



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 02:49 AM EDT

PDB ID : 9BMG / pdb_00009bmg
EMDB ID : EMD-44698
Title : State-2 of full-length human dynein-1 in 5mM ATPVi
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 2.86 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 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) : 2.50

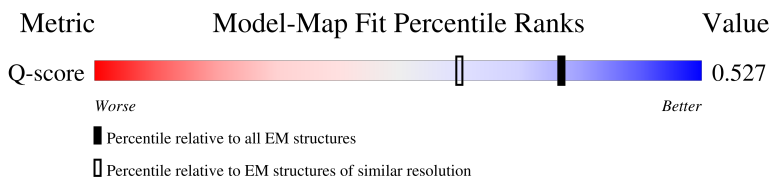
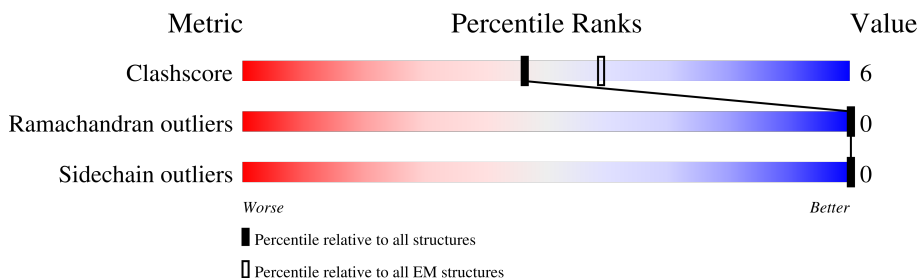
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.86 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	12017 (2.36 - 3.36)

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](#)

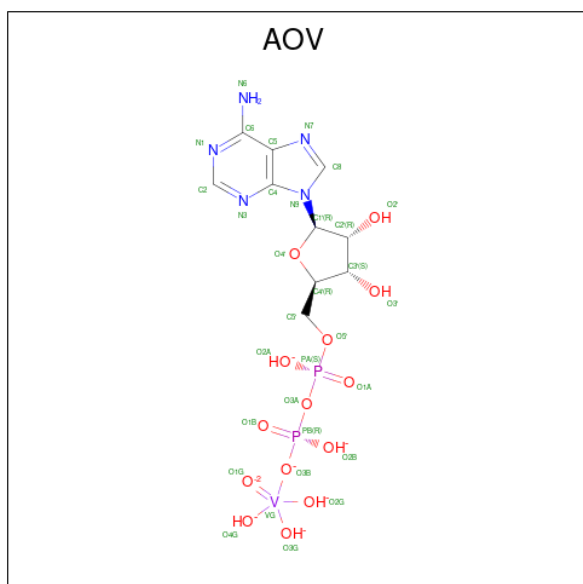
There are 5 unique types of molecules in this entry. The entry contains 23712 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

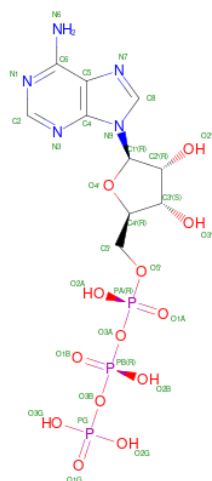
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2937	23593	15028	4070	4378	117	0	0

- Molecule 2 is ADP ORTHOVANADATE (CCD ID: AOV) (formula: $C_{10}H_{17}N_5O_{14}P_2V$) (labeled as "Ligand of Interest" by depositor).

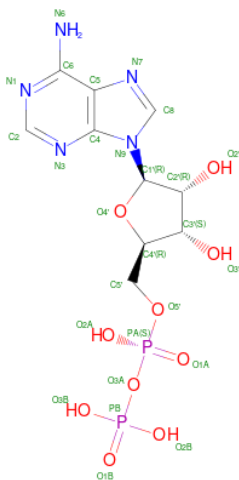


Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	V	
2	A	1	32	10	5	14	2	1	0

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



- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



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

Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total 2	Mg 2	0

V2006	P1848	K1649	T1565	S1503	LYS	ALA	VAL	TRP	ARG	GLU	ALA	ASN	GLU	ASN	GLU	ASN	PHE
K2007	K1849	K1650	Q1566	V1504	ASN	SER	ALA	GLU	PHE	PHE	GLN	LEU	ARG	LEU	LEU	LEU	PHE
P2010	Q1850	H1653	R1567	S1505	ALA	THR	GLU	THR	PHE	THR	GLU	THR	GLN	ASP	GLN	GLN	PHE
T2017	T1851	H1653	F1568	S1506	ILE	PHE	VAL	PRO	PRO	GLN	ILE	MET	ASN	GLU	GLU	GLU	LYS
T2018	D1852	E1668	Q1569	M1507	VAL	VAL	GLN	VAL	TRP	SER	ARG	PRO	VAL	VAL	VAL	VAL	VAL
T2028	V1853	E1668	S1572	K1508	LYS	GLN	ASP	THR	TRP	TRP	LYS	ASP	GLN	GLN	GLN	GLN	VAL
P2029	Q1856	S1671	T1573	L1509	ASP	ARG	LEU	THR	ARG	ARG	VAL	GLU	LEU	LEU	LEU	LEU	ILE
D2030	N1867	R1679	L1576	P1511	VAL	GLY	VAL	PRO	ASN	ASN	THR	GLU	PRO	GLY	GLY	GLY	ILE
D2031	D1877	T1693	A1577	Y1512	ALA	THR	TRP	GLU	ILE	ILE	PHE	GLU	PRO	VAL	VAL	VAL	ILE
L2032	K1878	T1698	L1578	Y1513	GLN	MET	SER	GLU	GLU	GLU	ASP	GLU	ARG	ARG	ARG	ARG	GLU
K2033	V1879	T1698	M1579	K1514	LYS	LYS	GLU	GLU	GLU	GLU	ASN	GLU	GLU	ILE	ILE	ILE	GLU
K2034	V1880	W1701	K1580	V1515	ASN	ASN	SER	LEU	GLU	SER	THR	TYR	GLU	ALA	ALA	ALA	ILE
M2041	Q1881	M1709	K1581	F1516	LEU	MET	VAL	GLN	TRP	GLN	THR	SER	CYS	GLY	GLY	GLY	ASP
T2042	T1882	E1725	V1582	E1517	LEU	VAL	TRP	ALA	GLY	GLY	THR	ALA	ARG	LEU	LEU	LEU	LEU
D2045	R1887	E1725	S1583	E1518	VAL	VAL	TRP	LEU	ALA	ALA	THR	VAL	TYR	ARG	ARG	ARG	GLU
R2046	P1904	G1728	K1584	D1519	ILE	ILE	GLU	THR	PHE	PHE	ALA	MET	LYS	VAL	VAL	VAL	VAL
R2047	E1914	K1729	S1585	A1520	LYS	GLU	GLN	ILE	ASN	ASN	PHE	GLY	THR	THR	THR	THR	ARG
L2048	R1925	L1587	P1586	L1521	SER	SER	ASP	GLY	ILE	ILE	THR	GLY	THR	GLN	GLN	GLN	SER
V2052	R1933	V1588	V1588	S1522	GLU	GLU	MET	LYS	ARG	ARG	VAL	SER	GLU	VAL	VAL	VAL	GLU
E2063	D1933	M1589	M1589	W1523	ALA	ALA	LYS	PHE	ILE	ILE	VAL	VAL	GLU	LEU	LEU	LEU	LEU
R2064	M1941	D1590	D1590	E1524	LEU	LEU	GLU	GLY	LYS	LYS	THR	THR	GLU	ALA	ALA	ALA	VAL
L2065	G1942	Q1595	Q1595	D1525	LYS	LYS	GLN	ARG	ASP	ASP	PHE	THR	THR	GLN	GLN	GLN	THR
A2066	R1943	G1596	G1596	K1526	ASP	ASP	PRO	LEU	SER	SER	ILE	TYR	TYR	ALA	ALA	ALA	ASP
N2067	V1936	V1597	V1597	N1528	TRP	TRP	TRP	ASP	ALA	ALA	THR	VAL	VAL	LYS	LYS	LYS	ASP
R2068	V1946	Q1598	Q1598	I1530	VAL	VAL	GLN	GLN	GLN	GLN	VAL	VAL	VAL	LEU	LEU	LEU	SER
T2069	F1960	R1599	R1599	M1531	LEU	LEU	PRO	CYS	ALA	ALA	LYS	PRO	PRO	ASP	ASP	ASP	GLU
V2070	E1964	S1600	S1600	E1532	ASN	MET	ARG	CYS	ASN	ASN	ASN	ARG	ARG	MET	MET	MET	LEU
L2075	E1964	L1601	L1601	L1532	LYS	LYS	LYS	ALA	LEU	LEU	LEU	ILE	ILE	ASP	ASP	ASP	ASN
L2080	E1985	E1602	E1602	L1533	ARG	ARG	LEU	ALA	GLN	GLN	GLN	TRP	TRP	THR	THR	THR	ARG
H2085	R1966	R1603	R1603	F1534	HIS	HIS	GLN	LYS	LYS	LYS	LYS	SER	SER	ASP	ASP	ASP	GLN
F2088	M1967	L1604	L1604	D1535	VAL	VAL	ASN	GLU	ILE	ILE	VAL	GLN	GLN	ALA	ALA	ALA	VAL
R2091	I1978	A1605	A1605	W1536	ASN	ASN	LEU	ALA	VAL	VAL	GLU	GLN	GLN	PRO	PRO	PRO	LYS
E2114	E1984	D1606	D1606	I1537	TRP	TRP	ASP	GLU	VAL	VAL	GLU	GLN	GLN	ARG	ARG	ARG	ALA
E2117	H1985	L1607	L1607	I1538	VAL	VAL	ALA	GLU	GLU	GLU	LYS	VAL	VAL	GLN	GLN	GLN	VAL
R2118	S1986	K1610	K1610	V1540	R1488	R1488	LEU	LEU	GLU	GLU	GLU	GLU	GLU	VAL	VAL	VAL	VAL
G2119	N1987	E1619	E1619	E1547	G1489	G1489	LEU	LEU	ASP	ASP	GLU	GLU	GLU	SER	SER	SER	ASP
E2120	P1988	R1621	R1621	E1548	W1490	W1490	THR	THR	VAL	VAL	VAL	ASN	ASN	GLY	GLY	GLY	GLY
A2121	N1989	E1622	E1622	F1551	D1491	D1491	ALA	SER	ARG	ARG	LEU	LEU	LEU	VAL	VAL	VAL	VAL
V2122	T1993	R1623	R1623	T1552	D1492	D1492	THR	THR	THR	THR	ALA	TYR	TYR	GLY	GLY	GLY	GLY
D2123	S1994	S1624	S1624	G1553	L1493	L1493	GLU	SER	ARG	ARG	LEU	SER	SER	ILE	ILE	ILE	ILE
E2124	A1995	F1625	F1625	S1554	F1494	F1494	LEU	GLY	VAL	VAL	LEU	ASN	ASN	PRO	PRO	PRO	ASN
G2125	I1997	Y1630	Y1630	A1555	M1495	M1495	LYS	LEU	GLU	GLU	THR	ARG	ARG	GLY	GLY	GLY	GLY
E2126	E2000	D1634	D1634	D1556	K1496	K1496	SER	LEU	SER	SER	ASN	LEU	LEU	GLU	GLU	GLU	GLU
I2127	L2001	E1635	E1635	I1557	V1497	V1497	PHE	SER	ARG	ARG	GLN	GLY	GLY	PRO	PRO	PRO	PRO
		L1638	L1638	K1558	E1499	E1499	THR	GLY	THR	THR	GLN	GLY	GLY	LYS	LYS	LYS	LYS
		E1639	E1639	H1559	H1559	H1559	ALA	SER	THR	THR	GLN	GLY	GLY	ILE	ILE	ILE	ILE
		I1640	I1640	L1560	L1560	L1560	ARG	GLU	THR	THR	LEU	ASP	ASP	GLU	GLU	GLU	GLU
				L1561	L1561	L1561	LEU	GLU	LEU	LEU	LEU	LEU	LEU	LYS	LYS	LYS	LYS
				P1562	P1562	P1562	ARG	ARG	ARG	ARG	VAL	ASN	ASN	ASN	ASN	ASN	ASN
				V1563	V1563	V1563	GLN	THR	THR	THR	LYS	TRP	TRP	VAL	VAL	VAL	VAL
				E1564	E1564	E1564			ASP	ASP	GLN	GLN	GLN	THR	THR	THR	THR

E3494	T3495	F3496	K3497	N3498	Q3499	T3502	S3510	F3520	Q3523	M3524	H3534	Q3542	F3543	R3544	T3545	D3546	I3547	T3550	L3553	D3557	E3558	R3561	W3562	L3567	E3575	I3578	M3579	L3580	K3581	R3585	D3591	T3597	I3600	R3607	R3608	R3611	D3617	A3618		
GLU	VAL	GLU	GLN	MET	ILE	ARG	ASP	ASN	TYR	GLU	ALA	GLU	GLU	GLU	GLU	GLU	GLU	GLY	GLU	GLU	THR	VAL	LYS	TRP	LYS	ASP	ARG	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
LYS	LYS	LYS	VAL	MET	SER	GLN	GLU	ILE	GLN	GLU	HIS	LYS	GLN	GLN	GLN	GLN	VAL	ILE	ALA	ASP	LYS	GLN	MET	LYS	VAL	GLU	GLU	GLN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	
ASN	PRO	PRO	ALA	ALA	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	
MET	SER	ASN	PRO	TYR	ASN	TYR	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
GLU	VAL	GLU	GLN	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	

