



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 11:11 PM UTC

PDB ID : 9BML / pdb_00009bml
EMDB ID : EMD-44702
Title : State-2 of the motor domain from full-length human dynein-1 in 5mM AMPPNP
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.30 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

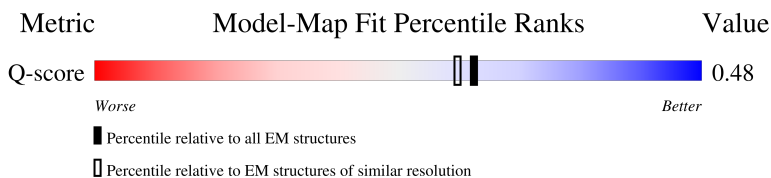
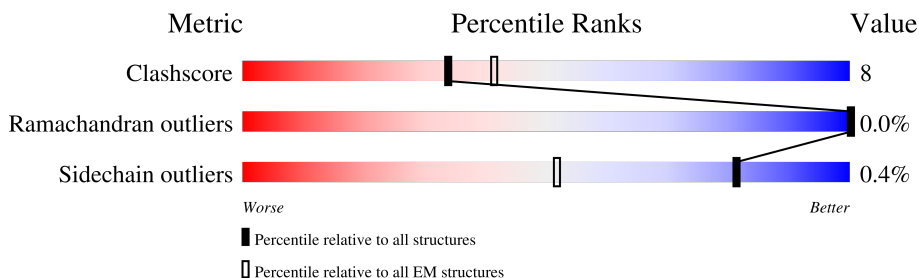
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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 23706 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.

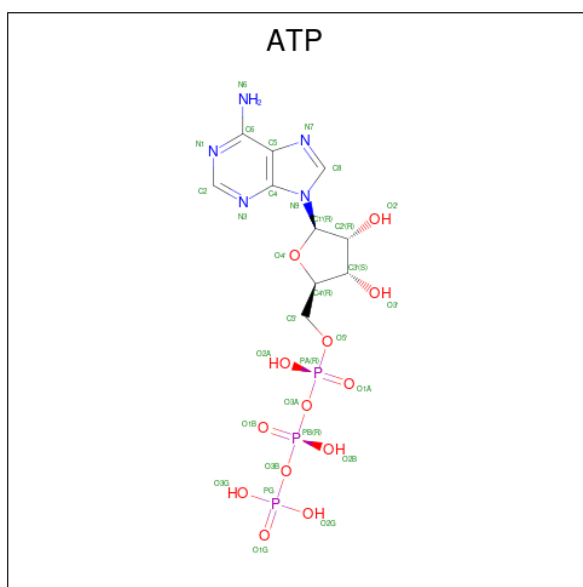
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2937	23593	15028	4070	4378	117	0	0

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



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

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



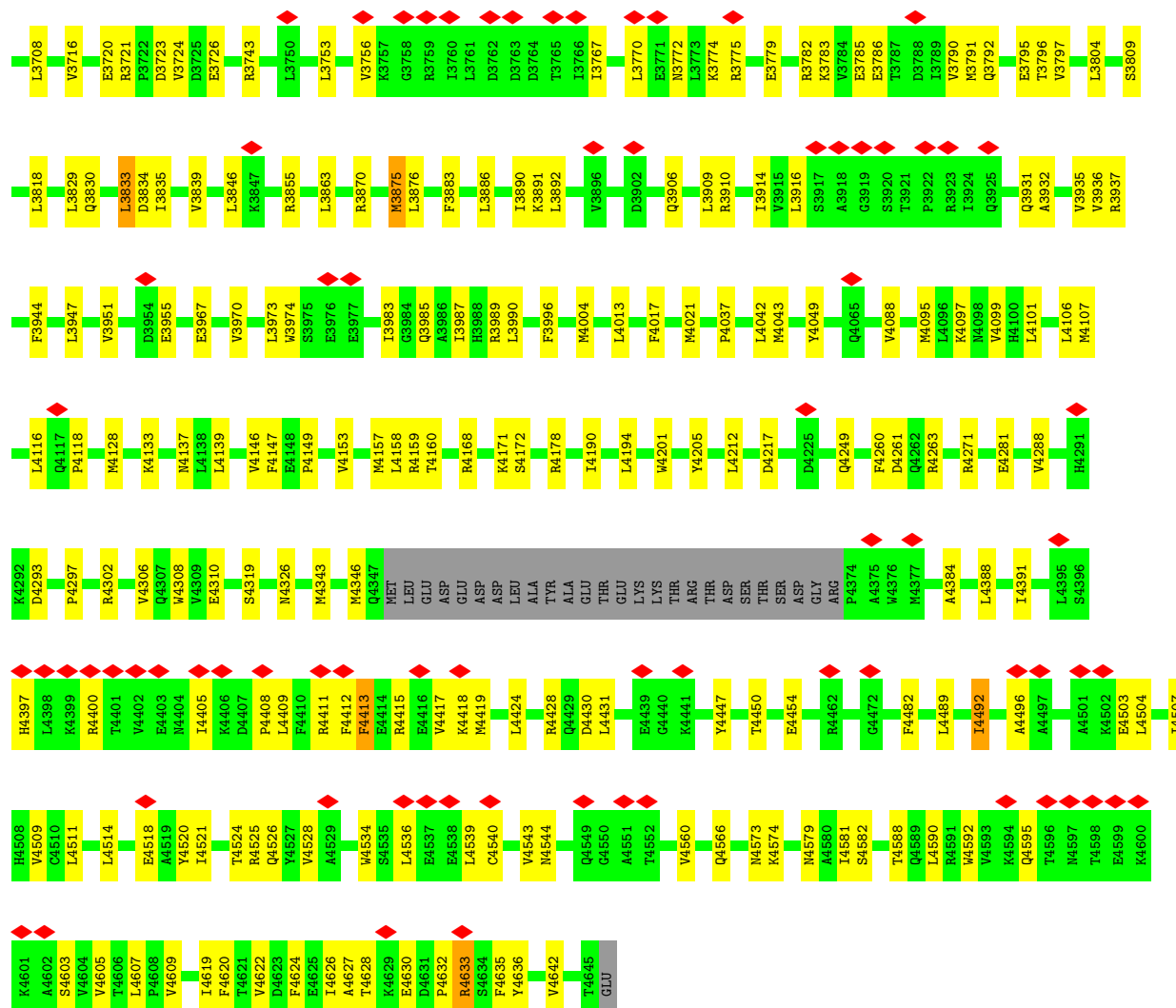
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0

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

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

V1971	Q1818	L1638	Q1566	LYS	VAL	TRP	ARG	GLU	ALA	ASN	GLU	ASN	PHE
E1980	R1819	E1639	Q1567	ASN	ALA	GLU	PHE	PHE	GLN	LEU	LEU	LEU	PHE
H1984	D1820	I1640	F1568	ALA	GLU	GLU	THR	THR	VAL	ASP	ILE	ARG	GLN
H1985	D1831	K1645	Q1569	ILE	VAL	VAL	PRO	GLN	ILE	MET	GLY	GLY	LYS
S1986	L1839	N1646	S1570	VAL	GLN	GLN	SER	SER	ARG	PRO	ASN	ASN	VAL
N1987	R1843	K1652	I1571	LYS	ASP	ASP	TRP	LYS	LYS	GLY	VAL	GLU	VAL
P1988		H1653	S1572	ASP	LEU	LEU	THR	SER	ALA	GLY	PRO	ILE	ASP
N1989	K1849	I1664	T1573	LEU	VAL	VAL	ARG	GLY	THR	VAL	LEU	LEU	LEU
Y1990	Q1850	L1576	L1576	VAL	GLY	GLY	ASN	GLU	THR	ALA	ASN	ILE	ILE
D1991	T1851	A1577	A1577	TYR	TYR	MET	PRO	GLU	GLU	ASP	PRO	VAL	GLU
K1992	D1852	L1578	L1578	GLN	GLN	GLY	SER	GLU	GLU	ASN	PRO	ARG	GLU
T1993	V1853	K1579	K1580	GLY	ILE	LYS	GLU	ALA	GLY	GLY	ILE	LEU	GLY
S1994	L1854	R1581	K1581	ASN	ASN	ASN	LEU	SER	LEU	TYR	GLY	ALA	ILE
A1995	Q1855	V1582	V1582	LEU	LEU	LEU	VAL	GLN	GLY	ALA	CYS	ARG	ASP
	Q1856	S1583	S1583	VAL	VAL	VAL	ALA	ALA	GLY	VAL	TYR	ARG	LEU
L2001	N1867	E1679	K1584	ILE	TRP	TRP	LEU	THR	ALA	VAL	LYS	LYS	GLU
L2002	Y1872	E1680	K1584	GLU	GLU	GLU	THR	ALA	PHE	GLY	GLY	ALA	VAL
I2016	L1873	G1681	S1585	LEU	ILE	ILE	THR	THR	ASP	GLY	TRP	ARG	THR
	D1877	E1682	P1586	LYS	ASP	ASP	GLY	SER	PRO	VAL	GLN	GLN	GLY
R2025	K1878	I1692	L1587	SER	GLN	GLN	GLY	GLY	MET	VAL	GLU	VAL	THR
	L1879	T1693	V1588	GLU	MET	GLY	LYS	LYS	ARG	ALA	LEU	ILE	CYS
D2030	C1888	E1706	M1589	ALA	LYS	GLY	PHE	GLY	ARG	VAL	VAL	ILE	MET
L2031	R1887	M1709	D1590	LEU	GLN	GLN	GLY	THR	ASP	GLN	GLN	ALA	GLY
L2032	C1888	I1713	V1591	LYS	PRO	PRO	ARG	ARG	ILE	VAL	VAL	VAL	TYR
M2041	S1903	L1717	L1592	ASP	TRP	TRP	LYS	LYS	ALA	LYS	ASN	ASN	GLY
D2045	P1907	K1729	N1593	ARG	VAL	VAL	ASP	ASP	ILE	VAL	VAL	VAL	GLY
R2046	T1910	A1730	Q1595	HIS	GLN	GLN	GLY	GLY	GLN	TRP	LEU	LEU	LEU
Q2047	G1911	I1731	G1596	LEU	ASN	ASN	PRO	GLY	GLN	GLN	GLN	GLN	GLY
L2048	K1912	T1731	V1597	TRP	VAL	VAL	ARG	GLY	GLY	TRP	LEU	LEU	GLY
L2049	T1913	S1732	Q1598	LYS	LYS	LYS	CYS	CYS	ALA	ASN	PRO	ARG	LEU
E2063	E1914	R1749	R1599	ARG	ARG	ARG	ALA	ALA	ASN	GLN	GLN	GLN	ILE
A2066	H1921	M1769	S1600	HIS	VAL	VAL	ILE	ILE	LYS	ASP	GLN	GLN	ASN
N2067	R1925	G1770	L1601	ASN	ASN	ASN	VAL	VAL	TRP	MET	ARG	PRO	LYS
K2068	F1930	D1606	E1602	TRP	VAL	VAL	ALA	ALA	ASP	GLN	GLN	GLN	ALA
L2069	F1930	L1607	R1603	VAL	VAL	VAL	GLU	GLU	VAL	ALA	GLN	VAL	VAL
V2070	G1771	L1608		SER	SER	SER	LEU	LEU	GLU	SER	VAL	SER	ASP
P2071	G1772	G1609		GLU	GLU	GLU	THR	THR	ASP	GLY	GLY	GLY	ASP
L2075	D1933	K1610		LEU	LEU	LEU	ALA	ALA	ARG	ILE	VAL	VAL	LEU
E1934	E1934	I1611		THR	THR	THR	VAL	VAL	VAL	TRP	GLY	GLY	ASN
T1935	T1935	Q1612		LEU	LEU	LEU	GLY	GLY	GLY	ASN	TYR	TYR	ASN
M1941	M1941	K1613		LEU	LEU	LEU	GLY	GLY	GLY	ASN	GLY	GLY	LEU
Q1950	Q1950	E1617		GLY	GLY	GLY	SER	SER	SER	ARG	GLY	GLY	HIS
E1959	E1959	Y1618		LEU	LEU	LEU	GLY	GLY	GLY	LEU	LEU	LEU	GLY
F1960	F1960	L1619		GLN	GLN	GLN	THR	THR	THR	GLY	GLY	GLY	TYR
R1966	R1966	E1620		ILE	ILE	ILE	PRO	PRO	PRO	GLY	GLY	GLY	LYS
		R1621		ASP	ASP	ASP	ALA	ALA	ALA	ASP	ASP	ASP	ASN
K2104	L1792	E1622		VAL	VAL	VAL	ARG	ARG	ARG	LEU	LEU	LEU	LEU
E2117	A1793			ASP	ASP	ASP	VAL	VAL	VAL	ASN	ASN	ASN	ASN
R2118	D1794			GLY	GLY	GLY	THR	THR	THR	GLY	GLY	GLY	GLY
G2119	L1811			LYS	LYS	LYS	THR	THR	THR	ASP	ASP	ASP	ASP
E2120	E1814			GLN	GLN	GLN	ALA	ALA	ALA	LEU	LEU	LEU	LEU
A2121	L1815			LYS	LYS	LYS	VAL	VAL	VAL	GLY	GLY	GLY	GLY

