



Full wwPDB EM Validation Report ⓘ

Aug 19, 2026 – 04:32 pm BST

PDB ID : 9TU9 / pdb_00009tu9
EMDB ID : EMD-56253
Title : CryoEM structure of DruE:ATPgammaS:DNA from Druantia type III - dimer 2
Authors : Grass, L.M.; Himpich, S.; Hilal, T.; Loll, B.; Wahl, M.C.
Deposited on : 2026-01-08
Resolution : 3.60 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:

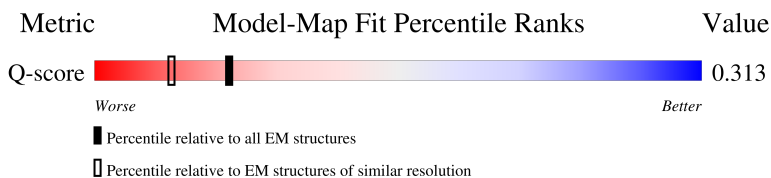
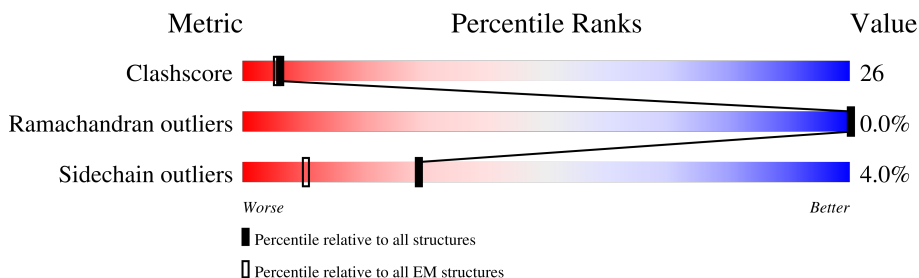
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	Y	2108	
1	y	2108	
2	G	30	
3	I	30	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33663 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 DEAD/DEAH box helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Y	2075	Total	C	N	O	S	0	0
			16471	10380	2939	3080	72		
1	y	2050	Total	C	N	O	S	0	0
			16275	10265	2912	3026	72		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP A0A4P8BDA5
Y	-2	ALA	-	expression tag	UNP A0A4P8BDA5
Y	-1	GLU	-	expression tag	UNP A0A4P8BDA5
Y	0	PHE	-	expression tag	UNP A0A4P8BDA5
y	-3	GLY	-	expression tag	UNP A0A4P8BDA5
y	-2	ALA	-	expression tag	UNP A0A4P8BDA5
y	-1	GLU	-	expression tag	UNP A0A4P8BDA5
y	0	PHE	-	expression tag	UNP A0A4P8BDA5

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*GP*AP*CP*CP*GP*TP*CP*GP*GP*AP*AP*GP*AP*GP*AP*CP*TP*AP*TP*CP*GP*AP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	24	Total	C	N	O	P	0	0
			497	235	98	140	24		

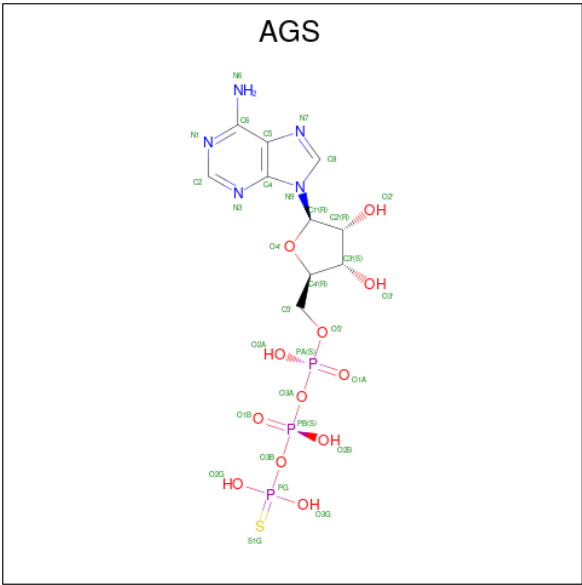
- Molecule 3 is a DNA chain called DNA (5'-D(P*AP*TP*CP*GP*AP*TP*AP*GP*TP*CP*TP*CP*TP*AP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	17	Total	C	N	O	P	0	0
			348	166	62	103	17		

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

Mol	Chain	Residues	Atoms		AltConf
4	Y	5	Total	Zn	0
			5	5	
4	y	5	Total	Zn	0
			5	5	

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).

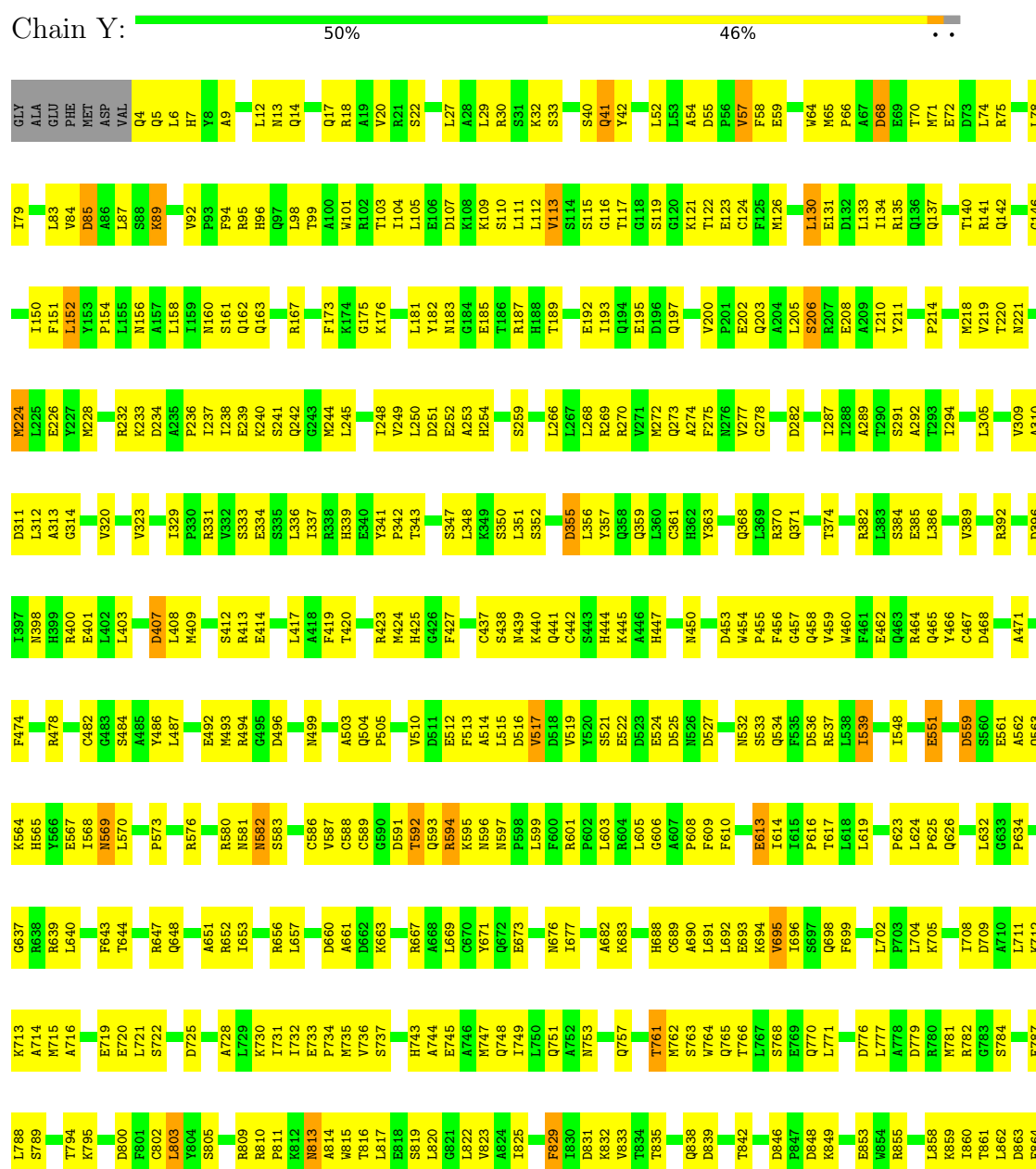


Mol	Chain	Residues	Atoms						AltConf
5	Y	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
5	y	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DEAD/DEAH box helicase

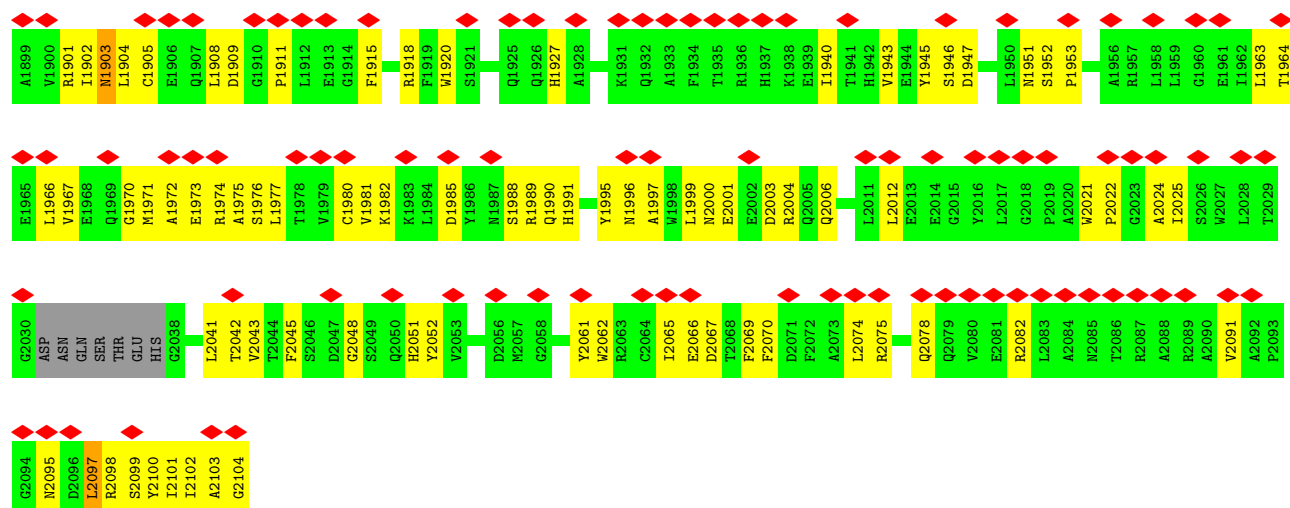




Chain y: 13% 48% 48% ..

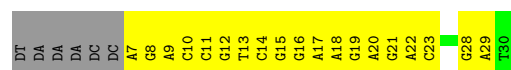


Q1827	S1757	F1672	I1602	T1541	A1468	M1400	Y1336	S1272	A1204	M1119	W1056	C982
L1828	L1758	C1681	R1603	P1542	S1473	L1401	L1337	Q1273	T1205	N1120	W1057	P983
M1829	V1759	E1605	D1604	E1543	M1474	G1402	T1338	L1274	K1206	N1121		Y984
R1834	A1761	C1683	E1606	N1544	P1475	K1403	A1339	A1275	L1207	V1122	S1060	R985
W1835	G1762	D1684	A1607	L1545	P1476	V1404	D1340	L1276	S1208	P1123	D1061	R986
Q1838	P1763	K1685	R1608	K1546	Q1477	L1405	E1341	L1277	G1209	P1124	E1062	R987
L1839	Q1764	F1686	R1609	N1547	P1479	L1406	E1342	L1278	K1210	P1125	L1063	A988
T1840	E1765	C1687	S1610	P1548	Q1477	A1406	L1342	L1279	K1210	P1126		L989
R1841	Q1766	H1688	L1611	E1549	P1478	G1408	E1343	E1279	F1213	W1069	K1066	D990
R1841	W1767	H1689	A1612	R1550	L1479	S1407	K1344	A1281	G1215	Y1070		Y991
E1842	P1691	C1690	V1613	E1551	W1480	Q1409	R1345	E1282	D1216	R1071		L992
L1843	L1691	L1614	L1615	E1552	K1481	Q1410	R1346	A1283	E1217	L1072		L993
Q1844	L1692	R1616	L1616	T1553	P1483	E1410	A1347	L1284	S1218	E1073		P1001
S1845	S1693	E1617	H1554	H1554	R1484	L1411	A1347	L1284	E1217	E1074		G1002
	Y1694		Y1555	Y1555	V1485	S1412	I1348	L1284	S1218	W1075		S1003
W1848	Q1697	K1622	L1556	L1556	L1486	G1413	K1349	K1285	A1143			K1004
	H1698		L1557	L1557	P1487	D1414	A1350	D1287	A1143			E1005
D1851	E1777	H1699	T1625	R1558	P1488	H1415	T1351	M1288	E1215			A1006
D1852	Y1699	V1700	I1625	G1559	S1489	H1416	GLN	S1289	G1215			A1007
T1855	Q1760	R1701	E1629	G1559	V1493	L1417	ALA	A1290	L1130			P1008
P1858	R1702	L1703	L1630	G1560	W1418	P1418	ASP	A1290	K1151			
G1859	L1703	L1703	G1631	S1561	W1419	Q1418	PRO	W1231	E1151			
L1859	D1704	D1704	V1632	N1562	F1420	W1420	ASN	E1292	N1152			
E1860	R1705	R1705	T1633	D1563	W1421	H1422	GLU	E1293	P1081			
	H1706	H1706	T1634	R1564	L1500		GLY	T1294	H1155			
G1863	H1707	H1707	Q1565	Q1565	G1501	G1427	GLU	P1295	G1156			
Q1864	A1708		S1566	S1566	R1502	A1428	SER	A1296	E1157			
S1868	L1711		D1639	S1567	S1506	G1429	PHE	A1299	E1158			
P1869	L1717		I1640	N1568	G1509	A1430	ARG	A1299	F1086			
V1870	Q1642		M1641	K1569	E1510	T1431	ARG	I1300	Q1085			
L1872	Y1643		Y1643	L1570	L1511	S1432	ILE	A1166	Q1085			
	L1722		G1645	C1571	F1512	T1433	GLU	T1169	F1086			
G1875	Y1726		Y1646	H1573	H1513	V1437	K1368	L1238	Q1087			
T1876	F1729		S1647	H1574	E1516	E1438	D1372	R1240	E1088			
S1877	G1730		I1648	V1575	G1517	C1439	R1374	R1240	L1164			
Q1878	D1731		F1649	H1576	E1518	A1439	D1373	R1305	K1095			
L1879	G1732		V1650	K1577	F1519	H1441	L1374	T1177	V1096			
H1880	R1804		D1652	D1578	G1520		P1375	F1178	N1097			
F1881	H1805		R1653	L1579	G1520	A1444	T1376	F1178	V1098			
S1882	Q1806		V1654	W1580	G1521	D1445	T1376	G1179	L1099			
S1882	L1807		E1736	L1581	G1522	D1446	A1377		M1100			
G1883	S1808		E1736	L1581	Y1523	Q1447	A1377		C1101			
Q1884	A1809		T1737	Y1583	A1524	Q1448	L1378		E1036			
L1886	L1810		S1584	Y1584	T1525	L1449	E1379		E1036			
S1887	P1814		G1859	S1585	G1526	D1450	E1380		R1307			
E1888	R1817		Y1660	R1586	L1527	Q1447	Y1381		T1103			
D1890	V1820		A1745	L1592	S1585	L1451	A1382		T1104			
L1891	K1821		L1748	E1591	L1527	K1452	D1386		H1187			
L1892	T1823		M1749	Q1593	S1528	R1453	V1387		M1105			
P1893	A1824		Y1753	L1594	C1529	Y1454	V1388		E1106			
A1894	T1825			D1596	G1530	R1461	L1389		M1107			
L1895	A1826			D1597	R1531	D1463	L1389		G1108			
P1896				N1598	A1532	R1465	G1390		V1109			
T1897				G1599	Q1535	Y1466	G1390		I1111			
G1898					T1536		P1392		L1195			
					D1670		K1391		F1196			
					V1671		Y1393		L1197			
							R1395		D1203			
							S1396					
							G1397					
							G1398					
							I1399					



- Molecule 2: DNA (5'-D(P*AP*GP*AP*CP*CP*GP*TP*CP*GP*GP*AP*AP*GP*AP*GP*A
P*CP*TP*AP*TP*CP*GP*AP*T)-3')

Chain G: 17% 63% 20%



- Molecule 3: DNA (5'-D(P*AP*TP*CP*GP*AP*TP*AP*GP*TP*CP*TP*CP*TP*AP*GP*G
P*C)-3')

Chain I: 13% 43% 43%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27507	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 ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.374	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	319.488, 319.488, 319.488	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1093334, 1.1093334, 1.1093334	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	Y	0.33	0/16840	0.42	0/22830
1	y	0.17	0/16641	0.35	0/22555
2	G	0.29	0/559	0.45	0/861
3	I	0.25	0/389	0.41	0/598
All	All	0.26	0/34429	0.39	0/46844

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	16471	0	16231	822	0
1	y	16275	0	16083	867	0
2	G	497	0	269	39	0
3	I	348	0	193	23	0
4	Y	5	0	0	0	0
4	y	5	0	0	0	0
5	Y	31	0	12	6	0
5	y	31	0	12	3	0
All	All	33663	0	32800	1721	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 26.