E3494	T3495	F3496	K3497	N3498	Q3499	T3502	S3510	F3520	Q3523	M3524	H3534	Q3542	F3543	R3544	T3545	D3546	I3547	T3550	L3553	D3557	E3558	R3561	W3562	L3567	E3575	I3578	M3579	L3580	K3581	R3585	D3591	T3597	I3600	R3607	R3608	R3611	D3617	A3618		
GLU	VAL	GLU	GLN	MET	ILE	ARG	ASP	ASN	TYR	GLU	ALA	GLU	GLU	GLU	GLU	GLU	GLU	GLY	GLU	GLU	THR	VAL	LYS	TRP	LYS	ASP	ARG	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
LYS	LYS	LYS	VAL	MET	SER	GLN	GLU	ILE	GLN	GLU	HIS	LYS	GLN	GLN	GLN	GLN	VAL	ILE	ALA	ASP	LYS	GLN	MET	LYS	VAL	GLU	GLU	GLN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
ASN	PRO	PRO	ALA	ALA	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	
MET	SER	ASN	PRO	TYR	ASN	TYR	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
GLU	VAL	GLU	GLN	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	

E3494	T3495	F3496	K3497	N3498	Q3499	T3502	S3510	F3520	Q3523	M3524	H3534	Q3542	F3543	R3544	T3545	D3546	I3547	T3550	L3553	D3557	E3558	R3561	W3562	L3567	E3575	I3578	M3579	L3580	K3581	R3585	D3591	T3597	I3600	R3607	R3608	R3611	D3617	A3618		
GLU	VAL	GLU	GLN	MET	ILE	ARG	ASP	ASN	TYR	GLU	ALA	GLU	GLU	GLU	GLU	GLU	GLU	GLY	GLU	GLU	THR	VAL	LYS	TRP	LYS	ASP	ARG	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
LYS	LYS	LYS	VAL	MET	SER	GLN	GLU	ILE	GLN	GLU	HIS	LYS	GLN	GLN	GLN	GLN	VAL	ILE	ALA	ASP	LYS	GLN	MET	LYS	VAL	GLU	GLU	GLN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
ASN	PRO	PRO	ALA	ALA	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	
MET	SER	ASN	PRO	TYR	ASN	TYR	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
GLU	VAL	GLU	GLN	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	

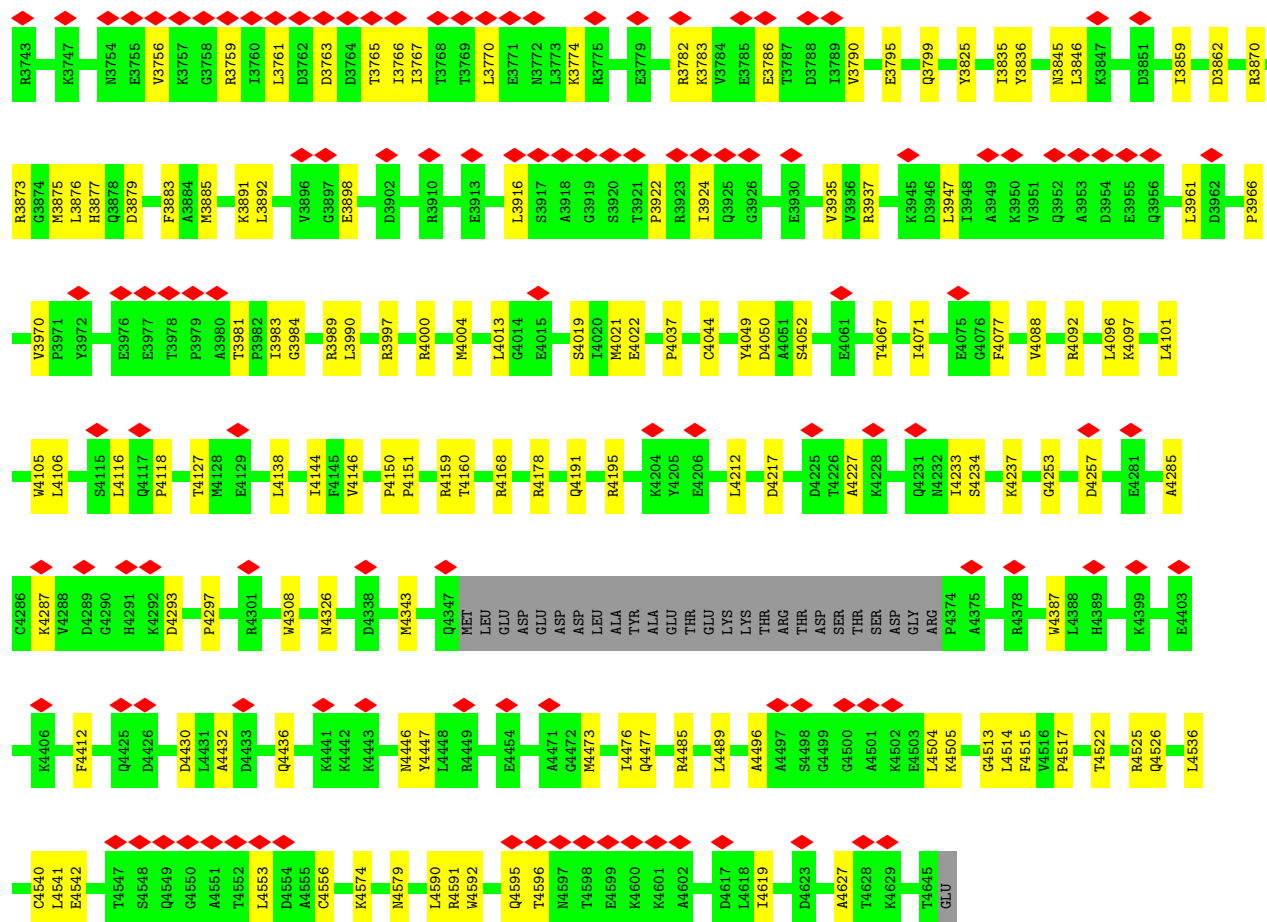
E3494	T3495	F3496	K3497	N3498	Q3499	T3502	S3510	F3520	Q3523	M3524	H3534	Q3542	F3543	R3544	T3545	D3546	I3547	T3550	L3553	D3557	E3558	R3561	W3562	L3567	E3575	I3578	M3579	L3580	K3581	R3585	D3591	T3597	I3600	R3607	R3608	R3611	D3617	A3618		
GLU	VAL	GLU	GLN	MET	ILE	ARG	ASP	ASN	TYR	GLU	ALA	GLU	GLU	GLU	GLU	GLU	GLU	GLY	GLU	GLU	THR	VAL	LYS	TRP	LYS	ASP	ARG	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
LYS	LYS	LYS	VAL	MET	SER	GLN	GLU	ILE	GLN	GLU	HIS	LYS	GLN	GLN	GLN	GLN	VAL	ILE	ALA	ASP	LYS	GLN	MET	LYS	VAL	GLU	GLU	GLN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
ASN	PRO	PRO	ALA	ALA	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	
MET	SER	ASN	PRO	TYR	ASN	TYR	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
GLU	VAL	GLU	GLN	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	

E3494	T3495	F3496	K3497	N3498	Q3499	T3502	S3510	F3520	Q3523	M3524	H3534	Q3542	F3543	R3544	T3545	D3546	I3547	T3550	L3553	D3557	E3558	R3561	W3562	L3567	E3575	I3578	M3579	L3580	K3581	R3585	D3591	T3597	I3600	R3607	R3608	R3611	D3617	A3618		
GLU	VAL	GLU	GLN	MET	ILE	ARG	ASP	ASN	TYR	GLU	ALA	GLU	GLU	GLU	GLU	GLU	GLU	GLY	GLU	GLU	THR	VAL	LYS	TRP	LYS	ASP	ARG	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
LYS	LYS	LYS	VAL	MET	SER	GLN	GLU	ILE	GLN	GLU	HIS	LYS	GLN	GLN	GLN	GLN	VAL	ILE	ALA	ASP	LYS	GLN	MET	LYS	VAL	GLU	GLU	GLN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
ASN	PRO	PRO	ALA	ALA	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	
MET	SER	ASN	PRO	TYR	ASN	TYR	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
GLU	VAL	GLU	GLN	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	

E3494	T3495	F3496	K3497	N3498	Q3499	T3502	S3510	F3520	Q3523	M3524	H3534	Q3542	F3543	R3544	T3545	D3546	I3547	T3550	L3553	D3557	E3558	R3561	W3562	L3567	E3575	I3578	M3579	L3580	K3581	R3585	D3591	T3597	I3600	R3607	R3608	R3611	D3617	A3618		
GLU	VAL	GLU	GLN	MET	ILE	ARG	ASP	ASN	TYR	GLU	ALA	GLU	GLU	GLU	GLU	GLU	GLU	GLY	GLU	GLU	THR	VAL	LYS	TRP	LYS	ASP	ARG	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
LYS	LYS	LYS	VAL	MET	SER	GLN	GLU	ILE	GLN	GLU	HIS	LYS	GLN	GLN	GLN	GLN	VAL	ILE	ALA	ASP	LYS	GLN	MET	LYS	VAL	GLU	GLU	GLN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
ASN	PRO	PRO	ALA	ALA	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	
MET	SER	ASN	PRO	TYR	ASN	TYR	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
GLU	VAL	GLU	GLN	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	

E3494	T3495	F3496	K3497	N3498	Q3499	T3502	S3510	F3520	Q3523	M3524	H3534	Q3542	F3543	R3544	T3545	D3546	I3547	T3550	L3553	D3557	E3558	R3561	W3562	L3567	E3575	I3578	M3579	L3580	K3581	R3585	D3591	T3597	I3600	R3607	R3608	R3611	D3617	A3618		
GLU	VAL	GLU	GLN	MET	ILE	ARG	ASP	ASN	TYR	GLU	ALA	GLU	GLU	GLU	GLU	GLU	GLU	GLY	GLU	GLU	THR	VAL	LYS	TRP	LYS	ASP	ARG	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
LYS	LYS	LYS	VAL	MET	SER	GLN	GLU	ILE	GLN	GLU	HIS	LYS	GLN	GLN	GLN	GLN	VAL	ILE	ALA	ASP	LYS	GLN	MET	LYS	VAL	GLU	GLU	GLN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
ASN	PRO	PRO	ALA	ALA	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	
MET	SER	ASN	PRO	TYR	ASN	TYR	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
GLU	VAL	GLU	GLN	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	

E3494	T3495	F3496	K3497	N3498	Q3499	T3502	S3510	F3520	Q3523	M3524	H3534	Q3542	F3543	R3544	T3545	D3546	I3547	T3550	L3553	D3557	E3558	R3561	W3562	L3567	E3575	I3578	M3579	L3580	K3581	R3585	D3591	T3597	I3600	R3607	R3608	R3611	D3617	A3618		
GLU	VAL	GLU	GLN	MET	ILE	ARG	ASP	ASN	TYR	GLU	ALA	GLU	GLU	GLU	GLU	GLU	GLU	GLY	GLU	GLU	THR	VAL	LYS	TRP	LYS	ASP	ARG	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
LYS	LYS	LYS																																						



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136324	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	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	2.050	Depositor
Minimum map value	-1.087	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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, AOV, ADP, ATP

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	0.10	0/24093	0.24	0/32651

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	23593	0	23657	287	0
2	A	32	0	12	3	0
3	A	31	0	12	0	0
4	A	54	0	24	2	0
5	A	2	0	0	0	0
All	All	23712	0	23705	287	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 6.