D3557	I3455	TRP	GLN	V3215	M3068	L2933	D2697	A2529	M2423	V2291	V2122
R3558	S3456	LYS	MET	E3216	N3069	G2937	V2701	P2530	V2433	R2292	D2123
R3559	E3457	ILE	SER	E3217	R3070	G2937	V2701	N2531	V2433		
R3560	A3458	ARG	LYS	L3218	E3073	L2961	Q2707	Y2537	E2444	K2297	E2126
R3562	Q3459	SER	GLU	R3219	D3077	R2962	F2708	E2538	L2449	D2308	N2130
Q3563	A3460	ILE	ASP	R3220	D3077	R2965	R2726	E2538	T2450		
D3570	I3461	ILE	LEU	R3221	T3081	R2966	R2729	T2541	R2451	D2308	L2131
D3571	A3462	MET	ASP	L3222	D3096	T2967	R2729	W2545	L2452	E2313	Q2134
E3575	A3463	GLN	LYS	R3223	M3097	T2968	V2731	W2548	R2453	N2316	
M3579	D3464	ASN	GLU	L3224	W3097	G2969	P2732	W2548	C2454		T2138
L3580	L3465	PRO	PRO	K3225	F3109	E2970		D2566	S2457	T2326	Q2139
L3588	A3466	ILE	VAL	S3226	M3113	E2974	L2759	T2571	M2461	N2338	M2145
R3582	A3467	THR	ILE	Q3227	D3114	D2975	M2773	T2571	L2462	F2343	L2149
	V3468	VAL	GLU	E3228	D3114	L2976	V2774	V2575	Q2464	E2344	V2150
R3585	A3469	ASN	GLN	L3229	Y3125	R2977	E2775	R2576	A2465	Q2346	L2156
L3588	A3470	PHE	ASN	E3230	V3125	L2980	I2793	L2581	A2466	D2347	L2157
	N3473	SER	ALA	R3231	V3129	L2980	W2802	P2590	R2467	L2348	F2158
R3474	R3474	GLU	VAL	V3231	V3129	D2985	P2802	P2590	Y2472	V2356	L2161
S3475	S3475	GLU	LYS	K3232	L3133	E2986	R2811	L2593	N2475	L2369	F2165
		LYS	SER	N3233	P3134	N2997	R2811	L2593	N2475	N2377	Y2170
		ILE	LYS	A3234	Q3135	N2998	L2816	L2593	Q2485	L2382	R2171
		LYS	LYS	A3235	Q3135	D3001	P2817	F2606	R2485	D2388	R2172
		ASP	LYS	A3236	P3136	S3002	V2818	V2617	R2488	E2389	G2173
		ALA	GLN	N3237	P3137	G3003	W2825	L2620	Y2489	GLY	E2174
		ALA	ILE	N3237	R3140	E3006	L2822	L2620	GLY	ASP	A2177
		ARG	LEU	D3238	E3141	R3007	W2825	S2623	GLY	ASP	
		LYS	GLU	K3239	A3142	R3007		S2624	GLY	ASP	E2181
		VAL	VAL	L3240	I3143	M3008			ALA	GLN	K2184
		LYS	ARG	K3241	V3144	N3009			ARG	ARG	E2188
		LYS	SER	K3242	V3148				ARG	ARG	M2189
		ASN	MET	K3242	F3149				LYS	LYS	Y2190
		ALA	ALA						LYS	LYS	E2205
		ASN	ASN						GLY	GLY	
		GLU	ASN						GLY	GLY	
		GLU	ASN						GLY	GLY	
		VAL	ASN						GLY	GLY	
		VAL	PRO						GLY	GLY	
		ASN	PRO						GLY	GLY	
		ASN	PRO						GLY	GLY	
		PRO	ALA						GLY	GLY	
		ALA	ALA						GLY	GLY	
		GLN	ALA						GLY	GLY	
		SER	ALA						GLY	GLY	
		TYR	VAL						GLY	GLY	
		ASN	ASN						GLY	GLY	
		ASP	GLU						GLY	GLY	
		ASP	GLU						GLY	GLY	
		GLU	LEU						GLY	GLY	
		LYS	LEU						GLY	GLY	
		ASN	ASN						GLY	GLY	
		ASN	ASN						GLY	GLY	
		ASN	ASN						GLY	GLY	
		ASN	ASN						GLY	GLY	
		ASN	ASN						GLY	GLY	
		ASN	ASN						GLY	GLY	
		ASN	ASN						GLY	GLY	
		ASN	ASN						GLY	GLY	
		ASN	ASN						GLY	GLY	
		ASN	ASN						GLY	GLY	
		ASN	ASN						GLY	GLY	
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		ASN	ASN						GLY	GLY	
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		ASN	ASN						GLY	GLY	
		ASN	ASN						GLY	GLY	
		ASN	ASN						GLY	GLY	
		ASN	ASN						GLY	GLY	
		ASN	ASN						GLY	GLY	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40850	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	1.898	Depositor
Minimum map value	-1.110	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.3	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, 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	0.15	0/24093	0.31	1/32651 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4628	THR	CB-CA-C	-5.07	110.71	116.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4633	ARG	Sidechain

5.2 Too-close contacts

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	23658	387	0
2	A	81	0	36	3	0
3	A	31	0	12	0	0
4	A	1	0	0	0	0
All	All	23706	0	23706	387	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 8.