All (1721) 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:Y:1529:CYS:SG	1:Y:1554:HIS:CD2	2.49	1.05
1:y:1622:LYS:HZ3	1:y:1671:VAL:HA	1.29	0.96
2:G:21:DG:N2	3:I:10:DC:O2	2.00	0.92
1:Y:65:MET:HE3	1:Y:66:PRO:HD2	1.51	0.92
2:G:21:DG:N1	3:I:10:DC:N3	2.19	0.90
2:G:28:DG:N2	3:I:3:DC:O2	2.04	0.90
1:Y:1526:CYS:SG	1:Y:1554:HIS:HE1	1.96	0.89
1:Y:2087:ARG:HE	1:Y:2089:ARG:HH22	1.21	0.88
1:y:916:TYR:HB2	3:I:12:DC:H5'	1.55	0.86
1:y:728:ALA:HA	1:y:731:ILE:HD12	1.59	0.85
2:G:28:DG:N1	3:I:3:DC:N3	2.24	0.84
1:Y:705:LYS:HZ2	1:Y:708:ILE:HG21	1.42	0.83
1:y:909:PRO:HB2	1:y:945:MET:HE2	1.60	0.82
1:y:684:LEU:HD23	1:y:692:LEU:HD11	1.61	0.81
1:Y:1943:VAL:HG13	1:Y:2043:VAL:HG12	1.64	0.80
1:Y:625:PRO:HG3	1:Y:639:ARG:HH22	1.45	0.80
1:y:1025:ARG:HA	1:y:1031:GLU:HA	1.62	0.79
1:y:492:GLU:O	1:y:494:ARG:NH1	2.16	0.79
1:Y:454:TRP:NE1	1:Y:456:PHE:O	2.14	0.79
1:y:1940:ILE:HD11	1:y:1971:MET:HE2	1.64	0.78
1:Y:1940:ILE:HG23	1:Y:1971:MET:HB3	1.66	0.77
1:y:166:LEU:HA	1:y:169:TRP:HD1	1.50	0.77
1:y:586:CYS:HB3	1:y:589:CYS:SG	2.25	0.77
1:y:1688:HIS:HA	1:y:1692:LEU:HB2	1.67	0.77
1:Y:588:CYS:SG	1:Y:589:CYS:N	2.57	0.77
1:Y:1293:GLU:O	1:Y:1298:LYS:NZ	2.18	0.77
1:Y:737:SER:HA	1:Y:744:ALA:HB2	1.66	0.77
1:Y:1379:ARG:NH1	1:Y:1478:LEU:O	2.19	0.76
1:y:692:LEU:HD12	1:y:715:MET:HG3	1.66	0.76
1:y:1609:ARG:HH21	1:y:1634:THR:H	1.34	0.76
1:Y:1115:SER:O	1:Y:1144:SER:OG	2.03	0.76
1:Y:1911:PRO:HD2	1:Y:1918:ARG:HH12	1.49	0.76
1:Y:75:ARG:HB2	1:Y:84:VAL:HG21	1.68	0.75
1:Y:1251:THR:HG21	1:Y:1255:LEU:H	1.51	0.75
1:Y:1767:TRP:CE3	1:Y:1858:PRO:HD2	2.21	0.75
1:y:1529:CYS:HB2	1:y:1556:LEU:HA	1.69	0.75
1:y:59:GLU:HG2	1:y:423:ARG:HG3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:906:GLN:NE2	1:y:907:LEU:O	2.20	0.75
1:Y:101:TRP:HA	1:Y:104:ILE:HG22	1.68	0.74
1:y:1607:ALA:HB2	1:y:1707:HIS:HB3	1.70	0.74
1:Y:1796:LEU:O	1:Y:1804:ARG:NH1	2.17	0.74
1:y:467:CYS:SG	1:y:468:ASP:N	2.60	0.74
1:y:622:SER:O	1:y:638:ARG:NH1	2.21	0.74
1:y:1840:THR:HG23	1:y:1845:SER:HB3	1.70	0.74
1:Y:1600:LEU:HD13	1:Y:1603:ARG:HH22	1.53	0.73
1:Y:731:ILE:HG12	1:y:734:PRO:HG3	1.71	0.73
1:Y:1219:GLN:N	1:Y:1219:GLN:OE1	2.21	0.73
1:Y:232:ARG:HE	1:Y:1198:ARG:HE	1.34	0.73
1:Y:1924:THR:HA	1:Y:1930:TRP:HB3	1.69	0.73
1:Y:1899:ALA:HA	1:Y:2104:GLY:H	1.53	0.73
1:y:700:SER:HA	1:y:708:ILE:HG12	1.71	0.73
1:Y:1267:ASP:OD1	1:Y:1271:ARG:NH1	2.22	0.73
1:Y:1107:MET:O	1:Y:1135:ARG:NH1	2.22	0.73
1:Y:1439:CYS:HB2	1:Y:1449:LEU:HD11	1.70	0.72
1:y:62:PHE:O	1:y:327:ARG:NH1	2.20	0.72
1:y:990:ASP:OD1	1:y:991:VAL:N	2.22	0.72
1:y:1126:PRO:HB3	1:y:1166:ALA:HA	1.69	0.72
1:y:1915:PHE:HA	1:y:1918:ARG:HE	1.54	0.72
1:y:66:PRO:HA	1:y:94:PHE:HA	1.71	0.72
1:Y:370:ARG:NH1	1:Y:419:PHE:O	2.21	0.72
1:y:45:PRO:HB2	1:y:48:GLN:HB2	1.71	0.72
1:Y:1411:LEU:HG	1:Y:1413:GLY:H	1.53	0.72
1:y:77:LYS:HG3	1:y:78:LEU:HG	1.72	0.72
1:Y:728:ALA:HA	1:Y:731:ILE:HD12	1.70	0.72
1:Y:1974:ARG:NH2	1:Y:2046:SER:OG	2.23	0.72
1:y:257:ILE:HG13	1:y:1174:PRO:HB3	1.71	0.72
1:y:736:VAL:HG22	1:y:743:HIS:HB3	1.72	0.72
1:Y:492:GLU:OE2	1:Y:494:ARG:NH1	2.23	0.71
1:y:64:TRP:HA	1:y:327:ARG:HA	1.72	0.71
1:y:147:THR:HA	1:y:216:SER:HA	1.70	0.71
1:y:1071:ARG:NH1	1:y:1072:LEU:O	2.22	0.71
1:Y:1900:VAL:H	1:Y:2103:ALA:H	1.37	0.71
1:y:665:THR:HG21	1:y:1069:TRP:HB2	1.73	0.71
1:Y:1368:LYS:NZ	2:G:10:DC:O2	2.23	0.71
1:Y:1813:MET:HG3	1:Y:1818:LEU:HD13	1.72	0.71
1:Y:637:GLY:O	1:Y:639:ARG:NH2	2.24	0.71
1:Y:1044:ASN:HD21	1:Y:1046:LEU:HB2	1.55	0.71
1:y:985:THR:O	1:y:987:ARG:NH1	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:445:LYS:HA	1:Y:458:GLN:HG3	1.71	0.71
1:Y:111:LEU:HD21	1:Y:113:VAL:HG13	1.71	0.71
1:y:151:PHE:HB2	1:y:219:VAL:HG12	1.72	0.71
1:y:1032:ILE:O	1:y:1037:ARG:NH2	2.22	0.70
1:Y:696:ILE:HG12	1:Y:708:ILE:HG23	1.71	0.70
1:Y:239:GLU:OE2	1:Y:240:LYS:NZ	2.18	0.70
1:Y:1184:VAL:HG11	1:Y:1245:THR:HG21	1.73	0.70
1:y:104:ILE:O	1:y:247:TYR:OH	2.09	0.70
1:Y:310:ALA:O	1:Y:314:GLY:N	2.25	0.70
1:Y:1226:TRP:CE2	1:Y:1230:GLN:HG3	2.27	0.70
1:Y:486:TYR:OH	1:Y:586:CYS:SG	2.50	0.69
1:Y:1738:ASN:OD1	1:Y:1743:ARG:NH1	2.25	0.69
1:y:1834:ARG:HE	1:y:1852:ASP:HA	1.57	0.69
1:y:466:TYR:HA	1:y:472:PRO:HA	1.73	0.69
1:Y:1417:ILE:O	1:Y:1453:ARG:NH2	2.26	0.69
1:Y:1024:TRP:HD1	1:Y:1066:LYS:H	1.39	0.69
1:y:868:GLU:OE2	1:y:869:ASN:ND2	2.26	0.69
1:y:1377:ALA:O	1:y:1381:TYR:N	2.23	0.69
1:Y:1250:LEU:HD23	1:Y:1251:THR:HG22	1.73	0.69
1:Y:239:GLU:OE1	1:Y:239:GLU:N	2.24	0.69
1:Y:1565:GLN:OE1	1:Y:1568:ASN:ND2	2.25	0.69
1:Y:1690:CYS:SG	1:Y:1691:LEU:N	2.66	0.69
1:Y:1940:ILE:HG13	1:Y:1975:ALA:H	1.56	0.69
1:y:1372:ARG:HE	1:y:1381:TYR:HE2	1.39	0.69
1:Y:1382:ALA:O	1:Y:1396:SER:OG	2.10	0.69
1:Y:1636:GLN:NE2	1:Y:1645:GLY:O	2.26	0.68
1:Y:339:HIS:NE2	1:Y:341:TYR:O	2.26	0.68
1:Y:1295:PRO:HD2	1:Y:1562:ASN:HD21	1.58	0.68
1:Y:1767:TRP:HE3	1:Y:1858:PRO:HD2	1.56	0.68
1:Y:224:MET:HE2	1:Y:224:MET:HA	1.75	0.68
1:y:1123:PRO:HB2	1:y:1128:ASN:HD22	1.59	0.68
1:Y:458:GLN:NE2	1:Y:459:VAL:O	2.27	0.68
1:y:713:LYS:HE2	1:y:719:GLU:HB3	1.75	0.68
1:y:1541:THR:OG1	1:y:1546:LYS:NZ	2.27	0.68
1:Y:59:GLU:OE2	1:Y:423:ARG:NH1	2.27	0.68
1:y:1417:ILE:O	1:y:1453:ARG:NH2	2.27	0.68
1:Y:214:PRO:HG2	1:Y:240:LYS:HG3	1.74	0.68
1:y:1415:HIS:HB2	1:y:1453:ARG:HH22	1.59	0.68
1:Y:732:ILE:HA	1:Y:735:MET:HE1	1.76	0.68
1:y:810:ARG:NH1	1:y:999:TYR:OH	2.27	0.68
1:y:18:ARG:O	1:y:22:SER:OG	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:1739:PRO:HG2	1:y:1742:LEU:HB3	1.75	0.67
1:y:228:MET:SD	1:y:228:MET:N	2.67	0.67
1:y:269:ARG:HA	1:y:272:MET:SD	2.34	0.67
1:Y:1829:MET:HE2	1:Y:1829:MET:HA	1.77	0.67
1:y:1210:LYS:HA	1:y:1214:GLU:HB2	1.75	0.67
1:Y:355:ASP:N	1:Y:355:ASP:OD1	2.27	0.67
1:Y:1540:ARG:HA	1:Y:1540:ARG:HH11	1.59	0.67
1:Y:1556:LEU:HG	1:Y:1571:CYS:HB2	1.75	0.67
1:Y:1492:TRP:HB3	1:Y:1504:ARG:HB2	1.77	0.67
1:y:1000:LEU:HD12	1:y:1001:PRO:HD2	1.77	0.67
1:Y:733:GLU:HA	1:Y:747:MET:SD	2.35	0.67
1:Y:1208:SER:OG	1:Y:1209:CYS:N	2.25	0.67
1:Y:458:GLN:OE1	1:Y:460:TRP:NE1	2.27	0.67
1:Y:1937:HIS:HE1	1:Y:1969:GLN:HG3	1.59	0.66
1:y:346:THR:HA	1:y:349:LYS:HD3	1.77	0.66
1:y:1396:SER:HA	1:y:1462:THR:HG22	1.77	0.66
1:Y:202:GLU:OE1	1:Y:202:GLU:N	2.28	0.66
1:Y:437:CYS:SG	1:Y:438:SER:N	2.69	0.66
1:y:369:LEU:HD21	1:y:390:ALA:HB2	1.75	0.66
1:y:878:GLN:HG3	1:y:881:ARG:HH12	1.60	0.66
1:y:1690:CYS:SG	1:y:1691:LEU:N	2.68	0.66
1:Y:413:ARG:NH2	1:Y:1142:SER:OG	2.28	0.66
1:Y:813:ASN:O	1:Y:987:ARG:NH2	2.22	0.66
1:Y:1247:LEU:HD22	1:Y:1250:LEU:HD13	1.78	0.66
5:Y:2206:AGS:O3G	5:Y:2206:AGS:O1A	2.13	0.66
1:y:549:SER:HB3	1:y:559:ASP:HB3	1.77	0.66
1:y:1535:GLN:NE2	1:y:1537:GLN:O	2.29	0.66
1:y:1940:ILE:HA	1:y:2045:PHE:HA	1.76	0.66
1:y:1976:SER:OG	1:y:2024:ALA:O	2.13	0.66
1:y:895:PRO:HD3	1:y:949:TRP:CE2	2.30	0.66
1:Y:27:LEU:HB3	1:Y:29:LEU:HD13	1.77	0.66
1:y:844:LEU:O	1:y:850:GLN:NE2	2.20	0.66
1:y:1175:ARG:NH2	1:y:1176:VAL:O	2.29	0.66
1:Y:57:VAL:HG12	1:Y:425:HIS:HB2	1.76	0.66
1:Y:1075:HIS:NE2	1:Y:1088:GLU:OE2	2.28	0.66
1:Y:1899:ALA:HB1	1:Y:2102:ILE:HB	1.76	0.66
1:y:624:LEU:HG	1:y:626:GLN:H	1.61	0.66
1:Y:1652:ASP:OD1	1:Y:1652:ASP:N	2.26	0.65
1:Y:688:HIS:HA	1:Y:691:LEU:HD12	1.76	0.65
1:Y:1851:ASP:OD1	1:Y:1852:ASP:N	2.28	0.65
1:Y:442:CYS:HB2	1:Y:445:LYS:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1073:GLU:HB3	1:Y:1087:ASN:HD21	1.61	0.65
1:Y:1423:CYS:SG	1:Y:1426:CYS:N	2.68	0.65
1:y:63:GLY:O	1:y:328:GLN:N	2.29	0.65
1:y:1019:LEU:HD22	1:y:1021:VAL:O	1.96	0.65
1:y:611:LEU:HA	1:y:614:ILE:HG12	1.78	0.65
1:y:1595:ASN:ND2	1:y:1599:GLY:O	2.25	0.65
1:Y:14:GLN:HB3	1:Y:18:ARG:HH12	1.60	0.65
1:Y:1218:SER:HB3	1:Y:1221:LEU:HB3	1.79	0.65
1:Y:1704:ASP:OD2	1:Y:1707:HIS:ND1	2.29	0.65
1:y:657:LEU:HD11	1:y:1072:LEU:HD22	1.79	0.65
1:y:490:LYS:NZ	1:y:492:GLU:OE1	2.29	0.65
1:Y:12:LEU:HD12	1:Y:403:LEU:HD11	1.77	0.65
1:Y:1488:PRO:O	1:Y:1504:ARG:NH2	2.30	0.65
2:G:20:DA:H2''	2:G:21:DG:H8	1.61	0.65
1:Y:183:ASN:HA	1:Y:224:MET:HG3	1.79	0.65
1:y:1506:SER:OG	1:y:1589:MET:SD	2.52	0.65
2:G:7:DA:N7	2:G:8:DG:N1	2.45	0.65
1:Y:813:ASN:N	1:Y:813:ASN:OD1	2.30	0.65
1:Y:1386:ASP:OD1	1:Y:1395:ARG:NE	2.27	0.65
1:Y:1953:PRO:HB2	1:Y:2083:LEU:HD11	1.78	0.65
1:y:1427:GLY:O	1:y:1484:ARG:NH2	2.28	0.65
1:Y:89:LYS:H	1:Y:89:LYS:HZ3	1.43	0.64
1:Y:745:GLU:OE2	1:Y:748:GLN:NE2	2.31	0.64
1:Y:1688:HIS:HA	1:Y:1692:LEU:HB2	1.79	0.64
1:y:1175:ARG:HH12	1:y:1177:ARG:HB2	1.62	0.64
1:y:848:ASP:OD1	1:y:849:LYS:NZ	2.29	0.64
1:Y:1110:ASP:OD1	1:Y:1135:ARG:NH2	2.30	0.64
1:Y:647:ARG:O	1:Y:651:ALA:N	2.30	0.64
1:Y:1909:ASP:O	1:Y:1918:ARG:NH1	2.31	0.64
1:Y:2044:THR:OG1	1:Y:2048:GLY:O	2.16	0.64
1:y:1374:LEU:HD22	1:y:1583:TYR:HD2	1.63	0.64
1:y:180:ALA:HB3	1:y:218:MET:HE1	1.78	0.64
1:y:672:GLN:O	1:y:1022:ARG:NH1	2.28	0.64
1:y:110:SER:HB3	1:y:320:VAL:HG22	1.80	0.64
1:y:586:CYS:SG	1:y:587:VAL:N	2.71	0.64
1:Y:110:SER:OG	1:Y:287:ILE:O	2.13	0.64
1:y:914:ARG:HA	1:y:920:ILE:HG21	1.79	0.64
2:G:13:DT:H2'	2:G:14:DC:C4	2.33	0.64
1:Y:121:LYS:NZ	5:Y:2206:AGS:S1G	2.66	0.64
1:Y:527:ASP:OD2	1:Y:580:ARG:NH2	2.30	0.64
1:y:18:ARG:HH11	1:y:617:THR:HG22	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:825:ILE:O	1:Y:859:LYS:NZ	2.30	0.64
1:Y:1976:SER:HB2	1:Y:2024:ALA:HB3	1.79	0.64
1:y:1341:GLU:O	1:y:1345:ARG:NH1	2.31	0.64
1:y:1550:ARG:NE	1:y:1555:TYR:OH	2.31	0.64
1:Y:1025:ARG:HA	1:Y:1031:GLU:HA	1.80	0.64
1:y:183:ASN:HA	1:y:224:MET:HG3	1.80	0.63
1:Y:117:THR:O	5:Y:2206:AGS:O2B	2.15	0.63
1:Y:562:ALA:HB1	1:Y:565:HIS:HB3	1.79	0.63
1:y:1629:GLU:O	1:y:1654:ASN:ND2	2.30	0.63
1:y:57:VAL:HG23	1:y:425:HIS:HB2	1.80	0.63
1:Y:1844:GLN:HA	1:Y:1876:THR:HA	1.79	0.63
1:y:171:ARG:NH2	1:y:202:GLU:OE2	2.31	0.63
1:y:978:GLN:HB3	1:y:1013:LEU:HD11	1.79	0.63
1:y:1227:LEU:HB2	1:y:1256:LEU:HD12	1.79	0.63
1:Y:7:HIS:ND1	1:Y:407:ASP:OD1	2.31	0.63
1:y:578:GLU:OE2	2:G:23:DC:N4	2.32	0.63
1:Y:1904:LEU:HB2	1:Y:2099:SER:H	1.64	0.63
1:y:552:GLU:HA	1:y:555:ALA:HB2	1.81	0.63
1:Y:1912:LEU:HD11	1:Y:1958:LEU:HA	1.80	0.63
1:y:1090:GLN:HG3	1:y:1095:LYS:HB2	1.81	0.63
1:Y:696:ILE:HA	1:Y:708:ILE:HD12	1.80	0.63
1:Y:1340:ASP:O	1:Y:1344:LYS:NZ	2.32	0.63
1:y:955:CYS:O	1:y:970:GLN:NE2	2.32	0.63
1:y:1079:ARG:HB3	1:y:1083:GLN:HE22	1.62	0.63
1:Y:242:GLN:NE2	1:Y:274:ALA:O	2.29	0.63
1:Y:1952:SER:HA	1:Y:1997:ALA:HA	1.81	0.63
1:y:1338:THR:HG22	1:y:1340:ASP:H	1.63	0.63
1:y:1771:GLN:H	1:y:1771:GLN:CD	2.05	0.63
1:Y:912:ARG:NH1	1:Y:913:ASP:OD1	2.32	0.62
1:y:97:GLN:NE2	1:y:119:SER:O	2.30	0.62
1:y:178:ARG:HB2	1:y:215:PRO:HB3	1.80	0.62
1:Y:1838:GLN:OE1	1:Y:1879:LYS:N	2.32	0.62
1:y:356:LEU:O	1:y:360:LEU:HG	1.98	0.62
1:Y:131:GLU:OE1	1:Y:135:ARG:NH2	2.32	0.62
1:y:30:ARG:HH11	1:y:482:CYS:HB2	1.65	0.62
1:y:309:VAL:HA	1:y:312:LEU:HD12	1.81	0.62
1:y:1603:ARG:HG3	1:y:1645:GLY:HA2	1.79	0.62
1:Y:1405:LEU:HB3	1:Y:1410:GLU:HB3	1.82	0.62
1:y:2102:ILE:HG22	1:y:2104:GLY:H	1.64	0.62
1:Y:1093:SER:OG	1:Y:1095:LYS:NZ	2.32	0.62
1:Y:1835:TRP:CZ2	1:Y:1838:GLN:HB2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:2071:ASP:OD1	1:Y:2071:ASP:N	2.32	0.62
1:y:886:ARG:NH2	2:G:17:DA:O4'	2.32	0.62
1:y:1101:CYS:HB3	1:y:1104:THR:HG23	1.81	0.62
1:y:1529:CYS:SG	1:y:1530:GLY:N	2.72	0.62
1:y:1780:GLN:NE2	1:y:1783:SER:OG	2.32	0.62
1:Y:156:ASN:ND2	2:G:8:DG:OP1	2.32	0.62
1:Y:1251:THR:OG1	1:Y:1252:ALA:N	2.31	0.62
1:Y:1338:THR:N	1:Y:1341:GLU:OE2	2.32	0.62
1:Y:877:GLU:OE1	1:Y:877:GLU:N	2.33	0.62
1:Y:1963:LEU:O	1:Y:1967:VAL:HG12	2.00	0.62
1:y:1157:MET:HE2	1:y:1689:HIS:CG	2.34	0.62
1:y:1403:LYS:HB2	1:y:1416:HIS:CD2	2.35	0.62
2:G:16:DG:H2'	2:G:16:DG:N3	2.15	0.62
1:Y:1403:LYS:HZ1	1:Y:1416:HIS:HA	1.65	0.61
1:Y:1988:SER:HB2	1:Y:1999:LEU:HD21	1.81	0.61
1:Y:831:ASP:O	1:Y:855:ARG:NH2	2.33	0.61
1:Y:2021:TRP:HZ3	1:Y:2025:ILE:HG12	1.65	0.61
2:G:20:DA:H2''	2:G:21:DG:C8	2.34	0.61
1:Y:1693:SER:N	1:Y:1696:SER:OG	2.33	0.61
1:Y:1911:PRO:O	1:Y:1915:PHE:N	2.32	0.61
1:y:269:ARG:NH1	1:y:1240:ARG:O	2.33	0.61
1:y:279:PRO:O	1:y:1240:ARG:NH2	2.31	0.61
1:y:1157:MET:HG3	1:y:1689:HIS:ND1	2.16	0.61
1:y:1807:LEU:HB3	1:y:1891:LEU:HD13	1.81	0.61
1:Y:591:ASP:OD1	1:Y:592:THR:N	2.33	0.61
1:y:110:SER:N	1:y:319:ASP:O	2.25	0.61
1:y:1465:ARG:HH12	1:y:1569:LYS:HE3	1.66	0.61
1:y:197:GLN:OE1	1:y:206:SER:OG	2.16	0.61
1:Y:59:GLU:OE2	1:Y:425:HIS:NE2	2.30	0.61
1:Y:1209:CYS:C	1:Y:1211:TRP:H	2.08	0.61
1:y:781:MET:N	1:y:781:MET:SD	2.74	0.61
1:y:934:GLN:OE1	1:y:937:TRP:N	2.26	0.61
1:y:1000:LEU:HD22	1:y:1008:PRO:HD3	1.83	0.61
1:y:1344:LYS:HE2	1:y:1346:ARG:HH12	1.66	0.61
1:y:1753:TYR:OH	1:y:1844:GLN:OE1	2.13	0.61
1:Y:150:ILE:HD13	1:Y:218:MET:HB3	1.83	0.61
1:Y:1998:TRP:HD1	1:Y:1999:LEU:H	1.49	0.61
1:y:479:CYS:SG	1:y:484:SER:OG	2.56	0.61
1:y:817:LEU:O	1:y:821:GLY:N	2.34	0.61
1:y:1016:MET:HE2	1:y:1016:MET:N	2.16	0.61
1:y:1183:ILE:HG22	1:y:1187:HIS:HE1	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:20:DA:H2	3:I:11:DT:H3	1.49	0.61
1:y:7:HIS:ND1	1:y:407:ASP:OD1	2.31	0.61
1:y:428:ILE:HG13	1:y:1149:LEU:HA	1.82	0.61
1:y:428:ILE:HG23	1:y:1147:ILE:HD11	1.83	0.61
1:Y:677:ILE:HG12	1:Y:1022:ARG:HH21	1.66	0.60
1:y:1446:ILE:HD13	1:y:1449:LEU:HD21	1.82	0.60
1:Y:537:ARG:HD2	1:Y:570:LEU:HD13	1.82	0.60
1:Y:1504:ARG:NH1	1:Y:1591:GLU:OE1	2.34	0.60
1:y:1421:TRP:HB2	1:y:1449:LEU:HD13	1.82	0.60
1:y:1535:GLN:NE2	1:y:1540:ARG:H	1.99	0.60
1:y:1592:LEU:HD21	1:y:1594:LEU:HG	1.82	0.60
1:Y:270:ARG:HD2	1:Y:1191:LEU:HB2	1.82	0.60
1:y:1074:GLU:O	1:y:1079:ARG:NH1	2.28	0.60
1:y:1909:ASP:O	1:y:1911:PRO:HD2	2.02	0.60
1:Y:734:PRO:HG2	1:y:731:ILE:HD11	1.84	0.60
1:Y:1843:GLY:O	1:Y:1876:THR:OG1	2.19	0.60
1:Y:1952:SER:O	1:Y:1955:THR:OG1	2.19	0.60
1:Y:259:SER:OG	1:Y:1659:GLY:N	2.35	0.60
1:Y:287:ILE:HD12	1:Y:313:ALA:HB2	1.82	0.60
1:Y:519:VAL:HG11	1:Y:809:ARG:HH22	1.67	0.60
1:y:750:LEU:O	1:y:754:SER:OG	2.18	0.60
1:y:777:LEU:HA	1:y:781:MET:SD	2.42	0.60
1:y:437:CYS:H	1:y:458:GLN:H	1.49	0.60
1:Y:510:VAL:HG13	1:Y:514:ALA:HB3	1.84	0.60
1:y:454:TRP:NE1	1:y:456:PHE:O	2.35	0.60
1:y:984:TYR:HE2	1:y:1008:PRO:HB3	1.67	0.60
1:y:1908:LEU:HD22	1:y:1918:ARG:HG3	1.83	0.60
1:Y:891:MET:HE2	1:Y:904:ARG:HH12	1.67	0.59
1:Y:2066:GLU:CD	1:Y:2089:ARG:H	2.10	0.59
1:y:827:TYR:CZ	1:y:862:LEU:HD11	2.36	0.59
1:y:1056:TRP:HE1	1:y:1061:ASP:HB3	1.67	0.59
1:Y:669:LEU:HD22	1:Y:771:LEU:HG	1.84	0.59
1:Y:2098:ARG:NH1	1:Y:2100:TYR:OH	2.35	0.59
1:y:684:LEU:HD11	1:y:746:ALA:HA	1.83	0.59
1:y:1073:GLU:HG2	1:y:1087:ASN:HB3	1.84	0.59
1:y:1082:GLU:O	1:y:1085:GLN:NE2	2.30	0.59
1:Y:1541:THR:H	1:Y:1577:LYS:HZ1	1.51	0.59
1:Y:1669:ALA:HA	1:Y:1720:LEU:HD23	1.83	0.59
1:y:148:GLN:HA	1:y:245:LEU:HD12	1.84	0.59
1:y:813:ASN:O	1:y:987:ARG:NH2	2.20	0.59
1:y:1177:ARG:HD3	1:y:1662:VAL:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:1450:ASP:OD1	1:y:1452:LYS:NZ	2.34	0.59
1:y:1541:THR:HG22	1:y:1577:LYS:HD3	1.84	0.59
1:Y:83:LEU:HD21	1:Y:130:LEU:HD11	1.84	0.59
1:Y:351:LEU:HD13	1:Y:359:GLN:HG3	1.83	0.59
1:y:662:ASP:OD1	1:y:1069:TRP:NE1	2.31	0.59
1:Y:910:GLN:N	1:Y:913:ASP:OD2	2.35	0.59
1:Y:1799:LEU:O	1:Y:1804:ARG:NH2	2.36	0.59
1:y:1541:THR:HB	1:y:1545:LEU:HD21	1.84	0.59
1:y:1903:ASN:HB3	1:y:2098:ARG:HH21	1.66	0.59
1:y:1927:HIS:HD1	1:y:2103:ALA:HB3	1.68	0.59
1:Y:1884:GLN:HE22	1:Y:1886:LEU:HD23	1.68	0.59
1:y:666:LEU:HD11	1:y:802:CYS:HB2	1.85	0.59
1:y:769:GLU:HA	1:y:772:VAL:HG12	1.84	0.59
1:y:1652:ASP:OD1	1:y:1654:ASN:ND2	2.34	0.59
1:Y:1946:SER:HA	1:Y:1980:CYS:HB2	1.83	0.59
1:y:979:VAL:HG21	1:y:988:ALA:HB1	1.83	0.59
1:y:1075:HIS:HB3	1:y:1084:ASN:HD21	1.68	0.59
1:y:1726:TYR:HE2	1:y:1868:SER:HB2	1.67	0.59
1:Y:1285:LYS:HD2	1:Y:1291:TRP:HB3	1.84	0.59
1:Y:1492:TRP:CE3	1:Y:1504:ARG:HD3	2.38	0.59
1:y:334:GLU:OE2	1:y:371:GLN:NE2	2.36	0.59
1:y:912:ARG:O	1:y:915:HIS:NE2	2.36	0.59
1:Y:195:GLU:OE1	1:Y:195:GLU:N	2.33	0.58
1:Y:1681:CYS:O	1:Y:1705:ARG:NH1	2.36	0.58
1:Y:902:GLN:N	1:Y:905:ASP:OD2	2.27	0.58
1:Y:979:VAL:HG11	1:Y:988:ALA:HB1	1.85	0.58
1:Y:1639:ASP:N	1:Y:1643:TYR:O	2.34	0.58
1:y:1604:ASP:OD2	1:y:1707:HIS:ND1	2.32	0.58
1:y:1661:ALA:O	1:y:1665:ILE:HG12	2.03	0.58
1:Y:1588:ASP:N	1:Y:1588:ASP:OD1	2.35	0.58
1:y:2003:ASP:HA	1:y:2006:GLN:OE1	2.03	0.58
1:Y:412:SER:OG	1:Y:419:PHE:N	2.36	0.58
1:y:648:GLN:NE2	3:I:17:DC:N3	2.51	0.58
1:y:816:THR:O	1:y:820:LEU:N	2.33	0.58
1:Y:1939:GLU:O	1:Y:1974:ARG:NH2	2.35	0.58
1:y:75:ARG:HA	1:y:84:VAL:HG21	1.83	0.58
1:y:1249:SER:HB2	1:y:1780:GLN:HB2	1.85	0.58
1:y:1386:ASP:OD1	1:y:1395:ARG:NE	2.26	0.58
1:Y:639:ARG:HD2	1:Y:1113:GLY:H	1.67	0.58
1:Y:829:PHE:HA	1:Y:832:LYS:HD3	1.84	0.58
1:Y:1072:LEU:HG	1:Y:1098:VAL:HG11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:181:LEU:HA	1:y:219:VAL:HG23	1.86	0.58
1:y:338:ARG:HH12	1:y:363:TYR:HE1	1.52	0.58
1:y:1528:SER:HB2	1:y:1573:GLY:HA3	1.84	0.58
1:Y:167:ARG:NH2	1:Y:203:GLN:OE1	2.36	0.58
1:y:437:CYS:HA	1:y:473:VAL:HG12	1.85	0.58
1:y:1420:PHE:HD1	1:y:1431:THR:HG22	1.69	0.58
1:y:934:GLN:HE22	1:y:936:HIS:HB3	1.68	0.58
1:y:1736:GLU:HB3	1:y:1870:VAL:HG13	1.86	0.58
1:y:2075:ARG:O	1:y:2078:GLN:NE2	2.35	0.58
1:Y:805:SER:HA	1:Y:883:MET:SD	2.43	0.58
1:Y:833:VAL:O	1:Y:855:ARG:NH2	2.36	0.58
1:Y:1895:LEU:HD23	1:Y:1901:ARG:HG2	1.86	0.58
1:y:916:TYR:OH	3:I:10:DC:O3'	2.21	0.58
1:y:917:ASN:O	1:y:921:LYS:NZ	2.37	0.58
2:G:16:DG:H5''	2:G:16:DG:C4	2.38	0.58
1:Y:594:ARG:HD3	1:Y:597:ASN:HD21	1.69	0.57
1:Y:863:ASP:OD1	1:Y:867:ARG:NH1	2.37	0.57
1:Y:1182:SER:OG	1:Y:1186:ARG:NH2	2.36	0.57
1:Y:1232:ASP:OD1	1:Y:1233:GLN:N	2.36	0.57
1:Y:1492:TRP:HE3	1:Y:1504:ARG:HD3	1.69	0.57
1:Y:1510:GLU:OE2	1:Y:1586:ARG:NE	2.37	0.57
1:y:442:CYS:HB3	1:y:445:LYS:HB2	1.86	0.57
1:Y:690:ALA:O	1:Y:694:LYS:HG3	2.04	0.57
1:y:1734:ARG:N	1:y:1872:THR:O	2.34	0.57
1:Y:9:ALA:HB1	1:Y:400:ARG:HH11	1.69	0.57
1:Y:1403:LYS:NZ	1:Y:1414:ASP:OD2	2.37	0.57
1:Y:1405:LEU:HD21	1:Y:1416:HIS:CD2	2.39	0.57
1:Y:1521:HIS:CD2	1:Y:1538:PRO:HD3	2.38	0.57
1:Y:1531:ARG:HE	1:Y:1554:HIS:HB2	1.69	0.57
1:y:227:TYR:O	1:y:231:ARG:N	2.33	0.57
1:y:491:GLU:OE2	1:y:499:ASN:ND2	2.37	0.57
1:y:1439:CYS:HB3	1:y:1444:ALA:H	1.70	0.57
1:Y:329:ILE:O	1:Y:331:ARG:NH1	2.33	0.57
1:Y:689:CYS:HA	1:Y:715:MET:CE	2.35	0.57
1:Y:1214:GLU:OE2	1:Y:1308:ARG:NH2	2.31	0.57
1:y:30:ARG:HA	1:y:986:ARG:HH21	1.70	0.57
1:y:182:TYR:OH	1:y:231:ARG:NH1	2.37	0.57
1:y:667:ARG:HB3	1:y:1063:LEU:HD11	1.85	0.57
1:y:913:ASP:OD1	1:y:916:TYR:OH	2.22	0.57
1:y:918:ARG:NH2	3:I:13:DT:OP2	2.38	0.57
1:y:1904:LEU:HB3	1:y:2099:SER:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:736:VAL:HG13	1:Y:743:HIS:HB3	1.86	0.57
1:y:1119:MET:HG3	1:y:1148:THR:HG23	1.85	0.57
1:Y:1400:MET:HE3	1:Y:1459:GLY:C	2.30	0.57
1:Y:1601:LEU:HD23	1:Y:1645:GLY:HA3	1.85	0.57
1:y:265:ALA:HB2	1:y:312:LEU:HD23	1.86	0.57
1:y:969:GLN:OE1	1:y:969:GLN:N	2.35	0.57
1:y:1605:GLU:OE2	1:y:1634:THR:OG1	2.21	0.57
1:y:1967:VAL:HG21	1:y:2021:TRP:HD1	1.70	0.57
1:Y:253:ALA:N	1:Y:291:SER:OG	2.38	0.57
1:Y:1123:PRO:HD2	1:Y:1129:TYR:HB2	1.87	0.57
1:y:575:SER:HA	1:y:582:ASN:HA	1.87	0.57
1:y:1609:ARG:NE	1:y:1634:THR:OG1	2.38	0.57
1:y:1973:GLU:HG2	1:y:2022:PRO:HD2	1.87	0.57
1:Y:779:ASP:OD1	1:Y:782:ARG:NH2	2.37	0.57
1:y:87:LEU:HD11	1:y:127:VAL:HG22	1.87	0.57
1:y:573:PRO:HB2	1:y:582:ASN:HD22	1.70	0.57
1:y:1782:ALA:O	1:y:1817:ARG:NE	2.36	0.57
1:Y:1119:MET:HE1	1:Y:1132:ARG:HD2	1.87	0.57
1:Y:1945:TYR:CZ	1:Y:1947:ASP:HB3	2.40	0.57
1:Y:1994:LEU:HD23	1:Y:2064:CYS:HB3	1.85	0.57
1:y:658:GLN:NE2	1:y:662:ASP:OD1	2.38	0.57
1:y:1605:GLU:OE2	1:y:1702:ARG:NH2	2.38	0.57
1:Y:1557:LEU:HB3	1:Y:1558:ARG:HD2	1.86	0.56
1:y:98:LEU:HD13	1:y:101:TRP:HE1	1.70	0.56
1:y:109:LYS:HD3	1:y:321:LYS:HD3	1.86	0.56
1:y:672:GLN:HB3	1:y:1023:HIS:HD2	1.69	0.56
1:Y:692:LEU:HB3	1:Y:711:LEU:HD21	1.86	0.56
1:y:1177:ARG:HG2	1:y:1662:VAL:HG11	1.88	0.56
1:Y:333:SER:HB3	1:Y:336:LEU:HD13	1.87	0.56
1:Y:389:VAL:HG22	1:Y:392:ARG:HH22	1.70	0.56
1:Y:1531:ARG:NH2	1:Y:1557:LEU:H	2.03	0.56
1:Y:1799:LEU:HD23	1:Y:1804:ARG:HG3	1.86	0.56
1:Y:1845:SER:OG	1:Y:1877:SER:O	2.15	0.56
1:y:33:SER:OG	1:y:448:GLU:O	2.23	0.56
1:y:1681:CYS:O	1:y:1705:ARG:NH1	2.38	0.56
1:Y:593:GLN:HG3	1:Y:599:LEU:H	1.67	0.56
1:Y:1024:TRP:HE1	1:Y:1065:LEU:HA	1.70	0.56
1:Y:1385:ALA:HB2	1:Y:1478:LEU:HD23	1.87	0.56
1:Y:1432:SER:OG	1:Y:1434:THR:O	2.23	0.56
1:y:424:MET:HE2	1:y:424:MET:HA	1.87	0.56
1:Y:1547:ASN:HB3	1:Y:1550:ARG:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1760:LEU:HD22	1:Y:1858:PRO:HG3	1.87	0.56
1:y:762:MET:SD	1:y:766:THR:HG23	2.46	0.56
1:Y:862:LEU:HD12	1:Y:866:ILE:HG13	1.86	0.56
1:Y:1841:ARG:HH21	1:Y:1844:GLN:H	1.54	0.56
1:y:1334:PHE:HD1	1:y:1460:PHE:HB3	1.71	0.56
1:Y:70:THR:HA	1:Y:92:VAL:HG12	1.88	0.56
1:Y:245:LEU:HD23	1:Y:277:VAL:HG21	1.86	0.56
1:Y:1760:LEU:HD11	1:Y:1790:LEU:HD11	1.86	0.56
1:Y:1940:ILE:O	1:Y:1974:ARG:NE	2.36	0.56
1:y:1483:PRO:HB3	1:y:1513:HIS:HA	1.87	0.56
1:Y:161:SER:OG	1:Y:162:GLN:NE2	2.35	0.56
1:Y:992:THR:OG1	1:Y:996:TYR:N	2.39	0.56
1:Y:1013:LEU:O	1:Y:1014:ILE:HD13	2.05	0.56
1:Y:1141:GLU:OE1	1:Y:1141:GLU:N	2.38	0.56
1:Y:1157:MET:O	1:Y:1161:LYS:HG2	2.06	0.56
1:y:211:TYR:HA	1:y:237:ILE:HD11	1.88	0.56
1:y:635:PHE:H	1:y:1097:ASN:HD21	1.54	0.56
1:y:1845:SER:OG	1:y:1877:SER:O	2.24	0.56
1:Y:789:SER:HG	1:Y:882:TRP:CG	2.23	0.56
1:Y:969:GLN:OE1	1:Y:969:GLN:N	2.39	0.56
1:Y:1091:PHE:HD1	1:Y:1096:VAL:HB	1.70	0.56
1:Y:1423:CYS:HB2	1:Y:1439:CYS:SG	2.45	0.56
1:Y:1737:THR:OG1	1:Y:1738:ASN:N	2.39	0.56
1:Y:2065:ILE:HB	1:Y:2089:ARG:HB2	1.87	0.56
1:y:14:GLN:OE1	1:y:1034:ARG:NH2	2.38	0.56
1:y:643:PHE:HE1	1:y:1105:MET:H	1.52	0.56
1:y:2069:PHE:O	1:y:2082:ARG:NE	2.39	0.56
1:Y:1760:LEU:HB3	1:Y:1858:PRO:HD3	1.88	0.56
1:Y:1946:SER:OG	1:Y:2040:GLU:O	2.19	0.56
1:y:130:LEU:O	1:y:134:ILE:HG12	2.05	0.56
1:y:1779:LEU:HD13	1:y:2095:ASN:HD22	1.71	0.56
1:Y:776:ASP:OD1	1:Y:776:ASP:N	2.36	0.55
1:Y:1930:TRP:CD1	1:Y:2051:HIS:HD1	2.24	0.55
1:y:639:ARG:HB3	1:y:1091:PHE:CZ	2.41	0.55
1:y:982:CYS:SG	1:y:985:THR:N	2.79	0.55
1:y:1603:ARG:HH12	1:y:1643:TYR:HB3	1.71	0.55
1:y:1764:GLN:HA	1:y:1767:TRP:CD1	2.40	0.55
1:y:2042:THR:HG22	1:y:2052:TYR:HB3	1.88	0.55
1:y:117:THR:O	5:y:2206:AGS:O2B	2.24	0.55
1:Y:695:VAL:HG21	1:Y:736:VAL:HG22	1.88	0.55
1:Y:748:GLN:NE2	1:Y:749:ILE:HG13	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:811:PRO:HG2	1:Y:814:ALA:HB3	1.87	0.55
1:Y:1835:TRP:HZ2	1:Y:1838:GLN:HB2	1.70	0.55
1:y:166:LEU:HA	1:y:169:TRP:CD1	2.37	0.55
1:y:762:MET:HG3	1:y:767:LEU:HB2	1.88	0.55
1:y:778:ALA:O	1:y:795:LYS:NZ	2.33	0.55
2:G:13:DT:H5"	2:G:13:DT:H6	1.70	0.55
1:Y:197:GLN:NE2	1:Y:200:VAL:O	2.39	0.55
1:y:131:GLU:OE2	1:y:135:ARG:NH1	2.40	0.55
1:y:297:ASP:OD1	1:y:324:ARG:NH1	2.39	0.55
1:y:816:THR:H	1:y:819:SER:HG	1.51	0.55
1:y:1613:VAL:HA	1:y:1616:ARG:HG2	1.87	0.55
1:Y:1056:TRP:HE1	1:Y:1061:ASP:HB3	1.71	0.55
1:y:252:GLU:O	1:y:255:SER:OG	2.21	0.55
1:y:253:ALA:HB3	1:y:291:SER:HB2	1.87	0.55
1:y:1554:HIS:O	1:y:1571:CYS:N	2.39	0.55
1:y:1605:GLU:HB2	1:y:1646:TYR:CZ	2.41	0.55
5:y:2206:AGS:O1B	5:y:2206:AGS:O3G	2.25	0.55
1:Y:1851:ASP:HB2	1:Y:1868:SER:OG	2.07	0.55
1:Y:2007:VAL:HG22	1:Y:2076:VAL:HG13	1.89	0.55
1:y:61:THR:HG21	1:y:423:ARG:HD3	1.89	0.55
1:y:152:LEU:HD23	1:y:250:LEU:HD23	1.89	0.55
1:y:1017:PRO:HG3	1:y:1047:ILE:HG23	1.89	0.55
1:Y:1069:TRP:CH2	1:Y:1072:LEU:HB2	2.42	0.55
1:Y:1157:MET:HE2	1:Y:1689:HIS:NE2	2.21	0.55
1:Y:1638:ARG:HH11	1:Y:1642:GLY:HA2	1.72	0.55
1:Y:1791:LEU:HD21	1:Y:1823:ILE:HG21	1.88	0.55
1:y:134:ILE:HD13	1:y:177:ILE:HD12	1.88	0.55
1:y:1219:GLN:OE1	1:y:1222:ARG:NH1	2.34	0.55
1:y:1270:TRP:O	1:y:1273:GLN:HG2	2.07	0.55
1:Y:54:ALA:HB3	1:Y:427:PHE:HB2	1.88	0.55
1:Y:409:MET:HG2	1:Y:419:PHE:HD2	1.71	0.55
1:Y:1277:LEU:O	1:Y:1281:ILE:HG22	2.07	0.55
1:Y:1616:ARG:HH22	1:Y:1695:ASP:CG	2.15	0.55
1:Y:1696:SER:HA	1:Y:1699:TYR:CZ	2.41	0.55
1:y:355:ASP:O	1:y:359:GLN:NE2	2.40	0.55
1:Y:846:ASP:OD2	1:Y:849:LYS:NZ	2.36	0.55
1:Y:1779:LEU:HD13	1:Y:2095:ASN:HD22	1.71	0.55
1:Y:1998:TRP:CD1	1:Y:1999:LEU:H	2.25	0.55
1:y:1036:GLU:O	1:y:1039:GLU:HG2	2.07	0.55
1:y:691:LEU:O	1:y:694:LYS:HG3	2.07	0.55
1:Y:482:CYS:SG	1:Y:484:SER:OG	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:137:GLN:HB2	1:y:177:ILE:HD11	1.89	0.54
1:y:812:LYS:NZ	3:I:13:DT:OP1	2.39	0.54
1:y:1402:GLY:HA2	1:y:1458:VAL:HG21	1.89	0.54
1:Y:30:ARG:HG3	1:Y:986:ARG:HH21	1.72	0.54
1:Y:409:MET:SD	1:Y:419:PHE:HB3	2.47	0.54
1:Y:886:ARG:HH12	1:Y:1469:HIS:CG	2.25	0.54
1:Y:1762:GLY:HA3	1:Y:1857:ALA:HB2	1.89	0.54
1:Y:2095:ASN:OD1	1:Y:2095:ASN:N	2.38	0.54
1:y:439:ASN:C	1:y:441:GLN:H	2.15	0.54
1:y:1553:THR:OG1	1:y:1571:CYS:O	2.20	0.54
1:y:1821:LYS:HE2	1:y:1885:THR:HG22	1.90	0.54
1:Y:1138:ARG:N	1:Y:1141:GLU:OE2	2.34	0.54
1:Y:1845:SER:OG	1:Y:1875:GLY:O	2.26	0.54
1:y:895:PRO:HB3	1:y:908:TRP:CD1	2.42	0.54
1:y:933:GLU:CD	1:y:933:GLU:H	2.14	0.54
1:Y:594:ARG:HH21	1:Y:596:ASN:CG	2.16	0.54
1:Y:1527:LEU:HD11	1:Y:1576:HIS:HB2	1.90	0.54
1:Y:2069:PHE:O	1:Y:2082:ARG:NH2	2.35	0.54
1:y:646:SER:O	1:y:1102:SER:OG	2.25	0.54
1:y:1234:LEU:O	1:y:1238:LEU:HB2	2.07	0.54
1:y:1740:LEU:HD22	1:y:1870:VAL:HG21	1.90	0.54
1:Y:730:LYS:HA	1:Y:733:GLU:HG2	1.89	0.54
1:Y:761:THR:OG1	1:Y:972:GLU:OE1	2.25	0.54
1:Y:1024:TRP:CD1	1:Y:1066:LYS:H	2.23	0.54
1:y:917:ASN:HD21	1:y:919:VAL:HG22	1.73	0.54
1:Y:160:ASN:O	1:Y:163:GLN:HG3	2.07	0.54
1:Y:493:MET:HE1	1:Y:499:ASN:OD1	2.07	0.54
1:Y:1035:GLU:HA	1:Y:1038:LEU:HD12	1.90	0.54
1:Y:1854:ALA:HB2	1:Y:1865:SER:HB2	1.89	0.54
1:y:111:LEU:HD11	1:y:323:VAL:HG12	1.88	0.54
1:y:577:GLY:HA2	2:G:21:DG:H3'	1.90	0.54
1:Y:173:PHE:HB3	1:Y:176:LYS:HB2	1.90	0.54
1:Y:689:CYS:HA	1:Y:715:MET:HE3	1.90	0.54
1:Y:735:MET:SD	1:Y:735:MET:N	2.80	0.54
1:Y:893:GLN:NE2	1:Y:905:ASP:OD1	2.41	0.54
1:Y:1603:ARG:HH21	1:Y:1643:TYR:HB3	1.72	0.54
1:Y:1904:LEU:HD12	1:Y:2099:SER:HB3	1.90	0.54
1:y:1238:LEU:O	1:y:1242:THR:OG1	2.12	0.54
1:y:1681:CYS:SG	1:y:1690:CYS:HB2	2.46	0.54
1:Y:185:GLU:OE1	1:Y:185:GLU:N	2.41	0.54
1:Y:704:LEU:HG	1:y:735:MET:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1788:VAL:HG13	1:Y:1818:LEU:HA	1.90	0.54
1:y:282:ASP:OD1	1:y:282:ASP:N	2.37	0.54
1:y:696:ILE:O	1:y:700:SER:N	2.41	0.54
1:y:1080:THR:HB	1:y:1083:GLN:HG3	1.90	0.54
1:y:1753:TYR:CD1	1:y:1841:ARG:HB2	2.43	0.54
1:y:2069:PHE:HB3	1:y:2082:ARG:HH21	1.73	0.54
