



Full wwPDB EM Validation Report ⓘ

May 26, 2025 – 04:11 PM EDT

PDB ID : 9BN1 / pdb_00009bn1
EMDB ID : EMD-44718
Title : State-8 of motor domain from full-length human dynein-1 in apo condition
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.80 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

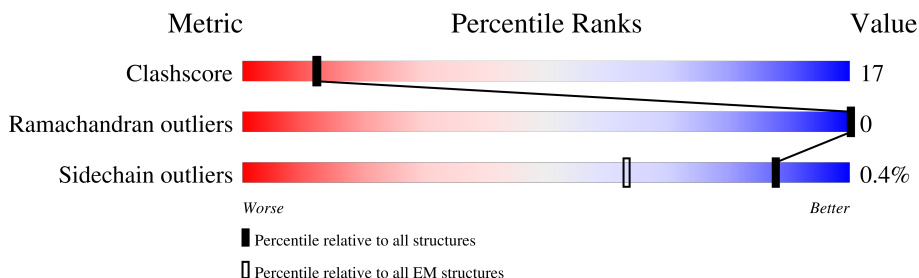
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	4646	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 24476 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 Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3029	24390	15542	4208	4518	122	0	0

- Molecule 2 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
			Total	C	N	O	P	
2	A	1	31	10	5	13	3	0

- Molecule 3 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
3	A	1	Total 27	C 10	N 5	O 10	P 2	0
3	A	1	Total 27	C 10	N 5	O 10	P 2	0

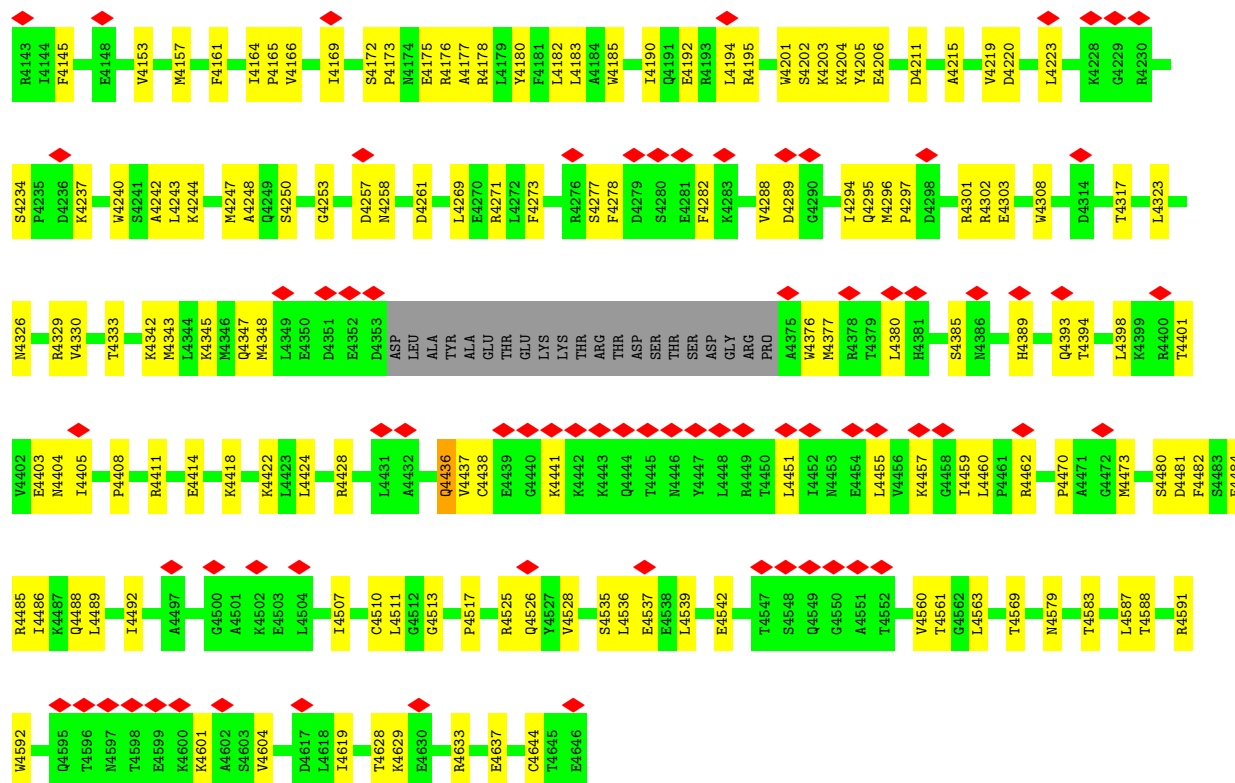
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Mg 1 1	0

V1880	A1898	A1908	G1909	E1914	L1923	G1924	R1925	F1926	V1927	L1928	V1929	F1930	D1933	E1934	F1938	Q1939	A1940	M1941	G1942	R1943	I1944	G1947	L1948	C1949	Q1950	V1951	W1954	N1961	R1962	L1963	E1964	E1965	R1966	M1967	V1971	Q1974	I1978	Q1979	L1982	R1983																			
S1796	L1803	R1804	R1805	K1806	L1807	L1808	E1809	H1810	L1811	L1812	L1815	H1816	H1817	D1820	V1821	T1822	I1826	I1830	S1835	F1836	E1837	K1849	Q1850	T1851	Q1856	L1857	S1858	I1859	Q1860	M1861	A1862	N1863	A1864	K1865	F1866	N1867	E1871	Y1872	G1873	V1875	Q1876	L1877	K1878	L1879															
K1697	M1698	N1699	E1700	W1701	L1702	V1705	E1706	K1707	E1708	V1711	K1715	A1718	E1719	S1720	V1721	V1724	K1729	A1730	T1731	S1732	I1733	Y1738	D1743	A1747	V1751	L1752	Q1755	I1756	A1765	L1766	M1769	G1770	G1771	G1772	G1773	D1774	V1785	E1786	L1789	L1792	A1793	D1794																	
Q1598	R1599	S1600	L1601	E1602	R1603	L1604	E1620	R1623	F1626	P1627	F1628	F1629	D1634	L1637	L1638	S1644	K1645	K1649	L1650	Q1651	H1652	F1653	F1654	K1655	M1656	M1657	V1661	N1667	E1668	V1672	V1673	L1674	G1675	I1676	R1679	V1684	M1685	F1686	K1687	V1690	S1691	I1692	T1693	E1694	H1695														
F1516	L1521	S1522	W1523	E1524	R1529	K1530	L1533	F1534	D1535	V1536	W1537	W1544	Y1545	Y1546	L1547	E1548	G1549	I1550	F1551	T1552	G1553	S1554	A1555	D1556	I1557	K1558	H1559	L1560	L1561	P1562	V1563	E1564	T1565	F1568	I1571	S1572	M1579	K1580	V1581	V1582	S1583	K1584	M1589	D1590	V1591	L1592	M1593	I1594	Q1595	G1596	V1597								
K1441	M1442	E1443	A1444	I1445	V1446	K1447	D1448	V1449	L1450	L1451	V1452	E1456	M1457	E1460	E1461	F1462	L1463	K1464	Q1465	L1466	R1467	N1471	T1472	Y1473	E1474	L1475	D1476	L1477	V1478	N1479	Y1480	Q1481	C1484	R1485	L1486	T1487	R1488	D1491	D1492	N1495	E1499	H1500	V1504	M1507	K1508	L1509	S1510	P1511	Y1512										
A1381	S1382	Y1383	E1384	F1385	V1386	Q1387	R1388	L1389	L1390	K1391	G1392	Y1393	M1394	K1395	I1396	N1397	M1398	L1399	V1400	I1401	E1402	L1403	K1404	S1405	E1406	A1407	L1408	K1409	D1410	R1411	H1412	V1413	K1414	Q1415	L1416	M1417	K1418	R1419	L1420	H1421	V1422	N1423	W1424	V1425	V1426	S1427	E1428	L1429	T1430	L1431	G1432	Q1433	I1434	W1435	D1436	V1437	D1438	L1439	Q1440
VAL	ALA	LEU	GLU	LEU	Q1327	D1328	L1329	K1330	G1331	V1332	W1333	S1334	E1335	L1336	S1337	K1338	V1339	W1340	E1341	Q1342	I1343	D1344	Q1345	M1346	K1347	E1348	Q1349	W1350	W1351	V1352	S1353	V1354	Q1355	P1356	R1357	K1358	L1359	R1360	Q1361	N1362	L1363	D1364	A1365	L1366	L1367	M1368	Q1369	L1370	K1371	S1372	F1373	P1374	A1375	R1376	L1377	R1378	Q1379	Y1380	
TRP	GLU	PHE	GLN	PHE	PRO	SER	TRP	THR	ASN	TYR	ILE	GLU	GLY	GLN	TRP	GLY	ALA	THR	ASP	GLY	LYS	PHE	ARG	GLY	THR	ILE	GLN	VAL	ALA	LYS	GLY	GLU	ALA	ILE	LYS	MET	ASP	ARG	GLN	TRP	THR	ASP	VAL	GLN	GLY	THR	ARG	GLY	THR	ARG	GLN								
ARG	PHE	GLN	PHE	PRO	PRO	SER	TRP	THR	ASN	TYR	ILE	GLU	GLY	GLN	TRP	GLY	ALA	THR	ASP	GLY	LYS	PHE	ARG	GLY	THR	ILE	GLN	VAL	ALA	LYS	GLY	GLU	ALA	ILE	LYS	MET	ASP	ARG	GLN	TRP	THR	ASP	VAL	GLN	GLY	THR	ARG	GLY	THR	ARG	GLN								
GLU	PHE	HIS	SER	GLN	ILE	SER	LYS	SER	GLN	GLU	LEU	GLU	HIS	SER	VAL	ASP	THR	ALA	THR	VAL	ASP	GLN	GLN	GLN	GLN	GLN	GLN	VAL	VAL	ASN	LEU	ARG	LYS	ILE	LYS	PHE	GLU	LYS	VAL	GLN	GLY	THR	ARG	GLY	THR	ARG	GLY	THR	ARG	GLN									
ASN	LYS	LEU	ASP	GLN	MET	GLN	ILE	GLU	VAL	ARG	PRO	GLU	ASP	GLY	VAL	VAL	ARG	LEU	GLU	VAL	ALA	TRP	ARG	LEU	GLY	VAL	VAL	VAL	VAL	ASP	MET	GLN	TRP	ASP	VAL	GLN	PRO	ALA	VAL	VAL	VAL	HIS	ASP	GLY	THR	ARG	GLY	THR	ARG	GLN									
PHE	ASN	PHE	GLN	GLY	LYS	VAL	ASP	ASP	LEU	ILE	ILE	GLU	GLY	GLN	GLY	ASP	LEU	GLU	VAL	GLU	VAL	GLY	TRP	ARG	LEU	GLY	VAL	VAL	VAL	ASP	MET	GLN	TRP	ASP	VAL	GLN	PRO	ALA	VAL	VAL	VAL	HIS	ASP	GLY	THR	ARG	GLY	THR	ARG	GLN									