All (387) 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:4574:LYS:HB3	1:A:4627:ALA:HB2	1.46	0.98
1:A:1480:TYR:HB2	1:A:1486:LEU:HD11	1.57	0.85
1:A:1526:LYS:HA	1:A:1529:ARG:HD3	1.62	0.82
1:A:2092:ALA:HB1	1:A:2145:MET:HE1	1.63	0.78
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.66	0.77
1:A:4260:PHE:HD1	1:A:4263:ARG:HH21	1.31	0.77
1:A:1523:TRP:HA	1:A:1526:LYS:HE3	1.70	0.74
1:A:1543:ARG:HA	1:A:1546:TYR:CE2	2.22	0.74
1:A:3502:THR:HG21	1:A:3544:ARG:HG3	1.70	0.71
1:A:4630:GLU:HB3	1:A:4635:PHE:HE1	1.55	0.71
1:A:3487:GLU:OE2	1:A:3491:LYS:NZ	2.22	0.71
1:A:2205:GLU:OE1	1:A:2209:GLN:NE2	2.24	0.71
1:A:1486:LEU:HA	1:A:1579:MET:HE1	1.73	0.70
1:A:3909:LEU:HD21	1:A:4343:MET:HE2	1.73	0.70
1:A:2075:LEU:HD13	1:A:2160:LEU:HD11	1.74	0.70
1:A:1497:VAL:HG13	1:A:1527:LEU:HD22	1.73	0.69
1:A:3481:SER:O	1:A:3774:LYS:NZ	2.26	0.68
1:A:3557:ASP:OD2	1:A:3743:ARG:NH1	2.26	0.68
1:A:2257:LYS:HE3	1:A:2676:THR:HG21	1.76	0.68
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.27	0.68
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.76	0.67
1:A:1652:LYS:HG3	1:A:1653:HIS:HD2	1.60	0.67
1:A:1930:PHE:HA	1:A:2326:THR:HG21	1.76	0.67
1:A:2080:LEU:HD23	1:A:2156:LEU:HD22	1.75	0.67
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.25	0.66
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	1.79	0.65
1:A:1477:LEU:HB3	1:A:1485:ARG:HB3	1.79	0.65
1:A:1546:TYR:CE1	1:A:1638:LEU:HB3	2.32	0.64
1:A:2615:MET:SD	1:A:2707:GLN:NE2	2.70	0.64
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.77	0.64
1:A:4088:VAL:HG11	1:A:4116:LEU:HD21	1.79	0.64
1:A:3931:GLN:O	1:A:3935:VAL:HG23	1.98	0.64
1:A:4525:ARG:HD3	1:A:4536:LEU:HD23	1.80	0.64
1:A:2083:GLN:HE21	1:A:2150:VAL:HG11	1.63	0.63
1:A:2313:GLU:OE1	1:A:2316:ASN:ND2	2.29	0.63
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.80	0.63
1:A:1587:LEU:HB3	1:A:1590:ASP:HB2	1.81	0.63
1:A:4409:LEU:O	1:A:4413:PHE:HB2	1.98	0.63
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.79	0.62
1:A:2847:ASP:OD1	1:A:2869:ARG:NH1	2.32	0.62
1:A:4518:GLU:OE2	1:A:4518:GLU:N	2.31	0.62
1:A:2581:LEU:HD11	1:A:2593:LEU:HD21	1.82	0.62
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.80	0.62
1:A:3830:GLN:NE2	1:A:3834:ASP:OD2	2.33	0.61
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.33	0.61
1:A:2075:LEU:HB3	1:A:2160:LEU:HD21	1.83	0.61
1:A:2864:GLU:OE2	1:A:2864:GLU:N	2.34	0.61
1:A:4605:VAL:HG23	1:A:4636:TYR:HE1	1.66	0.61
1:A:1497:VAL:HG11	1:A:1531:MET:HG2	1.83	0.61
1:A:1535:ASP:O	1:A:2292:ARG:NH2	2.34	0.61
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.81	0.60
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.84	0.60
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.33	0.60
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.83	0.60
1:A:3655:ARG:HG2	1:A:3660:VAL:HG22	1.82	0.60
1:A:3597:THR:HG23	1:A:3634:LEU:HD21	1.83	0.60
1:A:2925:ILE:HG21	1:A:2933:LEU:HG	1.83	0.59
1:A:2995:ASP:OD1	1:A:2996:GLU:N	2.35	0.59
1:A:3970:VAL:HB	1:A:3989:ARG:HD3	1.83	0.59
1:A:2624:SER:HB3	1:A:3081:THR:HA	1.85	0.59
1:A:2654:GLN:NE2	1:A:3048:GLU:OE2	2.35	0.59
1:A:3935:VAL:HG22	1:A:3996:PHE:HE1	1.67	0.59
1:A:1543:ARG:HA	1:A:1546:TYR:HE2	1.64	0.59
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.84	0.59
1:A:2517:TYR:HA	1:A:2520:ARG:HD3	1.86	0.58
1:A:4525:ARG:HG3	1:A:4592:TRP:CZ3	2.38	0.58
1:A:3611:ARG:NH1	1:A:3636:GLN:OE1	2.33	0.58
1:A:3792:GLN:O	1:A:3796:THR:HG23	2.03	0.58
1:A:2257:LYS:NZ	1:A:2308:ASP:OD2	2.36	0.58
1:A:1546:TYR:HE1	1:A:1638:LEU:HB3	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4607:LEU:HD13	1:A:4624:PHE:HD2	1.69	0.58
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.37	0.58
1:A:4525:ARG:NH2	1:A:4536:LEU:O	2.32	0.57
1:A:3207:LYS:NZ	1:A:3756:VAL:O	2.38	0.57
1:A:3581:LYS:HE3	1:A:3582:ARG:HG3	1.85	0.57
1:A:3721:ARG:HE	1:A:3724:VAL:HG21	1.69	0.57
1:A:3491:LYS:O	1:A:3495:THR:HG23	2.05	0.57
1:A:2495:VAL:HG21	1:A:2524:VAL:HG21	1.85	0.56
1:A:3967:GLU:HB2	1:A:4004:MET:HE2	1.87	0.56
1:A:2138:ILE:HD12	1:A:2161:LEU:HD22	1.88	0.56
1:A:3487:GLU:O	1:A:3491:LYS:HG2	2.05	0.56
1:A:4413:PHE:HE1	1:A:4492:ILE:HG23	1.70	0.55
1:A:1713:LEU:HD11	1:A:1872:TYR:HB2	1.88	0.55
1:A:1959:GLU:OE2	1:A:2025:ARG:NH1	2.40	0.55
1:A:4190:ILE:HD12	1:A:4201:TRP:HZ2	1.72	0.55
1:A:1539:ASP:OD2	1:A:1543:ARG:NH2	2.39	0.55
1:A:1589:MET:SD	1:A:1589:MET:N	2.80	0.55
1:A:1619:LEU:HD11	1:A:1638:LEU:HD13	1.89	0.55
1:A:2498:ILE:HG23	1:A:2502:LEU:HD22	1.89	0.55
1:A:2138:ILE:HD11	1:A:2165:PHE:CG	2.42	0.54
1:A:3990:LEU:HA	1:A:4004:MET:HG2	1.89	0.54
1:A:4503:GLU:O	1:A:4507:ILE:HG23	2.08	0.54
1:A:1792:LEU:HD21	1:A:1811:LEU:HB3	1.88	0.54
1:A:1914:GLU:HG3	2:A:4701:ADP:H2'	1.88	0.54
1:A:3951:VAL:HG12	1:A:3973:LEU:HD21	1.87	0.54
1:A:3779:GLU:O	1:A:3783:LYS:HG2	2.07	0.54
1:A:2517:TYR:CE2	1:A:2521:ILE:HD13	2.42	0.54
1:A:4107:MET:HG3	1:A:4137:ASN:HD21	1.72	0.54
1:A:3947:LEU:O	1:A:3951:VAL:HG13	2.08	0.54
1:A:2773:MET:HG2	1:A:2825:TRP:HE1	1.73	0.54
1:A:2159:SER:OG	1:A:4411:ARG:NH1	2.42	0.53
1:A:2968:THR:OG1	1:A:2969:GLY:N	2.40	0.53
1:A:1985:HIS:O	1:A:1985:HIS:ND1	2.40	0.53
1:A:4544:ASN:HA	1:A:4573:ASN:HD21	1.74	0.53
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.89	0.53
1:A:2449:LEU:HA	1:A:2453:ARG:HH21	1.73	0.53
1:A:2156:LEU:HG	1:A:4411:ARG:HD2	1.90	0.53
1:A:2623:SER:OG	1:A:3006:GLU:OE1	2.23	0.53
1:A:3045:ASP:OD1	1:A:3046:SER:N	2.42	0.53
1:A:3030:MET:HA	1:A:3030:MET:HE3	1.91	0.53
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4293:ASP:N	1:A:4293:ASP:OD1	2.40	0.52
1:A:3791:MET:O	1:A:3795:GLU:HG3	2.09	0.52
1:A:4400:ARG:HD2	1:A:4405:ILE:HD11	1.92	0.52
1:A:4560:VAL:HB	1:A:4588:THR:HB	1.92	0.52
1:A:1501:ILE:HG13	1:A:1527:LEU:HD13	1.91	0.52
1:A:2291:VAL:HG13	1:A:2292:ARG:HG3	1.92	0.52
1:A:3459:GLN:HA	1:A:3462:LYS:HD2	1.91	0.52
1:A:2461:MET:HE2	1:A:2497:ALA:HA	1.91	0.52
1:A:3782:ARG:HA	1:A:3785:GLU:OE2	2.08	0.52
1:A:2485:GLN:OE1	1:A:2488:ARG:NH2	2.42	0.52
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.45	0.52
1:A:4412:PHE:HZ	1:A:4514:LEU:HD13	1.75	0.52
1:A:1671:SER:HA	1:A:1692:ILE:HG12	1.92	0.52
1:A:3914:ILE:O	1:A:3937:ARG:NH1	2.43	0.52
1:A:1912:LYS:HG3	2:A:4701:ADP:O3B	2.09	0.51
1:A:1987:ASN:OD1	1:A:1989:ASN:ND2	2.44	0.51
1:A:2080:LEU:O	1:A:4415:ARG:NH1	2.43	0.51
1:A:3916:LEU:HD11	1:A:3937:ARG:HG3	1.91	0.51
1:A:3875:MET:HE1	1:A:3883:PHE:HB2	1.92	0.51
1:A:3559:ARG:O	1:A:3563:GLN:HG2	2.09	0.51
1:A:1543:ARG:O	1:A:1547:LEU:HB2	2.11	0.51
1:A:2644:THR:OG1	1:A:2647:GLY:O	2.28	0.51
1:A:1550:ILE:O	1:A:1554:SER:OG	2.27	0.51
1:A:3723:ASP:O	1:A:3726:GLU:HG2	2.11	0.51
1:A:1467:ARG:HB2	1:A:1523:TRP:HH2	1.75	0.51
1:A:1504:VAL:HG11	1:A:1524:GLU:HG3	1.92	0.51
1:A:1475:LEU:HG	1:A:1487:ILE:HG23	1.92	0.50
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.12	0.50
1:A:4153:VAL:O	1:A:4157:MET:HG3	2.11	0.50
1:A:1542:ARG:O	1:A:1546:TYR:HD2	1.94	0.50
1:A:4099:VAL:HG23	1:A:4106:LEU:HD11	1.93	0.50
1:A:4412:PHE:CZ	1:A:4514:LEU:HD13	2.47	0.50
1:A:1490:TRP:HZ3	1:A:1534:PHE:HD2	1.59	0.50
1:A:2463:HIS:O	1:A:2467:ARG:HG3	2.11	0.50
1:A:3154:LEU:HD21	1:A:3532:TRP:HZ2	1.75	0.50
1:A:3786:GLU:O	1:A:3790:VAL:HG23	2.12	0.50
1:A:4288:VAL:O	1:A:4319:SER:OG	2.28	0.50
1:A:4566:GLN:OE1	1:A:4582:SER:OG	2.27	0.50
1:A:2974:GLU:OE1	1:A:2977:ARG:NH1	2.44	0.50
1:A:4496:ALA:HB2	1:A:4504:LEU:HD21	1.94	0.50
1:A:2348:LEU:HD13	1:A:2356:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2620:LEU:HD11	1:A:2661:LEU:HD23	1.93	0.50
1:A:3008:MET:HE3	1:A:3008:MET:HA	1.93	0.50
1:A:4540:CYS:HB3	1:A:4595:GLN:HG2	1.93	0.50
1:A:1879:LEU:HB3	2:A:4701:ADP:C6	2.46	0.50
1:A:2172:ARG:NH1	1:A:2205:GLU:OE2	2.44	0.50
1:A:2461:MET:CE	1:A:2497:ALA:HA	2.42	0.50
1:A:2694:ARG:HG3	1:A:2701:VAL:HG21	1.94	0.50
1:A:3036:GLY:O	1:A:3040:GLU:HG2	2.12	0.50
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.93	0.50
1:A:1903:SER:HA	1:A:2016:ILE:O	2.12	0.49
1:A:1652:LYS:HG3	1:A:1653:HIS:CD2	2.45	0.49
1:A:3144:VAL:O	1:A:3148:VAL:HG23	2.11	0.49
1:A:4388:LEU:HD21	1:A:4431:LEU:HB3	1.94	0.49
1:A:2454:CYS:HB3	1:A:2502:LEU:HD12	1.95	0.49
1:A:2996:GLU:HG2	1:A:3068:MET:HA	1.94	0.49
1:A:1706:GLU:O	1:A:1709:MET:HG2	2.12	0.49
1:A:4509:VAL:HG11	1:A:4514:LEU:HD11	1.94	0.49
1:A:3114:ASP:O	1:A:3140:ARG:NH2	2.45	0.49
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.95	0.49
1:A:2818:VAL:O	1:A:2822:ILE:HG12	2.13	0.49
1:A:3932:ALA:O	1:A:3936:VAL:HG13	2.13	0.49
1:A:2495:VAL:CG2	1:A:2524:VAL:HG21	2.43	0.48
1:A:3499:GLN:O	1:A:3503:ILE:HG13	2.13	0.48
1:A:4171:LYS:HG3	1:A:4172:SER:H	1.77	0.48
1:A:2521:ILE:HG13	1:A:2522:THR:N	2.28	0.48
1:A:3154:LEU:HD11	1:A:3516:TYR:HB3	1.94	0.48
1:A:3775:ARG:O	1:A:3779:GLU:HG2	2.13	0.48
1:A:4397:HIS:CE1	1:A:4418:LYS:HG3	2.48	0.48
1:A:4520:TYR:O	1:A:4524:THR:HG23	2.13	0.48
1:A:3149:PHE:O	1:A:3153:THR:HG22	2.13	0.48
1:A:2045:ASP:O	1:A:2049:ILE:HG13	2.13	0.48
1:A:2418:ASP:O	1:A:2422:ILE:HG12	2.14	0.48
1:A:3211:THR:O	1:A:3215:VAL:HG13	2.13	0.48
1:A:3974:TRP:HZ2	1:A:3985:GLN:HG2	1.79	0.48
1:A:4042:LEU:HD22	1:A:4128:MET:HE1	1.95	0.48
1:A:4413:PHE:CE1	1:A:4492:ILE:HG23	2.48	0.48
1:A:3502:THR:HG23	1:A:3543:PHE:HA	1.95	0.48
1:A:2901:TYR:OH	1:A:2909:LEU:N	2.47	0.48
1:A:1980:GLU:O	1:A:1984:GLU:HG2	2.14	0.48
1:A:4397:HIS:NE2	1:A:4418:LYS:HA	2.29	0.47