1:Y:1487:VAL:HG13	1:Y:1504:ARG:HH22	1.72	0.53
2:G:9:DA:H8	2:G:9:DA:H5'	1.73	0.53
1:Y:58:PHE:CE1	1:Y:424:MET:HG3	2.44	0.53
1:Y:123:GLU:N	1:Y:123:GLU:OE1	2.40	0.53
1:Y:1490:SER:OG	1:Y:1491:VAL:N	2.42	0.53
1:Y:1535:GLN:NE2	1:Y:1577:LYS:O	2.34	0.53
1:y:80:SER:N	1:y:131:GLU:OE1	2.41	0.53
1:y:696:ILE:HG12	1:y:711:LEU:HD23	1.90	0.53
1:y:826:HIS:NE2	1:y:831:ASP:OD2	2.36	0.53
1:y:2061:TYR:OH	1:y:2097:LEU:O	2.26	0.53
1:Y:242:GLN:NE2	1:Y:275:PHE:HA	2.23	0.53
1:Y:1368:LYS:NZ	2:G:11:DC:N3	2.57	0.53
1:y:244:MET:N	1:y:244:MET:SD	2.82	0.53
1:y:1183:ILE:HG22	1:y:1187:HIS:CE1	2.43	0.53
1:y:1248:MET:HE1	1:y:1749:ASN:HA	1.90	0.53
1:Y:1761:ALA:H	1:Y:1856:VAL:HG23	1.73	0.53
1:Y:1937:HIS:CE1	1:Y:1969:GLN:HG3	2.42	0.53
1:y:539:ILE:HG12	1:y:568:ILE:HD11	1.90	0.53
1:y:541:SER:O	1:y:569:ASN:ND2	2.41	0.53
1:y:786:LYS:NZ	1:y:792:ASP:HB2	2.24	0.53
1:y:1943:VAL:HB	1:y:1977:LEU:HA	1.91	0.53
1:Y:1185:GLN:O	1:Y:1189:ASN:ND2	2.38	0.53
1:Y:1417:ILE:HD11	1:Y:1527:LEU:HD21	1.90	0.53
1:y:816:THR:N	1:y:819:SER:OG	2.28	0.53
1:y:876:ASN:HD21	1:y:878:GLN:HB2	1.72	0.53
1:y:912:ARG:O	1:y:912:ARG:NH1	2.42	0.53
1:y:1478:LEU:HG	1:y:1479:PRO:HD2	1.89	0.53
1:y:1540:ARG:HH22	1:y:1542:PRO:HG3	1.72	0.53
1:Y:1941:THR:H	1:Y:2045:PHE:HA	1.74	0.53
1:y:107:ASP:N	1:y:107:ASP:OD1	2.42	0.53
1:Y:206:SER:O	1:Y:210:ILE:HG12	2.08	0.53
1:y:122:THR:O	1:y:126:MET:HG3	2.09	0.53
1:y:167:ARG:O	1:y:171:ARG:NH2	2.41	0.53
1:y:1044:ASN:HD21	1:y:1046:LEU:HG	1.73	0.53
1:Y:513:PHE:HE1	1:Y:606:GLY:HA3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1175:ARG:HH12	1:Y:1177:ARG:HH22	1.56	0.53
1:Y:1927:HIS:HB3	1:Y:1930:TRP:HB2	1.91	0.53
1:y:387:LEU:HA	1:y:402:LEU:HD22	1.91	0.53
1:y:729:LEU:HD13	1:y:751:GLN:HE22	1.74	0.53
1:y:1266:VAL:HG12	1:y:1269:ARG:HH21	1.74	0.53
1:y:1699:TYR:HB3	1:y:1702:ARG:HD3	1.91	0.53
1:Y:14:GLN:HB3	1:Y:18:ARG:NH1	2.24	0.52
1:Y:140:THR:O	1:Y:142:GLN:NE2	2.30	0.52
1:Y:691:LEU:O	1:Y:743:HIS:NE2	2.42	0.52
1:Y:1106:GLU:OE1	1:Y:1132:ARG:NH2	2.41	0.52
1:Y:2021:TRP:CZ3	1:Y:2025:ILE:HG12	2.43	0.52
1:y:1119:MET:SD	1:y:1120:ASN:N	2.82	0.52
1:y:810:ARG:HH22	1:y:999:TYR:HE2	1.56	0.52
1:y:1422:HIS:HA	1:y:1429:GLY:HA2	1.92	0.52
1:y:1952:SER:HA	1:y:1997:ALA:HA	1.91	0.52
1:y:340:GLU:OE1	1:y:364:ARG:NH1	2.43	0.52
1:y:1403:LYS:HB2	1:y:1416:HIS:HD2	1.73	0.52
1:Y:409:MET:HE1	1:Y:420:THR:O	2.09	0.52
1:y:295:GLY:O	1:y:324:ARG:NH2	2.42	0.52
1:y:762:MET:HA	1:y:762:MET:HE2	1.91	0.52
1:y:1292:GLU:HG3	1:y:1349:LYS:HB3	1.91	0.52
1:y:182:TYR:HB3	1:y:220:THR:HG23	1.92	0.52
1:y:640:LEU:N	1:y:1097:ASN:O	2.42	0.52
1:y:1745:ALA:HA	1:y:1777:GLU:HG2	1.91	0.52
1:Y:908:TRP:CG	1:Y:909:PRO:HD2	2.45	0.52
1:Y:1695:ASP:OD1	1:Y:1695:ASP:N	2.30	0.52
1:y:692:LEU:O	1:y:696:ILE:HG13	2.09	0.52
1:y:1902:ILE:HG23	1:y:2101:ILE:HG13	1.92	0.52
1:Y:521:SER:HB2	1:Y:594:ARG:NH2	2.24	0.52
1:y:122:THR:OG1	5:y:2206:AGS:S1G	2.68	0.52
1:y:676:ASN:OD1	1:y:975:SER:HB2	2.10	0.52
1:y:902:GLN:H	1:y:905:ASP:CG	2.16	0.52
1:y:1844:GLN:NE2	1:y:1845:SER:O	2.42	0.52
1:Y:849:LYS:HB3	1:Y:853:GLU:HG2	1.91	0.52
1:y:187:ARG:NH2	1:y:205:LEU:O	2.41	0.52
1:y:268:LEU:O	1:y:271:VAL:HG22	2.09	0.52
1:y:545:LYS:HZ2	1:y:567:GLU:HB3	1.74	0.52
1:y:1071:ARG:N	1:y:1097:ASN:OD1	2.37	0.52
1:Y:113:VAL:HG12	1:Y:323:VAL:HB	1.92	0.52
1:Y:1044:ASN:HD22	1:Y:1047:ILE:HG12	1.74	0.52
1:Y:1793:ALA:HA	1:Y:1823:ILE:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:137:GLN:OE1	1:y:141:ARG:NH1	2.43	0.52
1:y:232:ARG:NH1	1:y:1197:LEU:O	2.43	0.52
1:y:423:ARG:NH2	1:y:1133:ALA:O	2.36	0.52
1:y:766:THR:HA	1:y:769:GLU:HG3	1.91	0.52
1:y:54:ALA:HB3	1:y:427:PHE:HB2	1.91	0.52
1:Y:777:LEU:H	1:Y:777:LEU:HD12	1.74	0.51
1:Y:1701:ASN:OD1	1:Y:1701:ASN:N	2.41	0.51
1:Y:1789:GLU:OE1	1:Y:1791:LEU:HB2	2.09	0.51
1:Y:1939:GLU:HG2	1:Y:1972:ALA:HB3	1.92	0.51
1:Y:2087:ARG:HE	1:Y:2089:ARG:NH2	2.00	0.51
1:y:174:LYS:HA	1:y:202:GLU:HB3	1.92	0.51
1:Y:1945:TYR:CD1	1:Y:2041:LEU:HD11	2.45	0.51
1:y:423:ARG:HH22	1:y:1133:ALA:C	2.18	0.51
1:y:542:ASP:N	1:y:542:ASP:OD1	2.42	0.51
1:y:1125:ALA:HB3	1:y:1128:ASN:HD21	1.74	0.51
1:y:1556:LEU:HG	1:y:1571:CYS:HB2	1.92	0.51
1:y:1733:SER:HB3	1:y:1871:VAL:HB	1.92	0.51
1:y:2043:VAL:O	1:y:2051:HIS:HB2	2.10	0.51
1:Y:689:CYS:O	1:Y:693:GLU:HG2	2.10	0.51
1:Y:1034:ARG:NH2	1:Y:1067:ASP:OD2	2.43	0.51
1:Y:1039:GLU:O	1:Y:1043:SER:OG	2.19	0.51
1:Y:1266:VAL:HG13	1:Y:1319:GLU:HG2	1.92	0.51
1:Y:1463:ASP:OD2	1:Y:1531:ARG:NH1	2.43	0.51
1:y:764:TRP:NE1	1:y:968:LYS:HG3	2.25	0.51
1:y:1638:ARG:HA	1:y:1644:THR:HA	1.92	0.51
1:y:1920:TRP:HE1	1:y:1966:LEU:HD13	1.74	0.51
1:y:2074:LEU:HB3	1:y:2078:GLN:NE2	2.24	0.51
1:Y:55:ASP:OD2	1:Y:384:SER:OG	2.29	0.51
1:Y:339:HIS:HD2	1:Y:363:TYR:HE1	1.58	0.51
1:Y:504:GLN:NE2	1:Y:505:PRO:O	2.35	0.51
1:Y:886:ARG:HH22	1:Y:1469:HIS:CE1	2.28	0.51
2:G:9:DA:C4	2:G:10:DC:C5	2.99	0.51
1:Y:1664:LEU:HD21	1:Y:1668:TRP:CH2	2.45	0.51
1:y:634:PRO:HB3	1:y:1069:TRP:CZ3	2.45	0.51
1:Y:1538:PRO:HB2	1:Y:1539:GLN:NE2	2.25	0.51
1:y:423:ARG:HH21	1:y:425:HIS:HE1	1.57	0.51
1:y:736:VAL:HA	1:y:739:LEU:HD12	1.91	0.51
1:y:900:LYS:HG3	1:y:905:ASP:HB2	1.92	0.51
1:y:1372:ARG:NH1	1:y:1376:THR:OG1	2.41	0.51
1:y:1418:PRO:HG2	1:y:1454:TYR:CZ	2.44	0.51
1:Y:1156:GLY:O	1:Y:1159:VAL:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1424:ARG:NH1	1:Y:1448:GLN:HA	2.26	0.51
1:Y:1564:ARG:HA	1:Y:1564:ARG:NE	2.25	0.51
1:Y:1547:ASN:HD22	1:Y:1550:ARG:HG3	1.75	0.51
1:y:1185:GLN:NE2	1:y:1189:ASN:OD1	2.43	0.51
1:y:1291:TRP:O	1:y:1297:GLY:HA3	2.09	0.51
1:y:2065:ILE:HD11	1:y:2091:VAL:HB	1.93	0.51
1:Y:239:GLU:HG2	1:Y:240:LYS:HD3	1.93	0.51
1:Y:605:LEU:HD12	1:Y:609:PHE:CD2	2.46	0.51
1:Y:1973:GLU:CD	1:Y:2022:PRO:HD2	2.35	0.51
1:y:150:ILE:HG23	1:y:248:ILE:HG23	1.91	0.51
1:y:912:ARG:HH12	1:y:915:HIS:CE1	2.29	0.51
2:G:10:DC:H2"	2:G:11:DC:C6	2.46	0.51
1:Y:653:ILE:O	1:Y:657:LEU:HG	2.11	0.51
1:Y:1528:SER:HB2	1:Y:1573:GLY:HA3	1.92	0.51
1:Y:1824:ALA:HB3	1:Y:1827:GLN:HG3	1.93	0.51
1:Y:2083:LEU:O	1:Y:2086:THR:OG1	2.28	0.51
1:y:348:LEU:HB3	1:y:356:LEU:HD13	1.93	0.51
1:y:1049:HIS:O	1:y:1052:GLU:HG2	2.11	0.51
1:y:1482:ASP:OD2	1:y:1609:ARG:NH2	2.44	0.51
1:y:1946:SER:HA	1:y:1980:CYS:HB2	1.93	0.51
1:y:1988:SER:HB2	1:y:1999:LEU:HD21	1.92	0.51
1:Y:1736:GLU:OE2	1:Y:1738:ASN:N	2.45	0.50
1:Y:2001:GLU:O	1:Y:2004:ARG:HG2	2.11	0.50
1:y:8:TYR:N	1:y:407:ASP:OD2	2.43	0.50
1:y:71:MET:SD	1:y:84:VAL:HG13	2.50	0.50
1:y:1420:PHE:CD1	1:y:1431:THR:HG22	2.46	0.50
1:Y:57:VAL:HG23	1:Y:382:ARG:HA	1.92	0.50
1:Y:1208:SER:O	1:Y:1312:LEU:N	2.44	0.50
1:y:844:LEU:HD23	1:y:850:GLN:HA	1.92	0.50
1:y:1250:LEU:HD21	1:y:1776:LYS:HE2	1.92	0.50
1:Y:294:ILE:HD11	1:Y:1174:PRO:HD2	1.93	0.50
1:Y:423:ARG:HA	1:Y:1144:SER:O	2.11	0.50
1:Y:462:GLU:HG3	1:Y:1689:HIS:HE1	1.77	0.50
1:Y:1139:ARG:HH22	5:Y:2206:AGS:H5'2	1.77	0.50
1:y:336:LEU:O	1:y:362:HIS:ND1	2.45	0.50
1:y:550:LEU:N	1:y:564:LYS:O	2.39	0.50
1:y:658:GLN:HE22	1:y:1069:TRP:HE1	1.59	0.50
1:y:793:LEU:HD12	1:y:797:GLN:HB3	1.93	0.50
1:y:836:CYS:HB2	1:y:841:LYS:HZ3	1.77	0.50
1:y:1545:LEU:HD13	1:y:1575:VAL:HG11	1.93	0.50
1:y:2070:PHE:HD1	1:y:2082:ARG:HD2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:208:GLU:O	1:Y:211:TYR:N	2.45	0.50
1:Y:647:ARG:HD2	1:Y:1078:GLN:HE22	1.75	0.50
1:Y:1263:MET:HE2	1:Y:1263:MET:HA	1.93	0.50
1:Y:1414:ASP:HB3	1:Y:1416:HIS:CE1	2.47	0.50
1:y:108:LYS:HG3	1:y:286:GLN:HG2	1.94	0.50
1:y:908:TRP:CD2	1:y:909:PRO:HD2	2.46	0.50
1:y:1119:MET:SD	1:y:1121:ASN:N	2.82	0.50
1:y:1329:VAL:HG13	1:y:1655:ALA:HB3	1.93	0.50
1:y:1610:SER:HB2	1:y:1708:ALA:HB2	1.94	0.50
2:G:21:DG:O6	3:I:10:DC:N4	2.30	0.50
1:Y:714:ALA:HB2	1:Y:721:LEU:HD21	1.93	0.50
1:Y:1034:ARG:NH1	1:Y:1070:TYR:OH	2.45	0.50
1:Y:1255:LEU:HD23	1:Y:1256:LEU:H	1.77	0.50
1:y:194:GLN:HA	1:y:197:GLN:HE21	1.76	0.50
1:y:607:ALA:HB1	1:y:611:LEU:HD23	1.93	0.50
1:y:747:MET:SD	1:y:751:GLN:NE2	2.84	0.50
1:y:1895:LEU:HD11	1:y:2102:ILE:HG12	1.94	0.50
1:Y:244:MET:N	1:Y:244:MET:SD	2.84	0.50
1:Y:624:LEU:HD12	1:Y:625:PRO:HD2	1.93	0.50
1:Y:716:ALA:HB3	1:Y:719:GLU:HB2	1.94	0.50
1:Y:1492:TRP:CD1	1:Y:1502:ARG:HD2	2.46	0.50
1:y:33:SER:N	1:y:453:ASP:OD2	2.32	0.50
1:y:772:VAL:HA	1:y:777:LEU:HD23	1.92	0.50
1:Y:846:ASP:N	1:Y:846:ASP:OD1	2.43	0.50
1:Y:911:ILE:HG12	1:Y:938:LYS:HG2	1.94	0.50
1:Y:1196:PHE:HB2	1:Y:1226:TRP:CZ3	2.47	0.50
1:Y:1733:SER:HB3	1:Y:1871:VAL:HG21	1.93	0.50
1:y:316:THR:O	1:y:318:ARG:HG2	2.12	0.50
1:y:1616:ARG:HB2	1:y:1630:LEU:HD11	1.94	0.50
1:Y:1487:VAL:HG13	1:Y:1504:ARG:NH2	2.26	0.50
1:y:277:VAL:HG12	1:y:285:VAL:HB	1.93	0.50
1:y:888:PRO:HG3	2:G:17:DA:C8	2.47	0.50
1:Y:146:GLY:HA3	1:Y:244:MET:SD	2.51	0.50
1:Y:154:PRO:HD3	1:Y:252:GLU:OE2	2.12	0.50
1:Y:576:ARG:NH2	1:Y:583:SER:O	2.32	0.50
1:Y:1904:LEU:HD13	1:Y:2061:TYR:CD2	2.47	0.50
1:y:188:HIS:HA	1:y:207:ARG:HB2	1.94	0.50
1:y:804:TYR:HB3	1:y:883:MET:HE1	1.94	0.50
1:y:1045:ALA:HA	1:y:1048:GLN:NE2	2.27	0.50
1:y:1302:TYR:HA	1:y:1305:ARG:HD2	1.93	0.50
1:y:1480:TRP:O	1:y:1481:LYS:NZ	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:1904:LEU:HD21	1:y:2062:TRP:CZ2	2.46	0.50
1:Y:339:HIS:O	1:Y:363:TYR:HA	2.11	0.49
1:y:122:THR:HA	1:y:125:PHE:CE2	2.47	0.49
1:y:673:GLU:HG2	1:y:770:GLN:HG3	1.94	0.49
1:y:870:SER:O	1:y:890:LYS:N	2.44	0.49
1:y:490:LYS:HB3	1:y:504:GLN:HB2	1.93	0.49
1:y:576:ARG:HH11	1:y:583:SER:HB3	1.77	0.49
1:y:757:GLN:HG3	1:y:977:LYS:HD2	1.93	0.49
1:y:1023:HIS:O	1:y:1025:ARG:HG3	2.12	0.49
1:Y:40:SER:OG	1:Y:41:GLN:NE2	2.46	0.49
1:Y:83:LEU:O	1:Y:87:LEU:N	2.46	0.49
1:Y:770:GLN:OE1	1:y:957:ARG:NH2	2.46	0.49
1:Y:1270:TRP:CD1	1:Y:1307:TYR:HH	2.31	0.49
1:y:427:PHE:HA	1:y:1148:THR:O	2.13	0.49
1:y:846:ASP:OD2	1:y:849:LYS:NZ	2.45	0.49
1:y:1417:ILE:HD12	1:y:1453:ARG:HB3	1.94	0.49
1:Y:311:ASP:HB3	1:Y:1176:VAL:HG21	1.93	0.49
1:Y:517:VAL:HG12	1:Y:656:ARG:HH22	1.78	0.49
1:y:635:PHE:HB2	1:y:1070:TYR:HB3	1.94	0.49
1:y:1940:ILE:HD12	1:y:1943:VAL:HG22	1.93	0.49
1:Y:464:ARG:HH12	1:Y:466:TYR:C	2.16	0.49
1:Y:1492:TRP:HE3	1:Y:1504:ARG:HH11	1.61	0.49
1:Y:2087:ARG:HG3	1:Y:2089:ARG:HH12	1.77	0.49
1:y:437:CYS:SG	1:y:471:ALA:HB3	2.52	0.49
1:y:1213:PHE:HB3	1:y:1270:TRP:CZ2	2.48	0.49
1:y:688:HIS:CG	1:y:746:ALA:HB2	2.48	0.49
2:G:18:DA:H2"	2:G:19:DG:N7	2.26	0.49
1:Y:107:ASP:OD2	1:Y:109:LYS:NZ	2.31	0.49
1:y:173:PHE:HB3	1:y:177:ILE:H	1.78	0.49
1:y:196:ASP:HA	1:y:199:LYS:HE2	1.95	0.49
1:y:252:GLU:HG3	1:y:1107:MET:HE2	1.94	0.49
1:y:1000:LEU:HD13	1:y:1008:PRO:HB3	1.94	0.49
1:y:1183:ILE:O	1:y:1187:HIS:ND1	2.39	0.49
1:y:1225:HIS:HB3	1:y:1229:HIS:CE1	2.47	0.49
1:y:1662:VAL:HA	1:y:1665:ILE:HD11	1.95	0.49
1:Y:886:ARG:HH12	1:Y:1469:HIS:CE1	2.30	0.49
1:Y:2057:MET:HE2	1:Y:2057:MET:O	2.12	0.49
1:y:463:GLN:HE21	1:y:1688:HIS:HE1	1.61	0.49
1:y:1845:SER:OG	1:y:1875:GLY:O	2.25	0.49
1:y:2012:LEU:HD11	1:y:2025:ILE:HD11	1.95	0.49
1:Y:816:THR:N	1:Y:819:SER:OG	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:858:LEU:O	1:Y:861:THR:OG1	2.29	0.49
1:Y:1027:SER:HB2	1:y:953:ARG:HH12	1.78	0.49
1:Y:1195:LEU:HD12	1:Y:1234:LEU:HD11	1.95	0.49
1:y:111:LEU:O	1:y:288:ILE:HA	2.12	0.49
1:y:831:ASP:O	1:y:855:ARG:NH2	2.45	0.49
1:y:1079:ARG:HB3	1:y:1083:GLN:NE2	2.28	0.49
1:y:1092:LYS:HE2	1:y:1111:ILE:HG23	1.94	0.49
1:y:1093:SER:O	1:y:1095:LYS:NZ	2.46	0.49
1:y:1226:TRP:O	1:y:1230:GLN:NE2	2.45	0.49
1:y:1556:LEU:O	1:y:1569:LYS:HD3	2.13	0.49
1:y:1726:TYR:CE2	1:y:1869:PRO:HD2	2.48	0.49
1:Y:864:PHE:CZ	1:Y:998:PRO:HG2	2.48	0.49
1:Y:1209:CYS:C	1:Y:1211:TRP:N	2.71	0.49
1:Y:1435:HIS:CG	1:Y:1436:PRO:HD2	2.48	0.49
1:y:170:THR:OG1	1:y:202:GLU:OE1	2.31	0.49
1:y:696:ILE:HD11	1:y:715:MET:HE1	1.95	0.49
1:y:1003:SER:OG	1:y:1005:GLU:OE2	2.27	0.49
1:Y:228:MET:O	1:Y:234:ASP:HB3	2.13	0.48
1:Y:802:CYS:O	1:Y:805:SER:OG	2.23	0.48
1:Y:1679:LEU:HD21	1:Y:1691:LEU:HD21	1.95	0.48
1:Y:1911:PRO:HA	1:Y:2089:ARG:NH2	2.27	0.48
1:y:97:GLN:NE2	1:y:123:GLU:OE2	2.46	0.48
1:y:966:ASP:O	1:y:970:GLN:HB2	2.13	0.48
1:y:1372:ARG:NH2	1:y:1380:GLU:OE1	2.46	0.48
1:y:1990:GLN:NE2	1:y:1997:ALA:O	2.43	0.48
1:Y:513:PHE:CE1	1:Y:606:GLY:HA3	2.47	0.48
1:Y:644:THR:HA	1:Y:1120:ASN:ND2	2.29	0.48
1:Y:1911:PRO:HG2	1:Y:1918:ARG:HH22	1.78	0.48
1:y:585:ALA:HB2	1:y:592:THR:HG22	1.95	0.48
1:y:688:HIS:O	1:y:692:LEU:HG	2.13	0.48
1:Y:788:LEU:HD12	1:Y:1392:LYS:HE2	1.95	0.48
1:Y:2089:ARG:NE	1:Y:2089:ARG:HA	2.27	0.48
1:y:148:GLN:HA	1:y:245:LEU:HA	1.94	0.48
1:y:979:VAL:HG12	1:y:1016:MET:HE1	1.95	0.48
1:y:1967:VAL:HG23	1:y:1971:MET:HE3	1.96	0.48
1:y:2048:GLY:HA3	1:y:2051:HIS:HE1	1.77	0.48
1:Y:163:GLN:HB3	1:Y:181:LEU:HD21	1.94	0.48
1:Y:733:GLU:OE2	1:Y:751:GLN:NE2	2.47	0.48
1:Y:1074:GLU:HG2	1:Y:1100:ASN:HD22	1.78	0.48
1:Y:1338:THR:HA	1:Y:1464:ILE:HD12	1.95	0.48
1:Y:1687:CYS:N	1:Y:1690:CYS:SG	2.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:926:VAL:HG22	1:y:996:TYR:HD2	1.78	0.48
1:y:1177:ARG:HE	1:y:1179:GLY:H	1.60	0.48
1:y:2000:ASN:HB2	1:y:2003:ASP:HB3	1.96	0.48
1:Y:163:GLN:OE1	1:Y:167:ARG:NH1	2.46	0.48
1:Y:765:GLN:O	1:Y:768:SER:OG	2.28	0.48
1:Y:1151:LYS:O	1:Y:1156:GLY:HA3	2.13	0.48
1:Y:1503:TYR:CE2	1:Y:1665:ILE:HD12	2.48	0.48
1:Y:1780:GLN:O	1:Y:1783:SER:OG	2.21	0.48
1:y:238:ILE:O	1:y:242:GLN:HG3	2.14	0.48
1:y:1616:ARG:HG3	1:y:1617:GLU:N	2.28	0.48
1:y:1693:SER:OG	1:y:1694:TYR:N	2.46	0.48
1:y:1759:VAL:HG23	1:y:1835:TRP:HZ3	1.78	0.48
1:Y:492:GLU:O	1:Y:493:MET:HE2	2.13	0.48
1:Y:1049:HIS:HA	1:Y:1052:GLU:CD	2.38	0.48
1:Y:1340:ASP:OD1	1:Y:1340:ASP:N	2.45	0.48
1:Y:1434:THR:OG1	1:Y:1435:HIS:N	2.46	0.48
1:Y:1998:TRP:HH2	1:Y:2007:VAL:HG21	1.79	0.48
1:y:465:GLN:HB2	1:y:1685:LYS:HD3	1.96	0.48
1:y:1805:HIS:CD2	1:y:1893:PRO:HG2	2.48	0.48
1:Y:524:GLU:H	1:Y:594:ARG:HH12	1.62	0.48
1:Y:1889:GLU:HA	1:Y:1892:LEU:HD12	1.95	0.48
1:y:1561:SER:HA	1:y:1569:LYS:HG3	1.94	0.48
1:y:1903:ASN:HA	1:y:2099:SER:O	2.13	0.48
3:I:12:DC:H2'	3:I:13:DT:C5	2.48	0.48
1:Y:1982:LYS:HA	1:Y:2030:GLY:H	1.78	0.48
1:y:843:LEU:HD12	1:y:927:PHE:CG	2.48	0.48
1:y:870:SER:OG	1:y:889:VAL:HA	2.14	0.48
1:y:1020:PRO:HD3	1:y:1040:TRP:CE2	2.48	0.48
1:y:1125:ALA:O	1:y:1128:ASN:ND2	2.47	0.48
1:y:1722:LEU:HD22	1:y:1735:VAL:HG13	1.95	0.48
1:y:1809:ALA:HB2	1:y:2100:TYR:HE1	1.79	0.48
1:Y:64:TRP:HB2	1:Y:94:PHE:CD1	2.49	0.48
1:Y:513:PHE:CZ	1:Y:608:PRO:HG2	2.48	0.48
1:Y:876:ASN:OD1	1:Y:877:GLU:N	2.47	0.48
1:Y:1245:THR:HG23	1:Y:1247:LEU:H	1.79	0.48
1:Y:1388:VAL:O	1:Y:1389:LEU:HD13	2.14	0.48
1:y:640:LEU:HB3	1:y:1098:VAL:HG13	1.94	0.48
1:Y:567:GLU:OE2	1:Y:567:GLU:N	2.41	0.48
1:Y:632:LEU:HB2	1:Y:1095:LYS:HE3	1.94	0.48
1:Y:1285:LYS:HZ2	1:Y:1291:TRP:HB3	1.79	0.48
1:Y:1529:CYS:HB2	1:Y:1556:LEU:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1902:ILE:HD12	1:Y:2101:ILE:O	2.13	0.48
1:Y:2087:ARG:HG3	1:Y:2089:ARG:NH1	2.28	0.48
1:y:64:TRP:HB2	1:y:94:PHE:CD1	2.49	0.48
1:y:628:ARG:HA	1:y:631:GLN:HG2	1.95	0.48
1:y:782:ARG:HG3	1:y:798:PHE:CG	2.49	0.48
1:y:1015:GLU:C	1:y:1016:MET:HE2	2.39	0.48
1:Y:233:LYS:O	1:Y:236:PRO:HD2	2.14	0.47
1:Y:251:ASP:OD1	1:Y:252:GLU:N	2.45	0.47
1:Y:487:LEU:HD12	1:Y:539:ILE:HG12	1.95	0.47
1:Y:624:LEU:O	1:Y:626:GLN:NE2	2.43	0.47
1:Y:652:ARG:NH2	1:Y:1473:SER:O	2.47	0.47
1:Y:908:TRP:CD2	1:Y:909:PRO:HD2	2.49	0.47
1:Y:1075:HIS:CD2	1:Y:1105:MET:HE2	2.49	0.47
1:Y:1509:GLY:HA3	1:Y:1589:MET:HE3	1.95	0.47
1:Y:1519:PHE:CD2	1:Y:1536:THR:HA	2.49	0.47
1:Y:1903:ASN:ND2	1:Y:1905:CYS:SG	2.87	0.47
1:Y:1909:ASP:HB2	1:Y:2090:ALA:O	2.14	0.47
1:y:342:PRO:HB3	1:y:363:TYR:CZ	2.49	0.47
1:y:534:GLN:HB3	1:y:573:PRO:HG2	1.96	0.47
1:y:763:SER:OG	1:y:766:THR:HG22	2.14	0.47
1:y:1452:LYS:HB3	1:y:1580:TRP:HE1	1.78	0.47
1:Y:158:LEU:HD12	1:Y:158:LEU:H	1.79	0.47
1:Y:487:LEU:HB2	1:Y:539:ILE:HG23	1.97	0.47
1:Y:515:LEU:O	1:Y:601:ARG:NH1	2.47	0.47
1:Y:886:ARG:HH12	1:Y:1469:HIS:CD2	2.31	0.47
1:y:251:ASP:OD2	1:y:290:THR:OG1	2.32	0.47
1:y:933:GLU:OE1	1:y:933:GLU:N	2.41	0.47
3:I:12:DC:O5'	3:I:13:DT:H72	2.14	0.47
1:Y:2000:ASN:ND2	1:Y:2002:GLU:OE1	2.47	0.47
1:Y:2006:GLN:HG3	1:Y:2076:VAL:HG11	1.95	0.47
1:y:1019:LEU:HD23	1:y:1021:VAL:H	1.79	0.47
1:y:1073:GLU:HB3	1:y:1099:LEU:HD22	1.97	0.47
1:y:1513:HIS:O	1:y:1582:GLY:HA2	2.13	0.47
1:y:1588:ASP:N	1:y:1588:ASP:OD1	2.46	0.47
1:Y:536:ASP:O	1:Y:537:ARG:NH1	2.47	0.47
1:Y:1438:GLU:OE2	1:Y:1444:ALA:N	2.47	0.47
1:y:337:ILE:HA	1:y:362:HIS:HA	1.96	0.47
1:y:352:SER:O	1:y:356:LEU:N	2.36	0.47
1:y:709:ASP:HA	1:y:712:LYS:HE2	1.95	0.47
1:y:1024:TRP:CZ2	1:y:1037:ARG:HB2	2.50	0.47
1:y:1114:MET:H	1:y:1114:MET:HE3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:1224:LEU:O	1:y:1227:LEU:HG	2.14	0.47
1:y:1740:LEU:HD11	1:y:1848:TRP:CE2	2.49	0.47
1:Y:1768:ASP:C	1:Y:1770:ALA:H	2.22	0.47
1:y:111:LEU:HB3	1:y:288:ILE:HG23	1.97	0.47
1:y:550:LEU:HB2	1:y:564:LYS:C	2.39	0.47
1:y:583:SER:OG	1:y:584:PHE:N	2.47	0.47
1:y:1974:ARG:HA	1:y:1974:ARG:HD2	1.72	0.47
1:Y:347:SER:O	1:Y:350:SER:OG	2.33	0.47
1:Y:624:LEU:HD12	1:Y:625:PRO:CD	2.44	0.47
1:Y:702:LEU:HD23	1:y:702:LEU:HD13	1.97	0.47
1:Y:1693:SER:N	1:Y:1696:SER:HG	2.12	0.47
1:Y:1763:PRO:HG2	1:Y:1766:GLN:HE22	1.79	0.47
1:y:537:ARG:HB3	1:y:570:LEU:HB2	1.95	0.47
3:I:11:DT:H3'	3:I:12:DC:C6	2.50	0.47
1:Y:33:SER:N	1:Y:453:ASP:OD2	2.38	0.47
1:Y:111:LEU:HD23	1:Y:112:LEU:N	2.30	0.47
1:Y:582:ASN:OD1	1:Y:582:ASN:N	2.45	0.47
1:Y:693:GLU:HA	1:Y:696:ILE:HD12	1.97	0.47
1:Y:1505:PHE:CE1	1:Y:1662:VAL:HG22	2.49	0.47
1:Y:2070:PHE:CE1	1:Y:2083:LEU:HG	2.50	0.47
1:y:776:ASP:OD1	1:y:777:LEU:N	2.48	0.47
1:y:984:TYR:CE2	1:y:1008:PRO:HB3	2.49	0.47
1:y:1036:GLU:HA	1:y:1039:GLU:OE2	2.14	0.47
2:G:12:DG:O5'	2:G:12:DG:H8	1.98	0.47
1:Y:6:LEU:HD13	1:Y:1116:LEU:HD11	1.97	0.47
1:Y:619:LEU:HD21	1:Y:1070:TYR:CD1	2.49	0.47
1:y:62:PHE:CZ	1:y:420:THR:HA	2.50	0.47
1:y:140:THR:O	1:y:142:GLN:NE2	2.30	0.47
1:y:934:GLN:NE2	1:y:936:HIS:HB3	2.29	0.47
1:y:1374:LEU:HD22	1:y:1583:TYR:CD2	2.47	0.47
1:Y:89:LYS:H	1:Y:89:LYS:NZ	2.11	0.47
1:Y:242:GLN:HE22	1:Y:275:PHE:HA	1.80	0.47
1:Y:534:GLN:O	1:Y:537:ARG:NH2	2.48	0.47
1:Y:1632:VAL:HG23	1:Y:1650:ILE:HG12	1.96	0.47
1:y:392:ARG:HA	1:y:392:ARG:CZ	2.45	0.47
1:y:406:LEU:HA	1:y:409:MET:HB3	1.97	0.47
1:y:548:ILE:HD13	1:y:558:ILE:HG23	1.97	0.47
1:y:1692:LEU:HD23	1:y:1703:LEU:HD11	1.97	0.47
1:y:1767:TRP:CZ3	1:y:1799:LEU:HB2	2.49	0.47
2:G:18:DA:N1	3:I:12:DC:N4	2.63	0.47
3:I:9:DT:H2''	3:I:10:DC:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:110:SER:O	1:Y:320:VAL:HA	2.15	0.47
1:Y:427:PHE:HB3	1:Y:1150:CYS:SG	2.55	0.47
1:Y:695:VAL:HG13	1:Y:699:PHE:CD2	2.50	0.47
1:Y:838:GLN:O	1:Y:842:THR:HG23	2.15	0.47
1:Y:1049:HIS:O	1:Y:1052:GLU:HG2	2.15	0.47
1:Y:1904:LEU:O	1:Y:2061:TYR:OH	2.17	0.47
1:Y:1983:LYS:NZ	1:Y:1984:LEU:O	2.47	0.47
1:y:11:LEU:HD12	1:y:621:PHE:CG	2.50	0.47
1:y:38:LEU:HA	1:y:41:GLN:HG2	1.96	0.47
1:y:64:TRP:HB2	1:y:94:PHE:CG	2.49	0.47
1:y:217:ILE:O	1:y:218:MET:HE2	2.14	0.47
1:y:365:VAL:HG21	1:y:394:TRP:HB2	1.97	0.47
1:y:636:ASN:HD22	1:y:638:ARG:HH21	1.63	0.47
1:y:1256:LEU:O	1:y:1259:THR:HG22	2.15	0.47
1:y:160:ASN:O	1:y:163:GLN:HG3	2.16	0.46
1:y:699:PHE:HA	1:y:702:LEU:HD21	1.96	0.46
1:Y:218:MET:HE2	1:Y:218:MET:HB2	1.73	0.46
1:Y:241:SER:HB3	1:Y:275:PHE:CD2	2.51	0.46
1:Y:386:LEU:HD23	1:Y:386:LEU:HA	1.73	0.46
1:Y:562:ALA:HB1	1:Y:565:HIS:CD2	2.51	0.46
1:Y:800:ASP:OD2	1:Y:968:LYS:NZ	2.44	0.46
1:Y:1075:HIS:CE1	1:Y:1084:ASN:HB3	2.51	0.46
1:Y:1245:THR:OG1	1:Y:1246:VAL:N	2.48	0.46
1:Y:1463:ASP:HA	1:Y:1557:LEU:HD12	1.97	0.46
1:Y:2074:LEU:HB3	1:Y:2078:GLN:NE2	2.30	0.46
1:y:447:HIS:HA	1:y:450:ASN:HB2	1.97	0.46
1:y:467:CYS:N	1:y:471:ALA:O	2.48	0.46
1:y:618:LEU:HD12	1:y:619:LEU:N	2.30	0.46
1:y:1080:THR:N	1:y:1083:GLN:HE21	2.14	0.46
1:y:1753:TYR:HA	1:y:1841:ARG:HG3	1.97	0.46
1:Y:175:GLY:H	1:Y:176:LYS:HZ3	1.62	0.46
1:Y:253:ALA:N	1:Y:291:SER:HG	2.12	0.46
1:Y:634:PRO:HD3	1:Y:1095:LYS:C	2.40	0.46
1:Y:911:ILE:HG22	1:Y:942:ASN:HD21	1.80	0.46
1:Y:1731:ASP:OD1	1:Y:1731:ASP:C	2.58	0.46
1:y:791:LEU:HD13	1:y:791:LEU:HA	1.81	0.46
1:y:948:VAL:O	1:y:952:ILE:HG12	2.16	0.46
3:I:6:DT:H2"	3:I:7:DA:H5"	1.97	0.46
1:Y:382:ARG:HB3	1:Y:385:GLU:OE1	2.15	0.46
1:Y:1902:ILE:O	1:Y:2100:TYR:HA	2.16	0.46
1:y:930:ILE:HD13	1:y:937:TRP:CZ3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:1187:HIS:CD2	1:y:1323:PRO:HG3	2.51	0.46
1:Y:18:ARG:HD2	1:Y:617:THR:HG22	1.96	0.46
1:Y:269:ARG:O	1:Y:273:GLN:N	2.47	0.46
1:Y:1092:LYS:HD3	1:Y:1092:LYS:HA	1.70	0.46
1:y:691:LEU:HB3	1:y:743:HIS:NE2	2.30	0.46
1:y:1273:GLN:O	1:y:1276:ILE:HG12	2.15	0.46
1:y:1545:LEU:O	1:y:1554:HIS:ND1	2.45	0.46
1:y:1590:VAL:HG13	1:y:1650:ILE:HB	1.96	0.46
1:y:1609:ARG:NH2	1:y:1634:THR:H	2.08	0.46
1:y:1778:LEU:HD22	1:y:1788:VAL:HG13	1.98	0.46
1:y:1810:LEU:HA	1:y:2097:LEU:HD11	1.97	0.46
1:Y:130:LEU:HA	1:Y:133:LEU:HB2	1.98	0.46
1:Y:652:ARG:NH2	1:Y:1472:VAL:O	2.46	0.46
1:Y:1767:TRP:O	1:Y:1767:TRP:HD1	1.99	0.46
1:Y:1874:LYS:HE2	1:Y:1874:LYS:HB3	1.73	0.46
1:Y:1937:HIS:ND1	1:Y:1970:GLY:HA3	2.31	0.46
1:y:645:ASP:H	1:y:1120:ASN:HD21	1.64	0.46
1:y:1161:LYS:HD3	1:y:1161:LYS:HA	1.64	0.46
1:y:1301:ALA:HB1	1:y:1305:ARG:NH2	2.29	0.46
1:y:1537:GLN:NE2	1:y:1538:PRO:O	2.49	0.46
1:y:1605:GLU:CD	1:y:1702:ARG:HH21	2.24	0.46
1:y:1613:VAL:HG22	1:y:1616:ARG:NH1	2.30	0.46
1:y:1827:GLN:OE1	1:y:1827:GLN:N	2.45	0.46
1:Y:648:GLN:H	1:Y:648:GLN:HG3	1.58	0.46
1:Y:1088:GLU:O	1:Y:1092:LYS:HG2	2.16	0.46
1:Y:1329:VAL:HG23	1:Y:1330:GLY:H	1.80	0.46
1:Y:1958:LEU:HD13	1:Y:2059:LEU:HD11	1.97	0.46
1:y:56:PRO:HD2	1:y:383:LEU:HD21	1.97	0.46
1:y:98:LEU:HA	1:y:101:TRP:NE1	2.31	0.46
1:y:272:MET:HE3	1:y:279:PRO:HD2	1.98	0.46
1:y:639:ARG:HH22	1:y:1092:LYS:HD3	1.81	0.46
1:y:1672:PHE:HB3	1:y:1717:LEU:HD11	1.98	0.46
1:Y:282:ASP:OD1	1:Y:282:ASP:N	2.46	0.46
1:Y:671:TYR:CZ	1:Y:822:LEU:HD12	2.51	0.46
1:Y:1061:ASP:OD1	1:Y:1062:ARG:N	2.49	0.46
1:y:9:ALA:HB1	1:y:400:ARG:CZ	2.46	0.46
1:y:342:PRO:HG3	1:y:348:LEU:HD11	1.97	0.46
1:y:1091:PHE:HB2	1:y:1099:LEU:HD21	1.98	0.46
1:Y:398:ASN:OD1	1:Y:401:GLU:N	2.41	0.46
1:Y:764:TRP:CH2	1:Y:803:LEU:HB3	2.51	0.46
1:Y:990:ASP:OD1	1:Y:991:VAL:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1373:ASP:C	1:Y:1373:ASP:OD2	2.59	0.46
1:Y:1904:LEU:HD23	1:Y:1904:LEU:HA	1.68	0.46
1:y:1947:ASP:O	1:y:1981:VAL:HG22	2.15	0.46
1:y:1985:ASP:OD1	1:y:1985:ASP:N	2.43	0.46
1:Y:1414:ASP:HB3	1:Y:1416:HIS:NE2	2.31	0.46
1:Y:1686:PHE:HA	1:Y:1690:CYS:SG	2.56	0.46
1:y:747:MET:O	1:y:751:GLN:HG2	2.16	0.46
1:y:1772:TRP:HD1	1:y:1773:PRO:HD2	1.81	0.46
2:G:14:DC:H2''	2:G:15:DG:N2	2.31	0.46
1:Y:1028:GLY:HA2	1:y:949:TRP:HZ3	1.80	0.45
1:Y:1036:GLU:H	1:Y:1036:GLU:CD	2.22	0.45
1:Y:1638:ARG:NH1	1:Y:1642:GLY:HA2	2.31	0.45
1:Y:1728:TYR:O	1:Y:1830:GLN:NE2	2.49	0.45
1:Y:1940:ILE:HG13	1:Y:1975:ALA:CB	2.46	0.45
1:y:149:ALA:HA	1:y:247:TYR:O	2.16	0.45
1:y:837:PRO:HB3	1:y:947:GLU:HG2	1.98	0.45
1:y:886:ARG:NH1	1:y:887:PHE:HA	2.31	0.45
1:y:1488:PRO:HD3	1:y:1509:GLY:HA2	1.97	0.45
1:y:1761:ALA:HB2	1:y:1793:ALA:HB3	1.98	0.45
1:y:1772:TRP:CE2	1:y:1774:LEU:HB2	2.51	0.45
1:y:1905:CYS:SG	1:y:2098:ARG:HG2	2.56	0.45
1:Y:643:PHE:CE2	1:Y:1132:ARG:HD3	2.51	0.45
1:Y:1452:LYS:HG3	1:Y:1580:TRP:CZ2	2.51	0.45
1:Y:1591:GLU:HB2	1:Y:1649:PHE:CE2	2.51	0.45
1:Y:1813:MET:HE1	1:Y:2096:ASP:O	2.16	0.45
1:Y:1904:LEU:HB3	1:Y:2061:TYR:CZ	2.51	0.45
1:y:427:PHE:CD2	1:y:1148:THR:HB	2.51	0.45
1:Y:54:ALA:HB2	1:Y:1160:PHE:CE1	2.51	0.45
1:Y:183:ASN:HA	1:Y:224:MET:CG	2.44	0.45
1:Y:1445:ASP:OD2	1:Y:1448:GLN:N	2.49	0.45
1:y:195:GLU:H	1:y:195:GLU:CD	2.24	0.45
1:y:785:PHE:HA	1:y:788:LEU:HG	1.97	0.45
1:y:802:CYS:O	1:y:805:SER:OG	2.24	0.45
1:y:1095:LYS:HA	1:y:1095:LYS:HD3	1.73	0.45
1:y:1220:CYS:O	1:y:1224:LEU:HG	2.16	0.45
1:y:1822:SER:HB3	1:y:1886:LEU:HD11	1.98	0.45
1:Y:437:CYS:SG	1:Y:471:ALA:HB3	2.57	0.45
1:Y:730:LYS:HA	1:Y:733:GLU:CG	2.47	0.45
1:Y:815:TRP:HE3	1:Y:820:LEU:HG	1.80	0.45
1:Y:817:LEU:HD12	1:Y:817:LEU:HA	1.72	0.45
1:Y:1497:ASP:OD2	1:Y:1719:ARG:NH2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:83:LEU:HG	1:y:87:LEU:HD12	1.98	0.45
1:y:403:LEU:HD12	1:y:406:LEU:HD11	1.99	0.45
1:y:1269:ARG:NH2	1:y:1319:GLU:HB3	2.31	0.45
1:y:1511:LEU:O	1:y:1584:SER:HA	2.16	0.45
1:y:1661:ALA:O	1:y:1664:LEU:HD12	2.16	0.45
1:y:1841:ARG:HH21	1:y:1844:GLN:HB2	1.80	0.45
1:y:2001:GLU:O	1:y:2004:ARG:HG2	2.17	0.45
2:G:9:DA:H2''	2:G:10:DC:H6	1.81	0.45
3:I:14:DA:H2''	3:I:15:DG:C4	2.52	0.45
1:Y:525:ASP:HA	1:Y:580:ARG:HG2	1.98	0.45
1:Y:1035:GLU:OE1	1:Y:1035:GLU:N	2.37	0.45
1:Y:1125:ALA:HB3	1:Y:1128:ASN:HB2	1.98	0.45
1:Y:1900:VAL:O	1:Y:2102:ILE:HA	2.16	0.45
1:Y:1950:LEU:HD23	1:Y:1981:VAL:HG21	1.98	0.45
1:y:14:GLN:HA	1:y:17:GLN:NE2	2.32	0.45
1:y:487:LEU:O	1:y:538:LEU:HA	2.17	0.45
1:y:913:ASP:HB3	1:y:916:TYR:CE1	2.52	0.45
1:y:934:GLN:O	1:y:938:LYS:HG3	2.17	0.45
1:y:1057:SER:O	1:y:1060:SER:OG	2.20	0.45
1:Y:226:GLU:OE2	1:Y:270:ARG:NH2	2.50	0.45
1:Y:273:GLN:HG3	1:Y:1240:ARG:HD2	1.99	0.45
1:Y:455:PRO:HG2	1:Y:456:PHE:CE2	2.52	0.45
1:Y:586:CYS:SG	1:Y:587:VAL:N	2.89	0.45
1:Y:1251:THR:OG1	1:Y:1253:THR:N	2.46	0.45
1:Y:1256:LEU:O	1:Y:1259:THR:OG1	2.29	0.45
1:Y:1880:THR:OG1	1:Y:1881:PHE:N	2.49	0.45
1:y:266:LEU:O	1:y:269:ARG:HB2	2.17	0.45
1:y:309:VAL:O	1:y:312:LEU:HB2	2.17	0.45
1:y:715:MET:HE2	1:y:715:MET:HB2	1.85	0.45
1:y:772:VAL:HG21	1:y:795:LYS:HB3	1.97	0.45
1:y:1299:ALA:HB2	1:y:1342:LEU:HD21	1.97	0.45
1:y:1394:TYR:HA	1:y:1466:TYR:CE1	2.52	0.45
1:y:1502:ARG:HH12	1:y:1640:ILE:HD11	1.82	0.45
1:y:1953:PRO:HD2	1:y:1996:ASN:O	2.17	0.45
1:Y:551:GLU:OE1	1:Y:563:GLN:HB2	2.16	0.45
1:Y:639:ARG:HD2	1:Y:1113:GLY:N	2.31	0.45
1:Y:869:ASN:O	1:Y:871:ALA:N	2.50	0.45
1:Y:1024:TRP:CE3	1:Y:1024:TRP:HA	2.51	0.45
1:Y:1905:CYS:N	1:Y:1907:GLN:OE1	2.49	0.45
1:y:833:VAL:O	1:y:855:ARG:NH2	2.50	0.45
1:y:1903:ASN:OD1	1:y:1903:ASN:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:98:LEU:HA	1:Y:101:TRP:NE1	2.32	0.45
1:Y:250:LEU:O	1:Y:289:ALA:HA	2.16	0.45
1:Y:1026:LEU:HD12	1:Y:1027:SER:H	1.82	0.45
1:Y:1220:CYS:O	1:Y:1223:PHE:HB3	2.17	0.45
1:Y:1955:THR:HA	1:Y:1958:LEU:HD12	1.99	0.45
1:y:182:TYR:HD1	1:y:224:MET:HB3	1.81	0.45
1:y:585:ALA:HA	1:y:591:ASP:O	2.16	0.45
1:y:931:GLN:HB2	1:y:934:GLN:HB2	1.98	0.45
1:y:1227:LEU:HD13	1:y:1256:LEU:HD12	1.98	0.45
1:y:1779:LEU:HD22	1:y:2095:ASN:HD21	1.82	0.45