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50945	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)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.817	Depositor
Minimum map value	-0.311	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	333.312, 333.312, 333.312	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: MG, 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	0/24908	0.40	1/33751 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1862	ALA	CB-CA-C	-5.13	110.68	116.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1603	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	24390	0	24462	826	0
2	A	31	0	12	4	0
3	A	54	0	24	7	0
4	A	1	0	0	0	0
All	All	24476	0	24498	826	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (826) 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:1457:MET:HE1	1:A:3659:ARG:HA	1.41	1.03
1:A:2444:GLU:H	1:A:2510:MET:HE1	1.33	0.92
1:A:2667:ASN:HD22	1:A:2712:CYS:HB2	1.35	0.91
1:A:1550:ILE:HG23	1:A:1638:LEU:HD21	1.51	0.90
1:A:3206:ARG:HH12	1:A:3209:LYS:HD3	1.35	0.89
1:A:2232:MET:HE3	1:A:2232:MET:H	1.37	0.88
1:A:2307:VAL:HA	1:A:2311:TRP:HE1	1.42	0.83
1:A:2238:LEU:HD11	1:A:2249:GLY:HA3	1.63	0.80
1:A:4169:ILE:HD11	1:A:4177:ALA:HA	1.63	0.80
1:A:3207:LYS:HZ1	1:A:3753:LEU:HB3	1.47	0.78
1:A:1360:ARG:NH2	1:A:2902:GLU:OE1	2.17	0.76
1:A:3889:ARG:HH22	1:A:4347:GLN:HG3	1.51	0.76
1:A:1411:ARG:HA	1:A:1414:LYS:HE2	1.66	0.75
1:A:1462:PHE:HB2	1:A:3628:ARG:HD3	1.69	0.75
1:A:3212:VAL:HG22	1:A:3482:LEU:HD13	1.69	0.75
1:A:4377:MET:HE3	1:A:4438:CYS:HA	1.67	0.75
1:A:4539:LEU:HD12	1:A:4592:TRP:HB3	1.68	0.74
1:A:3659:ARG:HE	1:A:3661:LEU:HD21	1.49	0.74
1:A:1417:MET:HE1	1:A:1424:TRP:HB2	1.70	0.73
1:A:2304:ASP:OD1	1:A:2726:ARG:NH2	2.21	0.73
1:A:3662:ILE:HD11	1:A:3671:LEU:HD12	1.69	0.73
1:A:3481:SER:HB3	1:A:3770:LEU:HD22	1.69	0.72
1:A:2294:GLU:O	1:A:2299:GLN:NE2	2.22	0.72
1:A:3951:VAL:HA	1:A:3957:PHE:CE2	2.25	0.72
1:A:2874:SER:HB2	1:A:2920:LEU:HD11	1.70	0.71
1:A:3115:LEU:HG	1:A:3143:ILE:HG13	1.72	0.70
1:A:3488:ARG:HA	1:A:3491:LYS:HD3	1.73	0.70
1:A:3536:LEU:HB3	1:A:3541:ILE:HB	1.71	0.70
1:A:1530:ILE:HD11	1:A:1589:MET:HE1	1.74	0.70
1:A:2581:LEU:HD12	1:A:2591:LEU:HD21	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2856:LYS:HG3	1:A:2857:HIS:HD2	1.56	0.70
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.73	0.69
1:A:1963:LEU:HB3	1:A:1967:MET:HG3	1.75	0.69
1:A:3838:ASN:OD1	1:A:3870:ARG:NH2	2.25	0.69
1:A:2606:PHE:HE1	1:A:2617:VAL:HG11	1.57	0.69
1:A:3885:MET:HE1	1:A:4008:PHE:HD2	1.56	0.68
1:A:4085:ASN:O	1:A:4089:LYS:NZ	2.26	0.68
1:A:4234:SER:HB3	1:A:4237:LYS:HG2	1.76	0.68
1:A:2845:TRP:O	1:A:2849:ASN:ND2	2.24	0.68
1:A:4173:PRO:HD2	1:A:4223:LEU:HD21	1.75	0.68
1:A:4244:LYS:NZ	1:A:4273:PHE:O	2.24	0.68
1:A:3835:ILE:HD12	1:A:3870:ARG:HG3	1.75	0.67
1:A:2964:HIS:HA	1:A:3643:PRO:HG2	1.76	0.67
1:A:2096:VAL:HG12	1:A:2097:LEU:HD23	1.76	0.67
1:A:3532:TRP:O	1:A:3536:LEU:HD12	1.94	0.67
1:A:1835:SER:OG	1:A:1837:GLU:OE1	2.11	0.67
1:A:1964:GLU:HG2	1:A:1967:MET:HE3	1.77	0.67
1:A:2377:ASN:OD1	2:A:4701:ATP:O2'	2.12	0.67
1:A:1861:MET:HE1	1:A:1889:TYR:HB3	1.76	0.67
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.77	0.67
1:A:1420:LEU:HD13	1:A:1437:VAL:HG11	1.76	0.67
1:A:2053:MET:HE2	1:A:2097:LEU:HB2	1.76	0.66
1:A:2652:PRO:HB3	1:A:2659:LEU:HD12	1.77	0.66
1:A:4003:ALA:O	1:A:4006:HIS:HB3	1.95	0.66
1:A:1356:PRO:HB2	1:A:1401:ILE:HD13	1.77	0.66
1:A:2577:HIS:O	1:A:2581:LEU:HD22	1.96	0.66
1:A:4180:TYR:OH	1:A:4220:ASP:OD2	2.12	0.66
1:A:3475:SER:O	1:A:3479:LEU:HD22	1.96	0.66
1:A:3559:ARG:NH2	1:A:3737:GLU:OE1	2.28	0.66
1:A:2775:GLU:O	1:A:2779:MET:HG3	1.96	0.66
1:A:1478:VAL:HG11	1:A:1488:ARG:HE	1.61	0.66
1:A:3133:LEU:HD11	1:A:3141:GLU:HB3	1.76	0.66
1:A:3731:LEU:HD13	1:A:3734:LEU:HD22	1.77	0.65
1:A:3973:LEU:HD12	1:A:3992:LEU:HD11	1.78	0.65
1:A:3875:MET:HE1	1:A:3883:PHE:HB2	1.76	0.65
1:A:1598:GLN:NE2	1:A:1602:GLU:OE2	2.28	0.65
1:A:2210:LEU:O	1:A:2214:THR:HG23	1.97	0.65
1:A:3856:LEU:O	1:A:3860:THR:HG23	1.96	0.65
1:A:1941:MET:SD	1:A:1942:GLY:N	2.70	0.65
1:A:2970:GLU:N	1:A:2970:GLU:OE1	2.26	0.65
1:A:2382:LEU:HD22	1:A:2420:ALA:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3186:LEU:HD21	1:A:3510:SER:HB2	1.77	0.64
1:A:3537:GLN:HB3	1:A:3543:PHE:HE1	1.62	0.64
1:A:1551:PHE:HB3	1:A:1558:LYS:HZ3	1.61	0.64
1:A:2043:LYS:HE3	1:A:2044:PRO:HD2	1.79	0.64
1:A:4075:GLU:O	1:A:4079:GLN:NE2	2.27	0.64
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.79	0.64
1:A:1510:SER:HB2	1:A:3629:PHE:HB3	1.79	0.63
1:A:3115:LEU:HD23	1:A:3140:ARG:HD3	1.79	0.63
1:A:4157:MET:HE1	1:A:4185:TRP:HA	1.79	0.63
1:A:2414:GLN:NE2	1:A:2418:ASP:OD1	2.22	0.63
1:A:3146:SER:O	1:A:3150:VAL:HG23	1.98	0.63
1:A:3879:ASP:OD2	1:A:4342:LYS:NZ	2.30	0.63
1:A:3585:ARG:NH1	1:A:3694:SER:O	2.32	0.62
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.64	0.62
1:A:3167:ARG:NH1	1:A:3519:TYR:OH	2.32	0.62
1:A:4097:LYS:HA	1:A:4127:THR:HG23	1.81	0.62
1:A:2987:ASN:OD1	1:A:3057:GLN:NE2	2.32	0.62
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.81	0.62
1:A:2346:GLN:HB2	1:A:2726:ARG:HD2	1.81	0.62
1:A:2752:ASN:ND2	1:A:2766:ALA:O	2.32	0.62
1:A:3553:LEU:HB2	1:A:3578:ILE:HD13	1.82	0.62
1:A:4206:GLU:N	1:A:4206:GLU:OE1	2.33	0.62
1:A:2536:ASP:OD1	1:A:2576:ARG:NH1	2.33	0.62
1:A:4247:MET:HE3	1:A:4247:MET:HA	1.81	0.62
1:A:4248:ALA:HB2	1:A:4269:LEU:HD12	1.81	0.62
1:A:4042:LEU:HD23	1:A:4128:MET:HE1	1.82	0.62
1:A:2312:VAL:HA	1:A:2315:LEU:HD12	1.81	0.62
1:A:1351:TRP:HE3	1:A:1429:LEU:HB3	1.65	0.62
1:A:1460:GLU:HA	1:A:1463:LEU:HG	1.81	0.62
1:A:2088:PHE:CE2	1:A:2145:MET:HE2	2.34	0.61
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	1.82	0.61
1:A:3211:THR:O	1:A:3215:VAL:HG22	1.99	0.61
1:A:1965:GLU:OE1	1:A:1965:GLU:N	2.32	0.61
1:A:2210:LEU:HD22	1:A:2222:MET:HE1	1.83	0.61
1:A:2222:MET:HB2	1:A:2344:GLU:HA	1.82	0.61
1:A:2603:MET:HE1	3:A:4702:ADP:N6	2.15	0.61
1:A:4247:MET:HB2	1:A:4269:LEU:HD11	1.83	0.61
1:A:2715:PRO:HA	1:A:2720:ARG:HB3	1.83	0.61
1:A:3828:SER:HB2	1:A:4140:ARG:HG3	1.81	0.61
1:A:1408:LEU:HD21	1:A:1450:LEU:HD22	1.81	0.61
1:A:3158:ASN:ND2	1:A:3169:MET:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4013:LEU:HB3	1:A:4017:PHE:CD2	2.36	0.61
1:A:4401:THR:OG1	1:A:4404:ASN:ND2	2.33	0.61
1:A:2386:PRO:HG3	1:A:2413:LEU:HD22	1.83	0.61
1:A:3917:SER:HB2	1:A:3920:SER:HB3	1.82	0.60
1:A:1477:LEU:HD11	1:A:1582:VAL:HG12	1.83	0.60
1:A:1816:VAL:HG11	1:A:2052:VAL:HG12	1.83	0.60
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.82	0.60
1:A:2940:GLY:HA3	1:A:3174:ARG:HG3	1.83	0.60
1:A:1650:LEU:HD21	1:A:1698:ILE:HD11	1.83	0.60
1:A:1923:LEU:O	1:A:1925:ARG:NH1	2.34	0.60
1:A:1701:TRP:O	1:A:1705:VAL:HG23	2.01	0.60
1:A:3206:ARG:NH1	1:A:3209:LYS:HD3	2.13	0.60
1:A:2088:PHE:HE2	1:A:2145:MET:HE2	1.67	0.60
1:A:2889:LEU:HD21	1:A:2920:LEU:HD21	1.83	0.60
1:A:1880:VAL:HG21	1:A:2052:VAL:HG21	1.83	0.60
1:A:2665:GLU:HB3	1:A:2668:LEU:HB2	1.82	0.60
1:A:2581:LEU:HD12	1:A:2591:LEU:CD2	2.32	0.60
1:A:3892:LEU:HD11	1:A:3983:ILE:HG21	1.84	0.60
1:A:4403:GLU:OE2	1:A:4403:GLU:N	2.33	0.60
1:A:2558:GLU:HG2	1:A:2560:HIS:H	1.67	0.59
1:A:3791:MET:SD	1:A:3791:MET:N	2.74	0.59
1:A:2683:ILE:O	1:A:2687:VAL:HG12	2.02	0.59
1:A:3606:ASP:N	1:A:3606:ASP:OD1	2.33	0.59
1:A:1419:ARG:NH2	1:A:1448:ASP:OD2	2.35	0.59
1:A:3107:LYS:NZ	1:A:3140:ARG:HB3	2.17	0.59
1:A:2747:ILE:HD11	3:A:4702:ADP:C6	2.36	0.59
1:A:4393:GLN:HG2	1:A:4394:THR:HG22	1.84	0.59
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.84	0.59
1:A:4525:ARG:HG2	1:A:4536:LEU:HD22	1.82	0.59
1:A:1674:LEU:HB3	1:A:1685:MET:HE1	1.85	0.59
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.35	0.59
1:A:4482:PHE:O	1:A:4486:ILE:HG12	2.02	0.59
1:A:2444:GLU:N	1:A:2510:MET:HE1	2.11	0.59
1:A:4105:TRP:CE2	1:A:4109:LEU:HD21	2.38	0.59
1:A:2423:MET:HE1	1:A:2462:LEU:HD13	1.85	0.58
1:A:2943:LYS:N	3:A:4703:ADP:O1B	2.36	0.58
1:A:3933:GLU:OE1	1:A:3937:ARG:NH2	2.34	0.58
1:A:1812:ILE:O	1:A:1816:VAL:HG12	2.02	0.58
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.84	0.58
1:A:2598:GLY:HA3	1:A:2795:SER:HB2	1.84	0.58
1:A:3148:VAL:O	1:A:3152:GLN:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3101:ALA:O	1:A:3105:VAL:HG23	2.03	0.58
1:A:3882:THR:O	1:A:3886:LEU:HD22	2.04	0.58
1:A:4202:SER:OG	1:A:4261:ASP:OD2	2.21	0.58
1:A:2503:SER:HB3	1:A:2514:LEU:HD13	1.85	0.58
1:A:2527:PRO:HD3	1:A:2545:TRP:CE2	2.38	0.58
1:A:4511:LEU:HG	1:A:4560:VAL:HG11	1.84	0.58
1:A:1331:GLY:O	1:A:1335:GLU:HG2	2.04	0.58
1:A:1589:MET:SD	1:A:1589:MET:N	2.77	0.58
1:A:2677:GLN:HB2	1:A:2680:ILE:HG12	1.84	0.58
1:A:3739:GLN:O	1:A:3743:ARG:HG2	2.03	0.58
1:A:3692:LEU:O	1:A:3696:VAL:HG12	2.04	0.58
1:A:3885:MET:HE3	1:A:3885:MET:HA	1.86	0.58
1:A:3910:ARG:HH21	1:A:4348:MET:HE2	1.67	0.58
1:A:1738:TYR:HE2	1:A:1792:LEU:HD21	1.69	0.57
1:A:2202:MET:SD	1:A:2202:MET:N	2.77	0.57
1:A:2816:LEU:HD23	1:A:2821:LEU:HD22	1.86	0.57
1:A:2889:LEU:O	1:A:2893:VAL:HG12	2.04	0.57
1:A:4398:LEU:HD12	1:A:4414:GLU:HG2	1.85	0.57
1:A:4436:GLN:HG3	1:A:4441:LYS:HB3	1.85	0.57
1:A:1484:CYS:HB2	1:A:1579:MET:HG3	1.87	0.57
1:A:1695:HIS:HB3	1:A:1700:GLU:HG3	1.87	0.57
1:A:1891:THR:HG22	1:A:4250:SER:HA	1.87	0.57
1:A:2581:LEU:O	1:A:2585:LEU:HG	2.04	0.57
1:A:2654:GLN:NE2	1:A:2655:LEU:O	2.37	0.57
1:A:4103:PRO:HA	1:A:4106:LEU:HD12	1.86	0.57
1:A:3871:VAL:HG12	1:A:3875:MET:HE2	1.86	0.57
1:A:1452:VAL:O	1:A:1456:GLU:HG2	2.04	0.57
1:A:1530:ILE:HG23	1:A:1534:PHE:CE1	2.39	0.57
1:A:1731:THR:OG1	1:A:1732:SER:N	2.37	0.57
1:A:2210:LEU:HG	1:A:2237:LEU:HD23	1.87	0.57
1:A:2964:HIS:ND1	1:A:2965:ARG:O	2.37	0.57
1:A:3040:GLU:OE1	1:A:3053:TRP:NE1	2.38	0.57
1:A:2096:VAL:HG22	1:A:2144:THR:HG21	1.87	0.56
1:A:3514:ILE:HD11	1:A:3582:ARG:HB2	1.86	0.56
1:A:1342:GLN:O	1:A:1346:MET:HG3	2.05	0.56
1:A:1425:VAL:HB	1:A:1428:GLU:HB3	1.87	0.56
1:A:1644:SER:OG	1:A:1645:LYS:NZ	2.38	0.56
1:A:2048:LEU:O	1:A:2052:VAL:HG22	2.05	0.56
1:A:3110:THR:HB	1:A:3113:MET:HG3	1.87	0.56
1:A:2839:GLU:OE1	1:A:2841:GLU:HB3	2.05	0.56
1:A:2028:LEU:HD23	1:A:2033:LYS:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2526:LEU:HG	1:A:2527:PRO:HD2	1.87	0.56
1:A:2679:VAL:O	1:A:2683:ILE:HG13	2.06	0.56
1:A:3731:LEU:HG	1:A:3791:MET:HE1	1.87	0.56
1:A:4288:VAL:HG11	1:A:4294:ILE:HD11	1.87	0.56
1:A:1628:ARG:HG2	1:A:1657:MET:SD	2.46	0.56
1:A:2808:GLU:OE2	1:A:2811:ARG:NH2	2.38	0.56
1:A:2999:VAL:HG13	1:A:3005:LEU:HD21	1.88	0.56
1:A:1933:ASP:OD1	1:A:1933:ASP:N	2.36	0.55
1:A:2573:ASP:O	1:A:2577:HIS:ND1	2.33	0.55
1:A:3654:ARG:HH22	1:A:3663:THR:H	1.54	0.55
1:A:2127:ILE:O	1:A:2131:LEU:HG	2.06	0.55
1:A:3483:SER:O	1:A:3487:GLU:HG2	2.06	0.55
1:A:2190:TYR:O	1:A:2377:ASN:ND2	2.39	0.55
1:A:1974:GLN:O	1:A:1978:ILE:HG12	2.06	0.55
1:A:2126:GLU:O	1:A:2130:ASN:ND2	2.40	0.55
1:A:2375:PHE:HE2	1:A:2455:LEU:HD11	1.72	0.55
1:A:4169:ILE:HG21	1:A:4302:ARG:HD3	1.89	0.55
1:A:2147:PRO:HG3	1:A:2209:GLN:HB3	1.89	0.55
1:A:2910:VAL:HG11	1:A:3105:VAL:HG22	1.89	0.55
1:A:3175:HIS:CE1	1:A:3585:ARG:HH12	2.25	0.55
1:A:2373:MET:HE3	2:A:4701:ATP:N3	2.21	0.55
1:A:3130:TYR:CZ	1:A:3132:LYS:HB3	2.42	0.55
1:A:1362:ASN:OD1	1:A:1363:LEU:N	2.38	0.55
1:A:1397:ASN:O	1:A:1401:ILE:HG12	2.07	0.55
1:A:2143:GLU:OE2	1:A:2170:TYR:OH	2.25	0.55
1:A:3126:MET:HG3	1:A:3128:VAL:HG23	1.88	0.55
1:A:3191:ARG:HG2	1:A:3503:ILE:HD13	1.89	0.55
1:A:4542:GLU:HB2	1:A:4591:ARG:HG2	1.89	0.55
1:A:2510:MET:HA	1:A:2513:GLU:HG2	1.89	0.55
1:A:3586:TYR:O	1:A:3696:VAL:HG23	2.06	0.55
1:A:2684:ARG:HH22	1:A:2726:ARG:HH21	1.55	0.54
1:A:2995:ASP:OD1	1:A:2996:GLU:N	2.34	0.54
1:A:4108:GLN:HA	1:A:4111:LYS:HD2	1.89	0.54
1:A:2229:GLY:N	2:A:4701:ATP:O1A	2.37	0.54
1:A:2277:ASP:OD1	1:A:2285:ARG:NH2	2.33	0.54
1:A:2961:ILE:HD11	1:A:2998:ASN:HD22	1.72	0.54
1:A:4023:GLN:HG2	1:A:4024:PRO:HD2	1.89	0.54
1:A:4088:VAL:HG23	1:A:4118:PRO:HA	1.89	0.54
1:A:2994:MET:HE2	1:A:3066:PHE:HE1	1.72	0.54
1:A:3807:ALA:O	1:A:3811:ILE:HG12	2.07	0.54
1:A:1466:ILE:HD12	1:A:1500:HIS:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2499:LEU:HD21	1:A:2518:ILE:HG21	1.89	0.54
1:A:2935:LEU:HD22	1:A:3094:PHE:HE1	1.73	0.54
1:A:4088:VAL:HG21	1:A:4116:LEU:HD11	1.89	0.54
1:A:2644:THR:OG1	1:A:2647:GLY:O	2.23	0.54
1:A:3505:GLY:O	1:A:3509:LEU:HD23	2.08	0.54
1:A:2224:GLY:O	1:A:2230:LYS:NZ	2.40	0.54
1:A:2366:GLU:OE2	1:A:2451:ARG:NH2	2.41	0.54
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.41	0.54
1:A:4408:PRO:O	1:A:4411:ARG:HG2	2.08	0.54
1:A:4042:LEU:HD21	1:A:4138:LEU:HG	1.89	0.54
1:A:2609:LEU:HD22	1:A:2615:MET:HG3	1.89	0.53
1:A:2664:ASP:OD1	1:A:2665:GLU:HG2	2.07	0.53
1:A:2873:TYR:CE2	1:A:2883:PRO:HD3	2.43	0.53
1:A:4051:ALA:HA	1:A:4054:HIS:CE1	2.43	0.53
1:A:4240:TRP:HB3	1:A:4244:LYS:NZ	2.23	0.53
1:A:2175:MET:HB3	1:A:2178:LEU:HD13	1.89	0.53
1:A:2299:GLN:O	1:A:2339:VAL:HA	2.07	0.53
1:A:2602:THR:HG22	1:A:2662:PHE:HZ	1.73	0.53
1:A:2614:ASP:O	1:A:2615:MET:HE2	2.07	0.53
1:A:4082:LYS:O	1:A:4086:THR:HG23	2.08	0.53
1:A:2175:MET:SD	1:A:2175:MET:N	2.82	0.53
1:A:3100:GLU:HG2	1:A:3130:TYR:HE1	1.74	0.53
1:A:3592:PRO:HB3	1:A:3684:PRO:HD3	1.90	0.53
1:A:2757:ARG:HG3	1:A:2763:ARG:HH22	1.74	0.53
1:A:2030:ASP:HA	1:A:2033:LYS:HB2	1.89	0.53
1:A:2438:GLU:O	1:A:2442:GLN:HG2	2.08	0.53
