



Full wwPDB EM Validation Report ⓘ

Dec 8, 2025 – 02:00 PM EST

PDB ID : 9MFW / pdb_00009mfw
EMDB ID : EMD-48240
Title : Motor domain with ADP AAA1 and ADP AAA3 from yeast full-length dynein-1 in 0.1 mM ATP condition
Authors : Geohring, I.C.; Chai, P.; Iyer, B.R.
Deposited on : 2024-12-10
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.47

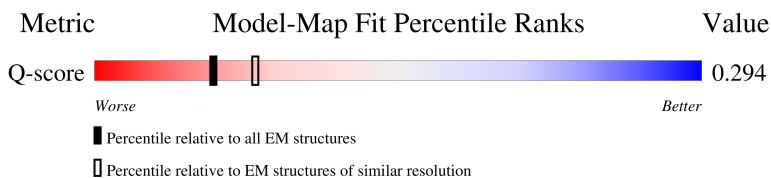
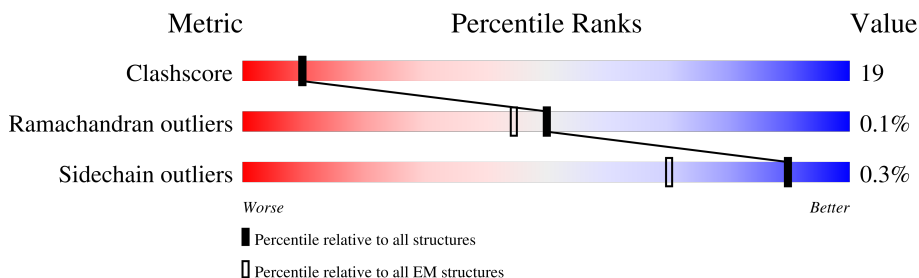
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

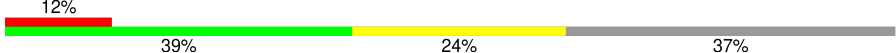
The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	6458 (3.60 - 4.60)

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

Mol	Chain	Length	Quality of chain
1	A	4092	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 21037 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 Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2583	20925	13431	3476	3920	98	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0
2	A	1	27	10	5	10	2	0
2	A	1	27	10	5	10	2	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

L1310	Q1736	E1637	R1536	V1443	A1381	D1321	L1261	MET	LYS	ASN	ARG	VAL	GLN	ASP	THR
Q1811	K1737	E1637	F1537	H1444	Q1382	I1322	Q1262	HIS	HIS	ASN	ILE	ILE	LYS	ILE	ASN
R1815	N1738	V1640	Y1538	W1445	E1383	G1323	S1263	VAL	ARG	ASN	ARG	VAL	GLU	ALA	VAL
V1816	D1739	V1640	Y1538	W1446	E1384	G1323	D1264	ALA	ARG	ASN	ARG	VAL	GLU	ALA	VAL
V1817	T1740	Q1646	D1543	V1448	V1385	K1324	R1265	ALA	LYS	ASN	ARG	VAL	GLU	ALA	VAL
V1818	L1741	W1656	D1544	V1448	I1386	R1325	A1266	ALA	LYS	ASN	ARG	VAL	GLU	ALA	VAL
V1819	L1742	W1656	L1545	V1448	V1386	R1325	A1266	ALA	LYS	ASN	ARG	VAL	GLU	ALA	VAL
F1820	D1743	W1660	L1546	V1448	H1388	Q1326	M1267	ALA	LYS	ASN	ARG	VAL	GLU	ALA	VAL
N1821	L1744	V1660	K1547	V1448	S1389	I1327	F1268	LYS	LYS	ASN	ARG	VAL	GLU	ALA	VAL
C1822	N1745	C1663	I1548	V1448	S1390	Q1328	F1269	LYS	LYS	ASN	ARG	VAL	GLU	ALA	VAL
D1823	S1746	C1663	G1550	V1448	G1391	K1329	R1270	ILE	ILE	ASN	ARG	VAL	GLU	ALA	VAL
D1824	V1747	L1664	S1551	V1448	L1392	L1331	R1271	PRO	PRO	ASN	ARG	VAL	GLU	ALA	VAL
S1825	I1748	N1667	H1554	V1448	L1393	L1332	A1272	VAL	VAL	ASN	ARG	VAL	GLU	ALA	VAL
F1826	S1750	N1667	H1555	V1448	L1394	L1332	D1273	VAL	VAL	ASN	ARG	VAL	GLU	ALA	VAL
D1827	L1755	S1670	H1556	V1448	V1395	D1333	E1274	ASN	ASN	ASN	ARG	VAL	GLU	ALA	VAL
Y1828	L1756	S1671	Q1557	V1448	R1396	D1334	L1275	ASP	ASP	ASN	ARG	VAL	GLU	ALA	VAL
Q1829	L1756	W1672	F1561	V1448	E1397	L1335	P1276	GLN	GLN	ASN	ARG	VAL	GLU	ALA	VAL
Q1830	Q1757	W1673	M1562	V1448	D1399	E1336	I1276	LEU	LEU	ASN	ARG	VAL	GLU	ALA	VAL
L1831	Y1758	K1674	K1563	V1448	V1400	F1337	A1277	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL
S1832	K1759	E1675	K1563	V1448	I1401	S1338	A1278	HIS	HIS	ASN	ARG	VAL	GLU	ALA	VAL
R1833	F1760	V1676	M1565	V1448	E1402	L1339	V1279	VAL	VAL	ASN	ARG	VAL	GLU	ALA	VAL
L1834	E1761	D1677	M1565	V1448	Q1403	K1340	K1280	VAL	VAL	ASN	ARG	VAL	GLU	ALA	VAL
L1835	Y1762	M1678	F1566	V1448	A1404	D1341	Q1281	GLU	GLU	ASN	ARG	VAL	GLU	ALA	VAL
I1838	I1765	K1679	I1569	V1448	C1405	V1342	Q1281	GLU	GLU	ASN	ARG	VAL	GLU	ALA	VAL
A1843	P1766	I1680	E1570	V1448	K1406	F1342	F1282	VAL	VAL	ASN	ARG	VAL	GLU	ALA	VAL
D1848	L1769	L1683	S1571	V1448	E1407	M1343	E1283	LYS	LYS	ASN	ARG	VAL	GLU	ALA	VAL
E1849	I1770	D1685	I1572	V1448	E1407	M1343	E1283	LYS	LYS	ASN	ARG	VAL	GLU	ALA	VAL
L1853	P1773	K1686	F1574	V1448	D1408	V1344	M1284	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL
K1855	I1777	M1688	L1493	V1448	L1409	L1346	Y1285	ASP	ASP	ASN	ARG	VAL	GLU	ALA	VAL
V1857	T1781	E1576	D1494	V1448	E1411	N1346	K1286	VAL	VAL	ASN	ARG	VAL	GLU	ALA	VAL
L1858	L1782	D1577	E1576	V1448	L1412	L1347	S1287	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL
N1864	T1783	F1578	F1578	V1448	L1413	T1348	L1288	ASP	ASP	ASN	ARG	VAL	GLU	ALA	VAL
I1865	D1784	V1582	V1582	V1448	N1350	L1349	F1289	SER	SER	ASN	ARG	VAL	GLU	ALA	VAL
L1868	S1785	E1586	E1586	V1448	E1351	E1351	Q1291	ILE	ILE	ASN	ARG	VAL	GLU	ALA	VAL
Q1869	L1786	G1587	G1587	V1448	I1352	I1352	V1292	PRO	PRO	ASN	ARG	VAL	GLU	ALA	VAL
K1789	H1787	E1588	E1588	V1448	L1353	L1353	M1293	GLU	GLU	ASN	ARG	VAL	GLU	ALA	VAL
L1872	Q1788	L1592	L1592	V1448	S1418	L1354	M1294	ALA	ALA	ASN	ARG	VAL	GLU	ALA	VAL
Q1873	Y1790	L1592	L1592	V1448	N1419	L1355	L1295	ASP	ASP	ASN	ARG	VAL	GLU	ALA	VAL
F1794	Y1794	D1600	D1600	V1448	Y1420	K1356	T1296	LYS	LYS	ASN	ARG	VAL	GLU	ALA	VAL
F1795	F1795	Q1603	Q1603	V1448	Y1421	I1357	S1297	ILE	ILE	ASN	ARG	VAL	GLU	ALA	VAL
G1796	G1796	A1604	A1604	V1448	K1422	I1357	S1297	PHE	PHE	ASN	ARG	VAL	GLU	ALA	VAL
T1800	T1800	Q1605	Q1605	V1448	F1423	E1359	M1299	ASP	ASP	ASN	ARG	VAL	GLU	ALA	VAL
G1801	G1801	E1606	E1606	V1448	F1424	E1359	M1299	GLU	GLU	ASN	ARG	VAL	GLU	ALA	VAL
K1802	K1802	W1607	W1607	V1448	E1425	R1360	K1300	GLU	GLU	ASN	ARG	VAL	GLU	ALA	VAL
T1803	T1803	L1608	L1608	V1448	Q1426	A1361	I1301	ILE	ILE	ASN	ARG	VAL	GLU	ALA	VAL
E1804	E1804	N1609	N1609	V1448	D1427	Q1362	L1302	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL
T1805	T1805	L1611	L1611	V1448	C1428	K1363	V1303	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL
K1807	K1807	L1611	L1611	V1448	L1429	E1364	E1304	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL
A1806	A1806	R1529	R1529	V1448	F1365	F1365	L1305	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL
F1809	F1809	Q1533	Q1533	V1448	L1431	V1366	K1306	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL
		F1534	F1534	V1448	E1432	I1367	D1307	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL
		P1535	P1535	V1448	E1432	E1368	G1308	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL
				V1448	L1435	K1369	A1309	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL
				V1448	L1436	S1370	L1310	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL
				V1448	S1439	L1371	K1311	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL
				V1448	E1440	N1372	P1312	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL
				V1448	I1441	R1373	R1313	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL
				V1448	Q1442	I1374	H1314	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL
				V1448		K1375	H1315	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL
				V1448		F1376	N1316	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL
				V1448		F1377	M1317	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL
				V1448		W1378	I1318	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL
				V1448		K1379	F1319	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL
				V1448		E1380	R1320	THR	THR	ASN	ARG	VAL	GLU	ALA	VAL





S4037	E4038	E4039	R4044	L4049	S4050	M4051	T4052	S4058	M4062	L4063	Q4064	L4065	Y4073	E4074	R4075	K4079	E4080	Y4081	A4082	S4083	S4084	T4085	E4086	L4089	Q4090	E4091	M4092

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53499	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.881	Depositor
Minimum map value	-0.306	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	333.312, 333.312, 333.312	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.302, 1.302, 1.302	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: ATP, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/21346	0.37	0/28844

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1373	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20925	0	21047	810	0
2	A	81	0	36	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	12	5	0
All	All	21037	0	21095	810	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 19.

