



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 07:36 AM UTC

PDB ID : 9BMP / pdb_00009bmp
EMDB ID : EMD-44706
Title : State-7 of the motor domain from full-length human dynein-1 in 5mM AMPPNP
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.50 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

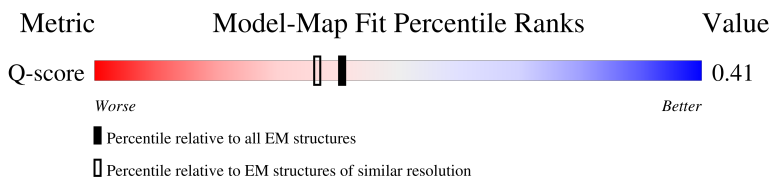
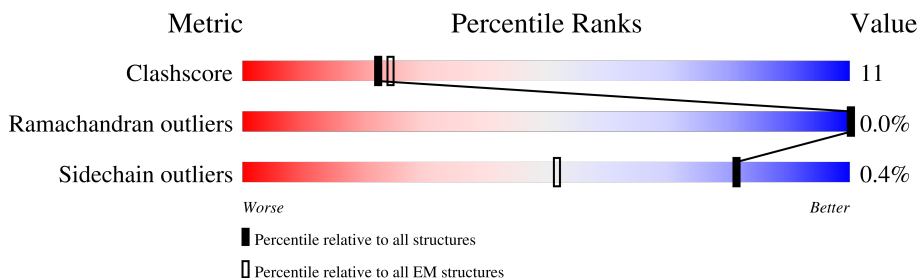
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	A	4646	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 23110 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	2858	22994	14663	3967	4249	115	0	0

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



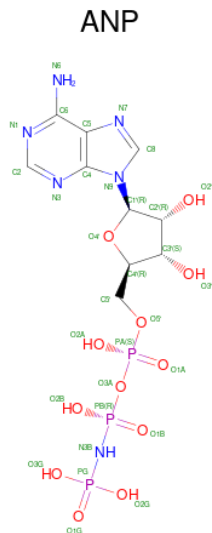
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0
2	A	1	27	10	5	10	2	0

- 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	

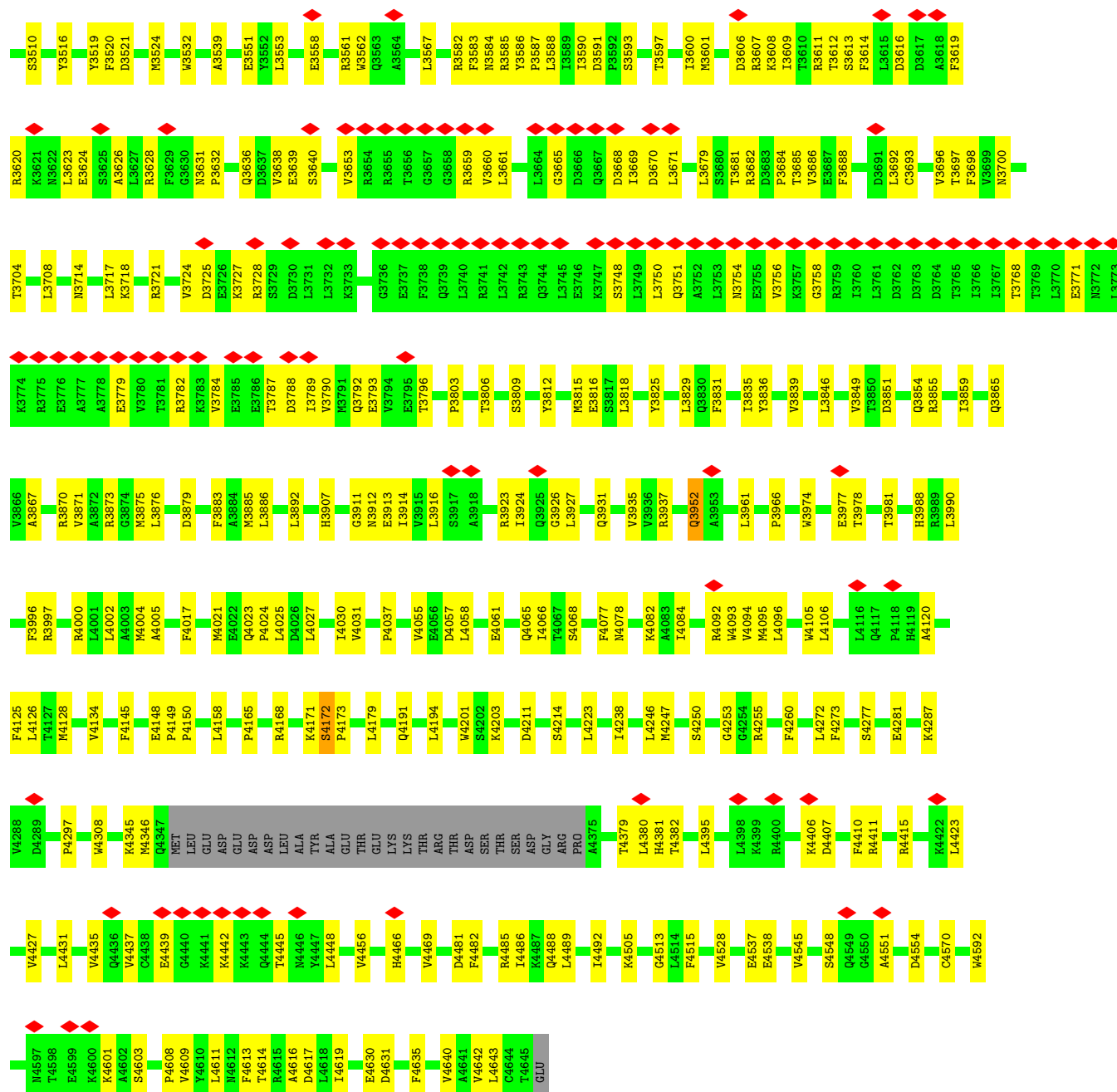
- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



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

Q2139	ALA	E1871	K1687	M1579	S1505	LYS	ASN	ALA	VAL	TRP	ARG	GLU	ALA	ASN	GLU	THR	LEU	ASP	ASN	PHE
Y2146	ARG	Y1872	K1698	K1580	A1506	ASN	TRP	TYR	SER	GLU	PHE	HIS	LEU	LEU	VAL	THR	LEU	ASP	GLN	PHE
L2149	N2027	V1875	W1701	K1582	M1507	ALA	GLU	GLU	GLU	LYS	THR	GLN	VAL	GLN	MET	THR	ILE	ASP	GLN	GLY
G2200	L2028	R1887	L1702	S1583	K1508	VAL	VAL	VAL	VAL	LYS	PRO	ILE	ILE	PRO	ASN	GLN	VAL	ASP	GLY	LYS
G2201	P2029	C1888	L1709	K1584	S1509	LYS	ASP	GLN	ASP	GLN	SER	SER	VAL	TRP	VAL	GLN	VAL	ASP	PRO	VAL
M2202	R2037	Y1889	M1709	S1585	L1510	ASP	P1511	GLN	ASP	GLN	TRP	LYS	VAL	TRP	VAL	GLN	VAL	GLU	ILE	GLY
Q2209	T2042	T1893	L1713	V1588	Y1512	LEU	Y1512	GLY	LEU	LYS	ARG	GLN	VAL	ASN	ASN	GLY	VAL	ILE	LEU	LEU
I2213	L2054	P1907	K1715	D1590	Y1514	VAL	Y1514	TYR	VAL	LYS	ILE	GLU	VAL	ASN	ASN	GLY	VAL	GLY	ILE	ILE
G2219	R2060	K1912	S1720	M1589	V1515	GLN	V1515	MET	SER	TRP	ILE	GLU	VAL	ASN	ASN	GLY	VAL	ARG	PRO	GLU
G2227	T2061	T1913	V1721	I1594	F1516	GLY	F1516	LYS	GLU	GLU	GLY	HIS	GLU	ASN	ASN	GLY	VAL	ILE	GLY	GLY
V2222	P2071	E1914	W1724	Q1595	E1517	MET	E1517	ASN	SER	LEU	TRP	VAL	GLU	TYR	TYR	GLY	VAL	ALA	ILE	ILE
M2223	V2070	K1917	D1734	G1596	D1519	ALA	D1519	LEU	VAL	ALA	GLY	ASP	VAL	TRP	GLY	VAL	VAL	ASP	LEU	LEU
S2226	P2072	Q1939	A1747	A1604	E1524	SER	E1524	GLU	SER	GLN	ARG	ALA	VAL	VAL	GLY	VAL	VAL	VAL	ARG	GLY
G2227	F2073	F1930	T1737	R1599	A1520	ALA	A1520	LEU	VAL	TRP	PHE	ALA	VAL	GLY	VAL	VAL	VAL	ALA	GLY	GLY
S2231	C2076	N1931	Y1738	S1600	L1521	GLU	L1521	GLU	GLU	ILE	LYS	PHE	GLY	ASN	ASN	GLY	TRP	THR	THR	THR
W2234	C2076	C1932	Y1738	L1601	S1522	LEU	S1522	LEU	ILE	ILE	ASP	THR	THR	ASP	ASP	GLY	THR	GLY	THR	THR
E2245	Q2079	D1933	A1747	L1604	W1523	SER	W1523	SER	SER	GLN	GLY	ILE	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
E2248	L2080	Q1939	L1749	A1605	E1524	GLU	E1524	GLU	GLU	MET	ARG	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
D2255	Y2086	F1945	S1753	D1606	I1528	LYS	I1528	LEU	ILE	GLU	ARG	LYS	VAL	GLY	GLY	VAL	VAL	VAL	VAL	VAL
T2259	L2090	V1946	G1772	L1615	M1531	LYS	M1531	LEU	GLN	TRP	ASP	GLN	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY
S2260	L2093	G1947	G1773	L1619	A1532	GLN	A1532	GLU	GLN	TRP	ASP	GLN	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY
K2261	L2097	V1951	D1774	L1623	L1533	LEU	L1533	GLU	GLN	SER	ASP	GLN	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY
Y2265	N2102	L1968	A1775	R1628	I1538	LYS	I1538	LEU	PRO	VAL	LYS	ILE	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
D2277	R2105	H1985	V1778	F1629	Q1541	ARG	Q1541	LEU	ARG	VAL	LYS	ILE	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
G2278	E2106	V1785	G1773	Y1629	R1542	LEU	R1542	LEU	GLN	TRP	ASP	GLN	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY
L2279	R2107	L1789	D1774	Y1630	R1543	GLN	R1543	LEU	GLN	SER	LYS	ILE	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
T2288	R2113	N1989	A1775	L1637	W1544	LYS	W1544	LEU	ASN	VAL	LYS	ILE	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
D2289	E2114	Y1990	L1792	I1640	Y1545	ASN	Y1545	LEU	ASN	TRP	ASP	GLY	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
S2290	LYS	D1991	L1803	I1641	Y1546	TRP	Y1546	ASP	ASN	GLU	GLU	LYS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
V2291	GLU	K1992	K1807	K1645	L1547	VAL	L1547	LEU	VAL	VAL	GLU	LYS	VAL	GLU	GLU	GLU	GLU	GLU	GLU	GLU
R2292	ARG	T1993	L1815	K1649	E1548	SER	E1548	LEU	VAL	VAL	ASP	GLN	VAL	GLU	GLU	GLU	GLU	GLU	GLU	GLU
L2295	GLY	S1994	L1815	L1650	G1549	GLU	G1549	ASN	GLU	ASN	ARG	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
Q2296	ALA	A1995	L1825	L1651	F1551	LEU	F1551	LEU	GLN	GLN	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
K2297	VAL	T1998	I1826	Q1651	T1552	LEU	T1552	LEU	GLN	GLN	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
R2298	ASP	C1999	L1827	K1652	G1553	LEU	G1553	LEU	LYS	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
Q2299	GLY	E2000	K1827	M1657	S1554	GLY	S1554	LEU	GLY	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
V2302	GLY	L2001	Q1850	M1667	A1555	GLY	A1555	LEU	GLY	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
E2310	GLU	Q2005	Q1855	N1667	K1558	GLY	K1558	LEU	ASP	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
N2314	GLY	T2017	Q1860	D1669	L1561	GLY	L1561	LEU	VAL	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	GLY	M2018	K1865	Y1672	E1564	GLY	E1564	LEU	ASP	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
	TYR	N2019	R1679	V1672	T1565	GLY	T1565	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
		PRO	E1680	R1679	Q1566	GLY	Q1566	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
		GLY			R1567	GLY	R1567	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
		TYR			F1568	GLY	F1568	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
					T1571	GLY	T1571	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
					S1572	GLY	S1572	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
					M1573	GLY	M1573	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
					V1574	GLY	V1574	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47831	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	1.499	Depositor
Minimum map value	-0.825	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	333.312, 333.312, 333.312	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.302, 1.302, 1.302	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.14	0/23487	0.35	1/31835 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	2387	LEU	N-CA-C	-5.24	107.18	113.21