1:A:2585:LEU:HB3	1:A:2707:GLN:HE22	1.73	0.53
1:A:1858:SER:HB3	1:A:1865:LYS:HE2	1.91	0.53
1:A:3133:LEU:HD12	1:A:3134:PRO:HD2	1.90	0.53
1:A:2124:GLU:HA	1:A:2127:ILE:HD12	1.90	0.53
1:A:2603:MET:HE1	3:A:4702:ADP:C6	2.43	0.53
1:A:3873:ARG:HH12	1:A:4021:MET:HA	1.73	0.53
1:A:2994:MET:HE2	1:A:3066:PHE:CE1	2.44	0.52
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.92	0.52
1:A:3654:ARG:CZ	1:A:3663:THR:HG23	2.38	0.52
1:A:1792:LEU:O	1:A:1796:VAL:HG12	2.08	0.52
1:A:1961:ASN:ND2	1:A:2019:ASN:O	2.43	0.52
1:A:2257:LYS:O	1:A:2678:ARG:NE	2.39	0.52
1:A:4459:ILE:HG22	1:A:4462:ARG:HH12	1.73	0.52
1:A:4535:SER:OG	1:A:4537:GLU:OE1	2.27	0.52
1:A:2307:VAL:HG13	1:A:2312:VAL:HG11	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2538:GLU:HB2	1:A:2548:TRP:CE2	2.44	0.52
1:A:2671:MET:HE2	1:A:2721:LYS:HG2	1.92	0.52
1:A:3851:ASP:HB3	1:A:3854:GLN:HB2	1.92	0.52
1:A:3989:ARG:O	1:A:4004:MET:HE1	2.10	0.52
1:A:2795:SER:OG	1:A:2798:GLU:OE1	2.21	0.52
1:A:3645:LEU:HD12	1:A:3648:VAL:HB	1.92	0.52
1:A:2503:SER:HB2	1:A:2511:ARG:HG2	1.91	0.52
1:A:1971:VAL:HA	1:A:1974:GLN:OE1	2.09	0.52
1:A:2445:HIS:NE2	1:A:2449:LEU:HD22	2.25	0.52
1:A:2515:GLY:O	1:A:2518:ILE:HG22	2.10	0.52
1:A:3789:ILE:HD12	1:A:3792:GLN:NE2	2.23	0.52
1:A:4080:ALA:O	1:A:4084:ILE:HG12	2.10	0.52
1:A:1410:ASP:O	1:A:1414:LYS:HG3	2.09	0.52
1:A:1530:ILE:HG23	1:A:1534:PHE:HE1	1.74	0.52
1:A:1667:ASN:HB2	1:A:1672:VAL:HG22	1.92	0.52
1:A:4108:GLN:O	1:A:4112:LYS:HG2	2.08	0.51
1:A:4561:THR:HG22	1:A:4587:LEU:HD23	1.92	0.51
1:A:1397:ASN:O	1:A:1397:ASN:ND2	2.37	0.51
1:A:2629:GLU:O	1:A:2633:LYS:HG2	2.10	0.51
1:A:3219:ARG:HD3	1:A:3479:LEU:HD21	1.92	0.51
1:A:3954:ASP:HB3	1:A:3957:PHE:CD2	2.45	0.51
1:A:1802:PRO:O	1:A:1806:ARG:HG2	2.11	0.51
1:A:3703:VAL:HG21	1:A:3829:LEU:HD22	1.93	0.51
1:A:1626:PHE:HB3	1:A:1629:PHE:CD2	2.45	0.51
1:A:1698:ILE:HA	1:A:1701:TRP:NE1	2.25	0.51
1:A:1938:PHE:HA	1:A:1941:MET:HG3	1.92	0.51
1:A:2893:VAL:HG11	1:A:2916:LEU:HD21	1.93	0.51
1:A:3208:ILE:O	1:A:3212:VAL:HG23	2.10	0.51
1:A:4569:THR:HG22	1:A:4583:THR:HG21	1.92	0.51
1:A:2134:GLN:O	1:A:2138:ILE:HG22	2.10	0.51
1:A:2666:ILE:HG22	1:A:2712:CYS:HB3	1.93	0.51
1:A:3886:LEU:O	1:A:3890:ILE:HG12	2.11	0.51
1:A:1769:MET:HE2	1:A:1774:ASP:O	2.11	0.51
1:A:1944:ILE:O	1:A:1948:LEU:HG	2.11	0.51
1:A:3139:HIS:O	1:A:3143:ILE:HG12	2.10	0.51
1:A:4488:GLN:O	1:A:4492:ILE:HG12	2.11	0.51
1:A:1961:ASN:ND2	1:A:2019:ASN:H	2.09	0.51
1:A:2660:VAL:HA	1:A:2707:GLN:O	2.10	0.51
1:A:3544:ARG:HB2	1:A:3547:ILE:HD11	1.92	0.51
1:A:1546:TYR:O	1:A:1550:ILE:HG12	2.11	0.51
1:A:1752:LEU:O	1:A:1756:ILE:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1810:HIS:NE2	1:A:1876:GLN:O	2.44	0.51
1:A:1817:HIS:O	1:A:1821:VAL:HG12	2.10	0.51
1:A:2791:HIS:HB3	1:A:3086:PHE:HE1	1.76	0.51
1:A:2028:LEU:HD23	1:A:2033:LYS:HG3	1.91	0.50
1:A:2057:GLN:NE2	1:A:2098:VAL:HA	2.27	0.50
1:A:2937:GLY:HA2	1:A:3095:GLY:HA2	1.92	0.50
1:A:1473:TYR:OH	1:A:1492:ASP:OD2	2.24	0.50
1:A:1816:VAL:HG11	1:A:2052:VAL:CG1	2.41	0.50
1:A:1850:GLN:HB2	1:A:1856:GLN:HG2	1.92	0.50
1:A:2290:SER:HA	1:A:2294:GLU:HG2	1.92	0.50
1:A:2569:VAL:HB	1:A:2747:ILE:HG13	1.94	0.50
1:A:3140:ARG:O	1:A:3144:VAL:HG13	2.11	0.50
1:A:1521:LEU:HD13	1:A:1524:GLU:OE1	2.10	0.50
1:A:1747:ALA:HB2	1:A:1807:LYS:HG2	1.92	0.50
1:A:1562:PRO:O	1:A:1564:GLU:N	2.42	0.50
1:A:1650:LEU:HA	1:A:1653:HIS:HD2	1.75	0.50
1:A:2888:GLU:OE1	1:A:2888:GLU:N	2.42	0.50
1:A:1836:PHE:CD2	1:A:4242:ALA:HA	2.47	0.50
1:A:2818:VAL:O	1:A:2822:ILE:HG12	2.11	0.50
1:A:3544:ARG:HH11	1:A:3544:ARG:HG3	1.76	0.50
1:A:3580:LEU:HD21	1:A:3699:VAL:HG11	1.93	0.50
1:A:4288:VAL:HG21	1:A:4294:ILE:HG12	1.94	0.50
1:A:2373:MET:HE3	2:A:4701:ATP:C4	2.47	0.50
1:A:2513:GLU:O	1:A:2516:GLU:HG3	2.11	0.50
1:A:2050:ALA:O	1:A:2054:LEU:HG	2.11	0.50
1:A:2319:LEU:HB3	1:A:2358:ARG:HB3	1.93	0.50
1:A:4424:LEU:HD12	1:A:4486:ILE:HG21	1.93	0.50
1:A:2310:GLU:N	1:A:2310:GLU:OE2	2.44	0.50
1:A:2635:PHE:HB3	1:A:2650:LEU:HD21	1.94	0.50
1:A:4164:ILE:HD12	1:A:4165:PRO:HD2	1.93	0.50
1:A:2455:LEU:HD12	1:A:2459:PHE:CZ	2.47	0.49
1:A:2880:ASP:HB2	1:A:2882:ILE:HD11	1.94	0.49
1:A:3491:LYS:O	1:A:3495:THR:HG23	2.11	0.49
1:A:4385:SER:O	1:A:4389:HIS:ND1	2.45	0.49
1:A:4485:ARG:NH1	1:A:4513:GLY:O	2.46	0.49
1:A:1687:LYS:HG3	1:A:1715:LYS:HE3	1.94	0.49
1:A:2323:LYS:HB3	1:A:2335:LEU:HB3	1.94	0.49
1:A:4480:SER:O	1:A:4484:GLU:HG2	2.12	0.49
1:A:2278:GLY:N	1:A:2281:THR:OG1	2.45	0.49
1:A:2373:MET:HE2	1:A:2374:ILE:N	2.26	0.49
1:A:4099:VAL:HG22	1:A:4128:MET:HB2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1457:MET:HA	1:A:1460:GLU:HG3	1.94	0.49
1:A:1891:THR:HG21	1:A:2039:LEU:HD13	1.94	0.49
1:A:2053:MET:HB3	1:A:2097:LEU:HD12	1.93	0.49
1:A:3811:ILE:O	1:A:3815:MET:HG3	2.13	0.49
1:A:3881:ILE:HD13	1:A:4018:MET:HE1	1.93	0.49
1:A:1500:HIS:O	1:A:1504:VAL:HG12	2.13	0.49
1:A:1544:TRP:HE1	1:A:1572:SER:HA	1.77	0.49
1:A:1794:ASP:OD2	1:A:2060:ARG:NH1	2.45	0.49
1:A:2041:MET:HE3	1:A:2042:THR:H	1.78	0.49
1:A:1537:TRP:CE3	1:A:1601:LEU:HD11	2.47	0.49
1:A:3486:ARG:O	1:A:3490:GLU:HG2	2.12	0.49
1:A:4082:LYS:HD3	1:A:4082:LYS:N	2.28	0.49
1:A:1398:MET:SD	1:A:1399:LEU:N	2.85	0.49
1:A:2109:GLN:HB3	1:A:2113:ARG:NH2	2.28	0.49
1:A:3588:LEU:HB2	1:A:3696:VAL:HG21	1.94	0.49
1:A:3622:ASN:O	1:A:3625:SER:OG	2.25	0.49
1:A:3967:GLU:HB2	1:A:4004:MET:HB2	1.95	0.49
1:A:4297:PRO:HB3	1:A:4308:TRP:CD1	2.48	0.49
1:A:2028:LEU:HD21	1:A:2036:PHE:HB2	1.94	0.49
1:A:2332:ARG:HH21	1:A:2334:SER:HB3	1.77	0.49
1:A:3478:LEU:O	1:A:3482:LEU:HG	2.13	0.49
1:A:3989:ARG:C	1:A:4004:MET:HE1	2.37	0.49
1:A:4073:SER:OG	1:A:4075:GLU:OE1	2.30	0.49
1:A:4563:LEU:HD23	1:A:4644:CYS:HA	1.94	0.49
1:A:3517:ALA:HA	1:A:3520:PHE:HD1	1.78	0.49
1:A:3891:LYS:HD3	1:A:4013:LEU:HD23	1.95	0.49
1:A:1667:ASN:HD22	1:A:1672:VAL:HG22	1.77	0.49
1:A:1720:SER:O	1:A:1724:VAL:HG23	2.13	0.49
1:A:3986:ALA:HA	1:A:3989:ARG:HE	1.78	0.49
1:A:4257:ASP:OD1	1:A:4258:ASN:N	2.46	0.49
1:A:4377:MET:HE1	1:A:4437:VAL:HG12	1.95	0.49
1:A:1947:GLY:O	1:A:1951:VAL:HG22	2.13	0.48
1:A:2049:ILE:HG21	1:A:2090:LEU:HD11	1.95	0.48
1:A:4510:CYS:SG	1:A:4561:THR:OG1	2.69	0.48
1:A:1676:ILE:HG12	1:A:1684:VAL:HB	1.95	0.48
1:A:2071:PRO:O	1:A:2075:LEU:HG	2.12	0.48
1:A:2297:LYS:HB2	1:A:2299:GLN:HE21	1.78	0.48
1:A:2363:TRP:HE1	1:A:2365:SER:HB3	1.76	0.48
1:A:2481:MET:HE2	1:A:2481:MET:HA	1.95	0.48
1:A:2773:MET:HE2	1:A:2802:TRP:CG	2.47	0.48
1:A:3756:VAL:HB	1:A:3759:ARG:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3801:TYR:HD2	1:A:3856:LEU:HD13	1.78	0.48
1:A:3973:LEU:HD12	1:A:3992:LEU:CD1	2.43	0.48
1:A:4042:LEU:HD13	1:A:4142:GLY:HA3	1.94	0.48
1:A:1495:ASN:O	1:A:1499:GLU:HG2	2.12	0.48
1:A:2094:LYS:O	1:A:2098:VAL:HG12	2.13	0.48
1:A:3737:GLU:O	1:A:3741:ARG:HG2	2.13	0.48
1:A:2590:PRO:HG2	1:A:2687:VAL:HG21	1.95	0.48
1:A:1928:LEU:HB3	1:A:1930:PHE:CE1	2.47	0.48
1:A:2752:ASN:HD22	1:A:2770:THR:HB	1.77	0.48
1:A:3197:GLN:HB3	1:A:3496:PHE:CE2	2.48	0.48
1:A:2419:ALA:O	1:A:2423:MET:HG2	2.14	0.48
1:A:2934:LEU:HD12	1:A:2935:LEU:N	2.28	0.48
1:A:3204:GLY:O	1:A:3208:ILE:HG12	2.13	0.48
1:A:3490:GLU:O	1:A:3494:GLU:HG2	2.14	0.48
1:A:3724:VAL:HG13	1:A:3793:GLU:OE2	2.13	0.48
1:A:3856:LEU:O	1:A:3859:ILE:HG22	2.13	0.48
1:A:1332:VAL:HG23	1:A:1377:LEU:HB3	1.95	0.48
1:A:1798:MET:SD	1:A:1799:GLU:N	2.87	0.48
1:A:1738:TYR:CE2	1:A:1792:LEU:HD21	2.48	0.48
1:A:1898:ALA:O	1:A:1983:ARG:NH1	2.47	0.48
1:A:3591:ASP:CG	1:A:3594:GLY:H	2.22	0.48
1:A:3885:MET:HE1	1:A:4008:PHE:CD2	2.45	0.48
1:A:4192:GLU:OE1	1:A:4195:ARG:NH1	2.45	0.48
1:A:4492:ILE:HG22	1:A:4507:ILE:HG12	1.95	0.48
1:A:1460:GLU:HB3	1:A:1516:PHE:CE1	2.49	0.48
1:A:1661:VAL:HG22	1:A:1676:ILE:HD12	1.95	0.48
1:A:1909:GLY:O	1:A:2043:LYS:NZ	2.47	0.48
1:A:2461:MET:HE1	1:A:2500:TRP:HB3	1.94	0.48
1:A:2942:GLY:O	1:A:2946:LEU:HD22	2.14	0.48
1:A:3588:LEU:HD13	1:A:3679:LEU:HB3	1.96	0.48
1:A:3810:SER:HB3	1:A:3890:ILE:HD12	1.94	0.48
1:A:2703:LEU:HD12	1:A:2706:ILE:HD13	1.96	0.47
1:A:1444:ALA:HA	1:A:1447:LYS:HE2	1.95	0.47
1:A:2232:MET:H	1:A:2232:MET:CE	2.18	0.47
1:A:4194:LEU:HD12	1:A:4194:LEU:H	1.80	0.47
1:A:1397:ASN:HD22	1:A:1397:ASN:C	2.15	0.47
1:A:2418:ASP:O	1:A:2422:ILE:HG12	2.14	0.47
1:A:2614:ASP:OD1	1:A:2614:ASP:N	2.47	0.47
1:A:1711:VAL:HG12	1:A:1715:LYS:HE2	1.96	0.47
1:A:2303:PHE:CD2	1:A:2341:ILE:HD11	2.49	0.47
1:A:4093:TRP:CD1	1:A:4123:ARG:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2000:GLU:HG2	1:A:2005:GLN:HE22	1.78	0.47
1:A:3189:GLU:OE1	1:A:3582:ARG:NH2	2.47	0.47
1:A:3769:THR:O	1:A:3773:LEU:HD12	2.14	0.47
1:A:1551:PHE:HB3	1:A:1558:LYS:NZ	2.28	0.47
1:A:2500:TRP:CD2	1:A:2580:LEU:HD11	2.49	0.47
1:A:2969:GLY:HA2	1:A:3004:PHE:HE1	1.78	0.47
1:A:2998:ASN:OD1	1:A:2998:ASN:N	2.45	0.47
1:A:3012:LEU:HD11	1:A:3066:PHE:HE2	1.79	0.47
1:A:4016:SER:O	1:A:4016:SER:OG	2.30	0.47
1:A:4405:ILE:O	1:A:4411:ARG:NH2	2.48	0.47
1:A:1504:VAL:HA	1:A:1507:MET:HE2	1.95	0.47
1:A:2080:LEU:HD13	1:A:2149:LEU:HD11	1.97	0.47
1:A:2308:ASP:OD1	1:A:2311:TRP:HD1	1.97	0.47
1:A:4271:ARG:HG2	1:A:4633:ARG:NH1	2.30	0.47
1:A:2329:ASN:OD1	1:A:2330:GLY:N	2.47	0.47
1:A:4563:LEU:HD12	1:A:4588:THR:HG21	1.97	0.47
1:A:2614:ASP:C	1:A:2657:LYS:HD2	2.41	0.47
1:A:2905:LEU:HD12	1:A:2906:ASP:N	2.30	0.47
1:A:3866:VAL:O	1:A:3870:ARG:HG2	2.15	0.47
1:A:3923:ARG:HD3	1:A:3924:ILE:N	2.30	0.47
1:A:1350:PRO:O	1:A:1354:VAL:HG13	2.15	0.46
1:A:1426:VAL:HA	1:A:1429:LEU:HD13	1.96	0.46
1:A:1691:SER:O	1:A:1695:HIS:ND1	2.31	0.46
1:A:1751:VAL:O	1:A:1755:GLN:HG3	2.16	0.46
1:A:2798:GLU:OE1	1:A:2798:GLU:N	2.41	0.46
1:A:4301:ARG:NH1	1:A:4303:GLU:OE1	2.48	0.46
1:A:2218:HIS:HA	1:A:2340:ARG:HH11	1.79	0.46
1:A:2108:ILE:HG12	1:A:2131:LEU:HD11	1.97	0.46
1:A:2127:ILE:HA	1:A:2130:ASN:HD21	1.80	0.46
1:A:2881:TYR:HE1	1:A:2927:ARG:HH22	1.63	0.46
1:A:3537:GLN:HB3	1:A:3543:PHE:CE1	2.46	0.46
1:A:3716:VAL:HG23	1:A:3836:TYR:OH	2.15	0.46
1:A:1332:VAL:HB	1:A:1377:LEU:HD22	1.96	0.46
1:A:1867:ASN:O	1:A:1925:ARG:NH2	2.28	0.46
1:A:2203:TRP:CH2	1:A:2236:VAL:HG11	2.50	0.46
1:A:2495:VAL:O	1:A:2498:ILE:HG13	2.16	0.46
1:A:3566:SER:O	1:A:3566:SER:OG	2.34	0.46
1:A:1551:PHE:CE2	1:A:1565:THR:HA	2.51	0.46
1:A:2145:MET:O	1:A:2149:LEU:HD23	2.15	0.46
1:A:2301:ILE:O	1:A:2341:ILE:HD12	2.15	0.46
1:A:3624:GLU:HB3	1:A:3628:ARG:HH22	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4088:VAL:O	1:A:4119:HIS:N	2.48	0.46
1:A:4414:GLU:O	1:A:4418:LYS:HG2	2.16	0.46
1:A:1822:THR:O	1:A:1826:ILE:HG13	2.15	0.46
1:A:1867:ASN:OD1	1:A:1867:ASN:N	2.49	0.46
1:A:2505:ASP:HB3	1:A:2733:VAL:HG23	1.98	0.46
1:A:3114:ASP:HB2	1:A:3191:ARG:HH12	1.81	0.46
1:A:3476:THR:HA	1:A:3479:LEU:HD23	1.97	0.46
1:A:3947:LEU:HD23	1:A:3948:ILE:HD12	1.96	0.46
1:A:1766:LEU:HD11	1:A:1830:ILE:HG22	1.97	0.46
1:A:2207:VAL:O	1:A:2210:LEU:HB3	2.16	0.46
1:A:2760:PRO:HA	1:A:2763:ARG:HD3	1.96	0.46
1:A:3107:LYS:HZ1	1:A:3140:ARG:HB3	1.79	0.46
1:A:3604:TYR:HA	1:A:3607:ARG:HH21	1.81	0.46
1:A:3985:GLN:O	1:A:3989:ARG:HG3	2.15	0.46
1:A:1837:GLU:H	1:A:1837:GLU:CD	2.19	0.46
1:A:2953:MET:O	1:A:2953:MET:HE3	2.15	0.46
1:A:3659:ARG:HE	1:A:3661:LEU:CD2	2.24	0.46
1:A:4457:LYS:HB2	1:A:4459:ILE:HG12	1.97	0.46
1:A:2948:ARG:HG2	1:A:2958:VAL:HG21	1.98	0.46
1:A:3646:ASN:OD1	1:A:3695:ARG:NH1	2.49	0.46
1:A:4330:VAL:O	1:A:4333:THR:OG1	2.22	0.46
1:A:4451:LEU:HD23	1:A:4455:LEU:HD23	1.97	0.45
1:A:1449:VAL:HG23	1:A:1450:LEU:HD23	1.99	0.45
1:A:1864:ALA:HB1	1:A:1866:PHE:CZ	2.51	0.45
1:A:2965:ARG:HD3	1:A:3642:ASP:CG	2.40	0.45
1:A:2979:VAL:HG21	1:A:2992:PHE:HE2	1.80	0.45
1:A:3753:LEU:O	1:A:3756:VAL:HG22	2.16	0.45
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.51	0.45
1:A:2472:TYR:CD1	1:A:2541:ILE:HG21	2.51	0.45
1:A:3100:GLU:HG2	1:A:3130:TYR:CE1	2.51	0.45
1:A:4104:GLY:HA2	1:A:4107:MET:HE3	1.98	0.45
1:A:4215:ALA:O	1:A:4219:VAL:HG12	2.15	0.45
1:A:4302:ARG:NH2	1:A:4303:GLU:HG3	2.31	0.45
1:A:4633:ARG:O	1:A:4637:GLU:HG3	2.17	0.45
1:A:1443:GLU:O	1:A:1447:LYS:HG3	2.17	0.45
1:A:3568:PRO:HB2	1:A:3570:ASP:OD2	2.17	0.45
1:A:4460:LEU:O	1:A:4462:ARG:NH1	2.47	0.45
1:A:1417:MET:SD	1:A:1422:VAL:HG23	2.56	0.45
1:A:1872:TYR:CZ	1:A:1874:GLY:HA2	2.51	0.45
1:A:2229:GLY:HA2	1:A:2232:MET:HE1	1.98	0.45
1:A:2855:LEU:HD11	1:A:2863:ARG:HE	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1424:TRP:CH2	1:A:1434:ILE:HG22	2.52	0.45
1:A:1887:ARG:HH12	1:A:4253:GLY:C	2.25	0.45
1:A:2077:ASP:HA	1:A:2088:PHE:HD1	1.82	0.45
1:A:2152:GLU:OE1	1:A:2152:GLU:N	2.43	0.45
1:A:2642:ARG:HH12	1:A:2651:ALA:HB3	1.81	0.45
1:A:3705:ARG:HA	1:A:3813:PHE:HE2	1.82	0.45
1:A:4628:THR:C	1:A:4629:LYS:HD2	2.41	0.45
1:A:1581:LYS:O	1:A:1584:LYS:NZ	2.44	0.45
1:A:4071:ILE:HD11	1:A:4096:LEU:HD22	1.98	0.45
1:A:1649:LYS:HE3	1:A:1649:LYS:HB3	1.85	0.45
1:A:2031:ASN:OD1	1:A:2031:ASN:N	2.47	0.45
1:A:2623:SER:OG	1:A:3081:THR:O	2.21	0.45
1:A:2654:GLN:OE1	1:A:2657:LYS:HB2	2.16	0.45
1:A:3691:ASP:O	1:A:3695:ARG:HG3	2.17	0.45
1:A:4203:LYS:NZ	1:A:4205:TYR:OH	2.49	0.45
1:A:4489:LEU:HD13	1:A:4492:ILE:HD11	1.99	0.45
1:A:2057:GLN:NE2	1:A:2101:GLY:HA3	2.32	0.45
1:A:2107:ARG:HD2	1:A:2110:LYS:NZ	2.31	0.45
1:A:2269:ASP:HB3	1:A:2274:GLU:HB2	1.99	0.45
1:A:2694:ARG:O	1:A:2698:GLN:N	2.42	0.45
1:A:2705:ARG:H	1:A:2706:ILE:HD12	1.81	0.45
1:A:1446:VAL:O	1:A:1450:LEU:HG	2.17	0.45
1:A:1461:GLU:HA	1:A:1464:LYS:HD3	1.99	0.45
