HG21	1:A:682:TYR:CZ	2.51	0.45
1:A:833:HIS:HA	1:A:836:LYS:HZ1	1.81	0.45
1:A:865:GLN:HG2	1:A:3170:ASP:HA	1.97	0.45
1:A:959:TYR:CE2	1:A:963:LYS:HD2	2.51	0.45
1:A:1619:ALA:O	1:A:1623:LEU:HD23	2.16	0.45
1:A:1863:PHE:HE2	1:A:1932:GLN:HE21	1.65	0.45
1:A:1992:VAL:HG21	1:A:2225:HIS:CD2	2.51	0.45
1:A:3361:GLU:C	1:A:3380:ARG:HH22	2.25	0.45
1:A:3460:GLU:H	1:A:3460:GLU:CD	2.24	0.45
1:A:3527:GLN:HG3	1:A:3700:GLU:OE1	2.17	0.45
1:A:4088:ASN:HB3	1:A:4109:ASP:OD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:462:MET:HE3	2:B:525:PHE:CD1	2.52	0.45
1:A:121:ALA:HB2	1:A:167:PRO:CG	2.44	0.45
1:A:139:ARG:NE	1:A:184:VAL:HG12	2.32	0.45
1:A:1067:ALA:O	1:A:1075:ARG:HG2	2.16	0.45
1:A:1653:LEU:HD13	1:A:1698:PHE:CG	2.52	0.45
1:A:2384:PHE:CD1	2:B:155:SER:HB2	2.51	0.45
1:A:3820:MET:HE3	1:A:3882:LEU:HD11	1.98	0.45
3:C:165:LEU:HD23	3:C:224:ILE:HD11	1.99	0.45
1:A:863:GLY:HA2	1:A:3167:ARG:HG3	1.98	0.45
1:A:1057:LYS:HG2	1:A:1061:LYS:NZ	2.31	0.45
1:A:1218:SER:O	1:A:1221:ILE:HG22	2.17	0.45
1:A:2097:LEU:HA	1:A:2100:LEU:CD2	2.47	0.45
1:A:2420:PHE:O	1:A:2423:VAL:HG12	2.17	0.45
1:A:2440:TYR:CD1	1:A:2476:ILE:HG22	2.50	0.45
1:A:2943:PHE:CD1	1:A:2949:THR:HG21	2.52	0.45
1:A:3585:PHE:CD1	1:A:3617:LEU:HD23	2.52	0.45
3:C:153:SER:HA	3:C:156:LYS:HG2	1.98	0.45
1:A:147:PHE:O	1:A:149:ILE:N	2.50	0.45
1:A:1930:GLU:HG2	1:A:1937:ARG:HH12	1.83	0.45
1:A:3512:VAL:C	1:A:3514:VAL:H	2.24	0.45
2:B:298:THR:HA	3:C:295:TYR:HA	1.98	0.45
3:C:528:ILE:HB	3:C:529:PRO:HD3	1.98	0.45
1:A:1438:GLY:O	1:A:1445:ARG:NH2	2.39	0.44
1:A:2202:PRO:HG3	1:A:2245:TRP:NE1	2.31	0.44
2:B:331:LYS:NZ	2:B:335:GLU:OE2	2.46	0.44
3:C:53:GLU:OE1	3:C:85:LEU:HD22	2.17	0.44
3:C:134:ILE:HB	3:C:163:PHE:HD1	1.82	0.44
3:C:659:LEU:HD13	3:C:662:LEU:HD21	1.99	0.44
1:A:1202:ARG:CB	1:A:1206:LEU:HD11	2.47	0.44
1:A:1525:CYS:HB2	1:A:1574:ASN:HD21	1.81	0.44
1:A:3117:ILE:HG23	1:A:3121:LEU:HD23	2.00	0.44
2:B:48:MET:HG2	2:B:59:PRO:HG2	2.00	0.44
2:B:362:LEU:HD11	2:B:409:TYR:OH	2.17	0.44
1:A:204:LEU:HD13	1:A:223:CYS:SG	2.57	0.44
1:A:1554:SER:C	1:A:1556:GLY:H	2.26	0.44
1:A:1655:ILE:HG13	1:A:1656:ASP:N	2.31	0.44
2:B:492:ALA:O	2:B:496:ASP:N	2.51	0.44
4:D:18:DT:H2"	4:D:19:DG:C8	2.52	0.44
1:A:208:MET:HG3	1:A:220:LEU:HD21	1.99	0.44
1:A:2201:THR:HG23	1:A:2201:THR:O	2.18	0.44
1:A:2943:PHE:HD1	1:A:2949:THR:HG21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3610:TYR:CE1	1:A:3652:LEU:HD13	2.53	0.44
2:B:259:LEU:HB3	2:B:344:GLY:HA2	1.98	0.44
3:C:544:LYS:C	3:C:545:LYS:HD2	2.43	0.44
3:C:597:ASN:OD1	3:C:598:PHE:N	2.50	0.44
1:A:158:GLY:O	1:A:162:LEU:HG	2.17	0.44
1:A:1424:THR:O	1:A:1428:ILE:HG12	2.18	0.44
1:A:1810:PRO:HB2	3:C:669:LYS:NZ	2.33	0.44
1:A:1955:VAL:O	1:A:1955:VAL:HG23	2.18	0.44
1:A:2085:MET:O	1:A:2085:MET:HG2	2.17	0.44
1:A:2216:LEU:HD13	1:A:2241:LEU:HD22	2.00	0.44
2:B:126:GLN:O	2:B:130:ARG:HG3	2.17	0.44
3:C:302:GLU:CD	3:C:302:GLU:N	2.75	0.44
1:A:240:GLU:OE1	1:A:240:GLU:N	2.51	0.44
1:A:484:HIS:HD2	1:A:574:LYS:HE3	1.83	0.44
1:A:928:VAL:HG11	1:A:2769:VAL:HG11	1.99	0.44
1:A:1592:MET:O	1:A:1596:VAL:HG23	2.18	0.44
1:A:1717:LEU:O	1:A:1721:HIS:HB2	2.18	0.44
1:A:1729:PHE:CE2	1:A:1736:PHE:HA	2.53	0.44
1:A:2560:ASN:O	1:A:2564:GLU:HG2	2.18	0.44
1:A:3269:ARG:HH21	1:A:3271:ASP:CG	2.23	0.44
1:A:3359:ILE:HG13	1:A:3360:LEU:N	2.31	0.44
1:A:3385:LEU:HB3	1:A:3416:LEU:CD2	2.48	0.44
2:B:290:ARG:HB3	3:C:309:ASP:OD1	2.18	0.44
2:B:422:ASP:OD1	2:B:422:ASP:N	2.51	0.44
3:C:616:LEU:HA	3:C:619:HIS:ND1	2.32	0.44
1:A:79:ARG:HG3	1:A:80:GLU:N	2.33	0.44
1:A:835:LYS:O	1:A:838:LYS:HG2	2.18	0.44
1:A:1257:LEU:HD11	1:A:1330:TYR:HE1	1.83	0.44
1:A:1373:VAL:HG23	1:A:1419:LEU:HD23	2.00	0.44
1:A:1684:LEU:HD11	1:A:1688:LEU:HD22	2.00	0.44
1:A:2481:HIS:O	1:A:2485:ARG:HG3	2.18	0.44
1:A:3020:ASP:HB2	1:A:3025:PRO:HD3	2.00	0.44
2:B:483:LEU:HG	2:B:487:PHE:CE2	2.53	0.44
1:A:330:ASN:O	1:A:334:HIS:HD2	2.01	0.44
1:A:1224:PHE:CE2	1:A:1267:TYR:HB3	2.52	0.44
1:A:1358:LEU:HD23	1:A:1358:LEU:H	1.83	0.44
1:A:1812:LEU:HG	3:C:625:ASP:OD1	2.18	0.44
1:A:1832:SER:HB3	1:A:1836:LEU:HD22	1.99	0.44
1:A:2886:GLN:HB2	1:A:2933:ILE:HD11	1.99	0.44
1:A:3620:PRO:HA	1:A:3633:ILE:HG12	1.99	0.44
2:B:40:PHE:HE2	2:B:83:LEU:HD12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:167:PHE:HB2	3:C:191:SER:O	2.18	0.44
3:C:365:PHE:O	3:C:377:LEU:HD23	2.17	0.44
3:C:380:LEU:O	3:C:384:LEU:HD23	2.17	0.44
1:A:392:CYS:HG	1:A:396:PHE:HD2	1.63	0.44
1:A:759:GLY:HA3	1:A:766:ALA:HB2	2.00	0.44
1:A:863:GLY:O	1:A:867:ASN:HB2	2.18	0.44
1:A:903:PRO:HB3	1:A:2819:GLU:HG3	1.99	0.44
1:A:3797:THR:HG23	1:A:3798:SER:O	2.17	0.44
1:A:3883:LEU:HD23	1:A:3883:LEU:HA	1.88	0.44
2:B:250:GLU:HB3	2:B:252:ARG:HH22	1.83	0.44
2:B:438:PRO:CG	3:C:267:ILE:HD11	2.48	0.44
2:B:447:PRO:HA	3:C:243:HIS:CE1	2.53	0.44
2:B:485:GLN:HG3	2:B:489:ASN:HD21	1.82	0.44
3:C:53:GLU:HG3	3:C:127:PHE:HZ	1.82	0.44
3:C:413:LYS:HB3	3:C:416:TYR:O	2.17	0.44
1:A:942:LEU:HD11	1:A:991:LEU:HD21	2.00	0.43
1:A:1195:VAL:HG23	1:A:1196:PRO:HD3	1.98	0.43
1:A:1212:LEU:HD21	1:A:1220:LEU:HD12	2.00	0.43
1:A:1966:LEU:O	1:A:1977:ILE:HD13	2.18	0.43
1:A:2500:LYS:HE3	1:A:2500:LYS:HB2	1.83	0.43
1:A:3887:PHE:O	1:A:3891:SER:HB3	2.18	0.43
2:B:348:MET:SD	3:C:518:PRO:HD3	2.58	0.43
3:C:261:ILE:CG1	3:C:364:VAL:HB	2.48	0.43
1:A:710:PHE:O	1:A:714:VAL:HG23	2.18	0.43
1:A:935:HIS:O	1:A:939:MET:HG2	2.19	0.43
1:A:1195:VAL:CG2	1:A:1196:PRO:HD3	2.48	0.43
1:A:1892:LYS:NZ	1:A:1907:GLU:HA	2.33	0.43
1:A:3103:ILE:HD12	1:A:3103:ILE:HA	1.88	0.43
1:A:3641:ASP:OD1	1:A:3641:ASP:N	2.52	0.43
1:A:3992:ARG:NH1	1:A:4103:GLN:OE1	2.50	0.43
1:A:4050:LYS:HE2	1:A:4059:ILE:HG21	2.00	0.43
3:C:280:ASP:N	3:C:280:ASP:OD1	2.49	0.43
1:A:167:PRO:O	4:D:12:DT:P	2.76	0.43
1:A:2568:MET:O	1:A:2568:MET:HG3	2.18	0.43
1:A:3019:ILE:HG13	1:A:3020:ASP:N	2.32	0.43
2:B:446:MET:HB3	2:B:447:PRO:HD2	1.99	0.43
3:C:537:PHE:HD1	3:C:538:PRO:HD2	1.84	0.43
1:A:149:ILE:HG23	1:A:181:LEU:HD22	2.00	0.43
1:A:248:ILE:O	1:A:252:VAL:HG23	2.19	0.43
1:A:969:LEU:HD23	1:A:969:LEU:HA	1.83	0.43
1:A:1731:PRO:HA	1:A:1736:PHE:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1880:MET:O	1:A:1884:LEU:HB2	2.19	0.43
1:A:2091:HIS:O	1:A:2091:HIS:CG	2.71	0.43
1:A:3271:ASP:HB3	1:A:3315:TYR:CE2	2.54	0.43
1:A:3387:GLU:OE2	1:A:3390:GLN:NE2	2.51	0.43
2:B:207:LYS:HB2	2:B:208:PRO:HD3	2.00	0.43
2:B:446:MET:HE1	3:C:363:LYS:HB2	2.00	0.43
2:B:458:GLN:HB3	2:B:525:PHE:HE1	1.83	0.43
3:C:385:ASP:OD1	3:C:386:ASP:N	2.51	0.43
1:A:528:VAL:HG13	1:A:529:ASP:H	1.82	0.43
1:A:1721:HIS:C	1:A:1722:PHE:HD1	2.27	0.43
1:A:3599:THR:HG22	1:A:3601:VAL:HG13	2.00	0.43
3:C:150:ILE:O	3:C:154:LEU:HG	2.18	0.43
3:C:524:THR:HA	3:C:527:GLN:OE1	2.19	0.43
1:A:14:ARG:O	1:A:17:GLU:HG2	2.18	0.43
1:A:79:ARG:HD3	1:A:122:LYS:HE2	2.00	0.43
1:A:1776:GLU:CD	1:A:1776:GLU:H	2.26	0.43
1:A:1802:TYR:CZ	1:A:1806:ARG:HD3	2.54	0.43
1:A:3412:ALA:HA	1:A:3415:THR:HG22	2.01	0.43
1:A:3961:PHE:CE1	1:A:4107:LEU:HG	2.50	0.43
4:D:5:DC:H2'	4:D:6:DT:H71	2.00	0.43
1:A:582:THR:C	1:A:615:ALA:HB2	2.44	0.43
1:A:1689:LYS:O	1:A:1693:VAL:HG13	2.19	0.43
1:A:1790:SER:O	1:A:1793:THR:HG22	2.18	0.43
1:A:1881:TYR:CE1	1:A:1889:VAL:HG11	2.49	0.43
1:A:2417:SER:OG	2:B:152:ASN:OD1	2.26	0.43
1:A:2763:MET:HA	1:A:2766:ASP:HB2	1.99	0.43
1:A:2952:ILE:HD11	1:A:2981:TRP:HH2	1.83	0.43
1:A:2987:THR:O	1:A:2991:LYS:HG2	2.19	0.43
1:A:3851:ASP:OD2	1:A:3851:ASP:N	2.51	0.43
2:B:518:LEU:HD12	2:B:519:GLY:N	2.32	0.43
3:C:14:MET:SD	3:C:58:LEU:HD22	2.59	0.43
1:A:1661:PHE:HA	1:A:1668:PHE:HE2	1.83	0.43
1:A:1984:LEU:HD11	1:A:2142:ILE:HD11	2.01	0.43
1:A:2140:LEU:HG	1:A:2144:LEU:HD13	2.01	0.43
1:A:2392:VAL:HG23	1:A:2393:LEU:HD12	2.00	0.43
1:A:3472:ILE:HG13	1:A:3483:MET:CE	2.49	0.43
1:A:346:TYR:O	1:A:350:ARG:HG2	2.17	0.43
1:A:579:LEU:HD23	1:A:581:LEU:HD21	2.00	0.43
1:A:732:PHE:CZ	1:A:736:LEU:HD11	2.54	0.43
1:A:810:LYS:HE3	1:A:2514:ASN:HA	2.00	0.43
1:A:2139:PRO:HG2	1:A:2142:ILE:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2253:TYR:C	1:A:2255:LEU:H	2.26	0.43
1:A:2300:PHE:HB3	1:A:2341:LEU:HD11	1.99	0.43
1:A:2517:LEU:O	1:A:2521:ILE:HD12	2.19	0.43
1:A:2806:LYS:HG2	1:A:2857:CYS:HB2	2.01	0.43
1:A:4120:THR:OG1	1:A:4126:PRO:HG3	2.19	0.43
2:B:43:ASP:OD2	2:B:170:THR:OG1	2.32	0.43
1:A:670:LEU:O	1:A:674:VAL:HG23	2.19	0.43
1:A:1282:LEU:HB3	1:A:1358:LEU:HD12	1.99	0.43
1:A:1820:VAL:O	1:A:1825:LEU:HG	2.19	0.43
1:A:2288:TYR:O	1:A:2289:ASP:C	2.62	0.43
3:C:365:PHE:HE1	3:C:418:CYS:HB3	1.84	0.43
1:A:135:LEU:HD12	1:A:177:LEU:HD11	1.99	0.42
1:A:249:PHE:HD1	1:A:282:PHE:CE2	2.37	0.42
1:A:900:GLU:HG3	1:A:901:MET:HG3	2.01	0.42
1:A:1775:GLU:O	1:A:1778:PHE:HB2	2.19	0.42
1:A:2259:LYS:O	1:A:2270:ASN:HA	2.19	0.42
1:A:3483:MET:N	7:A:4330:HOH:O	2.43	0.42
3:C:165:LEU:O	3:C:226:SER:HA	2.19	0.42
1:A:1650:ALA:O	1:A:1654:GLN:HB2	2.20	0.42
1:A:2745:ARG:O	1:A:2748:VAL:HG12	2.19	0.42
1:A:3484:THR:HG22	1:A:3513:ALA:CB	2.42	0.42
1:A:3820:MET:HB2	1:A:3825:LYS:HG3	2.00	0.42
1:A:3917:ILE:HD12	1:A:4051:LEU:HD13	2.01	0.42
1:A:4070:LYS:HD2	1:A:4070:LYS:O	2.19	0.42
2:B:355:LEU:HD12	3:C:475:ASP:HB3	2.01	0.42
3:C:9:ALA:HB1	3:C:83:LEU:HD22	2.01	0.42
3:C:311:ILE:HB	3:C:324:SER:HB3	2.01	0.42
4:D:16:DG:N2	5:E:28:DC:N3	2.62	0.42
1:A:1571:LEU:HD22	1:A:1578:ALA:HB1	2.01	0.42
1:A:1833:LEU:HD23	1:A:1835:ALA:C	2.45	0.42
1:A:1881:TYR:HE2	1:A:1915:LEU:HD21	1.85	0.42
1:A:2442:MET:HE2	1:A:2446:LEU:HD21	2.01	0.42
1:A:2476:ILE:HD13	7:A:4322:HOH:O	2.19	0.42
1:A:3680:LEU:CD1	1:A:3682:GLU:HB2	2.49	0.42
2:B:83:LEU:O	2:B:108:LEU:HA	2.19	0.42
2:B:352:PRO:O	2:B:355:LEU:HD23	2.19	0.42
3:C:165:LEU:HD12	3:C:166:PRO:O	2.19	0.42
3:C:666:VAL:HG23	3:C:675:TRP:NE1	2.34	0.42
1:A:89:LEU:HA	1:A:89:LEU:HD23	1.79	0.42
1:A:723:ASP:OD1	1:A:723:ASP:N	2.51	0.42
1:A:947:GLN:HB3	1:A:949:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1344:PHE:O	1:A:1348:LEU:HG	2.20	0.42
1:A:1825:LEU:HD23	1:A:1825:LEU:HA	1.90	0.42
1:A:1915:LEU:O	1:A:1918:LEU:HG	2.20	0.42
1:A:2785:ILE:HG12	1:A:2789:SER:OG	2.20	0.42
1:A:2788:SER:O	1:A:2792:THR:HB	2.19	0.42
1:A:3281:CYS:SG	1:A:3329:LEU:HD13	2.59	0.42
1:A:4076:ASP:O	1:A:4080:VAL:HG23	2.19	0.42
3:C:653:GLN:HG2	3:C:654:ARG:H	1.84	0.42
1:A:631:ARG:HH21	1:A:668:LYS:HD3	1.84	0.42
1:A:1102:GLU:O	1:A:1106:ILE:HG12	2.19	0.42
1:A:1812:LEU:HG	3:C:625:ASP:CG	2.44	0.42
