



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 04:49 PM UTC

PDB ID : 9DHA / pdb_00009dha
EMDB ID : EMD-46861
Title : State-7-Post-1 of the motor domain from full-length human dynein-1 in 5mM AMPPNP with 5mM Mg²⁺
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-09-03
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

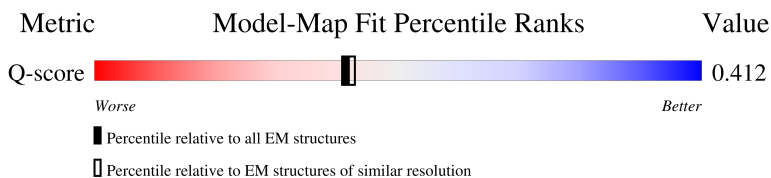
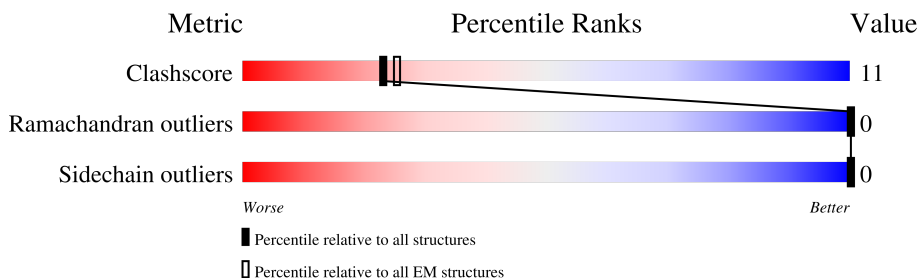
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	4646	

2 Entry composition [i](#)

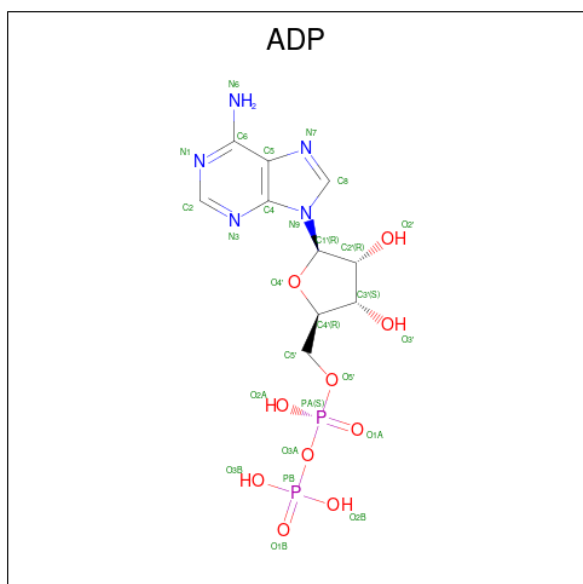
There are 5 unique types of molecules in this entry. The entry contains 24588 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

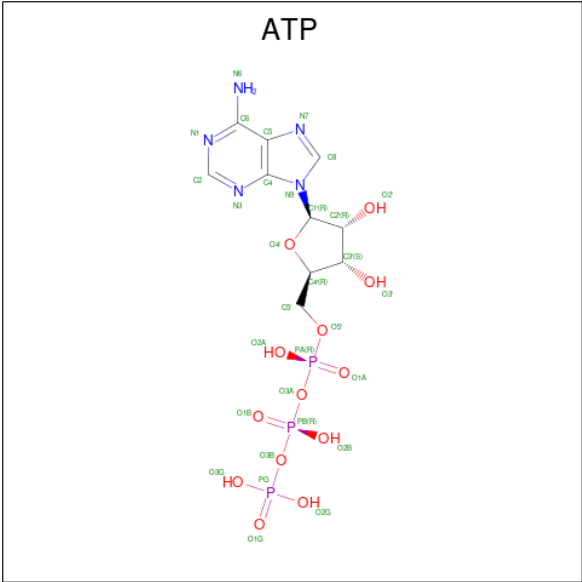
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3038	Total	C	N	O	S	0	0
			24471	15586	4225	4538	122		

- 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).



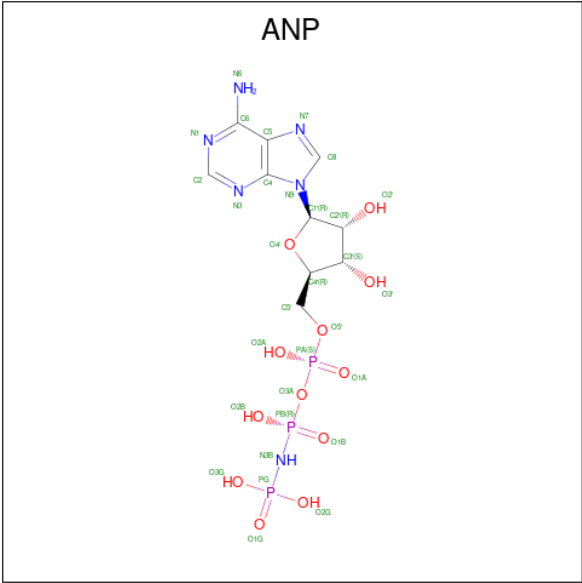
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

- 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	

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	6	12	3	

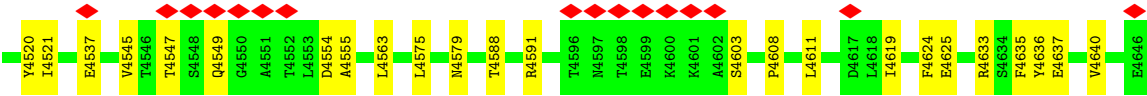
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

K1992	A1862	E1706	L1592	Y1513	K1441	A1381	VAL	TRP	ARG	GLU	ALA	ASN	GLU	ASN	PHE
T1993	L1879	R1710	N1593	K1514	N1442	S1382	ALA	GLU	PHE	PHE	LEU	LYS	LEU	LEU	ASN
S1994	V1880		I1594	Y1515	E1443	Y1383	GLU	THR	PHE	THR	VAL	GLN	ILE	ASP	PHE
A1995	Q1881	V1721	Q1596	F1516	A1444	E1384	GLU	LYS	PRO	GLN	ILE	MET	THR	GLY	GLY
P1996	T1862	V1724	G1596	E1518	I1445	F1385	LEU	VAL	PRO	ILE	ARG	PRO	ASN	VAL	LYS
I1997	T1895		V1597	E1519	V1446	V1386		THR	TRP	SER	LYS	GLY	VAL	ILE	GLY
L2001		G1728	Q1598	A1520	K1447	Q1387	Q1327	THR	VAL	THR	Q1327	ASN	VAL	GLY	GLY
L2002	C1888	K1729	R1599	L1521	D1448	R1388	D1328	GLY	ASN	THR	L1328	LEU	VAL	GLY	ASN
N2003	V1889	T1730	E1602	W1522	V1449	L1389	K1330	ILE	TYR	GLN	K1330	LEU	VAL	ILE	ASP
V2006	M1892	T1731	R1603	E1524	L1450	L1390	G1331	PRO	ASN	GLU	G1331	LEU	VAL	GLY	ILE
K2007	S1903	S1732	G1609	D1525	L1451	K1391	V1332	GLU	ILE	GLU	V1332	PRO	VAL	VAL	ILE
P2008	P1904	T1739	K1610	K1526	A1453	G1392	W1333	GLU	GLY	GLN	W1333	ILE	ARG	GLY	GLY
V2008	F1905	T1740	I1611	W1527	Q1454	Y1393	S1334	ALA	GLY	GLY	S1334	GLY	VAL	ALA	LYS
D2011	T1910	W1741	M1528	M1528	Q1455	M1394	E1335	THR	TRP	VAL	E1335	CYS	GLY	ASP	ASP
M2012	G1911	V1750	K1612	R1529	G1456	K1395	L1336	ALA	GLY	ASP	L1336	LEU	ARG	LEU	LEU
M2018			K1613	I1530	E1456	I1396	S1337	THR	ALA	THR	S1337	TYR	ARG	LEU	GLY
G2021	E1914	E1763	P1627	M1531	L1459	M1397	K1338	LEU	PHE	VAL	K1338	LYS	ALA	ARG	GLU
ALA	F1926	L1766	E1635	D1535	E1460	M1398	V1339	ALA	ILE	ALA	V1339	LYS	ALA	ALA	VAL
GLY			D1636	D1539	F1461	L1399	W1340	GLY	ASP	THR	W1340	THR	THR	THR	GLY
ARG	M1931	M1769	E1639	V1540	L1463	I1400	E1341	LYS	ILE	SER	E1341	VAL	GLN	VAL	GLY
S2026	C1932	G1770	E1639	Q1542	K1464	I1401	Q1342	PHE	ARG	VAL	Q1342	VAL	VAL	LEU	THR
N2027	D1933	G1771	K1645	R1543	Q1465	E1402	I1343	LYS	LYS	ILE	I1343	ASP	GLY	LEU	CYS
D2030	E1934	G1772	K1646	R1543	I1466	L1403	D1344	THR	ASP	PHE	D1344	TRP	GLN	ALA	THR
K2033	T1935	G1773	N1646	Y1546	R1467	L1404	Q1345	LYS	ALA	THR	Q1345	MET	LYS	GLY	HIS
L1946		D1774	K1649	L1547	E1468	S1405	M1346	ASP	ILE	VAL	M1346	VAL	VAL	ASP	LYS
L1947			H1653	L1547	N1471	E1406	K1347	ASP	GLN	VAL	K1347	VAL	VAL	LYS	THR
C1949	L1948	V1781	H1654	G1549	T1472	A1407	E1348	ARG	GLN	GLY	E1348	THR	ALA	ALA	PHE
Q1950	Q1950	M1784	F1654	I1550	L1475	L1408	Q1349	GLU	GLN	GLY	Q1349	SER	SER	GLY	LYS
V1951	V1951	V1785	K1655	F1551	D1476	K1409	P1350	CYS	VAL	VAL	P1350	LEU	VAL	VAL	GLY
G1952	G1952		K1656	T1552	L1477	D1410	W1351	ALA	ASN	LYS	W1351	ARG	PRO	ASP	ILE
D1958		T1788	A1659	G1553	L1477	R1411	V1352	LYS	LEU	ILE	V1352	ILE	ILE	ASP	ASN
N1961		L1792	G1660	S1554	V1478	H1412	S1353	GLN	GLN	LYS	S1353	TRP	GLN	ASP	VAL
R1962		Q1800	V1661	A1555	Q1481	W1413	V1354	GLY	LYS	GLN	V1354	ASP	ALA	GLN	ALA
R1966		R1804	E1668	D1557	N1482	K1414	Q1355	VAL	ILE	PHE	Q1355	MET	ARG	PRO	LYS
S1969		L1811	S1671	K1558	N1482	Q1415	P1356	GLU	VAL	LYS	P1356	GLN	GLN	VAL	ALA
Q1973		I1812	I1676	E1564	R1485	L1416	R1357	GLU	GLY	LYS	R1357	VAL	ALA	VAL	VAL
T1978		I1829	R1679	E1574	L1486	M1417	K1357	THR	ASP	GLN	K1357	GLY	SER	SER	ASP
E1984		I1830	M1685	F1575	L1487	K1418	L1359	THR	ARG	GLY	L1359	ILE	GLY	HIS	LYS
H1985		N1832	S1691	L1576	W1490	R1419	R1360	GLY	ALA	LEU	R1360	ASN	PRO	ASN	ASN
S1986		A1833	T1692	A1577	D1491	V1422	Q1361	THR	VAL	THR	Q1361	ARG	GLY	GLY	HIS
N1987		W1838	T1693	M1579	D1492	N1423	L1363	SER	THR	THR	L1363	THR	GLY	ILE	ASN
P1988		R1843	K1694	K1580	F1494	W1424	D1364	GLY	ASP	GLY	D1364	ASP	GLY	LEU	LEU
N1989		F1844	E1694	N1581	N1495	V1425	A1365	GLY	LEU	LEU	A1365	LEU	LEU	LYS	PRO
Y1990		Y1845	K1697	V1582	K1496	V1426	L1366	ARG	LEU	LEU	L1366	ASN	ASN	ASN	ILE
D2077		M1861	I1698	K1583	V1497	S1427	L1367	VAL	THR	THR	L1367	TRP	VAL	VAL	VAL
S2082			W1701	S1583	A1506	E1428	M1368	GLY	GLY	GLY	M1368	GLY	GLY	GLY	HIS
Q2083			V1705	K1584	M1507	L1429	Q1369	THR	ARG	GLY	Q1369	GLY	GLY	PRO	GLY
Y2086			D1590	L1587	K1508	T1430	L1370	THR	THR	GLY	L1370	GLY	GLY	PRO	GLY
			V1591	S1510	L1509	L1431	K1371	THR	THR	GLY	K1371	GLY	GLY	PRO	GLY
				P1511	S1511	G1432	S1372	THR	THR	GLY	S1372	GLY	GLY	PRO	GLY
				Y1512	Y1512	Q1433	F1373	THR	THR	GLY	F1373	GLY	GLY	PRO	GLY
						I1434	A1375	THR	THR	GLY	A1375	GLY	GLY	PRO	GLY
						W1435	R1376	THR	THR	GLY	R1376	GLY	GLY	PRO	GLY
						D1436	L1377	THR	THR	GLY	L1377	GLY	GLY	PRO	GLY
						V1437	R1378	THR	THR	GLY	V1437	GLY	GLY	PRO	GLY
						D1438	Q1379	THR	THR	GLY	D1438	GLY	GLY	PRO	GLY
						L1439	Y1380	THR	THR	GLY	L1439	GLY	GLY	PRO	GLY
						Q1440		THR	THR	GLY	Q1440	GLY	GLY	PRO	GLY







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40983	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	0.956	Depositor
Minimum map value	-0.343	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1573, 1.1573, 1.1573	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, ANP

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	0.12	0/24989	0.32	0/33856

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	24471	0	24527	545	0
2	A	54	0	24	10	0
3	A	31	0	12	6	0
4	A	31	0	13	5	0
5	A	1	0	0	0	0
All	All	24588	0	24576	546	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 11.