All (810) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:GLU:CG	1:A:1420:TYR:CD2	1.83	1.62
1:A:1364:GLU:CD	1:A:1420:TYR:C	1.84	1.46
1:A:1364:GLU:HG3	1:A:1420:TYR:CD2	1.41	1.42
1:A:1364:GLU:CD	1:A:1420:TYR:O	1.66	1.39
1:A:1364:GLU:CG	1:A:1420:TYR:O	1.69	1.38
1:A:1367:ILE:HG23	1:A:1415:MET:CE	1.51	1.37
1:A:1364:GLU:OE1	1:A:1421:TYR:CA	1.76	1.32
1:A:1364:GLU:HG3	1:A:1420:TYR:CE2	1.69	1.27
1:A:1313:ARG:NH1	1:A:1423:ILE:HG23	1.49	1.25
1:A:1364:GLU:CG	1:A:1420:TYR:CG	2.20	1.25
1:A:1313:ARG:CZ	1:A:1423:ILE:HG23	1.70	1.20
1:A:1364:GLU:HG2	1:A:1420:TYR:CG	1.77	1.20
1:A:1360:ARG:O	1:A:1420:TYR:CD2	1.99	1.14
1:A:1367:ILE:HD11	1:A:1418:SER:CB	1.78	1.12
1:A:1364:GLU:HG2	1:A:1420:TYR:CD2	1.66	1.11
1:A:1363:LYS:HB3	1:A:1419:ASN:OD1	1.54	1.08
1:A:1364:GLU:HG2	1:A:1420:TYR:O	1.46	1.07
1:A:1364:GLU:HG3	1:A:1420:TYR:CG	1.87	1.07
1:A:1364:GLU:CD	1:A:1421:TYR:HA	1.79	1.06
1:A:1367:ILE:HG21	1:A:1424:PHE:CZ	1.90	1.06
1:A:1367:ILE:HD11	1:A:1418:SER:OG	1.56	1.05
1:A:1367:ILE:CG2	1:A:1424:PHE:CZ	2.39	1.05
1:A:1367:ILE:HG23	1:A:1415:MET:HE2	1.37	1.04
1:A:1364:GLU:OE2	1:A:1420:TYR:C	1.97	1.04
1:A:1364:GLU:CD	1:A:1421:TYR:N	2.16	1.03
1:A:1364:GLU:OE2	1:A:1421:TYR:N	1.93	1.02
1:A:1364:GLU:OE1	1:A:1421:TYR:HA	0.84	1.01
1:A:1367:ILE:HD13	1:A:1421:TYR:CB	1.90	1.00
1:A:1367:ILE:HG23	1:A:1415:MET:HE3	1.43	0.98
1:A:1364:GLU:CD	1:A:1421:TYR:CA	2.34	0.98
1:A:1360:ARG:HG2	1:A:1420:TYR:HB2	1.41	0.98
1:A:1360:ARG:HG2	1:A:1420:TYR:CB	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1367:ILE:CG2	1:A:1424:PHE:HZ	1.77	0.92
1:A:1367:ILE:HD13	1:A:1421:TYR:HB2	1.53	0.90
1:A:1367:ILE:CG2	1:A:1415:MET:CE	2.46	0.89
1:A:3617:GLU:HB3	1:A:3671:VAL:HG11	1.53	0.89
1:A:1360:ARG:HG2	1:A:1420:TYR:CG	2.08	0.88
1:A:1364:GLU:CB	1:A:1420:TYR:CD2	2.56	0.88
1:A:1313:ARG:NH1	1:A:1423:ILE:CG2	2.35	0.88
1:A:1367:ILE:CD1	1:A:1421:TYR:HB3	2.03	0.87
1:A:1360:ARG:O	1:A:1420:TYR:HD2	1.54	0.86
1:A:1364:GLU:HG2	1:A:1420:TYR:CB	2.05	0.85
1:A:3569:GLU:HG3	1:A:3583:LEU:HD21	1.58	0.85
1:A:3395:SER:O	1:A:3399:ASN:HB2	1.78	0.82
1:A:1367:ILE:HD13	1:A:1421:TYR:HB3	1.63	0.81
1:A:1367:ILE:HG21	1:A:1424:PHE:CE1	2.16	0.80
1:A:2269:SER:HB2	1:A:2326:LEU:HD21	1.63	0.80
1:A:1367:ILE:HG21	1:A:1424:PHE:HZ	1.34	0.79
1:A:3534:LEU:HB2	1:A:3542:GLN:HG2	1.64	0.79
1:A:3785:TYR:HA	1:A:3873:MET:HB2	1.62	0.79
1:A:2282:ASN:HB3	1:A:2552:ARG:HG3	1.66	0.78
1:A:1361:ALA:HA	1:A:1420:TYR:CE2	2.19	0.77
1:A:1367:ILE:HD11	1:A:1418:SER:HB2	1.67	0.77
1:A:1364:GLU:HG2	1:A:1420:TYR:C	2.08	0.76
1:A:1392:LEU:HD21	1:A:1483:TYR:HE2	1.50	0.76
1:A:1364:GLU:CG	1:A:1420:TYR:C	2.40	0.76
1:A:2135:ARG:HE	1:A:2184:LEU:HD21	1.51	0.76
1:A:2759:ILE:HD11	1:A:2894:PRO:HG3	1.66	0.76
1:A:2124:GLU:HB3	1:A:2126:ARG:HH21	1.52	0.75
1:A:3631:MET:HA	1:A:3634:LYS:HD2	1.68	0.75
1:A:1364:GLU:CG	1:A:1420:TYR:CE2	2.48	0.75
1:A:3330:TYR:HE1	1:A:3346:LEU:HD21	1.52	0.75
1:A:1364:GLU:OE1	1:A:1420:TYR:O	2.04	0.75
1:A:1363:LYS:CB	1:A:1419:ASN:OD1	2.34	0.75
1:A:1789:LYS:O	1:A:1873:GLN:NE2	2.20	0.74
1:A:1929:ILE:HD11	1:A:1970:LEU:HD11	1.67	0.74
1:A:3374:ASP:HA	1:A:3377:MET:HE2	1.68	0.74
1:A:1360:ARG:HD3	1:A:1420:TYR:CZ	2.13	0.73
1:A:2552:ARG:NH2	3:A:4102:ATP:O3G	2.22	0.73
1:A:1313:ARG:CZ	1:A:1423:ILE:CG2	2.59	0.72
1:A:2009:THR:HA	1:A:2012:LEU:HD12	1.71	0.72
1:A:2800:LYS:HE3	1:A:2843:LEU:HD23	1.72	0.72
1:A:3631:MET:HE1	1:A:3698:MET:HG2	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1714:GLN:HE22	1:A:1727:LEU:HD13	1.54	0.71
1:A:3521:ASN:O	1:A:3528:ARG:NH2	2.24	0.71
1:A:1367:ILE:CD1	1:A:1418:SER:CB	2.66	0.70
1:A:1367:ILE:HD11	1:A:1418:SER:HG	1.53	0.70
1:A:1364:GLU:CB	1:A:1420:TYR:O	2.39	0.70
1:A:1551:SER:O	1:A:1557:GLN:NE2	2.24	0.70
1:A:2275:ILE:HG22	1:A:2276:LEU:HD12	1.73	0.70
1:A:4035:GLN:HE22	1:A:4037:SER:HB3	1.56	0.70
1:A:4033:LEU:HD21	1:A:4035:GLN:HE21	1.54	0.70
1:A:2040:ASP:HB3	1:A:2044:ARG:HH21	1.58	0.69
1:A:2744:ARG:HD3	1:A:2915:ASN:HD21	1.58	0.69
1:A:1905:ARG:NH1	1:A:1906:SER:O	2.26	0.68
1:A:1908:LEU:O	1:A:1913:LYS:NZ	2.26	0.68
1:A:3527:THR:HG23	1:A:3528:ARG:HD3	1.75	0.68
1:A:2084:TRP:HA	1:A:2087:VAL:HG12	1.74	0.68
1:A:2637:PRO:HD3	1:A:2703:ASP:HB3	1.76	0.68
1:A:1313:ARG:HH12	1:A:1423:ILE:HA	1.59	0.68
1:A:1364:GLU:HG3	1:A:1420:TYR:CZ	2.27	0.68
1:A:3741:ASN:OD1	1:A:3745:ARG:NH1	2.26	0.68
1:A:3350:LYS:HA	1:A:3353:LEU:HD12	1.75	0.68
1:A:1392:LEU:HD21	1:A:1483:TYR:CE2	2.29	0.67
1:A:2226:ILE:HD11	1:A:2284:LEU:HD22	1.76	0.67
1:A:2441:VAL:HB	1:A:2484:LEU:HA	1.76	0.67
1:A:2763:ARG:NH1	1:A:3511:SER:O	2.27	0.67
1:A:2468:SER:OG	1:A:2469:LYS:NZ	2.28	0.67
1:A:1685:ASP:O	1:A:1689:LYS:NZ	2.27	0.67
1:A:2177:THR:HA	1:A:2183:ARG:HD2	1.77	0.67
1:A:3629:PHE:HZ	1:A:3646:ILE:HG13	1.60	0.66
1:A:2127:ASP:O	1:A:2131:THR:OG1	2.12	0.66
1:A:3800:LEU:HG	1:A:3811:LEU:HD11	1.77	0.66
1:A:1364:GLU:CA	1:A:1420:TYR:O	2.44	0.66
1:A:2921:ASP:O	1:A:2924:THR:OG1	2.13	0.66
1:A:2650:TYR:HB2	1:A:2694:LEU:HD23	1.78	0.66
1:A:2762:SER:O	1:A:2988:SER:OG	2.13	0.66
1:A:2563:SER:OG	1:A:2564:GLY:N	2.27	0.65
1:A:2600:TYR:CZ	1:A:2604:LYS:HD2	2.31	0.65
1:A:3464:ARG:HH21	1:A:3481:ILE:HA	1.60	0.65
1:A:2549:ARG:NH1	3:A:4102:ATP:O2G	2.30	0.65
1:A:2106:THR:H	1:A:2156:SER:HB3	1.61	0.65
1:A:3330:TYR:CE1	1:A:3346:LEU:HD21	2.30	0.65
1:A:1815:ARG:HH22	1:A:1891:HIS:HB3	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1910:GLU:HA	1:A:1913:LYS:HD3	1.79	0.65
1:A:2118:MET:HA	1:A:2125:TRP:HA	1.78	0.65
1:A:3707:LYS:HA	1:A:3710:ILE:HG22	1.78	0.65
1:A:2174:LYS:HG3	1:A:2186:ILE:HG13	1.79	0.64
1:A:1562:MET:HA	1:A:1565:MET:HG3	1.78	0.64
1:A:4022:GLN:NE2	1:A:4024:VAL:O	2.29	0.64
1:A:3713:GLU:HA	1:A:3716:LYS:HE2	1.79	0.64
1:A:2333:GLU:HA	1:A:2336:ARG:HE	1.62	0.64
1:A:2446:SER:HG	1:A:2449:THR:HG1	1.37	0.64
1:A:1572:ILE:HG22	1:A:1582:VAL:HG12	1.78	0.64
1:A:1313:ARG:NH1	1:A:1423:ILE:HA	2.12	0.64
1:A:2286:THR:OG1	1:A:2412:ARG:NH1	2.31	0.64
1:A:1964:ASN:OD1	1:A:1965:HIS:N	2.32	0.64
1:A:4081:VAL:O	1:A:4085:THR:HG23	1.98	0.64
1:A:3547:ASP:HA	1:A:3550:LYS:HE3	1.80	0.63
1:A:1364:GLU:CG	1:A:1420:TYR:HD2	1.97	0.63
1:A:2836:ALA:O	1:A:2911:ARG:NH2	2.31	0.63
1:A:1853:LEU:HB2	1:A:1858:LEU:HD12	1.80	0.63
1:A:2723:PHE:CZ	1:A:2772:PHE:HA	2.34	0.63
1:A:3859:VAL:O	1:A:3891:ARG:NH1	2.32	0.63
1:A:3742:ASN:OD1	1:A:3745:ARG:NH2	2.30	0.63
1:A:3800:LEU:HD23	1:A:3840:LEU:HD22	1.81	0.63
1:A:2225:LYS:NZ	1:A:2281:PHE:O	2.32	0.62
1:A:3694:PHE:HA	1:A:3697:ILE:HG12	1.80	0.62
1:A:3312:GLN:HA	1:A:3315:LYS:HE3	1.80	0.62
1:A:3634:LYS:NZ	1:A:4092:MET:SD	2.72	0.62
1:A:1367:ILE:HG23	1:A:1415:MET:HE1	1.70	0.62
1:A:3862:THR:O	1:A:3891:ARG:NH2	2.32	0.62
1:A:2056:LYS:NZ	1:A:2214:TRP:O	2.30	0.62
1:A:2336:ARG:HA	1:A:2339:ILE:HD12	1.82	0.62
1:A:1756:LEU:HD11	1:A:1786:LEU:HD22	1.82	0.62
1:A:1367:ILE:CD1	1:A:1421:TYR:CB	2.63	0.61
1:A:1388:HIS:CD2	1:A:1394:LEU:HD23	2.35	0.61
1:A:4063:LEU:HB3	1:A:4065:LEU:HD23	1.82	0.61
1:A:2940:PHE:O	1:A:3318:GLN:NE2	2.30	0.61
1:A:4030:PRO:HD2	1:A:4044:ARG:HH12	1.65	0.61
1:A:2081:THR:N	3:A:4102:ATP:O2B	2.23	0.61
1:A:3621:ILE:HG12	1:A:3675:LEU:HD13	1.82	0.61
1:A:3823:ASN:HA	1:A:3826:GLN:HG2	1.82	0.61
1:A:3711:GLU:O	1:A:3716:LYS:NZ	2.33	0.61
1:A:2606:ARG:NH1	1:A:2668:SER:OG	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:GLU:HA	1:A:1420:TYR:O	2.00	0.61
1:A:1364:GLU:HB2	1:A:1420:TYR:CD2	2.35	0.61
1:A:1674:LYS:O	1:A:1678:MET:HG2	2.01	0.61
1:A:3306:TRP:O	1:A:3309:THR:OG1	2.19	0.61
1:A:2245:GLU:OE2	1:A:2299:ARG:NH1	2.34	0.61
1:A:2971:HIS:HB3	1:A:3352:LEU:HD11	1.81	0.61
1:A:3305:ARG:HH11	1:A:3308:ASN:HB3	1.66	0.61
1:A:1694:VAL:O	1:A:1698:ILE:HD12	2.01	0.60
1:A:3523:GLU:O	1:A:3528:ARG:NH2	2.28	0.60
1:A:3596:ASN:OD1	1:A:3599:LYS:NZ	2.29	0.60
1:A:2612:GLN:HE22	1:A:2661:VAL:HG13	1.66	0.60
1:A:3319:GLU:HB2	1:A:3360:TYR:HA	1.83	0.60
1:A:2423:GLY:O	1:A:2427:ILE:HG12	2.01	0.60
1:A:2810:GLU:OE1	1:A:2884:ASN:ND2	2.33	0.60
1:A:3665:ARG:H	1:A:3676:TRP:HZ3	1.48	0.60
1:A:1364:GLU:HB2	1:A:1420:TYR:CE2	2.37	0.60
1:A:3431:PHE:HD2	1:A:3454:ASP:HB2	1.66	0.60
1:A:1911:ASN:HB3	1:A:3846:MET:HB2	1.84	0.60
1:A:2100:VAL:HB	1:A:2150:ILE:HA	1.82	0.60
1:A:2857:ARG:HH12	1:A:2873:LEU:HD11	1.66	0.60
1:A:1865:ILE:HD11	1:A:1894:VAL:HG11	1.84	0.60
1:A:2075:LYS:NZ	1:A:2215:PHE:O	2.35	0.60
1:A:2252:LEU:O	1:A:2256:SER:HB3	2.02	0.60
1:A:3021:LEU:HD13	1:A:3307:LEU:HG	1.82	0.60
1:A:3743:ASP:HB2	1:A:3762:TRP:HZ2	1.65	0.60
1:A:1367:ILE:HG22	1:A:1424:PHE:CZ	2.33	0.60
1:A:2115:TYR:HE1	1:A:2166:MET:HE2	1.67	0.60
1:A:3506:PRO:HD2	1:A:3509:LEU:HD21	1.83	0.59
1:A:1692:ASP:HA	1:A:1695:LYS:HB2	1.85	0.59
1:A:2481:ASN:OD1	1:A:2528:ARG:NH1	2.35	0.59
1:A:2455:LEU:HG	1:A:2459:HIS:CE1	2.38	0.59
1:A:3509:LEU:O	1:A:3513:VAL:N	2.34	0.59
1:A:3728:GLU:HG2	1:A:4075:ARG:HH22	1.66	0.59
1:A:1800:THR:N	2:A:4101:ADP:O2A	2.36	0.59
1:A:2068:GLN:HG2	1:A:2174:LYS:HE3	1.84	0.59
1:A:3611:PHE:O	1:A:3615:VAL:HG13	2.03	0.59
1:A:3707:LYS:HB3	1:A:3715:TYR:HE2	1.68	0.59
1:A:3693:LYS:HG3	1:A:4081:VAL:HG12	1.85	0.58
1:A:1703:VAL:HG13	1:A:1770:ILE:HD12	1.85	0.58
1:A:1748:PHE:HA	1:A:1758:TYR:H	1.68	0.58
1:A:1822:CYS:SG	1:A:1853:LEU:HD21	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1360:ARG:HD3	1:A:1420:TYR:CE2	2.38	0.58
1:A:2414:ILE:HG23	1:A:2532:VAL:HG23	1.85	0.58
1:A:3476:ARG:NH2	1:A:3487:ASP:OD1	2.35	0.58
1:A:2822:ILE:HA	1:A:2827:PHE:HE2	1.68	0.58
1:A:1538:TYR:O	1:A:1833:ARG:NE	2.36	0.58
1:A:2766:LYS:NZ	1:A:2891:ILE:O	2.34	0.58
1:A:1258:VAL:HG11	1:A:1303:VAL:HA	1.84	0.58
1:A:1301:ILE:HD13	1:A:1347:LEU:HB3	1.85	0.58
1:A:1787:HIS:ND1	1:A:1788:GLN:OE1	2.29	0.58
1:A:2400:HIS:HA	1:A:2403:ILE:HG22	1.84	0.58
1:A:2733:VAL:HG11	1:A:2928:VAL:HA	1.86	0.58
1:A:3302:GLU:O	1:A:3591:LYS:NZ	2.32	0.57
1:A:2934:ASP:HA	1:A:2962:ARG:HH22	1.70	0.57
1:A:2422:SER:OG	1:A:2424:LYS:NZ	2.37	0.57
1:A:4022:GLN:NE2	1:A:4027:VAL:O	2.37	0.57
1:A:2870:GLU:HA	1:A:2873:LEU:HD12	1.84	0.57
1:A:3447:GLY:HA3	1:A:3489:SER:HB3	1.84	0.57
1:A:1445:TRP:HA	1:A:1448:VAL:HG22	1.86	0.57
1:A:1360:ARG:C	1:A:1420:TYR:CD2	2.82	0.57
1:A:2681:LEU:HD12	1:A:2682:PRO:HD2	1.87	0.57
1:A:1608:LEU:HD23	1:A:1611:LEU:HD21	1.85	0.57
1:A:2639:GLN:OE1	1:A:2643:SER:OG	2.22	0.57
1:A:2759:ILE:HA	1:A:2891:ILE:HG22	1.86	0.57
1:A:3384:LEU:HD21	1:A:3394:MET:HE3	1.86	0.57
1:A:1360:ARG:HD3	1:A:1420:TYR:CD2	2.39	0.57
1:A:3644:ILE:HD11	1:A:3686:PHE:CE2	2.40	0.57
1:A:1402:GLU:OE1	1:A:1442:GLN:HB3	2.04	0.56
1:A:2060:PHE:HE1	1:A:2072:LEU:HD21	1.70	0.56
1:A:2517:LYS:HB3	1:A:2520:GLU:HB3	1.85	0.56
1:A:3330:TYR:HE2	1:A:3364:TYR:HE2	1.51	0.56
1:A:3960:ASP:OD2	1:A:3997:LYS:NZ	2.38	0.56
1:A:1504:ASN:O	1:A:1508:THR:OG1	2.20	0.56
1:A:2500:GLN:HE22	1:A:2502:VAL:HG22	1.70	0.56
1:A:2081:THR:OG1	3:A:4102:ATP:O2A	2.23	0.56
1:A:2088:ILE:HG12	1:A:2099:ASN:ND2	2.20	0.56
1:A:2229:LEU:HB3	1:A:2288:VAL:HG11	1.85	0.56
1:A:2823:LEU:HD12	1:A:2824:GLU:HG3	1.86	0.56
1:A:1607:TRP:HA	1:A:1610:ILE:HG22	1.88	0.56
1:A:2792:LEU:HD11	1:A:2830:ARG:HG3	1.87	0.56
1:A:2523:TRP:HE1	1:A:2525:THR:HG22	1.70	0.56
1:A:1603:GLN:N	1:A:1606:GLU:OE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1664:LEU:O	1:A:1721:LYS:NZ	2.39	0.56
1:A:3315:LYS:HA	1:A:3359:LYS:HZ1	1.70	0.56
1:A:1396:ARG:HH22	1:A:2122:THR:HB	1.70	0.56
1:A:1801:GLY:O	1:A:1805:THR:N	2.38	0.56
1:A:2689:ILE:HD12	1:A:2694:LEU:HD11	1.87	0.56
1:A:2822:ILE:HD11	1:A:2828:LEU:HB2	1.87	0.56
1:A:1569:ILE:HG21	1:A:1582:VAL:HB	1.87	0.56
1:A:1367:ILE:CG2	1:A:1415:MET:HE3	2.25	0.56
1:A:2166:MET:O	1:A:2170:LEU:N	2.31	0.56
1:A:3430:SER:HB3	1:A:3433:GLU:HG2	1.88	0.56
1:A:3844:ILE:HG13	1:A:3875:MET:HB3	1.88	0.56
1:A:2640:THR:HG23	1:A:2643:SER:H	1.71	0.55
1:A:3826:GLN:HB3	1:A:3850:TRP:HZ2	1.71	0.55
1:A:1364:GLU:HG3	1:A:1420:TYR:CD1	2.39	0.55
1:A:1458:ILE:HG21	1:A:1523:LEU:HD21	1.88	0.55
1:A:2742:ILE:HG23	1:A:2773:VAL:HG22	1.88	0.55
1:A:3406:PHE:HB3	1:A:3515:LEU:HA	1.87	0.55
1:A:1504:ASN:OD1	1:A:1507:THR:OG1	2.24	0.55
1:A:3524:SER:HB3	1:A:3528:ARG:HH12	1.71	0.55
1:A:3845:GLN:HG2	1:A:3881:GLY:HA3	1.89	0.55
1:A:1784:ASP:OD2	1:A:3988:HIS:NE2	2.36	0.55
1:A:3844:ILE:HG23	1:A:3851:VAL:HG11	1.87	0.55
1:A:3934:TRP:HE1	1:A:4049:LEU:HD21	1.70	0.55
1:A:2289:GLN:NE2	1:A:2410:SER:O	2.32	0.54
1:A:3819:ILE:HA	1:A:3822:LEU:HD12	1.89	0.54
1:A:2163:VAL:O	1:A:2167:ASN:N	2.41	0.54
1:A:3690:LEU:HD12	1:A:3694:PHE:HB3	1.90	0.54
1:A:1241:LEU:HD22	1:A:1275:LEU:HD21	1.89	0.54
1:A:3987:ASP:O	1:A:3991:THR:OG1	2.20	0.54
1:A:2169:VAL:HG13	1:A:2186:ILE:HD13	1.90	0.54
1:A:1687:LEU:HD12	1:A:1695:LYS:HG2	1.90	0.54
1:A:1986:GLU:OE2	1:A:2030:ASN:ND2	2.41	0.54
1:A:1364:GLU:CB	1:A:1420:TYR:CE2	2.87	0.54
1:A:1562:MET:HE1	1:A:1569:ILE:HB	1.89	0.54
1:A:2081:THR:HA	1:A:2084:TRP:NE1	2.22	0.54
1:A:3542:GLN:HA	1:A:3545:ARG:HE	1.72	0.54
1:A:1745:ASN:O	1:A:1757:GLN:NE2	2.40	0.54
1:A:3654:LYS:O	1:A:3654:LYS:NZ	2.39	0.54
1:A:1360:ARG:CG	1:A:1420:TYR:CG	2.69	0.54
1:A:1404:ALA:O	1:A:1407:GLU:HG2	2.08	0.54
1:A:2612:GLN:HE22	1:A:2661:VAL:CG1	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:GLU:OE2	1:A:1421:TYR:CA	2.50	0.54
1:A:2828:LEU:HD13	1:A:2902:MET:HE1	1.89	0.54
1:A:1360:ARG:O	1:A:1420:TYR:CG	2.59	0.53
1:A:1387:GLU:HB2	1:A:1393:LYS:HZ3	1.73	0.53
1:A:3338:ASN:HD22	1:A:3523:GLU:HG2	1.73	0.53
1:A:3815:PRO:O	1:A:3821:ASN:ND2	2.35	0.53
1:A:1361:ALA:HA	1:A:1420:TYR:HE2	1.70	0.53
1:A:1489:ARG:O	1:A:1489:ARG:NH1	2.41	0.53
1:A:1884:GLU:OE1	1:A:1885:GLU:N	2.41	0.53
1:A:1935:GLN:HG2	1:A:1939:PHE:CE1	2.43	0.53
1:A:2773:VAL:HA	1:A:2776:LEU:HD12	1.91	0.53
1:A:3579:GLU:O	1:A:3583:LEU:HD23	2.09	0.53
1:A:1864:ASN:HB3	1:A:1881:LEU:HD21	1.90	0.53
1:A:2080:LYS:NZ	1:A:2196:THR:O	2.41	0.53
1:A:2444:ASN:HA	1:A:2487:ASP:HB2	1.91	0.53
1:A:2934:ASP:OD1	1:A:2962:ARG:NH1	2.41	0.53
1:A:2060:PHE:CD2	1:A:2087:VAL:HG11	2.42	0.53
1:A:1557:GLN:OE1	1:A:1557:GLN:N	2.31	0.53
1:A:1804:GLU:N	1:A:1804:GLU:OE1	2.41	0.53
1:A:2646:ARG:HH12	1:A:2687:GLY:H	1.56	0.53
1:A:2830:ARG:HH21	1:A:2840:ILE:HD12	1.73	0.53
1:A:3303:LYS:HD3	1:A:3587:LEU:HD22	1.90	0.53
1:A:3325:ILE:O	1:A:3329:ILE:HD12	2.09	0.53
1:A:1663:CYS:O	1:A:1667:ASN:N	2.34	0.53
1:A:1865:ILE:HA	1:A:1868:ILE:HG22	1.91	0.53
1:A:1998:LEU:HD13	1:A:2002:ILE:HD13	1.90	0.53
1:A:2536:ASN:OD1	1:A:2543:ARG:NH2	2.42	0.53
1:A:1586:GLU:OE2	1:A:1765:ILE:N	2.42	0.53
1:A:2621:GLU:N	1:A:2621:GLU:OE1	2.42	0.53
1:A:2792:LEU:HD22	1:A:2826:ALA:HB1	1.91	0.53
1:A:2920:TRP:HB3	1:A:2924:THR:OG1	2.09	0.52
1:A:3463:SER:HA	1:A:3466:ILE:HG22	1.91	0.52
1:A:1543:ASP:OD1	1:A:1544:ASP:N	2.43	0.52
1:A:2419:PRO:HD3	1:A:2558:TYR:HE1	1.74	0.52
1:A:1555:HIS:NE2	1:A:1577:ASP:OD1	2.42	0.52
1:A:3394:MET:HA	1:A:3397:VAL:HG12	1.91	0.52
1:A:1379:LYS:HD2	1:A:1380:GLU:HG3	1.91	0.52
1:A:1872:LEU:HD22	1:A:1888:LEU:HD21	1.91	0.52
1:A:1438:LEU:HD11	1:A:1497:ILE:HA	1.92	0.52
1:A:1773:PRO:O	1:A:1777:ILE:HD12	2.10	0.52
1:A:1828:TYR:OH	1:A:1864:ASN:ND2	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2757:MET:HB3	1:A:2914:ILE:HG22	1.92	0.52
1:A:2419:PRO:HD2	1:A:2422:SER:HB3	1.90	0.52
1:A:3408:LEU:HD11	1:A:3501:PRO:HB3	1.90	0.52
1:A:2107:LYS:HB2	1:A:2504:LEU:HD12	1.91	0.52
1:A:2932:MET:SD	1:A:2996:LEU:HD22	2.49	0.52
1:A:3384:LEU:HD11	1:A:3394:MET:HG2	1.92	0.52
1:A:2752:VAL:HG13	1:A:2753:GLN:HG2	1.92	0.52
1:A:3017:VAL:HG11	1:A:3313:PHE:HE2	1.75	0.52
1:A:1963:MET:HE1	1:A:1965:HIS:CD2	2.46	0.52
1:A:3986:ARG:HD2	1:A:4012:ALA:HA	1.92	0.52
1:A:1637:GLU:O	1:A:1640:VAL:HG22	2.10	0.51
1:A:2654:ARG:NH2	1:A:2658:ASP:OD1	2.37	0.51
1:A:3319:GLU:OE1	1:A:3361:ASP:N	2.43	0.51
1:A:3708:PHE:HA	1:A:3716:LYS:HG2	1.90	0.51
1:A:1917:ARG:HD3	1:A:3963:PHE:HE2	1.76	0.51
1:A:3788:MET:HB3	1:A:3876:THR:HA	1.92	0.51
1:A:1351:GLU:O	1:A:1355:THR:OG1	2.22	0.51
1:A:2780:LYS:O	1:A:2814:CYS:N	2.32	0.51
1:A:3509:LEU:O	1:A:3513:VAL:HG12	2.09	0.51
1:A:4082:ALA:O	1:A:4085:THR:OG1	2.16	0.51
1:A:1367:ILE:CG2	1:A:1424:PHE:CE1	2.83	0.51
1:A:1424:PHE:HB2	1:A:1427:ASP:HB3	1.92	0.51
1:A:1926:SER:HA	1:A:1929:ILE:HG12	1.91	0.51
1:A:2600:TYR:CG	1:A:2622:LEU:HD11	2.45	0.51
1:A:2294:LEU:HD11	1:A:2317:LEU:HB3	1.93	0.51
1:A:2893:ASP:OD2	1:A:2895:THR:OG1	2.28	0.51
1:A:2971:HIS:O	1:A:2974:ARG:NH1	2.44	0.51
1:A:2260:ALA:O	1:A:2263:THR:OG1	2.29	0.51
1:A:3593:GLU:HA	1:A:3596:ASN:HD22	1.76	0.51
1:A:4058:SER:HG	1:A:4062:TRP:CG	2.29	0.51
1:A:2619:PRO:HA	1:A:2622:LEU:HD13	1.93	0.51
1:A:2673:LEU:HD22	1:A:2689:ILE:HG21	1.91	0.51
1:A:2974:ARG:NH1	1:A:2975:ASN:HB2	2.26	0.51
1:A:3401:GLN:OE1	1:A:3401:GLN:N	2.44	0.51
1:A:3426:THR:HG23	1:A:3451:ILE:HD13	1.92	0.51
1:A:2759:ILE:HG23	1:A:2916:TRP:HA	1.92	0.51
1:A:1412:LEU:HD22	1:A:1435:LEU:HD12	1.93	0.51
1:A:1869:GLN:O	1:A:1873:GLN:HG2	2.11	0.51
1:A:2152:VAL:O	1:A:2193:LEU:N	2.39	0.51
1:A:2422:SER:HB2	1:A:2559:LEU:HD12	1.93	0.51
1:A:3454:ASP:HB3	1:A:3457:PHE:HD1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3948:HIS:HB2	1:A:4073:TYR:HD2	1.76	0.51
1:A:2697:SER:HB2	1:A:2743:LEU:HD22	1.93	0.50
1:A:3851:VAL:HA	1:A:3855:LEU:HB3	1.93	0.50
1:A:1927:GLY:HA2	1:A:1950:VAL:HG21	1.93	0.50
1:A:2661:VAL:HG12	1:A:2916:TRP:CD2	2.47	0.50
1:A:4051:ASN:OD1	1:A:4052:THR:N	2.44	0.50
1:A:2869:THR:O	1:A:2873:LEU:N	2.36	0.50
1:A:2259:MET:N	1:A:2259:MET:HE2	2.26	0.50
1:A:2824:GLU:HB2	1:A:2827:PHE:CE1	2.46	0.50
1:A:3330:TYR:CE2	1:A:3366:PHE:HB2	2.46	0.50
1:A:1398:TRP:HZ3	1:A:1446:VAL:HB	1.76	0.50
1:A:2280:THR:O	1:A:2284:LEU:HG	2.12	0.50
1:A:2674:TYR:HE1	1:A:2689:ILE:HG22	1.75	0.50
1:A:2930:ASN:OD1	1:A:2962:ARG:HD3	2.11	0.50
1:A:3741:ASN:ND2	1:A:3744:LEU:HD12	2.27	0.50
1:A:1604:ALA:HA	1:A:1607:TRP:NE1	2.27	0.50
1:A:2079:GLY:O	1:A:2083:THR:N	2.40	0.50
1:A:2538:PRO:HA	1:A:2543:ARG:HB2	1.93	0.50
1:A:2546:MET:HE2	1:A:2546:MET:HA	1.94	0.50
1:A:2968:ILE:HG13	1:A:3352:LEU:CD2	2.41	0.50
1:A:2475:PRO:HB3	1:A:2527:GLU:HB2	1.93	0.49
1:A:2891:ILE:HD11	1:A:2899:SER:HA	1.94	0.49
1:A:2567:LEU:HA	1:A:2570:ILE:HG22	1.94	0.49
1:A:3317:SER:HA	1:A:3320:LEU:HD23	1.94	0.49
1:A:3329:ILE:HG23	1:A:3333:TYR:HB2	1.94	0.49
1:A:2606:ARG:HH22	1:A:2671:GLN:HE22	1.60	0.49
1:A:2423:GLY:N	2:A:4103:ADP:O2A	2.36	0.49
1:A:2830:ARG:NH1	1:A:2842:ASP:OD2	2.46	0.49
1:A:2806:CYS:SG	1:A:2813:THR:OG1	2.65	0.49
1:A:3632:LEU:HB3	1:A:3644:ILE:HD13	1.94	0.49
1:A:2324:TYR:HB3	1:A:2403:ILE:HD11	1.93	0.49
1:A:2655:ILE:HD11	1:A:2747:ARG:HH22	1.78	0.49
1:A:2830:ARG:NH2	1:A:2842:ASP:OD1	2.44	0.49
1:A:2963:ASP:HA	1:A:2966:VAL:HG22	1.95	0.49
1:A:2690:SER:N	1:A:2693:SER:OG	2.46	0.49
1:A:1835:LEU:HD12	1:A:1838:ILE:HD11	1.95	0.49
1:A:1935:GLN:HA	1:A:1939:PHE:CD1	2.47	0.49
1:A:2695:LEU:HD11	1:A:2709:LYS:HE2	1.94	0.49
1:A:1314:HIS:HA	1:A:1317:MET:HE2	1.94	0.49
1:A:1371:LEU:HD13	1:A:1424:PHE:CE2	2.48	0.49
1:A:1592:LEU:HD11	1:A:1614:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2160:PRO:O	1:A:2164:GLU:N	2.46	0.49
1:A:1865:ILE:HD11	1:A:1894:VAL:HG21	1.95	0.49
1:A:2898:LYS:O	1:A:2902:MET:HG2	2.13	0.49
1:A:1313:ARG:HH12	1:A:1423:ILE:CA	2.26	0.48
1:A:2457:ALA:HA	1:A:2460:ARG:NE	2.27	0.48
1:A:3524:SER:C	1:A:3526:GLU:H	2.20	0.48
1:A:1365:PHE:HA	1:A:1368:GLU:HB3	1.95	0.48
1:A:3366:PHE:HE1	1:A:3370:LEU:HD12	1.78	0.48
1:A:2429:ASN:O	1:A:2433:ARG:HG2	2.14	0.48
1:A:2645:ILE:HD13	1:A:2681:LEU:HD21	1.95	0.48
1:A:3710:ILE:HG23	1:A:3711:GLU:HG2	1.95	0.48
1:A:3975:ASN:HD21	1:A:3980:ILE:HB	1.78	0.48
1:A:2575:TYR:O	1:A:2578:ILE:HG22	2.13	0.48
1:A:2167:ASN:O	1:A:2171:ASP:N	2.46	0.48