1:A:1946:ASN:ND2	1:A:2092:GLU:O	2.50	0.42
1:A:2363:CYS:O	1:A:2367:VAL:HG23	2.19	0.42
1:A:2394:LYS:HD3	1:A:2423:VAL:CG2	2.50	0.42
1:A:3577:GLN:NE2	1:A:3577:GLN:O	2.53	0.42
2:B:71:TYR:HB3	2:B:116:ILE:HG12	2.02	0.42
2:B:461:LYS:NZ	2:B:524:GLU:OE1	2.53	0.42
4:D:16:DG:OP2	7:D:101:HOH:O	2.22	0.42
1:A:275:PHE:HE2	1:A:319:PHE:HB2	1.84	0.42
1:A:1186:LYS:O	1:A:1190:LEU:HD23	2.19	0.42
1:A:2855:VAL:O	1:A:2859:GLN:HG3	2.19	0.42
1:A:3310:ASN:CG	1:A:3311:ASN:H	2.26	0.42
1:A:3772:ASN:HA	1:A:3775:LEU:HB3	2.01	0.42
2:B:302:THR:HA	3:C:291:LYS:HA	2.01	0.42
2:B:455:THR:OG1	2:B:458:GLN:OE1	2.32	0.42
1:A:1342:MET:HB3	1:A:1402:LEU:HD22	2.01	0.42
1:A:2166:SER:O	1:A:2170:GLN:HB3	2.20	0.42
1:A:2458:VAL:CG1	1:A:2476:ILE:HD11	2.45	0.42
1:A:2557:LEU:O	1:A:2560:ASN:HB3	2.20	0.42
1:A:3554:PHE:O	1:A:3557:ARG:HG2	2.20	0.42
2:B:78:SER:O	2:B:80:ARG:N	2.50	0.42
3:C:688:LYS:HE3	3:C:693:GLY:HA2	2.02	0.42
1:A:493:LYS:HE3	1:A:527:TYR:OH	2.19	0.42
1:A:753:GLN:HB2	1:A:795:CYS:SG	2.60	0.42
1:A:1185:HIS:O	1:A:1189:GLU:HG3	2.20	0.42
1:A:1189:GLU:O	1:A:1193:LYS:HG2	2.20	0.42
1:A:2124:SER:HA	1:A:2127:LYS:HE2	2.01	0.42
1:A:3118:ASP:OD2	1:A:3120:LEU:HD23	2.19	0.42
1:A:3819:THR:HG21	1:A:3882:LEU:O	2.20	0.42
3:C:39:THR:HA	3:C:42:VAL:HG12	2.02	0.42
3:C:250:ARG:HG2	3:C:260:ARG:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLN:O	1:A:139:ARG:HG2	2.20	0.42
1:A:431:TYR:O	1:A:434:VAL:HG12	2.19	0.42
1:A:758:LEU:HB2	1:A:765:LEU:HD23	2.01	0.42
1:A:774:GLU:O	1:A:778:ILE:HD12	2.20	0.42
1:A:1147:LYS:HE2	1:A:1149:LYS:HD3	2.00	0.42
1:A:1576:ASP:OD1	1:A:1577:LEU:N	2.51	0.42
1:A:1611:GLN:CD	1:A:1614:GLN:HB3	2.45	0.42
1:A:1777:LEU:HD23	1:A:1777:LEU:HA	1.76	0.42
1:A:1887:ASP:OD1	1:A:1888:ASP:N	2.52	0.42
1:A:2443:MET:HE1	1:A:2479:TRP:CD2	2.55	0.42
1:A:3356:ALA:HA	1:A:3359:ILE:HG12	2.02	0.42
1:A:3481:SER:HA	1:A:3484:THR:CG2	2.50	0.42
2:B:42:VAL:HA	2:B:169:PHE:HB2	2.01	0.42
2:B:143:LEU:HA	2:B:146:VAL:HG12	2.00	0.42
2:B:299:LYS:HB3	2:B:299:LYS:HE2	1.85	0.42
2:B:334:THR:HA	2:B:337:LEU:HD22	2.01	0.42
2:B:381:LEU:O	2:B:385:LEU:HD23	2.20	0.42
3:C:62:ASP:HA	3:C:103:GLN:OE1	2.20	0.42
3:C:484:ASN:HB3	3:C:487:PHE:CE1	2.55	0.42
1:A:381:VAL:HG22	1:A:424:LEU:HB3	2.00	0.42
1:A:989:MET:SD	1:A:1035:GLU:HG3	2.59	0.42
1:A:1143:VAL:HG13	1:A:1197:LEU:HD11	2.01	0.42
1:A:1992:VAL:HG21	1:A:2225:HIS:HD2	1.83	0.42
1:A:2432:GLN:OE1	1:A:2464:HIS:NE2	2.53	0.42
1:A:2533:SER:HA	1:A:2565:MET:CE	2.50	0.42
1:A:2870:SER:HB3	1:A:2899:ARG:HH12	1.84	0.42
1:A:3062:LEU:HD22	1:A:3093:GLN:NE2	2.35	0.42
1:A:3387:GLU:O	1:A:3390:GLN:HG3	2.20	0.42
3:C:64:THR:HG21	3:C:74:TYR:O	2.19	0.42
3:C:371:GLU:HB2	3:C:374:ALA:HB3	2.02	0.42
3:C:413:LYS:HD2	3:C:414:HIS:H	1.85	0.42
1:A:296:VAL:O	1:A:299:LYS:HG3	2.20	0.41
1:A:891:ARG:HD3	1:A:956:PRO:HB2	2.02	0.41
1:A:986:PRO:O	1:A:989:MET:N	2.53	0.41
1:A:1601:LEU:HD13	1:A:1651:LYS:HB3	2.02	0.41
1:A:1802:TYR:OH	1:A:1806:ARG:HD3	2.20	0.41
1:A:2126:MET:HE1	1:A:2160:TYR:CD2	2.54	0.41
1:A:2287:PRO:HG3	1:A:2326:ILE:HG23	2.02	0.41
1:A:3493:TRP:C	1:A:3495:PHE:H	2.28	0.41
1:A:3530:VAL:HG11	1:A:3568:ILE:HG21	2.02	0.41
2:B:219:ASP:OD1	2:B:220:ILE:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:409:PHE:HA	3:C:410:PRO:HD3	1.88	0.41
3:C:629:THR:OG1	3:C:630:PRO:HD3	2.19	0.41
1:A:208:MET:HE1	1:A:251:PHE:O	2.19	0.41
1:A:1088:GLU:C	1:A:1090:ARG:H	2.28	0.41
1:A:1148:ALA:CA	1:A:1164:CYS:HB3	2.50	0.41
1:A:1208:LEU:HD12	1:A:1208:LEU:HA	1.88	0.41
1:A:3725:ARG:H	1:A:3725:ARG:HD3	1.85	0.41
2:B:505:ASP:OD2	2:B:508:LEU:HG	2.20	0.41
3:C:364:VAL:HG22	3:C:419:LEU:O	2.20	0.41
3:C:512:ILE:HD13	3:C:512:ILE:HA	1.90	0.41
1:A:538:ASP:OD1	1:A:539:GLN:N	2.53	0.41
1:A:805:LEU:O	1:A:805:LEU:HD23	2.21	0.41
1:A:949:PRO:CB	1:A:954:GLY:O	2.68	0.41
1:A:2547:SER:O	1:A:2547:SER:OG	2.35	0.41
1:A:3530:VAL:HA	1:A:3562:LEU:HD23	2.02	0.41
1:A:3663:THR:O	1:A:3666:LEU:HG	2.20	0.41
1:A:3887:PHE:HZ	1:A:3904:PHE:CD1	2.39	0.41
2:B:279:LYS:HB2	3:C:357:MET:HE3	2.02	0.41
3:C:356:PHE:HB3	3:C:422:VAL:HG11	2.02	0.41
3:C:725:VAL:O	3:C:728:LEU:HB3	2.20	0.41
1:A:12:LEU:HD21	1:A:64:GLY:HA2	2.02	0.41
1:A:859:LEU:CD2	1:A:870:LEU:HD11	2.50	0.41
1:A:1538:LEU:HG	1:A:1555:HIS:HB2	2.01	0.41
1:A:1865:THR:O	1:A:1869:LYS:HG2	2.20	0.41
1:A:3873:LYS:HG3	1:A:3877:LYS:NZ	2.36	0.41
2:B:362:LEU:HD21	2:B:409:TYR:OH	2.20	0.41
1:A:440:VAL:HG23	1:A:482:VAL:HG23	2.02	0.41
1:A:2746:LYS:O	1:A:2749:ALA:HB3	2.21	0.41
1:A:3154:GLN:HG2	1:A:3227:ILE:HD11	2.02	0.41
1:A:3522:THR:HG21	1:A:3558:ILE:HG23	2.01	0.41
2:B:212:ASP:OD1	2:B:212:ASP:N	2.51	0.41
3:C:188:HIS:CD2	3:C:478:PRO:HD2	2.55	0.41
4:D:20:DG:H2"	4:D:21:DA:C8	2.56	0.41
1:A:1018:VAL:HG23	1:A:1018:VAL:O	2.20	0.41
1:A:1082:PHE:HB2	1:A:1107:TYR:OH	2.20	0.41
1:A:1960:LYS:HD3	1:A:2123:PRO:HG2	2.02	0.41
1:A:2146:LEU:O	1:A:2150:VAL:HG23	2.21	0.41
1:A:2894:GLU:OE2	1:A:3974:MET:HE1	2.21	0.41
1:A:3169:PRO:HG3	1:A:3182:ILE:HG13	2.01	0.41
1:A:3259:LEU:HD23	1:A:3259:LEU:HA	1.96	0.41
1:A:3361:GLU:C	1:A:3380:ARG:HH12	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3962:ARG:HE	1:A:3964:THR:HG21	1.86	0.41
3:C:42:VAL:HG13	3:C:91:LEU:HD13	2.03	0.41
1:A:253:LEU:HG	1:A:257:ARG:HD2	2.03	0.41
1:A:1247:PRO:HG3	1:A:1303:MET:SD	2.60	0.41
1:A:2253:TYR:HE2	1:A:2289:ASP:HB2	1.85	0.41
1:A:2386:LEU:HD13	1:A:2397:CYS:HB3	2.03	0.41
1:A:2506:LEU:HD23	1:A:2506:LEU:HA	1.84	0.41
1:A:3022:GLU:HG2	1:A:3022:GLU:O	2.21	0.41
1:A:3121:LEU:O	1:A:3124:SER:HB2	2.21	0.41
1:A:3542:PHE:HZ	1:A:3555:VAL:HG21	1.85	0.41
1:A:3634:GLN:HG3	1:A:3635:THR:N	2.36	0.41
2:B:484:GLN:HB3	2:B:488:ARG:NH1	2.35	0.41
2:B:511:VAL:HA	2:B:514:MET:HE2	2.02	0.41
3:C:163:PHE:CE2	3:C:165:LEU:HB3	2.56	0.41
3:C:537:PHE:CD1	3:C:538:PRO:HD2	2.55	0.41
3:C:672:ASN:OD1	3:C:673:HIS:ND1	2.54	0.41
1:A:678:LYS:NZ	1:A:735:SER:O	2.40	0.41
1:A:1146:ASN:HD21	1:A:1165:LEU:HB3	1.86	0.41
1:A:1563:PHE:C	1:A:1565:GLU:H	2.27	0.41
1:A:2104:MET:HA	1:A:2107:SER:HB3	2.03	0.41
1:A:3493:TRP:NE1	1:A:3710:LYS:HG3	2.36	0.41
1:A:3907:SER:O	1:A:3911:ILE:HG23	2.20	0.41
3:C:20:MET:HE1	3:C:31:PHE:HA	2.01	0.41
1:A:260:ILE:HG12	3:C:553:ILE:HG13	2.03	0.41
1:A:487:LEU:HD23	1:A:487:LEU:HA	1.91	0.41
1:A:660:LEU:HB3	7:A:4432:HOH:O	2.21	0.41
1:A:737:PRO:O	1:A:739:ASN:N	2.54	0.41
1:A:948:MET:H	1:A:949:PRO:HD2	1.80	0.41
1:A:1301:ILE:C	1:A:1303:MET:H	2.28	0.41
1:A:1817:GLN:HB2	1:A:1868:THR:HG23	2.03	0.41
1:A:2262:GLY:C	1:A:2263:LYS:HD2	2.45	0.41
1:A:2339:GLU:HG2	1:A:2340:SER:N	2.36	0.41
1:A:2371:PHE:CZ	1:A:2373:PRO:HG2	2.56	0.41
1:A:2439:ILE:O	1:A:2443:MET:CB	2.62	0.41
1:A:2533:SER:N	7:A:4353:HOH:O	2.48	0.41
1:A:2963:SER:HB2	1:A:3250:ASN:O	2.21	0.41
1:A:3026:ASP:OD2	1:A:3048:LYS:NZ	2.54	0.41
1:A:3421:ASP:O	1:A:3425:ARG:HG3	2.21	0.41
1:A:3526:PRO:HB2	1:A:3564:GLN:NE2	2.36	0.41
1:A:3735:PRO:HB3	1:A:3753:LYS:HB3	2.03	0.41
1:A:3842:TRP:O	1:A:3846:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3854:ALA:O	1:A:3858:MET:HB2	2.21	0.41
1:A:3871:PHE:O	1:A:3875:GLU:HG2	2.21	0.41
1:A:4044:ILE:O	1:A:4048:LYS:HG3	2.21	0.41
2:B:78:SER:C	2:B:80:ARG:H	2.28	0.41
2:B:312:LEU:C	2:B:314:SER:H	2.28	0.41
2:B:352:PRO:HG2	2:B:355:LEU:HD22	2.03	0.41
2:B:461:LYS:HE2	2:B:461:LYS:HB3	1.95	0.41
1:A:871:LEU:HD12	1:A:3122[B]:HIS:CD2	2.56	0.41
1:A:1184:ARG:O	1:A:1188:ILE:HG23	2.21	0.41
1:A:1333:SER:O	1:A:1336:THR:HG22	2.21	0.41
1:A:1538:LEU:HD11	1:A:1555:HIS:CD2	2.56	0.41
1:A:2746:LYS:O	1:A:2750:GLU:OE1	2.39	0.41
1:A:2855:VAL:HG12	7:A:4404:HOH:O	2.20	0.41
1:A:2931:ARG:HH22	1:A:3000:ASP:CB	2.34	0.41
1:A:3271:ASP:HB3	1:A:3315:TYR:HE2	1.86	0.41
1:A:3442:TYR:HB2	1:A:3443:PRO:HD3	2.02	0.41
2:B:179:ASP:OD2	2:B:182:LYS:N	2.42	0.41
2:B:351:LYS:HE2	2:B:355:LEU:HD11	2.02	0.41
1:A:1333:SER:HA	1:A:1336:THR:HG22	2.02	0.40
1:A:1758:LEU:HG	7:A:4360:HOH:O	2.21	0.40
1:A:2885:GLN:O	1:A:2888:VAL:HG22	2.22	0.40
1:A:3177:ASN:OD1	1:A:3177:ASN:N	2.54	0.40
1:A:3623:PRO:HG3	1:A:3633:ILE:HG21	2.03	0.40
3:C:610:GLU:C	3:C:612:ALA:H	2.29	0.40
1:A:142:ARG:HH11	1:A:145:ASP:HB2	1.86	0.40
1:A:215:PRO:HG3	3:C:553:ILE:HG21	2.02	0.40
1:A:410:MET:HB3	1:A:411:PRO:HD3	2.03	0.40
1:A:1062:ARG:HH22	1:A:3746:ARG:HH12	1.68	0.40
1:A:2929:LEU:HD23	1:A:2929:LEU:HA	1.87	0.40
1:A:3030:ILE:HG21	1:A:3041:LEU:HD13	2.04	0.40
1:A:3263:HIS:HB2	1:A:3276:TRP:CZ2	2.56	0.40
2:B:470:ARG:HG3	3:C:389:MET:HE1	2.02	0.40
3:C:73:GLN:H	3:C:73:GLN:HG2	1.76	0.40
3:C:129:LYS:HD2	3:C:239:LYS:HD3	2.03	0.40
3:C:653:GLN:HG2	3:C:654:ARG:N	2.36	0.40
1:A:252:VAL:HG22	1:A:274:LEU:HD23	2.04	0.40
1:A:531:PHE:CD1	1:A:534:LEU:HD12	2.57	0.40
1:A:1370:ARG:HD2	1:A:1370:ARG:C	2.45	0.40
1:A:1581:GLU:HA	1:A:1584:GLN:HB2	2.02	0.40
1:A:1873:TYR:HA	1:A:1876:ILE:HD12	2.02	0.40
1:A:2379:MET:CE	1:A:2404:ARG:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3198:THR:OG1	1:A:3199:PRO:HD3	2.21	0.40
1:A:3385:LEU:HB3	1:A:3416:LEU:HD21	2.03	0.40
3:C:386:ASP:OD1	3:C:387:LEU:N	2.54	0.40
3:C:501:PRO:HB2	3:C:502:ARG:NH1	2.36	0.40
1:A:1224:PHE:HD2	1:A:1267:TYR:CD1	2.39	0.40
1:A:1696:LEU:HA	1:A:1696:LEU:HD23	1.85	0.40
1:A:1797:LEU:O	1:A:1800:SER:OG	2.35	0.40
1:A:1837:ARG:HA	1:A:1840:PHE:CD2	2.56	0.40
1:A:1988:TYR:CE2	1:A:2088:LEU:HD13	2.56	0.40
1:A:2506:LEU:HD13	1:A:2524:PHE:CE2	2.57	0.40
1:A:2844:LEU:HD23	1:A:2844:LEU:HA	1.85	0.40
1:A:3007:GLU:HB3	7:A:4347:HOH:O	2.22	0.40
1:A:3334:TYR:HE1	1:A:3384:HIS:CE1	2.39	0.40
1:A:3493:TRP:CD1	1:A:3493:TRP:H	2.39	0.40
2:B:141:TYR:HE1	2:B:175:PRO:HB3	1.87	0.40
3:C:446:PRO:HB2	3:C:451:LEU:HD21	2.03	0.40
1:A:1920:TYR:CZ	1:A:1924:THR:HG21	2.57	0.40
1:A:3335:ARG:HH11	1:A:3385:LEU:HD11	1.85	0.40
3:C:347:LYS:HE3	3:C:347:LYS:HB3	1.97	0.40
3:C:465:LYS:O	3:C:474:GLU:HG3	2.20	0.40
3:C:641:ALA:O	3:C:644:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2131/4128 (52%)	1915 (90%)	215 (10%)	1 (0%)	100	100
2	B	488/609 (80%)	423 (87%)	65 (13%)	0	100	100
3	C	653/732 (89%)	580 (89%)	71 (11%)	2 (0%)	36	64
All	All	3272/5469 (60%)	2918 (89%)	351 (11%)	3 (0%)	49	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	949	PRO
3	C	322	PRO
3	C	410	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3211/3671 (88%)	3202 (100%)	9 (0%)	86	95
2	B	443/548 (81%)	440 (99%)	3 (1%)	76	91
3	C	583/649 (90%)	581 (100%)	2 (0%)	86	95
All	All	4237/4868 (87%)	4223 (100%)	14 (0%)	84	95