All (287) 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:1490:TRP:HH2	1:A:1537:TRP:HD1	1.34	0.74
1:A:4574:LYS:HB3	1:A:4627:ALA:HB2	1.70	0.72
1:A:1504:VAL:HG11	1:A:1524:GLU:HB2	1.71	0.72
1:A:2457:SER:HB2	1:A:2732:PRO:HB3	1.71	0.72
1:A:4049:TYR:OH	1:A:4191:GLN:NE2	2.24	0.71
1:A:2811:ARG:HB3	1:A:2812:PRO:HD3	1.72	0.69
1:A:3627:LEU:HD23	1:A:3662:ILE:HG21	1.74	0.69
1:A:2834:GLN:HE21	1:A:2843:ARG:HB3	1.58	0.67
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	1.76	0.67
1:A:2085:HIS:HB2	1:A:2361:MET:HG2	1.77	0.66
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.76	0.66
1:A:2758:LEU:HD13	1:A:2811:ARG:HA	1.78	0.65
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	1.79	0.64
1:A:2804:ARG:O	1:A:2808:GLU:HG2	1.98	0.64
1:A:1483:LYS:NZ	1:A:1548:GLU:OE2	2.29	0.64
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.80	0.63
1:A:3017:VAL:HB	1:A:3020:LEU:HB2	1.82	0.62
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.82	0.62
1:A:1490:TRP:CH2	1:A:1537:TRP:HD1	2.17	0.62
1:A:3178:ASP:OD1	1:A:3585:ARG:NE	2.33	0.62
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.81	0.62
1:A:2592:VAL:HG23	1:A:2731:VAL:HG11	1.82	0.61
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.82	0.61
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.33	0.61
1:A:1914:GLU:HG3	2:A:4701:AOV:H2'	1.83	0.61
1:A:2969:GLY:HA2	1:A:3004:PHE:HE1	1.66	0.61
1:A:2034:LYS:HE3	1:A:4050:ASP:HB3	1.84	0.60
1:A:1867:ASN:O	1:A:1925:ARG:NH1	2.28	0.60
1:A:3110:THR:O	1:A:3140:ARG:NH1	2.35	0.60
1:A:3981:THR:HG23	1:A:3984:GLY:H	1.66	0.60
1:A:2775:GLU:HG2	1:A:2779:MET:HE2	1.84	0.59
1:A:2449:LEU:HA	1:A:2453:ARG:HH21	1.67	0.58
1:A:3611:ARG:NH1	1:A:3636:GLN:OE1	2.36	0.58
1:A:4489:LEU:HD11	1:A:4515:PHE:HE2	1.67	0.58
1:A:4526:GLN:HA	1:A:4536:LEU:HD21	1.85	0.58
1:A:2358:ARG:NH2	2:A:4701:AOV:O3G	2.33	0.58
1:A:3222:LEU:HA	1:A:3225:LYS:HE3	1.86	0.58
1:A:1623:ARG:NH2	1:A:1634:ASP:OD1	2.37	0.57
1:A:3935:VAL:HG13	1:A:3947:LEU:HD23	1.85	0.57
1:A:4556:CYS:SG	1:A:4591:ARG:NH2	2.77	0.57
1:A:2221:MET:HE1	1:A:2348:LEU:HD21	1.86	0.57
1:A:1946:VAL:HG22	1:A:2006:VAL:HG21	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1978:ILE:HD11	1:A:2001:LEU:HD11	1.86	0.57
1:A:4150:PRO:HB3	1:A:4159:ARG:HH12	1.69	0.57
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.87	0.57
1:A:1491:ASP:O	1:A:1495:ASN:ND2	2.38	0.56
1:A:2717:ASP:O	1:A:4446:ASN:ND2	2.37	0.56
1:A:3203:VAL:HG23	1:A:3206:ARG:HH21	1.71	0.56
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.87	0.56
1:A:3044:LEU:HD22	1:A:3049:GLU:HG3	1.86	0.56
1:A:1589:MET:HE3	1:A:1589:MET:HA	1.87	0.56
1:A:3068:MET:HE1	1:A:3078:ARG:HG3	1.88	0.55
1:A:3731:LEU:HD11	1:A:3790:VAL:HG12	1.87	0.55
1:A:2312:VAL:HG13	1:A:2355:THR:HG21	1.88	0.55
1:A:3478:LEU:HD22	1:A:3767:ILE:HG23	1.89	0.54
1:A:1985:HIS:CD2	1:A:2010:PRO:HB3	2.42	0.54
1:A:3835:ILE:HG12	1:A:3870:ARG:HD2	1.90	0.54
1:A:4050:ASP:OD2	1:A:4052:SER:OG	2.24	0.54
1:A:2967:TYR:OH	1:A:2975:ASP:OD2	2.22	0.54
1:A:3546:ASP:OD2	1:A:3547:ILE:N	2.41	0.54
1:A:2644:THR:OG1	1:A:2647:GLY:O	2.24	0.54
1:A:1933:ASP:OD2	1:A:2314:ASN:ND2	2.38	0.54
1:A:3174:ARG:NH1	1:A:3650:ASN:OD1	2.41	0.53
1:A:3961:LEU:O	1:A:3997:ARG:NH1	2.42	0.53
1:A:2222:MET:HE2	1:A:2342:MET:HE2	1.91	0.53
1:A:3481:SER:O	1:A:3774:LYS:NZ	2.41	0.53
1:A:2686:MET:HE3	1:A:2708:PHE:CE1	2.43	0.53
1:A:3124:ASP:OD1	1:A:3125:TYR:N	2.42	0.53
1:A:4021:MET:HE3	1:A:4021:MET:HA	1.90	0.53
1:A:2872:LEU:HD22	1:A:2920:LEU:HD12	1.92	0.52
1:A:2909:LEU:HD11	1:A:2945:THR:HG21	1.90	0.52
1:A:2290:SER:HB2	1:A:2295:LEU:HG	1.92	0.52
1:A:3664:LEU:HB3	1:A:3669:ILE:HD12	1.91	0.52
1:A:3898:GLU:HG3	1:A:3981:THR:HG21	1.92	0.52
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.73	0.52
1:A:1619:LEU:HD21	1:A:1638:LEU:HD23	1.92	0.52
1:A:2075:LEU:HD22	1:A:4522:THR:HG23	1.92	0.52
1:A:2665:GLU:HB3	1:A:2668:LEU:HD12	1.91	0.52
1:A:1464:LYS:O	1:A:1468:GLU:HG3	2.10	0.52
1:A:3481:SER:OG	1:A:3774:LYS:NZ	2.40	0.51
1:A:2065:LEU:HD22	1:A:2137:LEU:HD22	1.92	0.51
1:A:2220:LEU:HD22	1:A:2342:MET:HE3	1.93	0.51
1:A:3618:ALA:O	1:A:3622:ASN:ND2	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4287:LYS:H	1:A:4293:ASP:HB3	1.74	0.51
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.92	0.51
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.11	0.51
1:A:2943:LYS:HG2	1:A:3094:PHE:HD2	1.76	0.51
1:A:2091:ARG:NH1	2:A:4701:AOV:O1G	2.42	0.50
1:A:2179:ARG:NH2	1:A:2195:ASP:OD1	2.33	0.50
1:A:2313:GLU:OE1	1:A:2316:ASN:ND2	2.43	0.50
1:A:2943:LYS:N	4:A:4704:ADP:O1B	2.44	0.50
1:A:3236:ALA:HB1	1:A:3455:ILE:HG22	1.94	0.50
1:A:4097:LYS:HA	1:A:4127:THR:HB	1.93	0.50
1:A:4430:ASP:OD2	1:A:4447:TYR:OH	2.29	0.50
1:A:2562:VAL:HG11	1:A:2755:MET:HB2	1.92	0.50
1:A:4505:LYS:HZ3	1:A:4553:LEU:HB3	1.76	0.50
1:A:2507:ARG:HE	1:A:2509:LYS:NZ	2.10	0.50
1:A:3225:LYS:HE2	1:A:3468:VAL:HG21	1.94	0.50
1:A:3763:ASP:OD2	1:A:3765:THR:OG1	2.29	0.50
1:A:3478:LEU:HD11	1:A:3770:LEU:HB3	1.93	0.50
1:A:1817:HIS:CE1	1:A:1881:GLN:HG2	2.47	0.50
1:A:2751:PHE:HB3	1:A:2803:VAL:HG11	1.94	0.50
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	1.92	0.49
1:A:4387:TRP:HZ2	1:A:4476:ILE:HD13	1.77	0.49
1:A:2686:MET:HG2	1:A:2703:LEU:HD11	1.93	0.49
1:A:2188:GLU:OE1	1:A:2243:ARG:NH2	2.43	0.49
1:A:3217:GLU:HB2	1:A:3220:ARG:HH21	1.77	0.49
1:A:2703:LEU:HD22	1:A:2706:ILE:HD12	1.95	0.49
1:A:1551:PHE:O	1:A:1558:LYS:NZ	2.45	0.49
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.46	0.49
1:A:2211:TYR:O	1:A:2214:THR:OG1	2.28	0.49
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.45	0.49
1:A:3475:SER:HB2	1:A:3761:LEU:HD11	1.94	0.49
1:A:3825:TYR:OH	1:A:3879:ASP:OD2	2.23	0.49
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.95	0.49
1:A:4071:ILE:HG23	1:A:4077:PHE:HE1	1.77	0.49
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.95	0.48
1:A:2686:MET:HE3	1:A:2708:PHE:CZ	2.48	0.48
1:A:3756:VAL:HG11	1:A:3766:ILE:HG13	1.95	0.48
1:A:2826:ALA:HB2	1:A:2867:MET:HE1	1.96	0.48
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.94	0.48
1:A:3922:PRO:HG2	1:A:3924:ILE:HD11	1.95	0.48
1:A:4088:VAL:HG11	1:A:4116:LEU:HD21	1.95	0.48
1:A:3154:LEU:HB3	1:A:3171:ILE:HG13	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4150:PRO:O	1:A:4195:ARG:NH2	2.37	0.48
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.46	0.48
1:A:2788:THR:HG22	1:A:2789:GLN:HG2	1.96	0.48
1:A:3970:VAL:HB	1:A:3989:ARG:HD3	1.94	0.48
1:A:2894:LYS:HD3	1:A:2911:LEU:HD12	1.96	0.48
1:A:3167:ARG:NH1	1:A:3687:GLU:OE2	2.43	0.48
1:A:3597:THR:HG23	1:A:3634:LEU:HD21	1.96	0.48
1:A:3885:MET:HE3	1:A:4343:MET:HE1	1.96	0.48
1:A:1879:LEU:HD11	1:A:1914:GLU:HB3	1.96	0.48
1:A:4517:PRO:HG2	1:A:4619:ILE:HD12	1.95	0.48
1:A:3639:GLU:HB3	1:A:3686:VAL:HG21	1.96	0.47
1:A:2297:LYS:O	1:A:2338:ASN:ND2	2.45	0.47
1:A:3209:LYS:HA	1:A:3209:LYS:HD3	1.68	0.47
1:A:2937:GLY:C	1:A:3070:PRO:HD3	2.40	0.47
1:A:2492:ARG:HG2	1:A:2545:TRP:NE1	2.29	0.47
1:A:3114:ASP:O	1:A:3116:GLU:HG2	2.14	0.47
1:A:3158:ASN:ND2	1:A:3169:MET:O	2.47	0.47
1:A:3738:PHE:CZ	1:A:3783:LYS:HE3	2.50	0.47
1:A:1850:GLN:HB3	1:A:1856:GLN:HG2	1.95	0.47
1:A:2042:THR:HG21	1:A:4257:ASP:HB2	1.95	0.47
1:A:1601:LEU:HD23	1:A:1604:LEU:HD12	1.96	0.47
1:A:2088:PHE:HD1	1:A:2145:MET:HE1	1.80	0.47
1:A:1960:PHE:HE2	1:A:2032:LEU:HD21	1.80	0.47
1:A:2810:LEU:O	1:A:2811:ARG:C	2.58	0.47
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.97	0.47
1:A:3130:TYR:CZ	1:A:3132:LYS:HB2	2.50	0.46
1:A:1623:ARG:HD3	1:A:1630:TYR:HA	1.98	0.46
1:A:1964:GLU:HB2	1:A:1967:MET:HG2	1.98	0.46
1:A:3916:LEU:HD11	1:A:3937:ARG:HG3	1.96	0.46
1:A:4234:SER:HB3	1:A:4237:LYS:HG2	1.97	0.46
1:A:2925:ILE:HG21	1:A:2933:LEU:HG	1.98	0.46
1:A:3239:LYS:HE3	1:A:3451:TYR:HD1	1.81	0.46
1:A:2769:LEU:HA	1:A:2858:PHE:HZ	1.81	0.46
1:A:1622:GLU:O	1:A:1625:SER:OG	2.34	0.46
1:A:1887:ARG:NH2	1:A:4253:GLY:O	2.48	0.46
1:A:4541:LEU:HD21	1:A:4590:LEU:HD22	1.97	0.46
1:A:3846:LEU:HD11	1:A:3859:ILE:HG13	1.98	0.46
1:A:4412:PHE:HZ	1:A:4514:LEU:HD13	1.81	0.46
1:A:1671:SER:HB2	1:A:1693:THR:HG23	1.98	0.45
1:A:1831:ASP:OD1	1:A:1831:ASP:N	2.48	0.45
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2488:ARG:NH2	1:A:2542:SER:O	2.49	0.45
1:A:2316:ASN:O	1:A:2320:ASP:HB2	2.16	0.45
1:A:2987:ASN:OD1	1:A:3057:GLN:NE2	2.38	0.45
1:A:2297:LYS:HB2	1:A:2299:GLN:HE21	1.82	0.45
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	1.98	0.45
1:A:4285:ALA:O	1:A:4293:ASP:HB2	2.17	0.45
1:A:4496:ALA:HB2	1:A:4504:LEU:HD21	1.98	0.45
1:A:2773:MET:HG3	1:A:2825:TRP:HE1	1.82	0.45
1:A:3611:ARG:HG3	1:A:3634:LEU:HD23	1.98	0.45
1:A:2201:GLY:O	1:A:2205:GLU:HG2	2.17	0.45
1:A:2374:ILE:HD13	1:A:2452:LEU:HD21	1.98	0.45
1:A:3502:THR:HG21	1:A:3544:ARG:HG3	1.99	0.45
1:A:2560:HIS:ND1	1:A:2561:LYS:HG3	2.32	0.45
1:A:3219:ARG:NH2	1:A:3476:THR:OG1	2.49	0.45
1:A:1508:LYS:HA	1:A:1513:TYR:CG	2.52	0.44
1:A:2830:LEU:HD11	1:A:2871:ILE:HD12	1.98	0.44
1:A:1984:GLU:OE2	1:A:1997:ILE:HD11	2.17	0.44
1:A:2063:GLU:O	1:A:2067:ASN:ND2	2.51	0.44
1:A:2075:LEU:HD13	1:A:4536:LEU:HD13	1.99	0.44
1:A:3214:GLN:O	1:A:3217:GLU:HG2	2.17	0.44
1:A:3135:GLN:HB2	1:A:3136:PRO:HD3	1.99	0.44
1:A:1996:PRO:HB2	1:A:2007:LYS:HG3	2.00	0.44
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	1.98	0.44
1:A:1853:VAL:HA	1:A:1856:GLN:HG3	2.00	0.44
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.51	0.44
1:A:2671:MET:HE3	1:A:2721:LYS:HB3	1.99	0.44
1:A:4297:PRO:HG3	1:A:4308:TRP:CD2	2.52	0.44
1:A:4542:GLU:HG2	1:A:4591:ARG:HB2	2.00	0.44
1:A:3845:ASN:ND2	1:A:3862:ASP:OD2	2.41	0.44
1:A:1543:ARG:HA	1:A:1546:TYR:CE2	2.53	0.43
1:A:1882:THR:HA	1:A:2048:LEU:HD23	1.99	0.43
1:A:3875:MET:HE1	1:A:3883:PHE:HB2	1.99	0.43
1:A:1882:THR:HB	1:A:2045:ASP:HB2	1.99	0.43
1:A:2666:ILE:HG22	1:A:2712:CYS:HB3	1.99	0.43
1:A:2185:VAL:HG13	1:A:2239:LYS:HD2	2.00	0.43
1:A:1796:VAL:O	1:A:1805:ARG:NH1	2.50	0.43
1:A:2316:ASN:O	1:A:2358:ARG:NE	2.48	0.43
1:A:1535:ASP:OD1	1:A:2292:ARG:NH1	2.52	0.43
1:A:2813:LEU:HD13	1:A:2816:LEU:HD13	2.00	0.43
1:A:2018:MET:HE1	1:A:2028:LEU:HD21	2.01	0.43
1:A:2863:ARG:O	1:A:2867:MET:N	2.45	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3799:GLN:OE1	1:A:3799:GLN:HA	2.19	0.43
1:A:1481:GLN:O	1:A:1483:LYS:HG3	2.18	0.43
1:A:2069:ILE:HB	1:A:2137:LEU:HD21	2.01	0.43
1:A:2493:TYR:O	1:A:2497:ALA:N	2.47	0.43
1:A:3873:ARG:HA	1:A:3873:ARG:HD3	1.78	0.43
1:A:1537:TRP:HA	1:A:1540:VAL:HG22	2.00	0.43
1:A:1698:ILE:HD12	1:A:1701:TRP:NE1	2.34	0.43
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.52	0.43
1:A:2519:ARG:HG3	1:A:2526:LEU:HD12	2.01	0.43
1:A:1599:ARG:O	1:A:1603:ARG:HG2	2.19	0.43
1:A:1943:ARG:NH1	1:A:2329:ASN:O	2.50	0.43
1:A:2626:THR:HB	1:A:2669:PRO:HG3	1.99	0.43
1:A:3558:GLU:OE1	1:A:3581:LYS:NZ	2.41	0.43
1:A:3990:LEU:HA	1:A:4004:MET:HG2	2.00	0.43
1:A:2943:LYS:HG2	1:A:3094:PHE:CD2	2.54	0.43
1:A:1478:VAL:HG21	1:A:1488:ARG:CZ	2.49	0.42
1:A:3795:GLU:O	1:A:3799:GLN:HG2	2.19	0.42
1:A:1564:GLU:CD	1:A:1567:ARG:HH21	2.27	0.42
1:A:3214:GLN:HB2	1:A:3759:ARG:NH1	2.34	0.42
1:A:2118:ARG:HD2	1:A:2118:ARG:C	2.43	0.42
1:A:3606:ASP:N	1:A:3606:ASP:OD1	2.51	0.42
1:A:4106:LEU:HD13	1:A:4138:LEU:HD22	2.00	0.42
1:A:4541:LEU:HD12	1:A:4592:TRP:CZ2	2.54	0.42
1:A:3782:ARG:O	1:A:3786:GLU:HG2	2.19	0.42
1:A:3892:LEU:HD13	1:A:3983:ILE:HG21	2.00	0.42
1:A:3032:GLN:HA	1:A:3035:GLU:HG2	2.02	0.42
1:A:2319:LEU:HD13	1:A:2359:CYS:SG	2.60	0.42
1:A:2818:VAL:O	1:A:2822:ILE:HG12	2.19	0.42
1:A:1966:ARG:HA	1:A:4101:LEU:HD13	2.02	0.42
1:A:3109:PHE:CG	1:A:3180:ILE:HD12	2.54	0.42
1:A:3114:ASP:O	1:A:3140:ARG:NH2	2.52	0.42
1:A:1904:PRO:HG2	1:A:2017:THR:HG22	2.02	0.42
1:A:2080:LEU:HD12	1:A:2088:PHE:CZ	2.55	0.42
1:A:4525:ARG:HB2	1:A:4592:TRP:CZ2	2.54	0.42
1:A:4485:ARG:HG2	1:A:4513:GLY:HA2	2.02	0.42
1:A:4540:CYS:SG	1:A:4595:GLN:NE2	2.93	0.42
1:A:3716:VAL:HB	1:A:3836:TYR:OH	2.20	0.42
1:A:2041:MET:HE2	1:A:2041:MET:HB3	1.98	0.41
1:A:2510:MET:HA	1:A:2513:GLU:HB2	2.01	0.41
1:A:3222:LEU:HD11	1:A:3469:GLU:HG3	2.02	0.41
1:A:3761:LEU:HD13	1:A:3767:ILE:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1733:ILE:HD11	1:A:1738:TYR:CD1	2.55	0.41
1:A:1941:MET:HE3	1:A:1941:MET:HB3	2.00	0.41
1:A:2869:ARG:HB3	1:A:2870:PRO:HD3	2.02	0.41
1:A:3763:ASP:HB3	1:A:3766:ILE:HG12	2.01	0.41
1:A:2793:ILE:O	1:A:2836:ARG:NH1	2.54	0.41
1:A:4473:MET:HG3	1:A:4477:GLN:HB2	2.02	0.41
1:A:1460:GLU:OE1	1:A:1460:GLU:N	2.52	0.41
1:A:2823:ARG:HH22	1:A:2868:SER:HB2	1.83	0.41
1:A:1640:ILE:HD11	1:A:1653:HIS:HB3	2.01	0.41
1:A:2797:ARG:HG2	4:A:4703:ADP:H4'	2.03	0.41
1:A:3591:ASP:O	1:A:3591:ASP:OD2	2.39	0.41
1:A:4019:SER:O	1:A:4022:GLU:HG2	2.21	0.41
1:A:1525:ASP:O	1:A:1529:ARG:HG3	2.21	0.41
1:A:2007:LYS:HE3	1:A:2007:LYS:HB3	1.78	0.41
1:A:2016:ILE:O	1:A:2016:ILE:HG13	2.20	0.41
1:A:2809:ALA:O	1:A:2812:PRO:HD2	2.21	0.41
1:A:4067:THR:HG23	1:A:4092:ARG:HH12	1.85	0.41
1:A:1709:MET:HE2	1:A:1709:MET:HB3	2.00	0.41
1:A:2671:MET:HG2	1:A:2677:GLN:HG3	2.03	0.41
1:A:2672:ASP:N	1:A:2672:ASP:OD2	2.54	0.41
1:A:2856:LYS:HB2	1:A:2856:LYS:HE3	1.82	0.41
1:A:2896:ARG:HD2	1:A:2896:ARG:HA	1.81	0.41
1:A:3873:ARG:HD3	1:A:4021:MET:HE1	2.02	0.41
1:A:3877:HIS:CE1	1:A:4151:PRO:HB3	2.55	0.41
1:A:4432:ALA:O	1:A:4436:GLN:HG2	2.20	0.41
1:A:2224:GLY:O	1:A:2346:GLN:HA	2.21	0.40
1:A:3550:THR:HG22	1:A:3575:GLU:HG3	2.02	0.40
1:A:4595:GLN:OE1	1:A:4596:THR:N	2.54	0.40
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.56	0.40
1:A:3553:LEU:HB2	1:A:3578:ILE:HD13	2.02	0.40
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	2.03	0.40
1:A:4044:CYS:SG	1:A:4144:ILE:HG23	2.61	0.40
1:A:2686:MET:CG	1:A:2703:LEU:HD11	2.50	0.40
1:A:3562:TRP:HB3	1:A:3567:LEU:HD22	2.03	0.40
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	2.03	0.40
1:A:3891:LYS:HD2	1:A:4013:LEU:HD23	2.03	0.40
1:A:1816:VAL:HG11	1:A:2052:VAL:HG22	2.03	0.40
1:A:3021:PHE:CG	1:A:3029:LEU:HD22	2.56	0.40
1:A:3072:SER:O	1:A:3076:LYS:HG3	2.22	0.40
1:A:3222:LEU:HD22	1:A:3472:VAL:HG21	2.03	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	2929/4646 (63%)	2886 (98%)	43 (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	2605/4125 (63%)	2605 (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 (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1593	ASN
1	A	1856	GLN
1	A	1867	ASN
1	A	1985	HIS
1	A	1989	ASN
1	A	2019	ASN
1	A	2047	GLN
1	A	2079	GLN
1	A	2134	GLN
1	A	2212	GLN
1	A	2263	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2637	HIS
1	A	2698	GLN
1	A	2730	HIS
1	A	2781	GLN
1	A	2786	GLN
1	A	2834	GLN
1	A	3063	HIS
1	A	3237	ASN
1	A	3498	ASN
1	A	3622	ASN
1	A	3877	HIS
1	A	3906	GLN
1	A	4029	HIS
1	A	4038	ASN
1	A	4114	HIS
1	A	4191	GLN
1	A	4335	GLN
1	A	4397	HIS
1	A	4429	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are 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	ADP	A	4703	-	28,29,29	1.40	4 (14%)	43,45,45	1.86	8 (18%)
3	ATP	A	4702	5	32,33,33	0.32	0	48,52,52	0.28	0
2	AOV	A	4701	5	32,34,34	5.09	7 (21%)	42,56,56	2.25	12 (28%)
4	ADP	A	4704	-	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)