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	22994	0	23055	524	0
2	A	54	0	24	2	0
3	A	31	0	12	1	0
4	A	31	0	13	1	0
All	All	23110	0	23104	524	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 (524) 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:3151:HIS:HD1	1:A:3516:TYR:HH	1.16	0.89
1:A:2836:ARG:HG3	1:A:3091:LEU:HB2	1.58	0.84
1:A:1698:ILE:HD12	1:A:1701:TRP:HE1	1.50	0.77
1:A:2762:LEU:HD13	1:A:2821:LEU:HD12	1.67	0.77
1:A:3727:LYS:HE2	1:A:3790:VAL:HG13	1.68	0.76
1:A:4423:LEU:HD12	1:A:4466:HIS:HB2	1.68	0.75
1:A:4128:MET:HE1	1:A:4134:VAL:HG11	1.70	0.74
1:A:2979:VAL:HG13	1:A:2990:ILE:HG21	1.70	0.73
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.70	0.73
1:A:2819:GLU:HG3	1:A:2865:LYS:HD2	1.69	0.73
1:A:3883:PHE:HA	1:A:3886:LEU:HD12	1.70	0.73
1:A:3638:VAL:HG12	1:A:3679:LEU:HD22	1.71	0.72
1:A:2519:ARG:HH21	1:A:2534:ILE:HD11	1.57	0.70
1:A:3885:MET:HE1	1:A:4005:ALA:HB1	1.71	0.70
1:A:1933:ASP:HA	1:A:1962:ARG:HH22	1.57	0.70
1:A:1709:MET:HE3	1:A:1872:TYR:H	1.57	0.69
1:A:2922:ILE:HD13	1:A:2933:LEU:HD21	1.75	0.69
1:A:3043:MET:N	1:A:3043:MET:SD	2.65	0.69
1:A:2919:VAL:HG23	1:A:2950:VAL:HG22	1.74	0.68
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.58	0.68
1:A:2847:ASP:HA	1:A:2850:ILE:HD12	1.76	0.68
1:A:4084:ILE:HG22	1:A:4094:VAL:HG21	1.76	0.67
1:A:3626:ALA:HA	1:A:3631:ASN:HB2	1.76	0.67
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.77	0.66
1:A:1548:GLU:O	1:A:1552:THR:OG1	2.11	0.66
1:A:4065:GLN:HE21	1:A:4092:ARG:HD3	1.61	0.66
1:A:2227:GLY:HA2	1:A:2452:LEU:HD12	1.77	0.65
1:A:2828:GLU:OE1	1:A:2924:ARG:NH2	2.28	0.65
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.79	0.65
1:A:3990:LEU:HD12	1:A:4004:MET:HG3	1.78	0.65
1:A:1561:LEU:O	1:A:1565:THR:OG1	2.14	0.65
1:A:4066:ILE:HG13	1:A:4093:TRP:HB2	1.78	0.65
1:A:2915:VAL:HG23	1:A:2946:LEU:HD11	1.79	0.63
1:A:3521:ASP:HB2	1:A:3704:THR:HG21	1.80	0.63
1:A:2925:ILE:HB	1:A:2933:LEU:HD22	1.81	0.63
1:A:3154:LEU:HB3	1:A:3171:ILE:HD13	1.80	0.63
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.81	0.63
1:A:2845:TRP:O	1:A:2849:ASN:ND2	2.30	0.63
1:A:3873:ARG:HD3	1:A:4021:MET:HE1	1.80	0.62
1:A:2643:ARG:O	1:A:2643:ARG:NH1	2.32	0.62
1:A:3167:ARG:NH2	1:A:3684:PRO:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3181:ASN:OD1	1:A:3584:ASN:ND2	2.32	0.61
1:A:2320:ASP:HB3	1:A:2358:ARG:HD3	1.83	0.61
1:A:2665:GLU:OE1	1:A:2720:ARG:NH1	2.30	0.61
1:A:1606:ASP:OD1	1:A:1607:LEU:N	2.34	0.61
1:A:3128:VAL:HG21	1:A:3149:PHE:HB2	1.82	0.61
1:A:2801:ARG:NH2	1:A:3087:ASN:O	2.32	0.61
1:A:3609:ILE:HA	1:A:3632:PRO:HG2	1.83	0.61
1:A:3727:LYS:NZ	1:A:3793:GLU:OE1	2.33	0.61
1:A:3923:ARG:HH11	1:A:3952:GLN:HG3	1.65	0.61
1:A:3005:LEU:HD11	1:A:3085:LEU:HD22	1.83	0.60
1:A:3653:VAL:HG13	1:A:3660:VAL:HG23	1.83	0.60
1:A:1477:LEU:HB3	1:A:1485:ARG:HB3	1.82	0.60
1:A:2512:ALA:O	1:A:2516:GLU:HG3	2.01	0.60
1:A:2950:VAL:HA	1:A:2953:MET:HG3	1.84	0.60
1:A:2102:ASN:OD1	1:A:2105:ARG:NH2	2.33	0.60
1:A:2248:GLU:HB2	1:A:2297:LYS:HG2	1.84	0.60
1:A:2487:GLU:O	1:A:2491:GLN:HG3	2.01	0.60
1:A:2836:ARG:HE	1:A:3091:LEU:HD23	1.67	0.60
1:A:2965:ARG:HH22	1:A:3614:PHE:HB3	1.67	0.60
1:A:2259:ILE:HD13	1:A:2279:LEU:HD12	1.81	0.59
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.82	0.59
1:A:3607:ARG:HG2	1:A:3632:PRO:HD3	1.85	0.59
1:A:1568:PHE:HA	1:A:1571:ILE:HG22	1.84	0.59
1:A:2813:LEU:HD21	1:A:2816:LEU:HB2	1.84	0.59
1:A:3067:THR:O	1:A:3068:MET:HE2	2.03	0.59
1:A:3779:GLU:OE2	1:A:3782:ARG:NH1	2.35	0.59
1:A:2302:VAL:HG12	1:A:2342:MET:HB2	1.83	0.59
1:A:2498:ILE:HG23	1:A:2502:LEU:HD13	1.84	0.59
1:A:3134:PRO:HG2	1:A:3137:PRO:HA	1.85	0.59
1:A:2419:ALA:O	1:A:2423:MET:HG3	2.03	0.59
1:A:4437:VAL:HG21	1:A:4448:LEU:HD21	1.84	0.59
1:A:2660:VAL:HG22	1:A:2707:GLN:HB2	1.83	0.59
1:A:3000:LEU:H	1:A:3004:PHE:HD1	1.51	0.59
1:A:3924:ILE:HG23	1:A:3926:GLY:H	1.68	0.59
1:A:2965:ARG:NH2	1:A:3640:SER:O	2.36	0.58
1:A:2921:ARG:HD3	1:A:3092:ASN:HD21	1.68	0.58
1:A:1889:TYR:O	1:A:1893:THR:HG23	2.03	0.58
1:A:3600:ILE:HG23	1:A:3601:MET:HE3	1.84	0.58
1:A:3913:GLU:OE2	1:A:3913:GLU:N	2.37	0.58
1:A:3037:ALA:HB1	1:A:3042:LEU:HB2	1.85	0.58
1:A:3907:HIS:HA	1:A:3911:GLY:HA3	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2851:ASP:OD1	1:A:2852:THR:N	2.38	0.57
1:A:3013:ALA:HB2	1:A:3088:ARG:HH11	1.70	0.57
1:A:3029:LEU:HD22	1:A:3032:GLN:HE21	1.70	0.57
1:A:1483:LYS:NZ	1:A:1548:GLU:OE2	2.38	0.57
1:A:2054:LEU:HG	1:A:2097:LEU:HD13	1.87	0.57
1:A:2623:SER:N	1:A:2626:THR:OG1	2.38	0.56
1:A:1720:SER:O	1:A:1724:VAL:HG12	2.05	0.56
1:A:2670:ASP:HA	1:A:2721:LYS:HE3	1.86	0.56
1:A:2992:PHE:HD2	1:A:3064:VAL:HG12	1.69	0.56
1:A:1558:LYS:HD2	1:A:1565:THR:HG21	1.88	0.56
1:A:3608:LYS:HD2	1:A:3631:ASN:HD21	1.70	0.56
1:A:3768:THR:O	1:A:3771:GLU:HG3	2.04	0.56
1:A:2354:ALA:HB1	1:A:2358:ARG:HH21	1.70	0.56
1:A:2290:SER:HB3	1:A:2295:LEU:HD13	1.88	0.56
1:A:2481:MET:HG3	1:A:2486:LEU:HB2	1.88	0.56
1:A:2759:ILE:HD12	1:A:2762:LEU:HD12	1.87	0.56
1:A:2299:GLN:HB2	1:A:2339:VAL:HG22	1.87	0.56
1:A:2346:GLN:HB2	1:A:2726:ARG:HD2	1.87	0.56
1:A:4172:SER:HB3	1:A:4173:PRO:HD2	1.87	0.55
1:A:2880:ASP:OD1	1:A:2880:ASP:N	2.38	0.55
1:A:4407:ASP:OD2	1:A:4410:PHE:N	2.36	0.55
1:A:3815:MET:O	1:A:3818:LEU:HB2	2.07	0.55
1:A:1486:LEU:HD13	1:A:1541:GLN:HE22	1.72	0.55
1:A:2517:TYR:CE2	1:A:2521:ILE:HD11	2.41	0.55
1:A:2961:ILE:HD11	1:A:2967:TYR:HE2	1.71	0.55
1:A:2852:THR:O	1:A:2856:LYS:HG2	2.07	0.55
1:A:1724:VAL:HG11	1:A:1753:SER:HB3	1.89	0.55
1:A:2231:SER:OG	3:A:4702:ATP:O1B	2.19	0.55
1:A:2932:HIS:NE2	1:A:3066:PHE:HB3	2.22	0.55
1:A:4096:LEU:HB2	1:A:4126:LEU:HD23	1.88	0.54
1:A:1470:TRP:HB2	1:A:1523:TRP:HH2	1.72	0.54
1:A:3558:GLU:HA	1:A:3561:ARG:NH1	2.22	0.54
1:A:3977:GLU:HG3	1:A:3978:THR:HG23	1.89	0.54
1:A:3784:VAL:HA	1:A:3787:THR:HG23	1.88	0.54
1:A:4411:ARG:O	1:A:4415:ARG:HG3	2.07	0.54
1:A:3871:VAL:HG12	1:A:3875:MET:HE2	1.88	0.54
1:A:1470:TRP:CE3	1:A:1588:VAL:HG11	2.42	0.54
1:A:1887:ARG:NH2	1:A:4253:GLY:O	2.41	0.54
1:A:1667:ASN:ND2	1:A:1669:ASP:OD1	2.32	0.54
1:A:2791:HIS:HD2	1:A:2836:ARG:HG2	1.73	0.54
1:A:3158:ASN:ND2	1:A:3169:MET:O	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3836:TYR:HA	1:A:3839:VAL:HG12	1.89	0.54
1:A:4201:TRP:O	1:A:4203:LYS:N	2.41	0.54
1:A:1985:HIS:O	1:A:1985:HIS:ND1	2.38	0.54
1:A:2134:GLN:O	1:A:2138:ILE:HG22	2.08	0.54
1:A:4380:LEU:HD21	1:A:4456:VAL:HG12	1.90	0.54
1:A:4281:GLU:OE2	1:A:4281:GLU:N	2.41	0.54
1:A:2356:VAL:HG13	1:A:2361:MET:HE1	1.89	0.53
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.90	0.53
1:A:2605:LEU:HD11	1:A:2709:VAL:HG11	1.90	0.53
1:A:2993:ILE:HG12	1:A:3065:VAL:CG2	2.39	0.53
1:A:3931:GLN:O	1:A:3935:VAL:HG23	2.09	0.53
1:A:1667:ASN:HB2	1:A:1672:VAL:HG22	1.91	0.53
1:A:2327:LEU:HD11	1:A:2333:LEU:HD23	1.91	0.53
1:A:1479:ASN:HD21	1:A:1482:ASN:HA	1.74	0.53
1:A:4272:LEU:O	1:A:4277:SER:OG	2.27	0.53
1:A:2897:LEU:HD13	1:A:2901:TYR:HE1	1.74	0.53
1:A:2079:GLN:OE1	1:A:4411:ARG:NH2	2.39	0.52
1:A:2209:GLN:O	1:A:2213:ILE:HG12	2.09	0.52
1:A:3924:ILE:HG22	1:A:3927:LEU:HD23	1.90	0.52
1:A:1504:VAL:HG11	1:A:1524:GLU:HB2	1.91	0.52
1:A:2073:PHE:HE2	1:A:2093:LEU:HA	1.75	0.52
1:A:2841:GLU:OE2	1:A:2844:ARG:NH1	2.40	0.52
1:A:4023:GLN:HG2	1:A:4024:PRO:HD2	1.91	0.52
1:A:2279:LEU:HD11	1:A:2693:TYR:HB3	1.90	0.52
1:A:3597:THR:O	1:A:3601:MET:HG2	2.09	0.52
1:A:1803:LEU:HD11	1:A:1875:VAL:HG21	1.92	0.52
1:A:2605:LEU:HD21	1:A:2709:VAL:HG12	1.91	0.52
1:A:3835:ILE:HD13	1:A:3867:ALA:HA	1.90	0.52
1:A:3037:ALA:O	1:A:3042:LEU:N	2.41	0.52
1:A:1513:TYR:CZ	1:A:1517:GLU:HG2	2.45	0.52
1:A:1601:LEU:HA	1:A:1604:LEU:HD12	1.91	0.52
1:A:1486:LEU:HD23	1:A:1579:MET:HE3	1.91	0.51
1:A:3012:LEU:HD13	1:A:3088:ARG:HB3	1.92	0.51
1:A:3055:THR:O	1:A:3059:ILE:HG23	2.10	0.51
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.31	0.51
1:A:2619:GLY:HA2	1:A:2662:PHE:HB3	1.92	0.51
1:A:3167:ARG:NH2	1:A:3685:THR:HA	2.26	0.51
1:A:3865:GLN:HA	1:A:4017:PHE:HE2	1.76	0.51
1:A:4057:ASP:OD2	1:A:4058:LEU:N	2.42	0.51
1:A:2245:GLU:OE1	1:A:2298:ARG:NH2	2.34	0.51
1:A:2592:VAL:HB	1:A:2733:VAL:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3133:LEU:HB3	1:A:3134:PRO:HD3	1.91	0.51
1:A:4021:MET:HE3	1:A:4021:MET:HA	1.91	0.51
1:A:4128:MET:CE	1:A:4134:VAL:HG11	2.40	0.51
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.91	0.51
1:A:4601:LYS:HE2	1:A:4603:SER:HB3	1.91	0.51
1:A:2202:MET:SD	1:A:2202:MET:N	2.84	0.51