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	LYS
1	A	165	LYS
1	A	166	ILE
1	A	946	THR
1	A	947	GLN
1	A	948	MET
1	A	2195	SER
1	A	2427	ARG
1	A	3577	GLN
2	B	58	THR
2	B	182	LYS
2	B	371	GLU
3	C	302	GLU
3	C	411	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	ASN
1	A	250	ASN
1	A	281	GLN
1	A	289	ASN
1	A	322	GLN
1	A	625	ASN
1	A	947	GLN
1	A	998	ASN
1	A	1125	GLN
1	A	1142	HIS
1	A	1466	ASN
1	A	1584	GLN
1	A	1589	ASN
1	A	1614	GLN
1	A	1716	GLN
1	A	1737	ASN
1	A	1738	ASN
1	A	1794	GLN
1	A	1890	HIS
1	A	2163	HIS
1	A	2365	ASN
1	A	2380	ASN
1	A	2496	GLN
1	A	2523	ASN
1	A	2560	ASN
1	A	2845	ASN
1	A	3249	GLN
1	A	3291	GLN
1	A	3339	ASN
1	A	3510	GLN
1	A	3516	HIS
1	A	3602	ASN
1	A	3951	GLN
1	A	3986	HIS
2	B	68	GLN
2	B	110	ASN
2	B	132	GLN
2	B	163	HIS
2	B	275	ASN
2	B	485	GLN
2	B	489	ASN
2	B	502	GLN
3	C	33	GLN