1:A:1420:TYR:CE1	1:A:1423:ILE:HD11	2.48	0.48
1:A:1572:ILE:HG13	1:A:1574:PHE:HE1	1.77	0.48
1:A:2738:MET:O	1:A:2742:ILE:HG13	2.13	0.48
1:A:2823:LEU:H	1:A:2827:PHE:HZ	1.61	0.48
1:A:2856:LEU:HD13	1:A:2873:LEU:HB3	1.96	0.48
1:A:2929:ALA:O	1:A:2932:MET:HG2	2.13	0.48
1:A:3799:LYS:O	1:A:3802:GLU:HG3	2.13	0.48
1:A:1941:ASP:OD2	1:A:1944:SER:HB2	2.14	0.48
1:A:3396:ILE:HD11	1:A:3516:VAL:HG23	1.96	0.48
1:A:3788:MET:HE1	1:A:3897:TYR:HB2	1.95	0.48
1:A:2822:ILE:HA	1:A:2827:PHE:CE2	2.46	0.48
1:A:3493:LYS:HB3	1:A:3495:PHE:CE1	2.49	0.48
1:A:1619:VAL:HG12	1:A:1760:PHE:HD2	1.78	0.48
1:A:1995:VAL:HG13	1:A:2018:LEU:HD11	1.95	0.48
1:A:2458:LEU:O	1:A:2462:THR:OG1	2.31	0.48
1:A:2935:VAL:HG13	1:A:2936:ILE:HG12	1.95	0.48
1:A:3714:GLN:NE2	1:A:3737:THR:OG1	2.47	0.48
1:A:3743:ASP:HB2	1:A:3762:TRP:CZ2	2.46	0.48
1:A:2129:LEU:HD11	1:A:2516:TRP:CD2	2.48	0.47
1:A:2492:PRO:HB2	1:A:2500:GLN:HG3	1.96	0.47
1:A:2218:ASP:OD1	1:A:2219:VAL:N	2.47	0.47
1:A:2230:LEU:HD21	1:A:2257:PHE:HZ	1.79	0.47
1:A:3312:GLN:O	1:A:3315:LYS:HG2	2.14	0.47
1:A:1743:ASP:O	1:A:1746:SER:OG	2.25	0.47
1:A:2008:ASP:OD1	1:A:2008:ASP:N	2.47	0.47
1:A:2072:LEU:HD13	1:A:2213:LEU:HB3	1.96	0.47
1:A:2407:LEU:HD12	1:A:2408:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3464:ARG:HE	1:A:3481:ILE:HD13	1.79	0.47
1:A:2456:SER:O	1:A:2460:ARG:HG3	2.14	0.47
1:A:2794:ASP:HA	1:A:2797:MET:SD	2.54	0.47
1:A:2975:ASN:HA	1:A:2978:GLN:HG2	1.95	0.47
1:A:3815:PRO:HA	1:A:3842:GLN:HG2	1.97	0.47
1:A:1918:GLU:OE1	1:A:1918:GLU:N	2.43	0.47
1:A:2285:GLU:HG3	1:A:2286:THR:N	2.30	0.47
1:A:1475:LYS:HE3	1:A:1515:SER:HB3	1.97	0.47
1:A:1545:LEU:HA	1:A:1548:ILE:HG12	1.95	0.47
1:A:2005:SER:OG	1:A:2212:LEU:O	2.32	0.47
1:A:3323:ASN:C	1:A:3323:ASN:HD22	2.23	0.47
1:A:1378:TRP:CZ2	1:A:1405:CYS:HB2	2.50	0.47
1:A:1676:VAL:O	1:A:1680:ILE:HG12	2.15	0.47
1:A:2661:VAL:HG12	1:A:2916:TRP:CE2	2.50	0.47
1:A:2046:GLY:O	1:A:2228:HIS:ND1	2.42	0.47
1:A:2088:ILE:O	1:A:2091:MET:HG2	2.15	0.47
1:A:2319:LYS:HB3	1:A:2353:LEU:HD22	1.95	0.47
1:A:2772:PHE:O	1:A:2776:LEU:HG	2.15	0.47
1:A:2857:ARG:NH1	1:A:2873:LEU:HD11	2.30	0.47
1:A:2930:ASN:OD1	1:A:2962:ARG:NH1	2.48	0.47
1:A:1364:GLU:CD	1:A:1423:ILE:CD1	2.89	0.46
1:A:1570:GLU:OE1	1:A:1570:GLU:N	2.48	0.46
1:A:1766:PRO:HG2	1:A:1811:GLN:CD	2.40	0.46
1:A:2851:LYS:HA	1:A:2854:ASN:ND2	2.29	0.46
1:A:2939:GLU:OE1	1:A:2961:ILE:HD13	2.14	0.46
1:A:1646:GLN:NE2	1:A:1762:TYR:HA	2.30	0.46
1:A:2160:PRO:HA	1:A:2163:VAL:HG22	1.98	0.46
1:A:3679:TYR:HD1	1:A:3702:MET:HE3	1.81	0.46
1:A:3975:ASN:OD1	1:A:3976:SER:N	2.48	0.46
1:A:3346:LEU:HD23	1:A:3346:LEU:HA	1.71	0.46
1:A:1981:SER:HA	1:A:1984:ILE:HD12	1.97	0.46
1:A:2315:THR:HA	1:A:2318:ILE:HG22	1.97	0.46
1:A:2952:LEU:HB2	1:A:3355:LYS:HZ1	1.79	0.46
1:A:3652:CYS:O	1:A:3656:VAL:HG23	2.16	0.46
1:A:2081:THR:HA	1:A:2084:TRP:CD1	2.51	0.46
1:A:2088:ILE:HD11	1:A:2151:TRP:CD1	2.51	0.46
1:A:2419:PRO:O	1:A:2424:LYS:NZ	2.48	0.46
1:A:2783:GLN:HB3	1:A:2816:ILE:HD11	1.97	0.46
1:A:3843:ASN:O	1:A:3846:MET:HG3	2.15	0.46
1:A:1750:SER:HB2	1:A:1755:LEU:HD13	1.96	0.46
1:A:1933:ILE:O	1:A:1936:ILE:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2176:LEU:HD23	1:A:2184:LEU:HB2	1.97	0.46
1:A:3541:MET:SD	1:A:3542:GLN:NE2	2.88	0.46
1:A:3640:TRP:HZ3	1:A:3884:LEU:HB2	1.78	0.46
1:A:1469:LEU:HB3	1:A:1472:GLU:HB2	1.98	0.46
1:A:2511:GLU:HG2	1:A:2512:LYS:HG3	1.97	0.46
1:A:3350:LYS:HE3	1:A:3360:TYR:HE2	1.81	0.46
1:A:3813:ILE:HD12	1:A:3840:LEU:HD23	1.97	0.46
1:A:1313:ARG:NH1	1:A:1423:ILE:CA	2.79	0.46
1:A:1984:ILE:HA	1:A:1993:THR:HG21	1.97	0.46
1:A:2068:GLN:OE1	1:A:2191:ARG:HD3	2.16	0.46
1:A:2514:GLY:HA2	1:A:2526:ILE:HG23	1.98	0.46
1:A:2714:ASN:O	1:A:2718:GLU:HG2	2.16	0.46
1:A:2780:LYS:HB3	1:A:2813:THR:HG22	1.97	0.46
1:A:3460:PRO:HA	1:A:3463:SER:HB2	1.97	0.46
1:A:1367:ILE:O	1:A:1415:MET:HE1	2.16	0.46
1:A:1534:PHE:HB3	1:A:1537:PHE:CD2	2.51	0.46
1:A:1781:THR:HG21	1:A:1919:PHE:CD2	2.51	0.46
1:A:3728:GLU:HA	1:A:3731:ASP:HB3	1.97	0.46
1:A:1534:PHE:CE2	1:A:1536:ARG:HB2	2.50	0.46
1:A:2070:LEU:HB2	1:A:2193:LEU:HD13	1.98	0.46
1:A:2937:PRO:O	1:A:2961:ILE:HG12	2.16	0.46
1:A:1395:VAL:HG11	1:A:1398:TRP:CD1	2.51	0.45
1:A:1440:GLU:HA	1:A:1443:VAL:HG22	1.98	0.45
1:A:2311:LYS:O	1:A:2314:ILE:HG22	2.16	0.45
1:A:1604:ALA:HA	1:A:1607:TRP:CE2	2.52	0.45
1:A:2204:PRO:HA	1:A:2207:ILE:HD12	1.98	0.45
1:A:2928:VAL:O	1:A:2932:MET:HE3	2.15	0.45
1:A:3592:LYS:O	1:A:3596:ASN:ND2	2.49	0.45
1:A:3700:MET:SD	1:A:3701:THR:N	2.90	0.45
1:A:3741:ASN:H	1:A:3745:ARG:HH12	1.64	0.45
1:A:1458:ILE:HG12	1:A:1546:LEU:HD13	1.99	0.45
1:A:2222:ILE:HD12	1:A:2284:LEU:HD11	1.98	0.45
1:A:3989:ILE:HD13	1:A:3993:VAL:HG21	1.98	0.45
1:A:4086:GLU:HA	1:A:4089:LEU:HG	1.97	0.45
1:A:1670:SER:O	1:A:1674:LYS:HG2	2.17	0.45
1:A:2615:TYR:CZ	1:A:2660:LEU:HD12	2.51	0.45
1:A:3822:LEU:HD22	1:A:3850:TRP:CG	2.51	0.45
1:A:2786:ILE:HG12	1:A:3460:PRO:HG2	1.99	0.45
1:A:3305:ARG:O	1:A:3305:ARG:NH1	2.50	0.45
1:A:3454:ASP:HB3	1:A:3457:PHE:CD1	2.52	0.45
1:A:3936:HIS:HA	1:A:3939:ILE:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1734:PHE:CE2	1:A:1749:ILE:HD13	2.52	0.45
1:A:1803:THR:HG21	1:A:1848:ASP:CG	2.41	0.45
1:A:3414:MET:HA	1:A:3414:MET:HE2	1.98	0.45
1:A:3540:GLU:O	1:A:3544:LYS:HB2	2.17	0.45
1:A:1782:LEU:HD11	1:A:1895:PHE:CD1	2.52	0.45
1:A:1820:PHE:CE2	1:A:1831:LEU:HD11	2.52	0.45
1:A:1933:ILE:HA	1:A:1936:ILE:HG22	1.98	0.45
1:A:1934:LEU:HD12	1:A:1946:ALA:HB2	1.98	0.45
1:A:2285:GLU:HG3	1:A:2412:ARG:HH12	1.82	0.45
1:A:2293:HIS:CE1	1:A:2409:ASN:HB3	2.52	0.45
1:A:1316:ASN:HB2	1:A:1332:LEU:HD21	1.98	0.45
1:A:4083:SER:HA	1:A:4086:GLU:OE1	2.17	0.45
1:A:1305:LEU:HG	1:A:1358:ILE:HD11	1.98	0.45
1:A:1364:GLU:OE2	1:A:1423:ILE:HD12	2.16	0.45
1:A:3023:LYS:HB3	1:A:3570:LEU:HD21	1.99	0.45
1:A:1367:ILE:CD1	1:A:1418:SER:OG	2.47	0.45
1:A:2079:GLY:HA2	3:A:4102:ATP:H5'2	1.99	0.45
1:A:3652:CYS:SG	1:A:3682:VAL:HG12	2.57	0.45
1:A:1736:GLN:OE1	1:A:1736:GLN:N	2.50	0.44
1:A:2765:GLY:N	2:A:4104:ADP:O1A	2.41	0.44
1:A:3305:ARG:NH1	1:A:3308:ASN:HB3	2.31	0.44
1:A:3400:SER:OG	1:A:3402:ASP:OD1	2.30	0.44
1:A:3664:THR:HB	1:A:3677:LEU:HD11	1.99	0.44
1:A:2476:LYS:HD2	1:A:2478:ASP:O	2.17	0.44
1:A:2932:MET:SD	1:A:2996:LEU:HD13	2.57	0.44
1:A:3583:LEU:O	1:A:3587:LEU:HG	2.17	0.44
1:A:3788:MET:CE	1:A:3897:TYR:HB2	2.47	0.44
1:A:1367:ILE:CG2	1:A:1415:MET:HE2	2.28	0.44
1:A:1413:VAL:HA	1:A:1416:LYS:HD2	2.00	0.44
1:A:2446:SER:HB2	1:A:2829:GLU:CG	2.47	0.44
1:A:2508:GLN:HG3	1:A:2512:LYS:HE2	1.99	0.44
1:A:2638:ARG:NH1	1:A:2638:ARG:HB2	2.32	0.44
1:A:2723:PHE:HZ	1:A:2775:TRP:HB3	1.82	0.44
1:A:3620:ILE:HA	1:A:3623:LYS:HZ2	1.82	0.44
1:A:1304:GLU:HB3	1:A:1358:ILE:HD13	1.99	0.44
1:A:1479:LEU:HD13	1:A:1516:LEU:HD22	1.98	0.44
1:A:3337:LEU:O	1:A:3389:TYR:OH	2.29	0.44
1:A:1397:GLU:O	1:A:1400:VAL:HG22	2.18	0.44
1:A:2232:LYS:O	1:A:2235:GLU:HG3	2.18	0.44
1:A:2486:CYS:O	1:A:2533:GLY:HA2	2.18	0.44
1:A:1245:VAL:HG21	1:A:1288:LEU:HG	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2068:GLN:HA	1:A:2191:ARG:HH11	1.83	0.44
1:A:2661:VAL:HG12	1:A:2916:TRP:CG	2.52	0.44
1:A:3639:HIS:CD2	1:A:3641:PHE:H	2.36	0.44
1:A:3688:THR:HB	1:A:3895:PHE:HD1	1.82	0.44
1:A:3790:SER:OG	1:A:3791:GLU:N	2.50	0.44
1:A:1505:PHE:O	1:A:1509:LEU:HG	2.17	0.44
1:A:1827:ASP:OD1	1:A:1828:TYR:N	2.51	0.44
1:A:2483:VAL:HG22	1:A:2530:HIS:HB2	2.00	0.44
1:A:2712:LEU:O	1:A:2716:ILE:HG12	2.18	0.44
1:A:3667:ALA:HB3	1:A:3673:GLU:CD	2.42	0.44
1:A:3934:TRP:O	1:A:3938:LEU:HD23	2.17	0.44
1:A:1385:VAL:HG12	1:A:1395:VAL:HG22	1.99	0.44
1:A:1527:LEU:HD13	1:A:1545:LEU:HD22	2.00	0.44
1:A:1683:LEU:HD22	1:A:1701:LEU:HD11	2.00	0.44
1:A:2073:VAL:HG21	1:A:2199:LEU:HD21	2.00	0.44
1:A:2768:ILE:HA	1:A:2771:ARG:HD3	2.00	0.44
1:A:3646:ILE:HD12	1:A:3646:ILE:H	1.83	0.44
1:A:1646:GLN:HE22	1:A:1762:TYR:HA	1.83	0.44
1:A:3780:ASN:C	1:A:3780:ASN:HD22	2.24	0.44
1:A:1383:TYR:HB3	1:A:1395:VAL:CG1	2.48	0.43
1:A:1465:ILE:HA	1:A:1468:PHE:HB2	2.00	0.43
1:A:1534:PHE:CZ	1:A:1608:LEU:HB3	2.53	0.43
1:A:1738:ASN:OD1	1:A:1739:ASP:N	2.51	0.43
1:A:1761:GLU:OE1	1:A:1816:VAL:HG23	2.17	0.43
1:A:2241:LEU:HD11	1:A:2299:ARG:HD3	2.00	0.43
1:A:2387:ARG:HB2	1:A:2390:ILE:HG12	1.99	0.43
1:A:2622:LEU:O	1:A:2626:VAL:HG13	2.18	0.43
1:A:3508:PHE:O	1:A:3512:ARG:HG2	2.18	0.43
1:A:3838:TRP:NE1	1:A:3872:LYS:HD3	2.32	0.43
1:A:4027:VAL:HG22	1:A:4052:THR:HG21	2.00	0.43
1:A:1380:GLU:O	1:A:1381:ALA:C	2.60	0.43
1:A:1459:LEU:HD23	1:A:1465:ILE:HG23	1.99	0.43
1:A:2170:LEU:HG	1:A:2209:ARG:HB3	2.00	0.43
1:A:2222:ILE:HG23	1:A:2284:LEU:HD11	1.99	0.43
1:A:3957:ASN:OD1	1:A:3958:ASP:N	2.51	0.43
1:A:3999:ASP:OD1	1:A:3999:ASP:N	2.51	0.43
1:A:1364:GLU:HG2	1:A:1420:TYR:CA	2.48	0.43
1:A:1708:PHE:O	1:A:1712:ILE:HG12	2.18	0.43
1:A:2506:LEU:O	1:A:2510:MET:HG3	2.17	0.43
1:A:3696:MET:HE2	1:A:3760:LEU:HB3	2.00	0.43
1:A:1330:ASN:O	1:A:1334:LYS:NZ	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1408:ASP:O	1:A:1411:GLU:HG3	2.18	0.43
1:A:1980:CYS:O	1:A:1984:ILE:HG13	2.18	0.43
1:A:3380:LEU:HD22	1:A:3386:LYS:HE3	2.00	0.43
1:A:3409:ASP:OD1	1:A:3409:ASP:N	2.50	0.43
1:A:1498:GLU:HA	1:A:1501:HIS:ND1	2.33	0.43
1:A:1769:LEU:HD11	2:A:4101:ADP:C5	2.53	0.43
1:A:2007:GLY:O	1:A:2010:ASP:N	2.51	0.43
1:A:2258:ASP:OD1	1:A:2258:ASP:N	2.45	0.43
1:A:2510:MET:SD	1:A:2553:HIS:HB3	2.59	0.43
1:A:1388:HIS:O	1:A:1389:SER:C	2.61	0.43
1:A:1917:ARG:HD3	1:A:3963:PHE:CE2	2.54	0.43
1:A:2416:LEU:HD13	1:A:2557:LEU:HB2	2.01	0.43
1:A:2442:GLY:HA2	1:A:2485:PHE:HB3	2.00	0.43
1:A:2637:PRO:C	1:A:2639:GLN:HE21	2.24	0.43
1:A:2804:SER:O	1:A:2808:LEU:N	2.36	0.43
1:A:2953:VAL:HA	1:A:2967:ASN:ND2	2.33	0.43
1:A:3316:THR:HA	1:A:3319:GLU:HG2	2.01	0.43
1:A:3428:LEU:HD12	1:A:3453:GLN:NE2	2.33	0.43
1:A:3747:LEU:HD11	1:A:3762:TRP:CZ3	2.53	0.43
1:A:1586:GLU:HG3	1:A:1765:ILE:HB	2.00	0.43
1:A:2305:LEU:HD23	1:A:2305:LEU:H	1.84	0.43
1:A:2943:PHE:CD2	1:A:2946:PRO:HB3	2.53	0.43
1:A:3470:PHE:HD1	1:A:3479:VAL:HB	1.83	0.43
1:A:3903:ILE:HD12	1:A:3941:ALA:HB2	2.00	0.43
1:A:4028:ARG:HE	1:A:4028:ARG:HB3	1.65	0.43
1:A:1796:GLY:O	1:A:1900:PRO:HD3	2.19	0.43
1:A:2447:LYS:H	1:A:2829:GLU:CD	2.26	0.43
1:A:1931:GLU:HG2	1:A:1932:MET:HE2	2.01	0.43
1:A:2696:PHE:HB3	1:A:2704:PHE:CZ	2.53	0.43
1:A:2831:MET:HE3	1:A:2834:LEU:HB3	2.01	0.43
1:A:3366:PHE:CE1	1:A:3370:LEU:HD12	2.54	0.43
1:A:3617:GLU:O	1:A:3620:ILE:HG22	2.19	0.43
1:A:3707:LYS:HA	1:A:3707:LYS:HD3	1.84	0.43
1:A:1868:ILE:HD11	1:A:1888:LEU:HD13	2.01	0.43
1:A:2077:GLY:HA3	1:A:2552:ARG:NE	2.33	0.43
1:A:2732:MET:HE1	2:A:4104:ADP:C4	2.54	0.43
1:A:1864:ASN:HA	1:A:1881:LEU:HD11	2.01	0.42
1:A:1934:LEU:HA	1:A:1937:MET:HG3	2.02	0.42
1:A:2081:THR:O	1:A:2085:LYS:HG2	2.18	0.42
1:A:2223:SER:HB2	1:A:2259:MET:HG3	2.01	0.42
1:A:2394:THR:H	1:A:2397:THR:HB	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3635:PHE:CZ	1:A:3698:MET:HB2	2.54	0.42
1:A:1384:GLU:OE1	1:A:1384:GLU:N	2.39	0.42
1:A:2294:LEU:HD13	1:A:2317:LEU:HD22	2.00	0.42
1:A:2929:ALA:HA	1:A:2932:MET:SD	2.59	0.42
1:A:2932:MET:HE2	1:A:2932:MET:HB3	1.73	0.42
1:A:3336:HIS:HA	1:A:3517:HIS:CE1	2.54	0.42
1:A:3651:SER:O	1:A:3655:ARG:HG2	2.19	0.42
1:A:3682:VAL:HG23	1:A:3702:MET:HE1	2.00	0.42
1:A:3767:PHE:HB3	1:A:3769:VAL:HG13	2.01	0.42
1:A:3841:LEU:HD12	1:A:3875:MET:HG3	2.01	0.42
1:A:1586:GLU:CD	1:A:1765:ILE:H	2.27	0.42
1:A:1671:LYS:HA	1:A:1671:LYS:HD3	1.76	0.42
1:A:1739:ASP:OD1	1:A:1740:THR:N	2.51	0.42
1:A:1910:GLU:HG2	1:A:3846:MET:HB3	2.00	0.42
1:A:2380:LEU:HD23	1:A:2380:LEU:H	1.84	0.42
1:A:2432:LEU:HG	1:A:2440:VAL:HG22	2.00	0.42
1:A:2785:LYS:NZ	1:A:3483:ASP:OD1	2.52	0.42
1:A:2972:PHE:CE1	1:A:3349:LEU:HD12	2.54	0.42
1:A:3512:ARG:NH2	2:A:4104:ADP:O5'	2.53	0.42
1:A:1766:PRO:HG2	1:A:1811:GLN:NE2	2.34	0.42
1:A:1933:ILE:O	1:A:1937:MET:HG3	2.19	0.42
1:A:2414:ILE:CG2	1:A:2532:VAL:HG23	2.48	0.42
1:A:2569:GLN:O	1:A:2573:ILE:HG12	2.20	0.42
1:A:1588:GLU:OE1	1:A:1762:TYR:OH	2.33	0.42
1:A:1673:TRP:HD1	1:A:1712:ILE:HG22	1.84	0.42
1:A:1378:TRP:O	1:A:1379:LYS:C	2.62	0.42
1:A:1827:ASP:O	1:A:1830:VAL:HG12	2.20	0.42
1:A:2050:SER:O	1:A:2054:LEU:N	2.33	0.42
1:A:3387:ASN:OD1	1:A:3390:PHE:HB2	2.20	0.42
1:A:3397:VAL:HG13	1:A:3398:MET:HE3	2.01	0.42
1:A:1258:VAL:HG23	1:A:1259:LEU:HD22	2.02	0.42
1:A:1687:LEU:HB2	1:A:1698:ILE:HG21	2.02	0.42
1:A:2831:MET:HE1	1:A:2834:LEU:HD23	2.01	0.42
1:A:2971:HIS:O	1:A:2974:ARG:HD3	2.20	0.42
1:A:3528:ARG:O	1:A:3532:ILE:HG12	2.20	0.42
1:A:1329:LYS:HB3	1:A:1329:LYS:HE2	1.85	0.42
1:A:2241:LEU:HD12	1:A:2241:LEU:HA	1.91	0.42
1:A:2426:MET:O	1:A:2430:ASN:ND2	2.52	0.42
1:A:2578:ILE:HD11	1:A:2630:TYR:N	2.35	0.42
1:A:2696:PHE:CZ	1:A:2706:GLU:HB2	2.55	0.42
1:A:2835:LEU:O	1:A:2911:ARG:NE	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3787:THR:HG23	1:A:3892:THR:HG21	2.01	0.42
1:A:1309:ALA:HA	1:A:1365:PHE:HB2	2.00	0.42
1:A:1371:LEU:HD11	1:A:1431:LEU:HD22	2.01	0.42
1:A:1801:GLY:H	2:A:4101:ADP:PA	2.41	0.42
1:A:1818:VAL:HG11	1:A:1838:ILE:HG21	2.01	0.42
1:A:2071:ILE:HG23	1:A:2212:LEU:HA	2.01	0.42
1:A:2190:PHE:CE2	1:A:2192:ILE:HD11	2.55	0.42
1:A:2526:ILE:HB	1:A:2529:ILE:HD13	2.02	0.42
1:A:2732:MET:HE2	1:A:2732:MET:HA	2.02	0.42
1:A:3380:LEU:HD21	1:A:3391:LEU:HD21	2.01	0.42
1:A:3402:ASP:OD1	1:A:3402:ASP:N	2.51	0.42
1:A:3460:PRO:O	1:A:3464:ARG:NH1	2.53	0.42
1:A:1801:GLY:HA3	2:A:4101:ADP:H8	1.84	0.42
1:A:2080:LYS:HE3	1:A:2195:GLU:HG3	2.01	0.42
1:A:2508:GLN:HA	1:A:2512:LYS:HZ1	1.84	0.42
1:A:3804:ALA:HB1	1:A:3809:GLU:HA	2.01	0.42
1:A:3840:LEU:HG	1:A:3842:GLN:OE1	2.20	0.42
1:A:1301:ILE:HD12	1:A:1351:GLU:HG3	2.01	0.41
1:A:1311:LYS:HB2	1:A:1314:HIS:HD1	1.84	0.41
1:A:1782:LEU:HD23	1:A:1809:PHE:CD2	2.55	0.41
1:A:2799:LEU:HD21	1:A:2834:LEU:HD22	2.01	0.41
1:A:3601:LEU:O	1:A:3605:GLU:HG2	2.20	0.41
1:A:3958:ASP:O	1:A:3961:PHE:N	2.53	0.41
1:A:1364:GLU:CB	1:A:1420:TYR:HD2	2.26	0.41
1:A:1563:LYS:HA	1:A:1569:ILE:O	2.20	0.41
1:A:1794:PHE:HB3	1:A:1802:LYS:HD2	2.01	0.41
1:A:2341:THR:O	1:A:2344:THR:OG1	2.33	0.41
1:A:3489:SER:OG	1:A:3491:ASP:OD1	2.34	0.41
1:A:3529:ILE:HD11	1:A:3622:GLY:HA2	2.02	0.41
1:A:3531:ASP:HA	1:A:3534:LEU:HG	2.02	0.41
1:A:4038:GLU:CD	1:A:4038:GLU:H	2.27	0.41
1:A:1406:LYS:HA	1:A:1409:LEU:HD12	2.02	0.41
1:A:1483:TYR:O	1:A:1487:THR:HG23	2.20	0.41
1:A:1523:LEU:O	1:A:1527:LEU:HD23	2.20	0.41
1:A:1566:PHE:O	1:A:1816:VAL:HG11	2.20	0.41
1:A:2527:GLU:C	1:A:2528:ARG:HG3	2.45	0.41
1:A:2905:SER:HB3	1:A:2908:LEU:HD12	2.03	0.41
1:A:3429:LEU:O	1:A:3452:ILE:HA	2.20	0.41
1:A:3430:SER:OG	1:A:3454:ASP:OD2	2.35	0.41
1:A:3547:ASP:O	1:A:3550:LYS:HG2	2.20	0.41
1:A:2153:VAL:HA	1:A:2193:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2489:ILE:O	1:A:2492:PRO:HD2	2.20	0.41
1:A:2893:ASP:HB2	1:A:2986:PRO:HB2	2.03	0.41
1:A:3336:HIS:HA	1:A:3517:HIS:ND1	2.35	0.41
1:A:3670:ARG:CZ	1:A:3674:ILE:HD11	2.50	0.41
1:A:1424:PHE:O	1:A:1428:CYS:N	2.33	0.41
1:A:3014:GLN:HA	1:A:3017:VAL:HG22	2.02	0.41
1:A:3629:PHE:CZ	1:A:3646:ILE:HG13	2.46	0.41
1:A:3845:GLN:CD	1:A:3878:HIS:H	2.28	0.41
1:A:3924:TRP:CD1	1:A:3977:THR:HG1	2.38	0.41
1:A:1820:PHE:CZ	1:A:1831:LEU:HD21	2.55	0.41
1:A:2485:PHE:CD1	1:A:2532:VAL:HG13	2.55	0.41
1:A:2999:LEU:HA	1:A:2999:LEU:HD12	1.81	0.41
1:A:3449:VAL:HG22	1:A:3493:LYS:HB2	2.02	0.41
1:A:1299:ASN:O	1:A:1303:VAL:HG23	2.21	0.41
1:A:1607:TRP:O	1:A:1610:ILE:HG22	2.20	0.41
1:A:1747:VAL:O	1:A:1757:GLN:NE2	2.53	0.41
1:A:1849:GLU:O	1:A:1849:GLU:HG3	2.21	0.41
1:A:2575:TYR:HA	1:A:2578:ILE:HG22	2.03	0.41
1:A:2664:LYS:NZ	1:A:2668:SER:HB2	2.36	0.41
1:A:2679:LYS:HD2	1:A:2680:TYR:CE2	2.56	0.41
1:A:2720:PHE:CE1	1:A:2732:MET:HB3	2.56	0.41
1:A:3900:ILE:HD13	1:A:3944:ARG:HD3	2.02	0.41
1:A:4033:LEU:HG	1:A:4035:GLN:HG3	2.03	0.41
1:A:2356:TYR:CG	1:A:2395:ILE:HD11	2.55	0.41
1:A:2520:GLU:HG3	1:A:2522:LYS:HB3	2.02	0.41
1:A:2622:LEU:HA	1:A:2625:LEU:HG	2.03	0.41
1:A:1821:ASN:HA	1:A:1848:ASP:HB3	2.03	0.41
1:A:2006:LEU:HB3	1:A:2010:ASP:HB2	2.02	0.41
1:A:2158:LEU:HD12	1:A:2163:VAL:HG11	2.03	0.41
1:A:2180:ASN:ND2	1:A:2181:GLY:N	2.69	0.41
1:A:2863:LEU:HB3	1:A:2865:LEU:HD13	2.03	0.41
1:A:2993:ILE:O	1:A:2996:LEU:HG	2.21	0.41
1:A:3376:LYS:HE2	1:A:3376:LYS:HA	2.03	0.41
1:A:2200:ASP:OD1	1:A:2201:HIS:N	2.53	0.41
1:A:2291:ALA:O	1:A:2295:ILE:HG23	2.21	0.41
1:A:2471:LEU:HD23	1:A:2522:LYS:HG2	2.03	0.41
1:A:2723:PHE:CZ	1:A:2775:TRP:HB3	2.56	0.41
1:A:2723:PHE:O	1:A:2727:GLU:N	2.54	0.41
1:A:2908:LEU:O	1:A:2912:CYS:HB2	2.21	0.41
1:A:3509:LEU:C	1:A:3513:VAL:HG12	2.46	0.41
1:A:3871:PHE:CD1	1:A:3873:MET:HE3	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3964:ALA:O	1:A:3968:LEU:HD23	2.22	0.41
1:A:4009:LYS:HG3	1:A:4010:LEU:N	2.36	0.41
1:A:1373:ARG:HA	1:A:1376:LYS:HE3	2.03	0.40
1:A:1656:TRP:O	1:A:1660:VAL:HG13	2.21	0.40
1:A:1790:TYR:CD2	1:A:3963:PHE:HZ	2.39	0.40
1:A:2085:LYS:O	1:A:2088:ILE:HG22	2.21	0.40
1:A:3743:ASP:OD1	1:A:3743:ASP:N	2.54	0.40
1:A:3897:TYR:CE2	1:A:3899:ASP:HB2	2.56	0.40
1:A:4039:GLU:H	1:A:4039:GLU:CD	2.26	0.40
1:A:1374:ILE:O	1:A:1375:LYS:C	2.64	0.40
1:A:1574:PHE:HA	1:A:1578:PHE:O	2.20	0.40
1:A:1608:LEU:O	1:A:1611:LEU:HG	2.21	0.40
1:A:1685:ASP:OD1	1:A:1686:LYS:N	2.53	0.40
1:A:1967:HIS:O	1:A:1972:THR:HG21	2.21	0.40
1:A:2661:VAL:HG12	1:A:2916:TRP:CD1	2.57	0.40
1:A:2734:ILE:HG23	1:A:2738:MET:SD	2.61	0.40
1:A:2754:GLY:HA3	1:A:2886:HIS:ND1	2.37	0.40
1:A:2869:THR:HB	1:A:2872:GLU:HB3	2.03	0.40
1:A:3447:GLY:HA2	1:A:3492:PHE:HB2	2.03	0.40
1:A:3997:LYS:HB2	1:A:3997:LYS:HE2	1.97	0.40
1:A:1383:TYR:HB3	1:A:1395:VAL:HG11	2.04	0.40
1:A:1554:HIS:O	1:A:1555:HIS:ND1	2.54	0.40
1:A:2163:VAL:HA	1:A:2166:MET:HB2	2.02	0.40
1:A:2305:LEU:HD11	1:A:2310:LEU:HD13	2.03	0.40
1:A:2386:MET:HG2	1:A:2627:ARG:CD	2.51	0.40
1:A:2943:PHE:HD2	1:A:2946:PRO:HB3	1.87	0.40
1:A:3464:ARG:HG3	1:A:3469:GLU:CD	2.46	0.40
1:A:3607:PHE:O	1:A:3611:PHE:N	2.45	0.40
1:A:1464:ASP:HB2	1:A:1550:GLY:HA2	2.04	0.40
1:A:1547:LYS:HD2	1:A:1561:PHE:CE2	2.56	0.40
1:A:1807:LYS:HD3	1:A:1819:VAL:HG21	2.04	0.40
1:A:2767:THR:HG22	2:A:4104:ADP:O2A	2.21	0.40
1:A:3008:GLN:O	1:A:3012:GLU:OE1	2.39	0.40
1:A:3439:ARG:HD2	1:A:3439:ARG:HA	1.93	0.40
1:A:4075:ARG:O	1:A:4079:LYS:HG2	2.21	0.40
1:A:1455:LEU:HD23	1:A:1458:ILE:HD12	2.04	0.40
1:A:1529:ARG:O	1:A:1533:GLN:HG2	2.22	0.40
1:A:2435:SER:O	1:A:2480:LYS:NZ	2.50	0.40
1:A:3388:ASP:OD1	1:A:3389:TYR:N	2.54	0.40
1:A:3592:LYS:HD2	1:A:3596:ASN:HD21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2579/4092 (63%)	2453 (95%)	124 (5%)	2 (0%)	48	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2499	SER
1	A	3525	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2358/3759 (63%)	2352 (100%)	6 (0%)	91	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1372	ASN
1	A	1374	ILE
1	A	1375	LYS
1	A	1376	LYS
1	A	1379	LYS
1	A	1380	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1246	GLN
1	A	1299	ASN
1	A	1542	ASN
1	A	1554	HIS
1	A	1717	ASN
1	A	1757	GLN
1	A	1866	GLN
1	A	1878	HIS
1	A	1925	GLN
1	A	2030	ASN
1	A	2138	ASN
1	A	2180	ASN
1	A	2270	ASN
1	A	2293	HIS
1	A	2513	GLN
1	A	2612	GLN
1	A	2671	GLN
1	A	2741	HIS
1	A	2832	ASN
1	A	2915	ASN
1	A	3574	GLN
1	A	3639	HIS
1	A	3714	GLN
1	A	3765	ASN
1	A	3984	GLN
1	A	4035	GLN
1	A	4064	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	4101	-	24,29,29	0.84	0	29,45,45	1.19	2 (6%)
3	ATP	A	4102	-	28,33,33	0.75	0	34,52,52	0.60	1 (2%)
2	ADP	A	4103	-	24,29,29	0.86	0	29,45,45	1.18	2 (6%)
2	ADP	A	4104	-	24,29,29	0.90	0	29,45,45	1.27	3 (10%)