1:A:3154:LEU:HG	1:A:3516:TYR:CD1	2.45	0.51
1:A:3606:ASP:OD2	1:A:3607:ARG:N	2.44	0.51
1:A:2925:ILE:HG13	1:A:2933:LEU:HD13	1.92	0.50
1:A:3031:THR:O	1:A:3034:LYS:HG2	2.11	0.50
1:A:3611:ARG:NH2	1:A:3636:GLN:OE1	2.44	0.50
1:A:1931:ASN:ND2	1:A:1933:ASP:OD2	2.43	0.50
1:A:1968:LEU:HD21	1:A:2029:PRO:HG3	1.93	0.50
1:A:3590:ILE:HA	1:A:3681:THR:HG22	1.93	0.50
1:A:4084:ILE:HA	1:A:4094:VAL:HG11	1.92	0.50
1:A:2113:ARG:HG2	1:A:2113:ARG:O	2.11	0.50
1:A:2830:LEU:HD22	1:A:2850:ILE:HD13	1.93	0.50
1:A:3612:THR:OG1	1:A:3613:SER:N	2.44	0.50
1:A:4171:LYS:NZ	1:A:4172:SER:OG	2.42	0.50
1:A:1547:LEU:HD13	1:A:1550:ILE:HD11	1.93	0.50
1:A:3659:ARG:NH1	1:A:3661:LEU:HD21	2.26	0.50
1:A:2933:LEU:HB3	1:A:3065:VAL:HG12	1.93	0.50
1:A:1999:CYS:SG	1:A:2001:LEU:HD13	2.52	0.50
1:A:2446:ILE:HG22	1:A:2505:ASP:O	2.12	0.50
1:A:2972:PHE:CD1	1:A:3004:PHE:HD2	2.30	0.50
1:A:3015:GLY:HA3	1:A:3059:ILE:HG22	1.94	0.50
1:A:3186:LEU:HD23	1:A:3190:LYS:HG2	1.94	0.50
1:A:1628:ARG:NH1	1:A:1871:GLU:OE2	2.45	0.49
1:A:3519:TYR:HA	1:A:3700:ASN:HB2	1.94	0.49
1:A:3661:LEU:HD12	1:A:3668:ASP:OD1	2.12	0.49
1:A:3624:GLU:O	1:A:3628:ARG:HG2	2.11	0.49
1:A:2060:ARG:HG3	1:A:2061:THR:HG23	1.92	0.49
1:A:4635:PHE:HD2	1:A:4640:VAL:HG11	1.76	0.49
1:A:1640:ILE:HG23	1:A:1650:LEU:HD21	1.93	0.49
1:A:2960:GLN:HB3	1:A:2962:LYS:HE3	1.93	0.49
1:A:2961:ILE:HD11	1:A:2967:TYR:CE2	2.47	0.49
1:A:1564:GLU:HG3	1:A:1567:ARG:HH21	1.76	0.49
1:A:1619:LEU:HD22	1:A:1637:LEU:HD23	1.94	0.49
1:A:1734:ASP:HB3	1:A:1737:THR:HG22	1.94	0.49
1:A:2497:ALA:O	1:A:2501:SER:HB2	2.12	0.49
1:A:3126:MET:HE2	1:A:3126:MET:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2656:GLY:H	1:A:2705:ARG:HH11	1.60	0.49
1:A:2603:MET:HE2	4:A:4703:ANP:C5	2.43	0.49
1:A:4246:LEU:O	1:A:4250:SER:OG	2.27	0.49
1:A:3178:ASP:OD2	1:A:3182:HIS:HD2	1.95	0.49
1:A:3113:MET:HE1	1:A:3183:TYR:CE2	2.47	0.49
1:A:2593:LEU:HD11	1:A:2605:LEU:HD13	1.94	0.48
1:A:3607:ARG:HG2	1:A:3607:ARG:O	2.13	0.48
1:A:3974:TRP:CG	1:A:3988:HIS:HD1	2.31	0.48
1:A:4002:LEU:O	1:A:4005:ALA:HB3	2.13	0.48
1:A:2037:ARG:NH2	1:A:4214:SER:OG	2.46	0.48
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	1.95	0.48
1:A:2960:GLN:OE1	1:A:2993:ILE:HB	2.13	0.48
1:A:3748:SER:O	1:A:3751:GLN:HG2	2.13	0.48
1:A:1850:GLN:HG2	1:A:1855:GLN:HB2	1.95	0.48
1:A:2776:PHE:HA	1:A:2779:MET:HE1	1.96	0.48
1:A:2870:PRO:O	1:A:2872:LEU:HD13	2.13	0.48
1:A:2875:ASN:OD1	1:A:2927:ARG:NH2	2.47	0.48
1:A:3109:PHE:HB3	1:A:3180:ILE:HG21	1.95	0.48
1:A:3551:GLU:OE1	1:A:3551:GLU:N	2.42	0.48
1:A:2387:LEU:O	1:A:2467:ARG:NH2	2.47	0.48
1:A:1486:LEU:HD22	1:A:1541:GLN:CD	2.39	0.48
1:A:2677:GLN:HB2	1:A:2680:ILE:HB	1.96	0.48
1:A:3167:ARG:HG3	1:A:3519:TYR:OH	2.14	0.48
1:A:3688:PHE:HB2	1:A:3693:CYS:SG	2.53	0.48
1:A:4548:SER:HB3	1:A:4551:ALA:HB2	1.96	0.48
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.47	0.48
1:A:2783:ARG:HG2	1:A:2784:PHE:N	2.29	0.48
1:A:2935:LEU:HD13	1:A:2943:LYS:HB3	1.95	0.48
1:A:3141:GLU:CD	1:A:3141:GLU:H	2.21	0.48
1:A:2516:GLU:O	1:A:2520:ARG:HG3	2.13	0.48
1:A:4395:LEU:HD23	1:A:4486:ILE:HG23	1.96	0.47
1:A:1645:LYS:HA	1:A:1645:LYS:HD3	1.69	0.47
1:A:1713:LEU:HD13	1:A:1749:LEU:HD21	1.96	0.47
1:A:2789:GLN:NE2	1:A:2838:VAL:HG21	2.29	0.47
1:A:2963:VAL:HG21	1:A:2998:ASN:HA	1.96	0.47
1:A:3558:GLU:HA	1:A:3561:ARG:HH12	1.78	0.47
1:A:2223:VAL:HG21	1:A:2348:LEU:HD12	1.95	0.47
1:A:3062:LEU:HD21	1:A:3064:VAL:HG13	1.96	0.47
1:A:3591:ASP:N	1:A:3591:ASP:OD1	2.47	0.47
1:A:4078:ASN:O	1:A:4082:LYS:HG2	2.14	0.47
1:A:1600:SER:O	1:A:1604:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1947:GLY:O	1:A:1951:VAL:HG12	2.15	0.47
1:A:2386:PRO:HG3	1:A:2413:LEU:HD13	1.95	0.47
1:A:2631:LEU:HD11	1:A:2683:ILE:HD11	1.97	0.47
1:A:3010:THR:HG23	1:A:3017:VAL:HG22	1.95	0.47
1:A:3714:ASN:OD1	1:A:3728:ARG:NH2	2.47	0.47
1:A:2797:ARG:O	1:A:2801:ARG:HG3	2.14	0.47
1:A:2892:TYR:O	1:A:2896:ARG:HG2	2.15	0.47
1:A:2915:VAL:O	1:A:2919:VAL:HG12	2.14	0.47
1:A:3208:ILE:HG22	1:A:3486:ARG:HH22	1.78	0.47
1:A:4381:HIS:CE1	1:A:4435:VAL:HG13	2.49	0.47
1:A:3066:PHE:CZ	1:A:3068:MET:HE3	2.49	0.47
1:A:4037:PRO:HG3	1:A:4120:ALA:HA	1.96	0.47
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	1.95	0.47
1:A:4058:LEU:O	1:A:4061:GLU:HG3	2.15	0.47
1:A:4211:ASP:OD1	1:A:4255:ARG:NH1	2.48	0.47
1:A:2219:GLY:HA2	1:A:2341:ILE:HG23	1.97	0.47
1:A:1615:LEU:O	1:A:1619:LEU:HG	2.15	0.46
1:A:2925:ILE:HG21	1:A:2933:LEU:HB2	1.97	0.46
1:A:3660:VAL:HG22	1:A:3671:LEU:HB3	1.97	0.46
1:A:3825:TYR:OH	1:A:3876:LEU:HB2	2.16	0.46
1:A:2938:VAL:HG23	1:A:2941:ALA:HB2	1.96	0.46
1:A:3751:GLN:HA	1:A:3754:ASN:HD21	1.80	0.46
1:A:1546:TYR:O	1:A:1550:ILE:HG12	2.14	0.46
1:A:2461:MET:HG2	1:A:2583:THR:CG2	2.42	0.46
1:A:3034:LYS:O	1:A:3038:GLN:HG2	2.15	0.46
1:A:3849:VAL:HG12	1:A:3855:ARG:HG2	1.97	0.46
1:A:1649:LYS:HA	1:A:1652:LYS:HE2	1.97	0.46
1:A:2966:LYS:HG2	1:A:3620:ARG:HH21	1.79	0.46
1:A:3558:GLU:H	1:A:3558:GLU:CD	2.22	0.46
1:A:1998:THR:HB	1:A:2005:GLN:HG2	1.98	0.46
1:A:3167:ARG:NH1	1:A:3519:TYR:OH	2.49	0.46
1:A:1917:LYS:HD2	1:A:1929:VAL:HG21	1.97	0.46
1:A:2648:VAL:HB	1:A:2701:VAL:HG12	1.98	0.46
1:A:2932:HIS:CD2	1:A:2933:LEU:N	2.83	0.46
1:A:3616:ASP:OD1	1:A:3619:PHE:N	2.48	0.46
1:A:4609:VAL:HG13	1:A:4642:VAL:HG12	1.96	0.46
1:A:1785:VAL:HG13	1:A:1815:LEU:HD12	1.97	0.46
1:A:2086:TYR:CE2	1:A:2149:LEU:HD23	2.51	0.46
1:A:2255:ASP:OD1	1:A:2685:GLN:HB2	2.15	0.46
1:A:2386:PRO:C	1:A:2388:ASP:H	2.24	0.46
1:A:1544:TRP:HE1	1:A:1572:SER:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1623:ARG:HB3	1:A:1630:TYR:CZ	2.51	0.46
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.97	0.46
1:A:3825:TYR:OH	1:A:3879:ASP:OD2	2.30	0.46
1:A:2743:SER:O	1:A:2747:ILE:HG22	2.16	0.46
1:A:2728:LEU:HD23	1:A:2728:LEU:HA	1.82	0.46
1:A:2862:ASP:OD1	1:A:2862:ASP:N	2.47	0.46
1:A:2987:ASN:OD1	1:A:3057:GLN:NE2	2.48	0.46
1:A:3123:PRO:HG3	1:A:3539:ALA:C	2.41	0.46
1:A:4537:GLU:HG2	1:A:4538:GLU:HG3	1.97	0.46
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.51	0.45
1:A:3914:ILE:O	1:A:3937:ARG:NE	2.50	0.45
1:A:4191:GLN:O	1:A:4194:LEU:HB2	2.15	0.45
1:A:1778:LEU:HB3	1:A:1827:LYS:NZ	2.31	0.45
1:A:2279:LEU:HD11	1:A:2693:TYR:CB	2.46	0.45
1:A:2834:GLN:NE2	1:A:2843:ARG:HD3	2.31	0.45
1:A:4489:LEU:HD11	1:A:4515:PHE:HE2	1.82	0.45
1:A:1508:LYS:HA	1:A:1513:TYR:CD1	2.52	0.45
1:A:1702:LEU:HD23	1:A:1702:LEU:HA	1.81	0.45
1:A:2102:ASN:O	1:A:2106:GLU:HG2	2.16	0.45
1:A:2261:LYS:HZ2	1:A:2310:GLU:C	2.23	0.45
1:A:2748:TYR:CZ	1:A:2799:MET:HB2	2.51	0.45
1:A:3194:LEU:HD22	1:A:3500:MET:SD	2.56	0.45
1:A:4106:LEU:HD23	1:A:4106:LEU:HA	1.84	0.45
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.99	0.45
1:A:3028:THR:O	1:A:3032:GLN:HG2	2.17	0.45
1:A:4423:LEU:CD1	1:A:4466:HIS:HB2	2.43	0.45
1:A:4437:VAL:HG21	1:A:4448:LEU:CD2	2.47	0.45
1:A:2452:LEU:HD23	1:A:2452:LEU:HA	1.83	0.45
1:A:3103:TYR:HB2	1:A:3129:VAL:HG21	1.99	0.45
1:A:4287:LYS:HG2	1:A:4287:LYS:O	2.16	0.45
1:A:2936:ILE:HD12	1:A:3068:MET:HB2	1.97	0.45
1:A:3141:GLU:HA	1:A:3144:VAL:HG22	1.99	0.45
1:A:4381:HIS:NE2	1:A:4439:GLU:OE2	2.50	0.45
1:A:2439:HIS:O	1:A:2442:GLN:HG2	2.16	0.45
1:A:2369:LEU:O	1:A:2451:ARG:NH1	2.47	0.45
1:A:2671:MET:HG3	1:A:2721:LYS:HG2	1.99	0.45
1:A:2894:LYS:HA	1:A:2897:LEU:HG	1.99	0.45
1:A:3519:TYR:HB2	1:A:3698:PHE:HB3	1.98	0.45
1:A:1912:LYS:HD2	1:A:2017:THR:HG23	1.99	0.45
1:A:2861:ILE:HD12	1:A:2865:LYS:HZ3	1.82	0.45
1:A:3029:LEU:HD22	1:A:3032:GLN:NE2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3169:MET:SD	1:A:3169:MET:N	2.90	0.45
1:A:3923:ARG:HA	1:A:3923:ARG:NE	2.30	0.45
1:A:1547:LEU:HA	1:A:1550:ILE:HG12	1.99	0.44
1:A:1914:GLU:HG3	2:A:4701:ADP:H3'	1.99	0.44
1:A:3588:LEU:HD22	1:A:3698:PHE:CD2	2.52	0.44
1:A:3692:LEU:O	1:A:3696:VAL:HG22	2.17	0.44
1:A:1637:LEU:O	1:A:1641:ILE:HG12	2.17	0.44
1:A:2226:SER:HB2	1:A:2726:ARG:HG2	2.00	0.44
1:A:2799:MET:HE3	1:A:2799:MET:HB3	1.81	0.44
1:A:3792:GLN:O	1:A:3796:THR:HG23	2.17	0.44
1:A:2500:TRP:CD2	1:A:2580:LEU:HD11	2.51	0.44
1:A:2596:PRO:HD3	1:A:2735:TYR:CE1	2.53	0.44
1:A:1912:LYS:N	2:A:4701:ADP:O1B	2.50	0.44
1:A:2000:GLU:O	1:A:2001:LEU:HD12	2.17	0.44
1:A:2922:ILE:HG22	1:A:2950:VAL:HG11	1.99	0.44
1:A:2369:LEU:HD12	1:A:2373:MET:SD	2.57	0.44
1:A:3086:PHE:O	1:A:3091:LEU:HD21	2.18	0.44
1:A:3497:LYS:HE2	1:A:3497:LYS:HB2	1.81	0.44
1:A:3876:LEU:HD22	1:A:4148:GLU:OE2	2.18	0.44
1:A:4031:VAL:HG21	1:A:4125:PHE:HZ	1.83	0.44