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Mol	Chain	Res	Type
3	C	119	GLN
3	C	432	GLN
3	C	452	ASN
3	C	510	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	1IX	A	4201	-	38,38,38	2.23	11 (28%)	53,54,54	2.18	18 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1IX	A	4201	-	-	2/18/26/26	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	4201	1IX	C14-C16	6.09	1.56	1.49
6	A	4201	1IX	C12-C13	5.44	1.47	1.37
6	A	4201	1IX	C11-CL1	4.36	1.83	1.73
6	A	4201	1IX	C21-C20	-3.90	1.36	1.42
6	A	4201	1IX	C24-N26	3.19	1.47	1.38
6	A	4201	1IX	C25-C20	2.90	1.46	1.41
6	A	4201	1IX	C20-N19	-2.55	1.33	1.37
6	A	4201	1IX	C10-C09	2.50	1.56	1.52
6	A	4201	1IX	C15-C14	2.28	1.43	1.39
6	A	4201	1IX	C14-C13	-2.22	1.35	1.39
6	A	4201	1IX	C15-C10	2.22	1.43	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	4201	1IX	C10-C09-C06	-6.03	105.48	111.20
6	A	4201	1IX	C18-N19-C20	5.13	121.27	115.43
6	A	4201	1IX	C21-C16-N17	-5.08	119.69	123.04
6	A	4201	1IX	N19-C18-N17	-4.56	122.48	128.67
6	A	4201	1IX	C21-C20-N19	-4.14	118.43	122.82
6	A	4201	1IX	C03-N04-N05	3.33	122.81	118.42
6	A	4201	1IX	C16-C21-C20	3.07	118.52	115.90
6	A	4201	1IX	C15-C10-C11	3.04	120.03	117.14
6	A	4201	1IX	C25-C20-N19	2.88	121.32	118.01
6	A	4201	1IX	C15-C14-C13	2.75	119.23	115.98
6	A	4201	1IX	C12-C11-C10	-2.73	119.51	122.46
6	A	4201	1IX	C14-C16-N17	2.65	119.89	115.17
6	A	4201	1IX	C01-O02-C03	-2.47	113.66	117.33
6	A	4201	1IX	C11-C12-C13	2.20	120.08	118.42
6	A	4201	1IX	C28-C27-N26	2.11	113.93	109.93
6	A	4201	1IX	C30-C31-N26	2.10	113.90	109.93
6	A	4201	1IX	C31-N26-C24	2.03	123.66	118.11
6	A	4201	1IX	C12-C13-C14	-2.03	120.34	123.59