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	ADP	A	4703	-	-	5/16/32/32	0/3/3/3
3	ATP	A	4702	5	-	3/22/38/38	0/3/3/3
2	AOV	A	4701	5	-	2/16/39/39	0/3/3/3
4	ADP	A	4704	-	-	1/16/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4701	AOV	O1G-VG	27.64	2.10	1.61
4	A	4703	ADP	C5-C4	4.71	1.47	1.39
4	A	4704	ADP	C5-C4	4.71	1.47	1.39
2	A	4701	AOV	C5-C4	4.63	1.47	1.39
4	A	4704	ADP	C5-C6	2.72	1.48	1.41
2	A	4701	AOV	C5-C6	2.71	1.48	1.41
4	A	4703	ADP	C5-C6	2.68	1.48	1.41
2	A	4701	AOV	C8-N9	-2.67	1.33	1.37
2	A	4701	AOV	C5-N7	-2.63	1.34	1.39
2	A	4701	AOV	PA-O3A	-2.57	1.56	1.59
4	A	4703	ADP	C5-N7	-2.33	1.34	1.39
4	A	4704	ADP	C8-N7	2.32	1.36	1.31
4	A	4704	ADP	C5-N7	-2.32	1.34	1.39
2	A	4701	AOV	C8-N7	2.24	1.36	1.31
4	A	4703	ADP	C8-N7	2.23	1.36	1.31

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	AOV	C5-C4-N3	-7.22	116.78	126.72
4	A	4703	ADP	C5-C4-N3	-6.10	118.32	126.72
4	A	4704	ADP	C5-C4-N3	-5.82	118.70	126.72
2	A	4701	AOV	N3-C4-N9	5.75	136.94	127.17
4	A	4703	ADP	N3-C4-N9	4.92	135.53	127.17
4	A	4704	ADP	N3-C4-N9	4.65	135.07	127.17
2	A	4701	AOV	C4-C5-N7	-4.38	105.58	110.58
2	A	4701	AOV	C2-N3-C4	4.26	122.23	111.83
4	A	4703	ADP	C2-N3-C4	3.79	121.09	111.83
2	A	4701	AOV	O2B-PB-O3A	3.71	117.30	107.27
4	A	4704	ADP	C2-N3-C4	3.70	120.86	111.83
2	A	4701	AOV	N3-C2-N1	-3.52	123.25	128.58
4	A	4704	ADP	C4-C5-N7	-3.38	106.72	110.58
2	A	4701	AOV	C5-N7-C8	3.33	108.69	103.45
4	A	4703	ADP	C4-C5-N7	-3.31	106.80	110.58
4	A	4704	ADP	N3-C2-N1	-3.27	123.63	128.58
4	A	4703	ADP	N3-C2-N1	-3.23	123.70	128.58
2	A	4701	AOV	C4-N9-C8	2.91	108.79	105.74
4	A	4704	ADP	C4-N9-C8	2.61	108.48	105.74
4	A	4703	ADP	C3'-C2'-C1'	2.56	106.30	101.46
4	A	4703	ADP	C5-N7-C8	2.48	107.35	103.45
4	A	4703	ADP	C4-N9-C8	2.48	108.34	105.74
4	A	4704	ADP	C5-N7-C8	2.48	107.34	103.45
4	A	4704	ADP	C3'-C2'-C1'	2.47	106.14	101.46
2	A	4701	AOV	O3A-PA-O1A	-2.37	103.56	110.70
2	A	4701	AOV	N9-C8-N7	-2.30	110.67	113.94
2	A	4701	AOV	C2'-C1'-N9	-2.16	107.94	113.30
2	A	4701	AOV	C6-C5-N7	2.14	136.22	132.09
4	A	4704	ADP	C6-C5-N7	2.02	135.98	132.09

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	4703	ADP	C5'-O5'-PA-O1A
4	A	4703	ADP	C5'-O5'-PA-O3A
3	A	4702	ATP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'
4	A	4703	ADP	O4'-C4'-C5'-O5'
2	A	4701	AOV	C5'-O5'-PA-O2A
2	A	4701	AOV	C5'-O5'-PA-O3A
4	A	4703	ADP	C5'-O5'-PA-O2A
4	A	4704	ADP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