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
2	ADP	A	4101	-	-	7/12/32/32	0/3/3/3
3	ATP	A	4102	-	-	9/18/38/38	0/3/3/3
2	ADP	A	4103	-	-	7/12/32/32	0/3/3/3
2	ADP	A	4104	-	-	1/12/32/32	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4101	ADP	N3-C2-N1	-3.64	123.73	128.67
2	A	4104	ADP	N3-C2-N1	-3.62	123.75	128.67
2	A	4103	ADP	N3-C2-N1	-3.57	123.83	128.67
2	A	4104	ADP	C4-C5-N7	-2.74	106.44	109.34
2	A	4103	ADP	C4-C5-N7	-2.55	106.64	109.34
2	A	4101	ADP	C4-C5-N7	-2.41	106.79	109.34
3	A	4102	ATP	C5-C6-N6	2.31	123.83	120.31
2	A	4104	ADP	C4'-O4'-C1'	2.12	111.86	109.92

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4101	ADP	PA-O3A-PB-O2B
2	A	4101	ADP	PA-O3A-PB-O3B
2	A	4101	ADP	C5'-O5'-PA-O1A
2	A	4101	ADP	C5'-O5'-PA-O3A
2	A	4103	ADP	PA-O3A-PB-O2B
2	A	4103	ADP	PA-O3A-PB-O3B
2	A	4103	ADP	C5'-O5'-PA-O1A
3	A	4102	ATP	PB-O3B-PG-O3G
3	A	4102	ATP	C5'-O5'-PA-O2A
2	A	4101	ADP	O4'-C4'-C5'-O5'
2	A	4101	ADP	C3'-C4'-C5'-O5'
3	A	4102	ATP	O4'-C4'-C5'-O5'
2	A	4103	ADP	O4'-C4'-C5'-O5'
2	A	4103	ADP	C3'-C4'-C5'-O5'
3	A	4102	ATP	C3'-C4'-C5'-O5'
3	A	4102	ATP	PA-O3A-PB-O1B
2	A	4103	ADP	C5'-O5'-PA-O3A
3	A	4102	ATP	C5'-O5'-PA-O1A
3	A	4102	ATP	C5'-O5'-PA-O3A
2	A	4104	ADP	C4'-C5'-O5'-PA
3	A	4102	ATP	PG-O3B-PB-O1B
2	A	4103	ADP	PA-O3A-PB-O1B
3	A	4102	ATP	PG-O3B-PB-O2B
2	A	4101	ADP	PA-O3A-PB-O1B