1:y:1893:PRO:HD2	1:y:1901:ARG:NH2	2.32	0.45
1:Y:5:GLN:HG2	1:Y:6:LEU:O	2.17	0.45
1:Y:224:MET:HE3	2:G:9:DA:H4'	1.97	0.45
1:Y:781:MET:HE2	1:Y:781:MET:HB2	1.75	0.45
1:y:805:SER:HA	1:y:883:MET:SD	2.57	0.45
1:y:980:TRP:CE2	1:y:1013:LEU:HD13	2.52	0.45
1:y:990:ASP:OD1	1:y:990:ASP:C	2.60	0.45
1:Y:181:LEU:HA	1:Y:219:VAL:HG13	1.98	0.45
1:Y:245:LEU:HD22	1:Y:275:PHE:HD2	1.81	0.45
1:Y:660:ASP:OD1	1:Y:661:ALA:N	2.50	0.45
1:Y:784:SER:O	1:Y:787:GLU:HG3	2.16	0.45
1:Y:876:ASN:CG	1:Y:878:GLN:HG2	2.42	0.45
1:Y:1267:ASP:OD1	1:Y:1267:ASP:C	2.60	0.45
1:Y:1424:ARG:NE	1:Y:1450:ASP:OD1	2.33	0.45
1:y:163:GLN:HG2	1:y:181:LEU:HD22	1.98	0.45
1:y:167:ARG:HH12	1:y:202:GLU:CD	2.25	0.45
1:y:886:ARG:HH11	1:y:887:PHE:HA	1.81	0.45
1:y:908:TRP:CD2	1:y:949:TRP:HD1	2.35	0.45
1:y:1157:MET:HE2	1:y:1689:HIS:ND1	2.32	0.45
1:y:1277:LEU:HA	1:y:1280:ASN:ND2	2.32	0.45
1:y:1297:GLY:HA2	1:y:1300:ILE:HG12	1.98	0.45
1:y:1632:VAL:HG22	1:y:1648:ILE:HD11	1.99	0.45
1:Y:137:GLN:HE22	1:Y:141:ARG:HH22	1.64	0.44
1:Y:762:MET:HE3	1:Y:762:MET:HB2	1.85	0.44
1:Y:873:PHE:N	1:Y:965:LEU:O	2.29	0.44
1:Y:960:GLU:OE1	1:Y:960:GLU:N	2.47	0.44
1:Y:1374:LEU:HD12	1:Y:1374:LEU:HA	1.76	0.44
1:Y:1804:ARG:HG2	1:Y:1891:LEU:O	2.16	0.44
1:Y:1957:ARG:HE	1:Y:2017:LEU:HD21	1.82	0.44
1:Y:1993:ALA:O	1:Y:1996:ASN:HB2	2.17	0.44
1:Y:2054:LEU:HG	1:Y:2102:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:571:LEU:HB3	1:y:584:PHE:CE2	2.52	0.44
1:y:643:PHE:CD1	1:y:1105:MET:HB3	2.51	0.44
1:y:1249:SER:HB3	1:y:1776:LYS:NZ	2.32	0.44
1:y:1927:HIS:ND1	1:y:2103:ALA:HB3	2.32	0.44
2:G:14:DC:H2"	2:G:15:DG:H21	1.81	0.44
1:Y:74:LEU:O	1:Y:79:ILE:N	2.50	0.44
1:Y:131:GLU:O	1:Y:134:ILE:HG12	2.17	0.44
1:Y:248:ILE:HB	1:Y:287:ILE:HG12	1.99	0.44
1:Y:692:LEU:HB2	1:Y:715:MET:HE2	1.99	0.44
1:Y:895:PRO:HD3	1:Y:949:TRP:CE2	2.52	0.44
1:Y:1665:ILE:HG22	1:Y:1737:THR:HB	1.98	0.44
1:y:696:ILE:HA	1:y:699:PHE:CE1	2.53	0.44
1:y:702:LEU:O	1:y:704:LEU:N	2.48	0.44
1:y:1155:HIS:HA	1:y:1158:GLU:HG3	1.99	0.44
1:y:1261:ALA:O	1:y:1265:GLN:HG2	2.17	0.44
1:y:1475:PRO:O	1:y:1477:GLN:NE2	2.50	0.44
1:y:1790:LEU:HD12	1:y:1820:VAL:HG22	2.00	0.44
1:Y:341:TYR:CE2	1:Y:343:THR:HG22	2.51	0.44
1:Y:865:PHE:CZ	1:Y:909:PRO:HD3	2.52	0.44
1:Y:881:ARG:NH1	1:Y:1468:ALA:O	2.50	0.44
1:Y:1139:ARG:NH2	5:Y:2206:AGS:H5'2	2.32	0.44
1:Y:1578:ASP:O	1:Y:1579:LEU:HD23	2.17	0.44
1:Y:1601:LEU:HB3	1:Y:1645:GLY:HA3	1.99	0.44
1:Y:1753:TYR:HA	1:Y:1841:ARG:HG3	1.99	0.44
1:Y:1887:SER:OG	1:Y:1888:ALA:N	2.50	0.44
1:Y:2052:TYR:O	1:Y:2104:GLY:HA3	2.18	0.44
1:y:110:SER:OG	1:y:287:ILE:HG13	2.18	0.44
1:Y:122:THR:HG23	5:Y:2206:AGS:S1G	2.57	0.44
1:Y:336:LEU:HB3	1:Y:361:CYS:HB3	1.99	0.44
1:Y:423:ARG:HD3	1:Y:1136:ALA:HB3	2.00	0.44
1:Y:519:VAL:HG12	1:Y:809:ARG:HH12	1.81	0.44
1:Y:1036:GLU:OE1	1:Y:1036:GLU:N	2.32	0.44
1:Y:1246:VAL:HG23	1:Y:1247:LEU:HD23	1.99	0.44
1:y:436:ALA:HA	1:y:458:GLN:O	2.17	0.44
1:y:445:LYS:NZ	1:y:454:TRP:O	2.46	0.44
1:y:494:ARG:HH11	1:y:500:TRP:HB2	1.82	0.44
1:y:658:GLN:HE22	1:y:1069:TRP:NE1	2.15	0.44
1:y:945:MET:O	1:y:948:VAL:HG12	2.17	0.44
1:y:1019:LEU:HD11	1:y:1024:TRP:CD1	2.52	0.44
1:y:1041:LEU:HD12	1:y:1047:ILE:HD12	2.00	0.44
1:y:1373:ASP:CG	1:y:1375:PRO:HD2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:64:TRP:HH2	1:Y:116:GLY:HA3	1.82	0.44
1:Y:1490:SER:C	1:Y:1504:ARG:HD2	2.43	0.44
1:Y:1802:SER:OG	1:Y:2039:ARG:NH2	2.41	0.44
1:Y:2045:PHE:HE2	1:Y:2051:HIS:CD2	2.35	0.44
1:y:542:ASP:C	1:y:569:ASN:HB3	2.42	0.44
1:y:740:SER:HB2	1:y:743:HIS:ND1	2.32	0.44
2:G:28:DG:H2"	2:G:29:DA:N7	2.33	0.44
1:Y:356:LEU:HD11	1:Y:408:LEU:HD12	1.98	0.44
1:Y:839:ASP:OD2	1:Y:943:HIS:ND1	2.51	0.44
1:Y:1004:LYS:HD3	1:Y:1004:LYS:HA	1.86	0.44
1:Y:1270:TRP:CG	1:Y:1307:TYR:HH	2.35	0.44
1:Y:1591:GLU:OE2	1:Y:1593:GLN:NE2	2.50	0.44
1:Y:1711:LEU:HD23	1:Y:1711:LEU:HA	1.67	0.44
1:Y:2066:GLU:OE1	1:Y:2066:GLU:N	2.50	0.44
1:Y:96:HIS:CE1	1:Y:119:SER:HB2	2.53	0.44
1:Y:671:TYR:CE1	1:Y:822:LEU:HD12	2.53	0.44
1:Y:1071:ARG:HB3	1:Y:1073:GLU:OE2	2.16	0.44
1:Y:1284:LEU:HB3	1:Y:1291:TRP:NE1	2.32	0.44
1:Y:1484:ARG:HA	1:Y:1484:ARG:HD2	1.78	0.44
1:Y:1841:ARG:HG2	1:Y:1842:GLU:H	1.82	0.44
1:y:91:PRO:O	1:y:93:PRO:HD3	2.18	0.44
1:y:571:LEU:HB3	1:y:584:PHE:HE2	1.83	0.44
1:y:1152:ASN:HD21	1:y:1689:HIS:CE1	2.36	0.44
1:y:1855:THR:O	1:y:1863:GLY:N	2.30	0.44
1:Y:462:GLU:O	1:Y:464:ARG:HG3	2.18	0.44
1:Y:639:ARG:HA	1:Y:1097:ASN:O	2.18	0.44
1:Y:673:GLU:OE2	1:Y:770:GLN:NE2	2.44	0.44
1:Y:1375:PRO:HB3	1:Y:1513:HIS:CD2	2.53	0.44
1:Y:1474:MET:HA	1:Y:1474:MET:HE3	2.00	0.44
1:Y:1944:GLU:HB2	1:Y:2042:THR:HG23	2.00	0.44
1:y:684:LEU:HD21	1:y:746:ALA:HB1	1.99	0.44
1:y:1105:MET:HE3	1:y:1108:GLY:HA2	2.00	0.44
1:y:1431:THR:HG21	1:y:1584:SER:OG	2.17	0.44
1:Y:13:ASN:O	1:Y:17:GLN:HG2	2.17	0.44
1:Y:32:LYS:HD2	1:Y:32:LYS:HA	1.74	0.44
1:Y:439:ASN:C	1:Y:441:GLN:H	2.25	0.44
1:Y:493:MET:HE2	1:Y:493:MET:HA	1.99	0.44
1:Y:880:PRO:HA	1:Y:883:MET:HB2	2.00	0.44
1:Y:913:ASP:OD1	1:Y:916:TYR:OH	2.26	0.44
1:Y:1029:GLY:HA2	1:y:896:ASP:CG	2.43	0.44
1:Y:1203:ASP:C	1:Y:1203:ASP:OD1	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1991:HIS:H	1:Y:1996:ASN:ND2	2.15	0.44
1:y:179:PHE:HB2	1:y:217:ILE:HB	1.99	0.44
1:y:721:LEU:HB3	1:y:725:ASP:HB2	1.99	0.44
1:y:961:SER:O	1:y:961:SER:OG	2.34	0.44
1:y:966:ASP:HB3	1:y:969:GLN:HE22	1.83	0.44
1:y:1191:LEU:O	1:y:1195:LEU:HG	2.17	0.44
1:Y:20:VAL:HG22	1:Y:42:TYR:HB3	2.00	0.43
1:Y:59:GLU:CD	1:Y:425:HIS:HE2	2.23	0.43
1:Y:580:ARG:HD2	1:Y:580:ARG:HA	1.64	0.43
1:Y:593:GLN:HE21	1:Y:593:GLN:HB3	1.64	0.43
1:Y:1900:VAL:HG11	1:Y:1926:GLN:HB3	2.00	0.43
1:y:71:MET:O	1:y:74:LEU:HD23	2.18	0.43
1:y:407:ASP:O	1:y:411:ARG:HG2	2.18	0.43
1:y:1697:GLN:HA	1:y:1700:VAL:HG22	2.00	0.43
2:G:22:DA:H2"	2:G:23:DC:C5	2.53	0.43
1:Y:254:HIS:HA	1:Y:294:ILE:HD12	1.99	0.43
1:Y:414:GLU:N	1:Y:414:GLU:OE1	2.51	0.43
1:Y:644:THR:H	1:Y:1102:SER:HA	1.83	0.43
1:Y:696:ILE:HD13	1:Y:712:LYS:NZ	2.33	0.43
1:Y:1210:LYS:O	1:Y:1210:LYS:HG2	2.18	0.43
1:Y:1967:VAL:CG2	1:Y:1973:GLU:HA	2.49	0.43
1:y:438:SER:HB2	1:y:472:PRO:HG2	1.99	0.43
1:y:607:ALA:N	1:y:608:PRO:HD2	2.33	0.43
1:y:691:LEU:O	1:y:695:VAL:HG23	2.17	0.43
1:y:764:TRP:CD1	1:y:764:TRP:C	2.95	0.43
1:y:1071:ARG:HB3	1:y:1096:VAL:HA	2.00	0.43
1:y:1101:CYS:HB2	1:y:1105:MET:HB2	2.00	0.43
1:Y:444:HIS:CG	1:Y:468:ASP:HB2	2.53	0.43
1:Y:731:ILE:CG1	1:y:734:PRO:HG3	2.46	0.43
1:Y:1344:LYS:HA	1:Y:1344:LYS:HD3	1.85	0.43
1:Y:2007:VAL:HG13	1:Y:2080:VAL:HG22	1.99	0.43
1:y:132:ASP:OD2	1:y:246:LYS:HD2	2.18	0.43
1:y:586:CYS:SG	1:y:588:CYS:N	2.73	0.43
1:y:634:PRO:HA	1:y:780:ARG:CZ	2.47	0.43
1:y:722:SER:O	1:y:726:ILE:HD12	2.18	0.43
1:y:725:ASP:O	1:y:729:LEU:HG	2.18	0.43
1:y:980:TRP:CD2	1:y:1013:LEU:HD13	2.53	0.43
1:y:1080:THR:HG22	1:y:1082:GLU:HG3	2.00	0.43
1:y:1125:ALA:HB3	1:y:1128:ASN:ND2	2.34	0.43
1:y:1302:TYR:O	1:y:1305:ARG:HG2	2.18	0.43
2:G:28:DG:O6	3:I:3:DC:N4	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:187:ARG:HB3	1:Y:192:GLU:OE2	2.18	0.43
1:Y:1027:SER:OG	1:Y:1028:GLY:N	2.51	0.43
1:Y:1940:ILE:HA	1:Y:2045:PHE:HA	2.01	0.43
1:y:114:SER:O	1:y:114:SER:OG	2.34	0.43
1:y:122:THR:HG22	1:y:126:MET:SD	2.58	0.43
1:y:140:THR:HB	1:y:142:GLN:HG2	2.01	0.43
1:y:197:GLN:HG2	1:y:205:LEU:HB2	1.99	0.43
1:y:534:GLN:O	1:y:537:ARG:NH1	2.38	0.43
1:y:704:LEU:O	1:y:707:SER:N	2.51	0.43
1:y:774:SER:OG	1:y:777:LEU:HB3	2.19	0.43
1:y:825:ILE:HG13	1:y:867:ARG:HH12	1.83	0.43
1:y:1089:LYS:HE3	1:y:1089:LYS:HB3	1.75	0.43
1:y:1386:ASP:CG	1:y:1476:ALA:H	2.25	0.43
1:y:1884:GLN:CD	1:y:1884:GLN:C	2.86	0.43
1:y:1991:HIS:ND1	1:y:1995:TYR:OH	2.43	0.43
3:I:8:DG:H3'	3:I:8:DG:OP2	2.19	0.43
1:Y:371:GLN:HA	1:Y:374:THR:HG22	2.01	0.43
1:Y:825:ILE:HG23	1:Y:971:ALA:HB1	2.00	0.43
1:y:392:ARG:HA	1:y:392:ARG:NH1	2.33	0.43
1:y:729:LEU:O	1:y:747:MET:HE3	2.17	0.43
1:y:878:GLN:NE2	1:y:881:ARG:HH22	2.15	0.43
1:y:1374:LEU:HD13	1:y:1583:TYR:CD2	2.54	0.43
1:y:1484:ARG:HA	1:y:1484:ARG:HD2	1.71	0.43
1:y:1543:GLU:OE2	1:y:1548:PRO:HD2	2.19	0.43
1:y:1757:SER:HB2	1:y:1838:GLN:HG2	2.00	0.43
2:G:10:DC:H2''	2:G:11:DC:H6	1.83	0.43
1:Y:478:ARG:HB2	1:Y:603:LEU:HD21	2.01	0.43
1:Y:936:HIS:O	1:Y:939:SER:OG	2.34	0.43
1:Y:1157:MET:HE2	1:Y:1689:HIS:CD2	2.54	0.43
1:y:331:ARG:NH2	1:y:332:VAL:O	2.43	0.43
1:y:382:ARG:HG3	1:y:1164:LEU:HD21	2.00	0.43
1:y:1221:LEU:HB3	1:y:1225:HIS:CE1	2.54	0.43
1:y:1288:ASN:ND2	1:y:1294:THR:HG21	2.34	0.43
1:y:1536:THR:HG22	1:y:1540:ARG:CZ	2.49	0.43
1:y:1855:THR:OG1	1:y:1864:GLN:N	2.44	0.43
1:y:1963:LEU:HG	1:y:1977:LEU:HD22	2.00	0.43
1:Y:75:ARG:NH1	1:Y:85:ASP:OD1	2.43	0.43
1:Y:152:LEU:HD12	1:Y:152:LEU:HA	1.73	0.43
1:Y:234:ASP:O	1:Y:237:ILE:N	2.49	0.43
1:Y:339:HIS:HD2	1:Y:363:TYR:CE1	2.36	0.43
1:Y:1026:LEU:HD23	1:Y:1029:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1564:ARG:HA	1:Y:1564:ARG:CZ	2.49	0.43
1:Y:1712:LEU:HD22	1:Y:1717:LEU:HD21	1.99	0.43
1:Y:2095:ASN:HB2	1:Y:2097:LEU:HD23	1.99	0.43
1:y:720:GLU:HA	1:y:755:GLY:HA2	2.00	0.43
1:y:1583:TYR:CD1	1:y:1584:SER:N	2.87	0.43
1:Y:151:PHE:CD1	1:Y:249:VAL:HB	2.54	0.43
1:Y:663:LYS:HG3	1:Y:667:ARG:HE	1.83	0.43
1:Y:1184:VAL:HG21	1:Y:1245:THR:OG1	2.19	0.43
1:Y:1601:LEU:HA	1:Y:1601:LEU:HD12	1.73	0.43
1:Y:1764:GLN:HG2	1:Y:1767:TRP:CZ2	2.54	0.43
1:Y:1840:THR:HG23	1:Y:1845:SER:HB3	1.99	0.43
1:y:138:LYS:HG2	1:y:141:ARG:NH2	2.34	0.43
1:y:259:SER:HB3	1:y:1658:ALA:HA	1.99	0.43
1:y:276:ASN:C	1:y:281:THR:HG21	2.44	0.43
1:y:896:ASP:N	1:y:896:ASP:OD1	2.51	0.43
1:y:1066:LYS:HE2	1:y:1066:LYS:HB2	1.81	0.43
1:y:1227:LEU:HD11	1:y:1260:GLN:HB2	2.01	0.43
1:y:1300:ILE:HA	1:y:1303:GLN:HG3	2.00	0.43
1:y:1497:ASP:HB3	1:y:1500:LEU:HB2	1.99	0.43
1:y:1665:ILE:O	1:y:1668:TRP:NE1	2.52	0.43
1:y:1748:LEU:HD13	1:y:1781:PHE:HB2	2.01	0.43
2:G:17:DA:C4	2:G:18:DA:C6	3.07	0.43
1:Y:193:ILE:HD13	1:Y:205:LEU:HB2	2.01	0.43
1:Y:533:SER:O	1:Y:573:PRO:HG3	2.19	0.43
1:Y:860:ILE:HD12	1:Y:998:PRO:HG3	2.00	0.43
1:Y:1916:GLY:CA	1:Y:1962:ILE:HG22	2.48	0.43
1:Y:2057:MET:HE1	1:Y:2060:SER:N	2.34	0.43
1:y:167:ARG:HH22	1:y:171:ARG:HH22	1.67	0.43
1:y:189:THR:OG1	1:y:192:GLU:OE2	2.22	0.43
1:y:401:GLU:HA	1:y:404:GLN:OE1	2.19	0.43
1:y:658:GLN:NE2	1:y:1069:TRP:HE1	2.17	0.43
1:y:779:ASP:OD1	1:y:780:ARG:N	2.51	0.43
1:Y:305:LEU:HD23	1:Y:305:LEU:HA	1.85	0.43
1:Y:551:GLU:HB3	1:Y:564:LYS:HG3	2.01	0.43
1:Y:2011:LEU:O	1:Y:2015:GLY:HA3	2.19	0.43
1:y:62:PHE:CD1	1:y:421:PRO:HD2	2.53	0.43
1:y:672:GLN:HB3	1:y:1023:HIS:CD2	2.49	0.43
1:y:684:LEU:HD12	1:y:685:SER:H	1.83	0.43
1:y:838:GLN:O	1:y:842:THR:HG23	2.18	0.43
1:y:934:GLN:HB3	1:y:937:TRP:HD1	1.84	0.43
1:y:1072:LEU:HD12	1:y:1073:GLU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:1284:LEU:HD12	1:y:1287:ASP:HB3	2.01	0.43
1:Y:72:GLU:OE1	1:Y:75:ARG:NE	2.35	0.42
1:Y:182:TYR:HB2	1:Y:218:MET:SD	2.59	0.42
1:Y:496:ASP:OD1	1:Y:496:ASP:N	2.42	0.42
1:Y:782:ARG:CZ	1:Y:795:LYS:HG2	2.49	0.42
1:Y:1114:MET:HG2	1:Y:1114:MET:O	2.18	0.42
1:Y:1374:LEU:HD23	1:Y:1583:TYR:CG	2.53	0.42
1:Y:1447:GLN:OE1	1:Y:1447:GLN:N	2.48	0.42
1:Y:1724:PRO:HA	1:Y:1727:GLN:NE2	2.34	0.42
1:Y:1948:ARG:HB3	1:Y:1982:LYS:HD3	2.00	0.42
1:y:111:LEU:HB3	1:y:288:ILE:HD12	2.01	0.42
1:y:613:GLU:O	1:y:616:PRO:HD2	2.19	0.42
1:y:721:LEU:HD22	1:y:725:ASP:HB3	2.00	0.42
1:y:912:ARG:HH11	1:y:914:ARG:HH12	1.65	0.42
1:y:1045:ALA:O	1:y:1048:GLN:HG2	2.19	0.42
1:y:1194:GLY:O	1:y:1197:LEU:HG	2.19	0.42
1:y:1331:VAL:HA	1:y:1373:ASP:HA	2.01	0.42
1:y:1417:ILE:HB	1:y:1454:TYR:O	2.19	0.42
1:Y:465:GLN:HG2	1:Y:466:TYR:CE2	2.54	0.42
1:Y:1128:ASN:HB3	1:Y:1132:ARG:HH12	1.85	0.42
1:Y:1452:LYS:HD3	1:Y:1452:LYS:HA	1.82	0.42
1:y:7:HIS:CE1	1:y:411:ARG:HE	2.37	0.42
1:y:151:PHE:HA	1:y:249:VAL:O	2.19	0.42
1:y:351:LEU:HD13	1:y:359:GLN:NE2	2.34	0.42
1:y:674:LEU:O	1:y:975:SER:OG	2.37	0.42
1:y:729:LEU:HD13	1:y:750:LEU:HD23	2.00	0.42
1:y:1510:GLU:HG3	1:y:1586:ARG:NE	2.34	0.42
2:G:7:DA:P	2:G:7:DA:H8	2.42	0.42
2:G:21:DG:H1'	2:G:22:DA:C8	2.54	0.42
3:I:10:DC:H1'	3:I:11:DT:O4'	2.19	0.42
1:Y:1251:THR:HG21	1:Y:1255:LEU:N	2.29	0.42
1:Y:1416:HIS:HB2	1:Y:1417:ILE:HD12	2.01	0.42
1:Y:1421:TRP:CZ3	1:Y:1429:GLY:HA2	2.55	0.42
1:Y:1439:CYS:O	1:Y:1443:LYS:N	2.42	0.42
1:Y:2000:ASN:O	1:Y:2004:ARG:HB3	2.18	0.42
1:Y:2076:VAL:HB	1:Y:2077:PRO:HD3	2.01	0.42
1:y:98:LEU:HD13	1:y:101:TRP:NE1	2.32	0.42
1:y:550:LEU:H	1:y:564:LYS:C	2.25	0.42
1:y:682:ALA:HB1	1:y:753:ASN:HB3	2.00	0.42
1:y:1772:TRP:CD1	1:y:1773:PRO:HD2	2.55	0.42
1:Y:83:LEU:HA	1:Y:83:LEU:HD23	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:115:SER:O	1:Y:292:ALA:HA	2.20	0.42
1:Y:259:SER:H	1:Y:1659:GLY:H	1.66	0.42
1:Y:521:SER:C	1:Y:522:GLU:OE1	2.62	0.42
1:Y:616:PRO:HA	1:Y:619:LEU:HD11	2.01	0.42
1:Y:676:ASN:ND2	1:Y:977:LYS:HE3	2.35	0.42
1:Y:722:SER:N	1:Y:725:ASP:OD2	2.49	0.42
1:Y:1801:ASP:OD1	1:Y:1801:ASP:N	2.53	0.42
1:Y:1955:THR:HG22	1:Y:2059:LEU:HG	2.00	0.42
1:Y:1999:LEU:HD23	1:Y:1999:LEU:HA	1.81	0.42
1:y:674:LEU:HG	1:y:975:SER:OG	2.19	0.42
1:y:917:ASN:OD1	1:y:920:ILE:HG22	2.20	0.42
1:y:1632:VAL:HG23	1:y:1650:ILE:HG13	2.01	0.42
1:y:1800:THR:O	1:y:1803:SER:OG	2.26	0.42
1:y:1940:ILE:O	1:y:1975:ALA:HB2	2.20	0.42
1:Y:1998:TRP:HA	1:Y:2072:PHE:CE1	2.54	0.42
1:y:657:LEU:CD1	1:y:1072:LEU:HD22	2.48	0.42
1:y:806:GLU:OE2	1:y:816:THR:OG1	2.37	0.42
1:y:1315:LYS:HG3	1:y:1319:GLU:OE2	2.19	0.42
1:y:1781:PHE:HD2	1:y:1788:VAL:HG22	1.84	0.42
1:y:1901:ARG:HA	1:y:2102:ILE:HG13	2.01	0.42
1:y:1945:TYR:CZ	1:y:1947:ASP:HB3	2.55	0.42
1:Y:660:ASP:OD1	1:Y:660:ASP:C	2.61	0.42
1:Y:699:PHE:HB2	1:Y:708:ILE:HD11	2.01	0.42
1:y:352:SER:HB2	1:y:355:ASP:HB2	2.01	0.42
1:y:1258:ARG:O	1:y:1262:MET:HG2	2.20	0.42
1:y:1258:ARG:HH22	1:y:1989:ARG:NH1	2.16	0.42
1:y:1951:ASN:OD1	1:y:2004:ARG:NH1	2.52	0.42
1:y:1981:VAL:HG12	1:y:1982:LYS:O	2.20	0.42
2:G:13:DT:H4'	2:G:14:DC:OP1	2.20	0.42
1:Y:245:LEU:HD22	1:Y:275:PHE:CD2	2.54	0.42
1:Y:272:MET:CE	1:Y:278:GLY:HA2	2.50	0.42
1:Y:689:CYS:HA	1:Y:715:MET:HE1	2.01	0.42
1:Y:1002:GLY:C	1:Y:1004:LYS:H	2.27	0.42
1:Y:1720:LEU:HD12	1:Y:1720:LEU:HA	1.83	0.42
1:Y:1953:PRO:HD2	1:Y:1996:ASN:O	2.19	0.42
1:y:639:ARG:NH2	1:y:1092:LYS:HD3	2.34	0.42
1:y:1006:ILE:HG13	1:y:1007:ALA:O	2.20	0.42
1:y:1189:ASN:HB3	1:y:1321:PHE:HD1	1.84	0.42
1:y:1208:SER:HA	1:y:1312:LEU:HB2	2.01	0.42
1:y:1553:THR:OG1	1:y:1554:HIS:N	2.42	0.42
1:y:1614:ALA:O	1:y:1617:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:1633:THR:O	1:y:1648:ILE:HD12	2.19	0.42
1:Y:268:LEU:HD13	1:Y:268:LEU:HA	1.90	0.42
1:Y:559:ASP:OD1	1:Y:561:GLU:N	2.53	0.42
1:Y:1464:ILE:HD12	1:Y:1464:ILE:HA	1.82	0.42
1:Y:1913:GLU:HA	1:Y:1961:GLU:OE2	2.20	0.42
1:Y:1922:LEU:HA	1:Y:1922:LEU:HD23	1.83	0.42
1:y:1266:VAL:HG21	1:y:1321:PHE:HE2	1.85	0.42
1:y:1660:TYR:O	1:y:1664:LEU:HG	2.19	0.42
1:y:1893:PRO:HD2	1:y:1901:ARG:HH21	1.85	0.42
3:I:5:DA:H1'	3:I:6:DT:H5'	2.02	0.42
1:Y:12:LEU:HA	1:Y:12:LEU:HD23	1.74	0.42
1:Y:176:LYS:H	1:Y:176:LYS:HE2	1.84	0.42
1:Y:1807:LEU:HA	1:Y:1807:LEU:HD23	1.78	0.42
1:y:260:GLN:HA	1:y:263:GLU:HB3	2.01	0.42
1:y:645:ASP:H	1:y:1120:ASN:ND2	2.17	0.42
1:y:917:ASN:OD1	1:y:919:VAL:N	2.53	0.42
1:y:1266:VAL:HA	1:y:1269:ARG:NE	2.35	0.42
1:y:1452:LYS:HE2	1:y:1580:TRP:CZ2	2.55	0.42
1:Y:512:GLU:O	1:Y:516:ASP:N	2.53	0.42
1:Y:909:PRO:O	1:Y:910:GLN:NE2	2.53	0.42
1:Y:1209:CYS:O	1:Y:1210:LYS:HD2	2.20	0.42
1:Y:1285:LYS:HZ1	1:Y:1291:TRP:H	1.68	0.42
1:Y:1984:LEU:CB	1:Y:2001:GLU:HB2	2.49	0.42
1:y:6:LEU:HD22	1:y:1116:LEU:HD21	2.02	0.42
1:y:639:ARG:NH2	1:y:1092:LYS:HA	2.35	0.42
1:y:914:ARG:CZ	1:y:915:HIS:HE1	2.32	0.42
1:y:1248:MET:SD	1:y:1248:MET:N	2.92	0.42
1:y:1270:TRP:CH2	1:y:1274:LEU:HD22	2.54	0.42
1:y:1446:ILE:HA	1:y:1449:LEU:HG	2.02	0.42
1:y:1516:GLU:HB3	1:y:1520:GLY:HA2	2.02	0.42
1:y:1630:LEU:HD12	1:y:1631:GLY:N	2.35	0.42
1:y:1835:TRP:HZ2	1:y:1838:GLN:HB3	1.85	0.42
1:y:1886:LEU:HD13	1:y:1891:LEU:HD21	2.02	0.42
1:y:1970:GLY:C	1:y:1972:ALA:H	2.28	0.42
1:Y:105:LEU:HD23	1:Y:105:LEU:HA	1.87	0.41
1:Y:334:GLU:O	1:Y:337:ILE:HG12	2.20	0.41
1:Y:342:PRO:HB3	1:Y:363:TYR:CE2	2.54	0.41
1:Y:357:TYR:CG	1:Y:414:GLU:HG3	2.55	0.41
1:Y:640:LEU:HD23	1:Y:640:LEU:HA	1.88	0.41
1:Y:1514:PHE:HA	1:Y:1581:LEU:O	2.20	0.41
1:Y:1554:HIS:NE2	1:Y:1571:CYS:HB3	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:911:ILE:HB	1:y:942:ASN:OD1	2.20	0.41
1:y:1277:LEU:HA	1:y:1280:ASN:HD21	1.86	0.41
1:y:1609:ARG:HD3	1:y:1609:ARG:HA	1.70	0.41
1:Y:22:SER:HB2	1:Y:613:GLU:HG3	2.02	0.41
1:Y:368:GLN:HA	1:Y:371:GLN:OE1	2.19	0.41
1:Y:440:LYS:H	1:Y:457:GLY:H	1.68	0.41
1:Y:548:ILE:O	1:Y:565:HIS:HA	2.19	0.41
1:Y:596:ASN:OD1	1:Y:597:ASN:N	2.53	0.41
1:Y:763:SER:HG	1:Y:766:THR:H	1.67	0.41
1:Y:1558:ARG:HD2	1:Y:1558:ARG:H	1.84	0.41
1:Y:1600:LEU:HD23	1:Y:1600:LEU:HA	1.83	0.41
1:y:167:ARG:NH2	1:y:171:ARG:HH22	2.18	0.41
1:y:266:LEU:HD21	1:y:1178:PHE:HE1	1.85	0.41
1:y:368:GLN:HA	1:y:371:GLN:OE1	2.20	0.41
1:y:397:ILE:HG22	1:y:401:GLU:HG2	2.01	0.41
1:y:641:LEU:O	1:y:1117:VAL:HA	2.20	0.41
1:y:688:HIS:NE2	1:y:742:GLU:HB2	2.35	0.41
1:y:1122:VAL:HA	1:y:1123:PRO:HD3	1.96	0.41
1:y:1233:GLN:HA	1:y:1236:ASP:OD2	2.20	0.41
1:y:1236:ASP:OD1	1:y:1237:LYS:N	2.53	0.41
1:y:1285:LYS:HA	1:y:1285:LYS:HD3	1.84	0.41
1:y:1415:HIS:ND1	1:y:1415:HIS:O	2.52	0.41
1:y:1767:TRP:CD1	1:y:1858:PRO:HD2	2.56	0.41
1:y:1807:LEU:HD22	1:y:1820:VAL:HG11	2.02	0.41
1:y:2066:GLU:HG2	1:y:2067:ASP:H	1.85	0.41
1:Y:610:PHE:O	1:Y:614:ILE:HB	2.20	0.41
1:Y:683:LYS:HA	1:Y:683:LYS:HD2	1.59	0.41
1:Y:945:MET:HE2	1:Y:945:MET:HA	2.02	0.41
1:Y:1254:GLN:O	1:Y:1257:THR:OG1	2.27	0.41
1:Y:1842:GLU:H	1:Y:1842:GLU:HG3	1.72	0.41
1:Y:1981:VAL:O	1:Y:2029:THR:HA	2.19	0.41
1:y:166:LEU:HD12	1:y:169:TRP:CD1	2.55	0.41
1:y:781:MET:H	1:y:781:MET:CE	2.33	0.41
1:y:1224:LEU:HD21	1:y:1263:MET:HB3	2.02	0.41
1:y:1230:GLN:HG2	1:y:1233:GLN:HE22	1.86	0.41
1:y:1259:THR:HA	1:y:1262:MET:HG2	2.02	0.41
1:y:1452:LYS:HE2	1:y:1580:TRP:CE2	2.55	0.41
1:y:1683:CYS:SG	1:y:1705:ARG:HD3	2.60	0.41
1:y:1967:VAL:HG21	1:y:2021:TRP:CD1	2.51	0.41
1:Y:348:LEU:HD21	1:Y:363:TYR:HE2	1.84	0.41
1:Y:352:SER:OG	1:Y:355:ASP:OD1	2.15	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:437:CYS:HB3	1:Y:442:CYS:SG	2.60	0.41
1:Y:581:ASN:OD1	1:Y:595:LYS:HD3	2.20	0.41
1:Y:682:ALA:HB1	1:Y:753:ASN:OD1	2.21	0.41
1:Y:709:ASP:O	1:Y:713:LYS:HG3	2.21	0.41
1:Y:803:LEU:HD13	1:Y:803:LEU:HA	1.75	0.41
1:Y:878:GLN:O	1:Y:882:TRP:HD1	2.03	0.41
1:Y:1028:GLY:HA2	1:y:949:TRP:CZ3	2.55	0.41
1:y:16:HIS:NE2	1:y:43:PHE:HA	2.35	0.41
1:y:996:TYR:CD1	1:y:1008:PRO:HG2	2.55	0.41
1:y:1298:LYS:HD2	1:y:1345:ARG:HB2	2.02	0.41
1:y:1736:GLU:OE2	1:y:1738:ASN:N	2.52	0.41
1:y:1763:PRO:HG2	1:y:1766:GLN:HE22	1.85	0.41
1:Y:95:ARG:O	1:Y:99:THR:HG22	2.20	0.41
1:Y:238:ILE:HD13	1:Y:238:ILE:HA	1.84	0.41
1:Y:424:MET:HE2	1:Y:424:MET:HB3	1.87	0.41
1:Y:862:LEU:HD12	1:Y:862:LEU:HA	1.83	0.41
1:Y:1903:ASN:HD22	1:Y:2098:ARG:HH21	1.68	0.41
1:y:21:ARG:NH1	1:y:1061:ASP:OD2	2.53	0.41
1:y:129:VAL:HG12	1:y:247:TYR:CD2	2.54	0.41
1:y:1130:LEU:CD2	1:y:1166:ALA:HB1	2.51	0.41
1:y:1314:SER:O	1:y:1317:ILE:HG22	2.21	0.41
3:I:7:DA:H5"	3:I:7:DA:H8	1.85	0.41
1:Y:208:GLU:H	1:Y:208:GLU:CD	2.28	0.41
1:Y:696:ILE:HG13	1:Y:711:LEU:HD23	2.01	0.41
1:Y:1284:LEU:HD12	1:Y:1284:LEU:HA	1.64	0.41
1:Y:1486:LEU:HB2	1:Y:1510:GLU:HB2	2.03	0.41
1:y:370:ARG:O	1:y:374:THR:HG22	2.20	0.41
1:y:492:GLU:HB3	1:y:494:ARG:HH22	1.86	0.41
1:y:1558:ARG:HD2	1:y:1558:ARG:HA	1.84	0.41
1:Y:594:ARG:HB2	1:Y:597:ASN:OD1	2.21	0.41
1:Y:757:GLN:HE21	1:Y:757:GLN:HB2	1.60	0.41
1:Y:810:ARG:HG3	1:Y:810:ARG:O	2.20	0.41
1:y:225:LEU:HA	1:y:228:MET:HG2	2.03	0.41
1:y:657:LEU:HD12	1:y:657:LEU:C	2.46	0.41
1:y:859:LYS:HE2	1:y:990:ASP:OD2	2.20	0.41
1:y:1526:CYS:HB2	1:y:1575:VAL:HG22	2.02	0.41
1:y:1612:ALA:O	1:y:1615:LEU:HG	2.21	0.41
1:Y:52:LEU:HD23	1:Y:52:LEU:HA	1.72	0.41
1:Y:68:ASP:OD1	1:Y:68:ASP:N	2.54	0.41
1:Y:121:LYS:O	1:Y:124:CYS:HB3	2.21	0.41
1:Y:695:VAL:HG23	1:Y:743:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1998:TRP:HD1	1:Y:1999:LEU:N	2.14	0.41
1:Y:2013:GLU:HA	1:Y:2021:TRP:HE3	1.85	0.41
1:Y:2071:ASP:OD2	1:Y:2079:GLN:HG3	2.21	0.41
1:y:427:PHE:HB3	1:y:1150:CYS:SG	2.60	0.41
1:y:809:ARG:HG3	1:y:868:GLU:HA	2.03	0.41
1:y:1256:LEU:HD13	1:y:1256:LEU:HA	1.91	0.41
1:y:1536:THR:H	1:y:1540:ARG:HH21	1.69	0.41
1:y:1759:VAL:HG21	1:y:1828:LEU:HD22	2.01	0.41
1:y:1773:PRO:O	1:y:1776:LYS:HG2	2.21	0.41
1:y:1964:THR:HA	1:y:1967:VAL:HG12	2.02	0.41
1:Y:163:GLN:CD	1:Y:167:ARG:HH12	2.28	0.41
1:Y:408:LEU:HD13	1:Y:408:LEU:HA	1.89	0.41
1:Y:447:HIS:HA	1:Y:450:ASN:ND2	2.36	0.41
1:Y:1339:ALA:O	1:Y:1342:LEU:HG	2.21	0.41
1:Y:1414:ASP:O	1:Y:1416:HIS:ND1	2.54	0.41
1:Y:1526:CYS:HB3	1:Y:1529:CYS:SG	2.61	0.41
1:Y:1790:LEU:HA	1:Y:1790:LEU:HD12	1.74	0.41
1:Y:1906:GLU:OE2	1:Y:2091:VAL:HG13	2.21	0.41
1:Y:1908:LEU:HD21	1:Y:1922:LEU:HD12	2.03	0.41
1:y:8:TYR:CE2	1:y:424:MET:HB2	2.56	0.41
1:y:134:ILE:HD12	1:y:173:PHE:CE1	2.56	0.41
1:y:178:ARG:NH2	1:y:213:ALA:O	2.48	0.41
1:y:237:ILE:HD12	1:y:237:ILE:H	1.85	0.41
1:y:550:LEU:N	1:y:565:HIS:HA	2.36	0.41
1:y:550:LEU:H	1:y:565:HIS:HA	1.85	0.41
1:y:640:LEU:HD11	1:y:1116:LEU:HB2	2.02	0.41
1:y:865:PHE:CD2	1:y:866:ILE:HG23	2.56	0.41
1:y:931:GLN:H	1:y:937:TRP:CG	2.38	0.41
1:y:1000:LEU:HD11	1:y:1005:GLU:OE1	2.20	0.41
1:y:1285:LYS:HD3	1:y:1291:TRP:CD1	2.56	0.41
1:y:1334:PHE:HA	1:y:1460:PHE:O	2.21	0.41
1:y:1521:HIS:CD2	1:y:1538:PRO:HD3	2.55	0.41
1:y:1556:LEU:HD13	1:y:1560:GLY:O	2.20	0.41
1:y:1584:SER:HB3	1:y:1586:ARG:HH22	1.85	0.41
1:y:1605:GLU:CD	1:y:1634:THR:HG1	2.25	0.41
1:y:1612:ALA:HB2	1:y:1648:ILE:HD13	2.02	0.41
1:y:1625:ILE:HD13	1:y:1660:TYR:CZ	2.56	0.41
1:y:1729:PHE:H	1:y:1733:SER:HG	1.69	0.41
1:Y:156:ASN:HD22	2:G:8:DG:P	2.44	0.41
1:Y:895:PRO:HB2	1:Y:946:ILE:HD13	2.02	0.41
1:Y:1966:LEU:HD12	1:Y:1966:LEU:HA	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:178:ARG:HB3	1:y:202:GLU:O	2.21	0.41
1:y:187:ARG:HE	1:y:193:ILE:HD11	1.86	0.41
1:y:539:ILE:HA	1:y:569:ASN:O	2.21	0.41
1:y:673:GLU:OE1	1:y:673:GLU:N	2.53	0.41
1:y:825:ILE:HG13	1:y:867:ARG:NH1	2.36	0.41
1:y:1265:GLN:O	1:y:1268:ILE:HG22	2.21	0.41
1:y:1602:ILE:HG12	1:y:1711:LEU:HD11	2.03	0.41
1:y:1824:ALA:HB3	1:y:1827:GLN:OE1	2.21	0.41
1:Y:71:MET:HA	1:Y:71:MET:HE3	2.02	0.40
1:Y:266:LEU:HA	1:Y:266:LEU:HD23	1.67	0.40
1:Y:551:GLU:CD	1:Y:564:LYS:H	2.24	0.40
1:Y:982:CYS:SG	1:Y:985:THR:N	2.76	0.40
1:Y:1243:GLN:HA	1:Y:1248:MET:HE3	2.02	0.40
1:Y:1285:LYS:NZ	1:Y:1291:TRP:HB3	2.35	0.40
1:Y:1535:GLN:HE21	1:Y:1535:GLN:HB2	1.55	0.40
1:Y:1592:LEU:HD22	1:Y:1668:TRP:CH2	2.56	0.40
1:Y:1680:ASP:OD1	1:Y:1709:LEU:HD11	2.21	0.40
1:Y:1758:LEU:HD23	1:Y:1862:TRP:CH2	2.56	0.40
1:y:762:MET:N	1:y:973:PHE:O	2.44	0.40
1:y:848:ASP:OD1	1:y:849:LYS:N	2.54	0.40
1:y:1041:LEU:HD21	1:y:1061:ASP:HB2	2.03	0.40
1:y:1523:TYR:HE2	1:y:1532:ALA:HB1	1.86	0.40
1:y:1658:ALA:HB3	1:y:1660:TYR:CE2	2.56	0.40
1:Y:74:LEU:O	1:Y:78:LEU:N	2.54	0.40
1:Y:1103:THR:HA	1:Y:1106:GLU:OE2	2.21	0.40
1:Y:1667:HIS:O	1:Y:1668:TRP:C	2.64	0.40
1:Y:1685:LYS:HE2	1:Y:1685:LYS:HB3	1.90	0.40
1:Y:1687:CYS:SG	1:Y:1689:HIS:ND1	2.94	0.40
1:y:186:THR:HG21	1:y:207:ARG:HG3	2.01	0.40
1:y:337:ILE:HD12	1:y:364:ARG:HG2	2.03	0.40
1:y:422:LEU:O	1:y:1143:ALA:HA	2.21	0.40
1:y:487:LEU:HD12	1:y:539:ILE:O	2.20	0.40
1:y:836:CYS:HB3	1:y:840:TRP:CD1	2.57	0.40
1:y:912:ARG:HD2	1:y:912:ARG:HA	1.89	0.40
1:y:1791:LEU:HD23	1:y:1821:LYS:HG3	2.03	0.40
1:Y:126:MET:HB2	1:Y:126:MET:HE2	1.79	0.40
1:Y:189:THR:HA	1:Y:208:GLU:OE2	2.20	0.40
1:Y:220:THR:HG22	1:Y:221:ASN:O	2.21	0.40
1:Y:619:LEU:HD21	1:Y:1070:TYR:HD1	1.87	0.40
1:Y:720:GLU:HG2	1:Y:721:LEU:N	2.35	0.40
1:Y:985:THR:O	1:Y:987:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1037:ARG:HB3	1:Y:1065:LEU:HD22	2.03	0.40
1:Y:1330:GLY:O	1:Y:1373:ASP:HA	2.21	0.40
1:Y:1473:SER:OG	1:Y:1474:MET:N	2.54	0.40
1:Y:2064:CYS:O	1:Y:2065:ILE:HD13	2.21	0.40
1:y:96:HIS:NE2	1:y:119:SER:HB3	2.36	0.40
1:y:224:MET:O	1:y:227:TYR:HB2	2.22	0.40
1:y:340:GLU:O	1:y:365:VAL:HG23	2.22	0.40
1:y:423:ARG:HH21	1:y:425:HIS:CE1	2.36	0.40
1:y:593:GLN:HG3	1:y:597:ASN:O	2.21	0.40
1:y:993:LEU:HD12	1:y:993:LEU:HA	1.90	0.40
1:y:1049:HIS:HA	1:y:1052:GLU:OE2	2.20	0.40
1:y:1105:MET:HE1	1:y:1109:VAL:N	2.36	0.40
1:y:1419:TRP:CD1	1:y:1453:ARG:HG2	2.56	0.40
1:y:1511:LEU:HD23	1:y:1511:LEU:HA	1.81	0.40
1:y:1524:ALA:O	1:y:1532:ALA:HA	2.21	0.40
1:y:1892:LEU:HD23	1:y:1892:LEU:HA	1.85	0.40
1:Y:224:MET:HA	1:Y:224:MET:CE	2.50	0.40
1:Y:474:PHE:CD1	1:Y:503:ALA:HA	2.56	0.40
1:Y:764:TRP:NE1	1:Y:800:ASP:OD1	2.52	0.40
1:Y:1616:ARG:NH2	1:Y:1695:ASP:OD2	2.51	0.40
1:Y:1732:GLY:O	1:Y:1734:ARG:HD2	2.21	0.40
1:y:62:PHE:HZ	1:y:420:THR:HG22	1.85	0.40
1:y:813:ASN:OD1	1:y:814:ALA:N	2.55	0.40
1:y:849:LYS:HE2	1:y:849:LYS:HB2	1.99	0.40
1:y:1249:SER:HB3	1:y:1776:LYS:HZ2	1.86	0.40
1:y:1317:ILE:HD12	1:y:1317:ILE:HA	1.85	0.40
1:y:1536:THR:H	1:y:1540:ARG:NH2	2.18	0.40
1:y:1687:CYS:N	1:y:1690:CYS:SG	2.82	0.40
1:y:1821:LYS:HB3	1:y:1885:THR:HA	2.04	0.40
1:Y:4:GLN:HE22	1:Y:623:PRO:HB3	1.87	0.40
1:Y:71:MET:HB3	1:Y:84:VAL:HG13	2.03	0.40
1:Y:239:GLU:O	1:Y:242:GLN:HB2	2.21	0.40
1:Y:569:ASN:OD1	1:Y:569:ASN:N	2.53	0.40
1:Y:848:ASP:OD1	1:Y:848:ASP:N	2.55	0.40
1:Y:864:PHE:CE2	1:Y:998:PRO:HG2	2.56	0.40
1:Y:1075:HIS:NE2	1:Y:1084:ASN:HB3	2.37	0.40
1:Y:1151:LYS:HA	1:Y:1151:LYS:HD2	1.93	0.40
1:Y:1230:GLN:OE1	1:Y:1233:GLN:NE2	2.50	0.40
1:Y:1959:LEU:HD12	1:Y:1960:GLY:N	2.36	0.40
1:y:105:LEU:HG	1:y:128:PRO:HB3	2.03	0.40
1:y:354:GLN:HG3	1:y:414:GLU:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:694:LYS:HE3	1:y:695:VAL:HG23	2.04	0.40
1:y:1188:VAL:HG22	1:y:1238:LEU:HD21	2.04	0.40
1:y:1561:SER:HB2	1:y:1568:ASN:O	2.21	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	Y	2069/2108 (98%)	1919 (93%)	149 (7%)	1 (0%)	100	100
1	y	2042/2108 (97%)	1934 (95%)	108 (5%)	0	100	100
All	All	4111/4216 (98%)	3853 (94%)	257 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	1208	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Y	1768/1795 (98%)	1683 (95%)	85 (5%)	23	50
1	y	1746/1795 (97%)	1691 (97%)	55 (3%)	34	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3514/3590 (98%)	3374 (96%)	140 (4%)	29 54