1:A:1486:LEU:HD23	1:A:1486:LEU:HA	1.81	0.45
1:A:1673:VAL:HG12	1:A:1686:PHE:HE1	1.81	0.45
1:A:1857:LEU:HD23	1:A:1857:LEU:HA	1.83	0.45
1:A:1860:GLN:HG2	1:A:1865:LYS:HD3	1.99	0.45
1:A:1979:GLN:HG3	1:A:2036:PHE:CE1	2.52	0.45
1:A:2219:GLY:HA2	1:A:2341:ILE:O	2.16	0.45
1:A:2755:MET:HG3	1:A:2807:PHE:HB2	1.98	0.45
1:A:4105:TRP:CZ2	1:A:4109:LEU:HD21	2.51	0.45
1:A:3107:LYS:O	1:A:3107:LYS:HD3	2.17	0.44
1:A:3132:LYS:HE2	1:A:3132:LYS:HB2	1.64	0.44
1:A:3557:ASP:OD1	1:A:3558:GLU:HG3	2.16	0.44
1:A:4172:SER:O	1:A:4176:ARG:NH1	2.49	0.44
1:A:1425:VAL:O	1:A:1428:GLU:N	2.44	0.44
1:A:2261:LYS:NZ	1:A:2310:GLU:O	2.51	0.44
1:A:2452:LEU:HD23	1:A:2452:LEU:HA	1.71	0.44
1:A:2481:MET:HE1	1:A:2485:GLN:OE1	2.17	0.44
1:A:2571:THR:HG23	1:A:2574:THR:H	1.83	0.44
1:A:2717:ASP:O	1:A:2720:ARG:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2849:ASN:O	1:A:2853:VAL:HG12	2.17	0.44
1:A:2891:ASP:O	1:A:2894:LYS:HG2	2.18	0.44
1:A:3044:LEU:HB3	1:A:3049:GLU:CD	2.43	0.44
1:A:4166:VAL:HA	1:A:4169:ILE:HG22	1.99	0.44
1:A:4257:ASP:OD1	1:A:4257:ASP:C	2.59	0.44
1:A:1392:GLY:HA2	1:A:1395:LYS:HE3	1.99	0.44
1:A:1445:ILE:O	1:A:1449:VAL:HG13	2.18	0.44
1:A:2308:ASP:HB2	1:A:2674:TYR:CD2	2.52	0.44
1:A:2792:TYR:CZ	1:A:2837:LEU:HD23	2.52	0.44
1:A:4027:LEU:HG	1:A:4058:LEU:HD22	1.99	0.44
1:A:2107:ARG:HA	1:A:2110:LYS:HG2	1.99	0.44
1:A:2439:HIS:O	1:A:2443:LEU:HG	2.17	0.44
1:A:3482:LEU:HD12	1:A:3483:SER:N	2.32	0.44
1:A:3750:LEU:O	1:A:3754:ASN:ND2	2.50	0.44
1:A:3831:PHE:O	1:A:3835:ILE:HG12	2.17	0.44
1:A:3835:ILE:HG23	1:A:3866:VAL:HG12	1.98	0.44
1:A:3944:PHE:O	1:A:3947:LEU:HD22	2.18	0.44
1:A:1529:ARG:O	1:A:1533:LEU:HD23	2.18	0.44
1:A:2527:PRO:HG3	1:A:2545:TRP:CG	2.52	0.44
1:A:3097:TRP:CZ3	1:A:3105:VAL:HG21	2.53	0.44
1:A:4025:LEU:HD23	1:A:4027:LEU:HB2	1.99	0.44
1:A:1392:GLY:HA2	1:A:1395:LYS:HG2	1.99	0.44
1:A:3524:MET:HE2	1:A:3524:MET:HA	1.99	0.44
1:A:2047:GLN:O	1:A:2051:GLN:HG3	2.18	0.44
1:A:1551:PHE:HE2	1:A:1565:THR:HA	1.83	0.44
1:A:2037:ARG:HH22	1:A:4211:ASP:HA	1.83	0.44
1:A:2133:GLU:H	1:A:2133:GLU:CD	2.26	0.44
1:A:3768:THR:O	1:A:3771:GLU:HG2	2.17	0.44
1:A:3776:GLU:O	1:A:3779:GLU:HG3	2.18	0.44
1:A:4470:PRO:HD2	1:A:4473:MET:SD	2.58	0.44
1:A:3757:LYS:HA	1:A:3757:LYS:HD2	1.84	0.44
1:A:4087:ALA:HA	1:A:4090:SER:OG	2.18	0.44
1:A:1456:GLU:CD	1:A:1512:TYR:HB3	2.42	0.43
1:A:3760:ILE:HD12	1:A:3766:ILE:HG21	1.99	0.43
1:A:3921:THR:HA	1:A:3936:VAL:HG21	2.00	0.43
1:A:3970:VAL:HG13	1:A:3992:LEU:HD22	1.99	0.43
1:A:1424:TRP:NE1	1:A:1433:GLN:HB3	2.32	0.43
1:A:2423:MET:HE1	1:A:2462:LEU:HD22	2.01	0.43
1:A:3219:ARG:HH11	1:A:3479:LEU:HD23	1.83	0.43
1:A:3733:LYS:HB2	1:A:3737:GLU:HB2	2.00	0.43
1:A:3787:THR:O	1:A:3790:VAL:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4113:LEU:HD11	1:A:4124:LEU:HD23	2.00	0.43
1:A:4536:LEU:HD23	1:A:4536:LEU:HA	1.81	0.43
1:A:1765:ALA:O	1:A:1769:MET:HG3	2.18	0.43
1:A:2041:MET:HE3	1:A:2041:MET:HA	2.00	0.43
1:A:2667:ASN:ND2	1:A:2712:CYS:HB2	2.17	0.43
1:A:2871:ILE:C	1:A:2872:LEU:HD23	2.43	0.43
1:A:2916:LEU:HD23	1:A:2916:LEU:HA	1.87	0.43
1:A:4178:ARG:O	1:A:4182:LEU:HG	2.19	0.43
1:A:4215:ALA:HB2	1:A:4247:MET:HE1	2.00	0.43
1:A:1363:LEU:HD11	1:A:1435:TRP:CZ2	2.53	0.43
1:A:1571:ILE:HG23	1:A:1604:LEU:HD22	2.01	0.43
1:A:2482:GLN:OE1	1:A:2483:ILE:N	2.51	0.43
1:A:2672:ASP:N	1:A:2676:THR:O	2.37	0.43
1:A:3511:ALA:O	1:A:3514:ILE:HG22	2.19	0.43
1:A:3731:LEU:CG	1:A:3791:MET:HE1	2.48	0.43
1:A:3983:ILE:O	1:A:3987:ILE:HG13	2.18	0.43
1:A:2238:LEU:HB2	1:A:2300:TRP:CZ3	2.53	0.43
1:A:2792:TYR:OH	1:A:2838:VAL:HG22	2.18	0.43
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.54	0.43
1:A:3102:LEU:HB3	1:A:3148:VAL:HG22	2.01	0.43
1:A:3167:ARG:CZ	1:A:3685:THR:HA	2.48	0.43
1:A:3557:ASP:OD1	1:A:3558:GLU:N	2.51	0.43
1:A:1697:LYS:O	1:A:1700:GLU:HG2	2.18	0.43
1:A:1967:MET:HE2	1:A:1967:MET:HB3	1.89	0.43
1:A:3544:ARG:HB2	1:A:3547:ILE:CD1	2.49	0.43
1:A:2606:PHE:CE1	1:A:2617:VAL:HG11	2.45	0.43
1:A:2622:PHE:CZ	1:A:2631:LEU:HD11	2.53	0.43
1:A:2651:ALA:HB1	1:A:2705:ARG:HH21	1.83	0.43
1:A:3129:VAL:HG11	1:A:3149:PHE:HD1	1.84	0.43
1:A:3612:THR:HB	1:A:3633:LEU:HD21	2.00	0.43
1:A:4190:ILE:HG22	1:A:4201:TRP:HZ2	1.84	0.43
1:A:4204:LYS:HE2	1:A:4204:LYS:HB2	1.89	0.43
1:A:1679:ARG:H	1:A:1679:ARG:HG3	1.69	0.43
1:A:2374:ILE:HD13	1:A:2374:ILE:HA	1.91	0.43
1:A:3721:ARG:HB3	1:A:3724:VAL:HG23	2.00	0.43
1:A:3903:ALA:HA	1:A:3906:GLN:NE2	2.33	0.43
1:A:4277:SER:HA	1:A:4282:PHE:CG	2.54	0.43
1:A:2237:LEU:HD12	1:A:2237:LEU:O	2.19	0.43
1:A:2992:PHE:O	1:A:3065:VAL:N	2.44	0.43
1:A:3012:LEU:HD11	1:A:3066:PHE:CE2	2.53	0.43
1:A:3174:ARG:NH1	1:A:3650:ASN:OD1	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3583:PHE:CD2	1:A:3587:PRO:HD3	2.54	0.43
1:A:3731:LEU:HA	1:A:3734:LEU:HB2	2.00	0.43
1:A:4206:GLU:H	1:A:4206:GLU:CD	2.26	0.43
1:A:4240:TRP:HB3	1:A:4244:LYS:HZ3	1.83	0.43
1:A:4376:TRP:O	1:A:4380:LEU:HG	2.18	0.43
1:A:1789:LEU:CD1	1:A:1815:LEU:HB3	2.49	0.43
1:A:2093:LEU:O	1:A:2097:LEU:HG	2.19	0.43
1:A:2616:GLU:HB2	1:A:2657:LYS:HE3	2.01	0.43
1:A:3073:GLU:OE2	1:A:3074:GLY:N	2.52	0.43
1:A:3644:VAL:O	1:A:3647:PRO:HD2	2.19	0.43
1:A:3793:GLU:O	1:A:3797:VAL:HG23	2.19	0.43
1:A:4401:THR:OG1	1:A:4403:GLU:OE2	2.21	0.43
1:A:2673:LYS:HB2	1:A:2674:TYR:CE1	2.54	0.42
1:A:3169:MET:SD	1:A:3169:MET:N	2.91	0.42
1:A:4095:MET:O	1:A:4096:LEU:HD23	2.19	0.42
1:A:4528:VAL:HG21	1:A:4592:TRP:HB2	2.01	0.42
1:A:4601:LYS:HB2	1:A:4604:VAL:HG13	2.01	0.42
1:A:1554:SER:O	1:A:1557:ILE:HG22	2.19	0.42
1:A:1667:ASN:OD1	1:A:1668:GLU:N	2.50	0.42
1:A:1718:ALA:O	1:A:1721:VAL:HG12	2.20	0.42
1:A:2104:LYS:HA	1:A:2136:ILE:HD13	2.01	0.42
1:A:3948:ILE:HD12	1:A:3948:ILE:H	1.84	0.42
1:A:1695:HIS:HB2	1:A:1701:TRP:HB3	2.00	0.42
1:A:1351:TRP:O	1:A:1354:VAL:HG22	2.19	0.42
1:A:2352:THR:HG23	1:A:2354:ALA:H	1.84	0.42
1:A:2609:LEU:HD13	1:A:2617:VAL:HG22	2.01	0.42
1:A:2943:LYS:HG2	1:A:3094:PHE:CE2	2.55	0.42
1:A:3024:ASP:OD1	1:A:3024:ASP:N	2.50	0.42
1:A:3619:PHE:CZ	1:A:3623:LEU:HD12	2.53	0.42
1:A:1467:ARG:HA	1:A:1523:TRP:CZ2	2.55	0.42
1:A:1533:LEU:HD11	1:A:1597:VAL:HG13	2.01	0.42
1:A:1789:LEU:HD11	1:A:1815:LEU:HB3	2.01	0.42
1:A:1878:LYS:HE3	1:A:1878:LYS:HB3	1.88	0.42
1:A:2186:CYS:HB3	1:A:2191:LEU:O	2.19	0.42
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.55	0.42
1:A:2684:ARG:NH2	1:A:2726:ARG:HH21	2.16	0.42
1:A:2910:VAL:HG12	3:A:4703:ADP:N1	2.35	0.42
1:A:2603:MET:SD	3:A:4702:ADP:C5	3.13	0.42
1:A:2880:ASP:OD2	1:A:2880:ASP:N	2.52	0.42
1:A:3544:ARG:HG3	1:A:3544:ARG:NH1	2.33	0.42
1:A:4077:PHE:HD1	1:A:4105:TRP:CE3	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2475:ASN:OD1	1:A:2475:ASN:C	2.62	0.42
1:A:2920:LEU:HD13	1:A:2920:LEU:HA	1.78	0.42
1:A:3001:ASP:OD1	1:A:3001:ASP:N	2.53	0.42
1:A:3888:ALA:O	1:A:3892:LEU:HD23	2.19	0.42
1:A:4111:LYS:HB2	1:A:4112:LYS:NZ	2.34	0.42
1:A:4153:VAL:HG22	1:A:4192:GLU:HG3	2.01	0.42
1:A:4183:LEU:HD22	1:A:4273:PHE:HZ	1.85	0.42
1:A:1344:ASP:O	1:A:1347:LYS:HG2	2.20	0.42
1:A:2435:LYS:HA	1:A:2438:GLU:HG3	2.02	0.42
1:A:2744:LEU:HA	1:A:2747:ILE:HG22	2.02	0.42
1:A:3207:LYS:HZ1	1:A:3753:LEU:CB	2.26	0.42
1:A:3730:ASP:HA	1:A:3733:LYS:HG2	2.02	0.42
1:A:4086:THR:HA	1:A:4089:LYS:NZ	2.34	0.42
1:A:4134:VAL:HG13	1:A:4139:LEU:HD11	2.01	0.42
1:A:4175:GLU:HG3	1:A:4278:PHE:HE2	1.85	0.42
1:A:4289:ASP:OD1	1:A:4317:THR:OG1	2.31	0.42
1:A:1785:VAL:O	1:A:1789:LEU:HD13	2.20	0.42
1:A:4025:LEU:HD21	1:A:4027:LEU:HD13	2.00	0.42
1:A:4323:LEU:HD12	1:A:4323:LEU:H	1.85	0.42
1:A:4329:ARG:O	1:A:4333:THR:HG23	2.20	0.42
1:A:2379:LEU:O	1:A:2383:ARG:HG3	2.20	0.42
1:A:3131:ASP:OD1	1:A:3132:LYS:N	2.52	0.42
1:A:3839:VAL:HG23	1:A:3862:ASP:HB3	2.00	0.42
1:A:4105:TRP:HA	1:A:4108:GLN:HG2	2.02	0.42
1:A:1509:LEU:HB3	1:A:3631:ASN:HD21	1.84	0.41
1:A:2458:LEU:O	1:A:2462:LEU:HG	2.20	0.41
1:A:2508:LEU:HB2	1:A:2509:LYS:NZ	2.36	0.41
1:A:2575:VAL:HA	1:A:2578:GLU:OE1	2.20	0.41
1:A:2755:MET:HE2	1:A:2755:MET:HB3	1.88	0.41
1:A:3480:LYS:HD2	1:A:3480:LYS:HA	1.85	0.41
1:A:4295:GLN:OE1	1:A:4296:MET:N	2.52	0.41
1:A:1686:PHE:HB3	1:A:1708:GLU:OE2	2.20	0.41
1:A:3633:LEU:O	1:A:3677:ILE:HD12	2.21	0.41
1:A:3655:ARG:HA	1:A:3659:ARG:O	2.20	0.41
1:A:3797:VAL:O	1:A:3800:GLN:HB3	2.20	0.41
1:A:1692:ILE:H	1:A:1692:ILE:HD12	1.85	0.41
1:A:1743:ASP:OD1	1:A:1804:ARG:NE	2.53	0.41
1:A:2048:LEU:HD23	1:A:2048:LEU:HA	1.87	0.41
1:A:2072:PHE:HB2	1:A:2164:VAL:HG21	2.02	0.41
1:A:2898:LYS:HD3	1:A:2898:LYS:C	2.44	0.41
1:A:3540:ASN:O	1:A:3540:ASN:ND2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3639:GLU:HG3	1:A:3686:VAL:HG21	2.02	0.41
1:A:1628:ARG:HH12	1:A:1706:GLU:CD	2.29	0.41
1:A:2020:PRO:HA	1:A:2026:SER:HA	2.02	0.41
1:A:3759:ARG:NH1	1:A:3763:ASP:OD2	2.54	0.41
1:A:2113:ARG:HA	1:A:2116:GLU:HG2	2.03	0.41
1:A:2169:GLN:OE1	1:A:2169:GLN:N	2.53	0.41
1:A:2279:LEU:HD21	1:A:2693:TYR:CD2	2.56	0.41
1:A:2579:ALA:O	1:A:2583:THR:HG23	2.20	0.41
1:A:3211:THR:HG21	1:A:3753:LEU:HD11	2.02	0.41
1:A:3825:TYR:OH	1:A:3879:ASP:OD1	2.21	0.41
1:A:3907:HIS:NE2	1:A:3938:LEU:HA	2.35	0.41
1:A:4517:PRO:HG2	1:A:4619:ILE:HD12	2.03	0.41
1:A:1645:LYS:HA	1:A:1645:LYS:HD3	1.91	0.41
1:A:1661:VAL:HG13	1:A:1676:ILE:HD12	2.02	0.41
1:A:2065:LEU:HD21	1:A:2134:GLN:HG2	2.02	0.41
1:A:2616:GLU:O	1:A:2660:VAL:HG22	2.20	0.41
1:A:2797:ARG:HA	3:A:4702:ADP:H4'	2.03	0.41
1:A:3677:ILE:HD12	1:A:3677:ILE:HA	1.85	0.41
1:A:4038:ASN:OD1	1:A:4038:ASN:N	2.52	0.41
1:A:4104:GLY:HA2	1:A:4107:MET:CE	2.50	0.41
1:A:4526:GLN:HG2	1:A:4536:LEU:HD11	2.02	0.41
1:A:1711:VAL:O	1:A:1715:LYS:HG3	2.20	0.41
1:A:1978:ILE:O	1:A:1982:LEU:HD22	2.20	0.41
1:A:2075:LEU:HD11	1:A:4536:LEU:HD12	2.02	0.41
1:A:2335:LEU:HD23	1:A:2336:PRO:O	2.21	0.41
1:A:2561:LYS:HE2	1:A:2561:LYS:HB2	1.98	0.41
1:A:3601:MET:HA	1:A:3609:ILE:HD13	2.02	0.41
1:A:3654:ARG:NH1	1:A:3663:THR:HG23	2.36	0.41
1:A:4297:PRO:HB3	1:A:4308:TRP:CG	2.55	0.41
1:A:4345:LYS:HB3	1:A:4345:LYS:HE2	1.76	0.41
1:A:1548:GLU:HG2	1:A:1568:PHE:HZ	1.85	0.41
1:A:1692:ILE:HG23	1:A:1701:TRP:CD1	2.55	0.41
1:A:2443:LEU:HB3	1:A:2510:MET:CE	2.51	0.41
1:A:2528:THR:O	1:A:2528:THR:OG1	2.36	0.41
1:A:1484:CYS:CB	1:A:1579:MET:HE2	2.51	0.41
1:A:1507:MET:HE2	1:A:1507:MET:HB3	1.95	0.41
1:A:1702:LEU:HD23	1:A:1702:LEU:HA	1.87	0.41
1:A:1809:GLU:HG2	1:A:2056:SER:HB2	2.02	0.41
1:A:2113:ARG:HA	1:A:2116:GLU:CD	2.46	0.41
1:A:2458:LEU:HD12	1:A:2458:LEU:HA	1.87	0.41
1:A:2580:LEU:O	1:A:2583:THR:OG1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2596:PRO:HB2	1:A:2738:TYR:CE1	2.55	0.41
1:A:2624:SER:OG	1:A:3081:THR:HA	2.20	0.41
1:A:2746:GLN:O	1:A:2750:THR:HG22	2.21	0.41
1:A:2825:TRP:HH2	1:A:2853:VAL:HG13	1.86	0.41
1:A:2864:GLU:OE1	1:A:2864:GLU:N	2.37	0.41
1:A:3106:GLY:O	1:A:3110:THR:HG23	2.21	0.41
1:A:3509:LEU:HD21	1:A:3536:LEU:HD13	2.02	0.41
1:A:3716:VAL:HG21	1:A:3804:LEU:HD23	2.02	0.41
1:A:3729:SER:O	1:A:3733:LYS:HE3	2.20	0.41
1:A:3885:MET:HB3	1:A:4343:MET:HE2	2.03	0.41
1:A:3959:ILE:HD12	1:A:3959:ILE:H	1.86	0.41
1:A:4018:MET:HE2	1:A:4018:MET:HB3	1.87	0.41
1:A:4105:TRP:O	1:A:4109:LEU:HG	2.20	0.41
1:A:4393:GLN:CD	1:A:4393:GLN:H	2.29	0.41
1:A:4393:GLN:HA	1:A:4428:ARG:HH12	1.85	0.41
1:A:1655:LYS:HE3	1:A:1655:LYS:HB3	1.81	0.41
1:A:1697:LYS:HB2	1:A:1700:GLU:HG2	2.03	0.41
1:A:1698:ILE:HA	1:A:1701:TRP:CD1	2.56	0.41
1:A:1914:GLU:H	1:A:1914:GLU:HG3	1.70	0.41
1:A:1923:LEU:HD12	1:A:1954:TRP:CH2	2.56	0.41
1:A:1923:LEU:HD23	1:A:1923:LEU:HA	1.86	0.41
1:A:2069:ILE:HD11	1:A:2137:LEU:HD21	2.02	0.41
1:A:2206:LYS:HD3	1:A:2206:LYS:HA	1.78	0.41
1:A:2374:ILE:HG21	1:A:2455:LEU:HG	2.02	0.41
1:A:3656:THR:O	1:A:3659:ARG:HB2	2.21	0.41
1:A:1509:LEU:HB3	1:A:3631:ASN:ND2	2.35	0.40
1:A:1626:PHE:CE2	1:A:1628:ARG:HB3	2.56	0.40
1:A:1954:TRP:CD2	1:A:2013:ALA:HB3	2.56	0.40
1:A:2001:LEU:HA	1:A:2001:LEU:HD12	1.73	0.40
1:A:2984:GLY:HA3	1:A:3054:PHE:CE2	2.56	0.40
1:A:3548:ALA:H	1:A:3735:GLN:HE22	1.69	0.40
1:A:3627:LEU:HD11	1:A:3648:VAL:HG22	2.02	0.40
1:A:1623:ARG:HB3	1:A:1630:TYR:CZ	2.56	0.40
1:A:1627:PRO:HB2	1:A:1951:VAL:HG12	2.04	0.40
1:A:2937:GLY:HA3	1:A:2943:LYS:HD3	2.03	0.40
1:A:3010:THR:HB	1:A:3017:VAL:HG12	2.03	0.40
1:A:3068:MET:HE2	1:A:3068:MET:HB3	1.82	0.40
1:A:3556:ALA:O	1:A:3560:LEU:HG	2.21	0.40
1:A:3825:TYR:CE1	1:A:3875:MET:HG2	2.55	0.40
1:A:4408:PRO:HA	1:A:4411:ARG:NE	2.36	0.40
1:A:3819:LYS:HE2	1:A:3826:GLN:HE22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4066:ILE:HD11	1:A:4095:MET:HB2	2.02	0.40
1:A:4118:PRO:HB3	1:A:4122:PHE:CD2	2.56	0.40
1:A:4481:ASP:CG	1:A:4485:ARG:HE	2.29	0.40
1:A:1676:ILE:HD11	1:A:1872:TYR:CD2	2.56	0.40
1:A:1940:ALA:O	1:A:1944:ILE:HG13	2.21	0.40
1:A:2449:LEU:HA	1:A:2453:ARG:NH2	2.37	0.40
1:A:2463:HIS:HA	1:A:2466:CYS:SG	2.62	0.40
1:A:2937:GLY:C	1:A:3070:PRO:HD3	2.46	0.40
1:A:3107:LYS:HZ2	1:A:3140:ARG:HB3	1.84	0.40
1:A:3117:LYS:HG3	1:A:3119:ASN:OD1	2.21	0.40
1:A:3551:GLU:OE2	1:A:3735:GLN:NE2	2.44	0.40
1:A:3880:HIS:ND1	1:A:4021:MET:HG3	2.36	0.40
1:A:4418:LYS:O	1:A:4422:LYS:HG2	2.22	0.40
1:A:1504:VAL:O	1:A:1508:LYS:HG3	2.21	0.40
1:A:1521:LEU:HA	1:A:1524:GLU:OE1	2.22	0.40
1:A:2382:LEU:O	1:A:2416:GLN:NE2	2.54	0.40
1:A:4243:LEU:O	1:A:4247:MET:HG2	2.22	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	3019/4646 (65%)	2946 (98%)	73 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	2696/4125 (65%)	2686 (100%)	10 (0%)	89 91