All (546) 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:3211:THR:HG21	1:A:3753:LEU:HD21	1.51	0.93
1:A:3208:ILE:HD11	1:A:3482:LEU:HD22	1.55	0.88
1:A:3202:ASN:HB3	1:A:3206:ARG:HH12	1.37	0.86
1:A:1511:PRO:O	1:A:1514:LYS:NZ	2.11	0.81
1:A:2481:MET:HE3	1:A:2485:GLN:HG2	1.61	0.81
1:A:3167:ARG:NH2	1:A:3169:MET:SD	2.55	0.79
1:A:3585:ARG:HB2	1:A:3697:THR:HG23	1.66	0.77
1:A:2386:PRO:HA	1:A:2416:GLN:HE22	1.51	0.76
1:A:3502:THR:HG21	1:A:3544:ARG:HG2	1.68	0.75
1:A:3167:ARG:NH1	1:A:3168:THR:O	2.20	0.75
1:A:2910:VAL:HG21	1:A:3105:VAL:HG22	1.68	0.74
1:A:2834:GLN:HE21	1:A:2843:ARG:HB3	1.51	0.74
1:A:3167:ARG:HH21	1:A:3687:GLU:HA	1.53	0.74
1:A:2804:ARG:HD3	1:A:2929:PRO:HG2	1.70	0.74
1:A:3817:SER:HB3	1:A:4349:LEU:HD21	1.71	0.73
1:A:2773:MET:HG2	1:A:2825:TRP:HE1	1.53	0.72
1:A:3202:ASN:HB3	1:A:3206:ARG:NH1	2.04	0.72
1:A:3654:ARG:HH11	1:A:3661:LEU:HD11	1.55	0.72
1:A:4192:GLU:OE1	1:A:4195:ARG:NH1	2.24	0.70
1:A:2994:MET:HE1	1:A:3008:MET:HE1	1.72	0.70
1:A:2601:LYS:NZ	4:A:4703:ANP:O3G	2.25	0.70
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.73	0.70
1:A:2839:GLU:HG3	1:A:2841:GLU:HG3	1.74	0.70
1:A:3724:VAL:HG11	1:A:3797:VAL:HG21	1.72	0.69
1:A:1397:ASN:O	1:A:1401:ILE:HD12	1.91	0.69
1:A:4193:ARG:NH2	1:A:4637:GLU:O	2.26	0.68
1:A:2148:LYS:HG2	1:A:2361:MET:HB3	1.75	0.68
1:A:2581:LEU:HD13	1:A:2591:LEU:HD21	1.73	0.68
1:A:2660:VAL:HG12	1:A:2707:GLN:HB2	1.75	0.68
1:A:4042:LEU:HD13	1:A:4139:LEU:HD23	1.74	0.68
1:A:2798:GLU:OE1	1:A:2836:ARG:NH2	2.26	0.68
1:A:2481:MET:HE2	1:A:2486:LEU:HA	1.77	0.67
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.25	0.66
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.77	0.66
1:A:2446:ILE:HG23	1:A:2447:MET:HG2	1.77	0.66
1:A:2768:PRO:HB2	1:A:2858:PHE:HE1	1.59	0.66
1:A:2793:ILE:O	1:A:2836:ARG:NH1	2.26	0.66
1:A:4545:VAL:HG22	1:A:4588:THR:HG22	1.75	0.66
1:A:2684:ARG:NH1	1:A:2688:GLU:OE1	2.29	0.65
1:A:3767:ILE:HA	1:A:3770:LEU:HD13	1.79	0.65
1:A:4107:MET:HE1	1:A:4137:ASN:HD21	1.61	0.65
1:A:2505:ASP:HB3	1:A:2733:VAL:HG13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2563:ALA:O	1:A:2804:ARG:NH2	2.29	0.65
1:A:2773:MET:HB3	1:A:2799:MET:HE1	1.79	0.65
1:A:1360:ARG:HB3	1:A:1397:ASN:HD21	1.62	0.64
1:A:4176:ARG:NH1	1:A:4220:ASP:OD1	2.30	0.64
1:A:2065:LEU:HD11	1:A:2133:GLU:HB3	1.79	0.64
1:A:4385:SER:O	1:A:4389:HIS:ND1	2.31	0.64
1:A:3044:LEU:HD11	1:A:3049:GLU:HB2	1.79	0.64
1:A:1438:ASP:OD1	1:A:1440:GLN:NE2	2.31	0.63
1:A:2287:ILE:HD12	1:A:2299:GLN:HG3	1.79	0.63
1:A:2413:LEU:HA	1:A:2416:GLN:HE21	1.63	0.63
1:A:1698:ILE:HD13	1:A:1701:TRP:HE1	1.63	0.63
1:A:3508:LEU:HD23	1:A:3536:LEU:HD21	1.80	0.63
1:A:1579:MET:HE2	1:A:1579:MET:HA	1.81	0.63
1:A:3584:ASN:O	1:A:3651:ARG:NH1	2.31	0.63
1:A:2918:HIS:O	1:A:2922:ILE:HG12	1.99	0.62
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.80	0.62
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	1.81	0.62
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	1.82	0.62
1:A:2915:VAL:HG13	1:A:2946:LEU:HD11	1.80	0.62
1:A:3638:VAL:HG22	1:A:3681:THR:HB	1.81	0.62
1:A:2485:GLN:HA	1:A:2488:ARG:HE	1.65	0.61
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.33	0.61
1:A:1491:ASP:O	1:A:1495:ASN:ND2	2.33	0.61
1:A:2665:GLU:HB3	1:A:2668:LEU:HD23	1.81	0.61
1:A:4554:ASP:OD2	1:A:4591:ARG:NH2	2.33	0.61
1:A:1766:LEU:HD13	1:A:1833:ALA:HA	1.83	0.60
1:A:3172:THR:HG21	1:A:3694:SER:HB2	1.81	0.60
1:A:1792:LEU:HB3	1:A:1812:ILE:HD11	1.81	0.60
1:A:3114:ASP:OD2	1:A:3191:ARG:NH2	2.34	0.60
1:A:4437:VAL:HG21	1:A:4444:GLN:HB3	1.84	0.60
1:A:4226:THR:HG21	1:A:4239:PRO:HD3	1.83	0.60
1:A:1486:LEU:HB3	1:A:1541:GLN:NE2	2.17	0.60
1:A:1395:LYS:NZ	1:A:1440:GLN:OE1	2.33	0.60
1:A:1905:PHE:HB3	1:A:2018:MET:HB3	1.82	0.60
1:A:2728:LEU:HA	1:A:2731:VAL:HG12	1.83	0.60
1:A:3835:ILE:HG12	1:A:3870:ARG:HD2	1.83	0.60
1:A:2138:ILE:HG23	1:A:2161:LEU:HD21	1.84	0.59
1:A:2488:ARG:NH1	1:A:2543:GLY:O	2.35	0.59
1:A:1531:MET:HE3	1:A:1535:ASP:HB2	1.85	0.59
1:A:4496:ALA:HB2	1:A:4504:LEU:HD21	1.84	0.59
1:A:1728:GLY:O	1:A:1784:ASN:ND2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4266:ASN:O	1:A:4270:GLU:HG2	2.03	0.59
1:A:1985:HIS:HD2	1:A:1997:ILE:HD12	1.67	0.59
1:A:2729:ARG:NH2	3:A:4702:ATP:O2A	2.33	0.59
1:A:3931:GLN:O	1:A:3935:VAL:HG23	2.03	0.59
1:A:3113:MET:O	1:A:3140:ARG:NH2	2.26	0.58
1:A:3808:CYS:HB3	1:A:3832:PHE:HZ	1.67	0.58
1:A:2488:ARG:O	1:A:2492:ARG:HG2	2.03	0.58
1:A:3544:ARG:NH2	1:A:3735:GLN:OE1	2.37	0.58
1:A:2875:ASN:OD1	1:A:2927:ARG:NH2	2.36	0.58
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.84	0.58
1:A:2112:LYS:HG3	1:A:2122:VAL:HG21	1.84	0.58
1:A:2593:LEU:HD12	1:A:2605:LEU:HG	1.86	0.58
1:A:3128:VAL:HG23	1:A:3145:ASN:HD21	1.68	0.58
1:A:3873:ARG:HH21	1:A:4020:ILE:HG22	1.68	0.58
1:A:2994:MET:O	1:A:3067:THR:OG1	2.20	0.58
1:A:1497:VAL:HG23	1:A:1527:LEU:HD12	1.85	0.58
1:A:2115:LYS:HE3	1:A:2122:VAL:HG12	1.86	0.57
1:A:3130:TYR:CZ	1:A:3132:LYS:HB2	2.39	0.57
1:A:1882:THR:HG22	1:A:1885:THR:HG23	1.85	0.57
1:A:4105:TRP:HZ3	1:A:4109:LEU:HD12	1.69	0.57
1:A:2275:TRP:NE1	1:A:2277:ASP:OD1	2.38	0.57
1:A:1396:ILE:HB	1:A:1439:LEU:HD12	1.86	0.57
1:A:1769:MET:HB3	1:A:1831:ASP:HB2	1.86	0.57
1:A:4100:HIS:NE2	1:A:4129:GLU:OE2	2.38	0.57
1:A:1376:ARG:NH1	1:A:1379:GLN:OE1	2.38	0.57
1:A:1486:LEU:HB3	1:A:1541:GLN:HE22	1.70	0.57
1:A:1985:HIS:CD2	1:A:1997:ILE:HD12	2.40	0.57
1:A:4377:MET:SD	1:A:4438:CYS:HA	2.45	0.57
1:A:1861:MET:HG2	1:A:1862:ALA:H	1.70	0.56
1:A:2257:LYS:NZ	1:A:2676:THR:OG1	2.29	0.56
1:A:1360:ARG:HB3	1:A:1397:ASN:ND2	2.20	0.56
1:A:2265:TYR:OH	1:A:2311:TRP:O	2.19	0.56
1:A:1414:LYS:HA	1:A:1417:MET:HE2	1.88	0.56
1:A:4554:ASP:OD1	1:A:4555:ALA:N	2.38	0.56
1:A:3947:LEU:O	1:A:3951:VAL:HG23	2.06	0.56
1:A:1763:GLU:OE2	1:A:1838:TRP:NE1	2.37	0.56
1:A:1574:GLU:OE1	1:A:1603:ARG:NH1	2.39	0.56
1:A:3766:ILE:O	1:A:3769:THR:OG1	2.24	0.56
1:A:1487:ILE:HD11	1:A:1579:MET:HE1	1.88	0.56
1:A:4129:GLU:O	1:A:4131:ASN:ND2	2.39	0.56
1:A:4537:GLU:OE2	1:A:4537:GLU:N	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.87	0.55
1:A:1523:TRP:HA	1:A:1526:LYS:HE3	1.89	0.55
1:A:1911:GLY:HA2	2:A:4701:ADP:H5'1	1.89	0.55
1:A:1409:LYS:HD2	1:A:1410:ASP:N	2.22	0.55
1:A:1429:LEU:HD21	1:A:1434:ILE:HD11	1.88	0.55
1:A:2729:ARG:NH1	3:A:4702:ATP:O3B	2.39	0.55
1:A:3824:LEU:HD11	1:A:4130:ILE:HG12	1.89	0.55
1:A:1911:GLY:HA3	2:A:4701:ADP:H8	1.71	0.55
1:A:4448:LEU:HD13	1:A:4451:LEU:HD23	1.88	0.55
1:A:2277:ASP:OD2	1:A:2285:ARG:NE	2.34	0.55
1:A:3194:LEU:O	1:A:3198:GLN:HG2	2.07	0.55
1:A:3817:SER:O	1:A:3820:GLN:NE2	2.40	0.55
1:A:3193:GLU:O	1:A:3196:GLU:HG3	2.07	0.54
1:A:3215:VAL:HG21	1:A:3478:LEU:HD22	1.89	0.54
1:A:1750:VAL:HG12	1:A:1811:LEU:HD21	1.90	0.54
1:A:1547:LEU:HD21	1:A:1612:GLN:HG3	1.88	0.54
1:A:2971:ASP:O	1:A:2974:GLU:HG2	2.06	0.54
1:A:2885:ASP:OD1	1:A:2886:GLN:N	2.40	0.54
1:A:3198:GLN:OE1	1:A:3496:PHE:HB3	2.08	0.54
1:A:4413:PHE:HE2	1:A:4504:LEU:HB3	1.72	0.54
1:A:2890:ARG:NH2	1:A:2913:ASN:OD1	2.41	0.54
1:A:4377:MET:HB3	1:A:4378:ARG:HH11	1.72	0.54
1:A:4603:SER:OG	1:A:4625:GLU:OE2	2.23	0.54
1:A:4071:ILE:HG13	1:A:4099:VAL:HG12	1.90	0.54
1:A:1578:LEU:O	1:A:1582:VAL:HG23	2.07	0.54
1:A:2283:VAL:O	1:A:2287:ILE:HG12	2.08	0.54
1:A:2499:LEU:O	1:A:2503:SER:OG	2.24	0.54
1:A:3688:PHE:HB3	1:A:3692:LEU:HD23	1.90	0.54
1:A:1363:LEU:O	1:A:1367:LEU:HG	2.08	0.54
1:A:1946:VAL:HG13	1:A:2006:VAL:HG21	1.89	0.54
1:A:3873:ARG:NH2	1:A:4020:ILE:O	2.41	0.53
1:A:4547:THR:O	1:A:4549:GLN:NE2	2.40	0.53
1:A:2628:PRO:HB3	1:A:2682:PHE:CD2	2.43	0.53
1:A:3484:ALA:HA	1:A:3487:GLU:OE1	2.09	0.53
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.89	0.53
1:A:1879:LEU:HB2	2:A:4701:ADP:C6	2.43	0.53
1:A:4002:LEU:O	1:A:4005:ALA:HB3	2.09	0.53
1:A:1701:TRP:O	1:A:1705:VAL:HG23	2.08	0.53
1:A:2231:SER:OG	1:A:2344:GLU:OE2	2.26	0.53
1:A:2601:LYS:NZ	4:A:4703:ANP:O2B	2.41	0.53
1:A:4350:GLU:N	1:A:4350:GLU:OE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1351:TRP:O	1:A:1404:LYS:NZ	2.40	0.53
1:A:1892:MET:HE3	1:A:1892:MET:HA	1.90	0.53
1:A:3889:ARG:HH22	1:A:4347:GLN:HE22	1.56	0.53
1:A:1910:THR:HG22	1:A:2044:PRO:HD3	1.90	0.53
1:A:2865:LYS:HD2	1:A:2865:LYS:O	2.09	0.53
1:A:3553:LEU:HB2	1:A:3578:ILE:HD13	1.90	0.53
1:A:4425:GLN:OE1	1:A:4429:GLN:NE2	2.41	0.53
1:A:3767:ILE:O	1:A:3770:LEU:HB2	2.08	0.52
1:A:4105:TRP:CZ3	1:A:4109:LEU:HD12	2.43	0.52
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.91	0.52
1:A:2729:ARG:HD3	1:A:2730:HIS:NE2	2.25	0.52
1:A:3558:GLU:HA	1:A:3561:ARG:NH1	2.25	0.52
1:A:2464:GLN:HG2	1:A:2583:THR:HA	1.90	0.52
1:A:3661:LEU:HD13	1:A:3668:ASP:HB3	1.91	0.52
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.74	0.52
1:A:4436:GLN:HG2	1:A:4441:LYS:HE2	1.91	0.52
1:A:2894:LYS:HG2	1:A:2911:LEU:HD23	1.91	0.52
1:A:3967:GLU:HB2	1:A:4004:MET:HB2	1.90	0.52
1:A:3558:GLU:HA	1:A:3561:ARG:HH12	1.74	0.52
1:A:3638:VAL:HG11	1:A:3679:LEU:HB3	1.92	0.52
1:A:3113:MET:SD	1:A:3184:ALA:HA	2.50	0.52
1:A:4088:VAL:HG21	1:A:4116:LEU:HD21	1.92	0.52
1:A:4452:ILE:O	1:A:4456:VAL:HG23	2.09	0.52
1:A:1880:VAL:HB	1:A:2049:ILE:HG12	1.92	0.52
1:A:3916:LEU:HD21	1:A:3936:VAL:HG13	1.91	0.52
1:A:4434:VAL:HA	1:A:4437:VAL:HG12	1.91	0.51
1:A:4055:VAL:HG11	1:A:4095:MET:SD	2.51	0.51
1:A:4271:ARG:HG3	1:A:4633:ARG:HH22	1.74	0.51
1:A:4469:VAL:HB	1:A:4473:MET:HE3	1.91	0.51
1:A:2996:GLU:HA	1:A:2999:VAL:HG22	1.91	0.51
1:A:4412:PHE:HE1	1:A:4516:VAL:HG23	1.75	0.51
1:A:1685:MET:HE3	1:A:1685:MET:HA	1.92	0.51
1:A:2218:HIS:HA	1:A:2340:ARG:HD3	1.93	0.51
1:A:2922:ILE:HB	1:A:2950:VAL:HG11	1.92	0.51
1:A:4431:LEU:HA	1:A:4434:VAL:HG12	1.91	0.51
1:A:2755:MET:HG2	1:A:2756:LEU:HD23	1.91	0.51
1:A:1952:GLY:HA2	1:A:2012:MET:HB3	1.93	0.50
1:A:2577:HIS:O	1:A:2581:LEU:HD23	2.10	0.50
1:A:2592:VAL:HG23	1:A:2731:VAL:HG21	1.93	0.50
1:A:4100:HIS:HB3	1:A:4128:MET:HG3	1.92	0.50
1:A:2729:ARG:HH22	3:A:4702:ATP:PA	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4008:PHE:O	1:A:4011:THR:OG1	2.27	0.50
1:A:1351:TRP:HZ3	1:A:1400:VAL:HG13	1.77	0.50
1:A:1832:ASN:OD1	1:A:1833:ALA:N	2.45	0.50
1:A:3514:ILE:HD11	1:A:3553:LEU:HD13	1.94	0.50
1:A:2363:TRP:CD1	1:A:2365:SER:HG	2.30	0.50
1:A:3846:LEU:HB3	1:A:3855:ARG:HH21	1.77	0.50
1:A:1800:GLN:OE1	1:A:1804:ARG:NH1	2.44	0.50
1:A:1947:GLY:O	1:A:1951:VAL:HG12	2.12	0.50
1:A:2026:SER:OG	1:A:2027:ASN:N	2.44	0.50
1:A:2925:ILE:HG12	1:A:2933:LEU:HB2	1.93	0.50
1:A:4274:THR:O	1:A:4277:SER:OG	2.27	0.50
1:A:1357:ARG:HD3	1:A:1357:ARG:N	2.27	0.50
1:A:2566:ASP:OD1	1:A:2566:ASP:N	2.45	0.50
1:A:2901:TYR:OH	1:A:2909:LEU:O	2.30	0.50
1:A:2335:LEU:HD12	1:A:2336:PRO:HD2	1.94	0.50
1:A:1447:LYS:O	1:A:1451:LEU:HG	2.13	0.49
1:A:3497:LYS:HD2	1:A:3497:LYS:O	2.13	0.49
1:A:1335:GLU:HG3	1:A:1377:LEU:HD13	1.94	0.49
1:A:3757:LYS:HB2	1:A:3759:ARG:HE	1.78	0.49
1:A:1408:LEU:O	1:A:1413:TRP:HD1	1.96	0.49
1:A:1459:LEU:HD22	1:A:1507:MET:HE2	1.94	0.49
1:A:1706:GLU:OE2	1:A:1710:ARG:NH2	2.45	0.49
1:A:3591:ASP:HB3	1:A:3701:PHE:HB2	1.92	0.49
1:A:4002:LEU:HD21	1:A:4336:GLY:HA2	1.93	0.49
1:A:1385:PHE:HA	1:A:1388:ARG:NH1	2.28	0.49
1:A:2175:MET:HE2	1:A:2208:LEU:HB3	1.94	0.49
1:A:3026:TYR:CE1	1:A:3030:MET:HE3	2.47	0.49
1:A:2302:VAL:HG12	1:A:2342:MET:HE3	1.95	0.49
1:A:2759:ILE:HG21	1:A:2762:LEU:HD12	1.95	0.49
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.94	0.49
1:A:3762:ASP:OD1	1:A:3763:ASP:N	2.42	0.49
1:A:1463:LEU:O	1:A:1467:ARG:HG3	2.13	0.48
1:A:1910:THR:N	2:A:4701:ADP:O1B	2.46	0.48
1:A:1984:GLU:HG2	1:A:1997:ILE:HD13	1.94	0.48
1:A:3954:ASP:OD1	1:A:3957:PHE:N	2.46	0.48
1:A:3961:LEU:O	1:A:3997:ARG:NH1	2.42	0.48
1:A:1478:VAL:HG21	1:A:1488:ARG:HH21	1.78	0.48
1:A:2324:LEU:HD11	1:A:2332:ARG:HB3	1.94	0.48
1:A:3113:MET:HE3	1:A:3115:LEU:HD11	1.94	0.48
1:A:2527:PRO:HD3	1:A:2545:TRP:CE2	2.48	0.48
1:A:3196:GLU:HA	1:A:3199:MET:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4353:ASP:OD1	1:A:4375:ALA:N	2.46	0.48
1:A:2150:VAL:HG12	1:A:2363:TRP:CE2	2.48	0.48
1:A:2299:GLN:O	1:A:2339:VAL:HA	2.13	0.48
1:A:4068:SER:OG	1:A:4097:LYS:NZ	2.37	0.48
1:A:2104:LYS:HA	1:A:2136:ILE:HD13	1.94	0.48
1:A:2395:GLN:HB2	1:A:2396:ARG:HH21	1.78	0.48
1:A:2999:VAL:HB	1:A:3005:LEU:HD21	1.95	0.48
1:A:4407:ASP:OD2	1:A:4410:PHE:N	2.45	0.48
1:A:1548:GLU:O	1:A:1552:THR:OG1	2.22	0.48
1:A:1378:ARG:HG2	1:A:1383:TYR:CZ	2.49	0.48
1:A:2964:HIS:NE2	1:A:2967:TYR:HA	2.28	0.48
1:A:3783:LYS:O	1:A:3787:THR:OG1	2.27	0.48
1:A:2796:PRO:O	1:A:2800:THR:HG23	2.14	0.47
1:A:2944:THR:OG1	2:A:4704:ADP:O2A	2.32	0.47
1:A:4563:LEU:HD12	1:A:4588:THR:HG21	1.95	0.47
1:A:3026:TYR:CZ	1:A:3030:MET:HE3	2.49	0.47
1:A:3110:THR:O	1:A:3140:ARG:NH2	2.46	0.47
1:A:4088:VAL:HG13	1:A:4118:PRO:HA	1.95	0.47
1:A:1509:LEU:HB3	1:A:3608:LYS:HG2	1.97	0.47
1:A:2222:MET:HG2	1:A:2364:PHE:HE2	1.80	0.47
1:A:2752:ASN:HA	1:A:2755:MET:HB3	1.96	0.47
1:A:3659:ARG:NE	1:A:3670:ASP:OD2	2.46	0.47
1:A:3769:THR:O	1:A:3772:ASN:HB3	2.14	0.47
1:A:1359:LEU:HD11	1:A:1435:TRP:HZ2	1.80	0.47
1:A:2422:ILE:HD13	1:A:2487:GLU:HA	1.97	0.47
1:A:4454:GLU:OE2	1:A:4461:PRO:HG3	2.15	0.47
1:A:1351:TRP:H	1:A:1430:THR:HA	1.80	0.47
1:A:1477:LEU:O	1:A:1485:ARG:NH2	2.40	0.47
1:A:1880:VAL:N	2:A:4701:ADP:N1	2.60	0.47
1:A:2278:GLY:N	1:A:2281:THR:OG1	2.48	0.47
1:A:1399:LEU:HD22	1:A:1439:LEU:HB3	1.97	0.47