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	41	GLN
1	Y	57	VAL
1	Y	68	ASP
1	Y	85	ASP
1	Y	89	LYS
1	Y	103	THR
1	Y	113	VAL
1	Y	130	LEU
1	Y	152	LEU
1	Y	206	SER
1	Y	224	MET
1	Y	309	VAL
1	Y	312	LEU
1	Y	355	ASP
1	Y	396	ASP
1	Y	407	ASP
1	Y	417	LEU
1	Y	467	CYS
1	Y	517	VAL
1	Y	532	ASN
1	Y	539	ILE
1	Y	551	GLU
1	Y	559	ASP
1	Y	568	ILE
1	Y	569	ASN
1	Y	582	ASN
1	Y	592	THR
1	Y	594	ARG
1	Y	613	GLU
1	Y	695	VAL
1	Y	698	GLN
1	Y	761	THR
1	Y	794	THR
1	Y	803	LEU
1	Y	813	ASN
1	Y	823	VAL
1	Y	829	PHE

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Mol	Chain	Res	Type
1	Y	835	THR
1	Y	889	VAL
1	Y	936	HIS
1	Y	941	VAL
1	Y	945	MET
1	Y	948	VAL
1	Y	982	CYS
1	Y	1058	THR
1	Y	1107	MET
1	Y	1130	LEU
1	Y	1153	THR
1	Y	1201	VAL
1	Y	1205	THR
1	Y	1210	LYS
1	Y	1242	THR
1	Y	1248	MET
1	Y	1399	ILE
1	Y	1423	CYS
1	Y	1426	CYS
1	Y	1431	THR
1	Y	1432	SER
1	Y	1458	VAL
1	Y	1464	ILE
1	Y	1487	VAL
1	Y	1511	LEU
1	Y	1536	THR
1	Y	1541	THR
1	Y	1587	THR
1	Y	1652	ASP
1	Y	1664	LEU
1	Y	1666	ASP
1	Y	1670	ASP
1	Y	1689	HIS
1	Y	1715	VAL
1	Y	1760	LEU
1	Y	1788	VAL
1	Y	1792	VAL
1	Y	1841	ARG
1	Y	1874	LYS
1	Y	1890	ASP
1	Y	1908	LEU
1	Y	1915	PHE