1:A:3113:MET:SD	1:A:3184:ALA:HA	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3724:VAL:HG21	1:A:3797:VAL:HG11	1.97	0.47
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.96	0.47
1:A:3154:LEU:HB3	1:A:3171:ILE:HD13	1.96	0.47
1:A:4450:THR:HG22	1:A:4454:GLU:OE2	2.14	0.47
1:A:4511:LEU:HD11	1:A:4521:ILE:HD11	1.96	0.47
1:A:1709:MET:HE2	1:A:1872:TYR:H	1.80	0.47
1:A:1853:VAL:HA	1:A:1856:GLN:HG3	1.97	0.47
1:A:1526:LYS:O	1:A:1530:ILE:HG13	2.15	0.47
1:A:1985:HIS:HD1	1:A:1985:HIS:C	2.22	0.47
1:A:2606:PHE:HE1	1:A:2617:VAL:HG21	1.80	0.47
1:A:2527:PRO:HD3	1:A:2545:TRP:CE2	2.50	0.47
1:A:3585:ARG:NH1	1:A:3694:SER:O	2.38	0.47
1:A:3779:GLU:O	1:A:3782:ARG:HG2	2.14	0.47
1:A:4415:ARG:HB3	1:A:4419:MET:HE3	1.96	0.47
1:A:1466:ILE:HB	1:A:1523:TRP:HZ3	1.80	0.47
1:A:1619:LEU:HD21	1:A:1638:LEU:HD12	1.97	0.47
1:A:4302:ARG:O	1:A:4306:VAL:HG23	2.14	0.47
1:A:4626:ILE:HD12	1:A:4630:GLU:O	2.15	0.47
1:A:1477:LEU:HA	1:A:1486:LEU:O	2.16	0.46
1:A:3225:LYS:HZ1	1:A:3464:ASP:HB3	1.79	0.46
1:A:2571:THR:O	1:A:2575:VAL:HG22	2.15	0.46
1:A:4525:ARG:HH21	1:A:4536:LEU:C	2.20	0.46
1:A:2967:TYR:OH	1:A:2975:ASP:OD2	2.27	0.46
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	1.97	0.46
1:A:2816:LEU:HD23	1:A:2817:PRO:O	2.16	0.46
1:A:4049:TYR:OH	1:A:4149:PRO:HG3	2.15	0.46
1:A:3653:VAL:HG12	1:A:3662:ILE:HB	1.97	0.46
1:A:2457:SER:OG	1:A:2732:PRO:HB3	2.14	0.46
1:A:3650:ASN:HD21	1:A:3695:ARG:HH11	1.63	0.46
1:A:4408:PRO:HG3	1:A:4526:GLN:HB3	1.98	0.46
1:A:3753:LEU:HD21	1:A:3770:LEU:HD21	1.97	0.46
1:A:2063:GLU:O	1:A:2067:ASN:ND2	2.48	0.46
1:A:3039:LYS:HB3	1:A:3039:LYS:HE3	1.75	0.46
1:A:4384:ALA:O	1:A:4388:LEU:HG	2.16	0.46
1:A:4205:TYR:OH	1:A:4261:ASP:OD2	2.25	0.46
1:A:2612:LEU:HB3	1:A:2615:MET:HG3	1.98	0.45
1:A:2905:LEU:HD11	1:A:3652:GLU:HB3	1.98	0.45
1:A:4489:LEU:HA	1:A:4492:ILE:HB	1.98	0.45
1:A:2548:TRP:CD1	1:A:2576:ARG:HG2	2.51	0.45
1:A:3154:LEU:HB3	1:A:3171:ILE:CD1	2.46	0.45
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1599:ARG:O	1:A:1603:ARG:HG2	2.17	0.45
1:A:1645:LYS:HD2	1:A:1645:LYS:HA	1.76	0.45
1:A:3229:LEU:HD11	1:A:3462:LYS:HG3	1.99	0.45
1:A:2423:MET:HG2	1:A:2494:LEU:HD13	1.98	0.45
1:A:4194:LEU:HD21	1:A:4205:TYR:O	2.16	0.45
1:A:4391:ILE:O	1:A:4428:ARG:NH1	2.50	0.45
1:A:1486:LEU:HD12	1:A:1486:LEU:H	1.82	0.45
1:A:2665:GLU:HB3	1:A:2668:LEU:HD12	1.98	0.45
1:A:3143:ILE:HD13	1:A:3541:ILE:HD13	1.99	0.45
1:A:2419:ALA:O	1:A:2423:MET:HE2	2.17	0.45
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.52	0.44
1:A:3558:GLU:HG3	1:A:3561:ARG:HH12	1.82	0.44
1:A:3720:GLU:OE1	1:A:3855:ARG:NE	2.47	0.44
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.52	0.44
1:A:4413:PHE:O	1:A:4417:VAL:HG23	2.17	0.44
1:A:2423:MET:HE3	1:A:2423:MET:HB2	1.86	0.44
1:A:2297:LYS:O	1:A:2338:ASN:ND2	2.47	0.44
1:A:2872:LEU:HD22	1:A:2920:LEU:HD12	1.99	0.44
1:A:1814:GLU:O	1:A:1818:GLN:HG3	2.17	0.44
1:A:4430:ASP:OD2	1:A:4447:TYR:OH	2.34	0.44
1:A:4574:LYS:HB3	1:A:4627:ALA:CB	2.33	0.44
1:A:1581:LYS:HE3	1:A:1594:ILE:HD13	2.00	0.44
1:A:1640:ILE:HD11	1:A:1653:HIS:HB3	2.00	0.44
1:A:2472:TYR:HB2	1:A:2541:ILE:HG12	1.99	0.44
1:A:1527:LEU:HD23	1:A:1530:ILE:HD12	2.00	0.44
1:A:1888:CYS:HB2	1:A:2041:MET:HE3	2.00	0.44
1:A:3457:GLU:O	1:A:3461:ILE:HG12	2.18	0.44
1:A:3575:GLU:O	1:A:3579:MET:HG3	2.18	0.44
1:A:4528:VAL:HG21	1:A:4592:TRP:CD1	2.53	0.44
1:A:3478:LEU:HD22	1:A:3767:ILE:HG23	1.99	0.43
1:A:4408:PRO:HB3	1:A:4411:ARG:HH21	1.83	0.43
1:A:1769:MET:HG2	1:A:1777:PRO:HD2	2.00	0.43
1:A:1960:PHE:HE2	1:A:2032:LEU:HD21	1.83	0.43
1:A:2369:LEU:O	1:A:2451:ARG:NH1	2.47	0.43
1:A:1664:ILE:HG22	1:A:1676:ILE:HG22	2.01	0.43
1:A:2177:ALA:O	1:A:2181:GLU:HG2	2.18	0.43
1:A:2444:GLU:HB2	1:A:2510:MET:HE3	2.00	0.43
1:A:4581:ILE:HD13	1:A:4581:ILE:HA	1.90	0.43
1:A:2495:VAL:HG21	1:A:2524:VAL:CG2	2.49	0.43
1:A:2623:SER:HB3	1:A:3009:ASN:HD22	1.82	0.43
1:A:4021:MET:HA	1:A:4021:MET:HE2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1462:PHE:HB2	1:A:1507:MET:HE1	2.01	0.43
1:A:1850:GLN:HB3	1:A:1856:GLN:HG2	2.00	0.43
1:A:2184:LYS:O	1:A:2188:GLU:HG3	2.18	0.43
1:A:1457:MET:HE3	1:A:1457:MET:HA	1.99	0.43
1:A:3891:LYS:HD2	1:A:4013:LEU:HD23	2.00	0.43
1:A:3944:PHE:HD1	1:A:3947:LEU:HD13	1.84	0.43
1:A:1487:ILE:HB	1:A:1490:TRP:CZ2	2.54	0.43
1:A:3818:LEU:HA	1:A:4346:MET:HE3	2.00	0.43
1:A:3829:LEU:HG	1:A:3833:LEU:HD23	2.01	0.43
1:A:4159:ARG:HE	1:A:4159:ARG:HB2	1.64	0.43
1:A:1933:ASP:OD1	1:A:1935:THR:HG22	2.19	0.43
1:A:3109:PHE:HB3	1:A:3180:ILE:HG21	2.00	0.43
1:A:3570:ASP:OD2	1:A:3571:ASP:N	2.52	0.43
1:A:3846:LEU:HD22	1:A:3855:ARG:HG2	2.00	0.43
1:A:4603:SER:O	1:A:4626:ILE:HG12	2.18	0.43
1:A:3835:ILE:HG12	1:A:3870:ARG:HD2	2.01	0.43
1:A:4281:GLU:OE2	1:A:4281:GLU:N	2.52	0.43
1:A:2344:GLU:HG2	1:A:2726:ARG:HH22	1.84	0.43
1:A:2530:PRO:HG2	1:A:2531:ASN:H	1.84	0.42
1:A:4042:LEU:HD13	1:A:4139:LEU:HD23	2.00	0.42
1:A:1671:SER:HB2	1:A:1693:THR:HG23	2.02	0.42
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.54	0.42
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.19	0.42
1:A:1572:SER:O	1:A:1576:LEU:HG	2.19	0.42
1:A:2970:GLU:OE1	1:A:2970:GLU:N	2.51	0.42
1:A:3133:LEU:HD11	1:A:3141:GLU:HB3	2.01	0.42
1:A:4543:VAL:HG21	1:A:4622:VAL:HG12	2.01	0.42
1:A:1467:ARG:HB2	1:A:1523:TRP:CH2	2.53	0.42
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.55	0.42
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	2.01	0.42
1:A:2758:LEU:HD13	1:A:2811:ARG:HA	2.00	0.42
1:A:3077:ASP:O	1:A:3081:THR:HG22	2.20	0.42
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	2.01	0.42
1:A:3716:VAL:HG21	1:A:3804:LEU:HD23	2.00	0.42
1:A:3833:LEU:HD13	1:A:3833:LEU:HA	1.91	0.42
1:A:1493:LEU:O	1:A:1497:VAL:HG23	2.20	0.42
1:A:1873:LEU:HD13	1:A:1921:HIS:HB3	2.01	0.42
1:A:2104:LYS:HG3	1:A:2131:LEU:HD21	2.02	0.42
1:A:2134:GLN:O	1:A:2138:ILE:HG12	2.19	0.42
1:A:2452:LEU:HD23	1:A:2452:LEU:HA	1.76	0.42
1:A:2686:MET:HE3	1:A:2708:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3017:VAL:HB	1:A:3020:LEU:HB2	2.02	0.42
1:A:3026:TYR:O	1:A:3030:MET:HG2	2.18	0.42
1:A:4424:LEU:HA	1:A:4482:PHE:HZ	1.85	0.42
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	2.00	0.42
1:A:4626:ILE:CD1	1:A:4632:PRO:HD3	2.50	0.42
1:A:3886:LEU:O	1:A:3890:ILE:HG12	2.19	0.42
1:A:4534:TRP:HE3	1:A:4539:LEU:HD21	1.84	0.42
1:A:1792:LEU:HD22	1:A:1815:LEU:HD22	2.02	0.42
1:A:3772:ASN:HA	1:A:3775:ARG:HH11	1.85	0.42
1:A:2190:TYR:O	1:A:2377:ASN:ND2	2.34	0.42
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	2.01	0.42
1:A:2002:LEU:HD23	1:A:2002:LEU:HA	1.85	0.42
1:A:2980:LEU:HB3	1:A:3054:PHE:HZ	1.85	0.42
1:A:3487:GLU:C	1:A:3491:LYS:HZ3	2.28	0.42
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	2.02	0.42
1:A:3207:LYS:HD3	1:A:3207:LYS:HA	1.86	0.42
1:A:3454:LEU:O	1:A:3457:GLU:HG2	2.19	0.42
1:A:3906:GLN:NE2	1:A:3910:ARG:HD2	2.35	0.42
1:A:4297:PRO:HG3	1:A:4308:TRP:CD2	2.54	0.42
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.52	0.41
1:A:2697:ASP:OD1	1:A:2697:ASP:N	2.51	0.41
1:A:3753:LEU:HD23	1:A:3753:LEU:HA	1.81	0.41
1:A:4619:ILE:HD13	1:A:4619:ILE:HA	1.93	0.41
1:A:1466:ILE:HG23	1:A:1500:HIS:CE1	2.55	0.41
1:A:1985:HIS:ND1	1:A:1985:HIS:C	2.78	0.41
1:A:2382:LEU:HG	1:A:2420:ALA:HB2	2.02	0.41
1:A:3983:ILE:O	1:A:3987:ILE:HG13	2.19	0.41
1:A:1547:LEU:HD23	1:A:1547:LEU:HA	1.79	0.41
1:A:1887:ARG:HD2	1:A:4249:GLN:HG2	2.02	0.41
1:A:2529:ALA:HB2	1:A:2537:TYR:OH	2.20	0.41
1:A:3692:LEU:O	1:A:3696:VAL:HG22	2.20	0.41
1:A:1907:PRO:HG2	1:A:1910:THR:HG21	2.03	0.41
1:A:4095:MET:HE3	1:A:4097:LYS:HG2	2.02	0.41
1:A:2452:LEU:HD13	1:A:2729:ARG:HE	1.85	0.41
1:A:3955:GLU:OE2	1:A:3955:GLU:N	2.50	0.41
1:A:4590:LEU:HD12	1:A:4590:LEU:O	2.20	0.41
1:A:1546:TYR:CD1	1:A:1638:LEU:HB3	2.55	0.41
1:A:1831:ASP:OD1	1:A:1831:ASP:N	2.52	0.41
1:A:1854:LEU:H	1:A:1854:LEU:HD12	1.86	0.41
1:A:2507:ARG:HH22	1:A:2510:MET:HE2	1.85	0.41
1:A:1544:TRP:CZ2	1:A:1576:LEU:HD21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1717:LEU:HB2	1:A:1749:LEU:HD22	2.02	0.41
1:A:3892:LEU:HD13	1:A:3983:ILE:HG21	2.02	0.41
1:A:1500:HIS:HB3	1:A:1527:LEU:HD11	2.03	0.41
1:A:1547:LEU:HD12	1:A:1608:LEU:HD22	2.02	0.41
1:A:1564:GLU:HA	1:A:1567:ARG:HB2	2.03	0.41
1:A:1966:ARG:HA	1:A:4101:LEU:HD13	2.02	0.41
1:A:2490:ILE:HD13	1:A:2490:ILE:HA	1.90	0.41
1:A:2509:LYS:HE3	1:A:2509:LYS:HB3	1.75	0.41
1:A:2937:GLY:C	1:A:3070:PRO:HD3	2.46	0.41
1:A:1527:LEU:HD23	1:A:1527:LEU:HA	1.86	0.40
1:A:2793:ILE:O	1:A:2793:ILE:HG13	2.21	0.40
1:A:3003:GLY:O	1:A:3007:ARG:HG3	2.21	0.40
1:A:3588:LEU:HD11	1:A:3638:VAL:HG11	2.03	0.40
1:A:2139:GLN:HG3	1:A:2170:TYR:CE1	2.56	0.40
1:A:2224:GLY:O	1:A:2346:GLN:HA	2.21	0.40
1:A:4013:LEU:HD13	1:A:4017:PHE:CZ	2.56	0.40
1:A:1471:ASN:HA	1:A:1589:MET:HE1	2.03	0.40
1:A:1941:MET:HE3	1:A:1971:VAL:HG11	2.01	0.40
1:A:4271:ARG:HD3	1:A:4633:ARG:HH12	1.87	0.40
1:A:1513:TYR:HE1	1:A:1520:ALA:HB3	1.87	0.40
1:A:1867:ASN:O	1:A:1925:ARG:NH1	2.44	0.40
1:A:3045:ASP:OD1	1:A:3045:ASP:C	2.64	0.40
1:A:4043:MET:HE2	1:A:4147:PHE:CE1	2.57	0.40
1:A:4158:LEU:HD21	1:A:4310:GLU:HG3	2.04	0.40
1:A:1606:ASP:OD1	1:A:1610:LYS:HE3	2.21	0.40
1:A:2890:ARG:O	1:A:2894:LYS:HG3	2.21	0.40
1:A:3096:ASP:OD2	1:A:3097:TRP:N	2.54	0.40
1:A:4133:LYS:HB2	1:A:4133:LYS:HE2	1.82	0.40
1:A:4418:LYS:HE3	1:A:4418:LYS:HB2	1.82	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%)	2888 (99%)	40 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2530	PRO