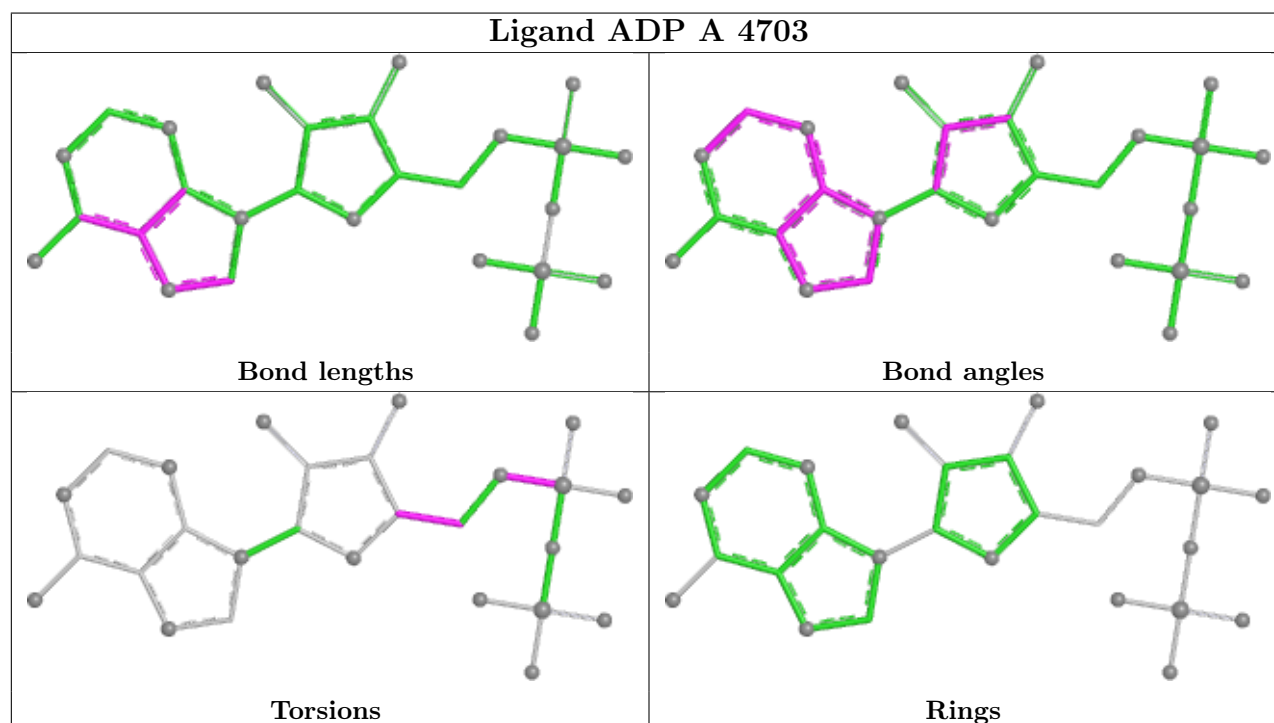
Mol	Chain	Res	Type	Atoms
3	A	4702	ATP	PA-O3A-PB-O2B
4	A	4703	ADP	C3'-C4'-C5'-O5'

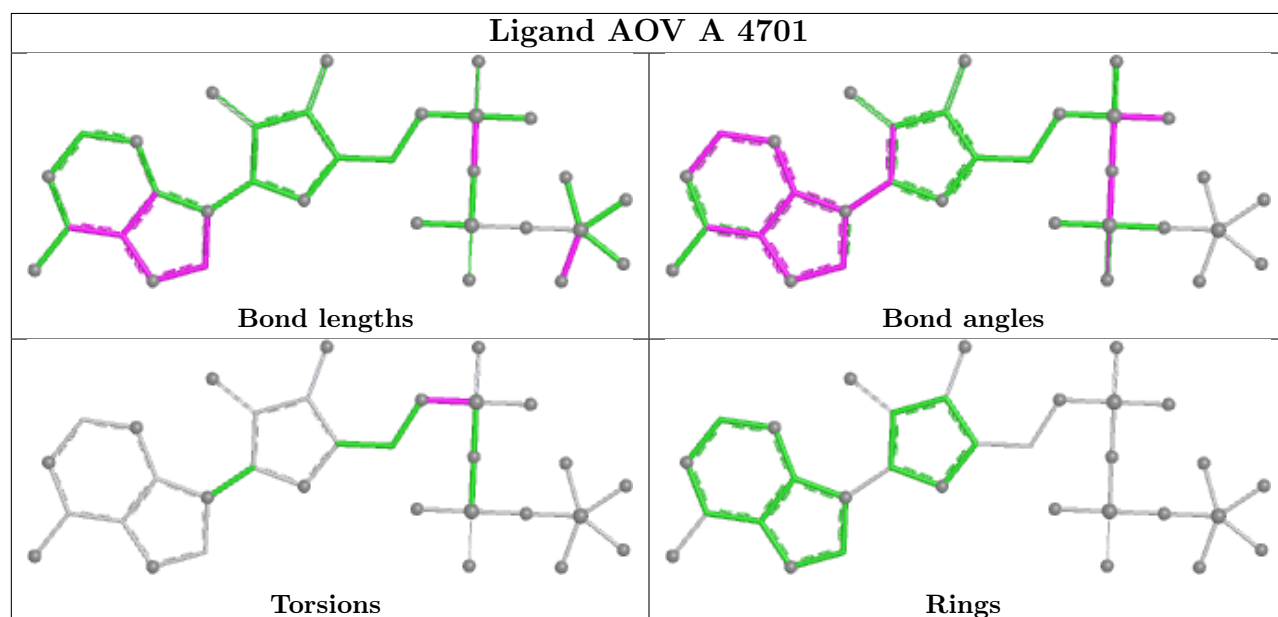
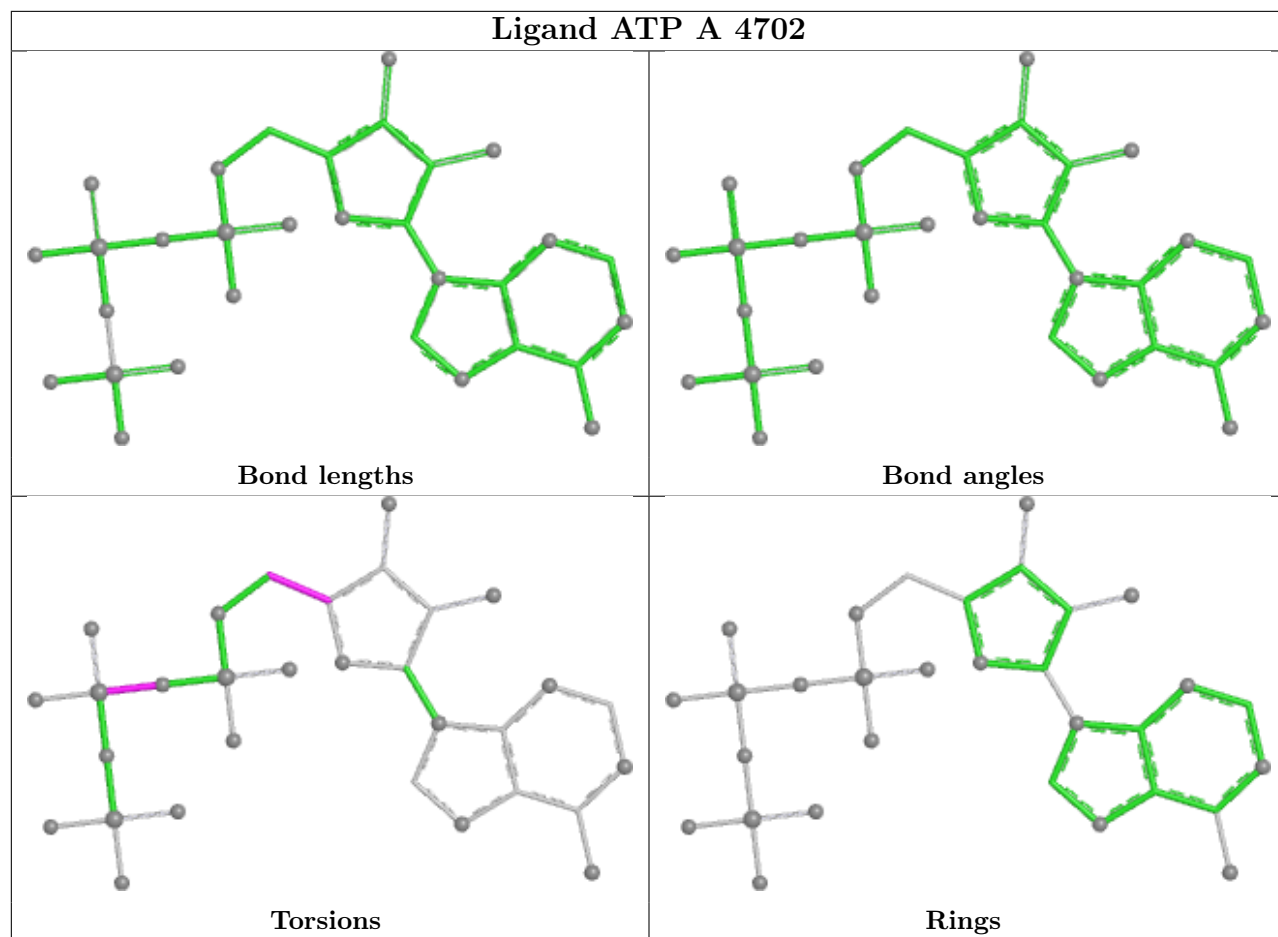
There are no ring outliers.

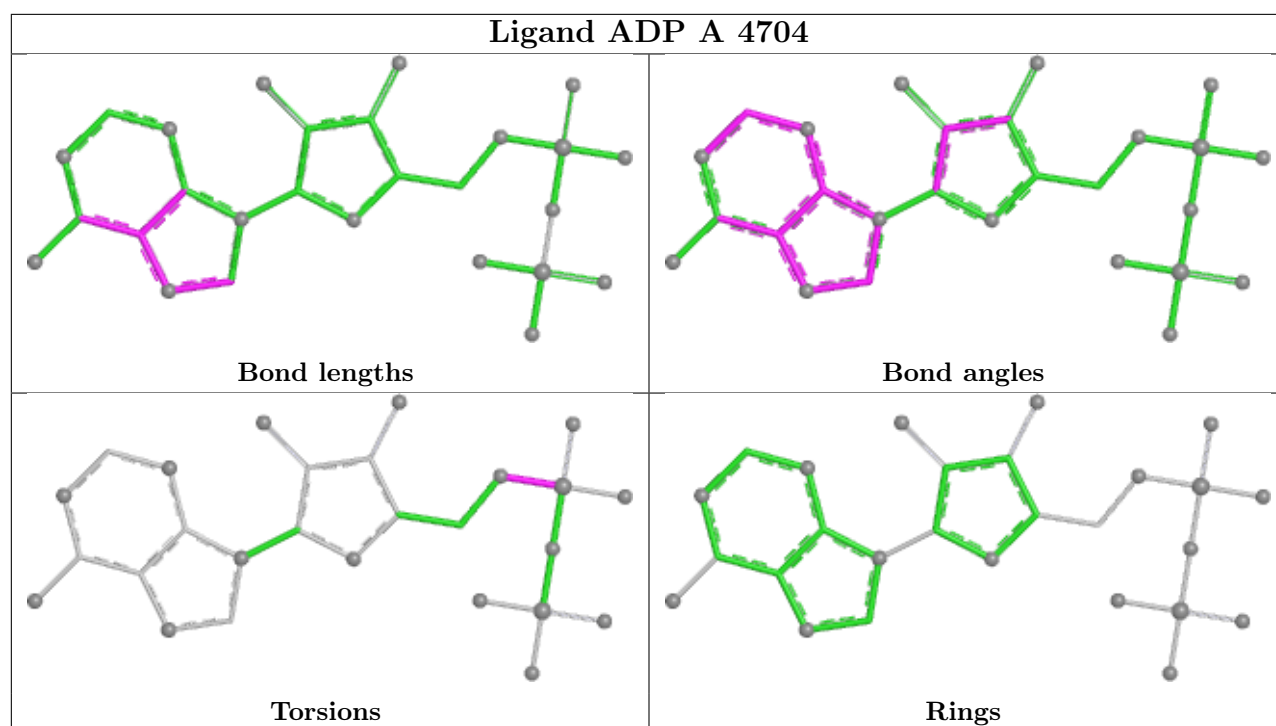
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4703	ADP	1	0
2	A	4701	AOV	3	0
4	A	4704	ADP	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

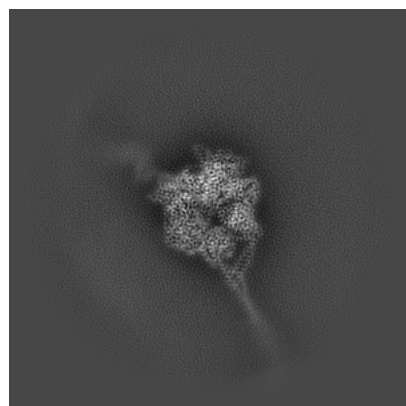
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44698. These allow visual inspection of the internal detail of the map and identification of artifacts.