1:A:4260:PHE:CE2	1:A:4608:PRO:HB3	2.51	0.44
1:A:4297:PRO:HB3	1:A:4308:TRP:CD1	2.53	0.44
1:A:3005:LEU:C	1:A:3007:ARG:H	2.25	0.44
1:A:3803:PRO:O	1:A:3806:THR:OG1	2.28	0.44
1:A:4004:MET:HE2	1:A:4004:MET:HA	2.00	0.44
1:A:4223:LEU:HD12	1:A:4223:LEU:HA	1.76	0.44
1:A:3175:HIS:HD2	1:A:3585:ARG:HH22	1.64	0.44
1:A:3209:LYS:HG2	1:A:3486:ARG:HH21	1.81	0.44
1:A:1738:TYR:HE2	1:A:1792:LEU:HD21	1.82	0.44
1:A:2495:VAL:HG21	1:A:2524:VAL:HG11	2.00	0.44
1:A:4631:ASP:OD1	1:A:4631:ASP:N	2.51	0.44
1:A:2793:ILE:HG21	1:A:3087:ASN:HB2	2.00	0.44
1:A:4545:VAL:HG11	1:A:4570:CYS:SG	2.58	0.44
1:A:2324:LEU:HD21	1:A:2332:ARG:HE	1.82	0.43
1:A:3116:GLU:N	1:A:3116:GLU:OE2	2.51	0.43
1:A:1860:GLN:HG2	1:A:1865:LYS:HG2	1.99	0.43
1:A:3626:ALA:HB1	1:A:3631:ASN:O	2.19	0.43
1:A:1571:ILE:HD11	1:A:1604:LEU:HD23	2.00	0.43
1:A:1578:LEU:O	1:A:1582:VAL:HG12	2.18	0.43
1:A:2571:THR:H	1:A:2574:THR:HB	1.82	0.43
1:A:2978:THR:HG22	1:A:2982:ARG:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3851:ASP:O	1:A:3855:ARG:HG3	2.18	0.43
1:A:2994:MET:SD	1:A:3066:PHE:CD1	3.11	0.43
1:A:4025:LEU:HD11	1:A:4027:LEU:HB3	2.01	0.43
1:A:4488:GLN:O	1:A:4492:ILE:HG12	2.19	0.43
1:A:1992:LYS:HA	1:A:1992:LYS:HD2	1.90	0.43
1:A:2903:GLU:O	1:A:2904:GLU:HB3	2.18	0.43
1:A:3718:LYS:HE3	1:A:3718:LYS:HB2	1.72	0.43
1:A:3812:TYR:CZ	1:A:3829:LEU:HD13	2.54	0.43
1:A:1511:PRO:HB3	1:A:3659:ARG:HH22	1.83	0.43
1:A:2277:ASP:O	1:A:2698:GLN:NE2	2.52	0.43
1:A:2439:HIS:HB2	1:A:2517:TYR:CE2	2.54	0.43
1:A:2444:GLU:HB3	1:A:2510:MET:HE3	2.01	0.43
1:A:2789:GLN:HE21	1:A:2838:VAL:HG21	1.83	0.43
1:A:3052:LYS:HE3	1:A:3052:LYS:HB3	1.84	0.43
1:A:2288:ILE:HD12	1:A:2288:ILE:HA	1.82	0.43
1:A:2932:HIS:HE1	1:A:3008:MET:SD	2.42	0.43
1:A:3659:ARG:NH2	1:A:3670:ASP:OD2	2.52	0.43
1:A:3835:ILE:HG12	1:A:3870:ARG:HD3	2.00	0.43
1:A:4179:LEU:HD23	1:A:4179:LEU:HA	1.85	0.43
1:A:4379:THR:HA	1:A:4382:THR:HG22	2.00	0.43
1:A:3148:VAL:O	1:A:3152:GLN:HG2	2.18	0.43
1:A:3178:ASP:OD2	1:A:3178:ASP:C	2.62	0.43
1:A:2897:LEU:HD21	1:A:2911:LEU:HD23	2.01	0.42
1:A:3851:ASP:HB3	1:A:3854:GLN:HB3	1.99	0.42
1:A:1547:LEU:HA	1:A:1550:ILE:CG1	2.50	0.42
1:A:1698:ILE:HA	1:A:1701:TRP:NE1	2.34	0.42
1:A:3056:SER:HB2	1:A:3060:ARG:NH2	2.35	0.42
1:A:3661:LEU:HD13	1:A:3669:ILE:O	2.19	0.42
1:A:3725:ASP:OD1	1:A:3728:ARG:NH1	2.52	0.42
1:A:1715:LYS:HD3	1:A:1715:LYS:HA	1.81	0.42
1:A:2822:ILE:HD11	1:A:2858:PHE:CD2	2.53	0.42
1:A:2919:VAL:HG21	1:A:2949:PHE:HE2	1.85	0.42
1:A:2922:ILE:HD11	1:A:2935:LEU:HD11	2.01	0.42
1:A:3616:ASP:OD1	1:A:3616:ASP:C	2.61	0.42
1:A:1990:TYR:OH	1:A:1995:ALA:N	2.52	0.42
1:A:2869:ARG:N	1:A:2870:PRO:HD2	2.34	0.42
1:A:3021:PHE:CD1	1:A:3029:LEU:HG	2.55	0.42
1:A:3912:ASN:O	1:A:3937:ARG:HD2	2.20	0.42
1:A:4613:PHE:HA	1:A:4643:LEU:HD13	2.00	0.42
1:A:2200:GLY:HA2	1:A:2373:MET:CE	2.49	0.42
1:A:2921:ARG:O	1:A:2925:ILE:HG12	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2995:ASP:CG	1:A:2996:GLU:H	2.26	0.42
1:A:3012:LEU:HB3	1:A:3088:ARG:CG	2.49	0.42
1:A:3114:ASP:HB3	1:A:3191:ARG:HH12	1.84	0.42
1:A:3873:ARG:HD3	1:A:3873:ARG:HA	1.90	0.42
1:A:1789:LEU:HG	1:A:1815:LEU:HB3	2.01	0.42
1:A:1993:THR:O	1:A:1993:THR:OG1	2.38	0.42
1:A:1747:ALA:HB2	1:A:1807:LYS:HG2	2.01	0.42
1:A:2911:LEU:HA	1:A:2915:VAL:HG11	2.02	0.42
1:A:3046:SER:HB3	1:A:3049:GLU:HB2	2.02	0.42
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.53	0.42
1:A:4485:ARG:NH1	1:A:4513:GLY:O	2.53	0.42
1:A:3154:LEU:HD21	1:A:3532:TRP:HZ2	1.85	0.42
1:A:1486:LEU:CD2	1:A:1579:MET:HE3	2.50	0.42
1:A:3916:LEU:HD23	1:A:3916:LEU:HA	1.91	0.42
1:A:3927:LEU:HD11	1:A:3996:PHE:HE1	1.84	0.42
1:A:1466:ILE:HG12	1:A:1500:HIS:CE1	2.55	0.42
1:A:2686:MET:HG2	1:A:2692:PHE:HB3	2.02	0.42
1:A:3961:LEU:O	1:A:3997:ARG:NH1	2.45	0.42
1:A:4158:LEU:HD12	1:A:4158:LEU:HA	1.93	0.42
1:A:4345:LYS:HB2	1:A:4345:LYS:HE3	1.77	0.42
1:A:1571:ILE:HD11	1:A:1604:LEU:HA	2.01	0.41
1:A:2453:ARG:HD3	1:A:2728:LEU:O	2.19	0.41
1:A:2642:ARG:HG2	1:A:2645:PRO:HD3	2.00	0.41
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	2.01	0.41
1:A:2900:PHE:CD2	1:A:2949:PHE:HD1	2.38	0.41
1:A:2993:ILE:HG12	1:A:3065:VAL:HG23	2.02	0.41
1:A:3012:LEU:HD23	1:A:3012:LEU:HA	1.75	0.41
1:A:2538:GLU:HB3	1:A:2548:TRP:NE1	2.35	0.41
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	2.02	0.41
1:A:3717:LEU:HD23	1:A:3717:LEU:HA	1.91	0.41
1:A:4223:LEU:HD11	1:A:4238:ILE:HD12	2.01	0.41
1:A:4406:LYS:H	1:A:4406:LYS:HD2	1.85	0.41
1:A:1568:PHE:O	1:A:1571:ILE:HG22	2.21	0.41
1:A:2146:VAL:HA	1:A:2149:LEU:HD12	2.03	0.41
1:A:4077:PHE:HD2	1:A:4105:TRP:CD1	2.39	0.41
1:A:4630:GLU:OE1	1:A:4630:GLU:N	2.52	0.41
1:A:2090:LEU:HD12	1:A:2090:LEU:HA	1.78	0.41
1:A:2455:LEU:HD23	1:A:2455:LEU:HA	1.89	0.41
1:A:3125:TYR:C	1:A:3127:PRO:HD3	2.45	0.41
1:A:3553:LEU:O	1:A:3582:ARG:NH1	2.54	0.41
1:A:3812:TYR:OH	1:A:3816:GLU:OE1	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3846:LEU:HD11	1:A:3859:ILE:HG13	2.02	0.41
1:A:4055:VAL:O	1:A:4058:LEU:HG	2.20	0.41
1:A:2595:GLY:O	1:A:2601:LYS:NZ	2.52	0.41
1:A:3750:LEU:O	1:A:3754:ASN:ND2	2.53	0.41
1:A:4171:LYS:HZ3	1:A:4171:LYS:HG2	1.64	0.41
1:A:1687:LYS:H	1:A:1687:LYS:HG2	1.73	0.41
1:A:2222:MET:HE1	1:A:2234:TRP:CD1	2.56	0.41
1:A:2432:LEU:HD11	1:A:2518:ILE:HG13	2.03	0.41
1:A:2464:GLN:NE2	1:A:2468:ASN:OD1	2.53	0.41
1:A:3178:ASP:OD1	1:A:3585:ARG:NH2	2.51	0.41
1:A:1678:SER:OG	1:A:1679:ARG:N	2.54	0.41
1:A:2076:CYS:O	1:A:2080:LEU:HB2	2.20	0.41
1:A:2231:SER:HA	1:A:2234:TRP:NE1	2.35	0.41
1:A:2265:TYR:CE1	1:A:2314:ASN:HB2	2.55	0.41
1:A:2962:LYS:HB2	1:A:3665:GLY:HA2	2.01	0.41
1:A:2975:ASP:O	1:A:2979:VAL:HG23	2.21	0.41
1:A:3135:GLN:HB2	1:A:3136:PRO:HD3	2.03	0.41
1:A:3207:LYS:O	1:A:3211:THR:HG23	2.21	0.41
1:A:4481:ASP:O	1:A:4485:ARG:HG3	2.19	0.41
1:A:2981:ARG:HD2	1:A:3032:GLN:HE22	1.86	0.41
1:A:3186:LEU:HD22	1:A:3507:CYS:SG	2.60	0.41
1:A:3195:GLU:OE2	1:A:3195:GLU:HA	2.21	0.41
1:A:1907:PRO:HD2	1:A:2042:THR:HA	2.03	0.41
1:A:2227:GLY:O	1:A:2369:LEU:HD23	2.21	0.41
1:A:2324:LEU:HD11	1:A:2332:ARG:HB3	2.03	0.41
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.20	0.41
1:A:2599:SER:OG	1:A:2736:VAL:HG12	2.21	0.41
1:A:2627:THR:HG23	1:A:2629:GLU:HB2	2.03	0.41
1:A:2932:HIS:CD2	1:A:2933:LEU:H	2.38	0.41
1:A:2963:VAL:HG11	1:A:2998:ASN:HA	2.03	0.41
1:A:3056:SER:HB2	1:A:3060:ARG:CZ	2.50	0.41
1:A:3099:THR:HG22	1:A:3129:VAL:HG22	2.02	0.41
1:A:3209:LYS:HD2	1:A:3209:LYS:HA	1.88	0.41
1:A:3562:TRP:HB3	1:A:3567:LEU:HD22	2.02	0.41
1:A:3583:PHE:CD2	1:A:3587:PRO:HD3	2.56	0.41
1:A:3608:LYS:HG3	1:A:3608:LYS:O	2.21	0.41
1:A:3756:VAL:HG23	1:A:3758:GLY:H	1.84	0.41
1:A:3831:PHE:HZ	1:A:3870:ARG:HB3	1.86	0.41
1:A:1657:MET:HE3	1:A:1657:MET:HB2	1.85	0.41
1:A:2631:LEU:HD23	1:A:2631:LEU:HA	1.86	0.41
1:A:3639:GLU:HG3	1:A:3686:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4165:PRO:HD2	1:A:4168:ARG:HD3	2.03	0.41
1:A:4442:LYS:HE3	1:A:4442:LYS:HB2	1.88	0.41
1:A:4614:THR:O	1:A:4616:ALA:N	2.54	0.41
1:A:1680:GLU:OE2	1:A:1875:VAL:HB	2.21	0.40
1:A:1721:VAL:HA	1:A:1724:VAL:CG1	2.52	0.40
1:A:2086:TYR:HE2	1:A:2149:LEU:HD23	1.86	0.40
1:A:2496:TYR:CE1	1:A:2500:TRP:HD1	2.39	0.40
1:A:2693:TYR:CE1	1:A:2700:TRP:HB2	2.56	0.40
1:A:2927:ARG:CZ	1:A:2927:ARG:HB2	2.51	0.40
1:A:3585:ARG:HB2	1:A:3697:THR:HG23	2.03	0.40
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.57	0.40
1:A:2783:ARG:HD2	1:A:2845:TRP:CZ3	2.56	0.40
1:A:2867:MET:HA	1:A:2869:ARG:HH21	1.86	0.40
1:A:2928:GLN:HB3	1:A:2930:GLN:OE1	2.21	0.40
1:A:3593:SER:C	1:A:3682:ARG:HH12	2.29	0.40
1:A:3892:LEU:HD12	1:A:3892:LEU:HA	1.85	0.40
1:A:4149:PRO:HA	1:A:4150:PRO:HD3	1.96	0.40
1:A:2410:SER:N	1:A:2411:PRO:HD2	2.36	0.40
1:A:2462:LEU:HD13	1:A:2462:LEU:HA	1.87	0.40
1:A:3721:ARG:HE	1:A:3724:VAL:HG21	1.87	0.40
1:A:3788:ASP:OD1	1:A:3789:ILE:N	2.52	0.40
1:A:4427:VAL:HG21	1:A:4482:PHE:HE2	1.87	0.40
1:A:2603:MET:C	1:A:2603:MET:SD	3.05	0.40
1:A:2872:LEU:HD21	1:A:2917:ASP:OD1	2.22	0.40
1:A:3586:TYR:HA	1:A:3587:PRO:HD3	1.95	0.40
1:A:3751:GLN:HA	1:A:3754:ASN:ND2	2.36	0.40
1:A:4066:ILE:HG21	1:A:4095:MET:HB2	2.03	0.40
1:A:4247:MET:HE1	1:A:4273:PHE:CZ	2.57	0.40
1:A:4445:THR:HG23	1:A:4448:LEU:H	1.86	0.40
1:A:2500:TRP:CE3	1:A:2580:LEU:HD11	2.57	0.40
1:A:3619:PHE:O	1:A:3623:LEU:HB2	2.21	0.40
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	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	2844/4646 (61%)	2762 (97%)	81 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4172	SER