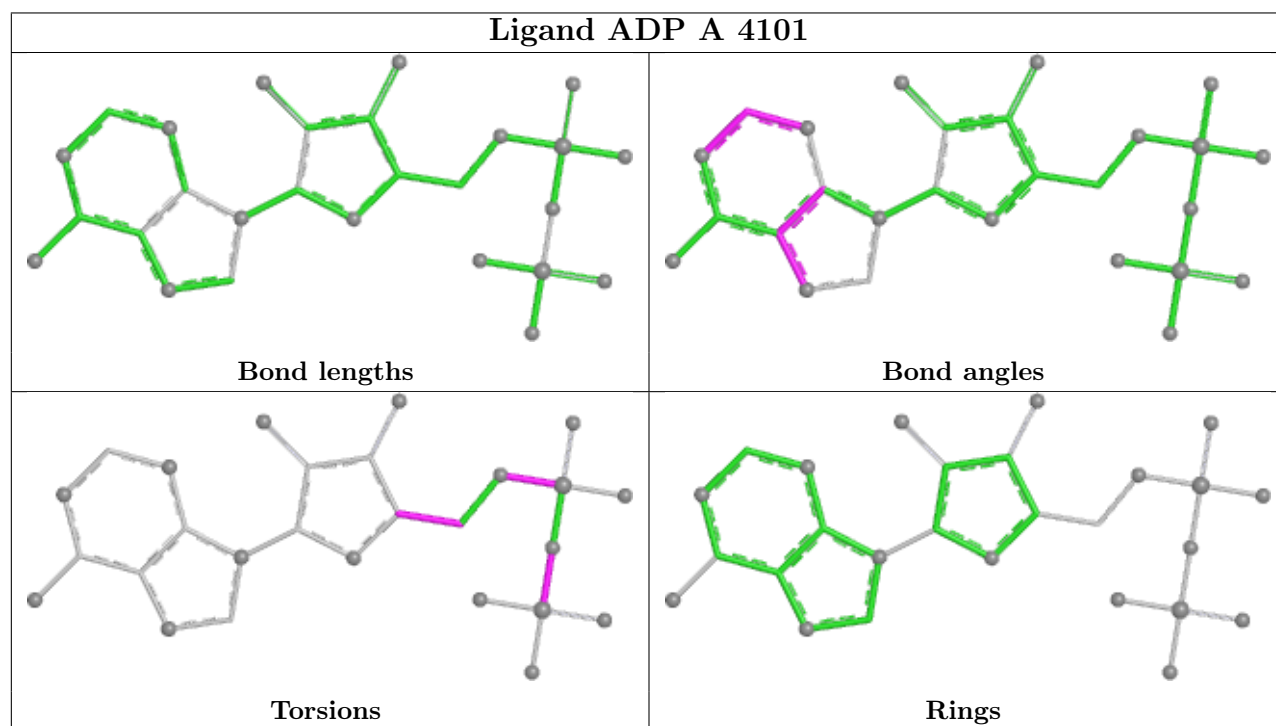
There are no ring outliers.