1:A:1460:GLU:HG2	1:A:1464:LYS:HE3	1.96	0.47
1:A:1661:VAL:HG22	1:A:1676:ILE:HD12	1.96	0.47
1:A:2590:PRO:HB3	1:A:2708:PHE:HB2	1.97	0.46
1:A:3879:ASP:OD1	1:A:4342:LYS:NZ	2.45	0.46
1:A:1343:ILE:HG22	1:A:1347:LYS:HD3	1.98	0.46
1:A:2191:LEU:HD21	1:A:2232:MET:HE3	1.96	0.46
1:A:2737:ASP:OD1	1:A:2738:TYR:N	2.44	0.46
1:A:2755:MET:HE2	1:A:2807:PHE:HB2	1.97	0.46
1:A:3117:LYS:NZ	1:A:3119:ASN:OD1	2.36	0.46
1:A:3176:TYR:O	1:A:3180:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2752:ASN:OD1	1:A:2770:THR:OG1	2.21	0.46
1:A:3476:THR:O	1:A:3480:LYS:NZ	2.48	0.46
1:A:1396:ILE:O	1:A:1400:VAL:HG23	2.16	0.46
1:A:1741:TRP:CH2	1:A:1750:VAL:HG13	2.50	0.46
1:A:1843:ARG:NH1	1:A:1845:TYR:OH	2.48	0.46
1:A:1978:ILE:HD11	1:A:2001:LEU:HD11	1.97	0.46
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.96	0.46
1:A:4451:LEU:HD12	1:A:4454:GLU:OE2	2.15	0.46
1:A:1781:VAL:O	1:A:1785:VAL:HG23	2.15	0.46
1:A:1911:GLY:HA3	2:A:4701:ADP:C8	2.51	0.46
1:A:2666:ILE:HB	1:A:2712:CYS:SG	2.56	0.46
1:A:2797:ARG:NH2	4:A:4703:ANP:O1A	2.49	0.46
1:A:3886:LEU:O	1:A:3890:ILE:HG12	2.15	0.46
1:A:4388:LEU:HD11	1:A:4435:VAL:HG21	1.97	0.46
1:A:4461:PRO:HD3	1:A:4475:VAL:HG12	1.97	0.46
1:A:1671:SER:HA	1:A:1692:ILE:HD12	1.97	0.46
1:A:4267:THR:HG21	1:A:4636:TYR:HD2	1.80	0.46
1:A:4603:SER:OG	1:A:4603:SER:O	2.34	0.46
1:A:1546:TYR:O	1:A:1550:ILE:HG12	2.16	0.46
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.96	0.46
1:A:1911:GLY:N	2:A:4701:ADP:O1B	2.48	0.46
1:A:4031:VAL:O	1:A:4123:ARG:NH2	2.44	0.46
1:A:4297:PRO:HB3	1:A:4308:TRP:CD1	2.51	0.46
1:A:1523:TRP:O	1:A:1527:LEU:HD23	2.16	0.46
1:A:2063:GLU:HG2	1:A:2064:VAL:N	2.31	0.46
1:A:4485:ARG:NH1	1:A:4513:GLY:O	2.49	0.46
1:A:4178:ARG:CZ	1:A:4296:MET:HE1	2.45	0.45
1:A:1609:GLY:O	1:A:1613:LYS:HG2	2.16	0.45
1:A:2593:LEU:HD23	1:A:2734:VAL:HB	1.99	0.45
1:A:3601:MET:CE	1:A:3611:ARG:HB2	2.47	0.45
1:A:2231:SER:HA	1:A:2234:TRP:NE1	2.31	0.45
1:A:2614:ASP:O	1:A:2615:MET:HE2	2.16	0.45
1:A:2729:ARG:HD3	1:A:2730:HIS:CD2	2.50	0.45
1:A:1455:GLY:O	1:A:1459:LEU:HG	2.16	0.45
1:A:2299:GLN:HB2	1:A:2339:VAL:HG22	1.98	0.45
1:A:4423:LEU:HD13	1:A:4466:HIS:ND1	2.31	0.45
1:A:2594:CYS:O	1:A:2735:TYR:HA	2.15	0.45
1:A:2808:GLU:OE2	1:A:2808:GLU:HA	2.16	0.45
1:A:4517:PRO:HG3	1:A:4611:LEU:HD13	1.98	0.45
1:A:1888:CYS:O	1:A:1892:MET:HG2	2.16	0.45
1:A:2571:THR:O	1:A:2575:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3485:GLU:CD	1:A:3488:ARG:HH22	2.25	0.45
1:A:1653:HIS:HA	1:A:1656:LYS:HE2	1.98	0.45
1:A:3851:ASP:O	1:A:3855:ARG:HG3	2.16	0.45
1:A:2509:LYS:HE2	1:A:2509:LYS:HB3	1.67	0.45
1:A:2616:GLU:HG3	1:A:2657:LYS:HD3	1.99	0.45
1:A:2963:VAL:HG22	1:A:2998:ASN:HB3	1.98	0.45
1:A:1373:PHE:HD2	1:A:1383:TYR:HE1	1.64	0.45
1:A:1409:LYS:HD2	1:A:1410:ASP:H	1.82	0.45
1:A:1464:LYS:O	1:A:1468:GLU:HG2	2.17	0.45
1:A:1539:ASP:CG	1:A:1543:ARG:HE	2.25	0.45
1:A:2239:LYS:HE2	1:A:2239:LYS:HB3	1.91	0.45
1:A:4086:THR:OG1	1:A:4092:ARG:NH2	2.50	0.45
1:A:4482:PHE:O	1:A:4486:ILE:HG12	2.17	0.45
1:A:1914:GLU:CD	2:A:4701:ADP:H3'	2.42	0.45
1:A:2182:LEU:HD23	1:A:2236:VAL:HG22	1.99	0.45
1:A:2361:MET:HE2	1:A:2361:MET:HB2	1.90	0.45
1:A:4387:TRP:HZ2	1:A:4476:ILE:HG22	1.82	0.45
1:A:1598:GLN:O	1:A:1602:GLU:HG2	2.16	0.44
1:A:2518:ILE:O	1:A:2522:THR:N	2.51	0.44
1:A:3554:SER:OG	1:A:3555:ASN:N	2.50	0.44
1:A:3779:GLU:O	1:A:3782:ARG:HG2	2.17	0.44
1:A:2210:LEU:O	1:A:2214:THR:HG23	2.18	0.44
1:A:2658:TRP:CE3	1:A:2705:ARG:HA	2.53	0.44
1:A:2822:ILE:HD12	1:A:2861:ILE:HG21	1.99	0.44
1:A:3101:ALA:O	1:A:3105:VAL:HG23	2.16	0.44
1:A:3618:ALA:HA	1:A:3621:LYS:HE2	2.00	0.44
1:A:3983:ILE:HD12	1:A:4012:ASN:ND2	2.31	0.44
1:A:1903:SER:O	1:A:1903:SER:OG	2.29	0.44
1:A:2813:LEU:HD21	1:A:2816:LEU:HG	2.00	0.44
1:A:2232:MET:O	1:A:2236:VAL:HG12	2.18	0.44
1:A:2943:LYS:NZ	2:A:4704:ADP:O3B	2.48	0.44
1:A:3813:PHE:O	1:A:3816:GLU:HG3	2.18	0.44
1:A:4336:GLY:O	1:A:4340:ILE:HG12	2.17	0.44
1:A:4575:LEU:HG	1:A:4624:PHE:HB3	1.99	0.44
1:A:1788:THR:O	1:A:1792:LEU:HD23	2.18	0.44
1:A:2030:ASP:OD1	1:A:2030:ASP:N	2.47	0.44
1:A:2107:ARG:O	1:A:2111:ILE:HG12	2.17	0.44
1:A:2451:ARG:O	1:A:2455:LEU:HD23	2.18	0.44
1:A:3030:MET:HE1	1:A:3047:HIS:O	2.18	0.44
1:A:3175:HIS:CD2	1:A:3585:ARG:HH12	2.35	0.44
1:A:1356:PRO:HD3	1:A:1404:LYS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1698:ILE:HA	1:A:1701:TRP:NE1	2.32	0.44
1:A:2540:SER:OG	1:A:2542:SER:O	2.32	0.44
1:A:2827:HIS:O	1:A:2831:ARG:HG2	2.18	0.44
1:A:2868:SER:OG	1:A:2870:PRO:O	2.35	0.44
1:A:3875:MET:HE3	1:A:3879:ASP:HB2	1.99	0.44
1:A:4153:VAL:O	1:A:4157:MET:HG3	2.18	0.44
1:A:4412:PHE:CE2	1:A:4520:TYR:HB2	2.53	0.44
1:A:1382:SER:O	1:A:1386:VAL:HG22	2.18	0.44
1:A:1905:PHE:HE2	1:A:2038:SER:HB3	1.82	0.44
1:A:3502:THR:HG23	1:A:3543:PHE:HA	1.99	0.44
1:A:3904:GLU:OE2	1:A:3904:GLU:N	2.40	0.44
1:A:2214:THR:HG22	1:A:2220:LEU:HD21	1.99	0.43
1:A:2230:LYS:HG2	1:A:2364:PHE:CD2	2.53	0.43
1:A:2449:LEU:HA	1:A:2453:ARG:NH2	2.32	0.43
1:A:2589:LYS:NZ	1:A:2730:HIS:O	2.45	0.43
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.53	0.43
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	2.00	0.43
1:A:4635:PHE:HD2	1:A:4640:VAL:HG11	1.83	0.43
1:A:1861:MET:HE1	1:A:1889:TYR:HB3	2.00	0.43
1:A:2485:GLN:HG3	1:A:2488:ARG:HH21	1.83	0.43
1:A:2301:ILE:HB	1:A:2341:ILE:HD13	2.00	0.43
1:A:2924:ARG:O	1:A:2928:GLN:HG2	2.18	0.43
1:A:1402:GLU:HG3	1:A:3655:ARG:HH22	1.83	0.43
1:A:1467:ARG:NH1	1:A:1523:TRP:HE1	2.16	0.43
1:A:2787:ASP:OD1	1:A:2787:ASP:N	2.51	0.43
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	2.00	0.43
1:A:2919:VAL:HG13	1:A:2950:VAL:HG22	2.00	0.43
1:A:4031:VAL:HA	1:A:4035:VAL:HG12	2.01	0.43
1:A:4077:PHE:HB3	1:A:4105:TRP:HE1	1.83	0.43
1:A:1335:GLU:O	1:A:1339:VAL:HG13	2.18	0.43
1:A:1415:GLN:HA	1:A:1418:LYS:HG2	2.01	0.43
1:A:2600:GLY:HA2	4:A:4703:ANP:H5'1	2.00	0.43
1:A:2884:VAL:HG13	1:A:2889:LEU:HD11	1.99	0.43
1:A:3485:GLU:HA	1:A:3488:ARG:NH1	2.34	0.43
1:A:3776:GLU:O	1:A:3779:GLU:HB3	2.18	0.43
1:A:4077:PHE:HB3	1:A:4105:TRP:NE1	2.33	0.43
1:A:4347:GLN:HA	1:A:4350:GLU:HB2	1.99	0.43
1:A:1460:GLU:O	1:A:1463:LEU:HG	2.19	0.43
1:A:2930:GLN:NE2	1:A:3012:LEU:O	2.46	0.43
1:A:3928:THR:HB	1:A:3931:GLN:HB2	2.01	0.43
1:A:1354:VAL:HG11	1:A:1431:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	2.01	0.43
1:A:2295:LEU:HA	1:A:2338:ASN:HD21	1.83	0.43
1:A:2914:GLU:OE1	1:A:2914:GLU:N	2.44	0.43
1:A:3138:SER:OG	1:A:3139:HIS:N	2.52	0.43
1:A:4107:MET:HE1	1:A:4137:ASN:ND2	2.32	0.43
3:A:4702:ATP:O5'	3:A:4702:ATP:H8	2.02	0.43
1:A:1659:ALA:HB2	1:A:1926:PHE:CD1	2.54	0.43
1:A:1933:ASP:HB3	1:A:1962:ARG:NH2	2.34	0.43
1:A:2213:ILE:HG22	1:A:2220:LEU:HD22	2.01	0.43
1:A:2668:LEU:HD12	1:A:3006:GLU:OE1	2.19	0.43
1:A:2930:GLN:HB2	1:A:3059:ILE:HG23	1.99	0.43
1:A:3510:SER:HB2	1:A:3553:LEU:HD21	2.01	0.43
1:A:3893:LYS:HE2	1:A:3893:LYS:HB3	1.73	0.43
1:A:4193:ARG:NH1	1:A:4321:LEU:O	2.52	0.43
1:A:2230:LYS:NZ	3:A:4702:ATP:O3G	2.44	0.43
1:A:2348:LEU:HB3	1:A:2351:ALA:HB3	2.01	0.43
1:A:2445:HIS:NE2	1:A:2449:LEU:HD22	2.34	0.43
1:A:2775:GLU:O	1:A:2778:THR:OG1	2.34	0.43
1:A:2847:ASP:CG	1:A:2869:ARG:HH22	2.26	0.43
1:A:3088:ARG:NH1	4:A:4703:ANP:O1G	2.51	0.43
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	2.00	0.43
1:A:4071:ILE:HD11	1:A:4096:LEU:HD22	2.01	0.43
1:A:1329:LEU:HA	1:A:1332:VAL:HG12	2.00	0.42
1:A:1843:ARG:NH2	1:A:1861:MET:O	2.52	0.42
1:A:2083:GLN:N	1:A:2083:GLN:OE1	2.52	0.42
1:A:2287:ILE:HD13	1:A:2294:GLU:HG2	2.01	0.42
1:A:2635:PHE:HB3	1:A:2650:LEU:HD21	2.00	0.42
1:A:2831:ARG:HA	1:A:2835:ASP:OD1	2.18	0.42
1:A:2927:ARG:HG3	1:A:2928:GLN:HE21	1.84	0.42
1:A:2934:LEU:HB2	1:A:3089:CYS:SG	2.59	0.42
1:A:4185:TRP:O	1:A:4189:ILE:HG12	2.19	0.42
1:A:2229:GLY:N	3:A:4702:ATP:O2B	2.52	0.42
1:A:2512:ALA:O	1:A:2516:GLU:HG2	2.19	0.42
1:A:2569:VAL:HB	1:A:2747:ILE:HG12	2.00	0.42
1:A:2592:VAL:O	1:A:2733:VAL:HA	2.19	0.42
1:A:4031:VAL:HG21	1:A:4058:LEU:HD21	2.02	0.42
1:A:1969:SER:O	1:A:1973:GLN:HG2	2.20	0.42
1:A:2630:LEU:O	1:A:2634:THR:HG23	2.19	0.42
1:A:4080:ALA:O	1:A:4084:ILE:HG13	2.19	0.42
1:A:4474:THR:OG1	1:A:4477:GLN:HG3	2.19	0.42
1:A:4517:PRO:O	1:A:4521:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1671:SER:O	1:A:1692:ILE:N	2.50	0.42
1:A:2784:PHE:HB3	1:A:2792:TYR:CD2	2.53	0.42
1:A:3212:VAL:HG21	1:A:3486:ARG:HH12	1.84	0.42
1:A:4169:ILE:HD12	1:A:4302:ARG:HE	1.84	0.42
1:A:4431:LEU:O	1:A:4435:VAL:HG23	2.19	0.42
1:A:4476:ILE:HA	1:A:4479:VAL:HG22	2.02	0.42
1:A:2759:ILE:HG22	1:A:2762:LEU:H	1.85	0.42
1:A:3200:HIS:NE2	1:A:3747:LYS:HD3	2.34	0.42
1:A:4635:PHE:CD2	1:A:4640:VAL:HG11	2.55	0.42
1:A:1485:ARG:HE	1:A:1485:ARG:HB3	1.74	0.42
1:A:1949:CYS:HB3	1:A:2008:VAL:HA	2.02	0.42
1:A:2437:LEU:HD22	1:A:2455:LEU:HD21	2.01	0.42
1:A:2981:ARG:O	1:A:2985:CYS:HB3	2.19	0.42
1:A:3597:THR:O	1:A:3600:ILE:HG22	2.20	0.42
1:A:4257:ASP:OD1	1:A:4257:ASP:N	2.52	0.42
1:A:2569:VAL:HG11	1:A:2747:ILE:HA	2.00	0.42
1:A:2870:PRO:HB2	1:A:2872:LEU:HD11	2.01	0.42
1:A:2967:TYR:HE1	1:A:2972:PHE:HB2	1.85	0.42
1:A:3928:THR:O	1:A:3932:ALA:N	2.39	0.42
1:A:4379:THR:O	1:A:4383:THR:HG23	2.20	0.42
1:A:2054:LEU:HG	1:A:2097:LEU:HD22	2.02	0.42
1:A:2972:PHE:CE2	1:A:2976:LEU:HD11	2.55	0.42
1:A:4490:GLN:O	1:A:4494:LEU:HG	2.20	0.42
1:A:2238:LEU:HD11	1:A:2249:GLY:HA3	2.02	0.41
1:A:2775:GLU:HG3	1:A:2779:MET:HE3	2.02	0.41
1:A:2994:MET:HB3	1:A:2998:ASN:OD1	2.20	0.41
1:A:3208:ILE:O	1:A:3212:VAL:HG23	2.20	0.41
1:A:3477:ALA:HA	1:A:3480:LYS:HG2	2.01	0.41
1:A:3567:LEU:HB2	1:A:3599:PHE:CD1	2.55	0.41
1:A:4265:LEU:O	1:A:4269:LEU:HD23	2.20	0.41
1:A:1356:PRO:HA	1:A:1359:LEU:HB3	2.02	0.41
1:A:1450:LEU:O	1:A:1454:GLN:HG2	2.21	0.41
1:A:2147:PRO:HB3	1:A:2362:VAL:HG12	2.01	0.41
1:A:2323:LYS:HE2	1:A:2323:LYS:HB3	1.85	0.41
1:A:2933:LEU:HD11	1:A:3092:ASN:HB2	2.02	0.41
1:A:3003:GLY:HA2	1:A:3006:GLU:HG2	2.02	0.41
1:A:3500:MET:O	1:A:3503:ILE:HG22	2.20	0.41
1:A:3586:TYR:HA	1:A:3587:PRO:HD3	1.96	0.41
1:A:3909:LEU:HD21	1:A:4343:MET:HE3	2.03	0.41
1:A:4088:VAL:HG11	1:A:4116:LEU:HD11	2.02	0.41
1:A:3570:ASP:O	1:A:3574:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3716:VAL:HG23	1:A:3836:TYR:OH	2.20	0.41
1:A:4235:PRO:HB3	1:A:4278:PHE:CD2	2.55	0.41
1:A:1391:LYS:HE2	1:A:1391:LYS:HB3	1.93	0.41
1:A:1587:LEU:O	1:A:1591:VAL:HG22	2.20	0.41
1:A:2395:GLN:HB2	1:A:2396:ARG:NH2	2.35	0.41
1:A:2739:PRO:HB2	1:A:2744:LEU:HG	2.03	0.41
1:A:3488:ARG:NH2	1:A:3489:TRP:HE1	2.19	0.41
1:A:4113:LEU:HD23	1:A:4116:LEU:HD23	2.02	0.41
1:A:1961:ASN:HB3	1:A:2018:MET:HE1	2.03	0.41
1:A:2294:GLU:N	1:A:2294:GLU:OE1	2.53	0.41
1:A:2900:PHE:CE1	1:A:2904:GLU:HG3	2.56	0.41
1:A:2922:ILE:HA	1:A:2925:ILE:HG22	2.02	0.41
1:A:3684:PRO:HB3	1:A:3702:THR:HG21	2.02	0.41
1:A:4018:MET:SD	1:A:4018:MET:N	2.93	0.41
1:A:4113:LEU:HD23	1:A:4113:LEU:HA	1.89	0.41
1:A:4377:MET:HB3	1:A:4378:ARG:NH1	2.35	0.41
1:A:1518:GLU:HG2	1:A:1519:ASP:N	2.36	0.41
1:A:1521:LEU:O	1:A:1524:GLU:HG3	2.21	0.41
1:A:2203:TRP:CH2	1:A:2236:VAL:HG11	2.55	0.41
1:A:2486:LEU:O	1:A:2490:ILE:HG12	2.21	0.41
1:A:1393:TYR:HE2	1:A:1435:TRP:CG	2.38	0.41
1:A:1691:SER:OG	1:A:1694:GLU:OE1	2.37	0.41
1:A:4133:LYS:HB2	1:A:4133:LYS:HE3	1.89	0.41
1:A:2082:SER:HA	1:A:2086:TYR:CD2	2.55	0.41
1:A:2396:ARG:HA	1:A:2399:LYS:HG3	2.02	0.41
1:A:2412:MET:HE1	1:A:2467:ARG:HA	2.02	0.41
1:A:2496:TYR:CE1	1:A:2500:TRP:HD1	2.39	0.41
1:A:2879:LYS:HB3	1:A:2879:LYS:HE3	1.88	0.41
1:A:4425:GLN:O	1:A:4426:ASP:C	2.64	0.41
1:A:1447:LYS:HE3	1:A:1447:LYS:HB2	1.79	0.41
1:A:1452:VAL:O	1:A:1456:GLU:HG2	2.20	0.41
1:A:1481:GLN:HE21	1:A:2273:ARG:NH1	2.18	0.41
1:A:1491:ASP:OD1	1:A:1492:ASP:N	2.53	0.41
1:A:2123:ASP:O	1:A:2127:ILE:HG13	2.21	0.41
1:A:2514:LEU:O	1:A:2518:ILE:HG12	2.20	0.41
1:A:2863:ARG:HD2	1:A:2863:ARG:HA	1.87	0.41
1:A:3485:GLU:OE1	1:A:3773:LEU:HD23	2.21	0.41
1:A:3757:LYS:HE3	1:A:3757:LYS:HB3	1.83	0.41
1:A:3871:VAL:O	1:A:3875:MET:HB2	2.21	0.41
1:A:1739:ILE:HG23	1:A:1804:ARG:HD3	2.02	0.41
1:A:2772:ALA:HA	1:A:2857:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3498:ASN:O	1:A:3501:SER:OG	2.30	0.41
1:A:4157:MET:HE2	1:A:4157:MET:HB3	1.88	0.41
1:A:2668:LEU:HD21	1:A:2720:ARG:NH1	2.36	0.40
1:A:4260:PHE:CE2	1:A:4608:PRO:HB3	2.56	0.40
1:A:3203:VAL:O	1:A:3207:LYS:HG2	2.21	0.40
1:A:2912:PHE:CE1	1:A:2915:VAL:HG23	2.57	0.40
1:A:2073:PHE:HE2	1:A:2093:LEU:HA	1.86	0.40
1:A:2300:TRP:CE3	1:A:2342:MET:HE1	2.57	0.40
1:A:2648:VAL:HG11	1:A:2694:ARG:NH2	2.36	0.40
1:A:1399:LEU:O	1:A:1403:LEU:HD23	2.21	0.40
1:A:2686:MET:HG2	1:A:2703:LEU:HD11	2.04	0.40
1:A:3154:LEU:HG	1:A:3516:TYR:CD1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3028/4646 (65%)	2940 (97%)	88 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2703/4125 (66%)	2703 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1355	GLN
1	A	1397	ASN
1	A	1495	ASN
1	A	1569	GLN
1	A	1598	GLN
1	A	1670	ASN
1	A	1736	ASN
1	A	1985	HIS
1	A	2057	GLN
1	A	2085	HIS
1	A	2212	GLN
1	A	2416	GLN
1	A	2439	HIS
1	A	2549	GLN
1	A	2637	HIS
1	A	2834	GLN
1	A	2954	ASN
1	A	3145	ASN
1	A	3185	ASN
1	A	3214	GLN
1	A	3526	GLN
1	A	3540	ASN
1	A	3595	GLN
1	A	3622	ASN
1	A	3931	GLN
1	A	4062	GLN
1	A	4078	ASN
1	A	4137	ASN
1	A	4156	ASN
1	A	4174	ASN
1	A	4191	GLN
1	A	4231	GLN
1	A	4347	GLN
1	A	4381	HIS
1	A	4530	GLN
1	A	4532	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	4549	GLN
1	A	4566	GLN