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	2544/4125 (62%)	2534 (100%)	10 (0%)	84	81

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

Mol	Chain	Res	Type
1	A	1541	GLN
1	A	1945	PHE
1	A	2872	LEU
1	A	3188	HIS
1	A	3952	GLN
1	A	3981	THR
1	A	4346	MET
1	A	4431	LEU
1	A	4469	VAL
1	A	4617	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1736	ASN

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Mol	Chain	Res	Type
1	A	1748	GLN
1	A	1973	GLN
1	A	1974	GLN
1	A	1979	GLN
1	A	2051	GLN
1	A	2414	GLN
1	A	2464	GLN
1	A	2549	GLN
1	A	2834	GLN
1	A	3057	GLN
1	A	3069	ASN
1	A	3092	ASN
1	A	3200	HIS
1	A	3202	ASN
1	A	3754	ASN
1	A	3772	ASN
1	A	3985	GLN
1	A	4029	HIS
1	A	4065	GLN
1	A	4490	GLN
1	A	4530	GLN
1	A	4549	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ANP	A	4703	-	33,33,33	0.93	4 (12%)	45,52,52	0.59	0
3	ATP	A	4702	-	32,33,33	0.39	0	48,52,52	0.29	0
2	ADP	A	4701	-	28,29,29	1.40	4 (14%)	43,45,45	1.84	9 (20%)
2	ADP	A	4704	-	28,29,29	1.41	4 (14%)	43,45,45	1.85	10 (23%)

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	-	-	4/18/38/38	0/3/3/3
3	ATP	A	4702	-	-	9/22/38/38	0/3/3/3
2	ADP	A	4701	-	-	3/16/32/32	0/3/3/3
2	ADP	A	4704	-	-	5/16/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4704	ADP	C5-C4	4.63	1.47	1.39
2	A	4701	ADP	C5-C4	4.63	1.47	1.39
2	A	4704	ADP	C5-C6	2.69	1.48	1.41
2	A	4701	ADP	C5-C6	2.62	1.48	1.41
4	A	4703	ANP	PG-O1G	2.53	1.50	1.46
4	A	4703	ANP	PB-O3A	-2.42	1.56	1.59
4	A	4703	ANP	PG-N3B	2.42	1.69	1.63
2	A	4704	ADP	C8-N7	2.37	1.36	1.31
4	A	4703	ANP	PB-O1B	2.36	1.49	1.46
2	A	4701	ADP	C5-N7	-2.36	1.34	1.39
2	A	4704	ADP	C5-N7	-2.30	1.34	1.39
2	A	4701	ADP	C8-N7	2.26	1.36	1.31

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	ADP	C5-C4-N3	-5.79	118.75	126.72
2	A	4704	ADP	C5-C4-N3	-5.76	118.78	126.72
2	A	4701	ADP	N3-C4-N9	4.62	135.02	127.17
2	A	4704	ADP	N3-C4-N9	4.44	134.72	127.17
2	A	4701	ADP	C2-N3-C4	3.70	120.86	111.83
2	A	4704	ADP	C2-N3-C4	3.68	120.83	111.83
2	A	4704	ADP	C4-C5-N7	-3.56	106.51	110.58
2	A	4701	ADP	C4-C5-N7	-3.39	106.71	110.58
2	A	4701	ADP	N3-C2-N1	-3.31	123.57	128.58
2	A	4704	ADP	N3-C2-N1	-3.24	123.67	128.58
2	A	4701	ADP	C4-N9-C8	2.65	108.52	105.74
2	A	4704	ADP	C4-N9-C8	2.60	108.46	105.74
2	A	4704	ADP	C5-N7-C8	2.53	107.42	103.45
2	A	4701	ADP	C5-N7-C8	2.45	107.31	103.45
2	A	4704	ADP	O4'-C1'-N9	2.43	112.76	108.09
2	A	4704	ADP	C6-C5-N7	2.15	136.24	132.09
2	A	4701	ADP	C3'-C2'-C1'	2.13	105.49	101.46
2	A	4701	ADP	C6-C5-N7	2.03	136.00	132.09
2	A	4704	ADP	C3'-C2'-C1'	2.02	105.29	101.46

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C5'-O5'-PA-O2A
3	A	4702	ATP	C5'-O5'-PA-O3A
4	A	4703	ANP	PB-N3B-PG-O1G
4	A	4703	ANP	PG-N3B-PB-O1B
4	A	4703	ANP	PG-N3B-PB-O3A
2	A	4704	ADP	C3'-C4'-C5'-O5'
4	A	4703	ANP	PB-O3A-PA-O1A
3	A	4702	ATP	PB-O3B-PG-O1G
2	A	4701	ADP	C5'-O5'-PA-O1A
3	A	4702	ATP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'
3	A	4702	ATP	O4'-C1'-N9-C8
3	A	4702	ATP	O4'-C1'-N9-C4

Continued on next page...

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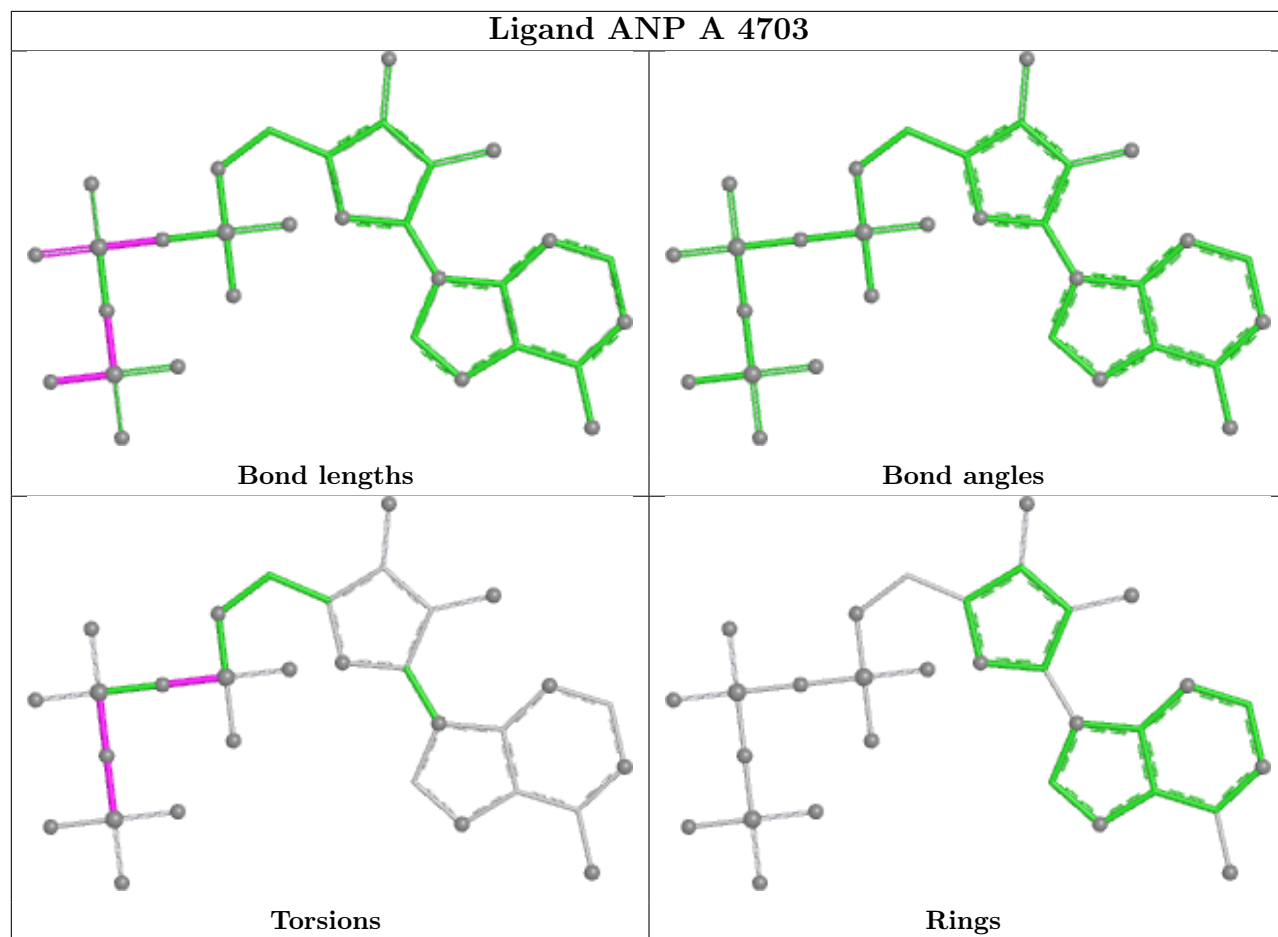
Mol	Chain	Res	Type	Atoms
3	A	4702	ATP	PG-O3B-PB-O1B
3	A	4702	ATP	PG-O3B-PB-O2B

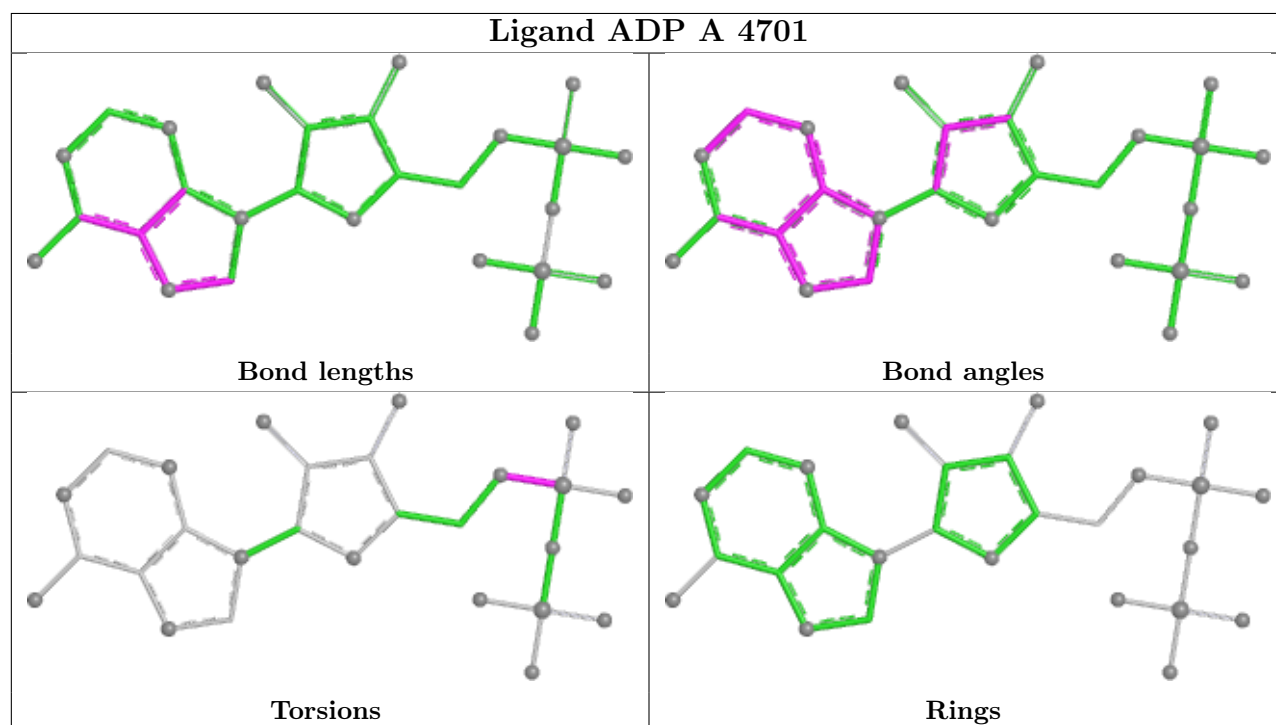
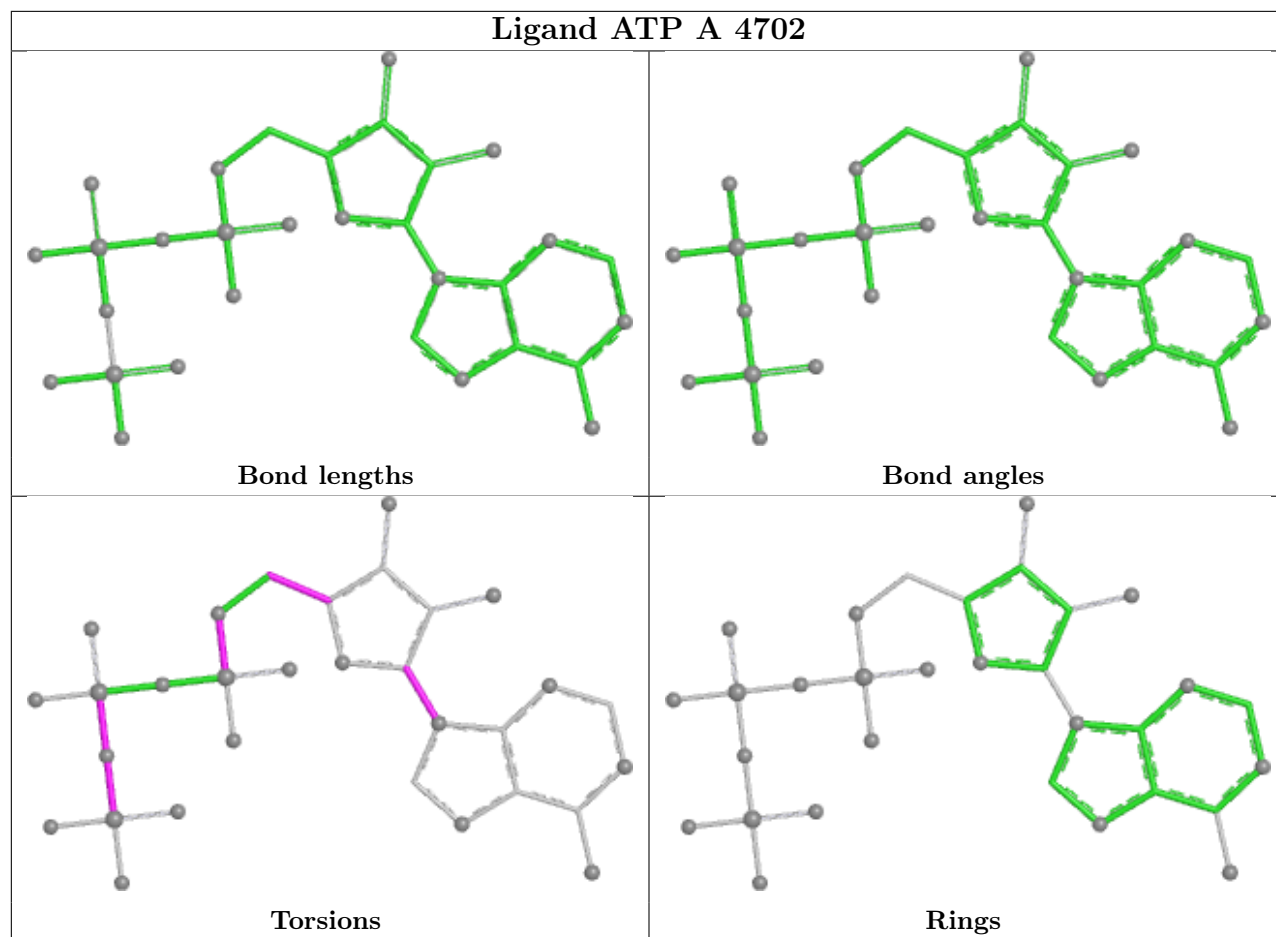
There are no ring outliers.