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1637	LEU
1	A	2359	CYS
1	A	2374	ILE
1	A	2787	ASP
1	A	3572	LEU
1	A	3676	VAL
1	A	3957	PHE
1	A	4127	THR
1	A	4161	PHE
1	A	4436	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1454	GLN
1	A	1790	ASN
1	A	2005	GLN
1	A	2057	GLN
1	A	2109	GLN
1	A	2130	ASN
1	A	2299	GLN
1	A	2689	HIS
1	A	2707	GLN
1	A	2752	ASN
1	A	2834	GLN
1	A	2857	HIS
1	A	2930	GLN
1	A	2954	ASN
1	A	2960	GLN
1	A	3061	ASN
1	A	3198	GLN
1	A	3555	ASN
1	A	3584	ASN
1	A	3667	GLN

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Mol	Chain	Res	Type
1	A	3792	GLN
1	A	3845	ASN
1	A	4262	GLN
1	A	4266	ASN
1	A	4526	GLN
1	A	4612	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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z > 2$
2	ATP	A	4701	4	28,33,33	0.88	1 (3%)	34,52,52	0.65	1 (2%)
3	ADP	A	4702	-	24,29,29	0.86	0	29,45,45	1.27	2 (6%)
3	ADP	A	4703	-	24,29,29	0.85	0	29,45,45	1.19	2 (6%)