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Mol	Chain	Res	Type
1	Y	1919	PHE
1	Y	1950	LEU
1	Y	1995	TYR
1	Y	2010	THR
1	Y	2016	TYR
1	Y	2079	GLN
1	y	13	ASN
1	y	22	SER
1	y	29	LEU
1	y	57	VAL
1	y	150	ILE
1	y	189	THR
1	y	193	ILE
1	y	225	LEU
1	y	271	VAL
1	y	383	LEU
1	y	571	LEU
1	y	641	LEU
1	y	650	THR
1	y	670	CYS
1	y	700	SER
1	y	709	ASP
1	y	730	LYS
1	y	736	VAL
1	y	763	SER
1	y	806	GLU
1	y	809	ARG
1	y	833	VAL
1	y	862	LEU
1	y	887	PHE
1	y	936	HIS
1	y	1014	ILE
1	y	1047	ILE
1	y	1052	GLU
1	y	1122	VAL
1	y	1128	ASN
1	y	1169	THR
1	y	1216	ASP
1	y	1232	ASP
1	y	1238	LEU
1	y	1251	THR
1	y	1292	GLU

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Mol	Chain	Res	Type
1	y	1348	ILE
1	y	1387	VAL
1	y	1404	VAL
1	y	1437	VAL
1	y	1441	HIS
1	y	1493	VAL
1	y	1519	PHE
1	y	1541	THR
1	y	1553	THR
1	y	1574	HIS
1	y	1590	VAL
1	y	1641	ASN
1	y	1740	LEU
1	y	1823	ILE
1	y	1870	VAL
1	y	1884	GLN
1	y	1903	ASN
1	y	2041	LEU
1	y	2097	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	4	GLN
1	Y	17	GLN
1	Y	162	GLN
1	Y	367	GLN
1	Y	658	GLN
1	Y	698	GLN
1	Y	757	GLN
1	Y	869	ASN
1	Y	878	GLN
1	Y	910	GLN
1	Y	970	GLN
1	Y	1048	GLN
1	Y	1636	GLN
1	Y	1673	ASN
1	Y	1688	HIS
1	Y	1721	ASN
1	Y	1903	ASN
1	Y	1990	GLN
1	Y	2050	GLN