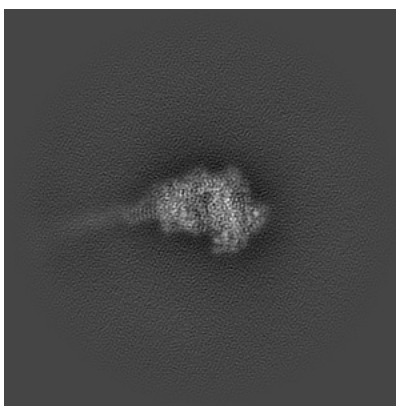
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

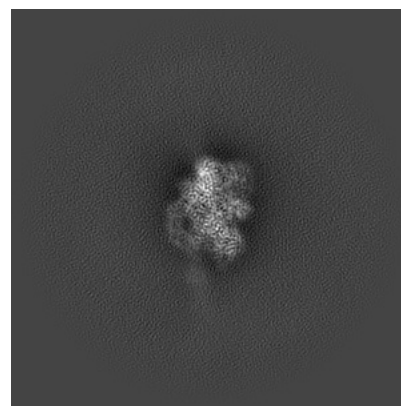
6.1.1 Primary map



X

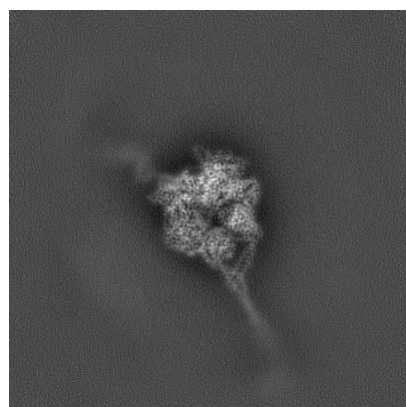


Y

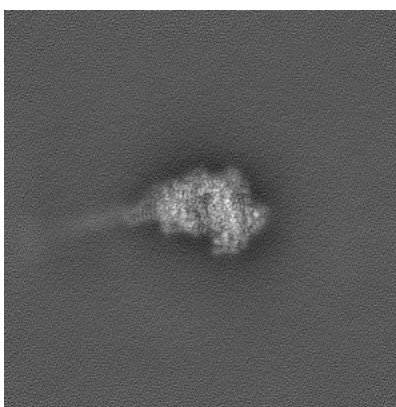


Z

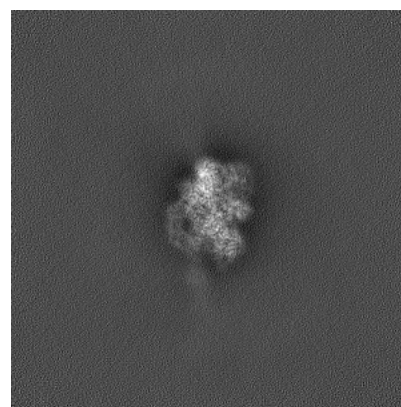
6.1.2 Raw map



X



Y

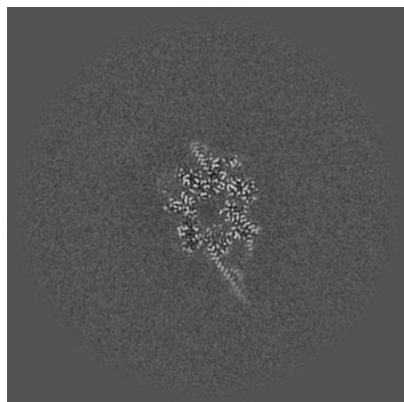


Z

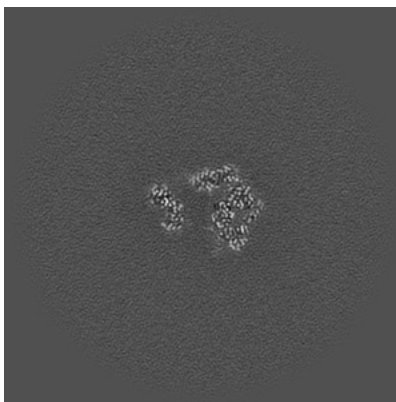
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

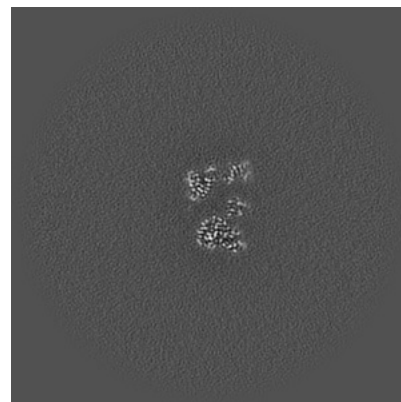
6.2.1 Primary map



X Index: 192

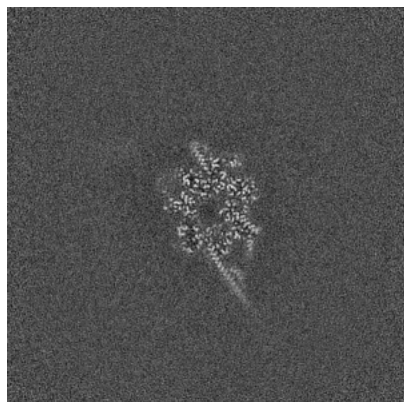


Y Index: 192

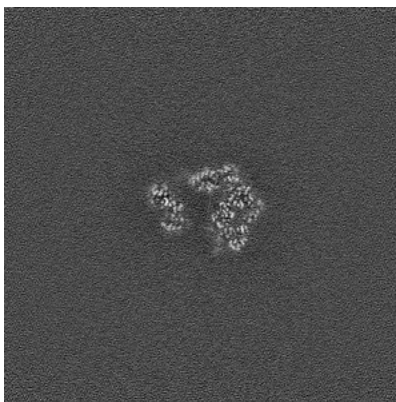


Z Index: 192

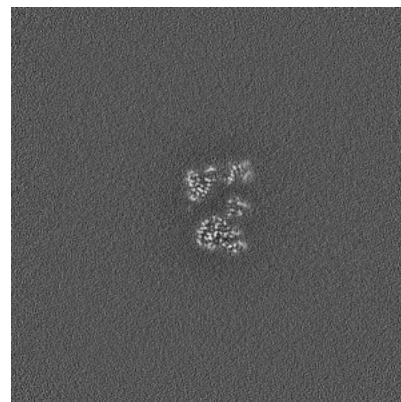
6.2.2 Raw map



X Index: 192



Y Index: 192

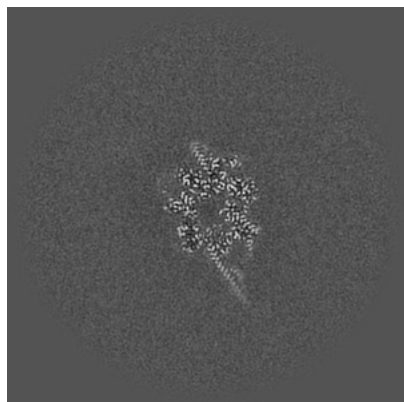


Z Index: 192

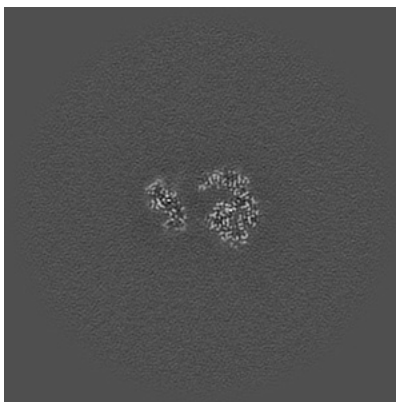
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

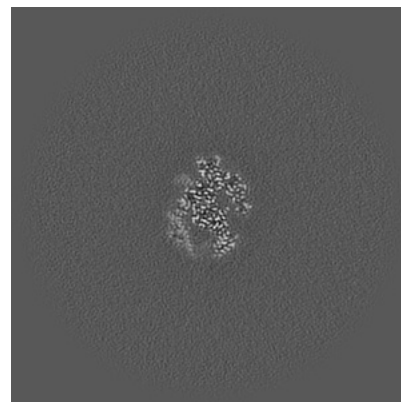
6.3.1 Primary map



X Index: 192

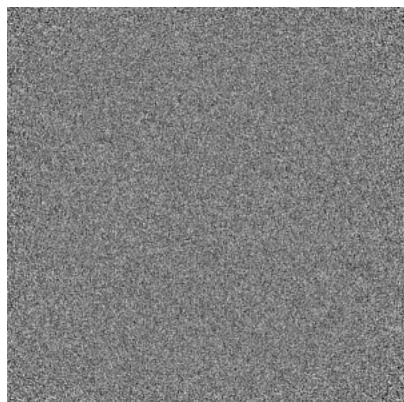


Y Index: 197

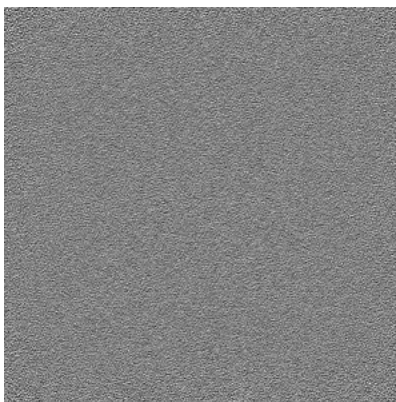


Z Index: 213

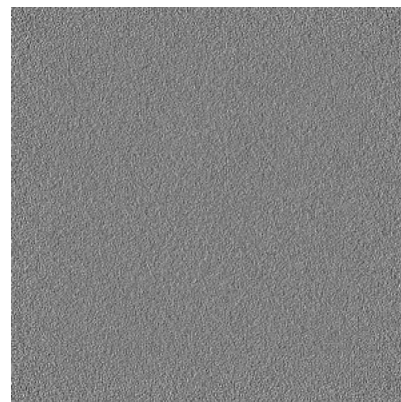
6.3.2 Raw map



X Index: 0



Y Index: 0

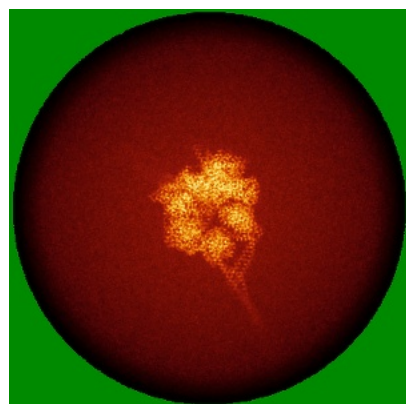


Z Index: 0

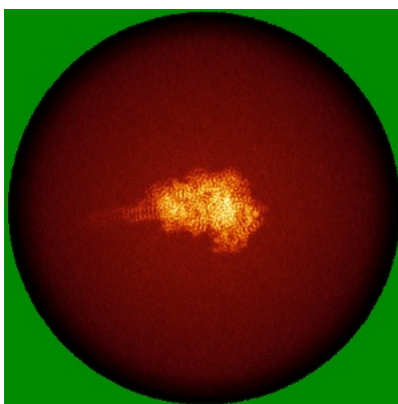
The images above show the largest variance slices of the map in three orthogonal directions.

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

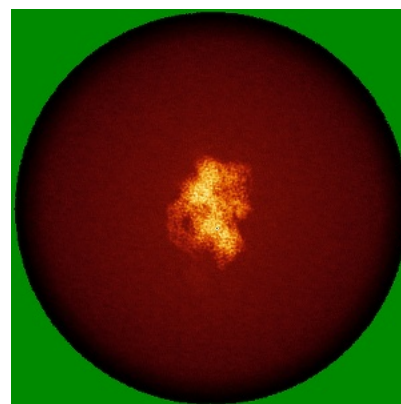
6.4.1 Primary map



X

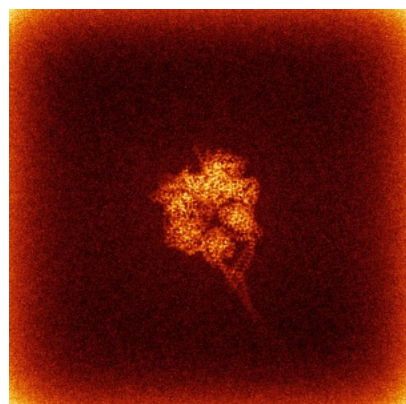


Y

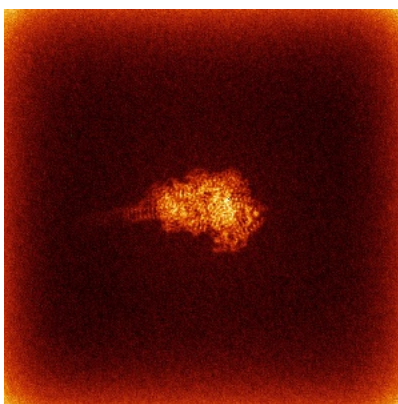


Z

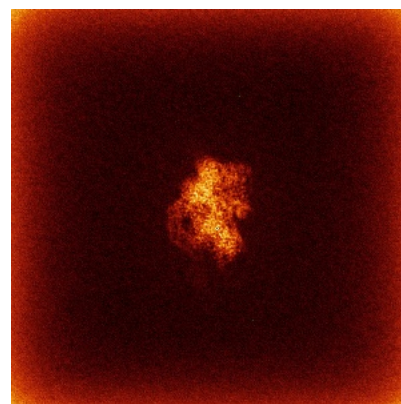
6.4.2 Raw map



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.