4 monomers are involved in 14 short contacts:

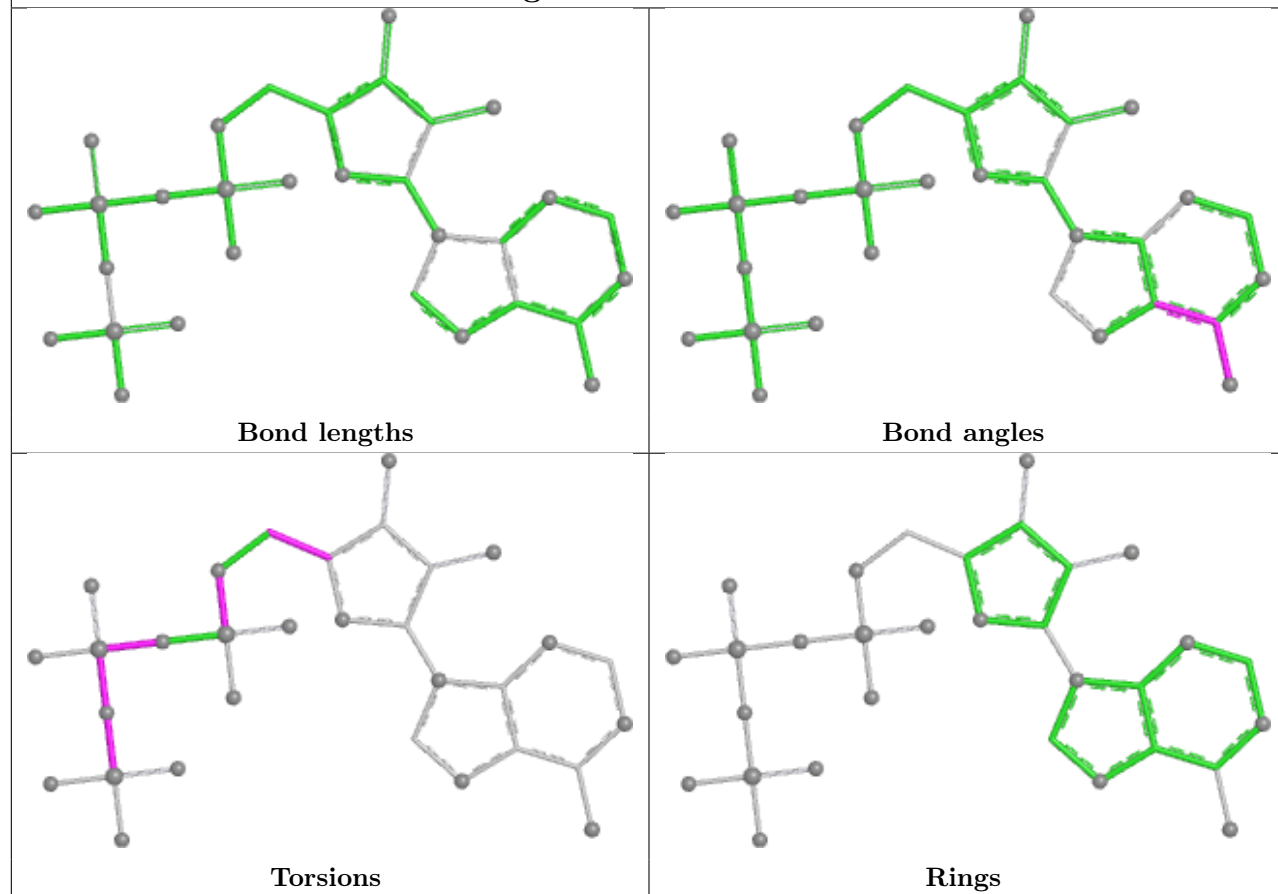
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4101	ADP	4	0
3	A	4102	ATP	5	0
2	A	4103	ADP	1	0
2	A	4104	ADP	4	0

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

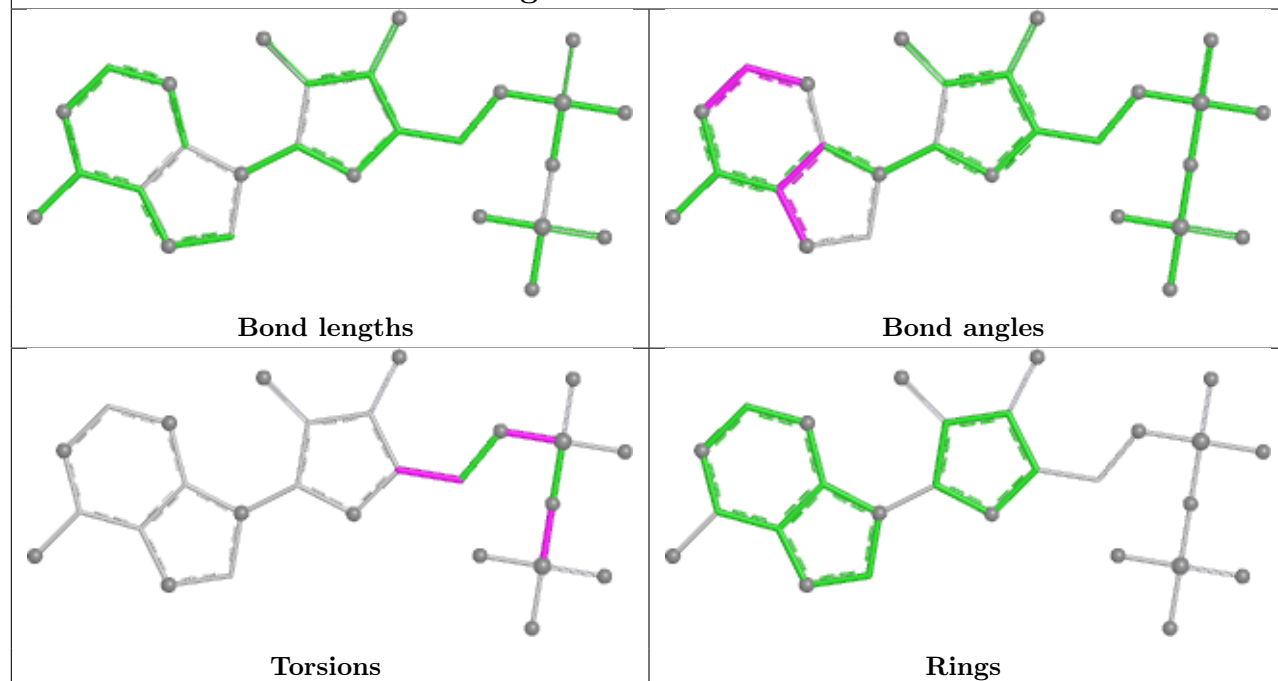
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

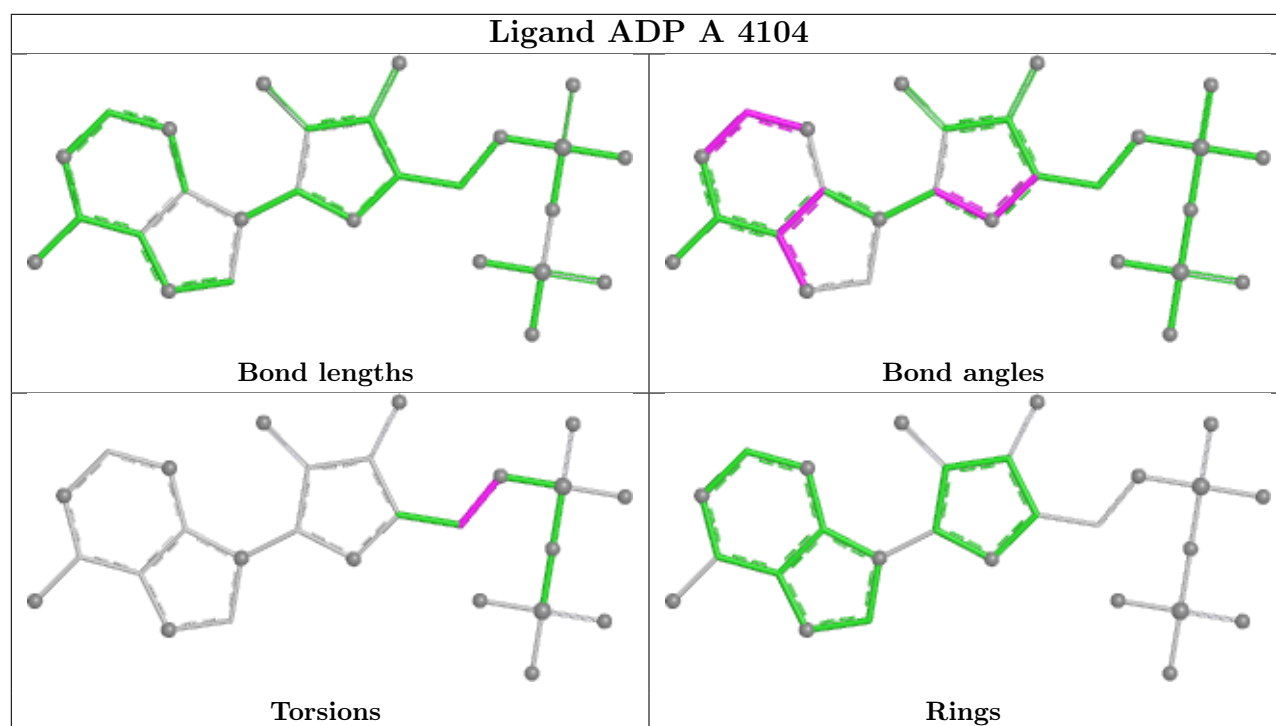


Ligand ATP A 4102



Ligand ADP A 4103





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

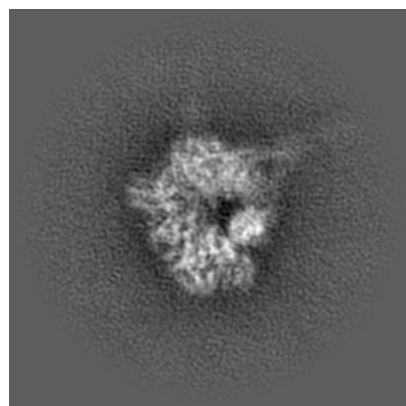
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48240. These allow visual inspection of the internal detail of the map and identification of artifacts.

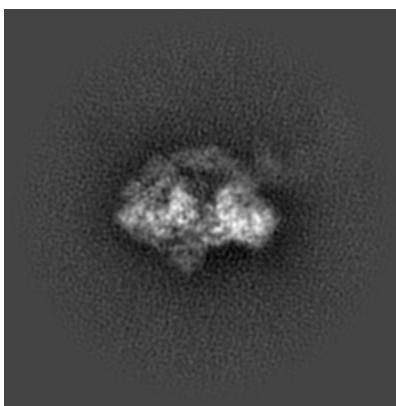
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

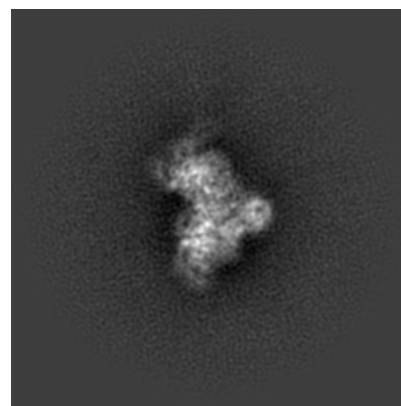
6.1.1 Primary map



X

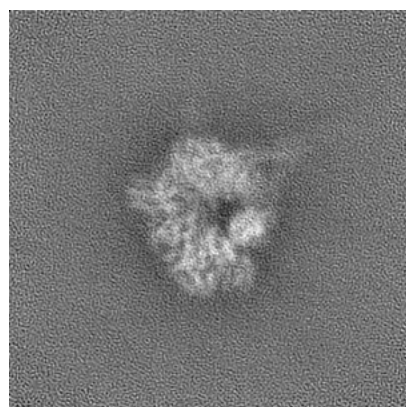


Y

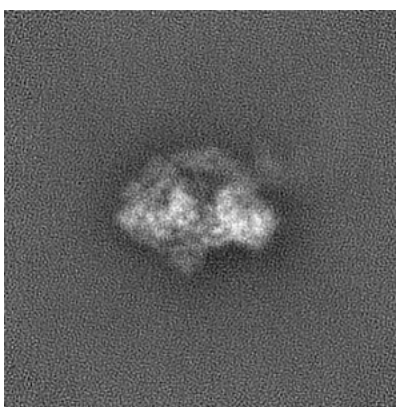


Z

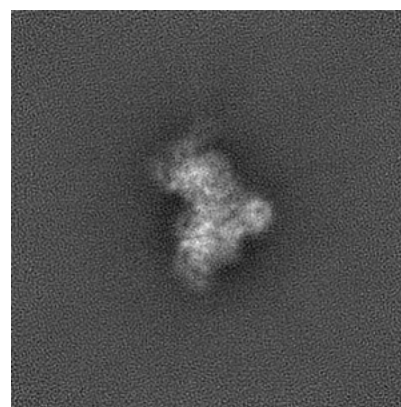
6.1.2 Raw map



X



Y

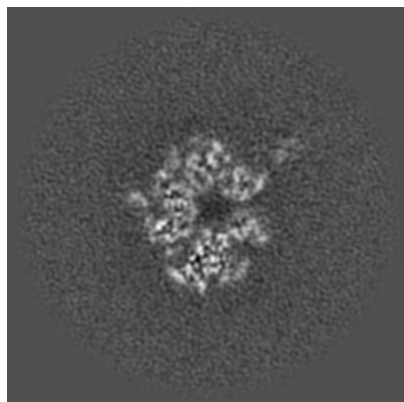


Z

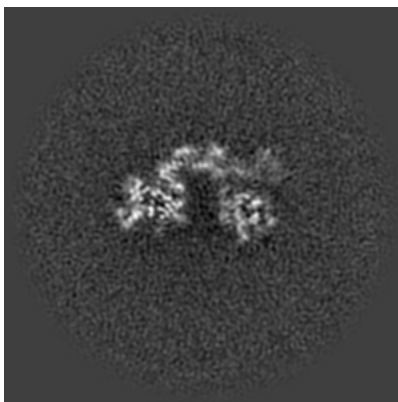
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

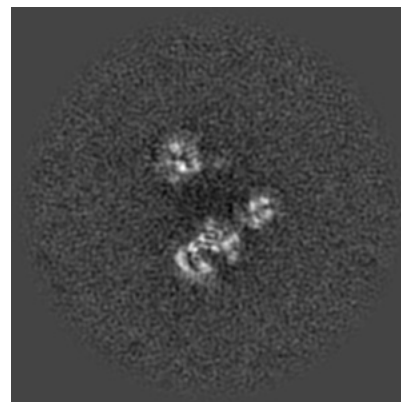
6.2.1 Primary map



X Index: 128

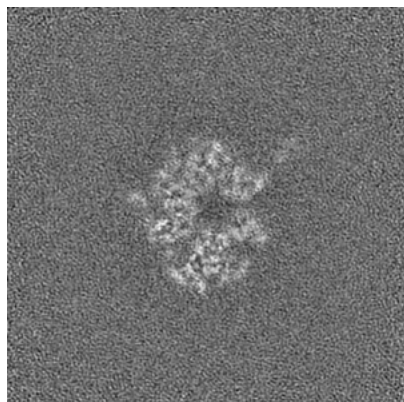


Y Index: 128

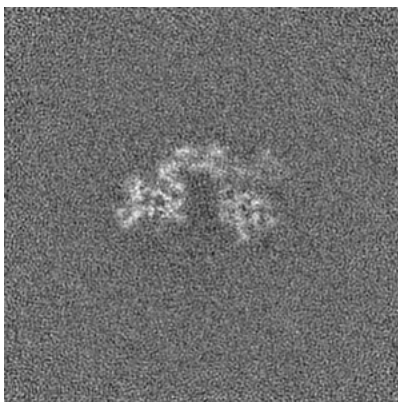


Z Index: 128

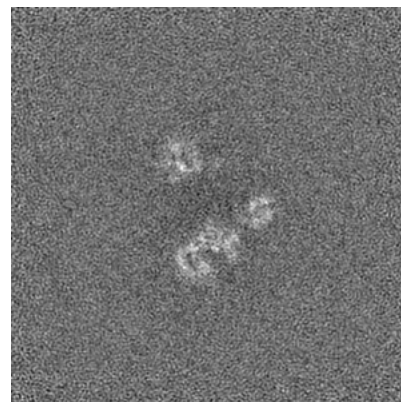
6.2.2 Raw map



X Index: 128



Y Index: 128

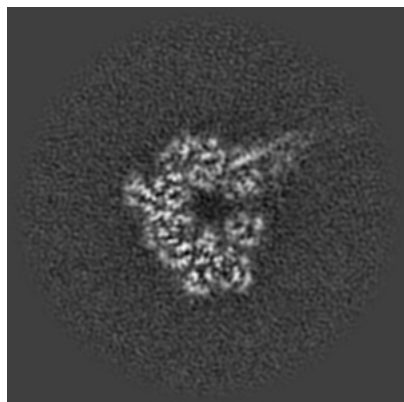


Z Index: 128

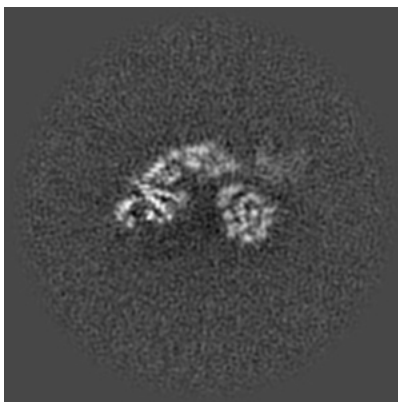
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