There are no chirality outliers.

All (2) torsion outliers are listed below:

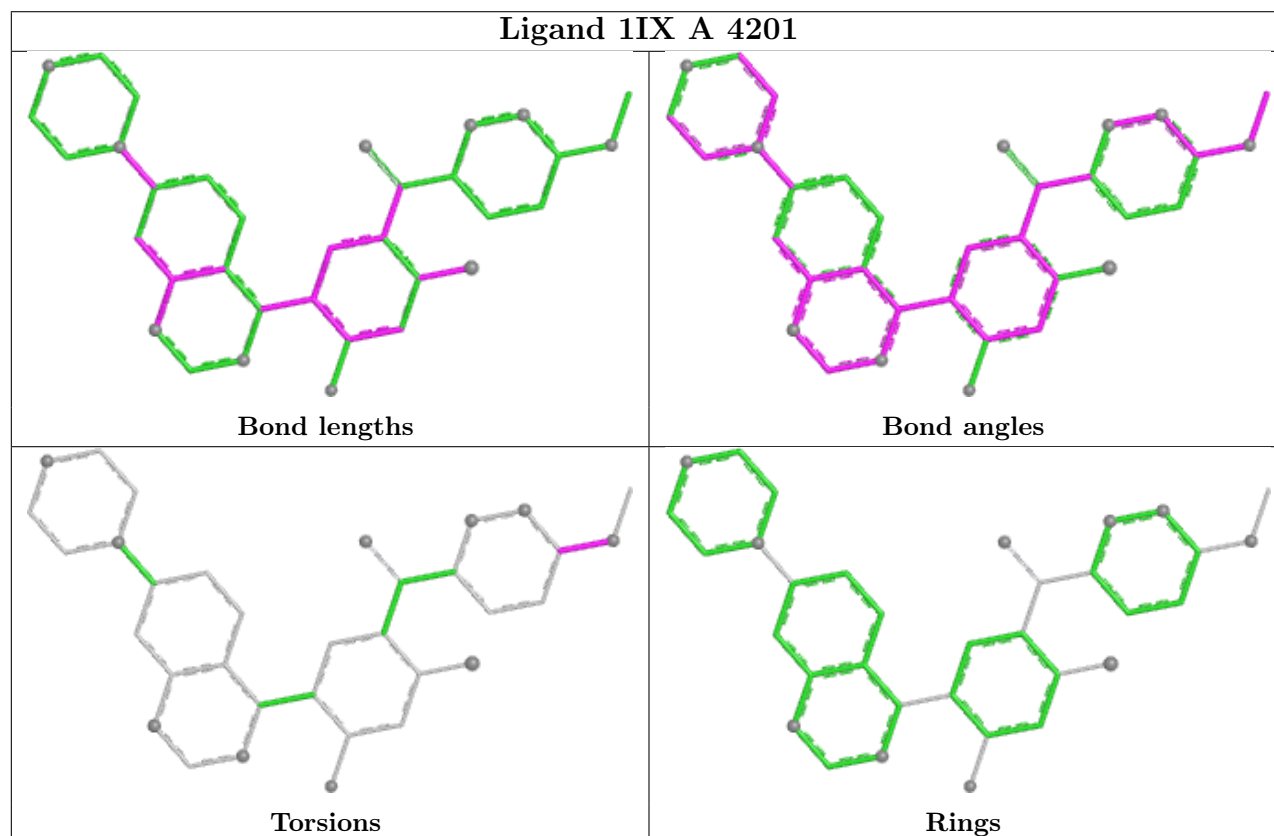
Mol	Chain	Res	Type	Atoms
6	A	4201	1IX	N04-C03-O02-C01
6	A	4201	1IX	C08-C03-O02-C01

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	4201	1IX	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

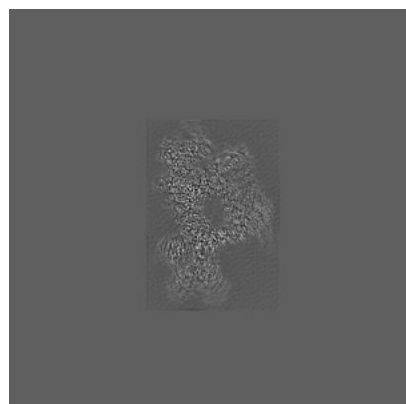
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14545. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