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%)	2595 (100%)	10 (0%)	84	84

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

Mol	Chain	Res	Type
1	A	1634	ASP
1	A	1709	MET
1	A	2001	LEU
1	A	2247	VAL
1	A	2522	THR
1	A	2671	MET
1	A	3833	LEU
1	A	3875	MET
1	A	4413	PHE
1	A	4492	ILE

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

Mol	Chain	Res	Type
1	A	1465	GLN
1	A	1643	ASN
1	A	1653	HIS
1	A	1755	GLN
1	A	1922	GLN

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Mol	Chain	Res	Type
1	A	1979	GLN
1	A	1989	ASN
1	A	2067	ASN
1	A	2217	ASN
1	A	2263	HIS
1	A	2677	GLN
1	A	2960	GLN
1	A	3069	ASN
1	A	3200	HIS
1	A	3233	ASN
1	A	3237	ASN
1	A	3526	GLN
1	A	3744	GLN
1	A	3820	GLN
1	A	3838	ASN
1	A	3968	GLN
1	A	4029	HIS
1	A	4114	HIS
1	A	4156	ASN
1	A	4191	GLN
1	A	4307	GLN
1	A	4444	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	4701	-	28,29,29	0.46	0	43,45,45	0.49	0
2	ADP	A	4704	-	28,29,29	1.40	4 (14%)	43,45,45	1.82	8 (18%)
2	ADP	A	4703	-	28,29,29	1.39	4 (14%)	43,45,45	1.85	8 (18%)
3	ATP	A	4702	4	32,33,33	0.34	0	48,52,52	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	4701	-	-	2/16/32/32	0/3/3/3
2	ADP	A	4704	-	-	1/16/32/32	0/3/3/3
2	ADP	A	4703	-	-	2/16/32/32	0/3/3/3
3	ATP	A	4702	4	-	4/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4704	ADP	C5-C4	4.64	1.47	1.39
2	A	4703	ADP	C5-C4	4.62	1.47	1.39
2	A	4704	ADP	C5-C6	2.69	1.48	1.41
2	A	4703	ADP	C5-C6	2.66	1.48	1.41
2	A	4703	ADP	C5-N7	-2.36	1.34	1.39
2	A	4704	ADP	C5-N7	-2.30	1.34	1.39
2	A	4704	ADP	C8-N7	2.30	1.36	1.31
2	A	4703	ADP	C8-N7	2.23	1.36	1.31

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	C5-C4-N3	-5.95	118.52	126.72
2	A	4704	ADP	C5-C4-N3	-5.88	118.62	126.72
2	A	4703	ADP	N3-C4-N9	4.75	135.25	127.17
2	A	4704	ADP	N3-C4-N9	4.66	135.10	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	C2-N3-C4	3.75	120.99	111.83
2	A	4704	ADP	C2-N3-C4	3.71	120.89	111.83
2	A	4704	ADP	C4-C5-N7	-3.40	106.69	110.58
2	A	4703	ADP	C4-C5-N7	-3.35	106.76	110.58
2	A	4703	ADP	N3-C2-N1	-3.26	123.65	128.58
2	A	4704	ADP	N3-C2-N1	-3.19	123.76	128.58
2	A	4704	ADP	C4-N9-C8	2.57	108.43	105.74
2	A	4703	ADP	C3'-C2'-C1'	2.55	106.29	101.46
2	A	4703	ADP	C4-N9-C8	2.52	108.39	105.74
2	A	4703	ADP	C5-N7-C8	2.50	107.38	103.45
2	A	4704	ADP	C5-N7-C8	2.44	107.28	103.45
2	A	4704	ADP	C3'-C2'-C1'	2.35	105.91	101.46

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

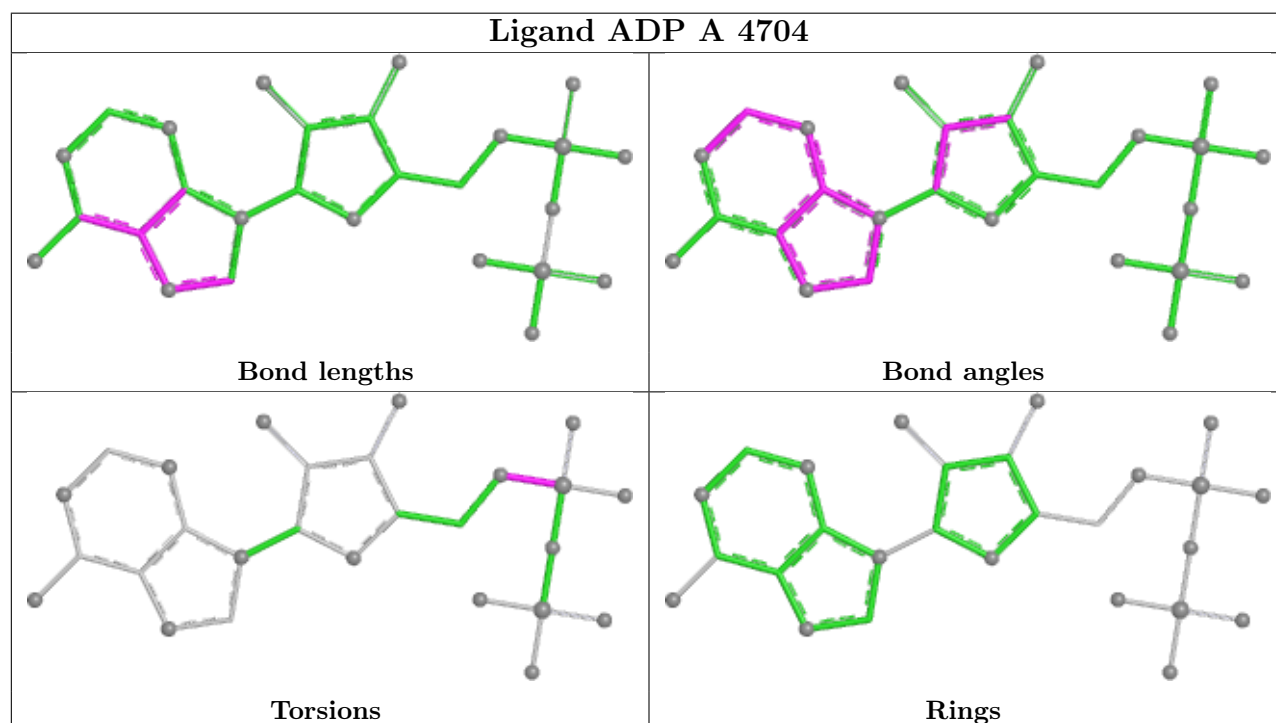
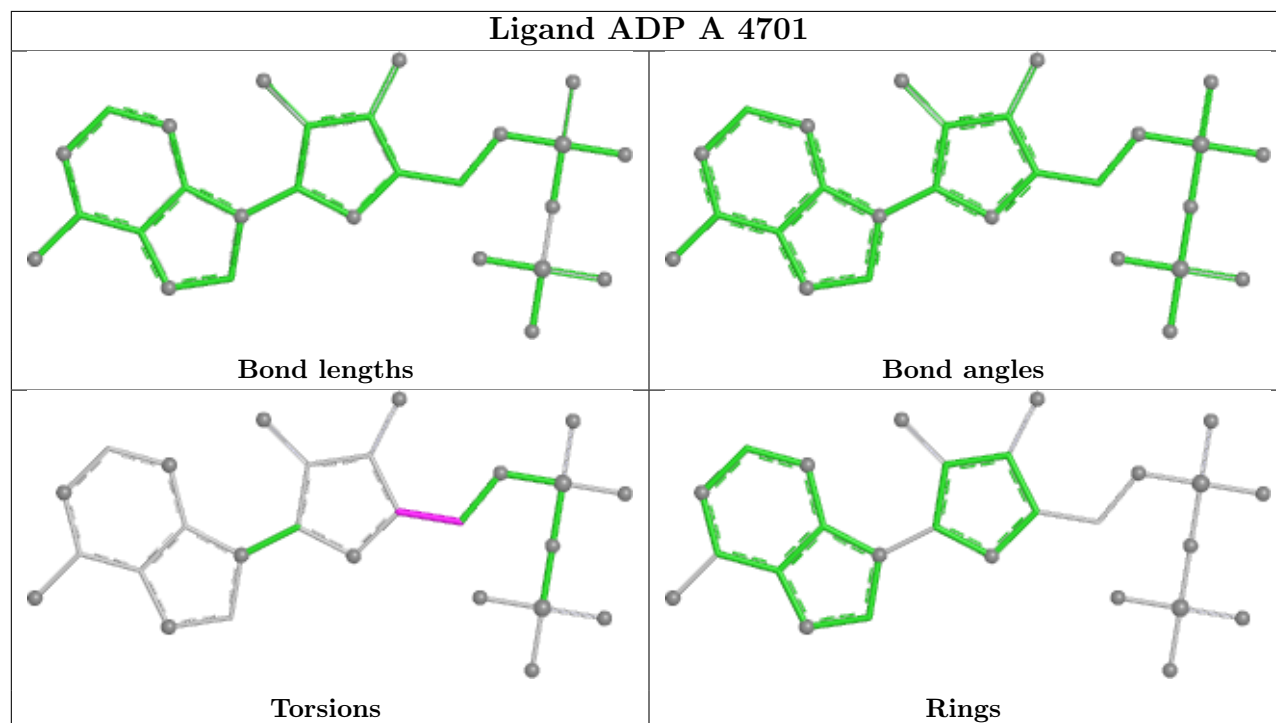
There are no ring outliers.