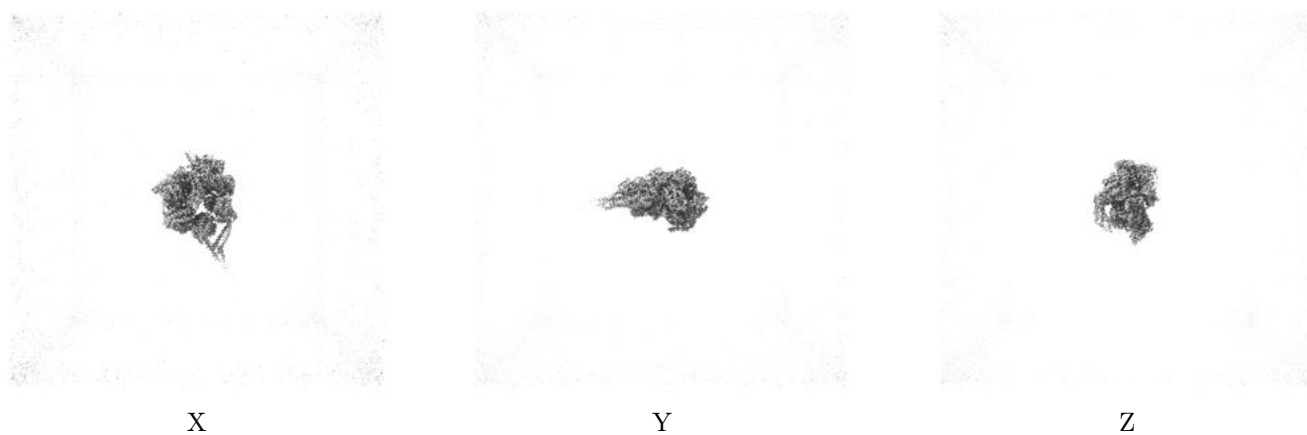
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

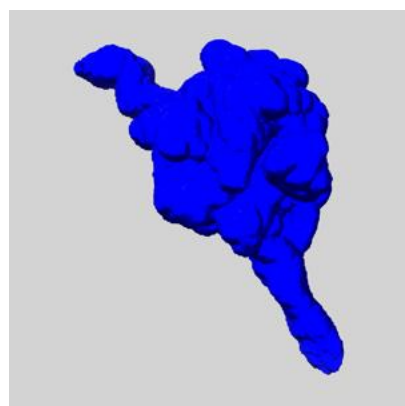
6.6 Mask visualisation [i](#)

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

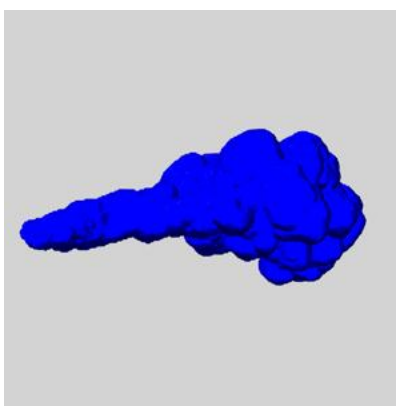
A mask typically either:

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

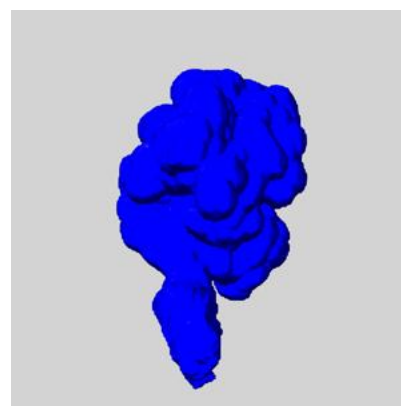
6.6.1 emd_44698_msk_1.map [i](#)



X



Y

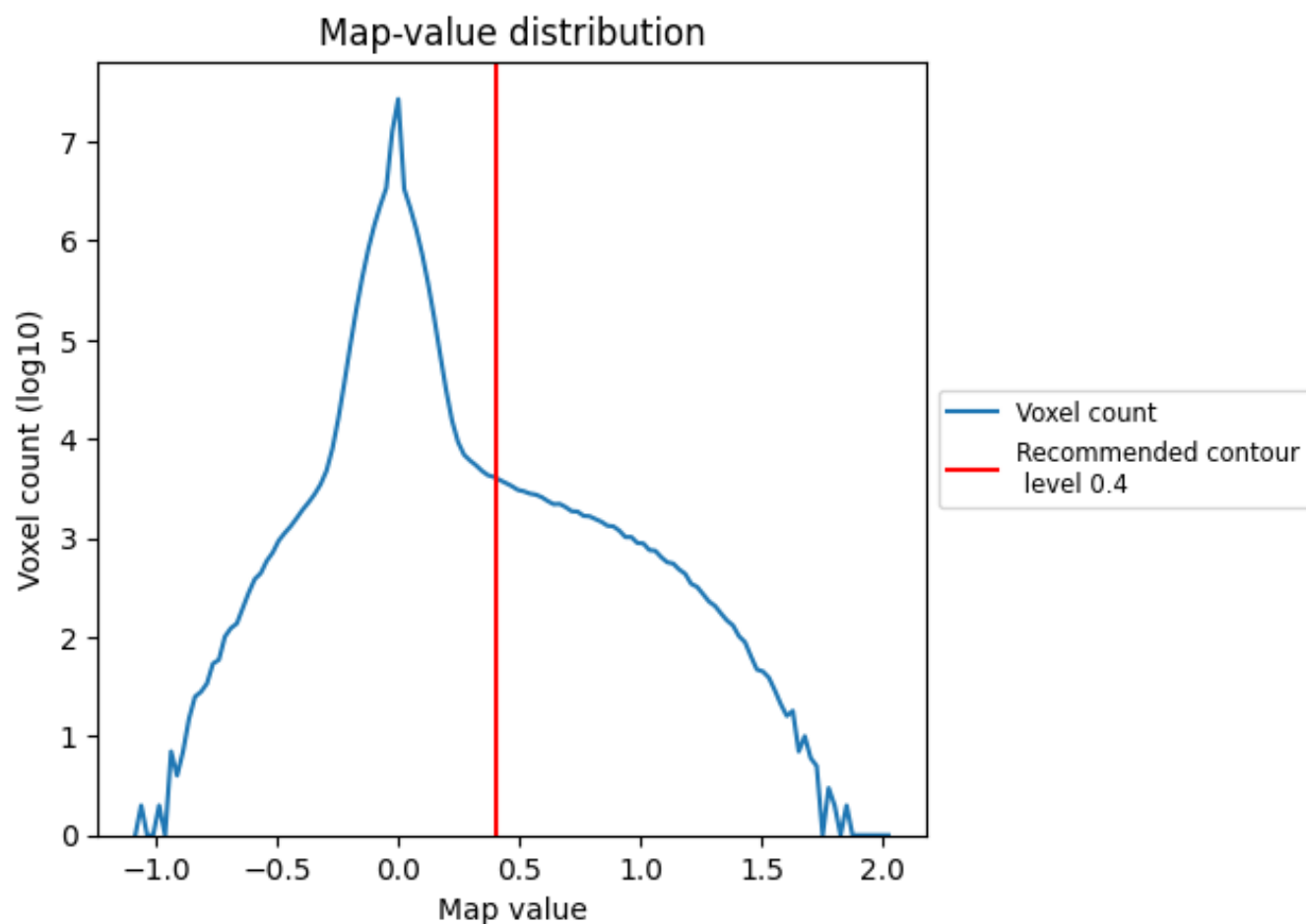


Z

7 Map analysis [i](#)

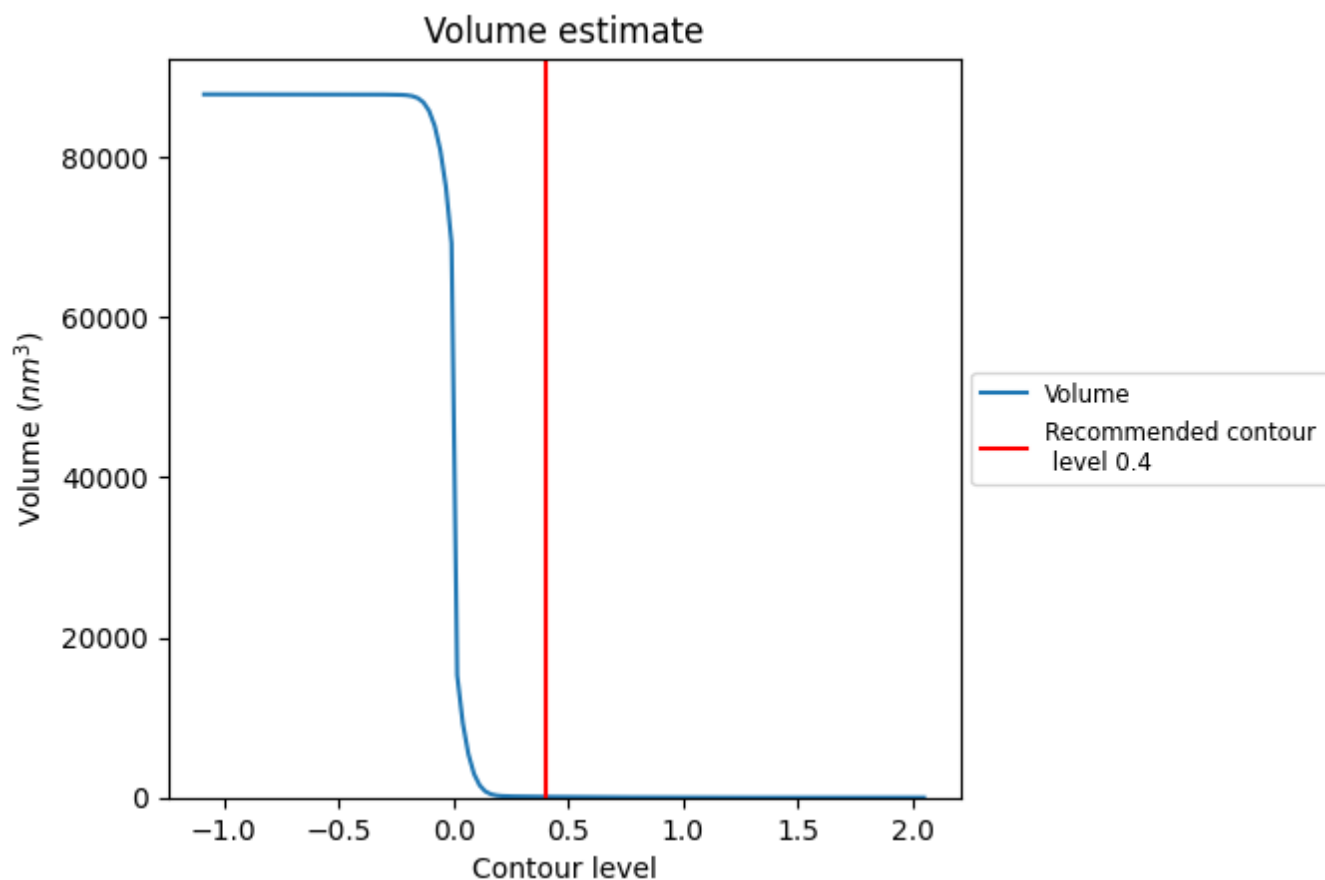
This section contains the results of statistical analysis of the map.

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.

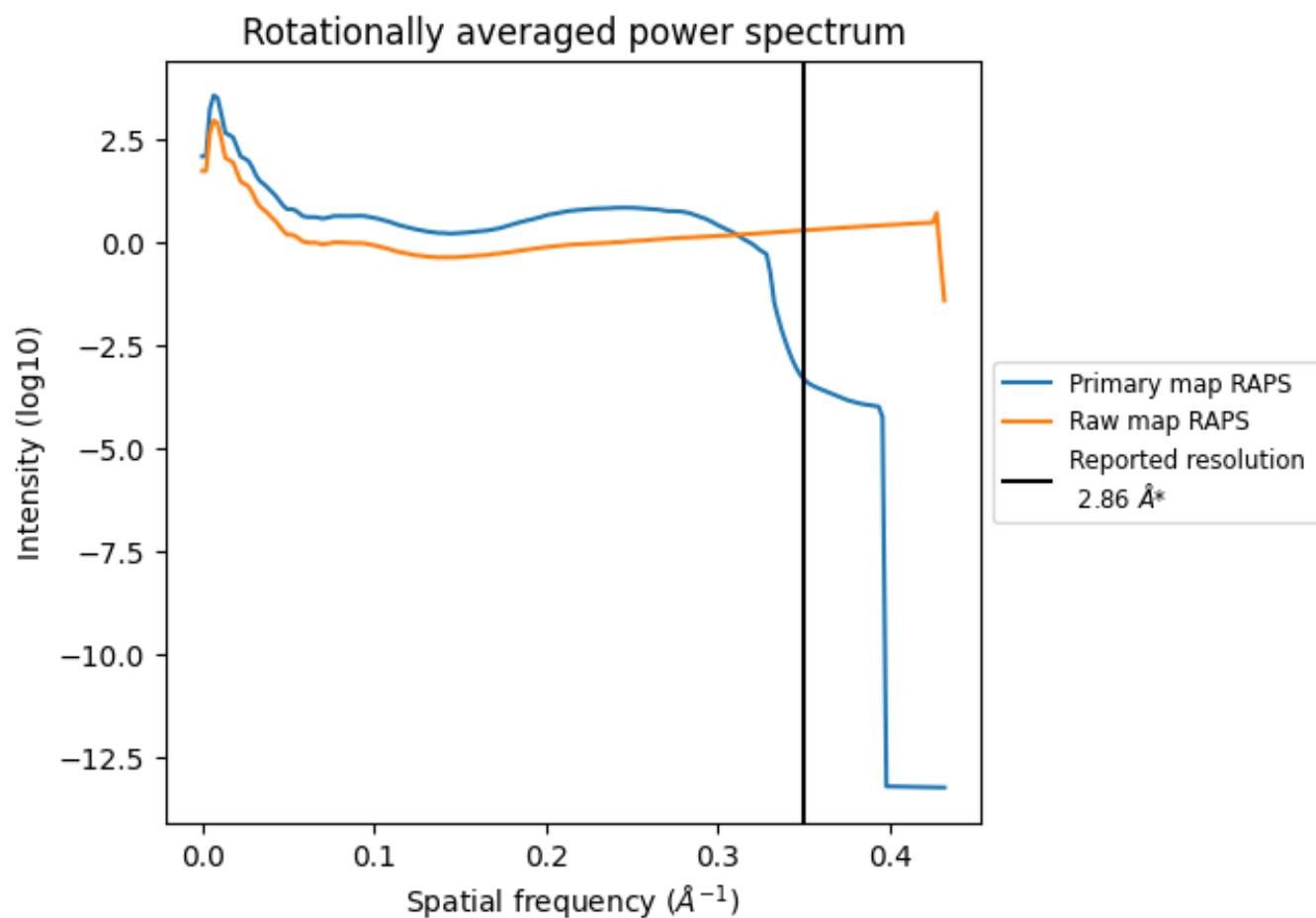
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 95 nm³; this corresponds to an approximate mass of 86 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 ⓘ