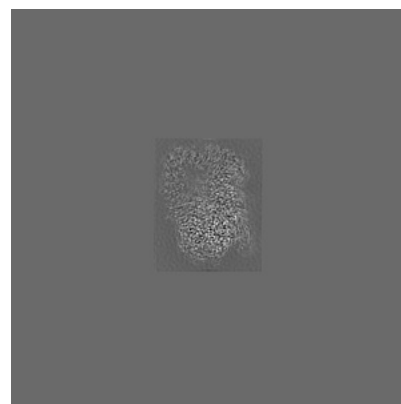
6.1.1 Primary map



X

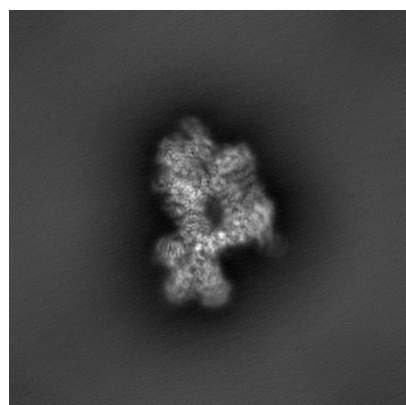


Y

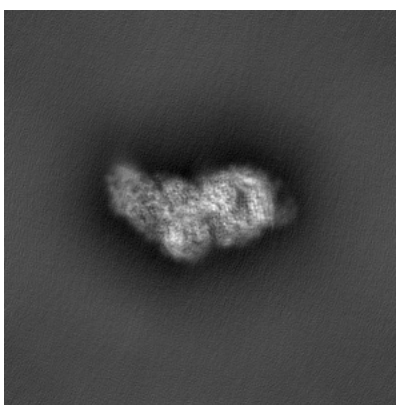


Z

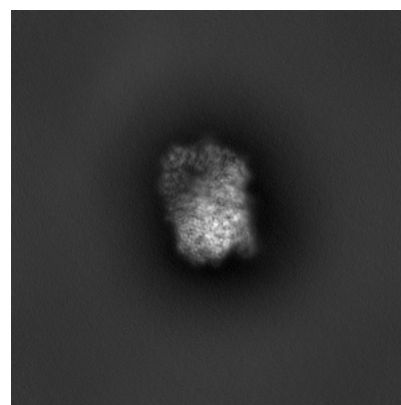
6.1.2 Raw map



X



Y

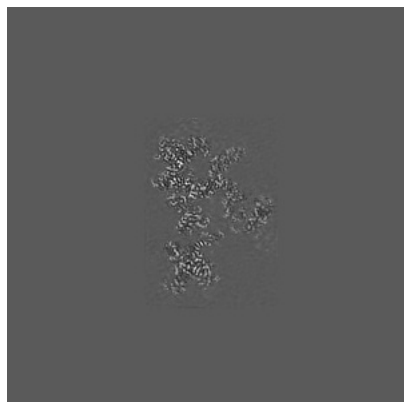


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 175

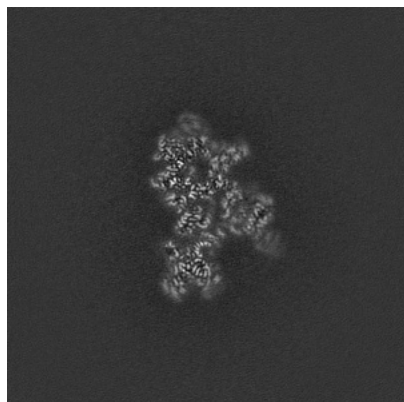


Y Index: 175

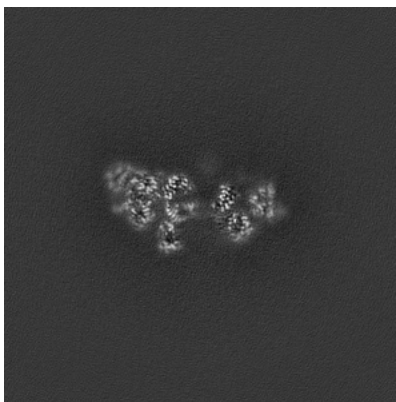


Z Index: 175

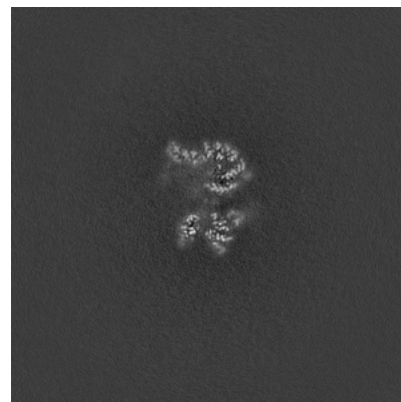
6.2.2 Raw map



X Index: 175



Y Index: 175

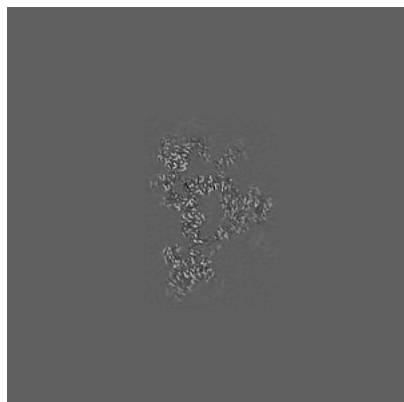


Z Index: 175

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

6.3 Largest variance slices [i](#)

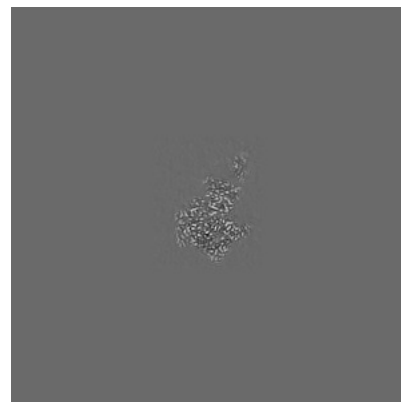
6.3.1 Primary map



X Index: 180

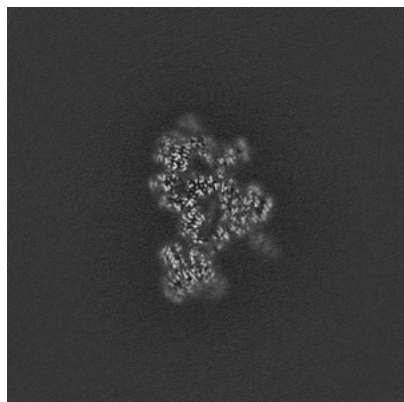


Y Index: 156

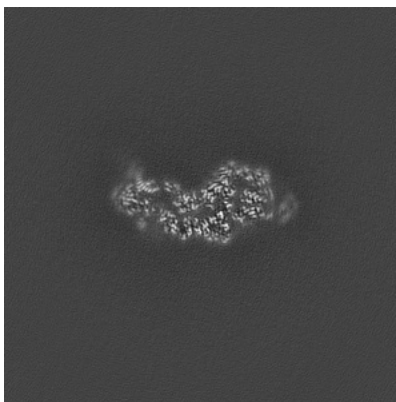


Z Index: 194

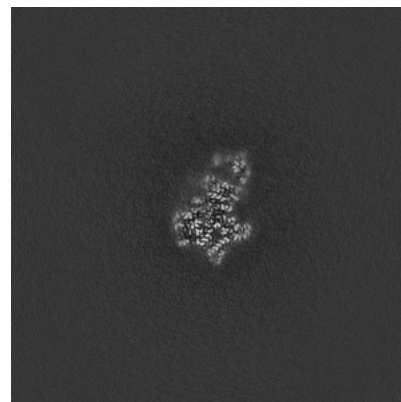
6.3.2 Raw map



X Index: 180



Y Index: 156

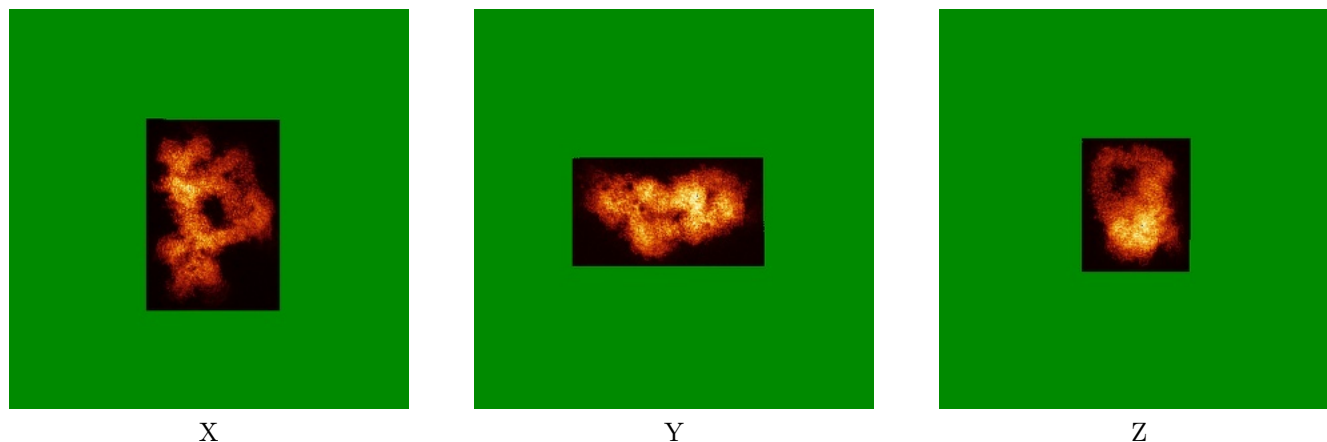


Z Index: 192

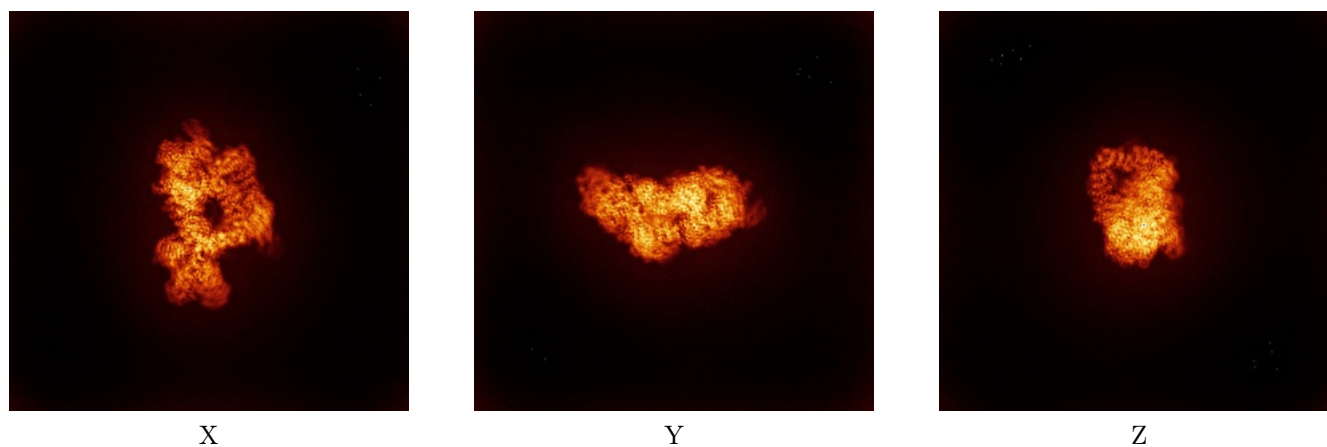
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



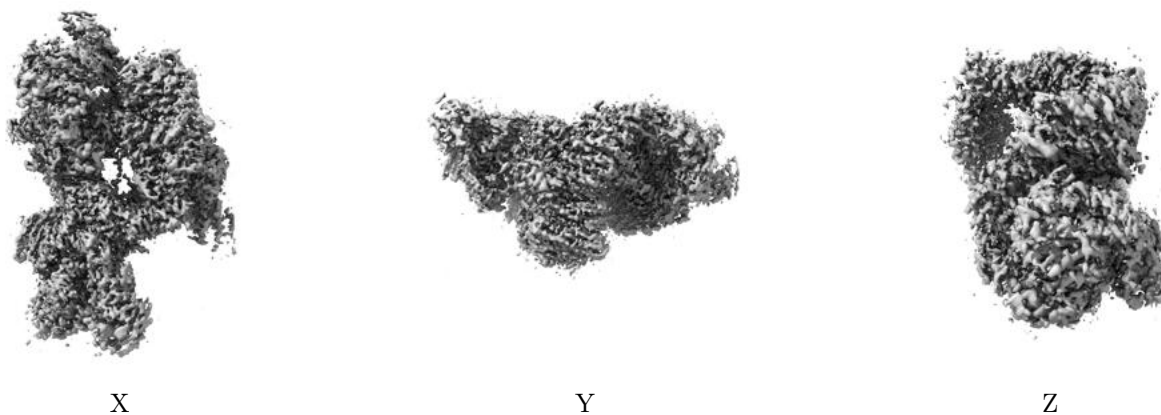
6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

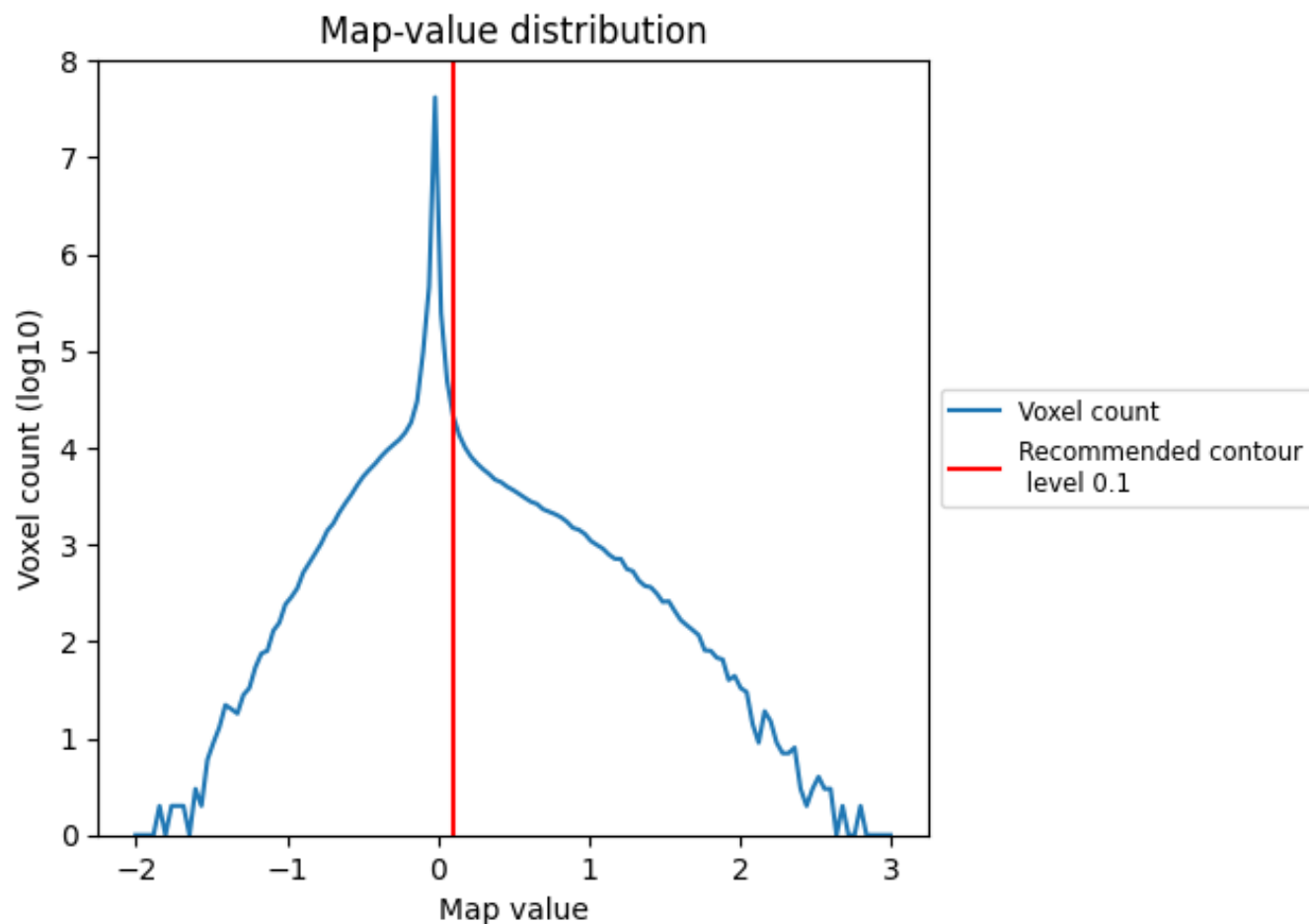
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