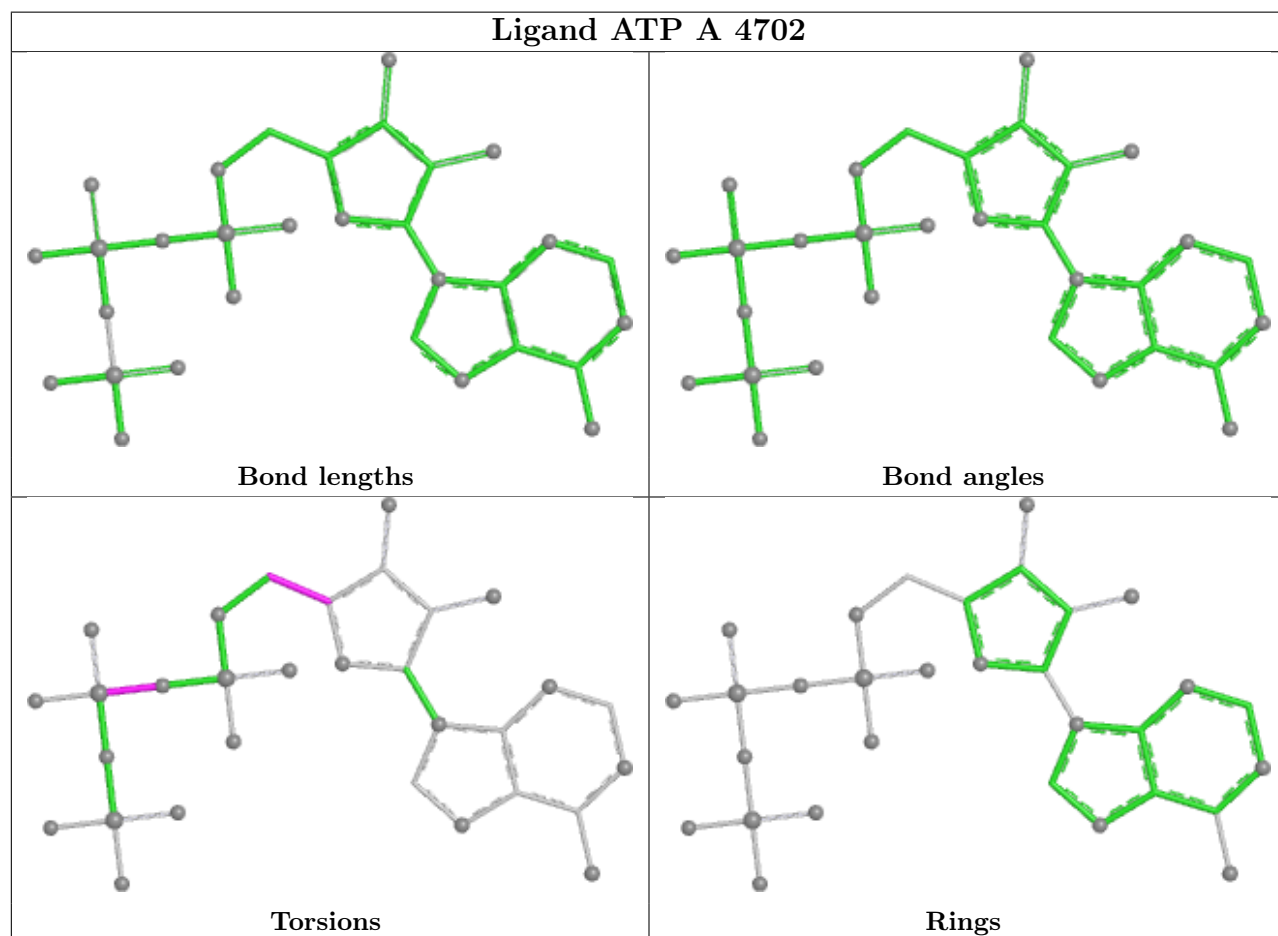
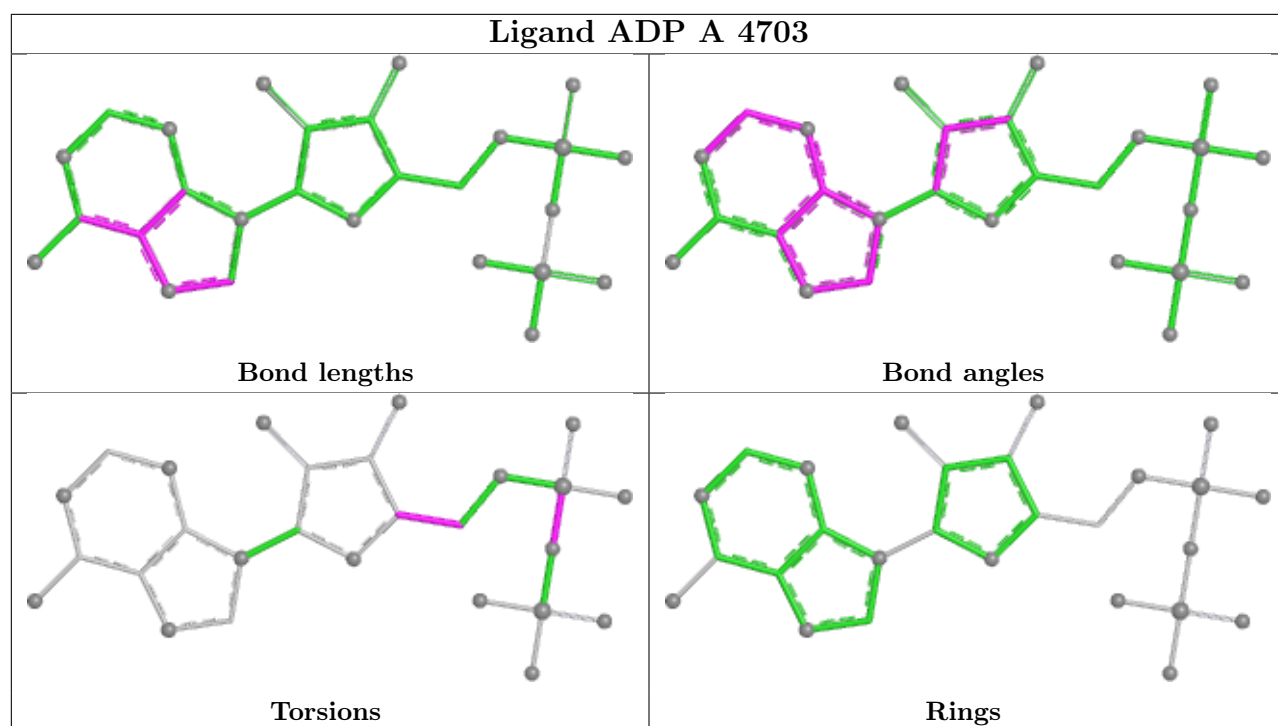
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	3	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.

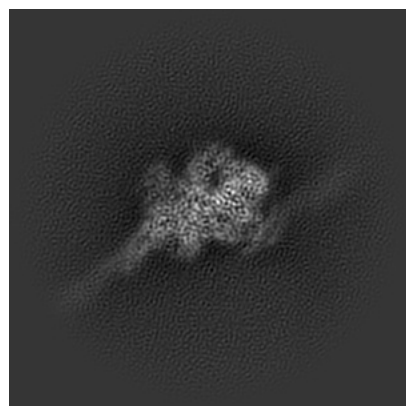
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44702. These allow visual inspection of the internal detail of the map and identification of artifacts.