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	ATP	A	4701	4	-	4/18/38/38	0/3/3/3
3	ADP	A	4702	-	-	0/12/32/32	0/3/3/3
3	ADP	A	4703	-	-	3/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4701	ATP	PA-O3A	-2.70	1.56	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4702	ADP	N3-C2-N1	-3.75	123.58	128.67
3	A	4703	ADP	N3-C2-N1	-3.64	123.73	128.67
3	A	4703	ADP	C4-C5-N7	-2.56	106.63	109.34
3	A	4702	ADP	C4-C5-N7	-2.32	106.88	109.34
2	A	4701	ATP	C5-C6-N6	2.28	123.78	120.31

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4701	ATP	O4'-C4'-C5'-O5'
2	A	4701	ATP	C3'-C4'-C5'-O5'
3	A	4703	ADP	C5'-O5'-PA-O1A
2	A	4701	ATP	PG-O3B-PB-O2B
2	A	4701	ATP	PA-O3A-PB-O1B
3	A	4703	ADP	C3'-C4'-C5'-O5'
3	A	4703	ADP	O4'-C4'-C5'-O5'

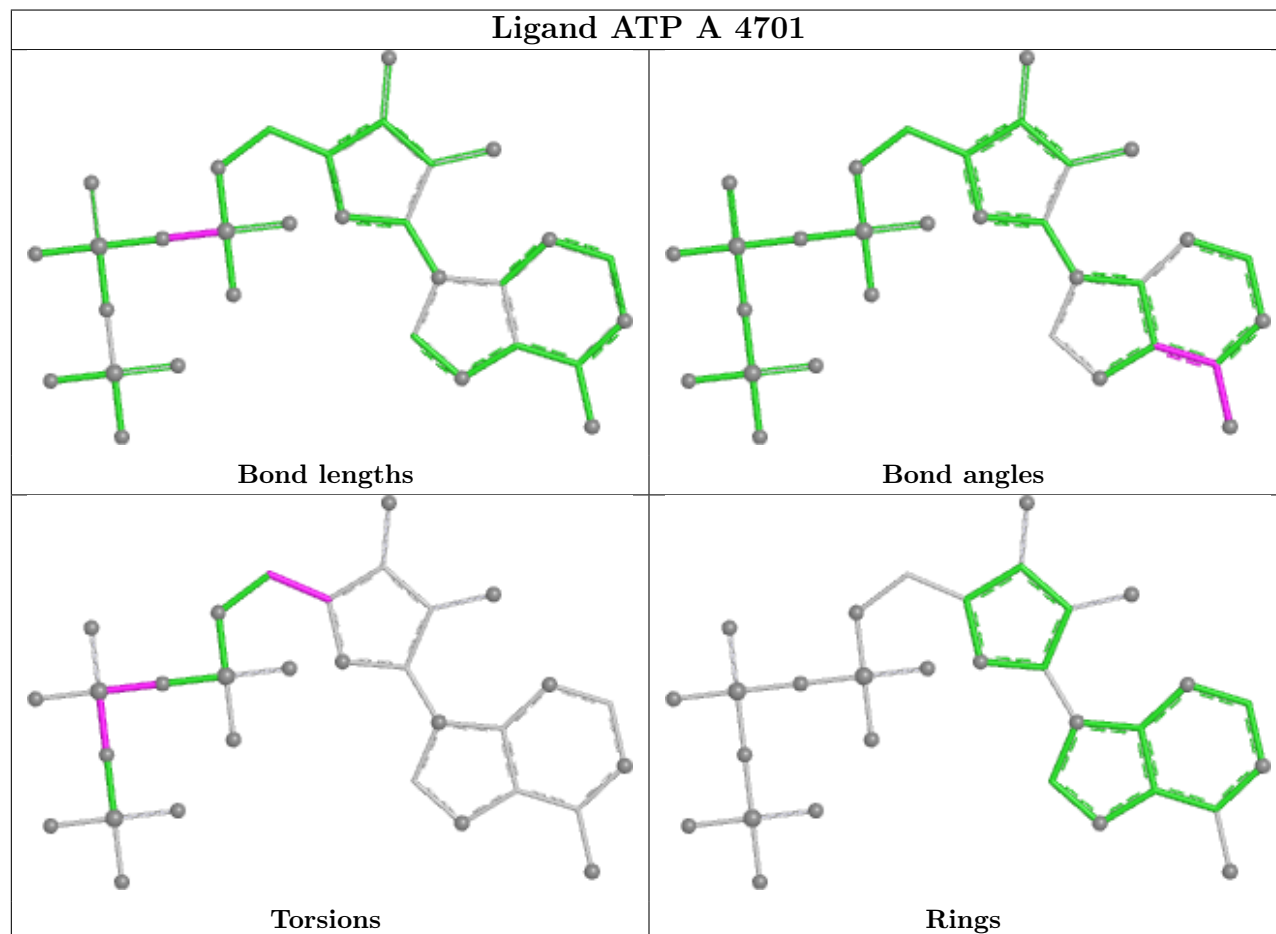
There are no ring outliers.

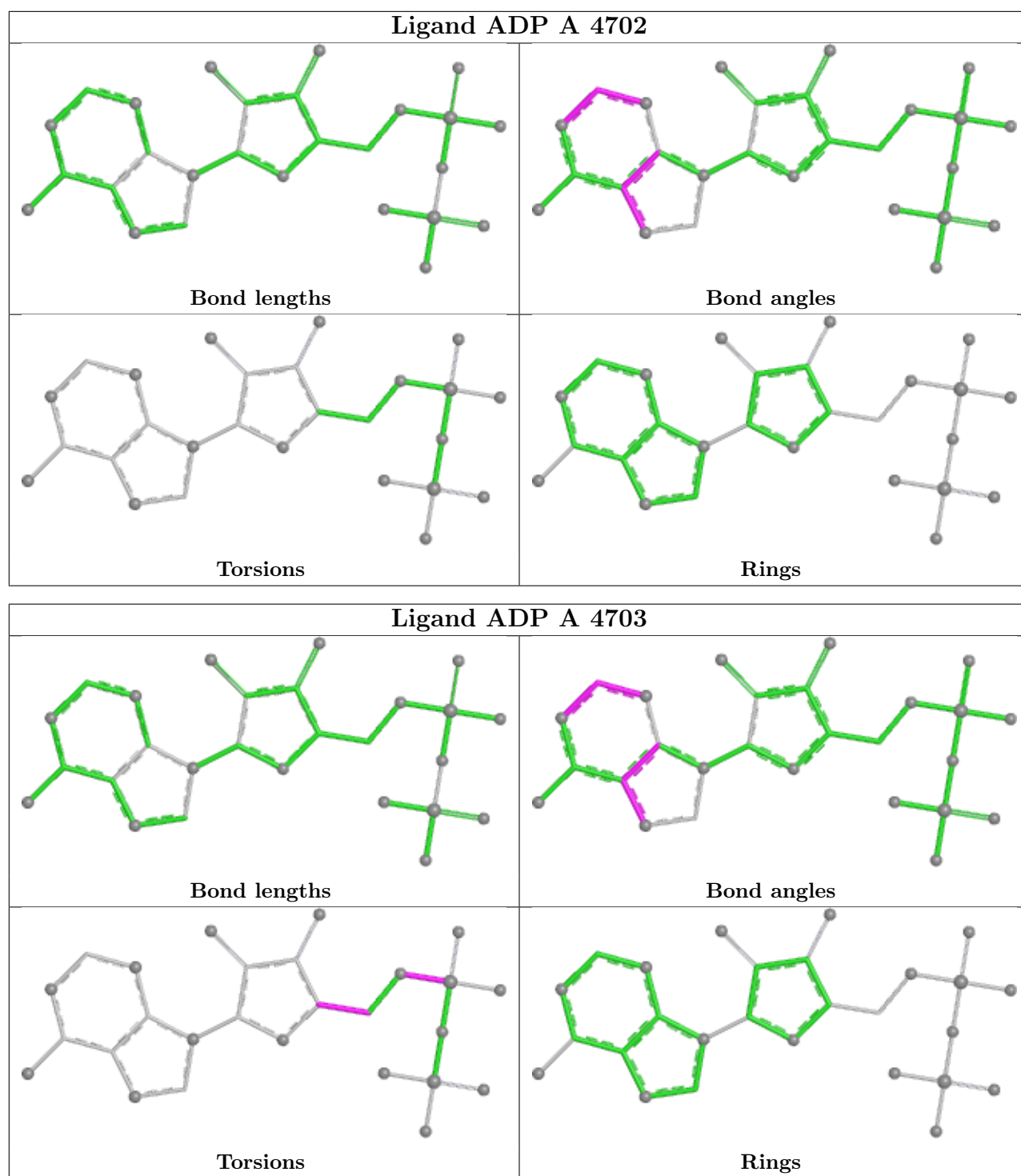
3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ATP	4	0
3	A	4702	ADP	5	0
3	A	4703	ADP	2	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.

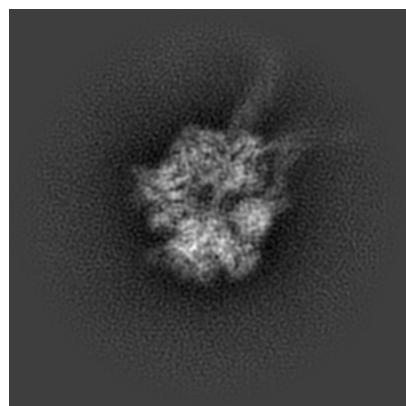
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44718. These allow visual inspection of the internal detail of the map and identification of artifacts.

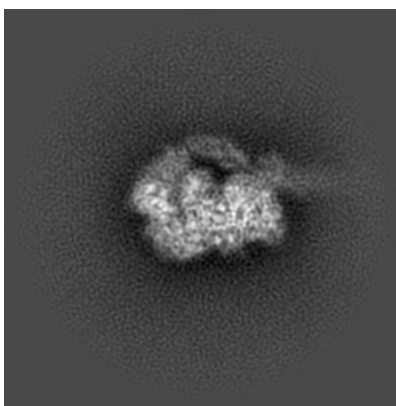
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

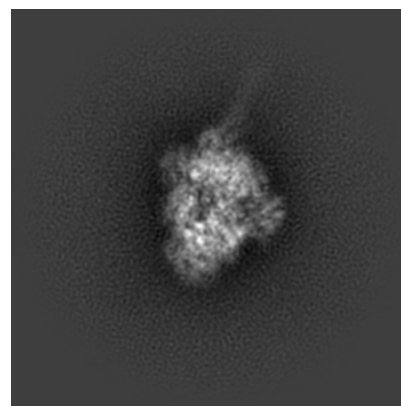
6.1.1 Primary map



X

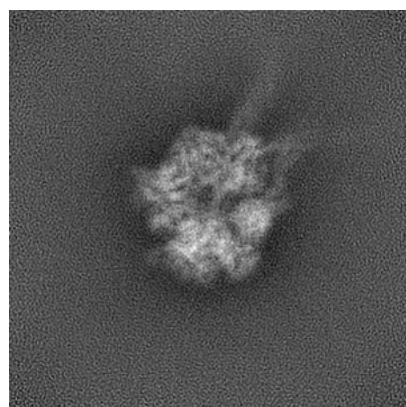


Y

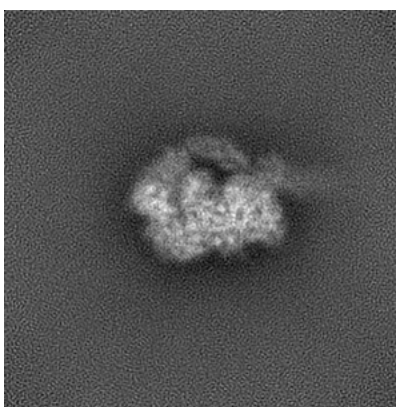


Z

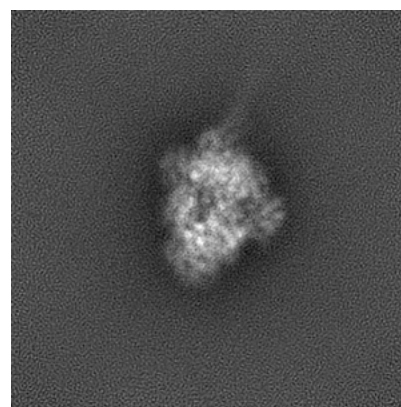
6.1.2 Raw map



X



Y

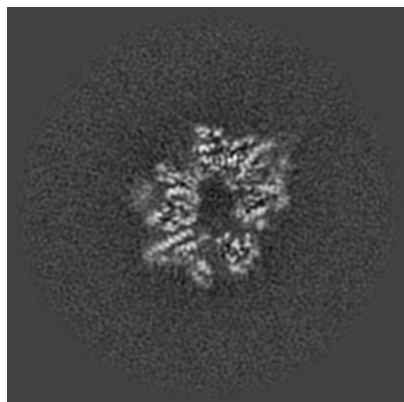


Z

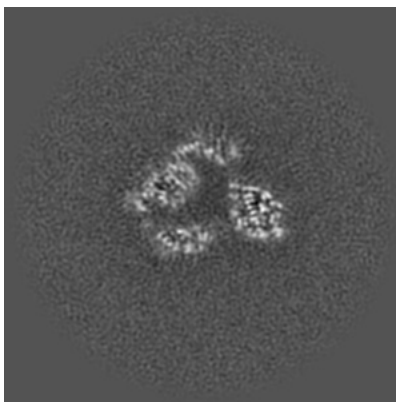
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

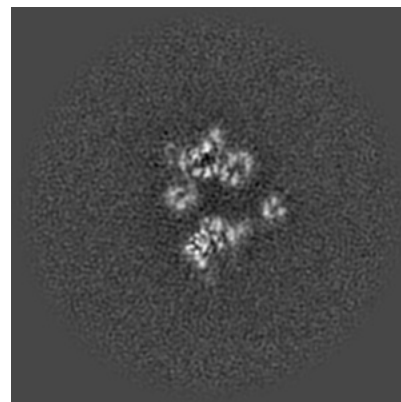
6.2.1 Primary map



X Index: 128

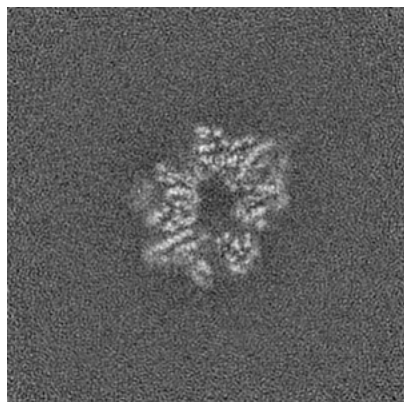


Y Index: 128

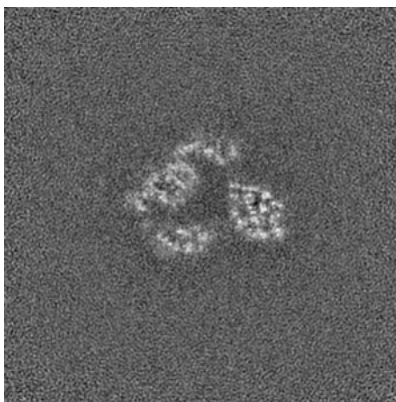


Z Index: 128

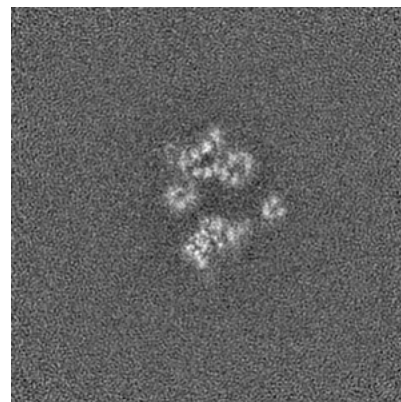
6.2.2 Raw map



X Index: 128



Y Index: 128

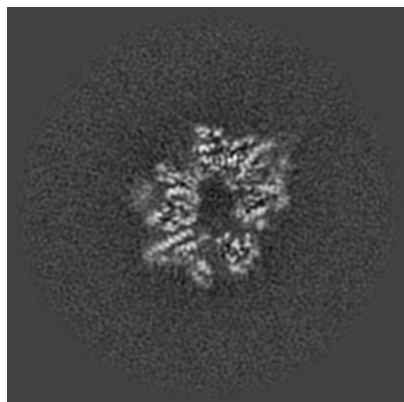


Z Index: 128

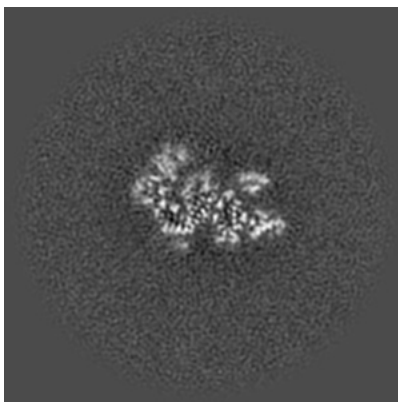
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