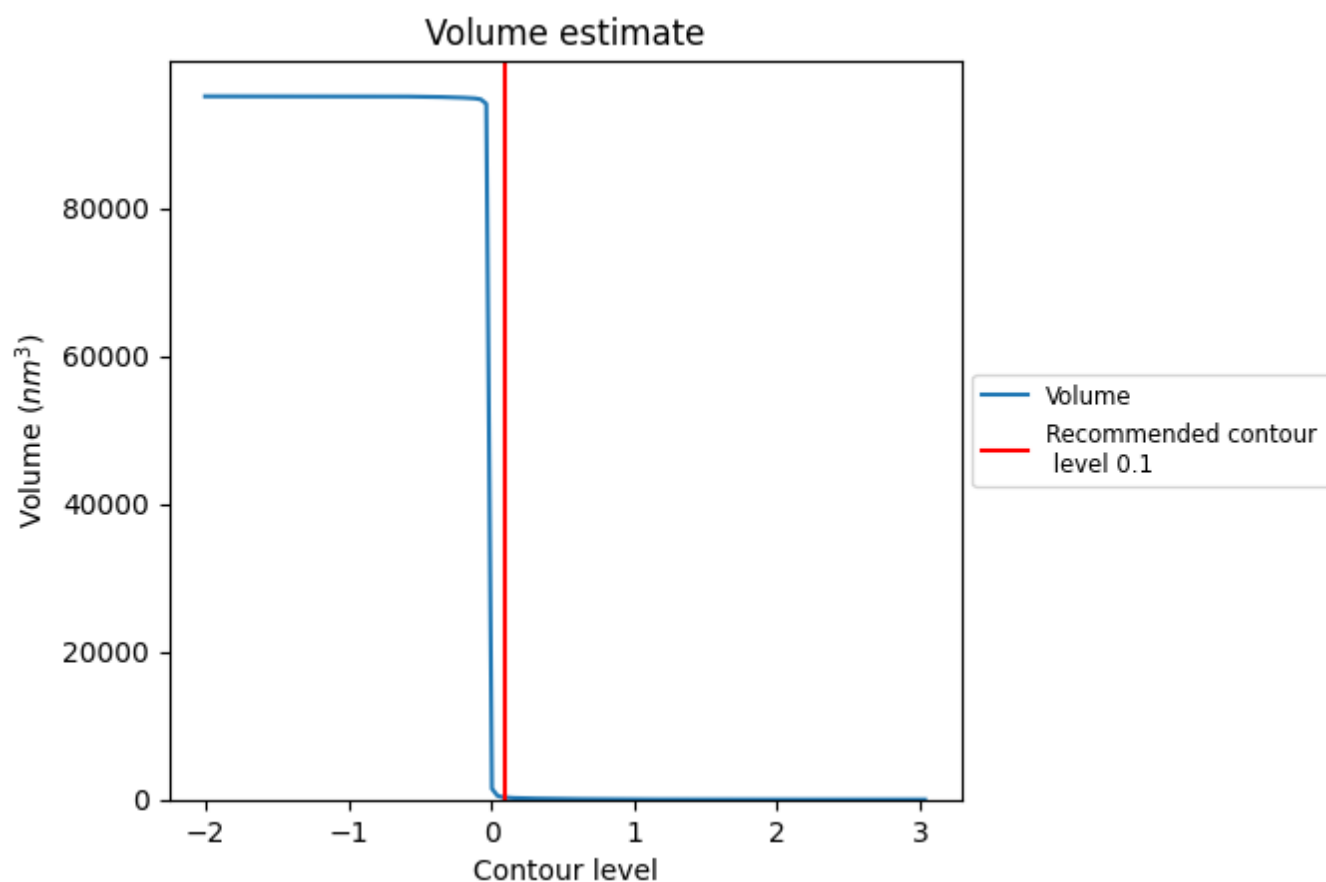
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

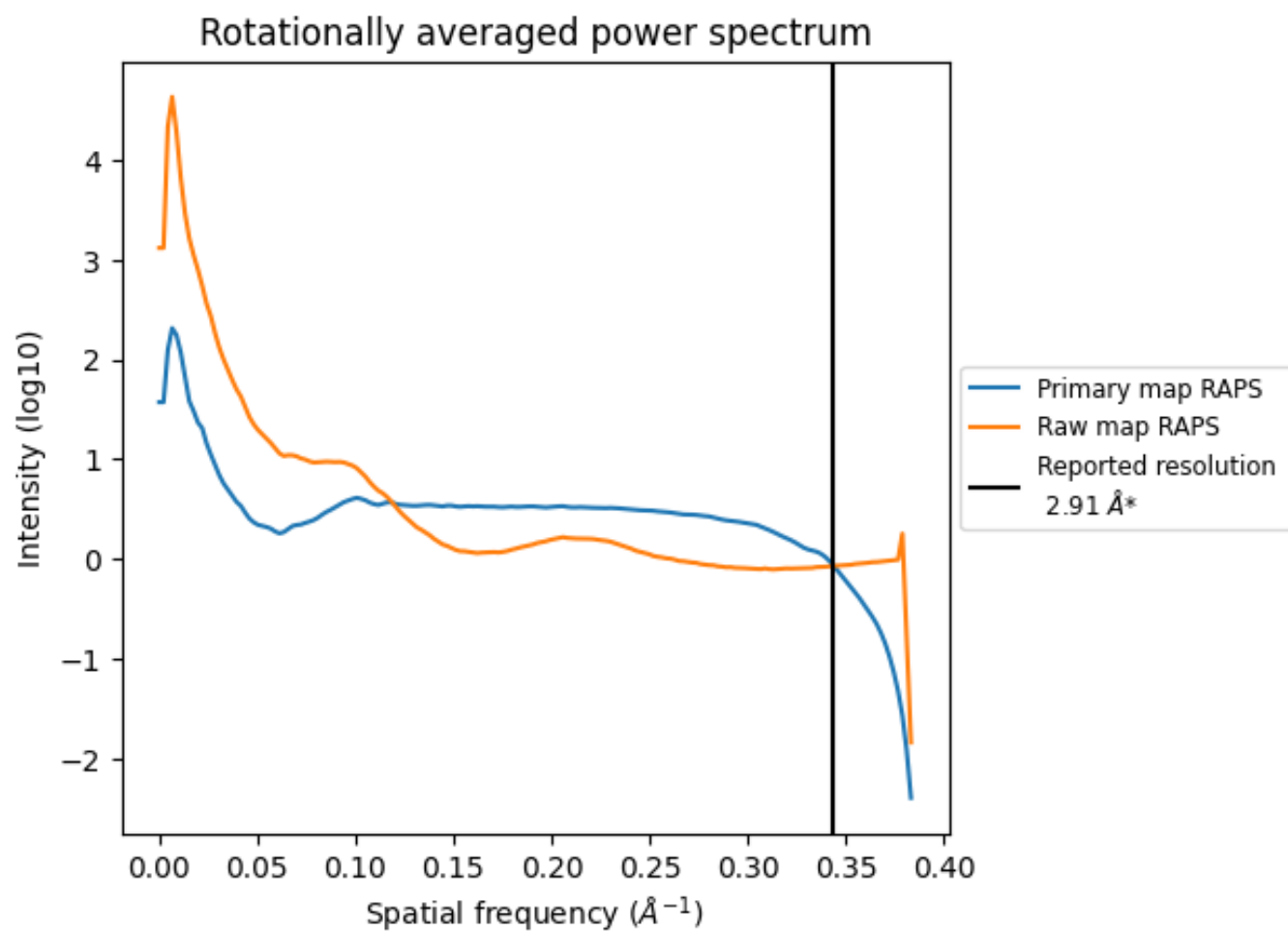
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 280 nm³; this corresponds to an approximate mass of 253 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 ⓘ

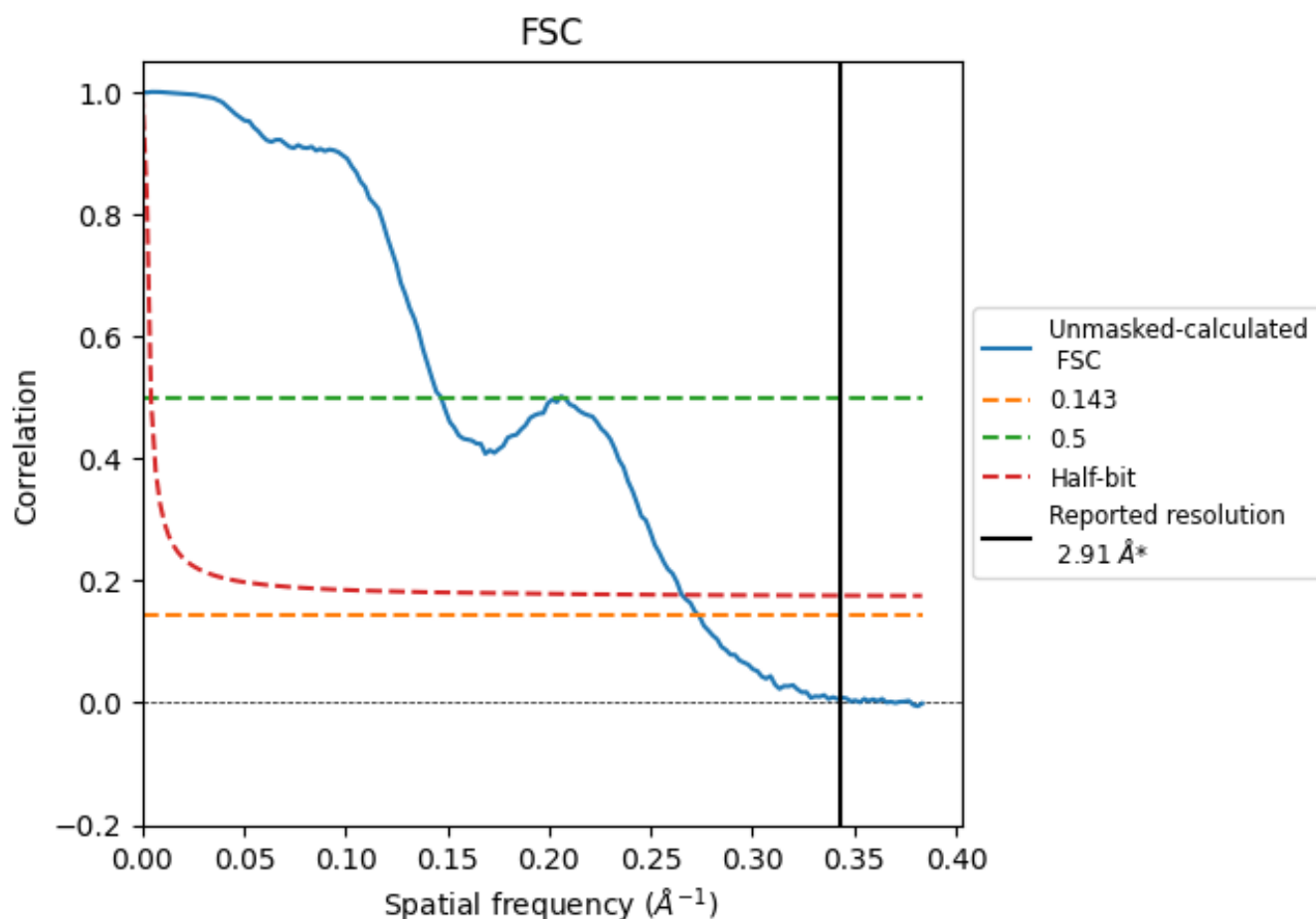


*Reported resolution corresponds to spatial frequency of 0.344 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.344 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