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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
4	ANP	A	4703	-	33,33,33	0.91	4 (12%)	45,52,52	0.61	0
2	ADP	A	4704	-	28,29,29	1.42	4 (14%)	43,45,45	1.84	9 (20%)
3	ATP	A	4702	5	32,33,33	0.34	0	48,52,52	0.30	0
2	ADP	A	4701	-	28,29,29	1.44	5 (17%)	43,45,45	1.80	7 (16%)

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
4	ANP	A	4703	-	-	2/18/38/38	0/3/3/3
2	ADP	A	4704	-	-	4/16/32/32	0/3/3/3
3	ATP	A	4702	5	-	3/22/38/38	0/3/3/3
2	ADP	A	4701	-	-	5/16/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4704	ADP	C5-C4	4.69	1.47	1.39
2	A	4701	ADP	C5-C4	4.67	1.47	1.39
2	A	4704	ADP	C5-C6	2.69	1.48	1.41
2	A	4701	ADP	C5-C6	2.66	1.48	1.41
4	A	4703	ANP	PG-O1G	2.45	1.49	1.46
4	A	4703	ANP	PG-N3B	2.41	1.69	1.63
2	A	4704	ADP	C8-N7	2.37	1.36	1.31
4	A	4703	ANP	PB-O1B	2.35	1.49	1.46
2	A	4701	ADP	C5-N7	-2.33	1.34	1.39
2	A	4704	ADP	C5-N7	-2.33	1.34	1.39
4	A	4703	ANP	PB-O3A	-2.32	1.56	1.59
2	A	4701	ADP	C8-N7	2.31	1.36	1.31
2	A	4701	ADP	PA-O3A	2.27	1.61	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	ADP	C5-C4-N3	-5.86	118.64	126.72
2	A	4704	ADP	C5-C4-N3	-5.81	118.72	126.72
2	A	4701	ADP	N3-C4-N9	4.65	135.08	127.17
2	A	4704	ADP	N3-C4-N9	4.54	134.90	127.17
2	A	4704	ADP	C2-N3-C4	3.68	120.82	111.83
2	A	4701	ADP	C2-N3-C4	3.68	120.81	111.83
2	A	4704	ADP	C4-C5-N7	-3.54	106.53	110.58
2	A	4701	ADP	C4-C5-N7	-3.36	106.74	110.58
2	A	4704	ADP	N3-C2-N1	-3.24	123.67	128.58
2	A	4701	ADP	N3-C2-N1	-3.17	123.79	128.58
2	A	4704	ADP	C4-N9-C8	2.63	108.50	105.74
2	A	4704	ADP	C5-N7-C8	2.56	107.48	103.45
2	A	4701	ADP	C4-N9-C8	2.54	108.41	105.74
2	A	4701	ADP	C5-N7-C8	2.42	107.25	103.45
2	A	4704	ADP	C3'-C2'-C1'	2.17	105.57	101.46
2	A	4704	ADP	C6-C5-N7	2.12	136.17	132.09