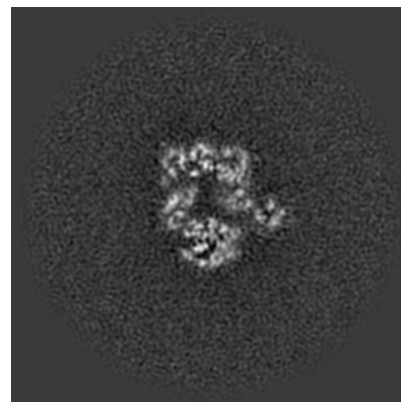
6.3.1 Primary map



X Index: 128

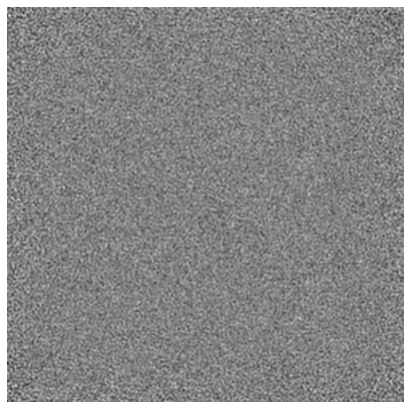


Y Index: 111

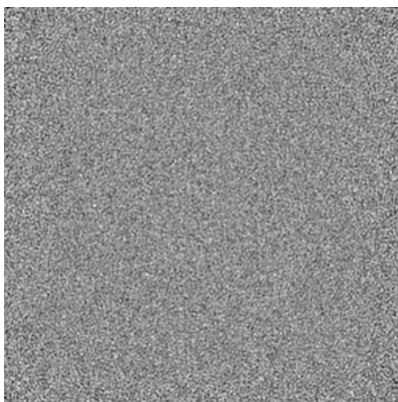


Z Index: 119

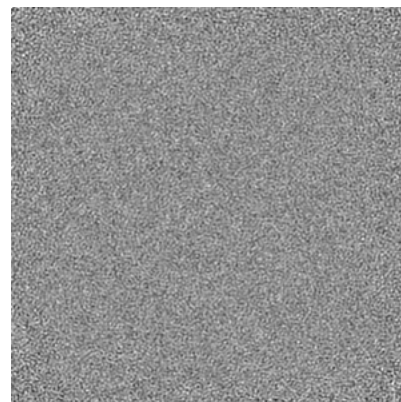
6.3.2 Raw map



X Index: 0



Y Index: 0

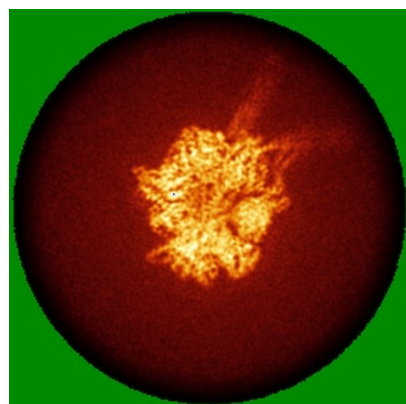


Z Index: 0

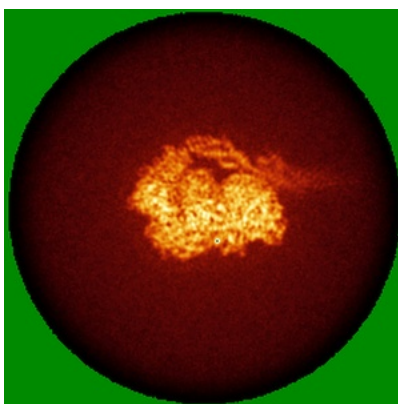
The images above show the largest variance slices of the map in three orthogonal directions.

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

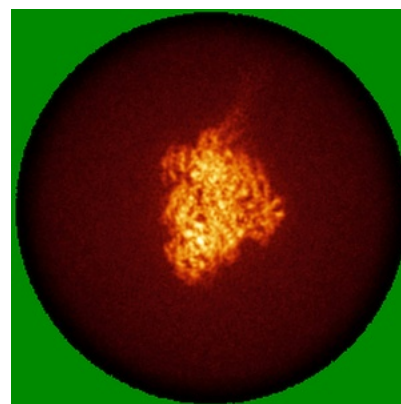
6.4.1 Primary map



X

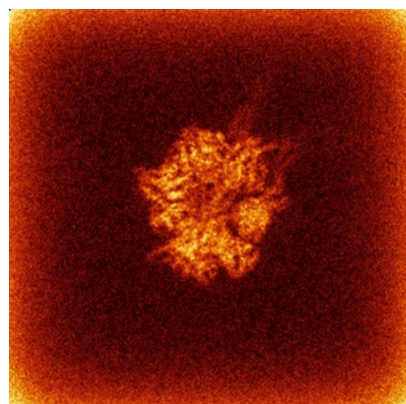


Y

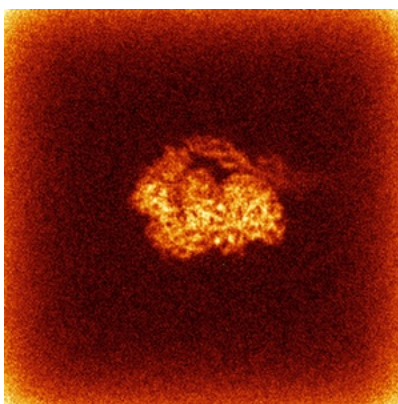


Z

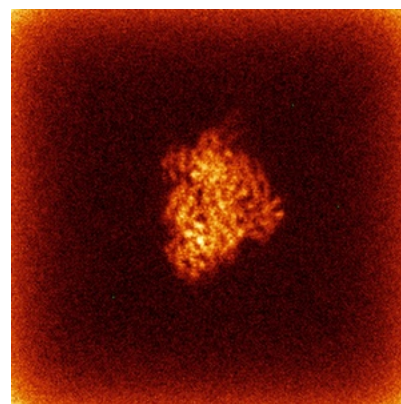
6.4.2 Raw map



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.

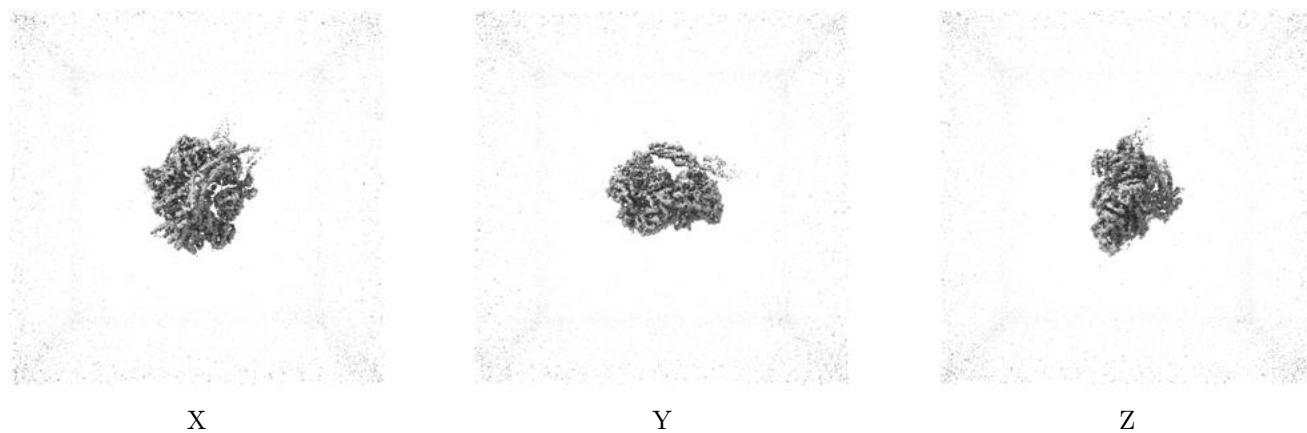
6.5 Orthogonal surface views [i](#)

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.

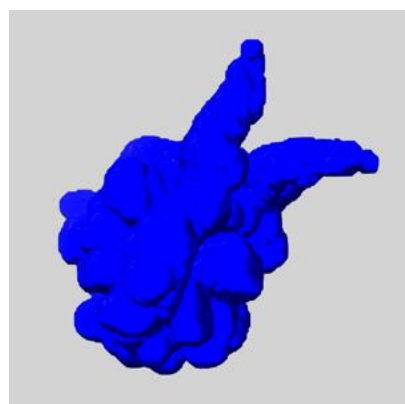
6.6 Mask visualisation [i](#)

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

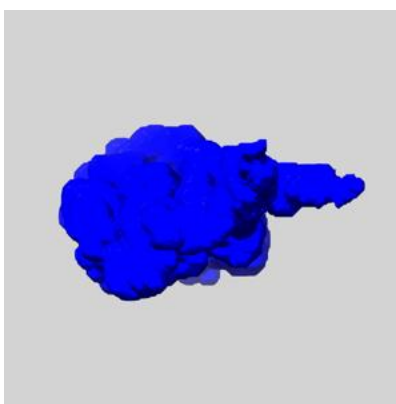
A mask typically either:

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

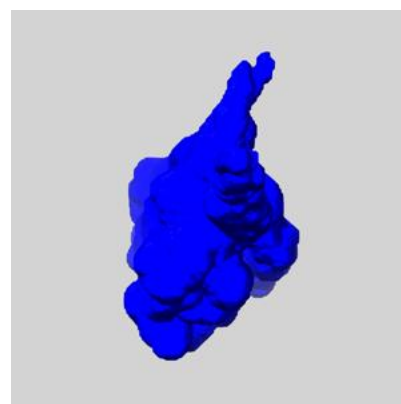
6.6.1 emd_44718_msk_1.map [i](#)



X



Y

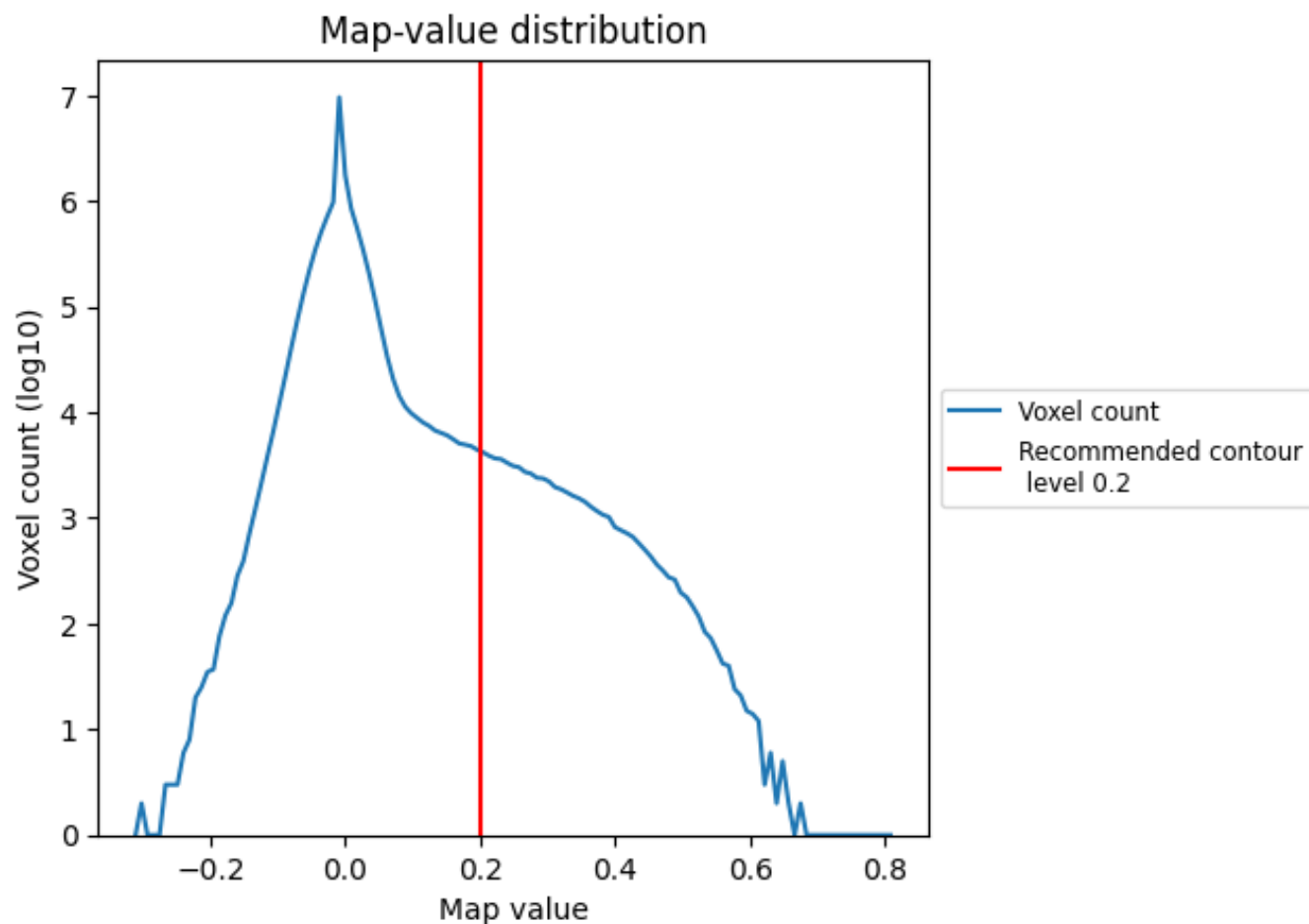


Z

7 Map analysis [i](#)

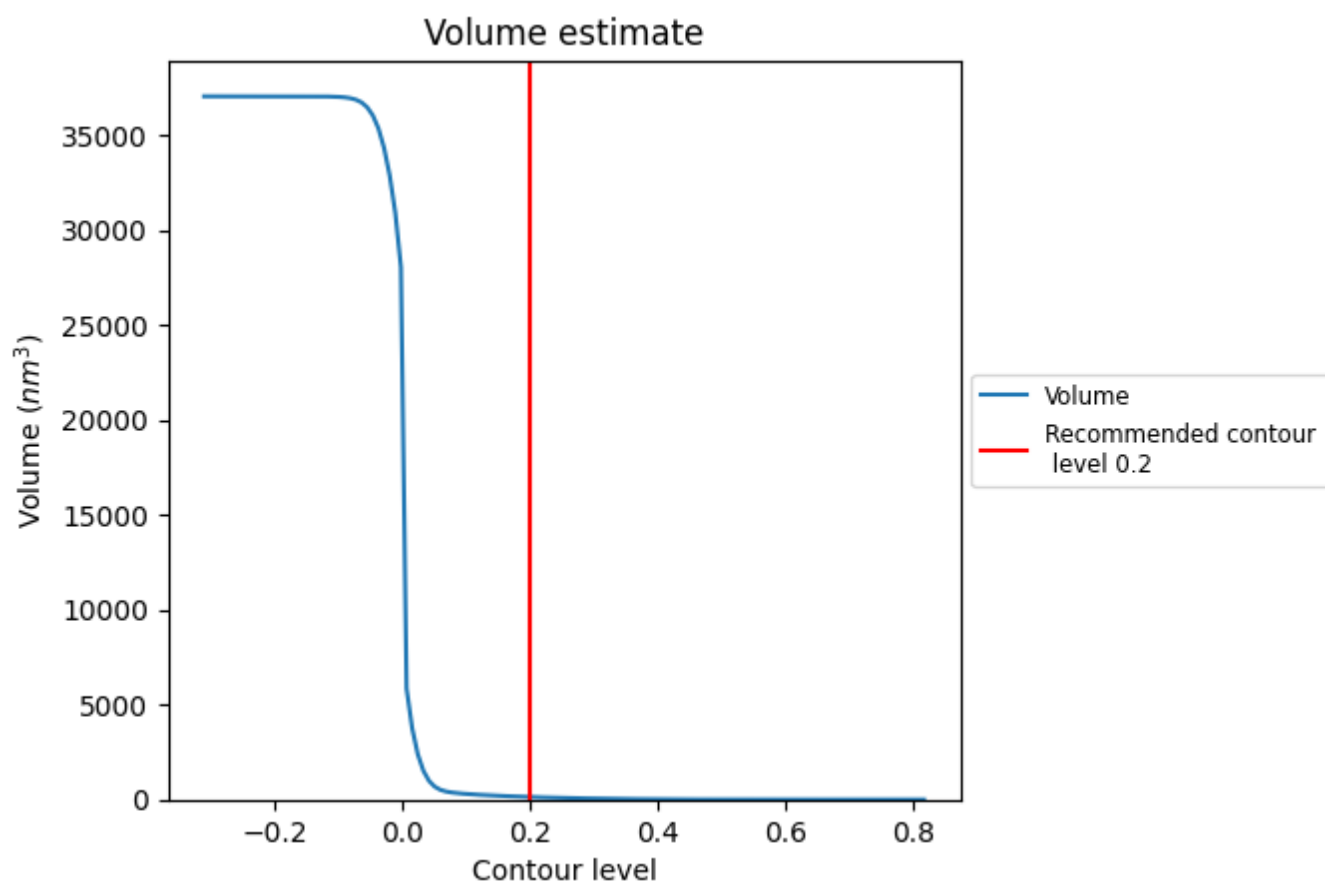
This section contains the results of statistical analysis of the map.

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.