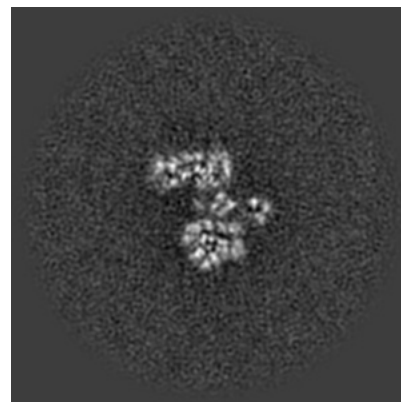
6.3.1 Primary map



X Index: 122

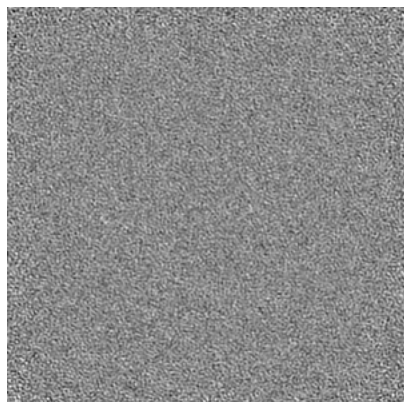


Y Index: 124

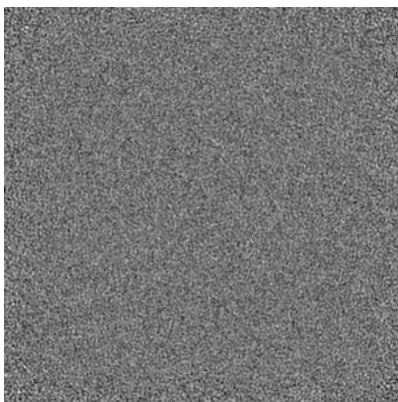


Z Index: 113

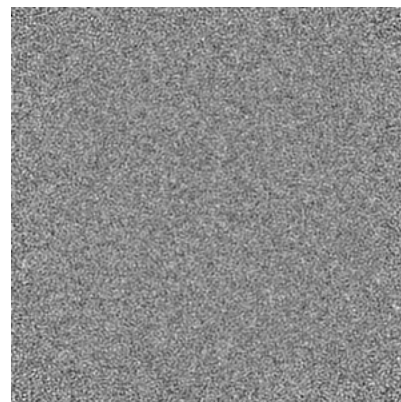
6.3.2 Raw map



X Index: 0



Y Index: 0

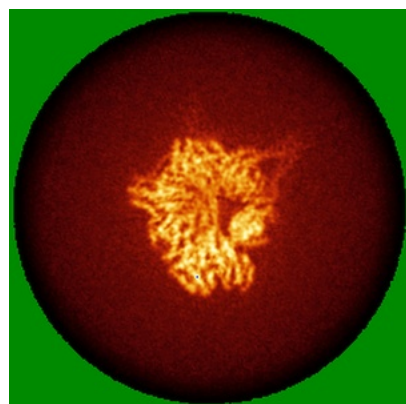


Z Index: 0

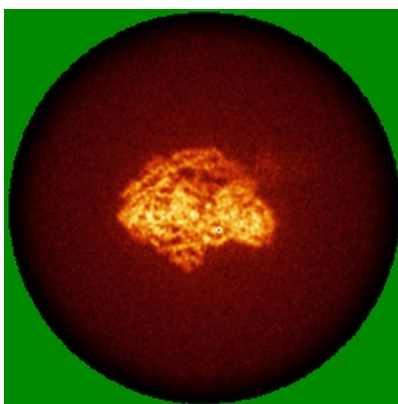
The images above show the largest variance slices of the map in three orthogonal directions.

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

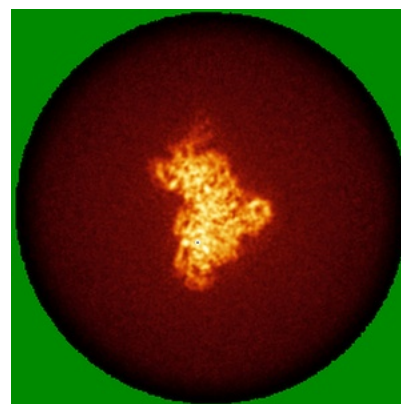
6.4.1 Primary map



X

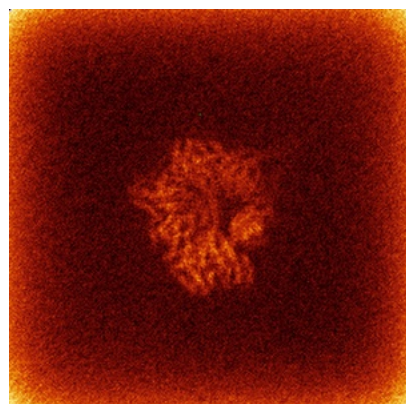


Y

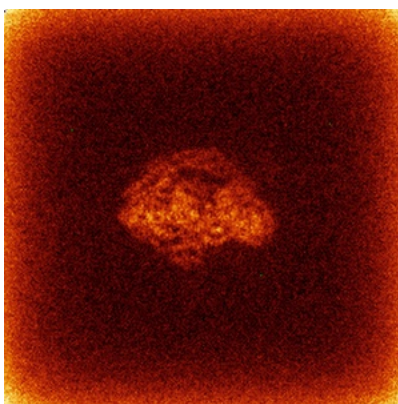


Z

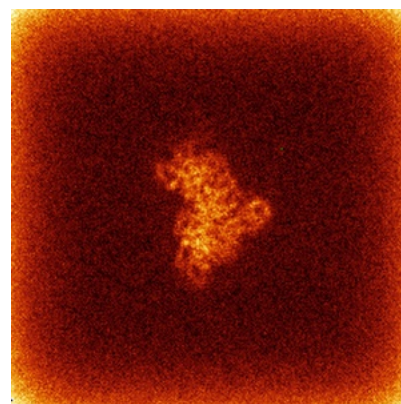
6.4.2 Raw map



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.

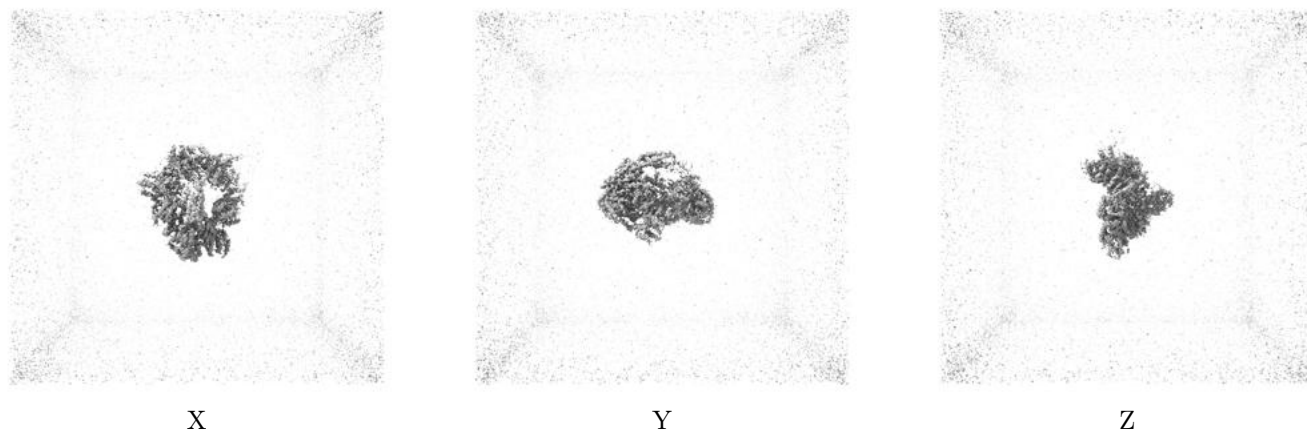
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

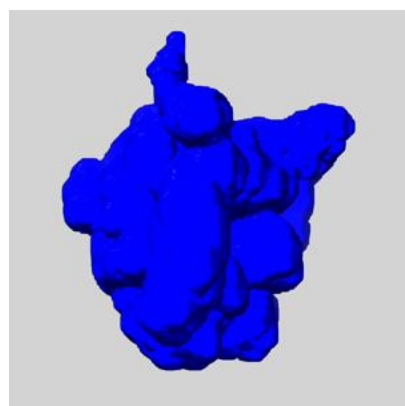
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

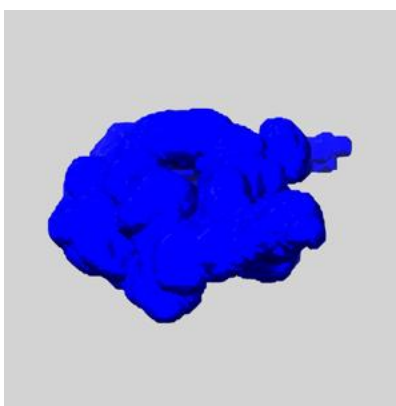
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

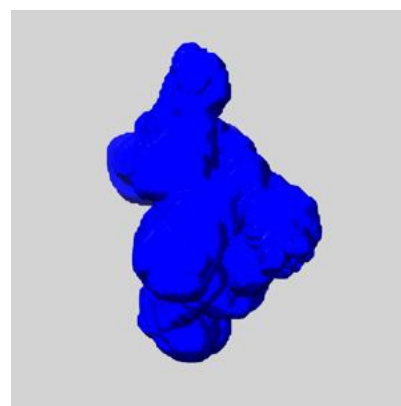
6.6.1 emd_48240_msk_1.map [i](#)



X



Y

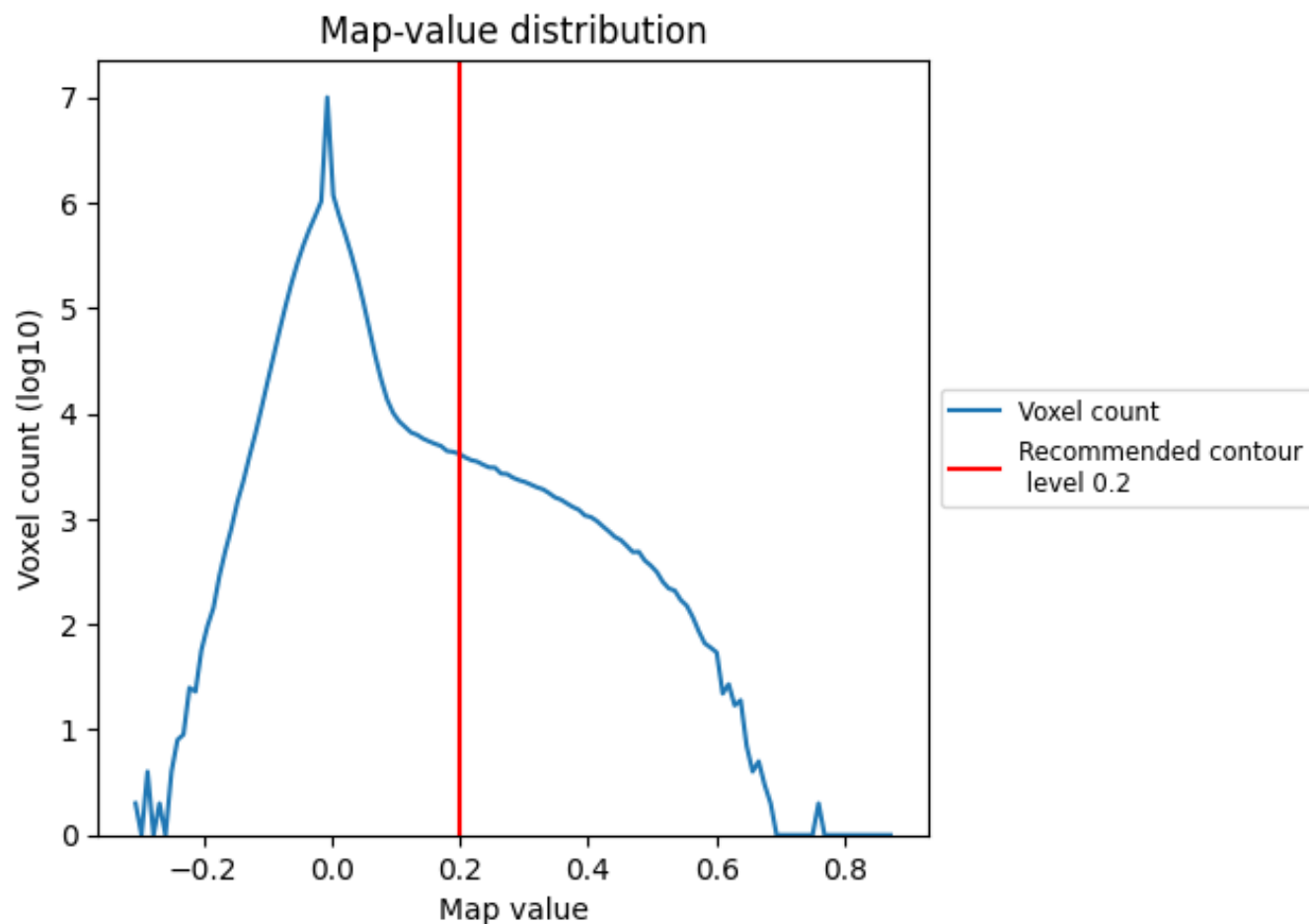


Z

7 Map analysis [i](#)

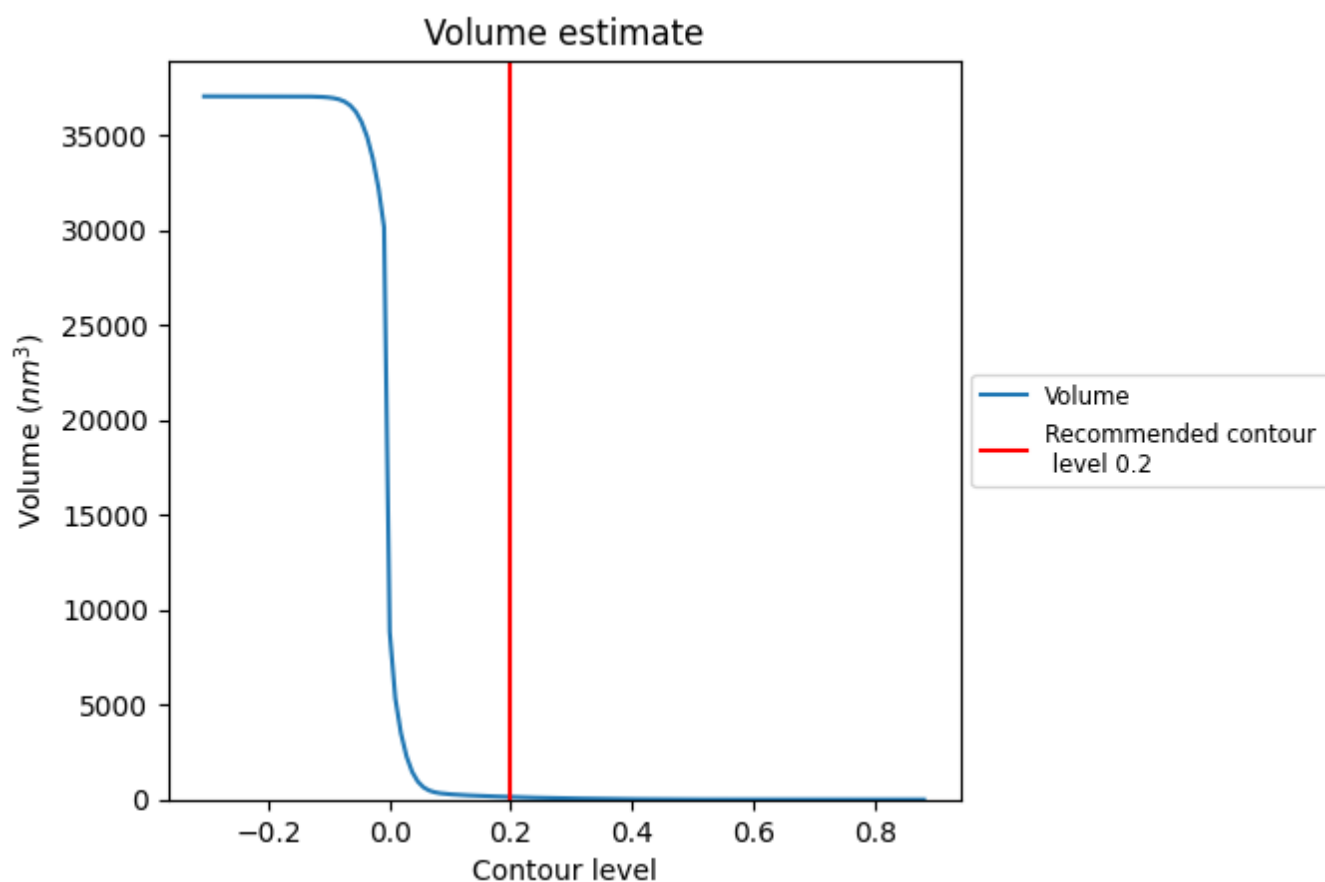
This section contains the results of statistical analysis of the map.