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O1A
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4704	ADP	C5'-O5'-PA-O3A
3	A	4702	ATP	C5'-O5'-PA-O3A
4	A	4703	ANP	PG-N3B-PB-O1B
3	A	4702	ATP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'
2	A	4701	ADP	C5'-O5'-PA-O3A
2	A	4701	ADP	PB-O3A-PA-O1A
2	A	4701	ADP	PB-O3A-PA-O2A
4	A	4703	ANP	C4'-C5'-O5'-PA
2	A	4704	ADP	PA-O3A-PB-O2B
2	A	4704	ADP	C4'-C5'-O5'-PA

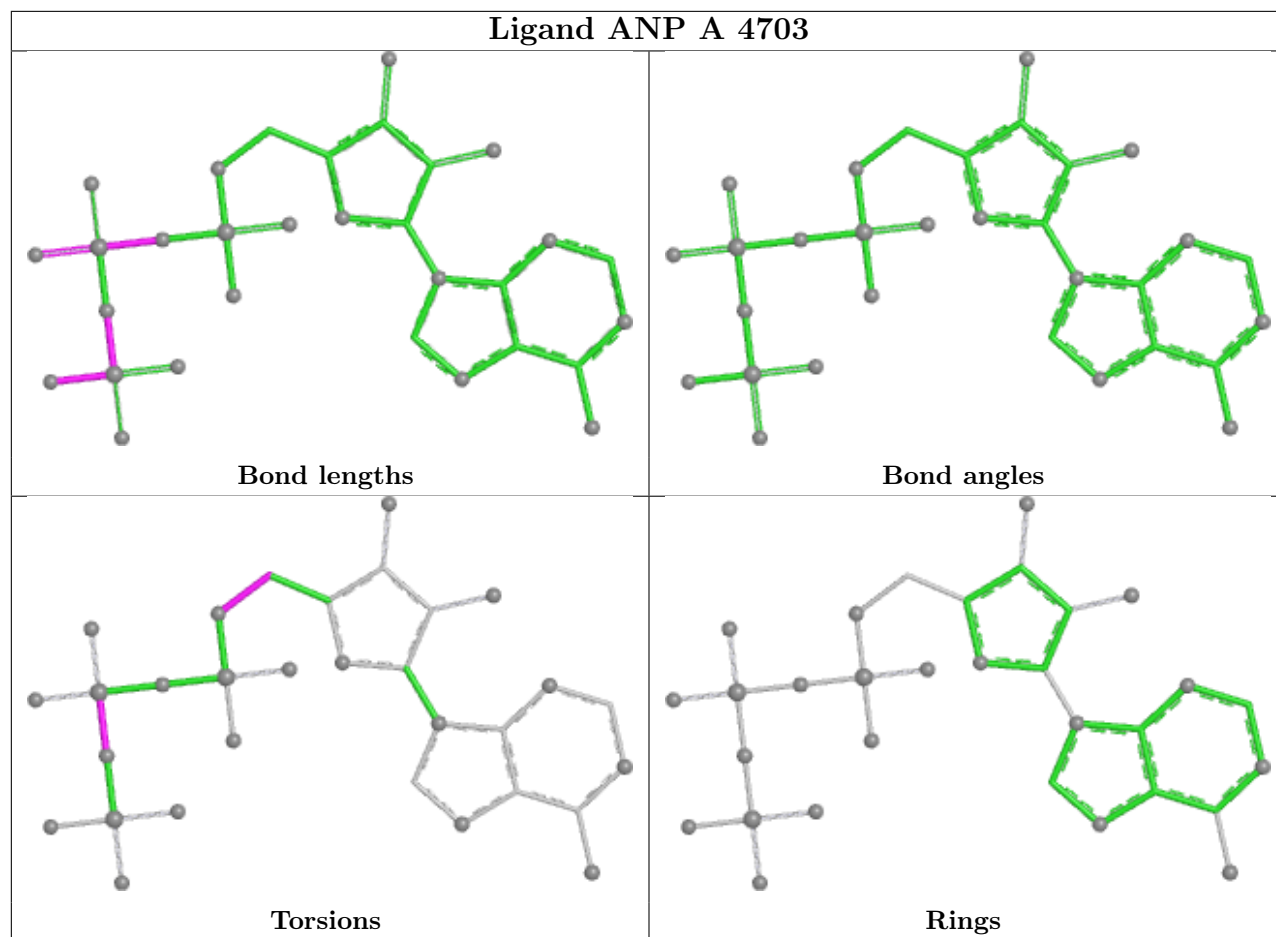
There are no ring outliers.

4 monomers are involved in 21 short contacts:

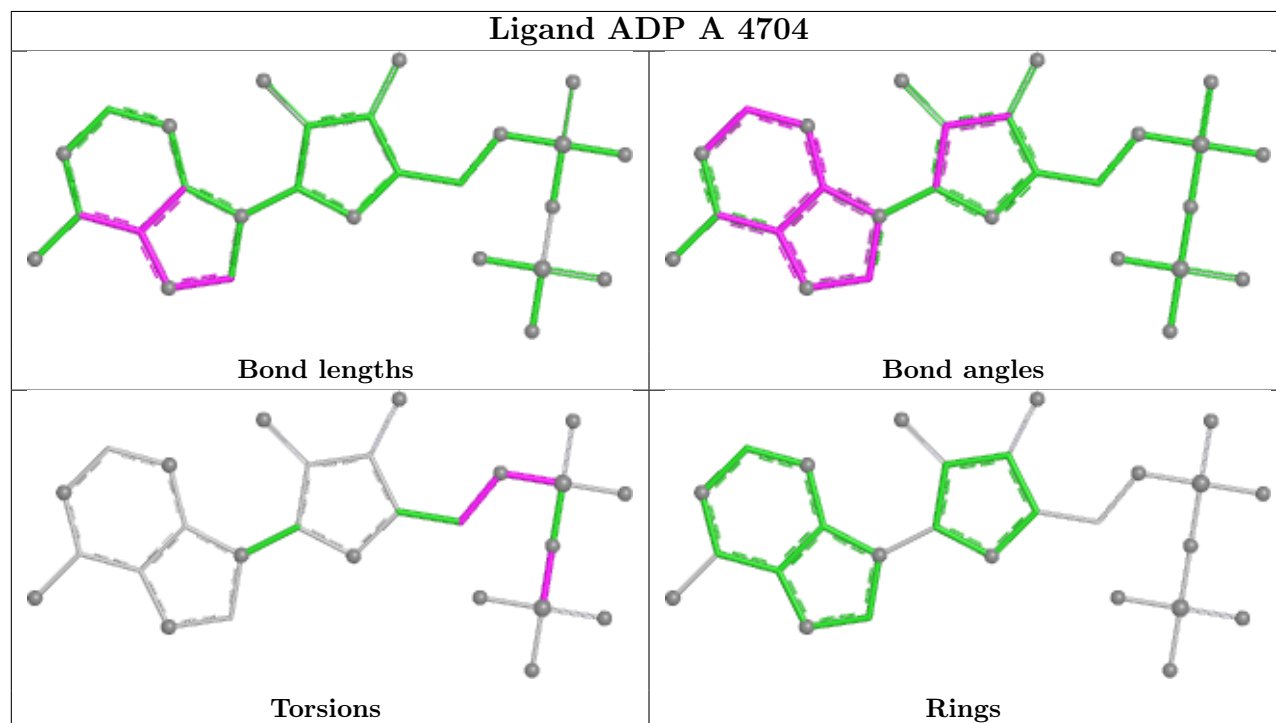
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4703	ANP	5	0
2	A	4704	ADP	2	0
3	A	4702	ATP	6	0
2	A	4701	ADP	8	0

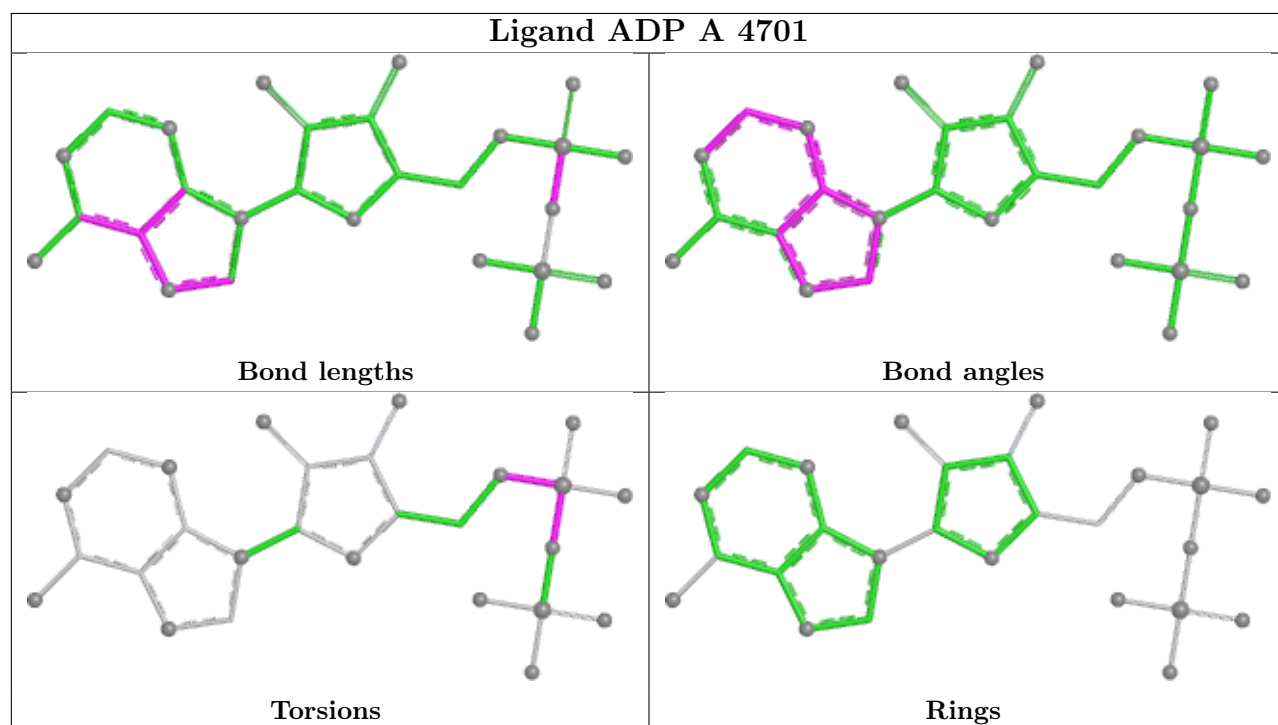
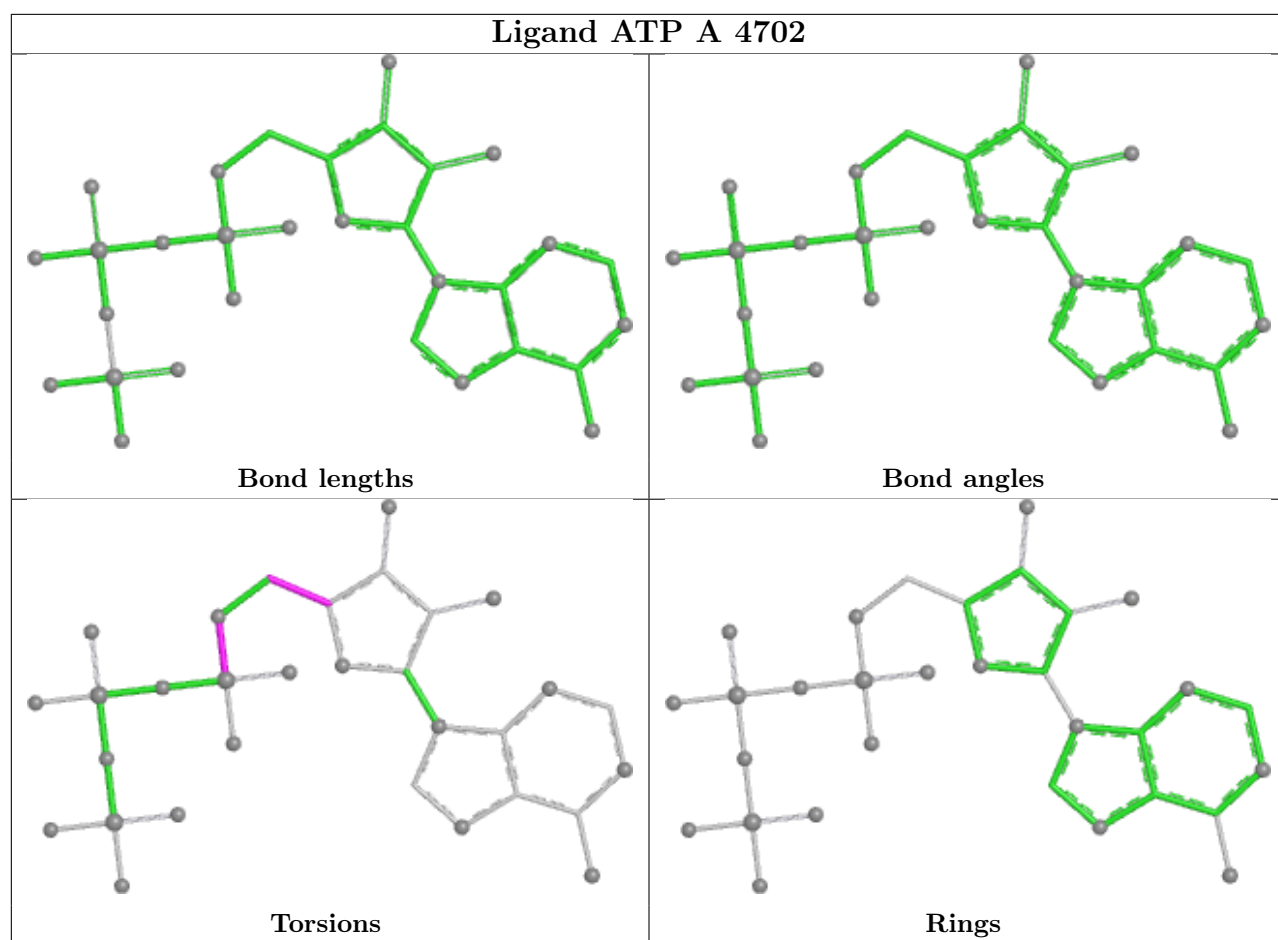
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ANP A 4703