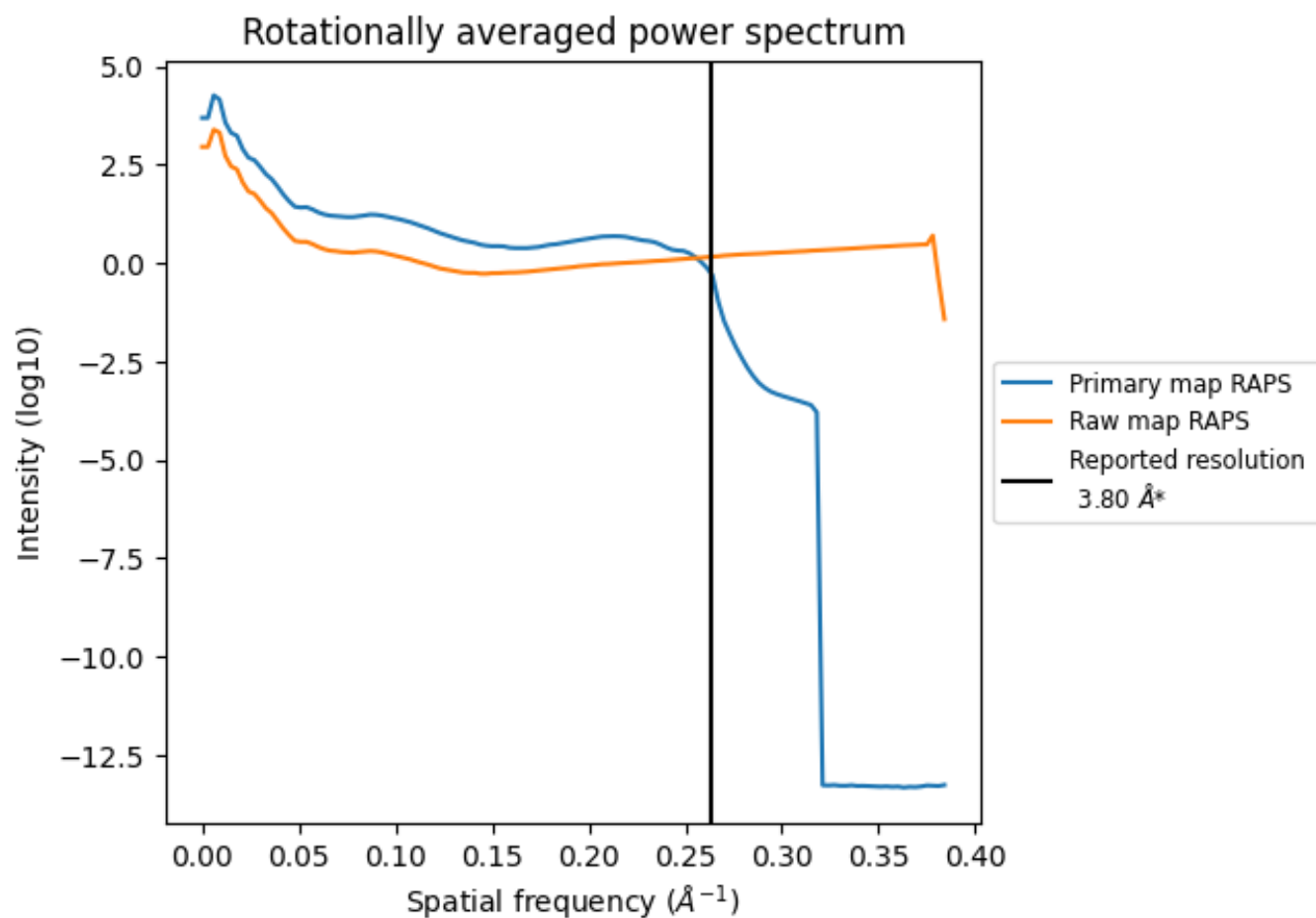
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 134 nm^3 ; this corresponds to an approximate mass of 121 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 ⓘ

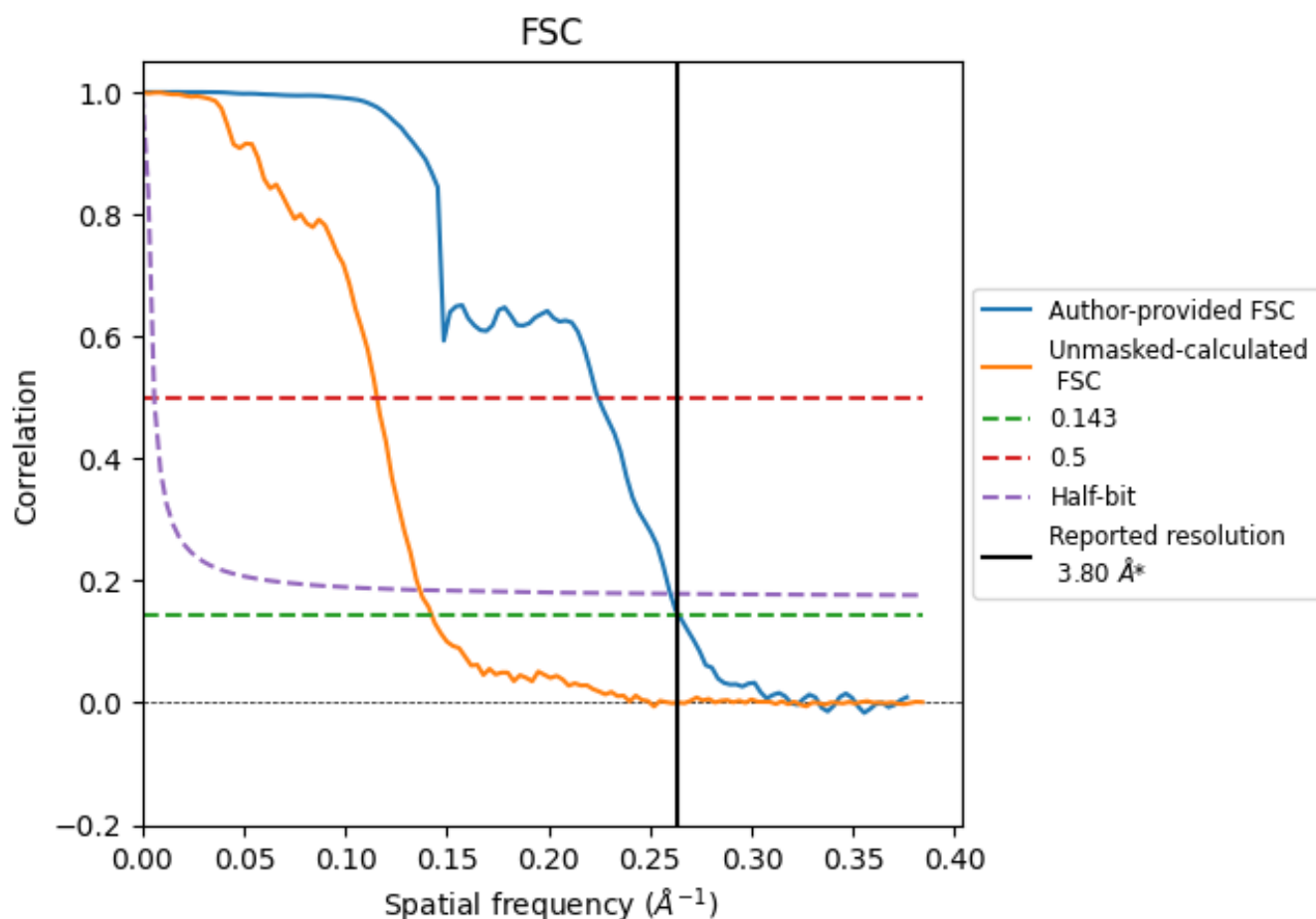


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 \AA^{-1}

8.2 Resolution estimates [i](#)

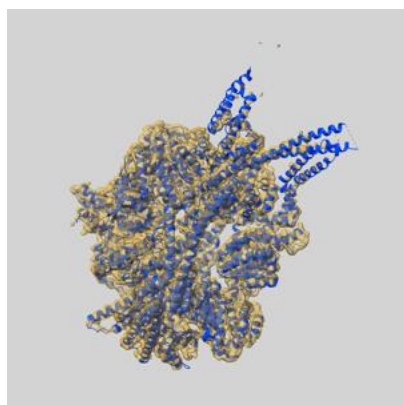
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.78	4.46	3.84
Unmasked-calculated*	7.01	8.65	7.31

*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 7.01 differs from the reported value 3.8 by more than 10 %

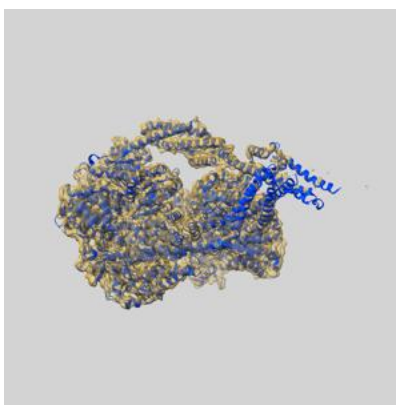
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44718 and PDB model 9BN1. Per-residue inclusion information can be found in section [3](#) on page [5](#).

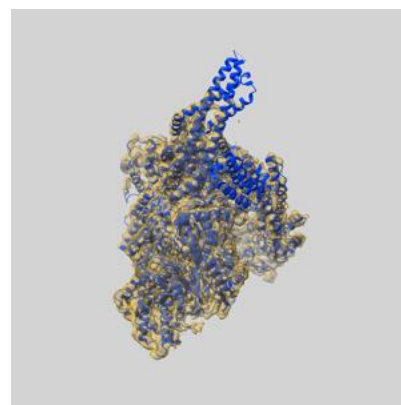
9.1 Map-model overlay [i](#)



X



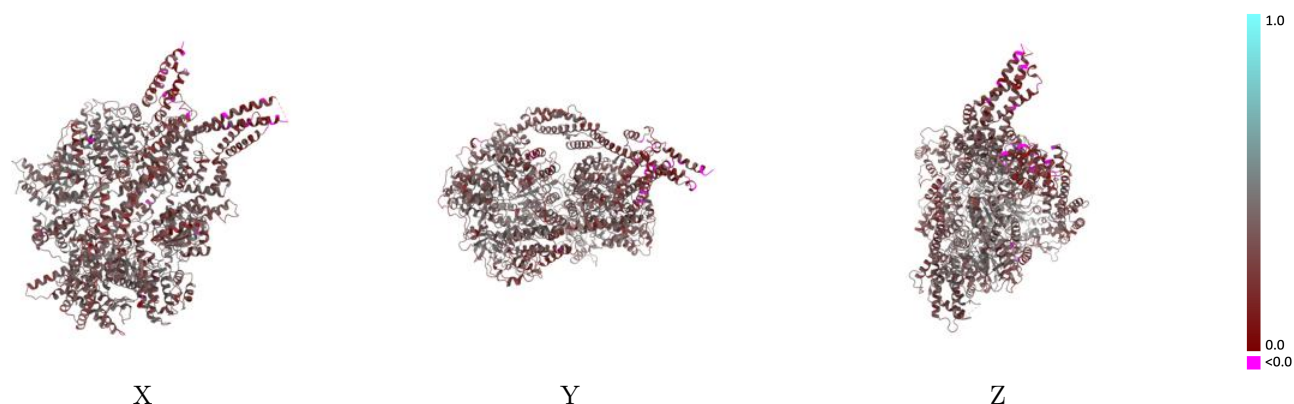
Y



Z

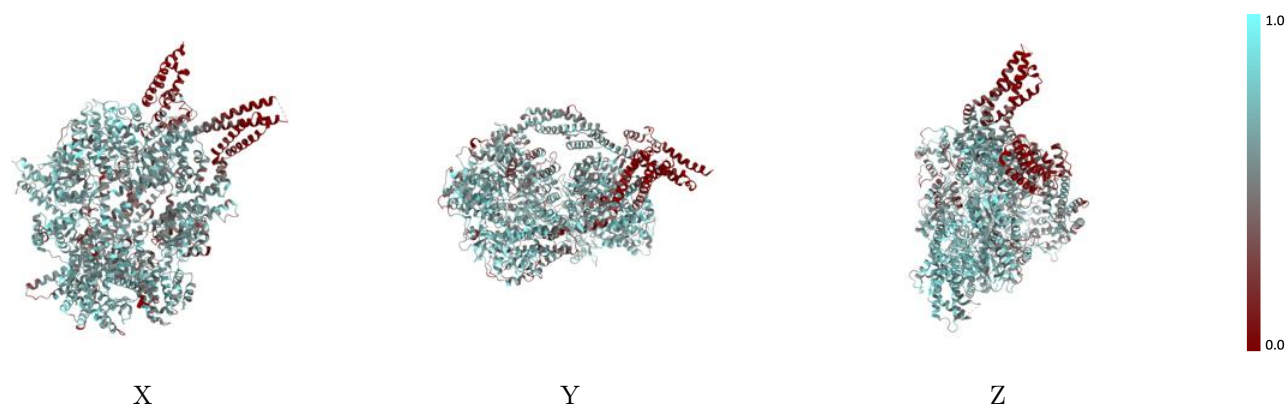
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



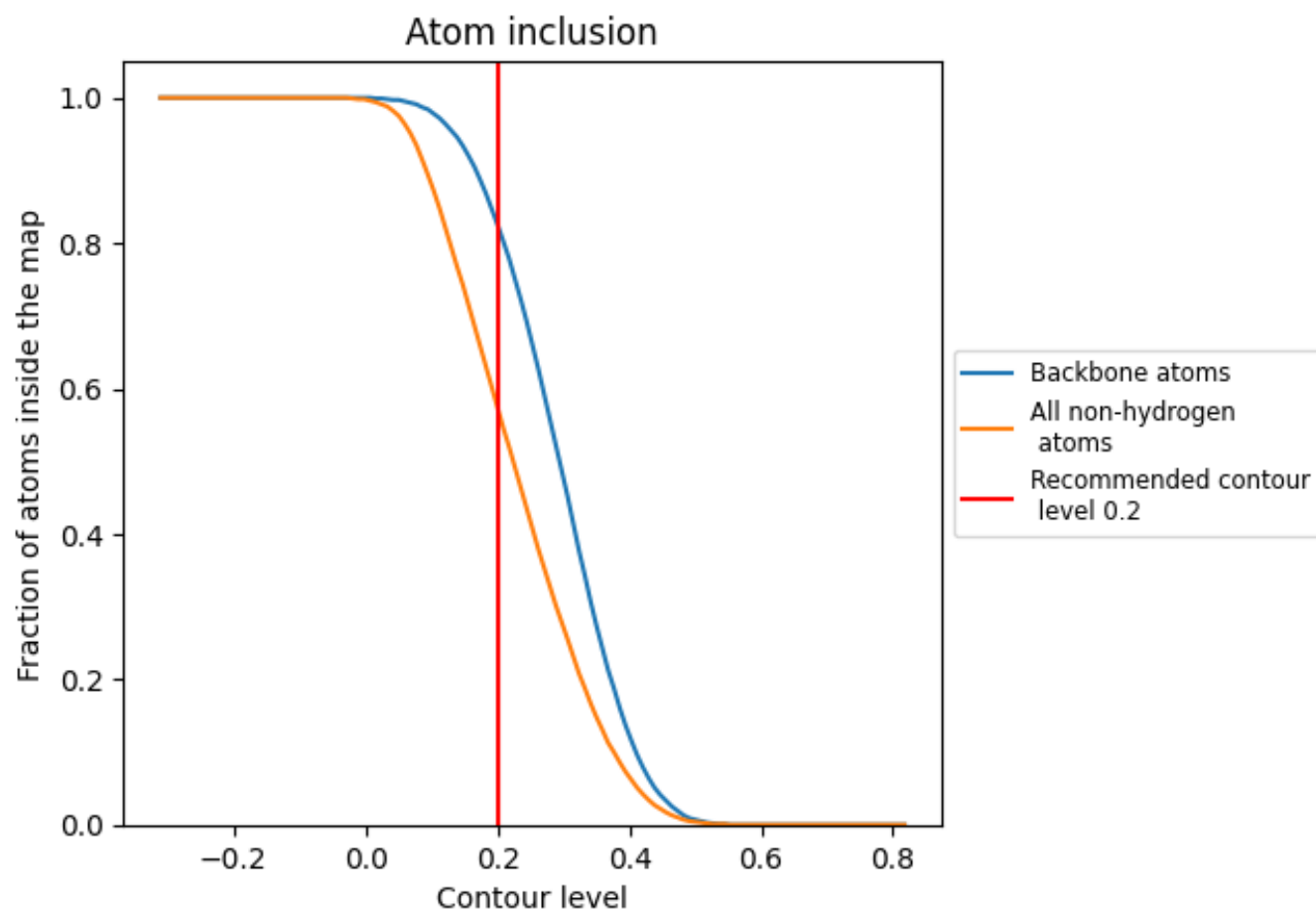
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 83% of all backbone atoms, 57% 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> 0.5750	<div></div> 0.3490
A	<div></div> 0.5750	<div></div> 0.3490