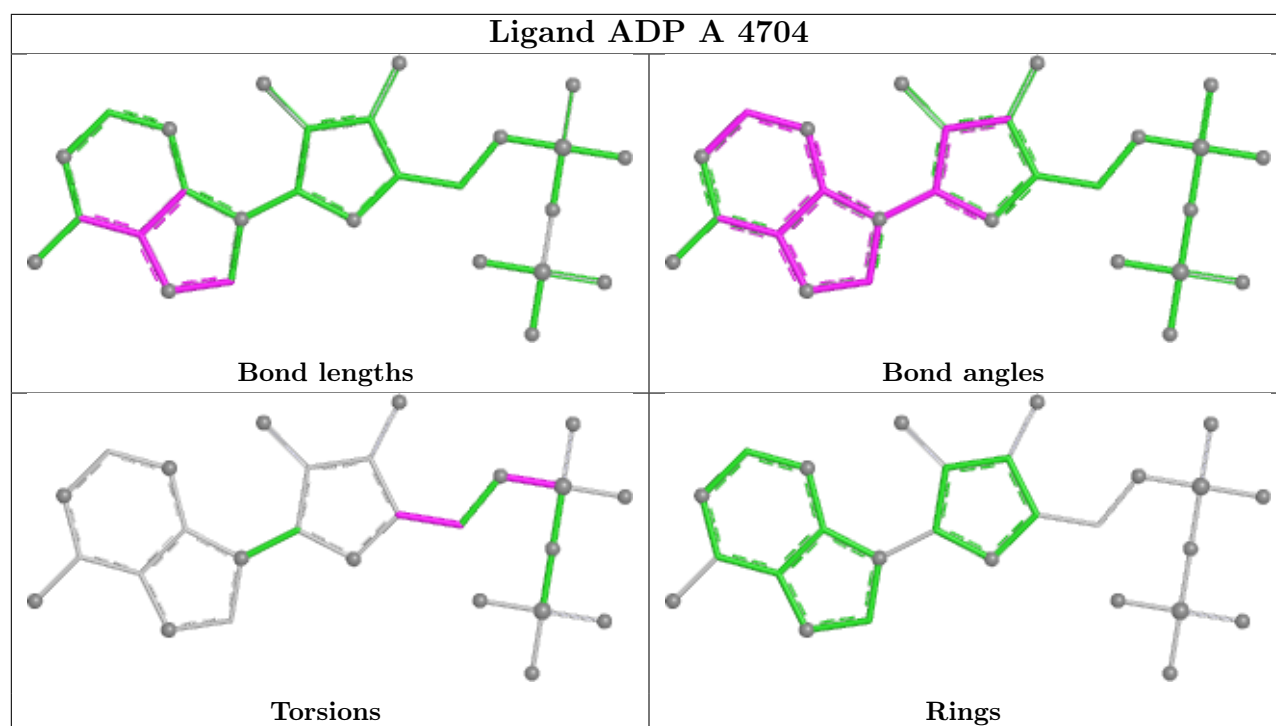
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4703	ANP	1	0
3	A	4702	ATP	1	0
2	A	4701	ADP	2	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

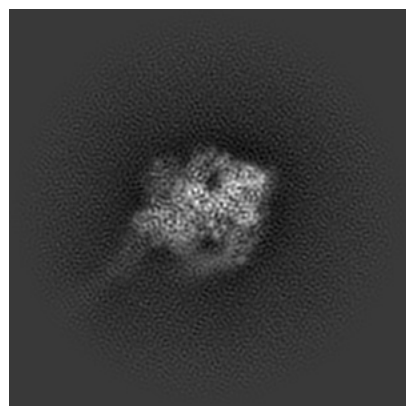
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44706. These allow visual inspection of the internal detail of the map and identification of artifacts.

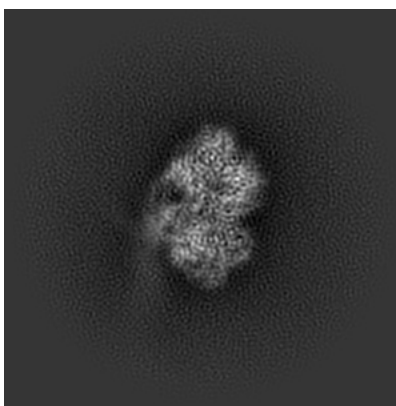
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

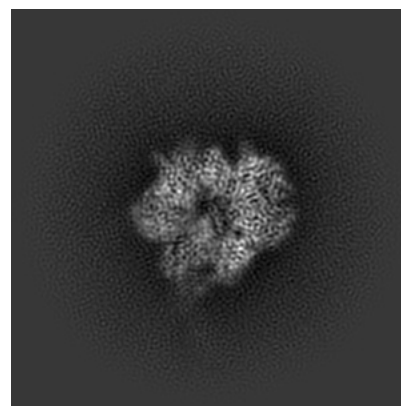
6.1.1 Primary map



X

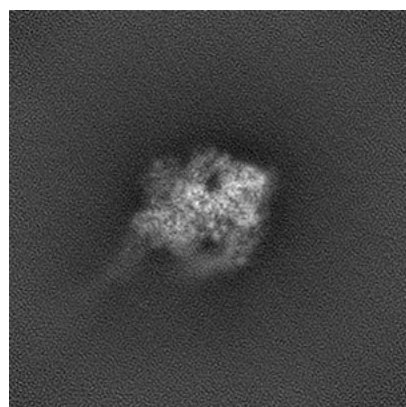


Y

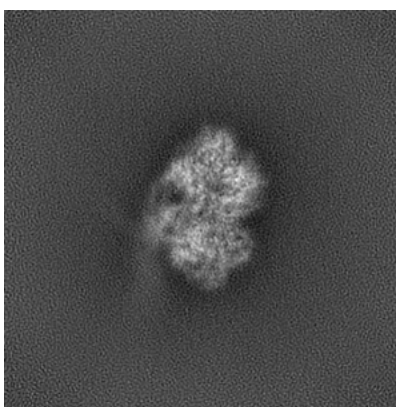


Z

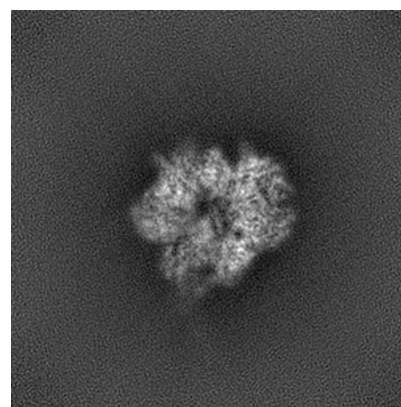
6.1.2 Raw map



X



Y

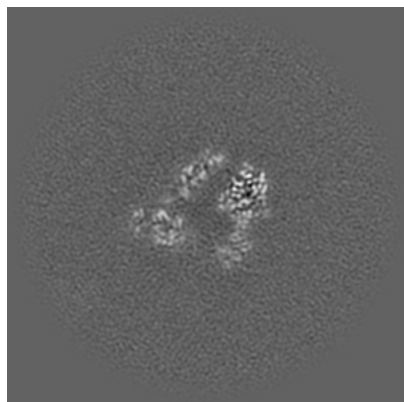


Z

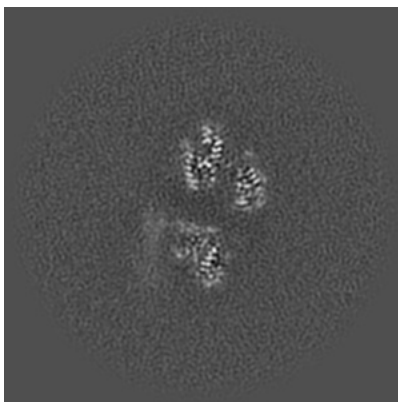
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

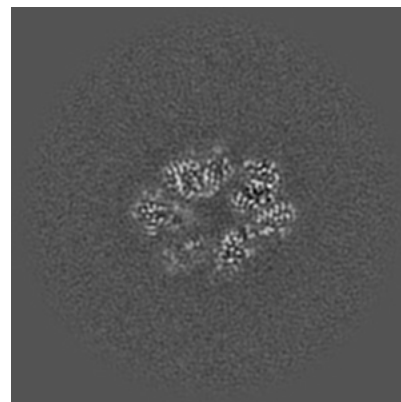
6.2.1 Primary map



X Index: 128

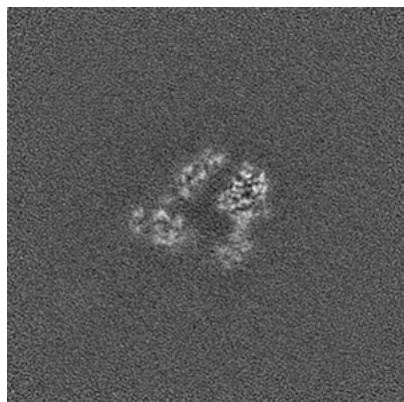


Y Index: 128

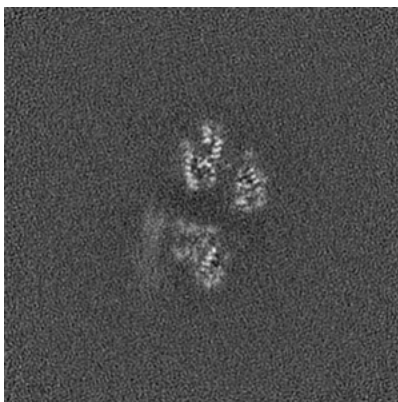


Z Index: 128

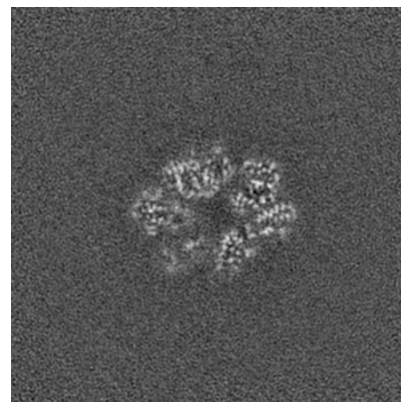
6.2.2 Raw map



X Index: 128



Y Index: 128

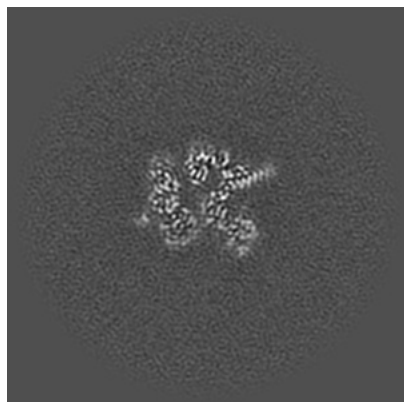


Z Index: 128

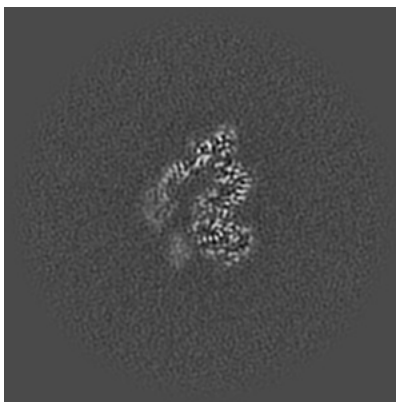
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

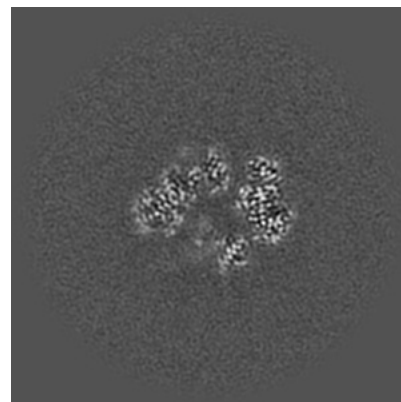
6.3.1 Primary map



X Index: 147

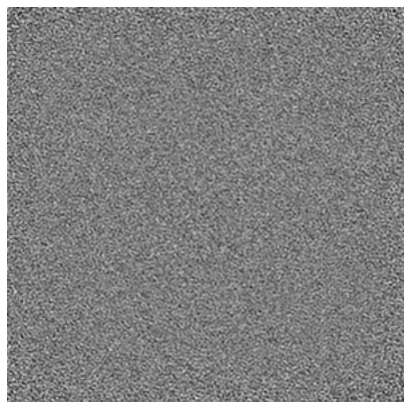


Y Index: 143

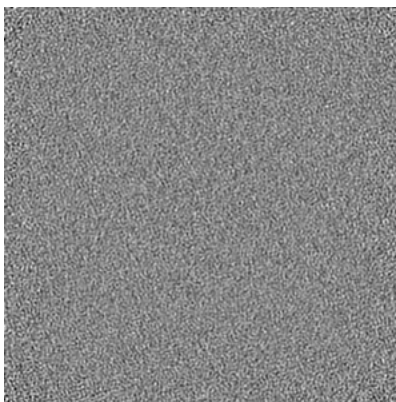


Z Index: 133

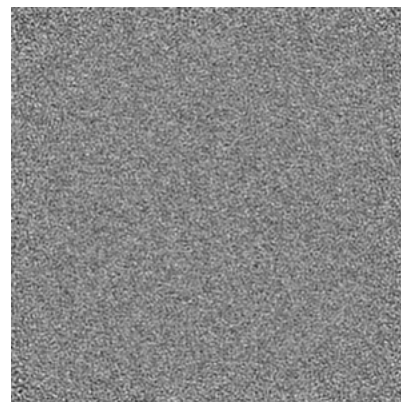
6.3.2 Raw map



X Index: 0



Y Index: 0

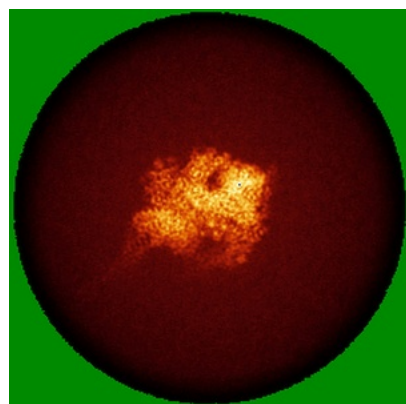


Z Index: 0

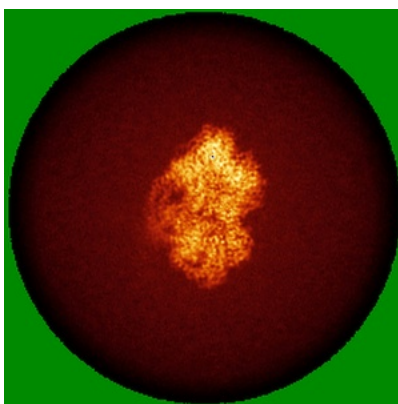
The images above show the largest variance slices of the map in three orthogonal directions.