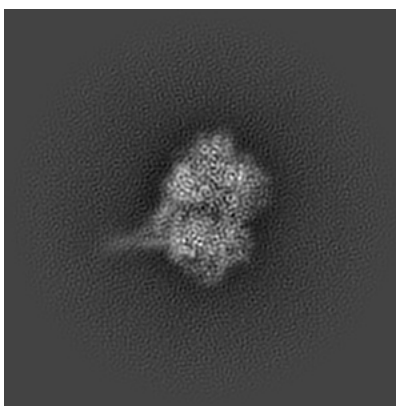
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

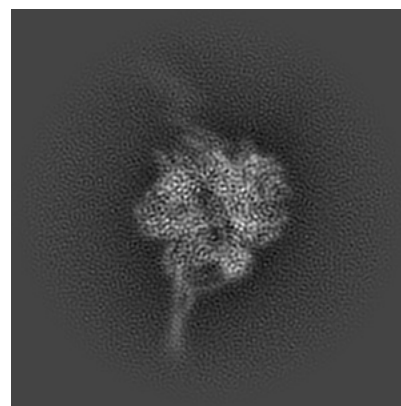
6.1.1 Primary map



X

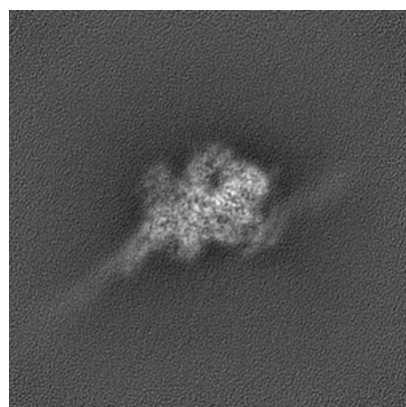


Y

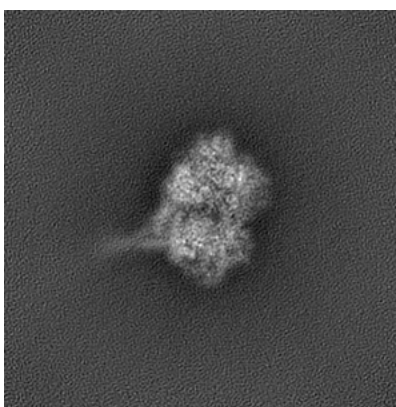


Z

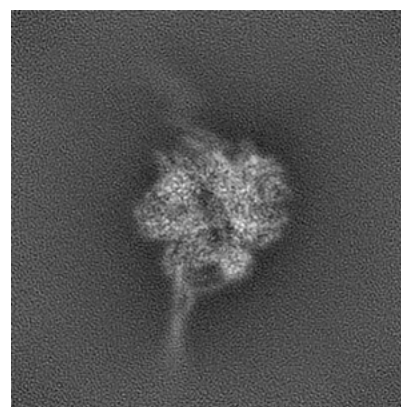
6.1.2 Raw map



X



Y

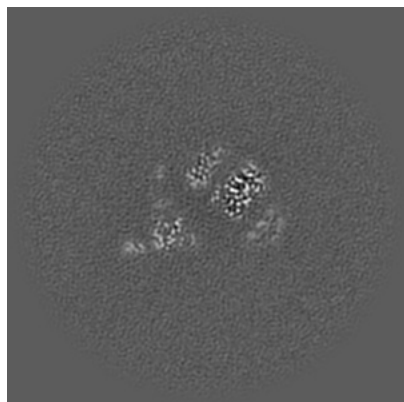


Z

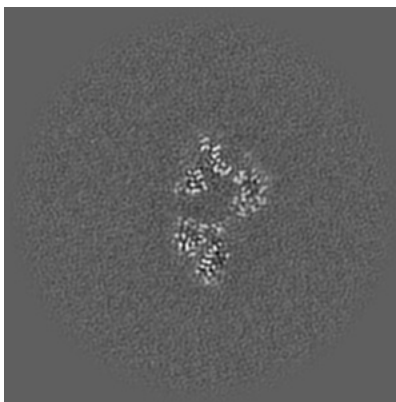
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

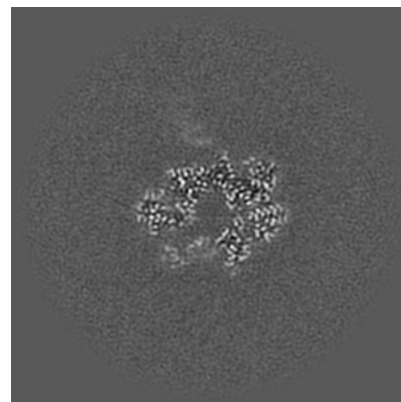
6.2.1 Primary map



X Index: 128

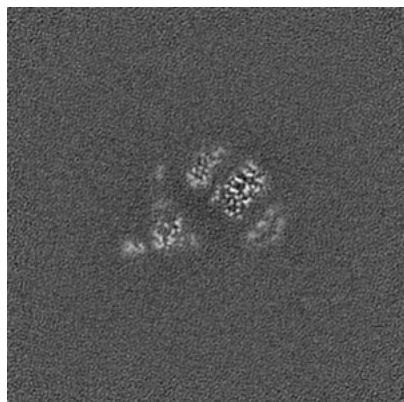


Y Index: 128

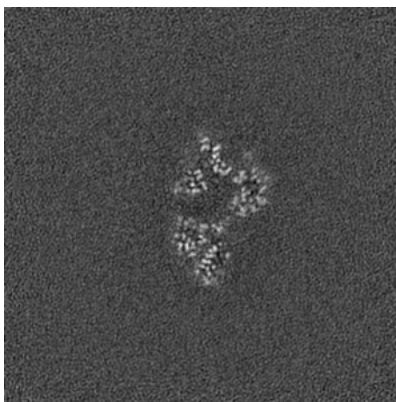


Z Index: 128

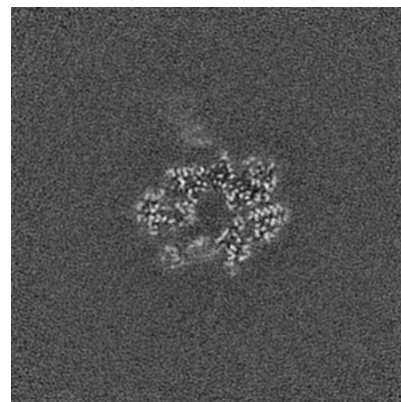
6.2.2 Raw map



X Index: 128



Y Index: 128

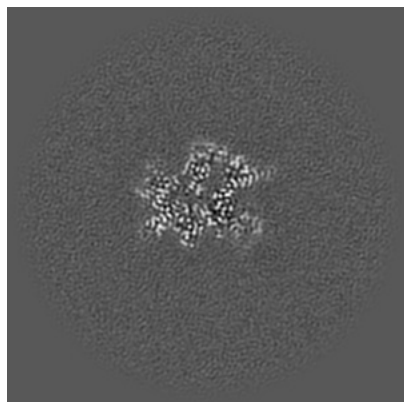


Z Index: 128

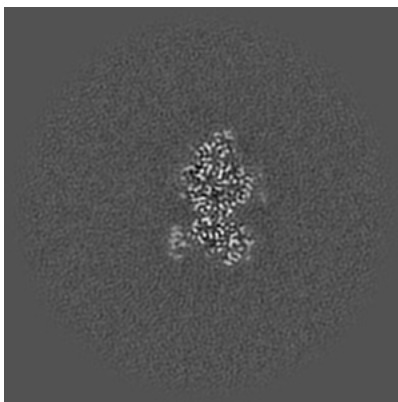
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

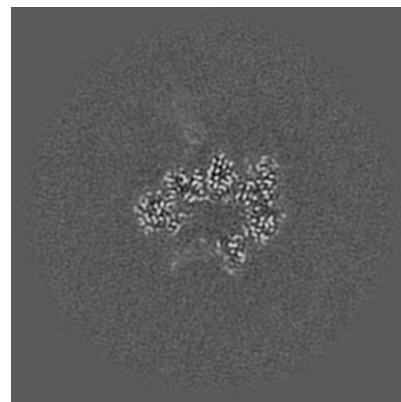
6.3.1 Primary map



X Index: 146

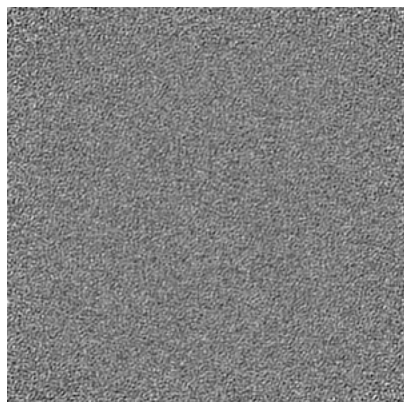


Y Index: 143

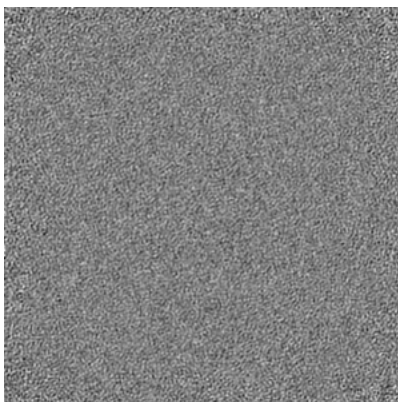


Z Index: 131

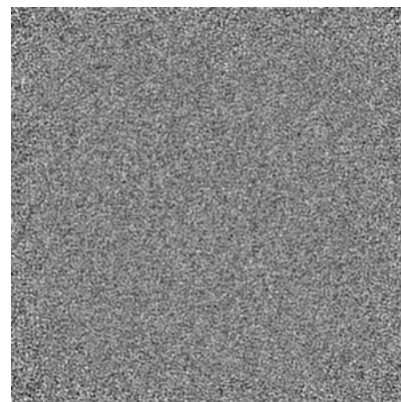
6.3.2 Raw map



X Index: 0



Y Index: 0

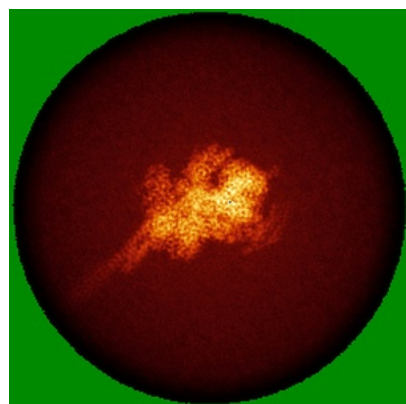


Z Index: 0

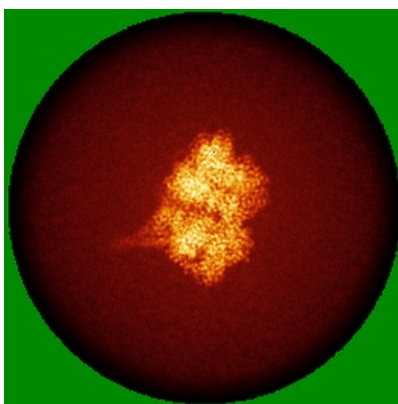
The images above show the largest variance slices of the map in three orthogonal directions.

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

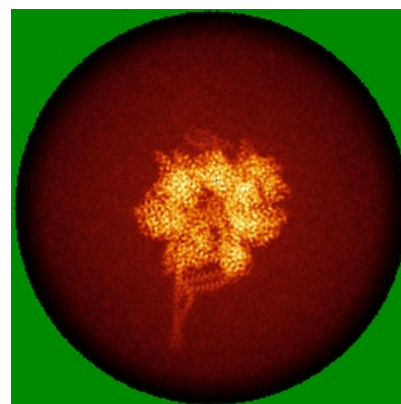
6.4.1 Primary map



X

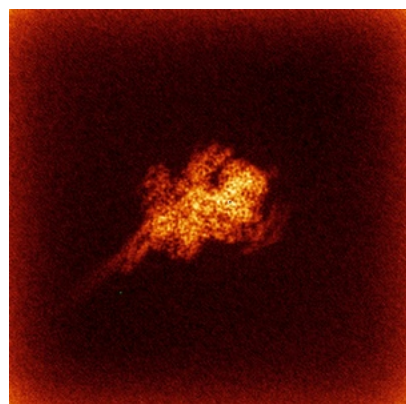


Y

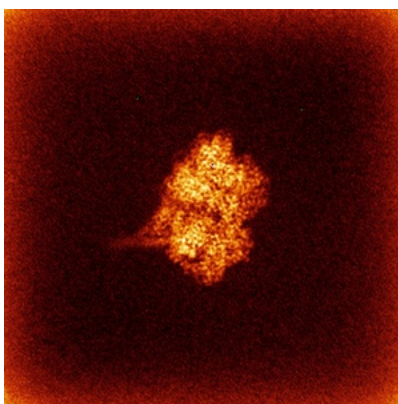


Z

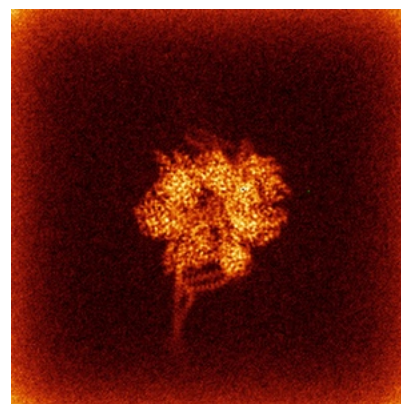
6.4.2 Raw map



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.