Ligand ADP A 4704





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.

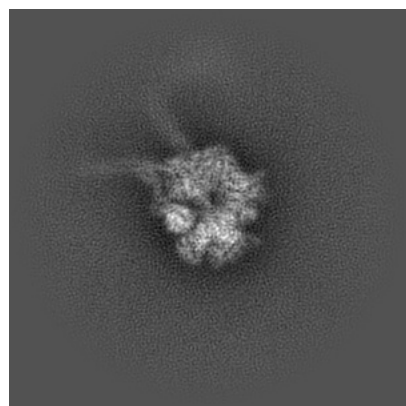
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46861. These allow visual inspection of the internal detail of the map and identification of artifacts.

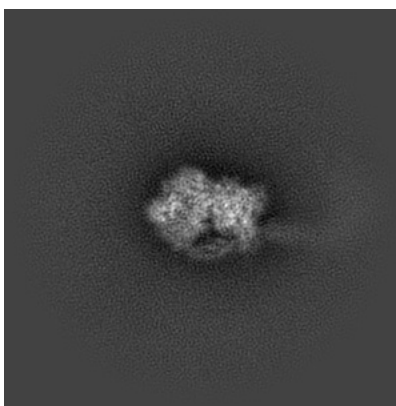
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

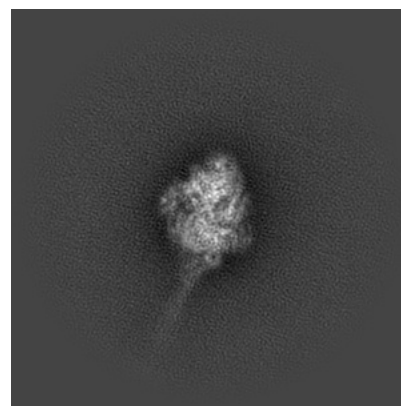
6.1.1 Primary map



X

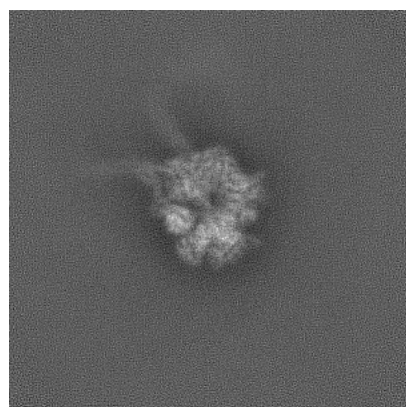


Y

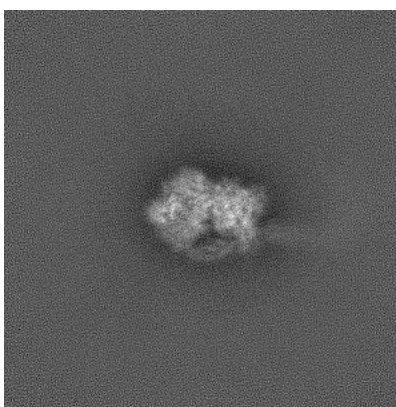


Z

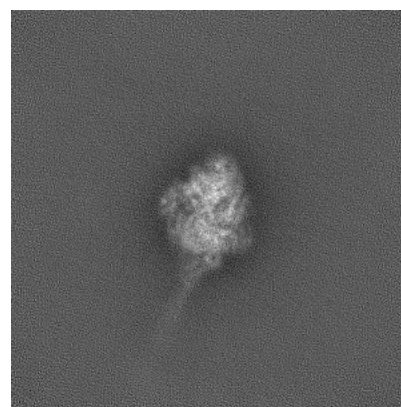
6.1.2 Raw map



X



Y

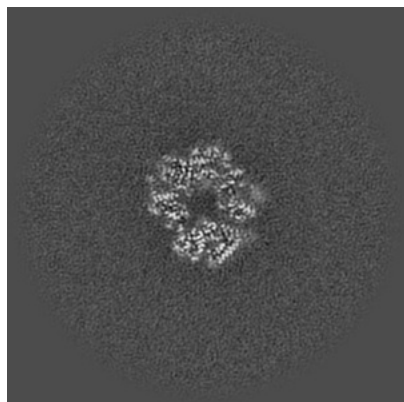


Z

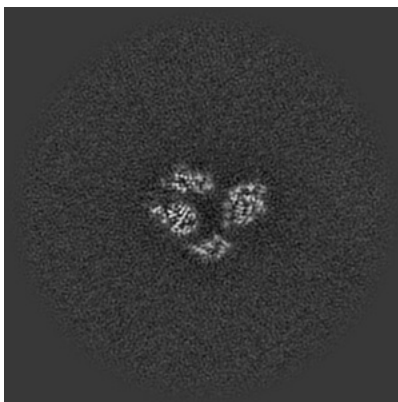
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

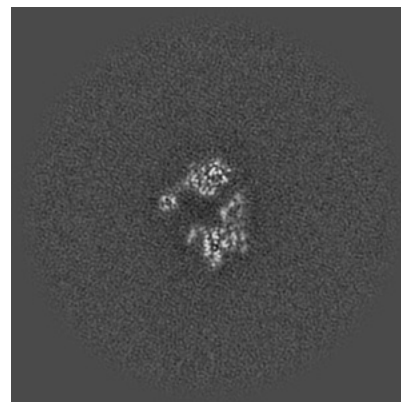
6.2.1 Primary map



X Index: 192

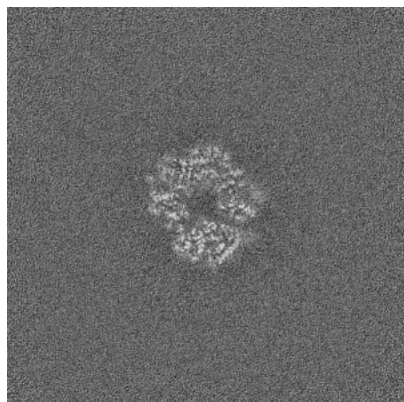


Y Index: 192

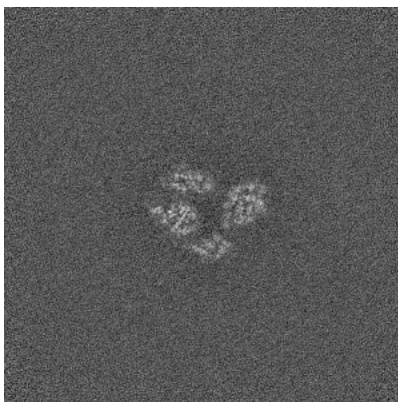


Z Index: 192

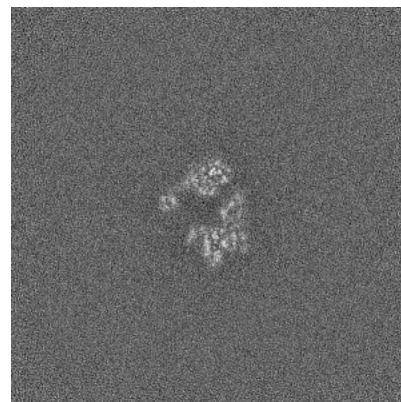
6.2.2 Raw map



X Index: 192



Y Index: 192

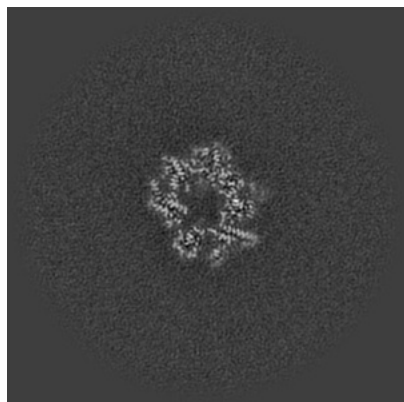


Z Index: 192

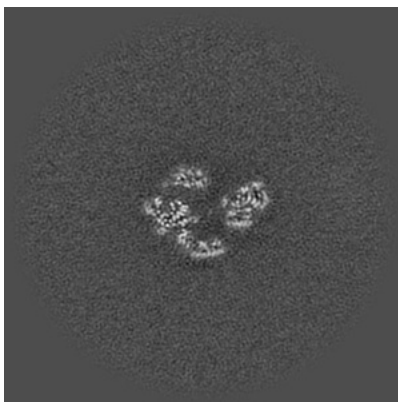
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

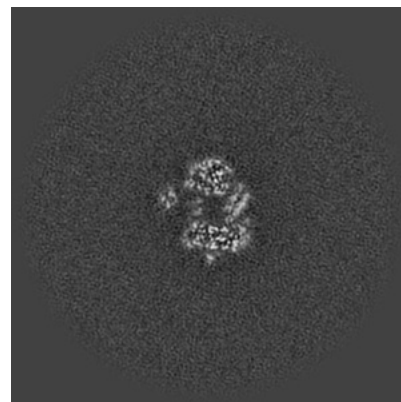
6.3.1 Primary map



X Index: 196

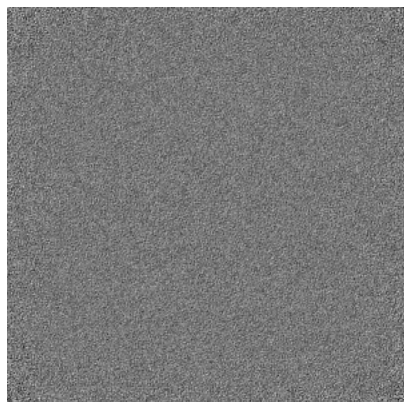


Y Index: 199

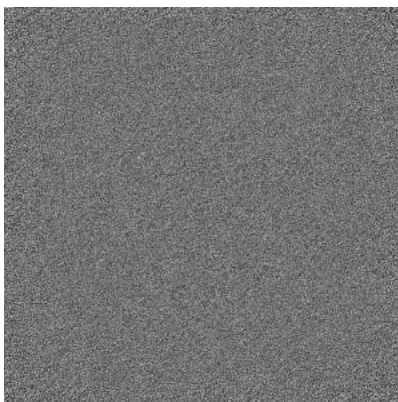


Z Index: 186

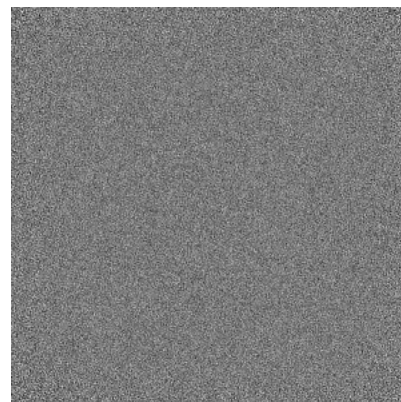
6.3.2 Raw map



X Index: 0



Y Index: 0

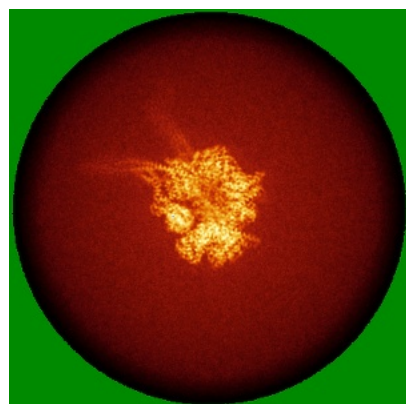


Z Index: 0

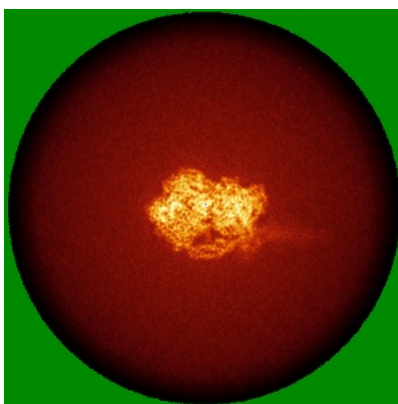
The images above show the largest variance slices of the map in three orthogonal directions.