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.

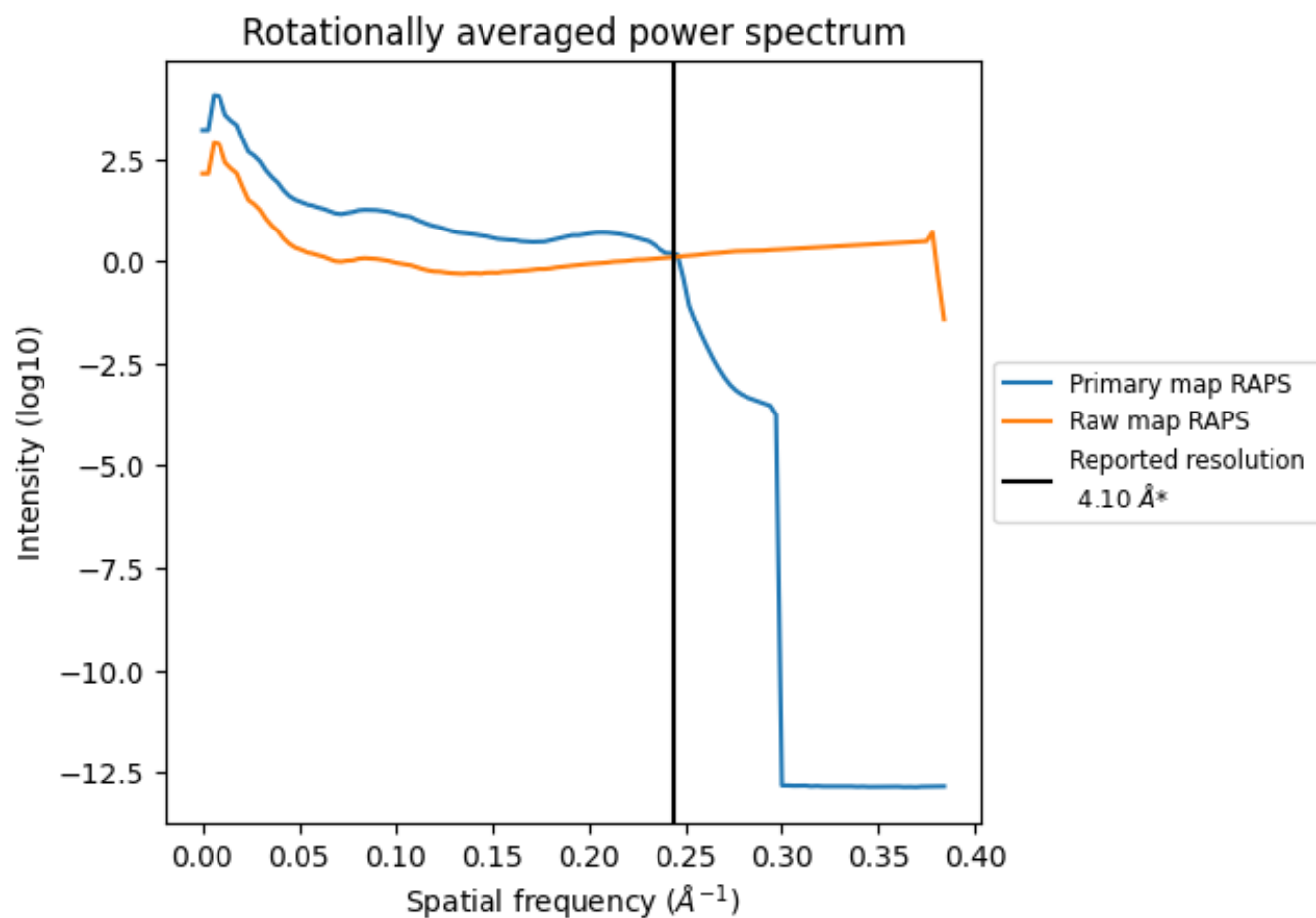
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 135 nm^3 ; this corresponds to an approximate mass of 122 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

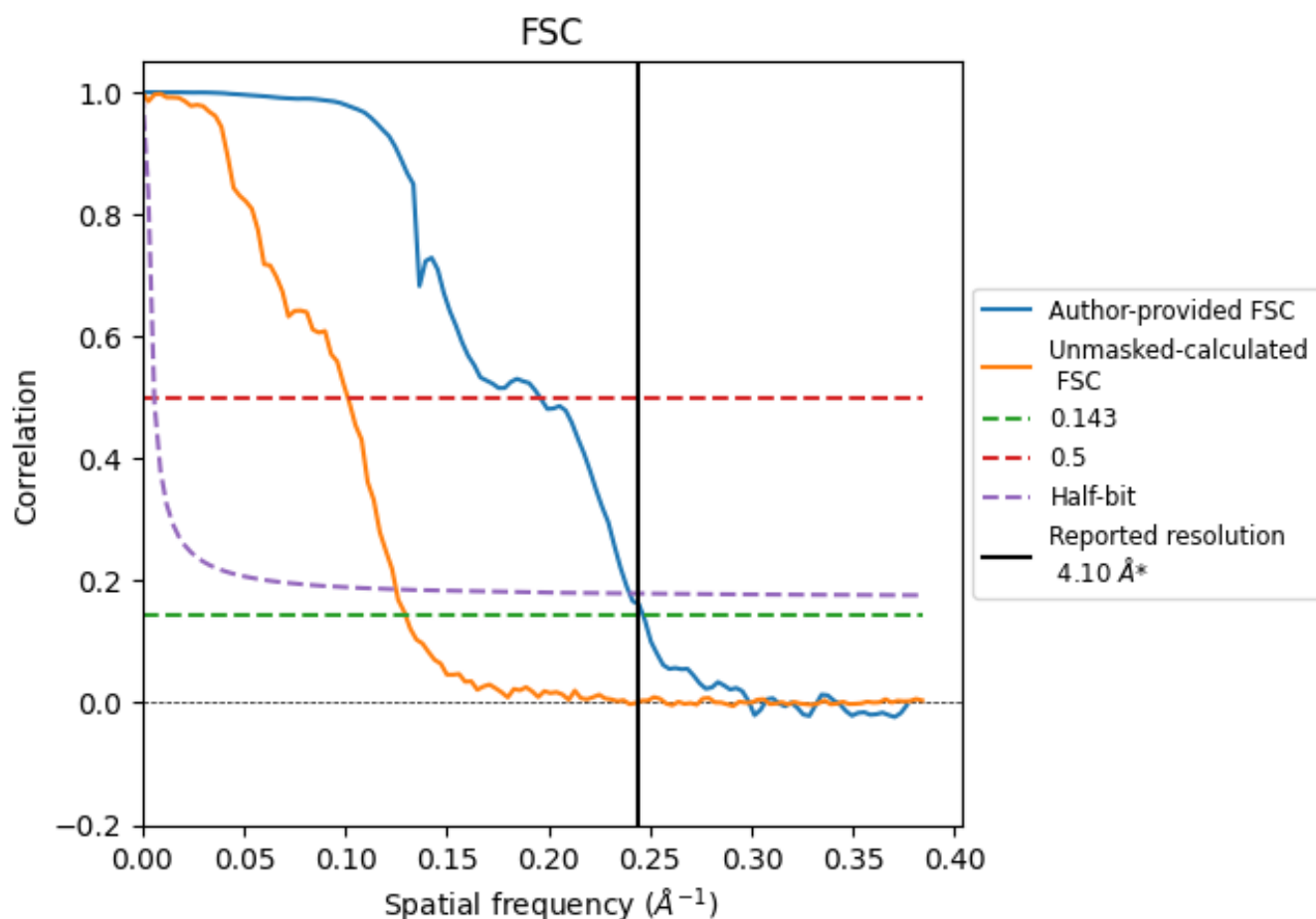


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.244 \AA^{-1}

8.2 Resolution estimates [i](#)

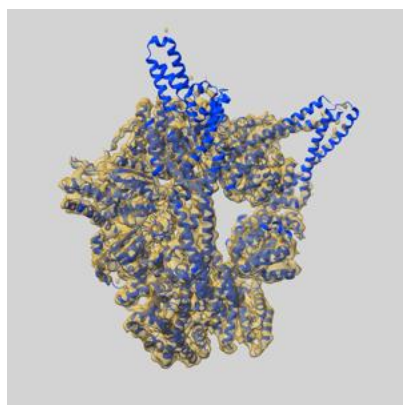
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.06	5.11	4.17
Unmasked-calculated*	7.71	9.88	8.00

*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 7.71 differs from the reported value 4.1 by more than 10 %

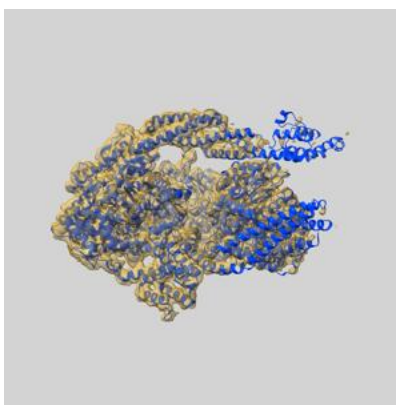
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48240 and PDB model 9MFW. Per-residue inclusion information can be found in section 3 on page 5.

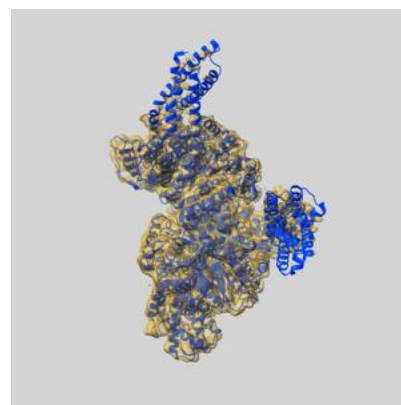
9.1 Map-model overlay [i](#)



X



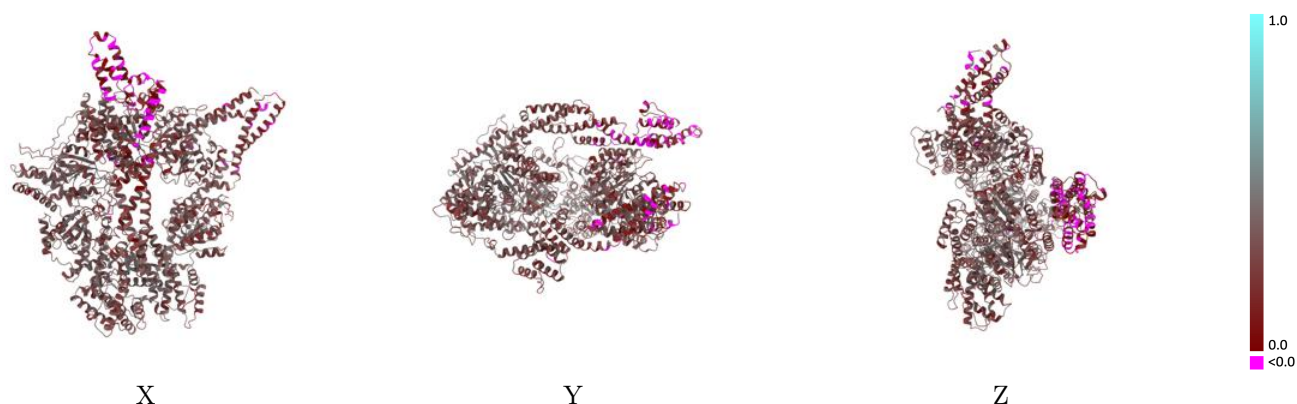
Y



Z

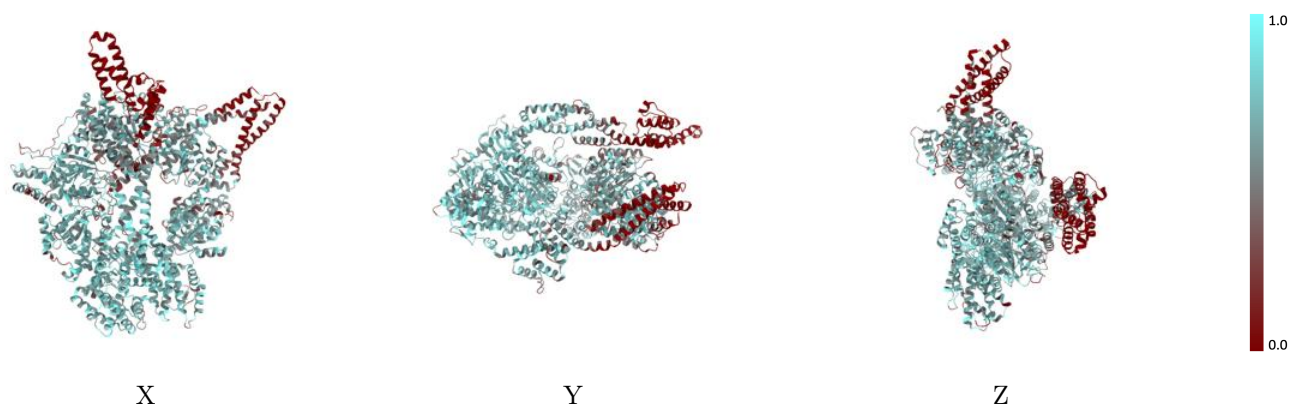
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



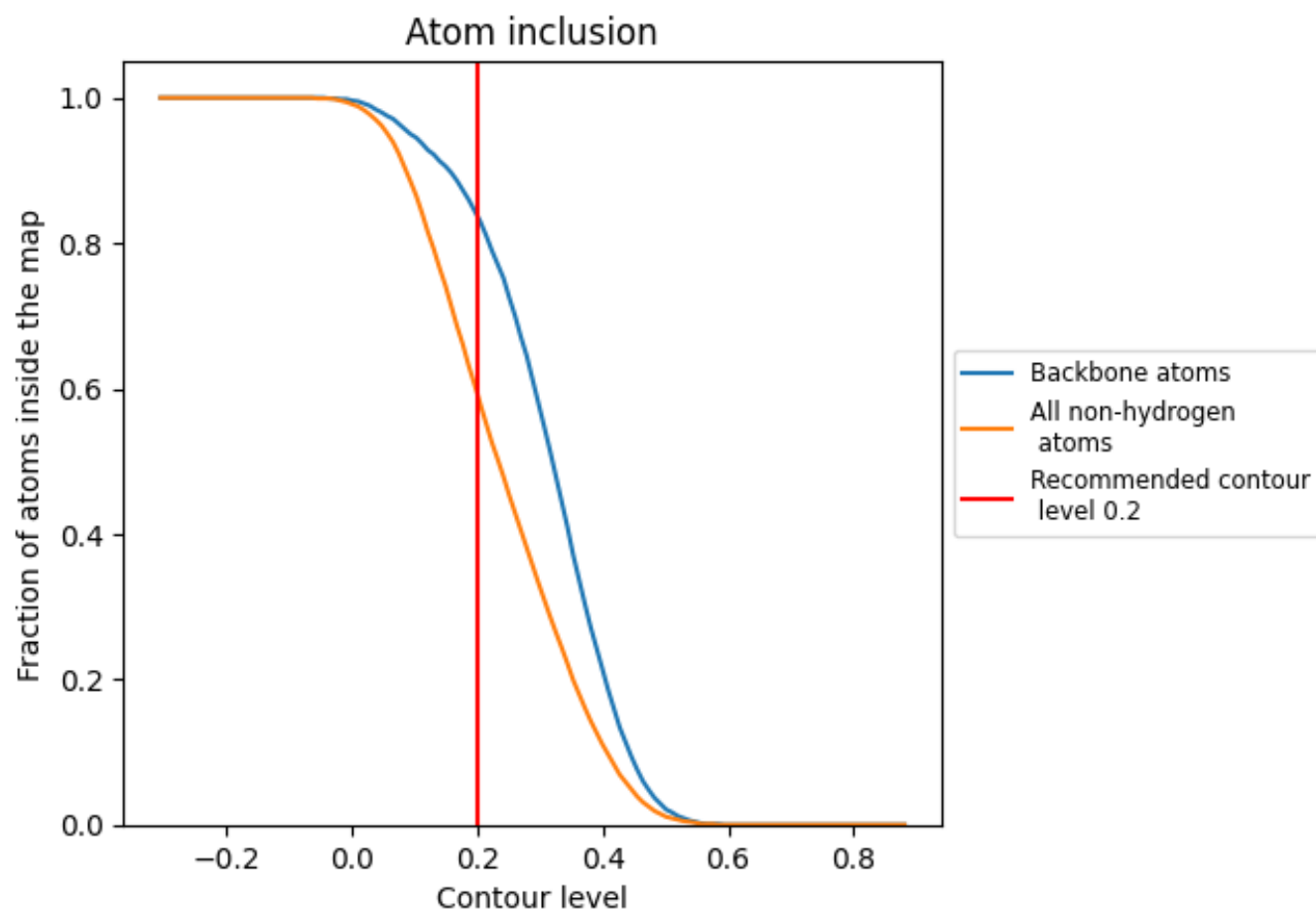
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 59% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5920	<div></div> 0.2940
A	<div></div> 0.5920	<div></div> 0.2940