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Mol	Chain	Res	Type
1	y	13	ASN
1	y	286	GLN
1	y	359	GLN
1	y	425	HIS
1	y	626	GLN
1	y	658	GLN
1	y	751	GLN
1	y	856	ASN
1	y	869	ASN
1	y	1083	GLN
1	y	1128	ASN
1	y	1229	HIS
1	y	1562	ASN
1	y	1576	HIS
1	y	1598	ASN
1	y	1635	GLN
1	y	1688	HIS
1	y	1689	HIS
1	y	1805	HIS
1	y	1969	GLN
1	y	2050	GLN
1	y	2095	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 for Mogul analysis.

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
5	AGS	Y	2206	-	29,33,33	0.46	0	39,52,52	0.75	1 (2%)
5	AGS	y	2206	-	29,33,33	0.47	1 (3%)	39,52,52	0.75	1 (2%)

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
5	AGS	Y	2206	-	-	6/21/38/38	0/3/3/3
5	AGS	y	2206	-	-	7/21/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	y	2206	AGS	PG-S1G	2.09	1.95	1.90

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	2206	AGS	PA-O3A-PB	-3.90	119.45	132.83
5	y	2206	AGS	PA-O3A-PB	-3.76	119.93	132.83

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Y	2206	AGS	C5'-O5'-PA-O2A
5	y	2206	AGS	PB-O3B-PG-O2G
5	y	2206	AGS	PB-O3B-PG-O3G
5	Y	2206	AGS	O4'-C4'-C5'-O5'
5	y	2206	AGS	O4'-C4'-C5'-O5'
5	Y	2206	AGS	C3'-C4'-C5'-O5'
5	y	2206	AGS	C3'-C4'-C5'-O5'
5	y	2206	AGS	C4'-C5'-O5'-PA

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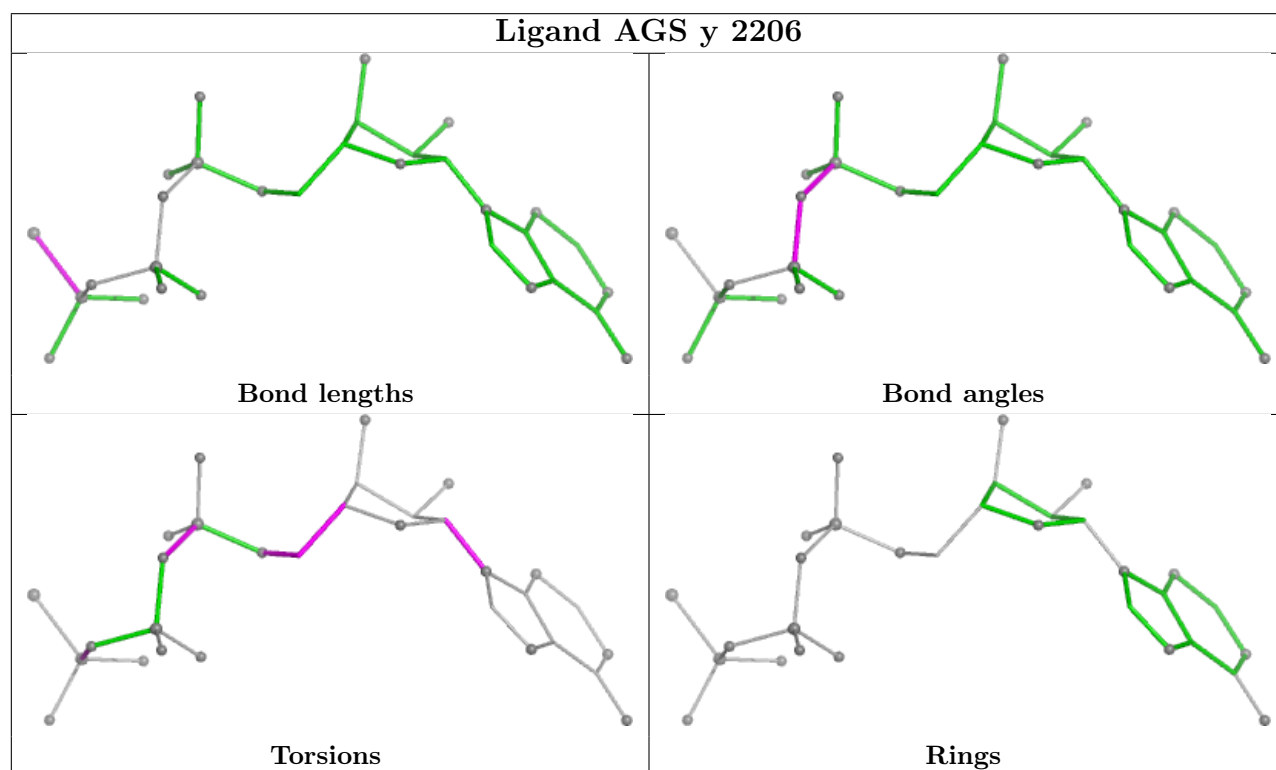
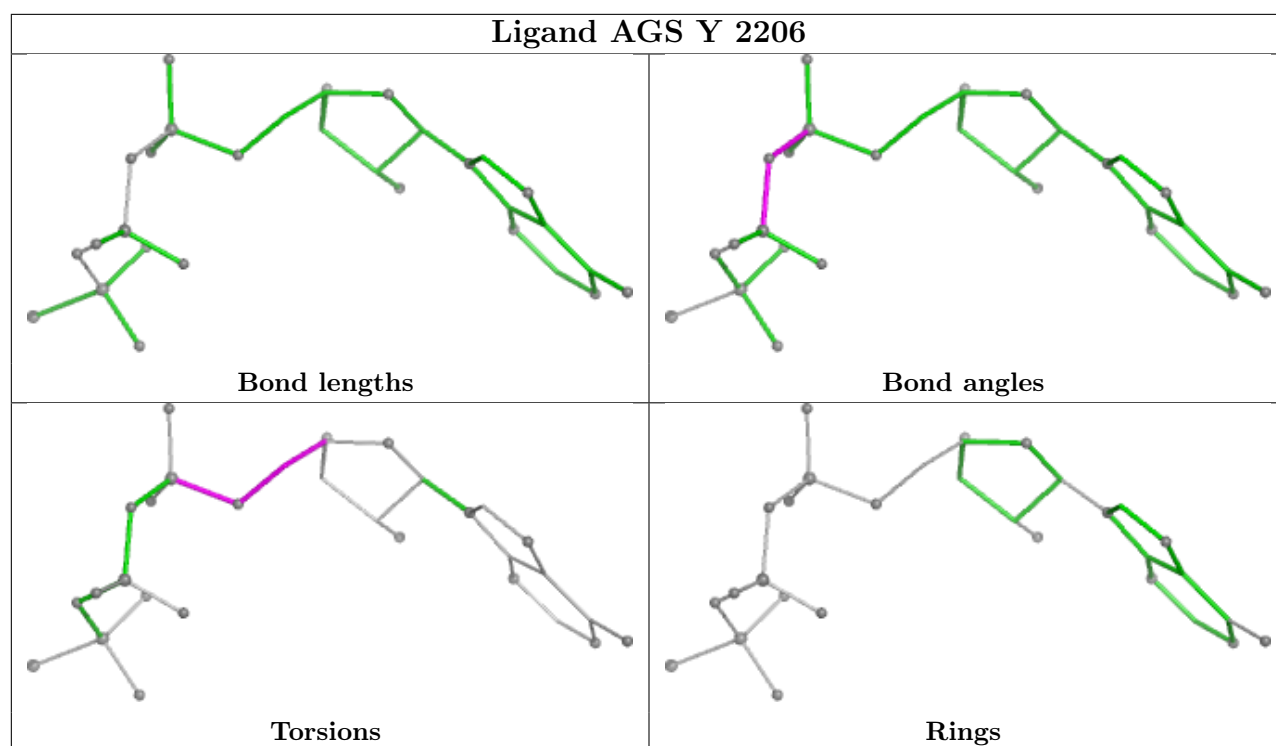
Mol	Chain	Res	Type	Atoms
5	y	2206	AGS	PB-O3A-PA-O5'
5	Y	2206	AGS	C4'-C5'-O5'-PA
5	Y	2206	AGS	C5'-O5'-PA-O3A
5	Y	2206	AGS	C5'-O5'-PA-O1A
5	y	2206	AGS	C2'-C1'-N9-C8

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Y	2206	AGS	6	0
5	y	2206	AGS	3	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

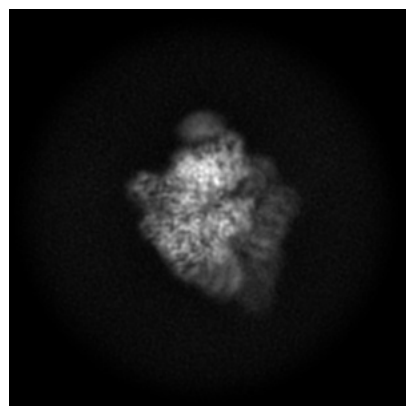
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56253. These allow visual inspection of the internal detail of the map and identification of artifacts.

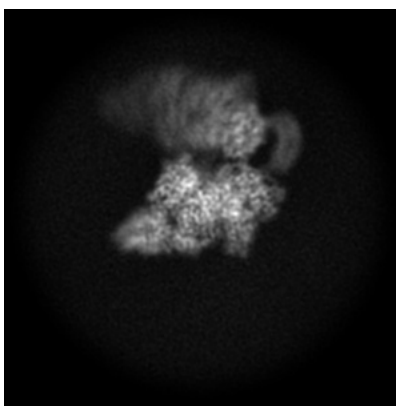
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

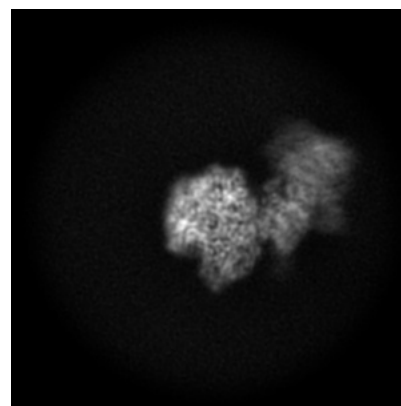
6.1.1 Primary map



X

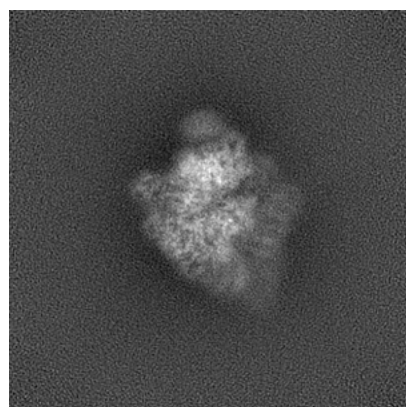


Y

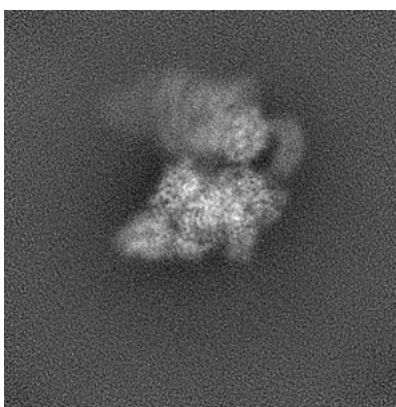


Z

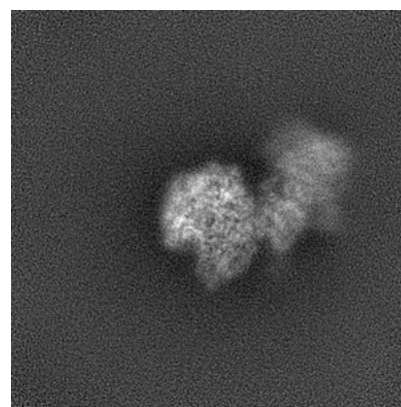
6.1.2 Raw map



X



Y

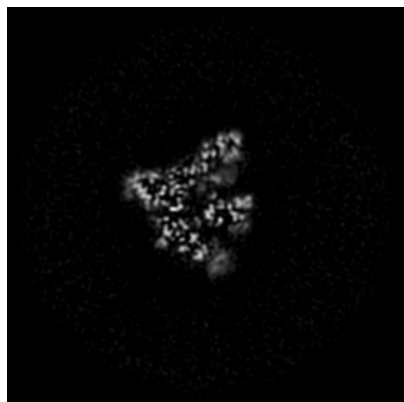


Z

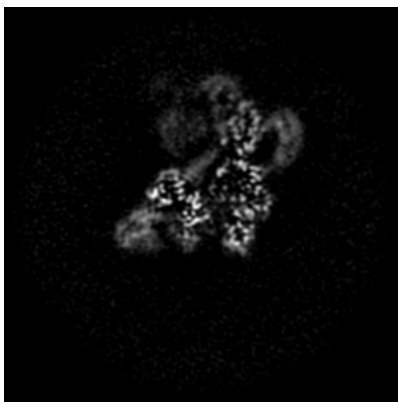
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

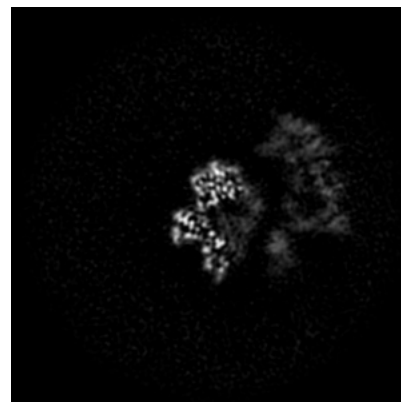
6.2.1 Primary map



X Index: 144

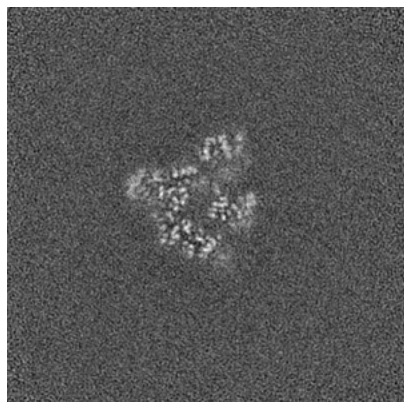


Y Index: 144

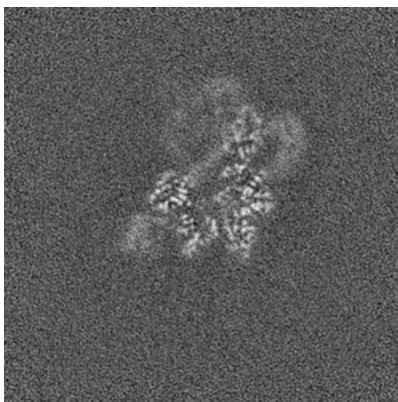


Z Index: 144

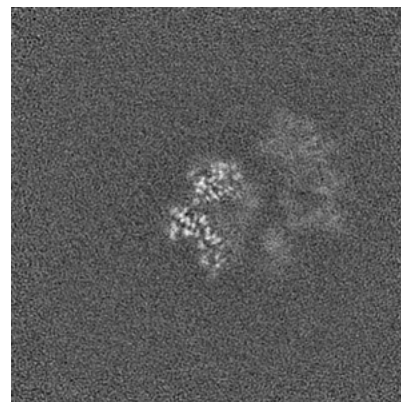
6.2.2 Raw map



X Index: 144



Y Index: 144

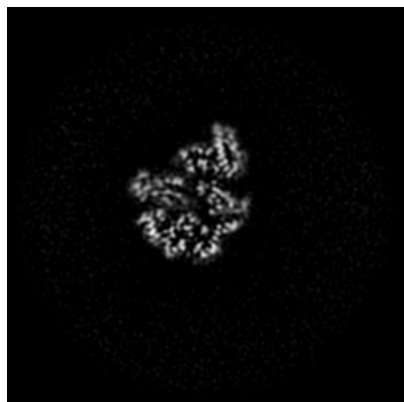


Z Index: 144

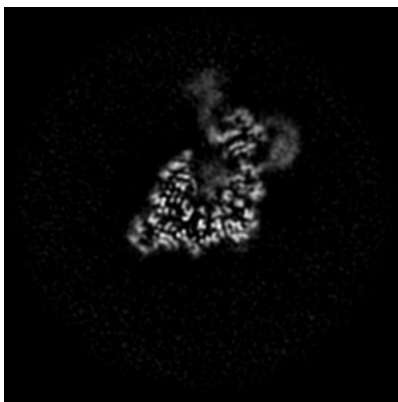
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

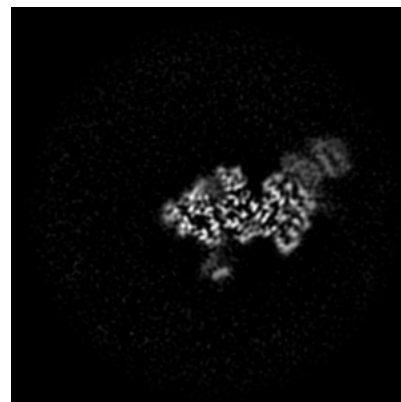
6.3.1 Primary map



X Index: 157

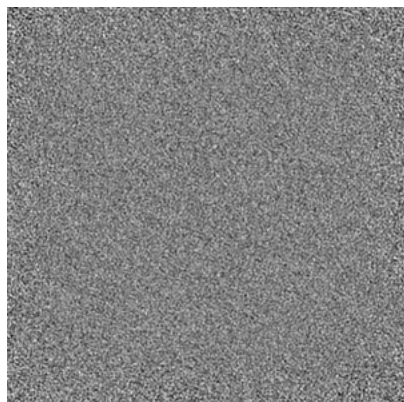


Y Index: 129

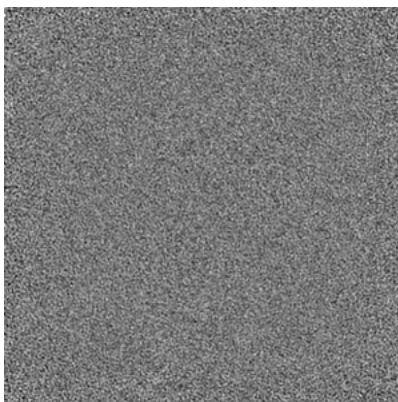


Z Index: 170

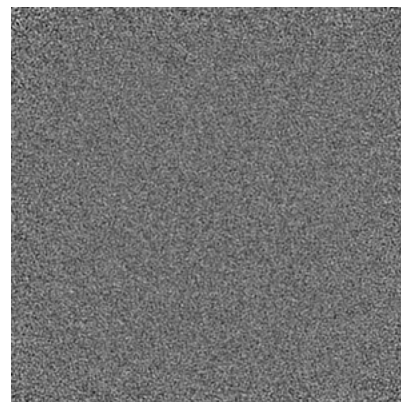
6.3.2 Raw map



X Index: 0



Y Index: 0

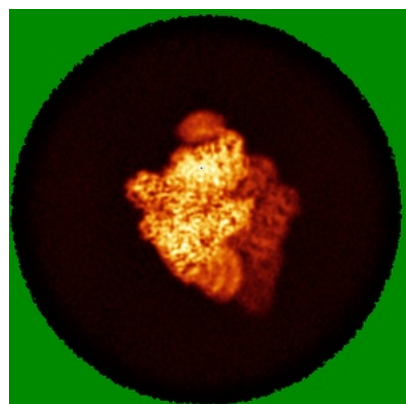


Z Index: 0

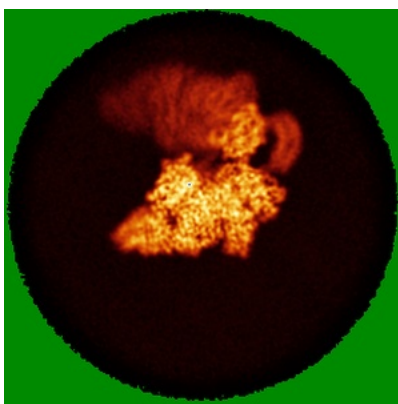
The images above show the largest variance slices of the map in three orthogonal directions.