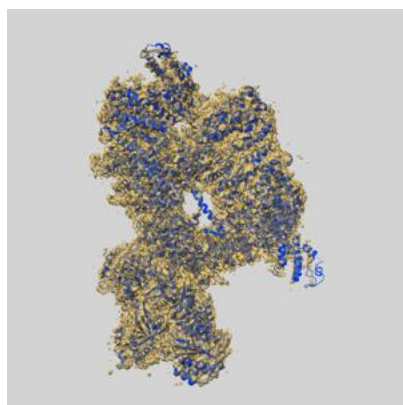
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.66	6.81	3.77

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.66 differs from the reported value 2.91 by more than 10 %

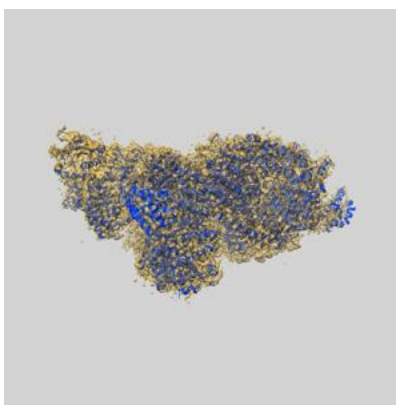
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14545 and PDB model 7Z87. Per-residue inclusion information can be found in section 3 on page 6.

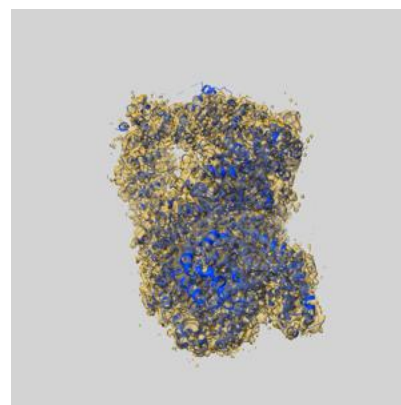
9.1 Map-model overlay [i](#)



X



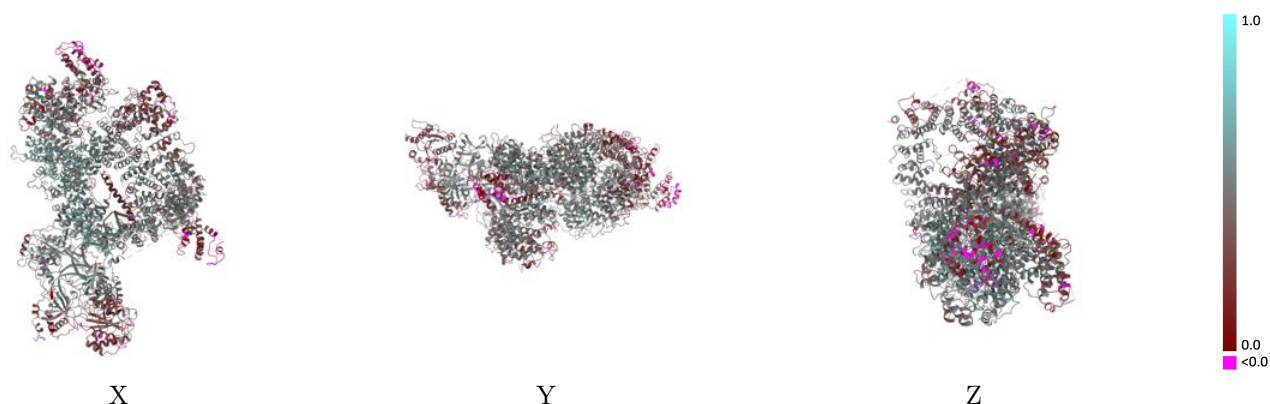
Y



Z

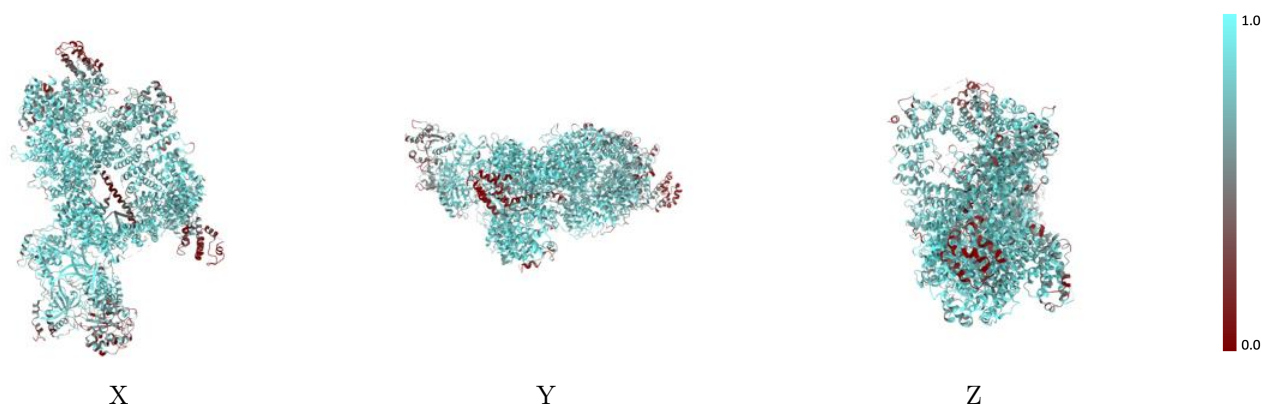
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



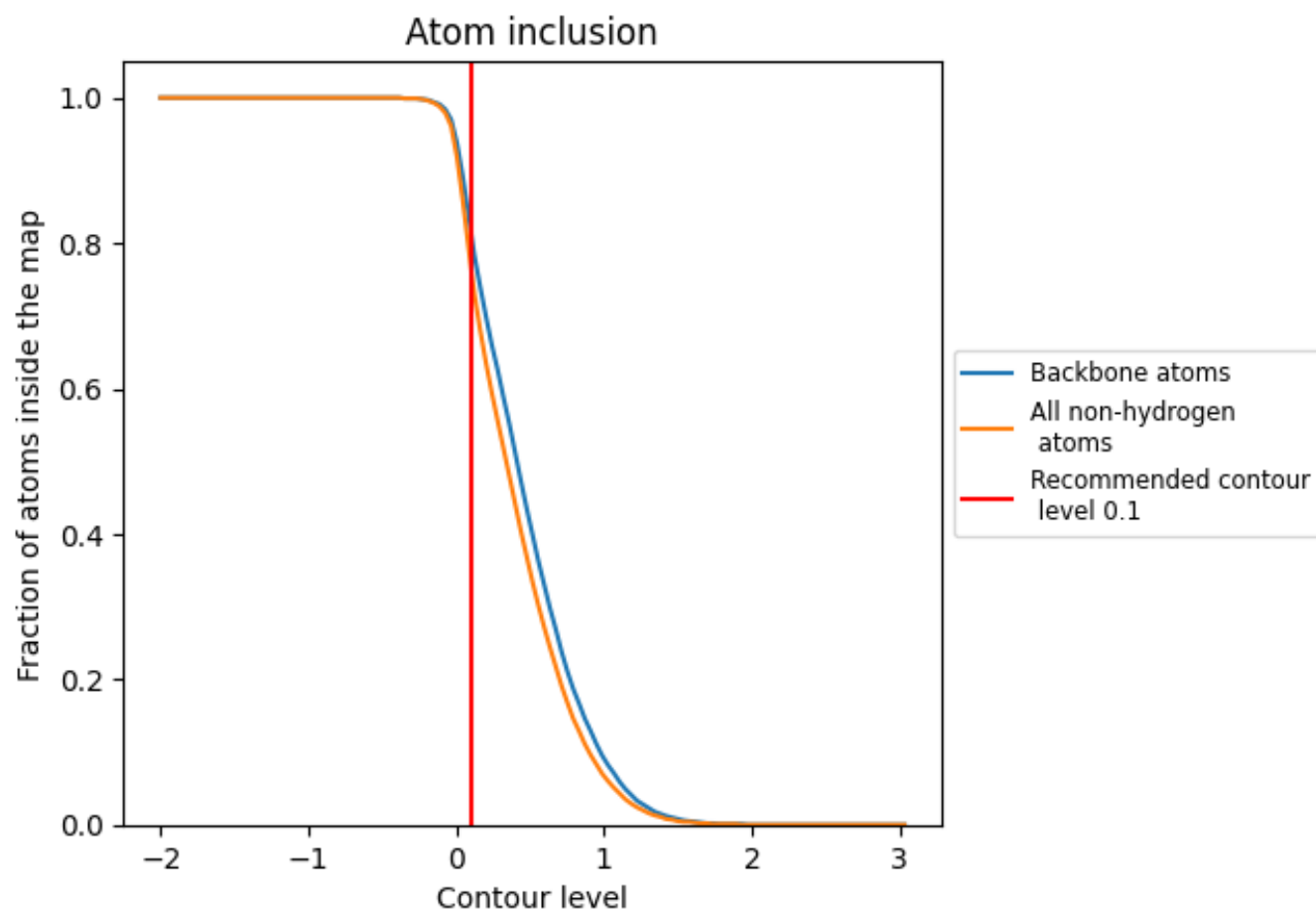
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 76% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7650	0.4260
A	0.7980	0.4450
B	0.7830	0.4200
C	0.5500	0.3080
D	0.9070	0.5050
E	0.8810	0.5250