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

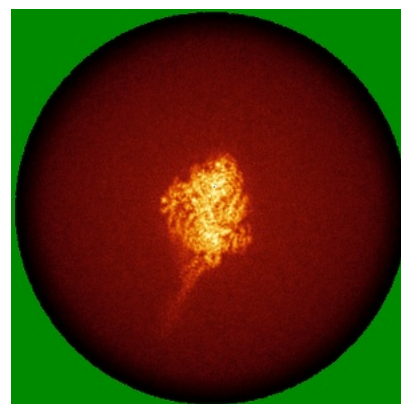
6.4.1 Primary map



X

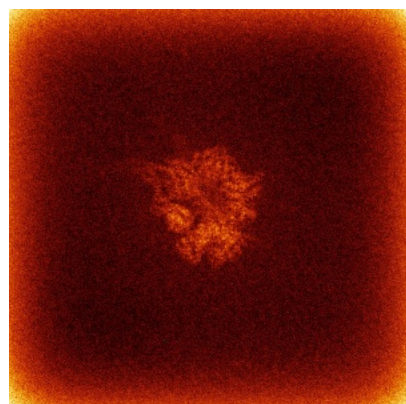


Y

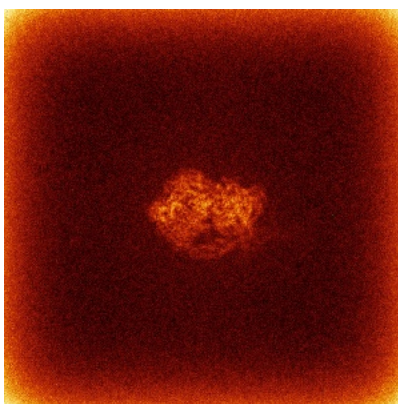


Z

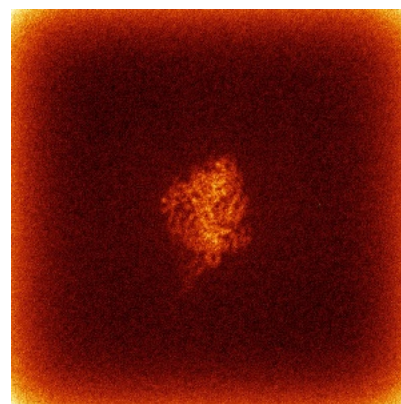
6.4.2 Raw map



X



Y

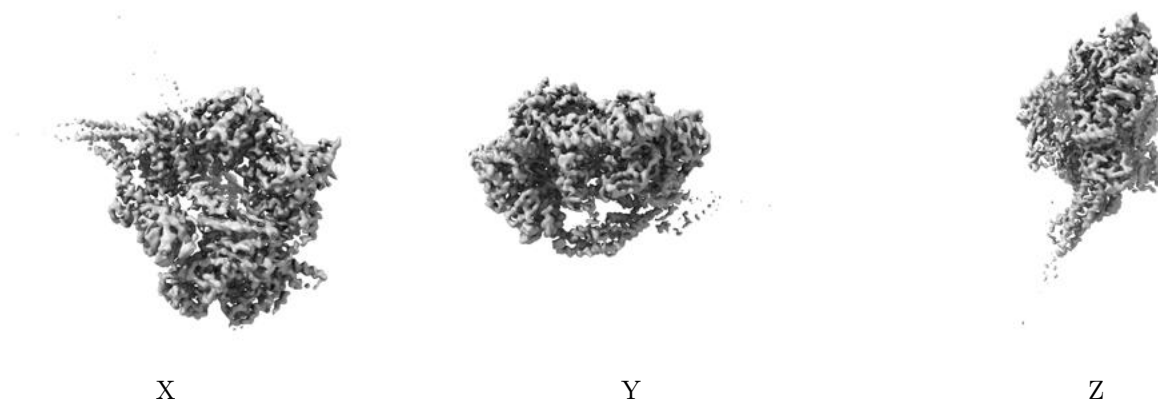


Z

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.

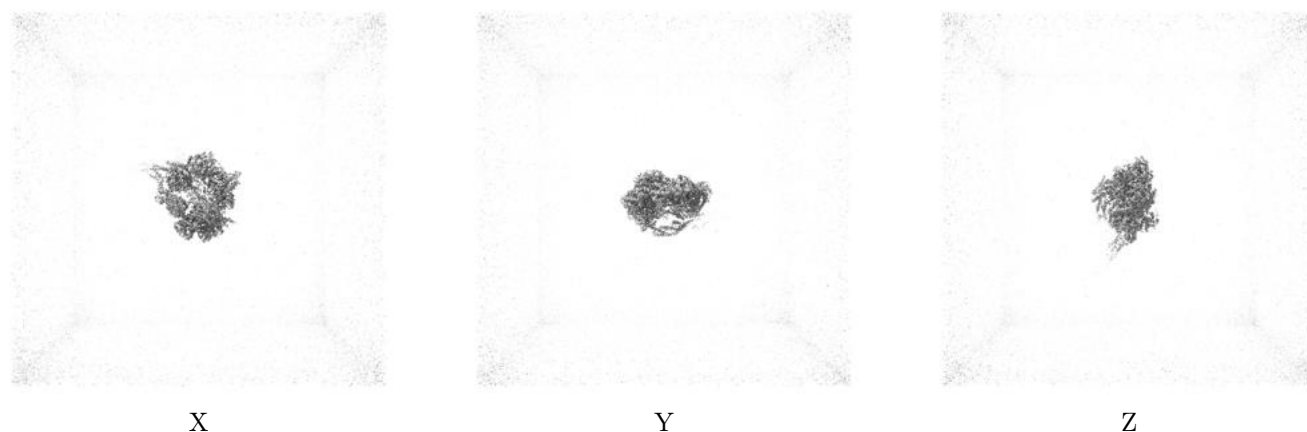
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

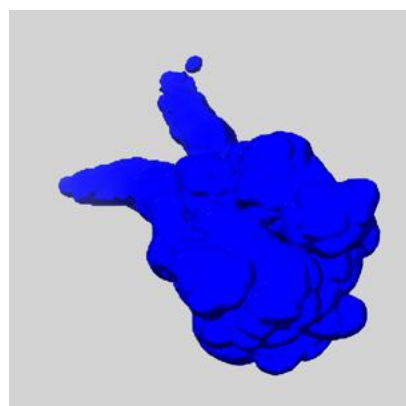
6.6 Mask visualisation [i](#)

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

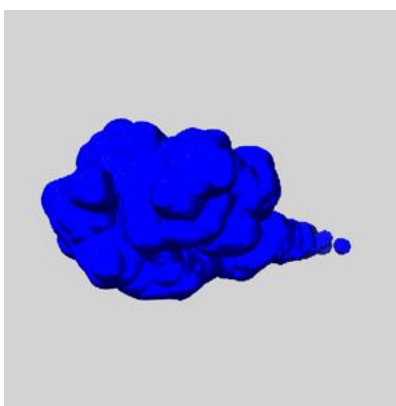
A mask typically either:

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

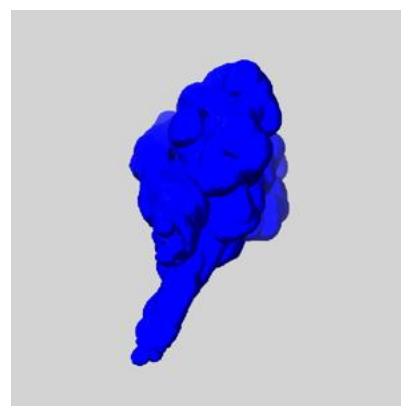
6.6.1 emd_46861_msk_1.map [i](#)



X



Y

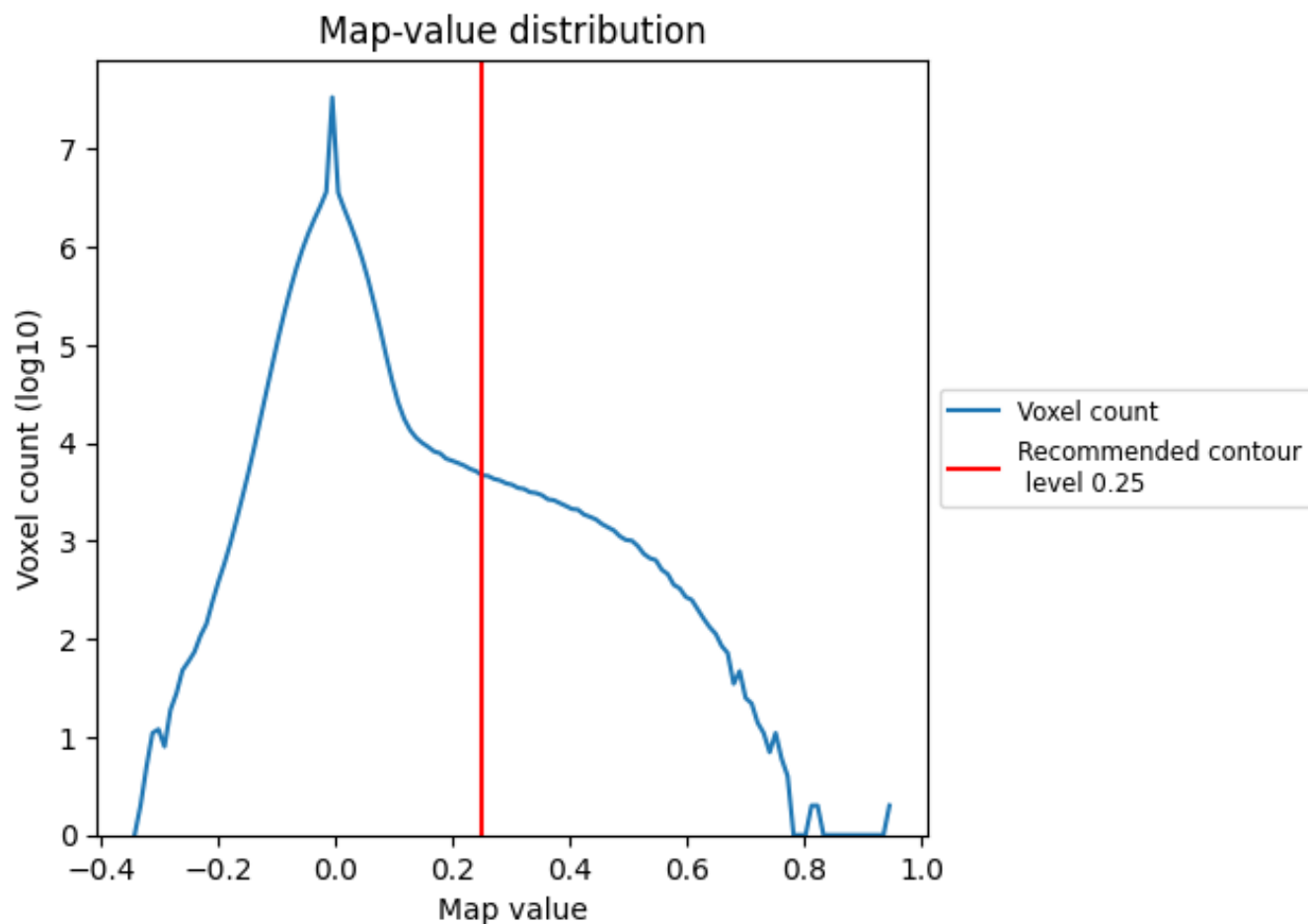


Z

7 Map analysis [i](#)

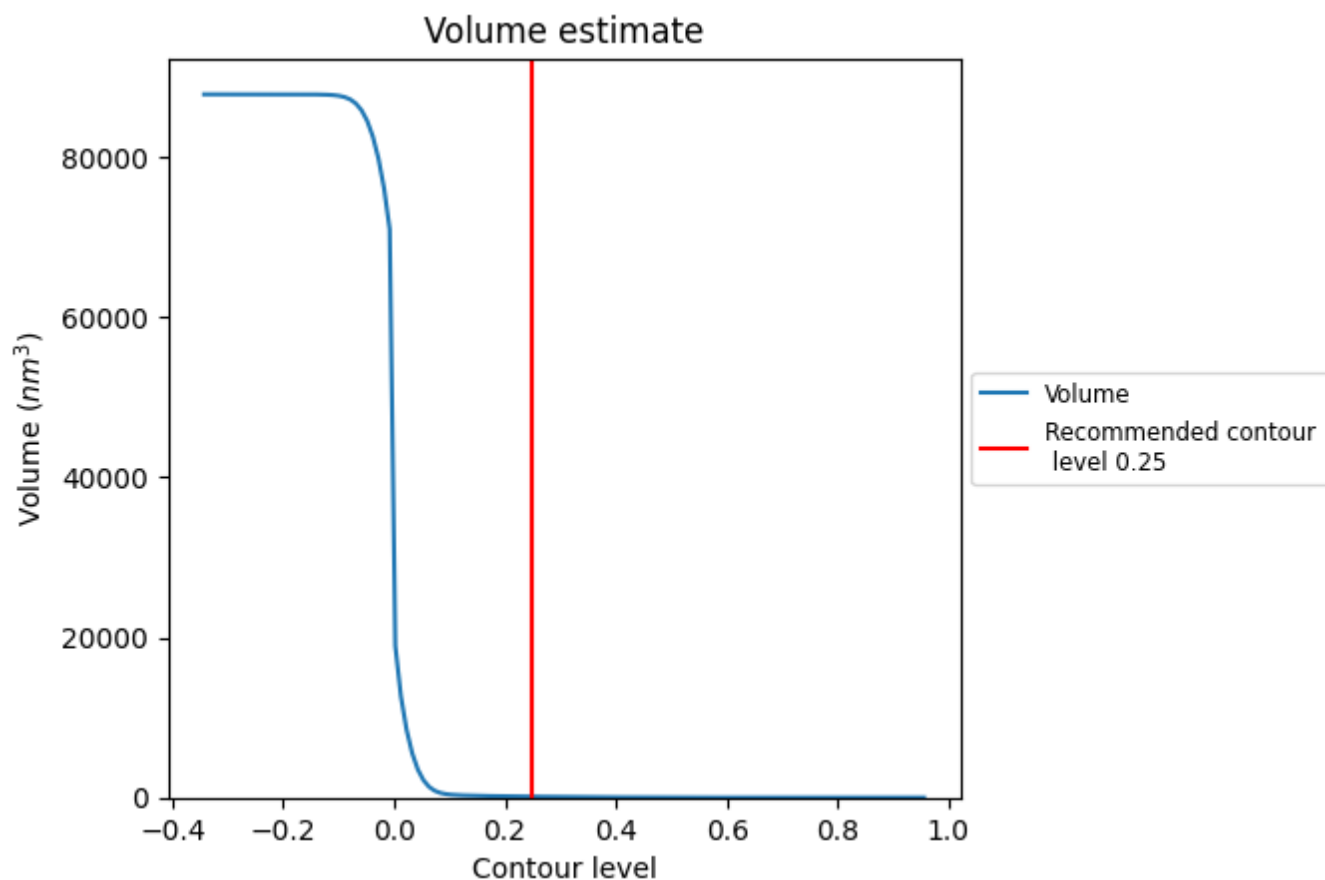
This section contains the results of statistical analysis of the map.

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.