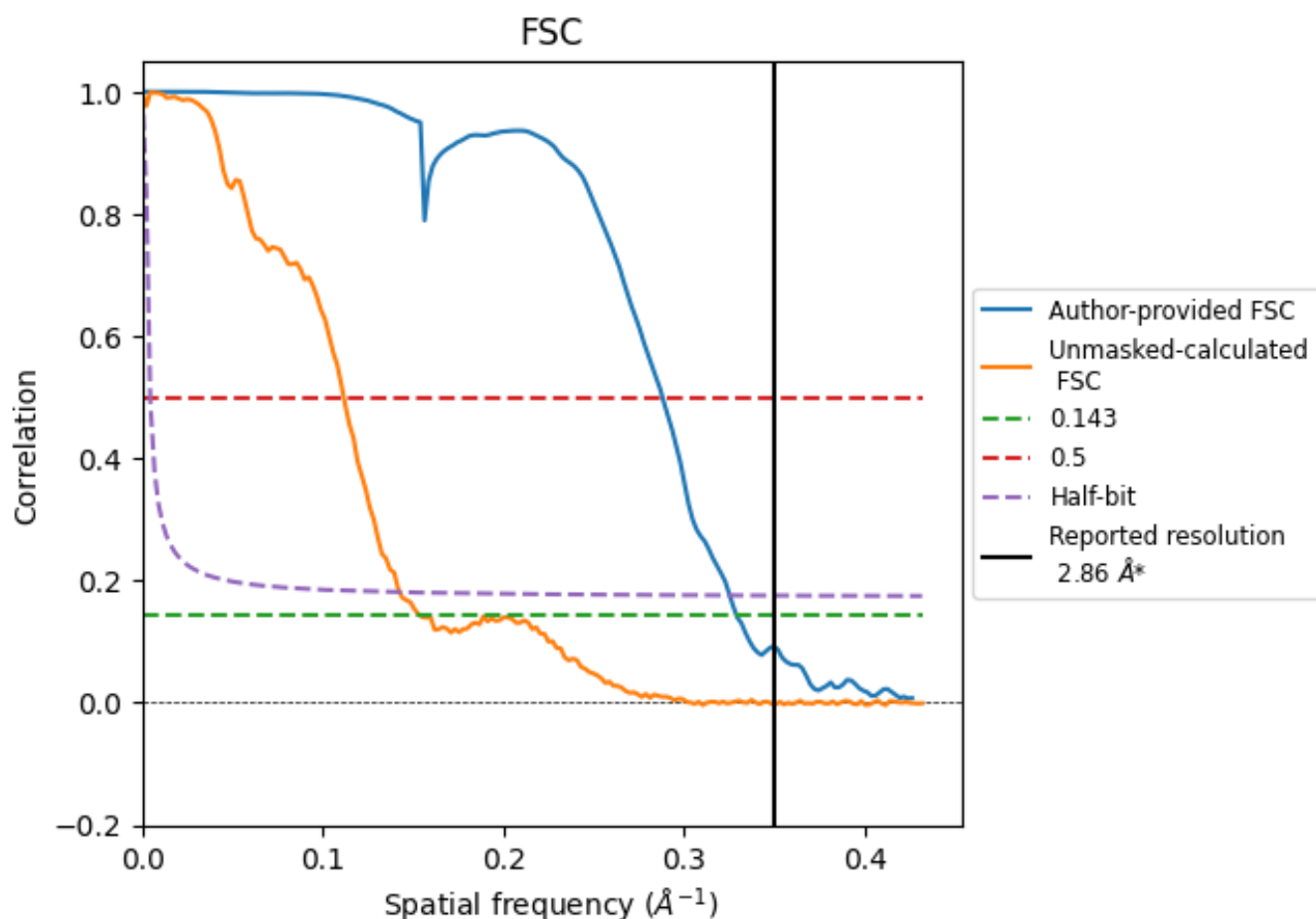


*Reported resolution corresponds to spatial frequency of 0.350 Å⁻¹

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 0.350 Å⁻¹

8.2 Resolution estimates [i](#)

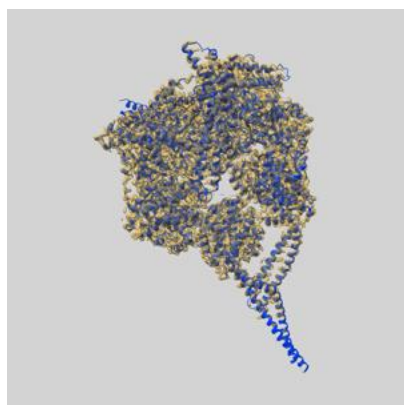
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	3.04	3.47	3.07
Unmasked-calculated*	6.50	8.96	7.01

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.50 differs from the reported value 2.86 by more than 10 %

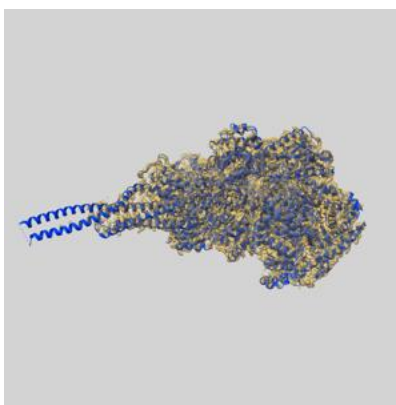
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44698 and PDB model 9BMG. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

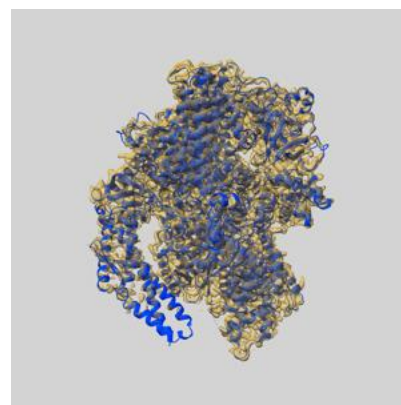
9.1 Map-model overlay [i](#)



X



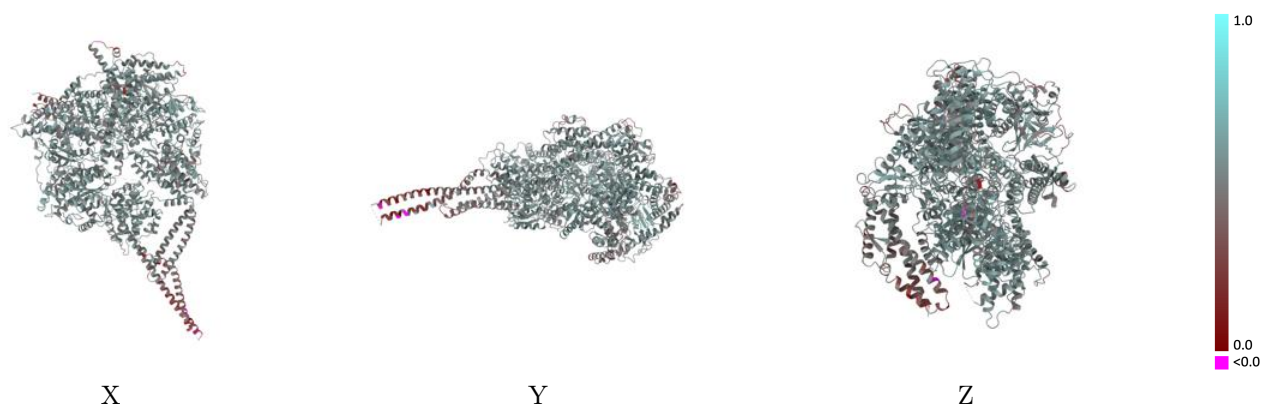
Y



Z

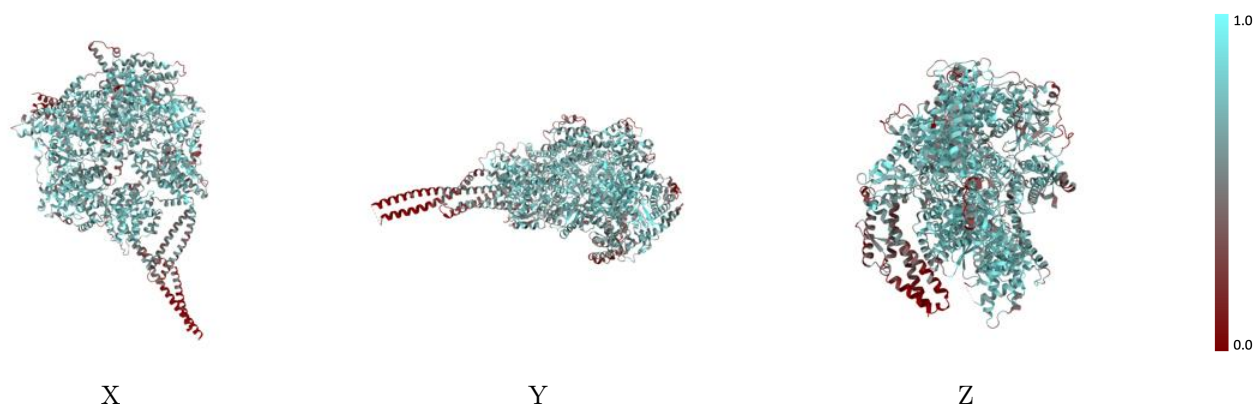
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



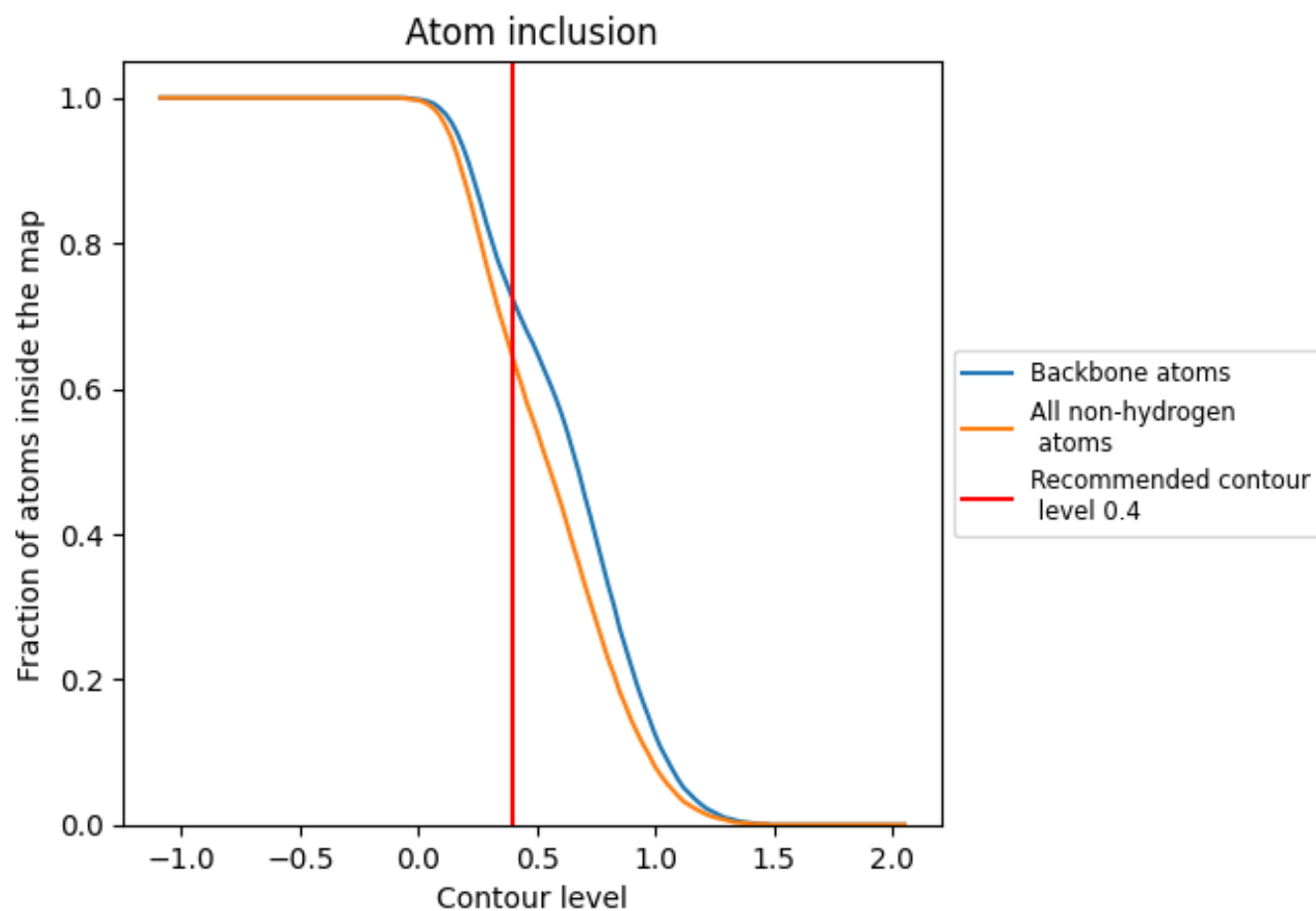
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 64% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6410	0.5270
A	0.6410	0.5270