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

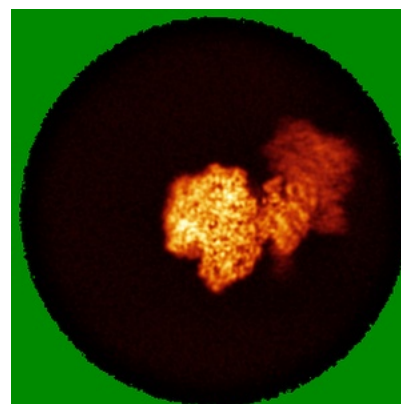
6.4.1 Primary map



X

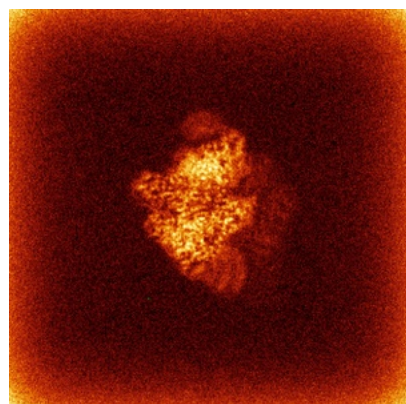


Y

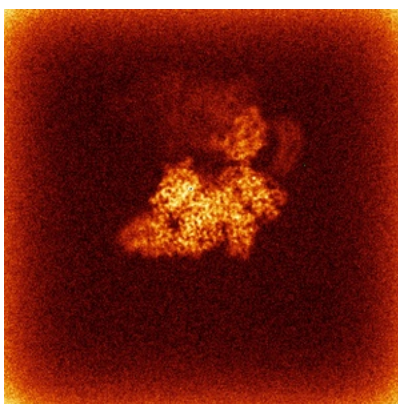


Z

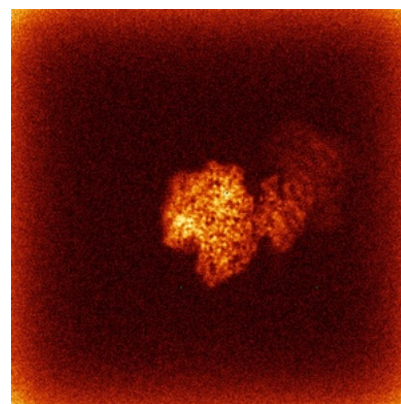
6.4.2 Raw map



X



Y

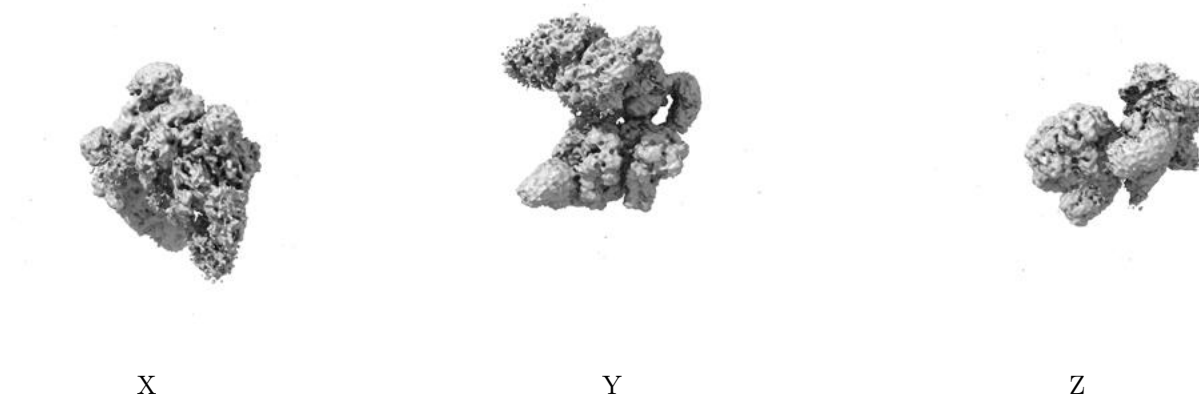


Z

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

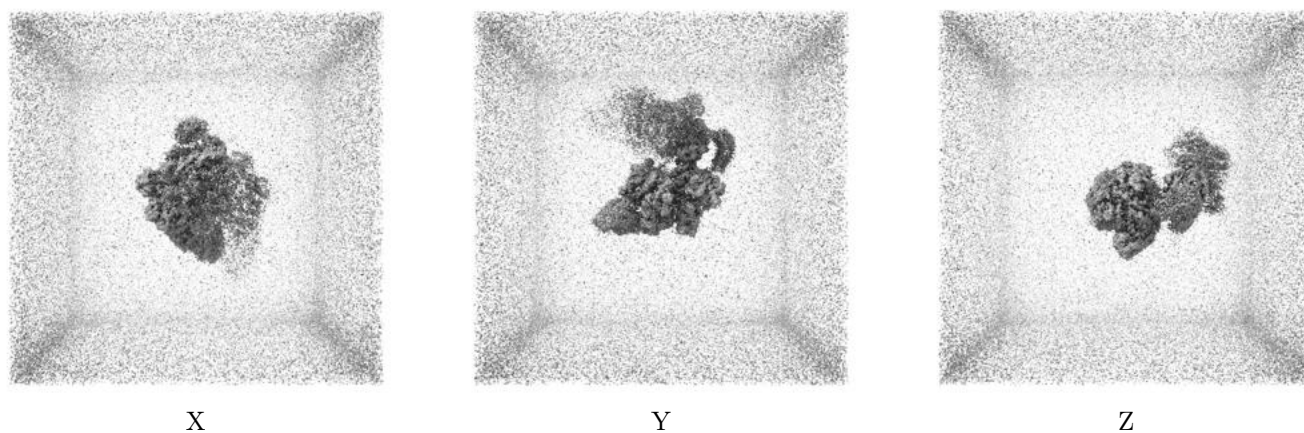
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

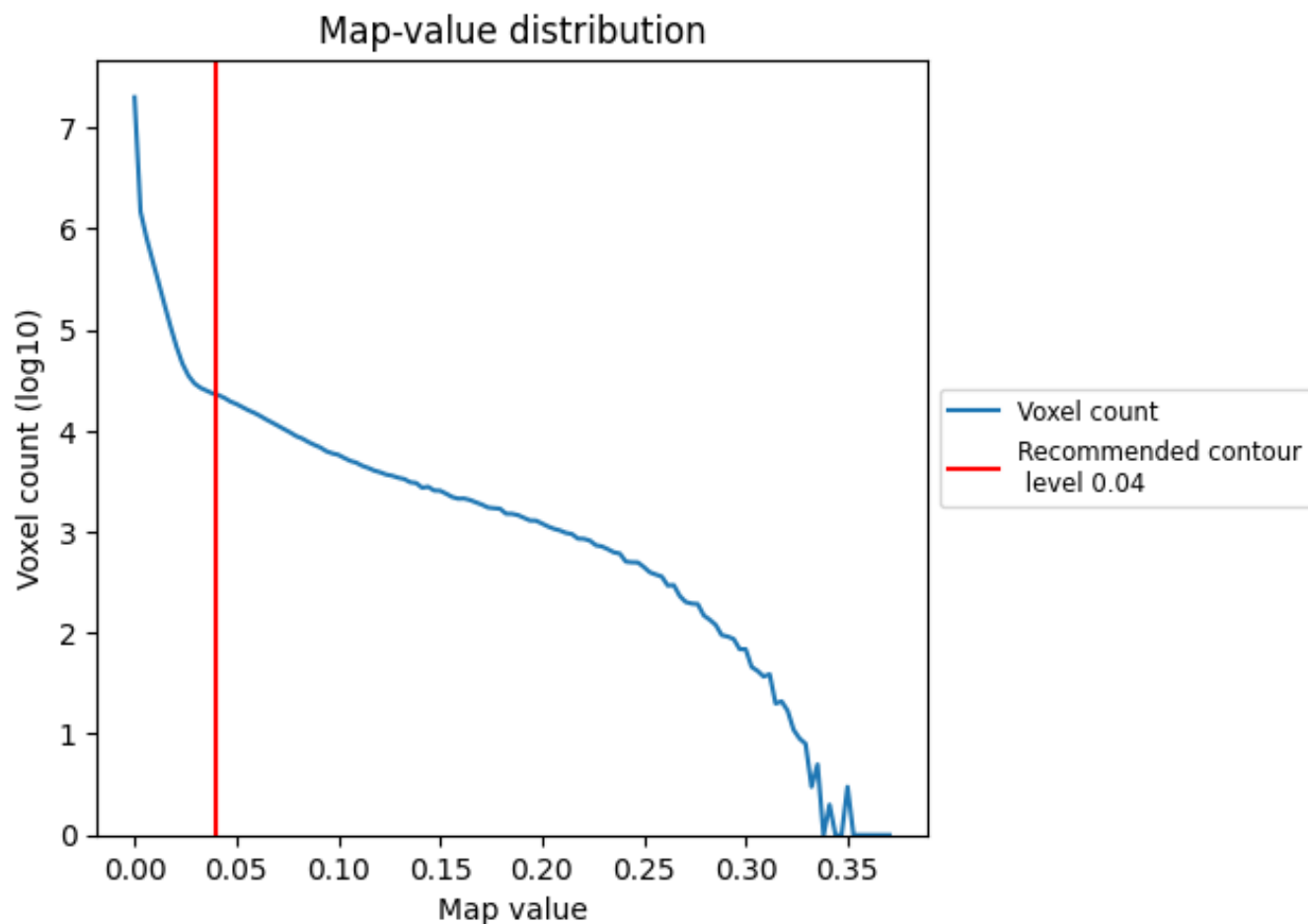
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

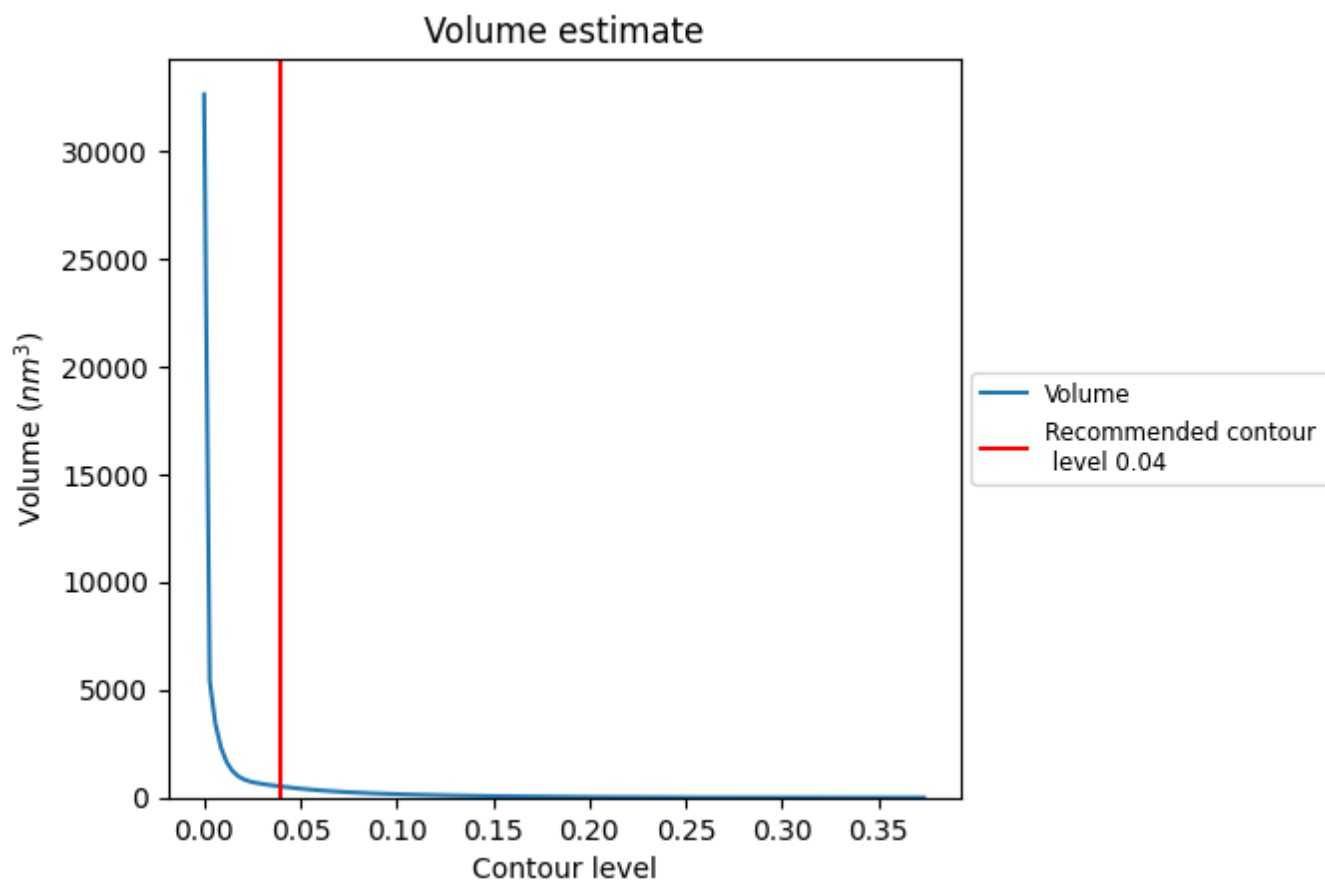
This section contains the results of statistical analysis of the map.

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.

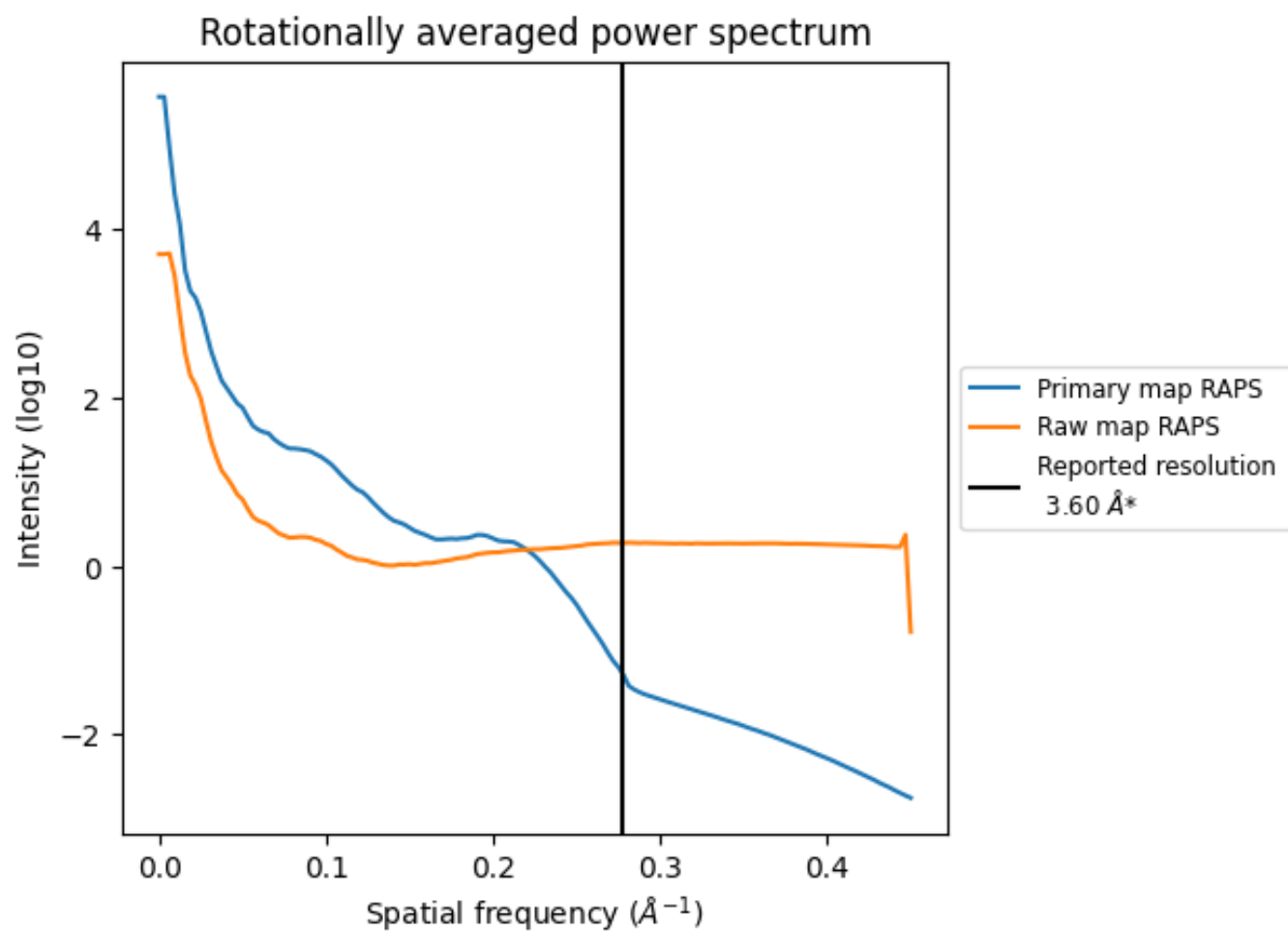
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 512 nm^3 ; this corresponds to an approximate mass of 463 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 [i](#)

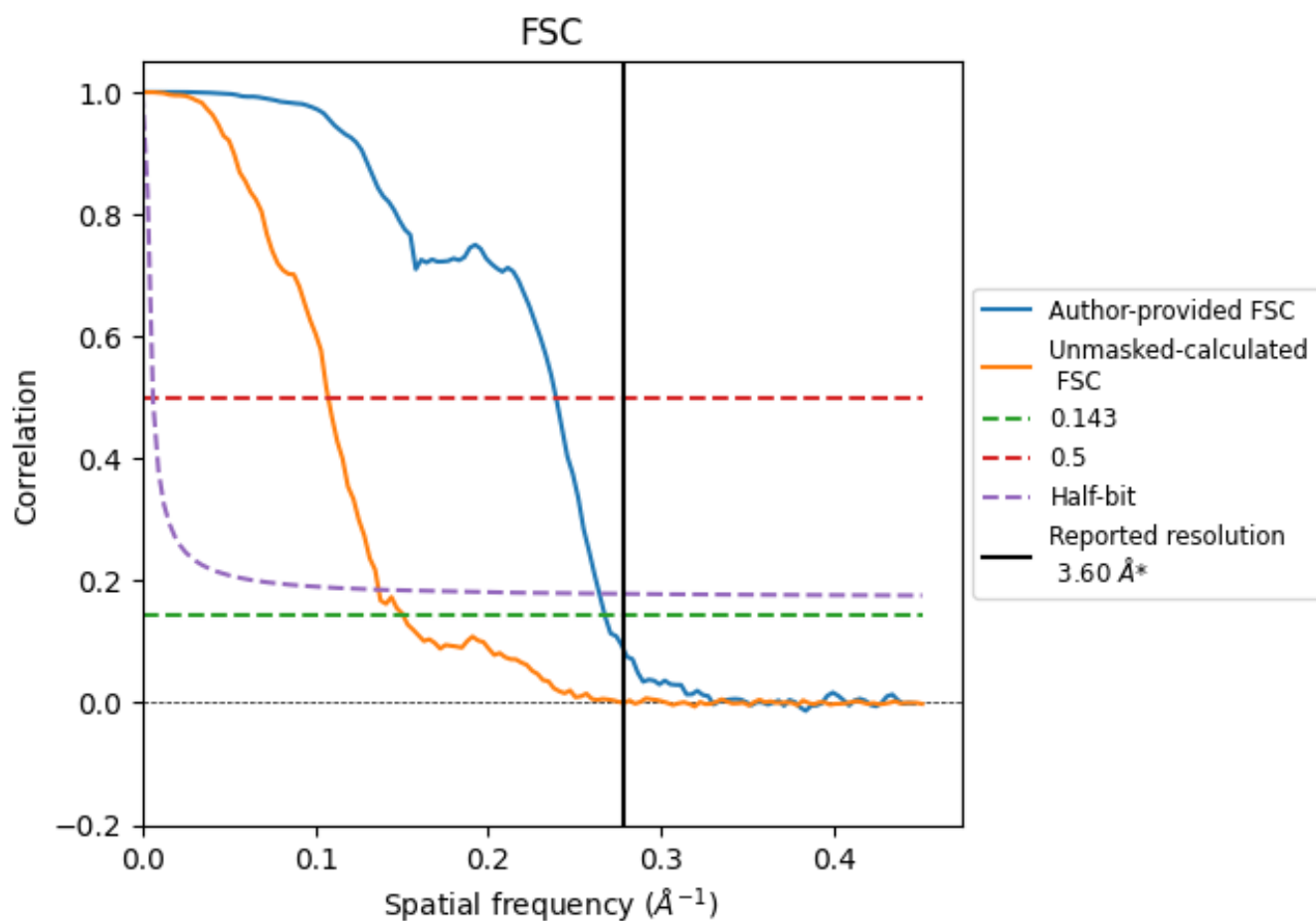


*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

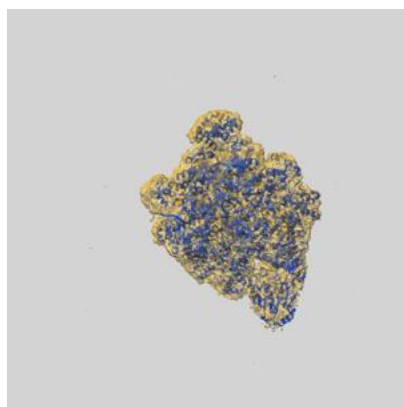
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.74	4.18	3.79
Unmasked-calculated*	6.63	9.31	7.32

*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 6.63 differs from the reported value 3.6 by more than 10 %

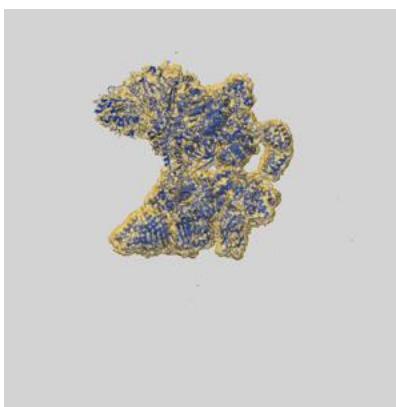
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56253 and PDB model 9TU9. Per-residue inclusion information can be found in section [3](#) on page [5](#).

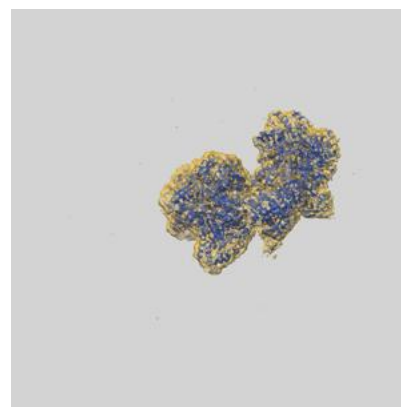
9.1 Map-model overlay [i](#)



X



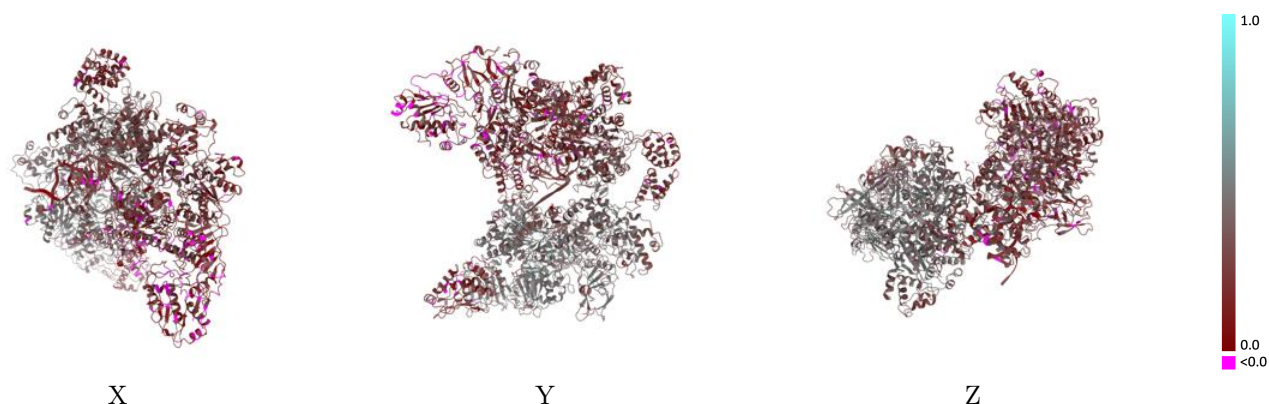
Y



Z

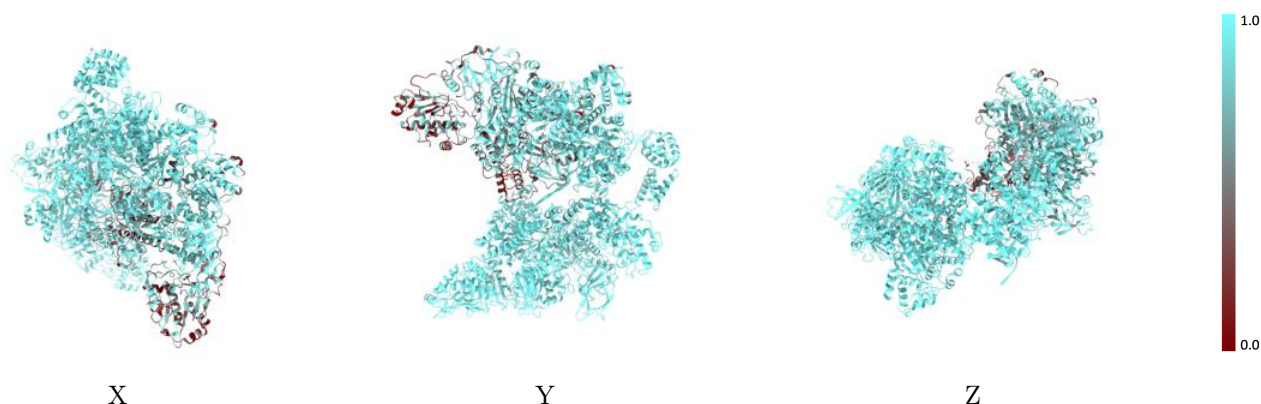
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



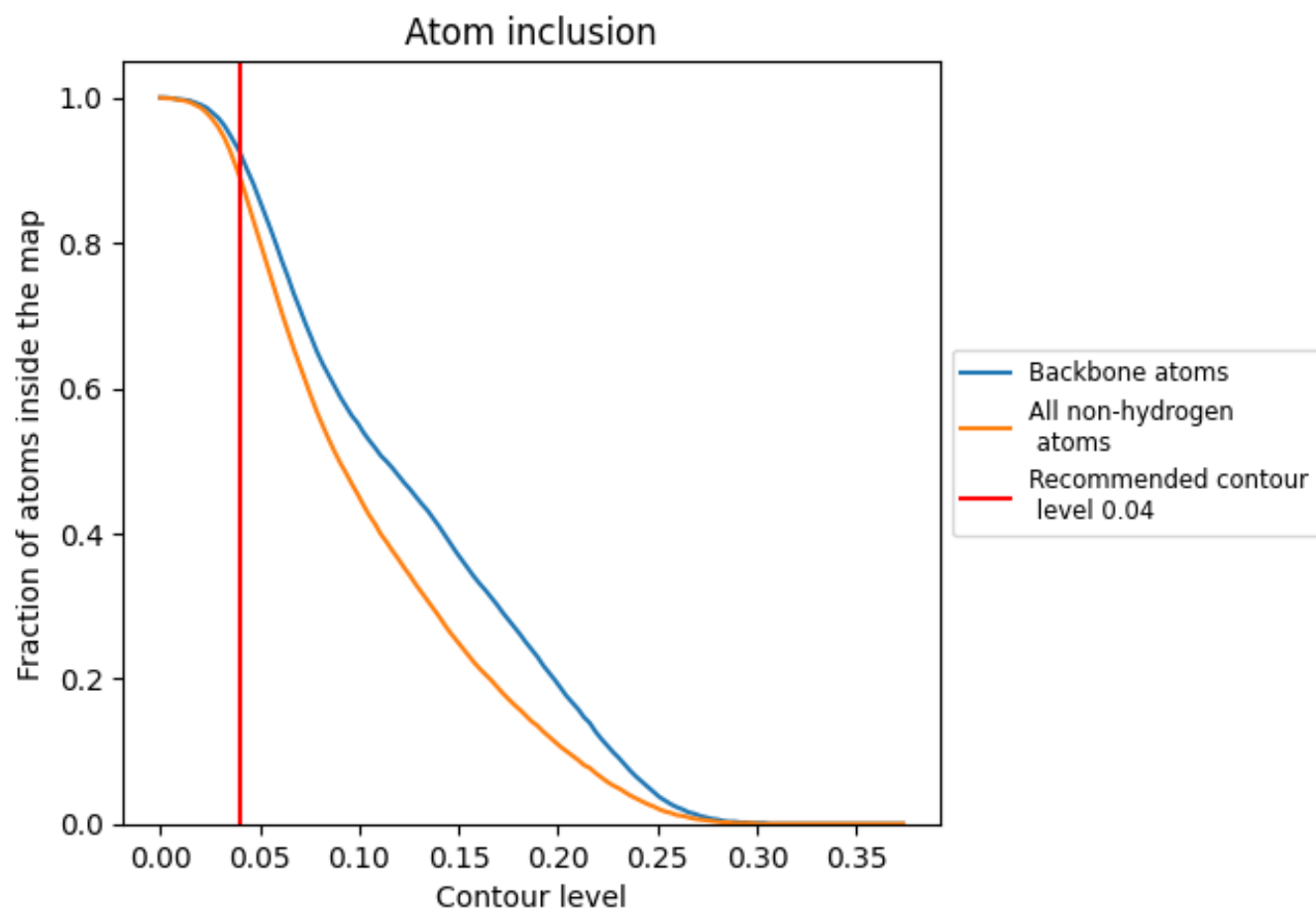
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 89% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8910	0.3130
G	0.9380	0.2590
I	0.9400	0.2340
Y	0.9890	0.3870
y	0.7890	0.2420