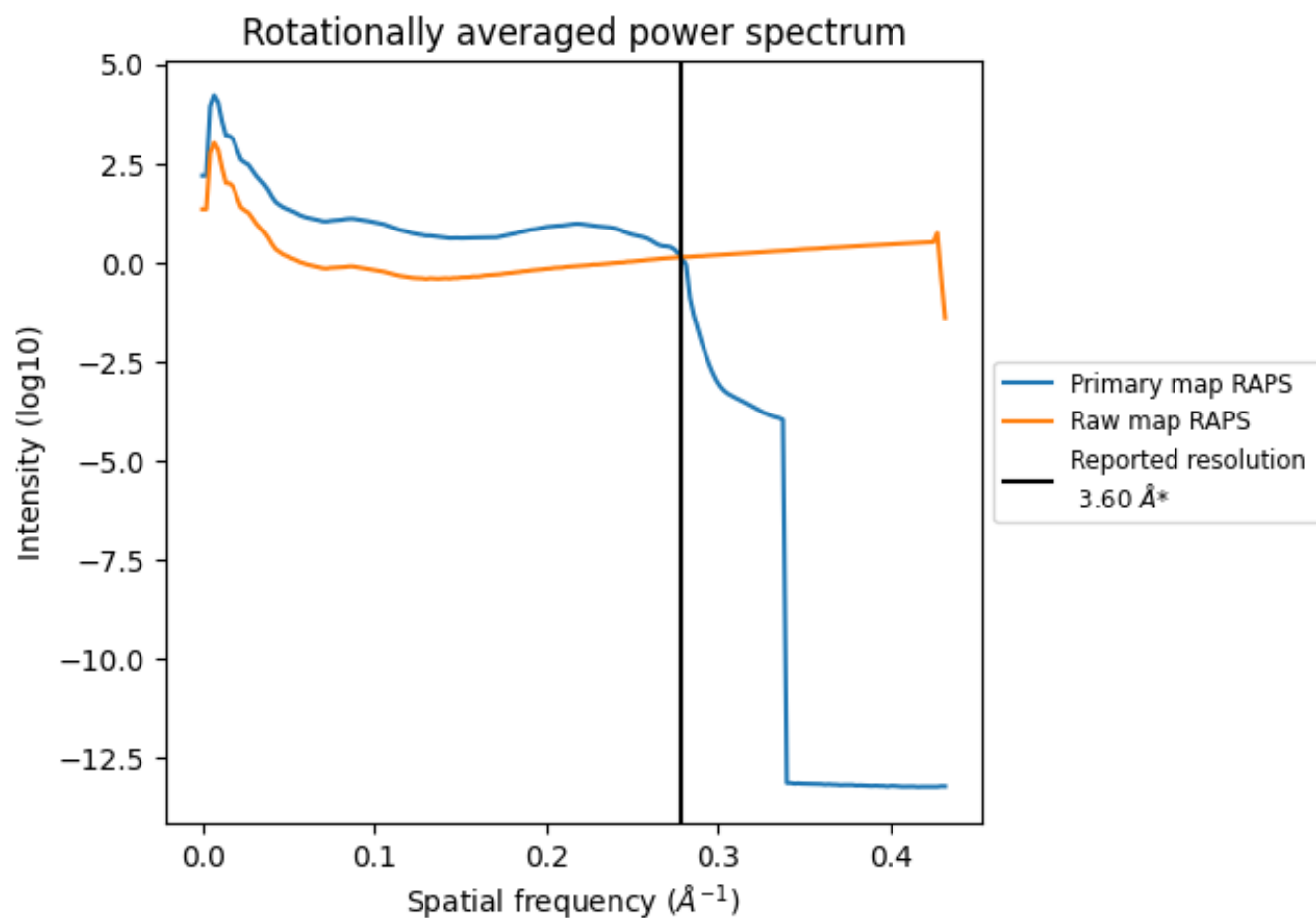
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 116 nm³; this corresponds to an approximate mass of 105 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 ⓘ

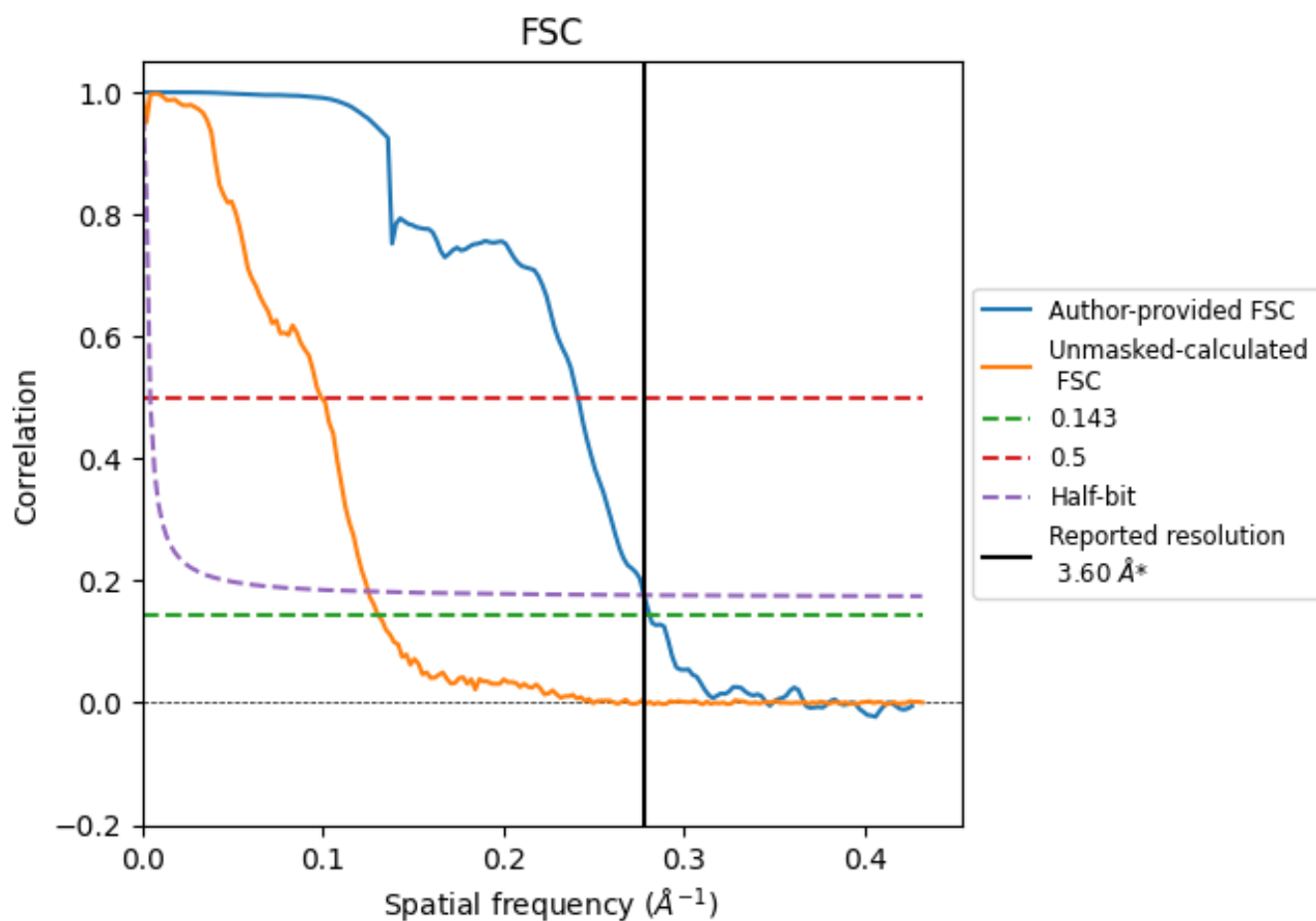


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

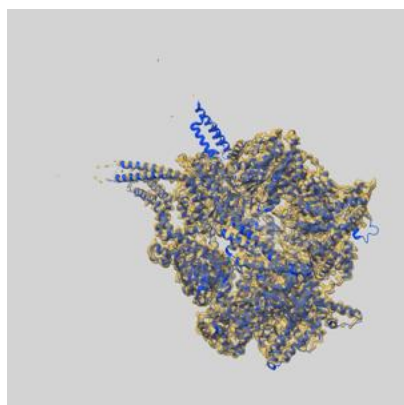
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.56	4.14	3.60
Unmasked-calculated*	7.65	10.09	7.99

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

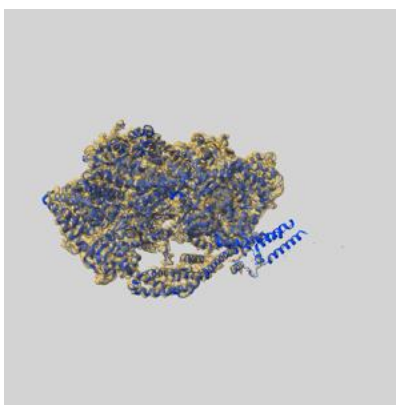
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46861 and PDB model 9DHA. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

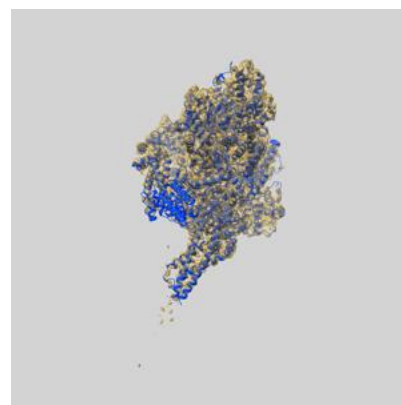
9.1 Map-model overlay [i](#)



X



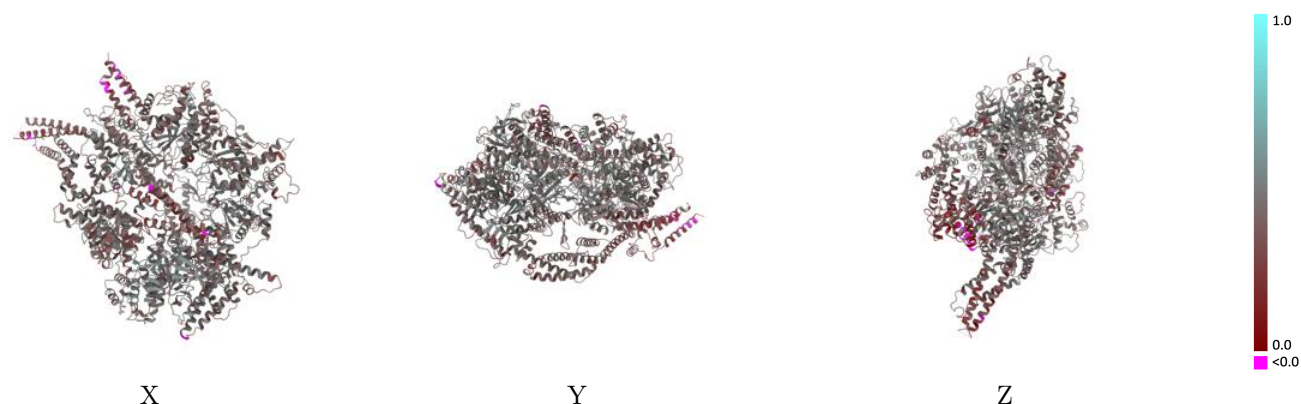
Y



Z

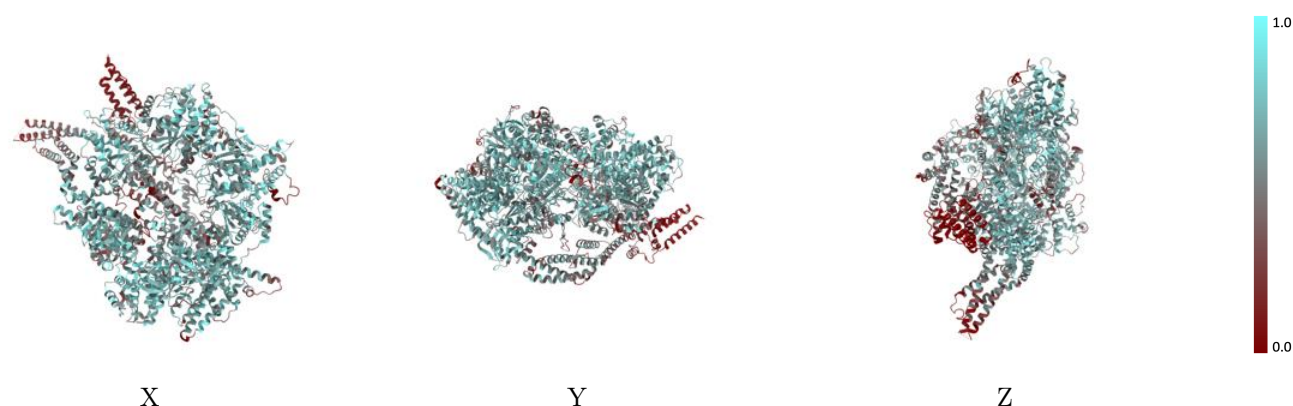
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



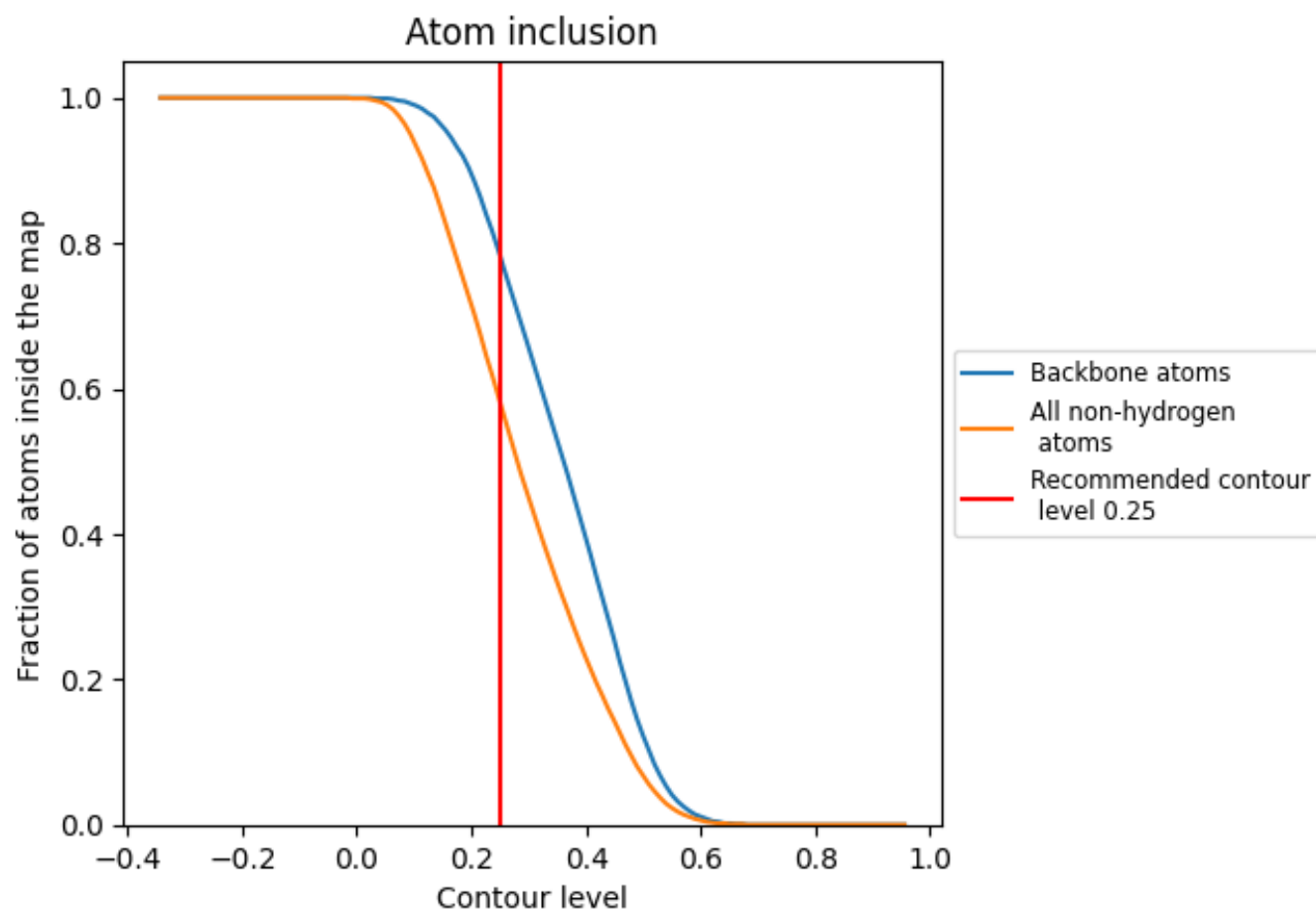
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 58% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5810	0.4120
A	0.5810	0.4120