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

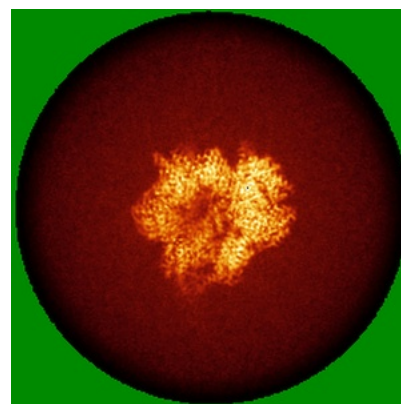
6.4.1 Primary map



X

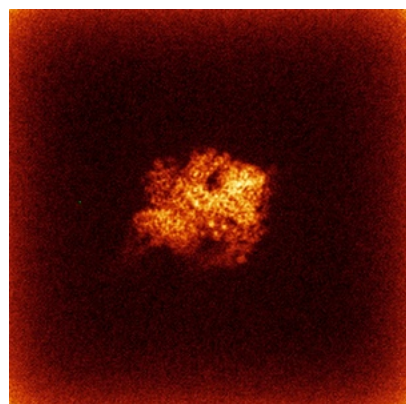


Y

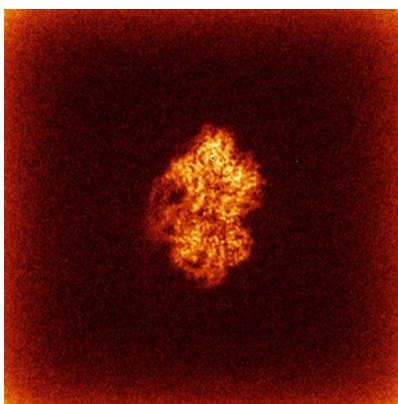


Z

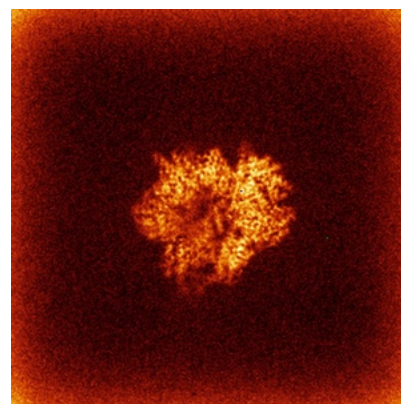
6.4.2 Raw map



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](#)

This section was not generated.

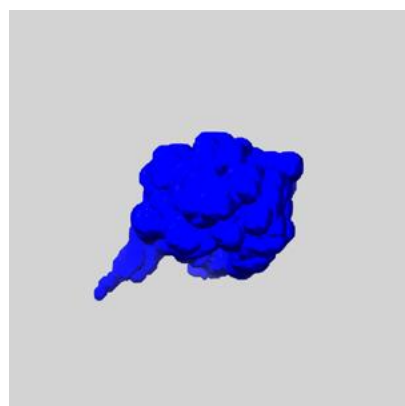
6.6 Mask visualisation [i](#)

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

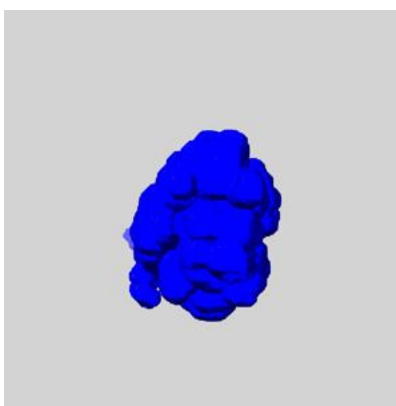
A mask typically either:

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

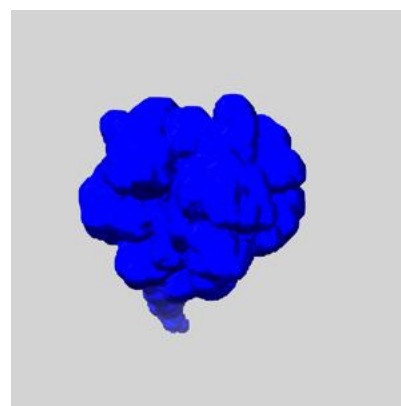
6.6.1 emd_44706_msk_1.map [i](#)



X



Y

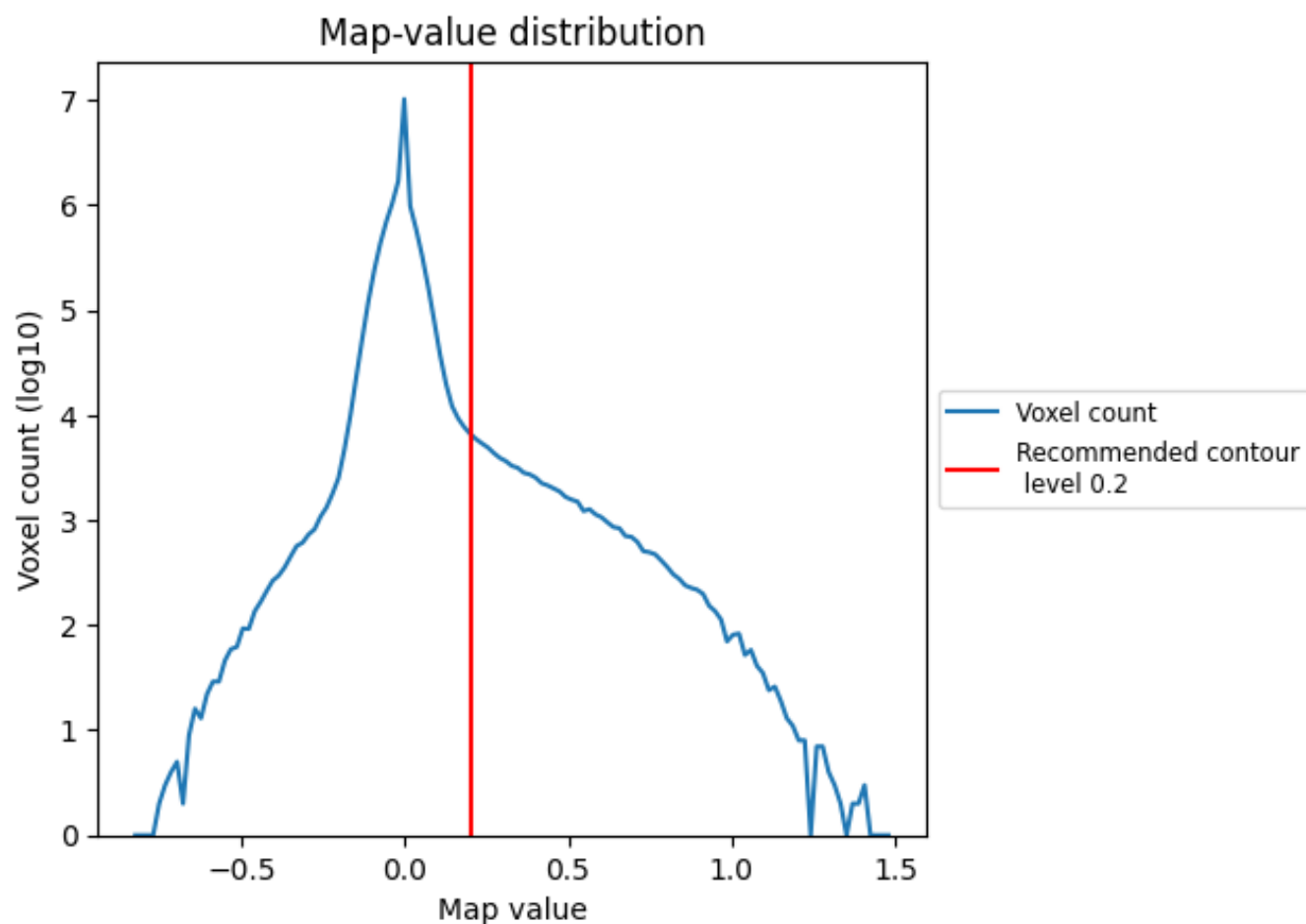


Z

7 Map analysis [i](#)

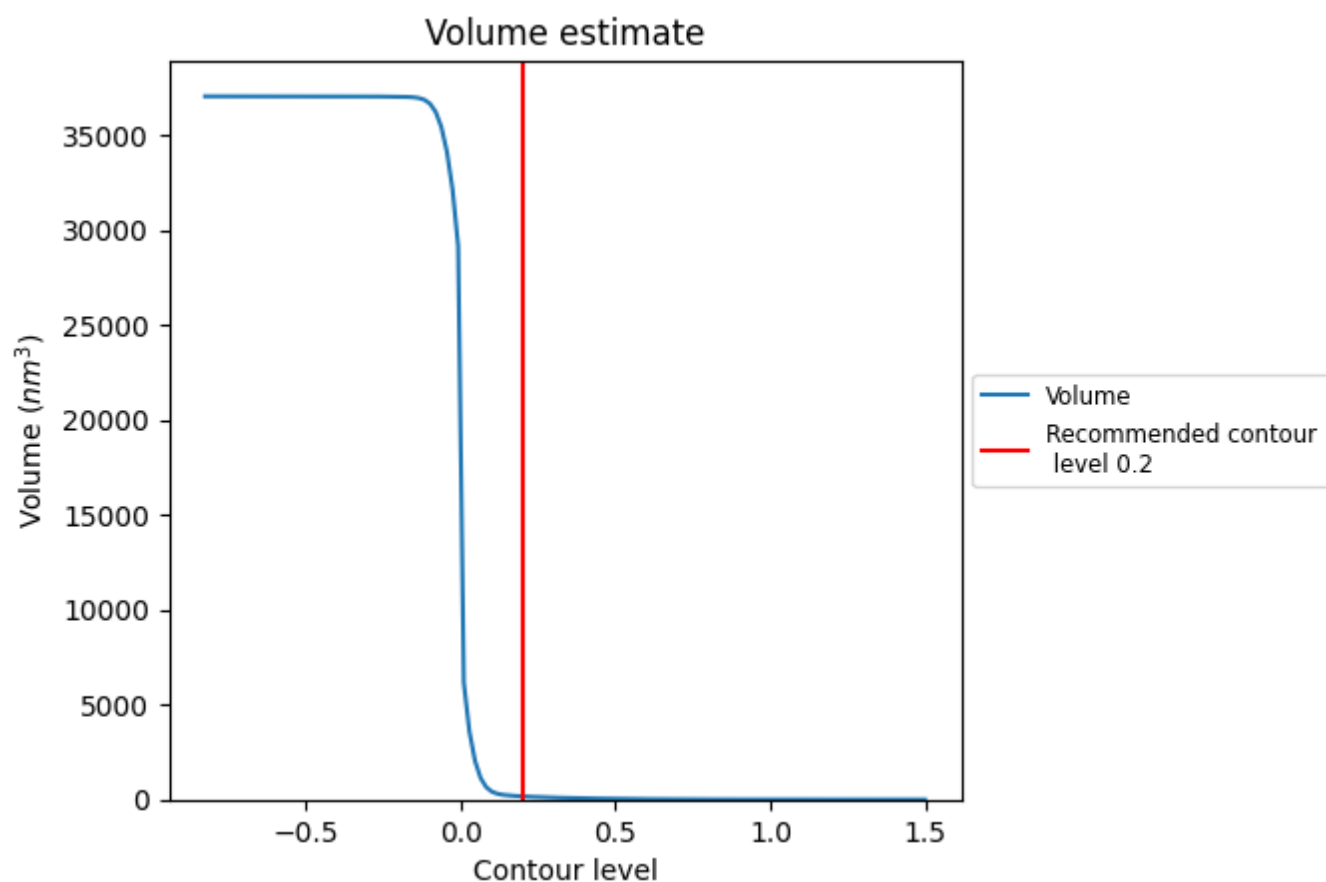
This section contains the results of statistical analysis of the map.

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.

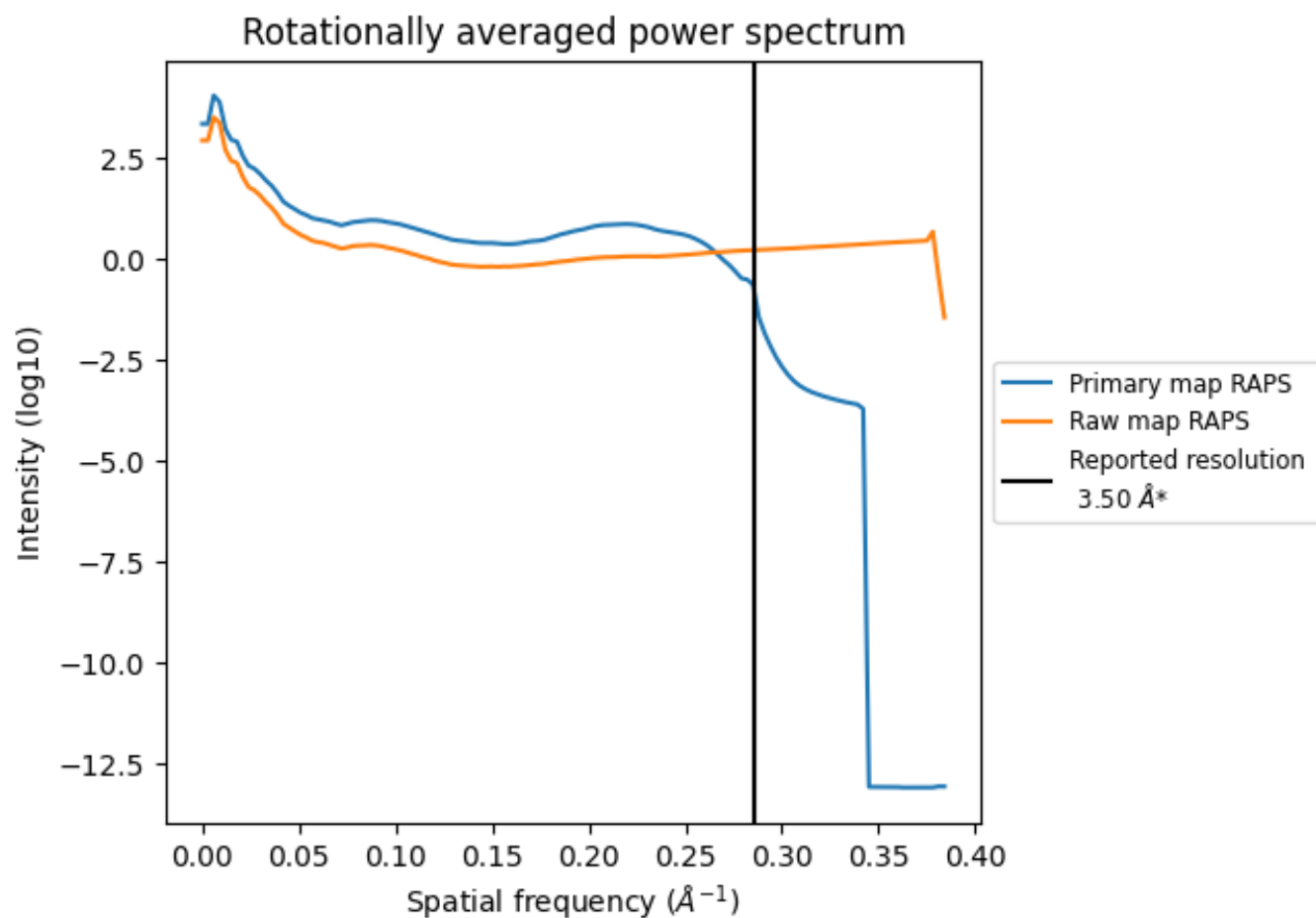
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 168 nm³; this corresponds to an approximate mass of 152 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 ⓘ

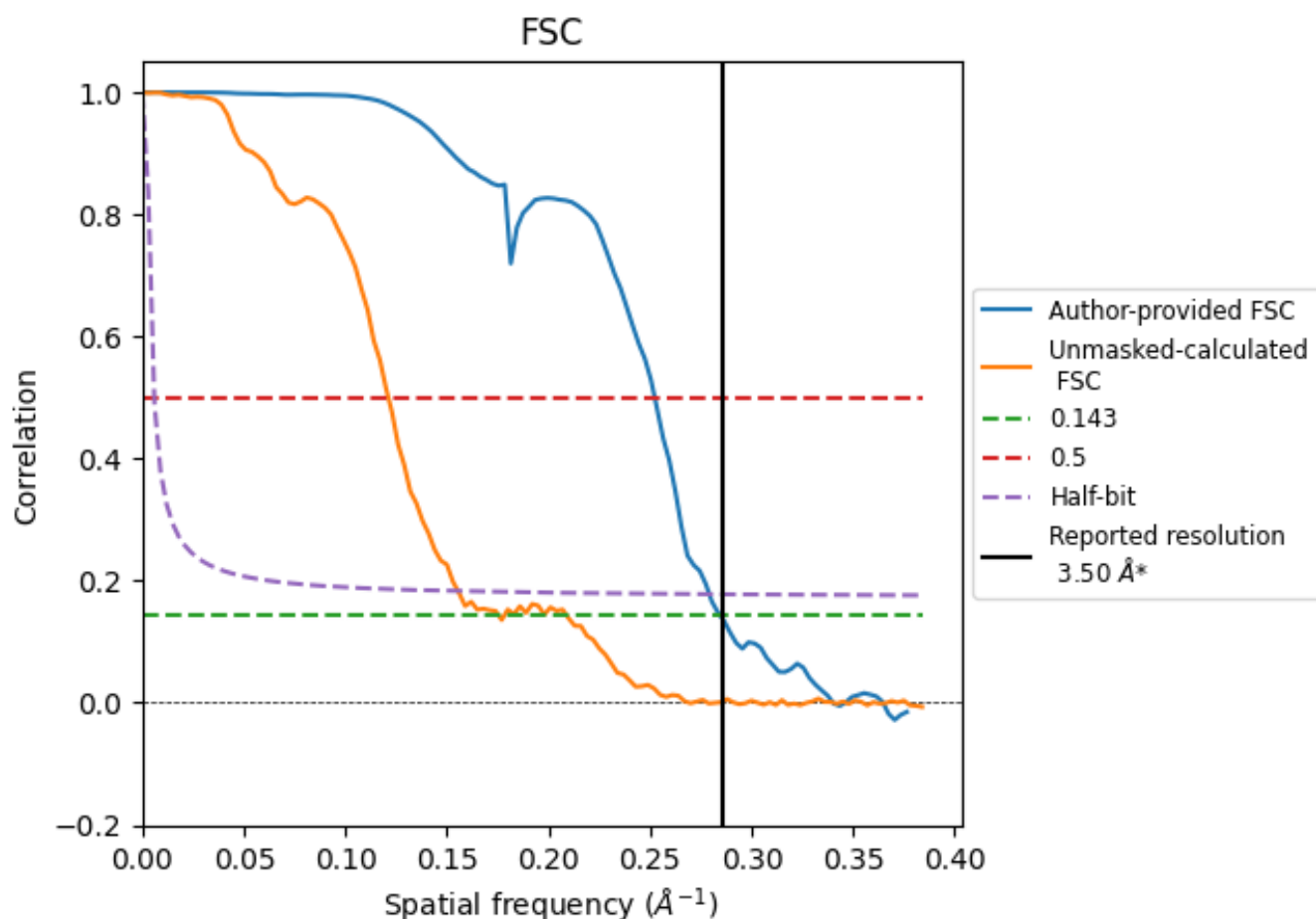


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 $0.286 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

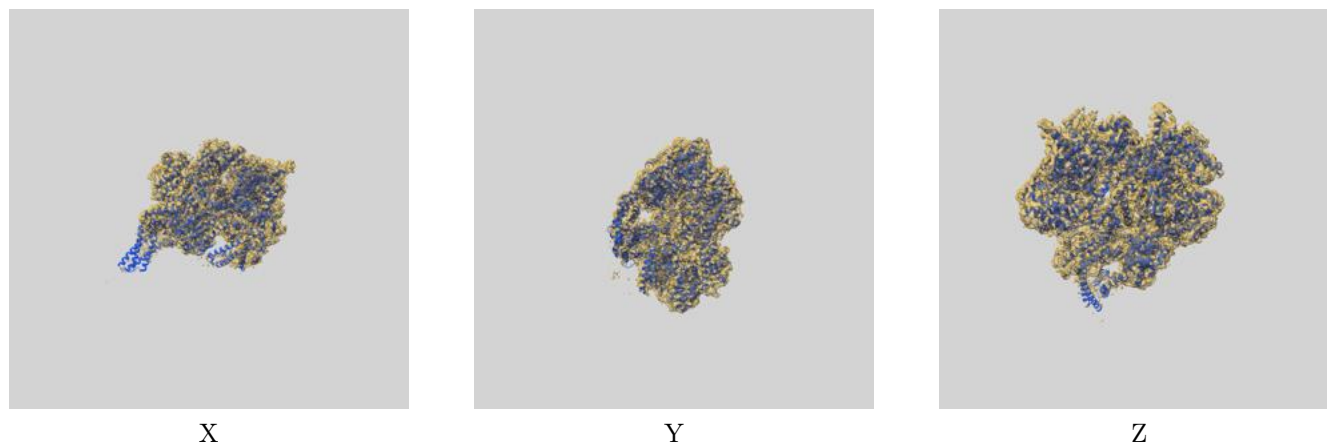
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.51	3.96	3.58
Unmasked-calculated*	5.70	8.25	6.43

*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 5.70 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

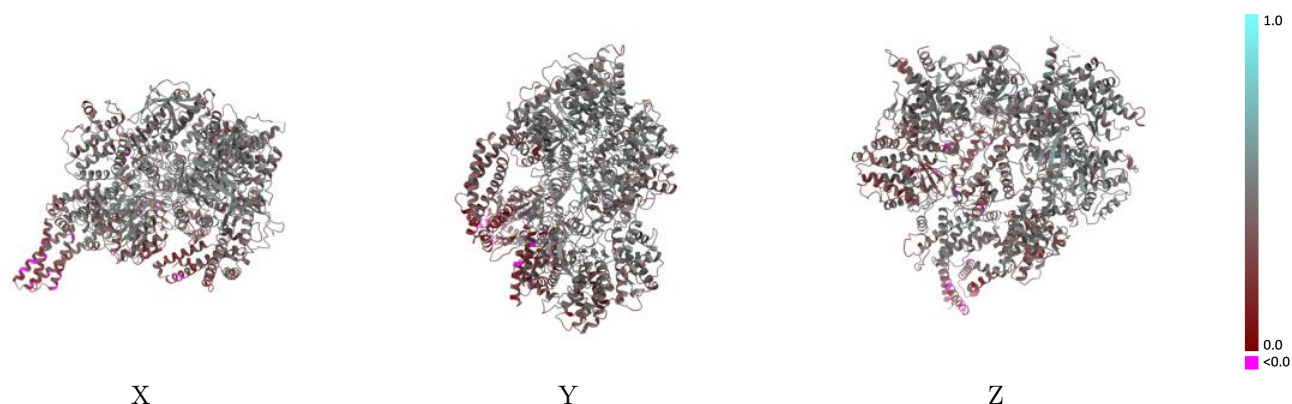
This section contains information regarding the fit between EMDB map EMD-44706 and PDB model 9BMP. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



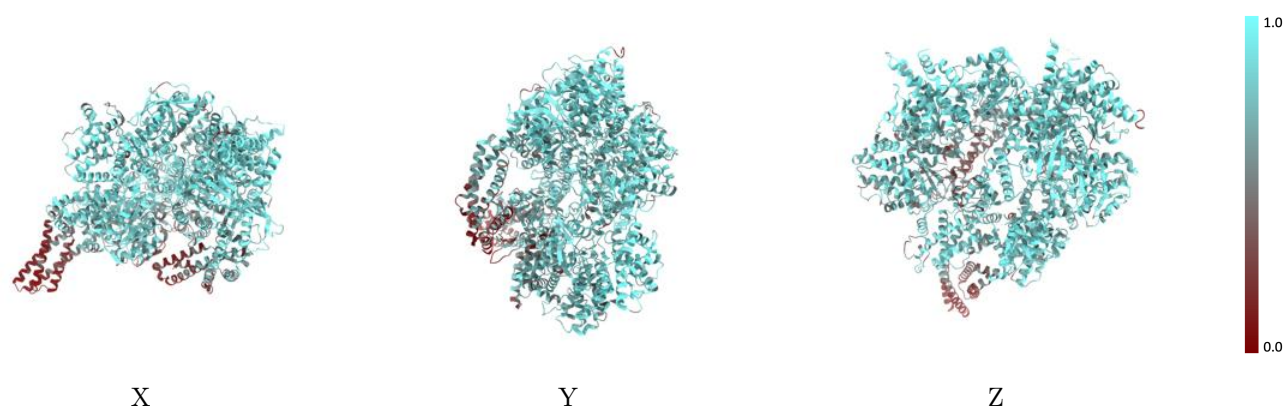
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



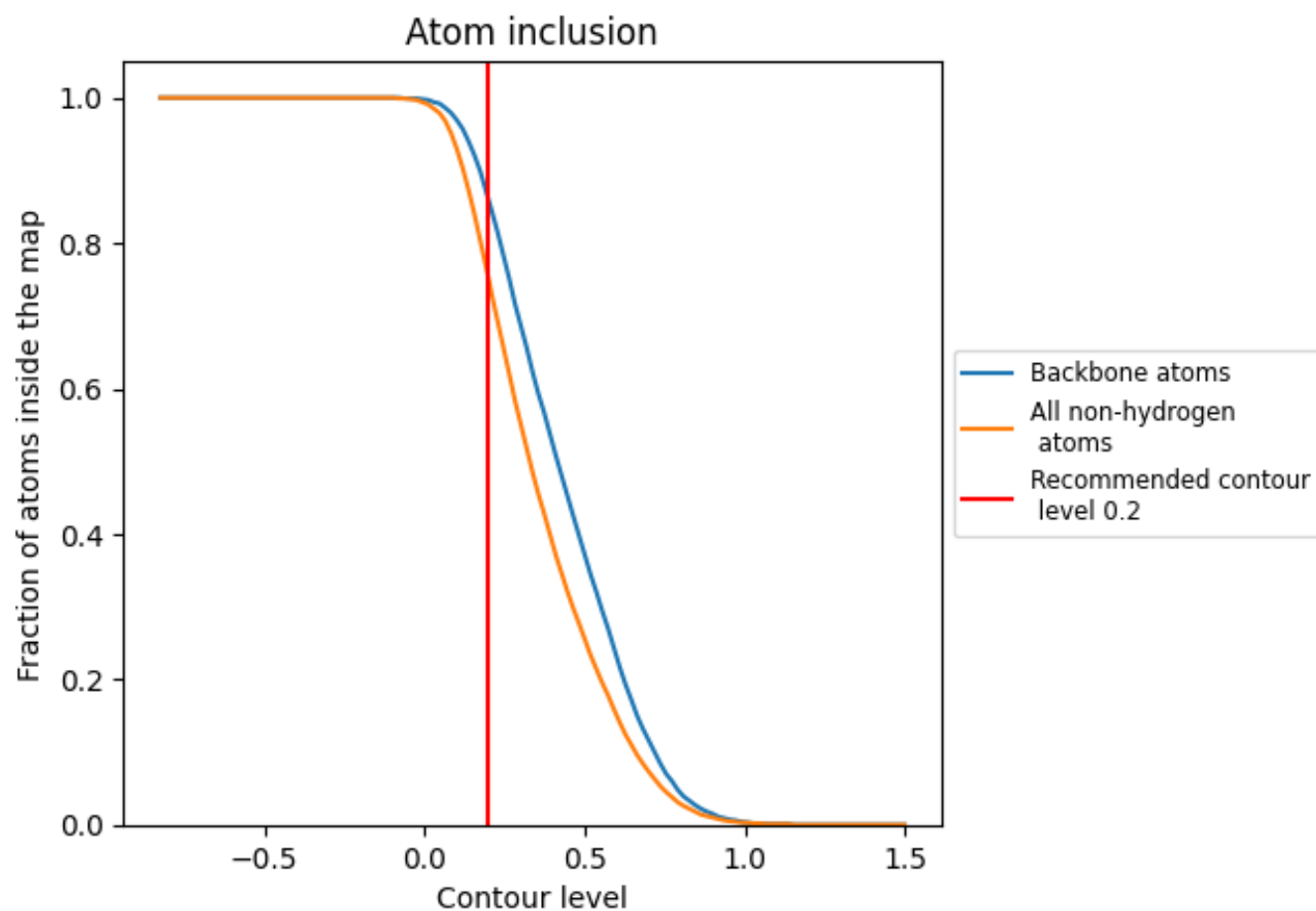
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7510	0.4100
A	0.7510	0.4100