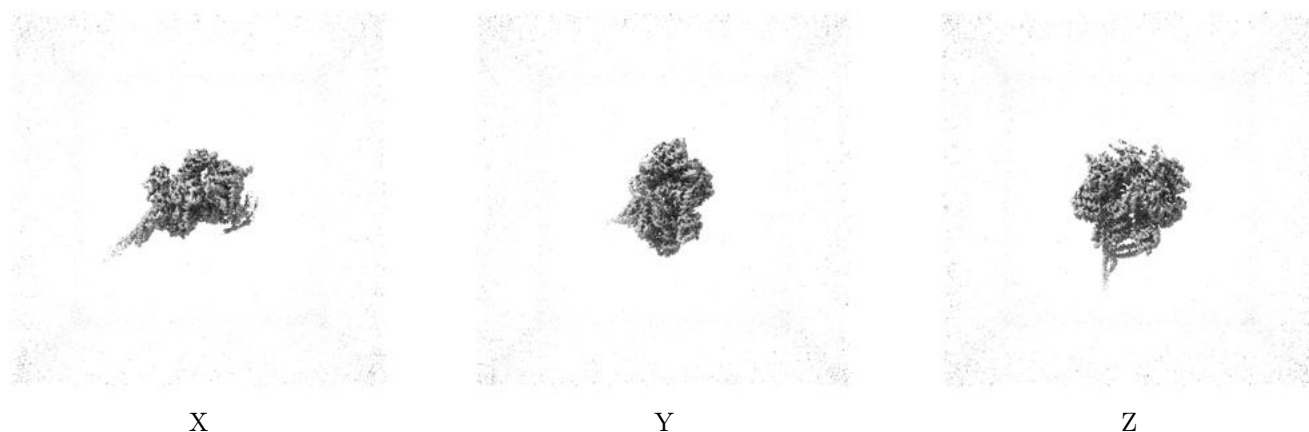
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

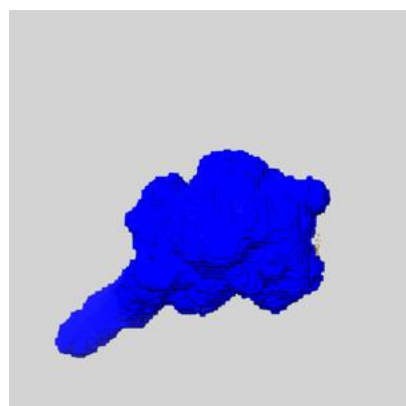
6.6 Mask visualisation [i](#)

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

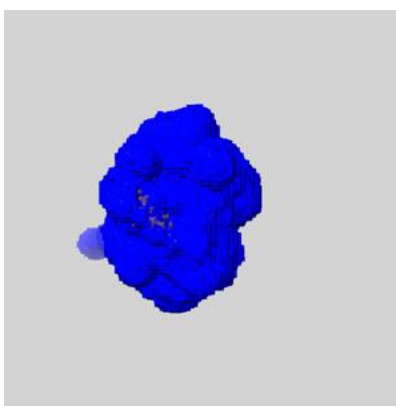
A mask typically either:

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

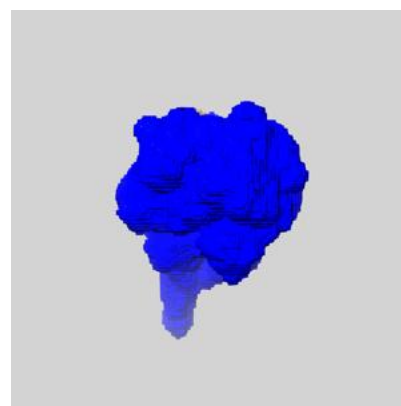
6.6.1 emd_44702_msk_1.map [i](#)



X



Y

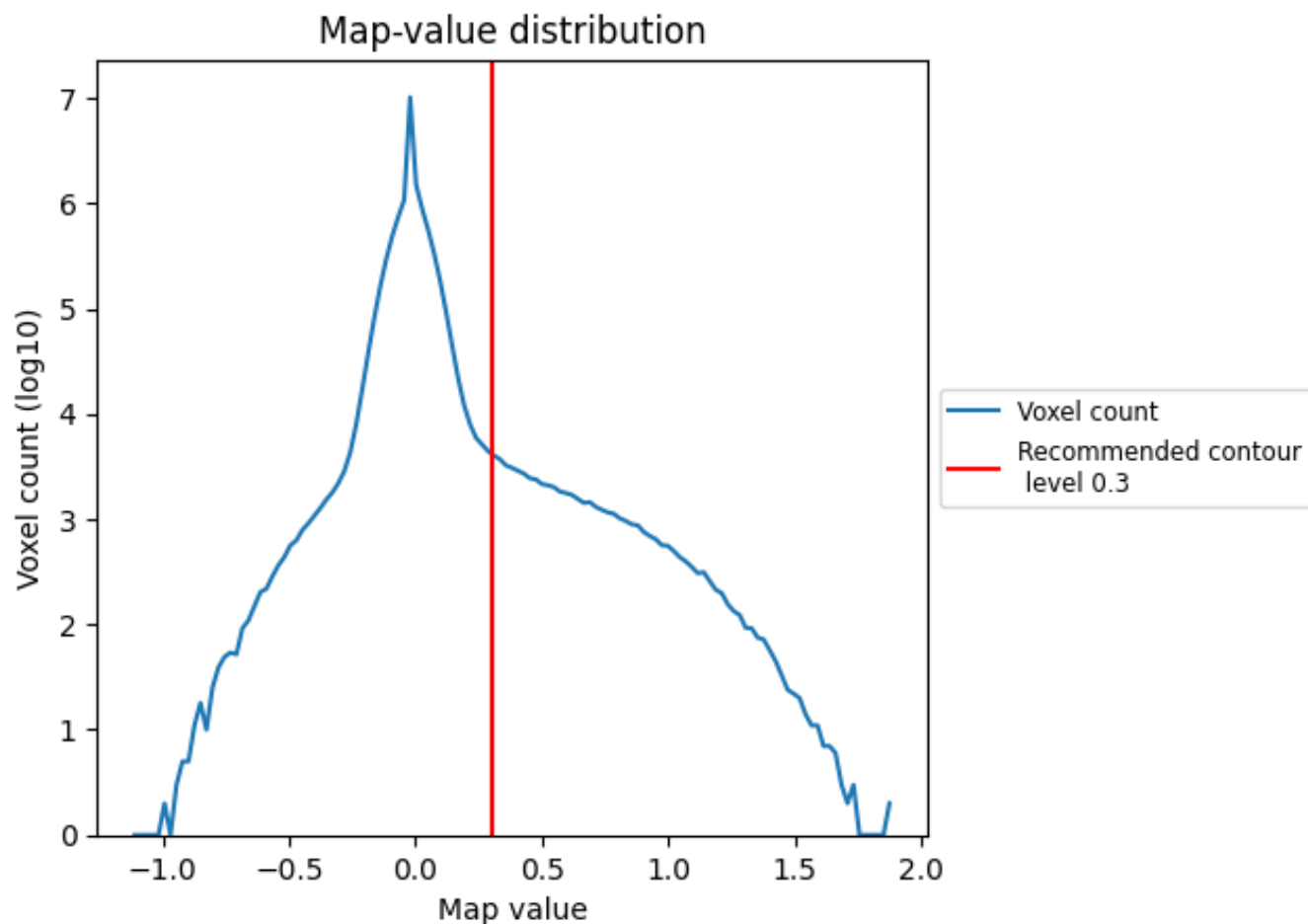


Z

7 Map analysis [i](#)

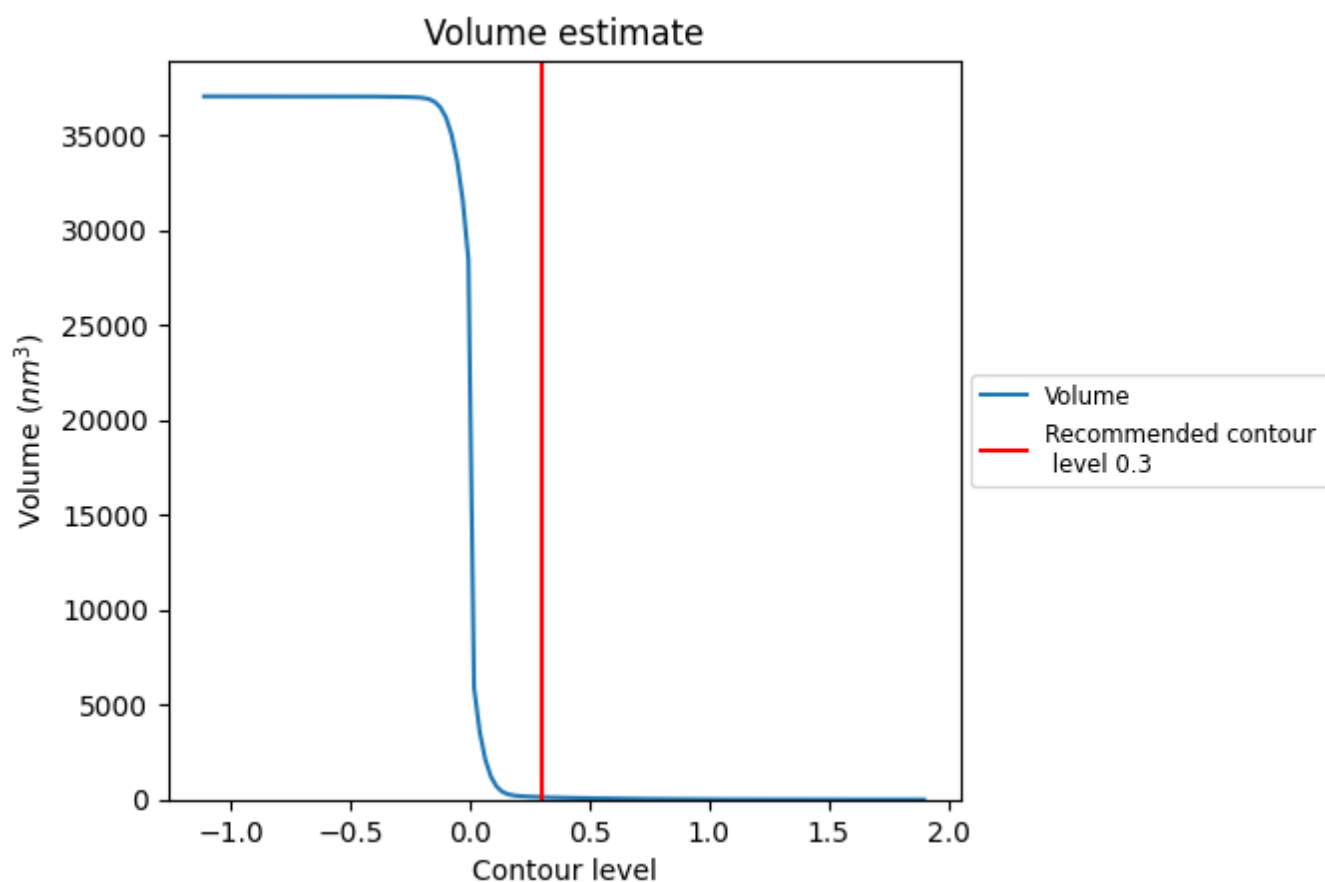
This section contains the results of statistical analysis of the map.

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.

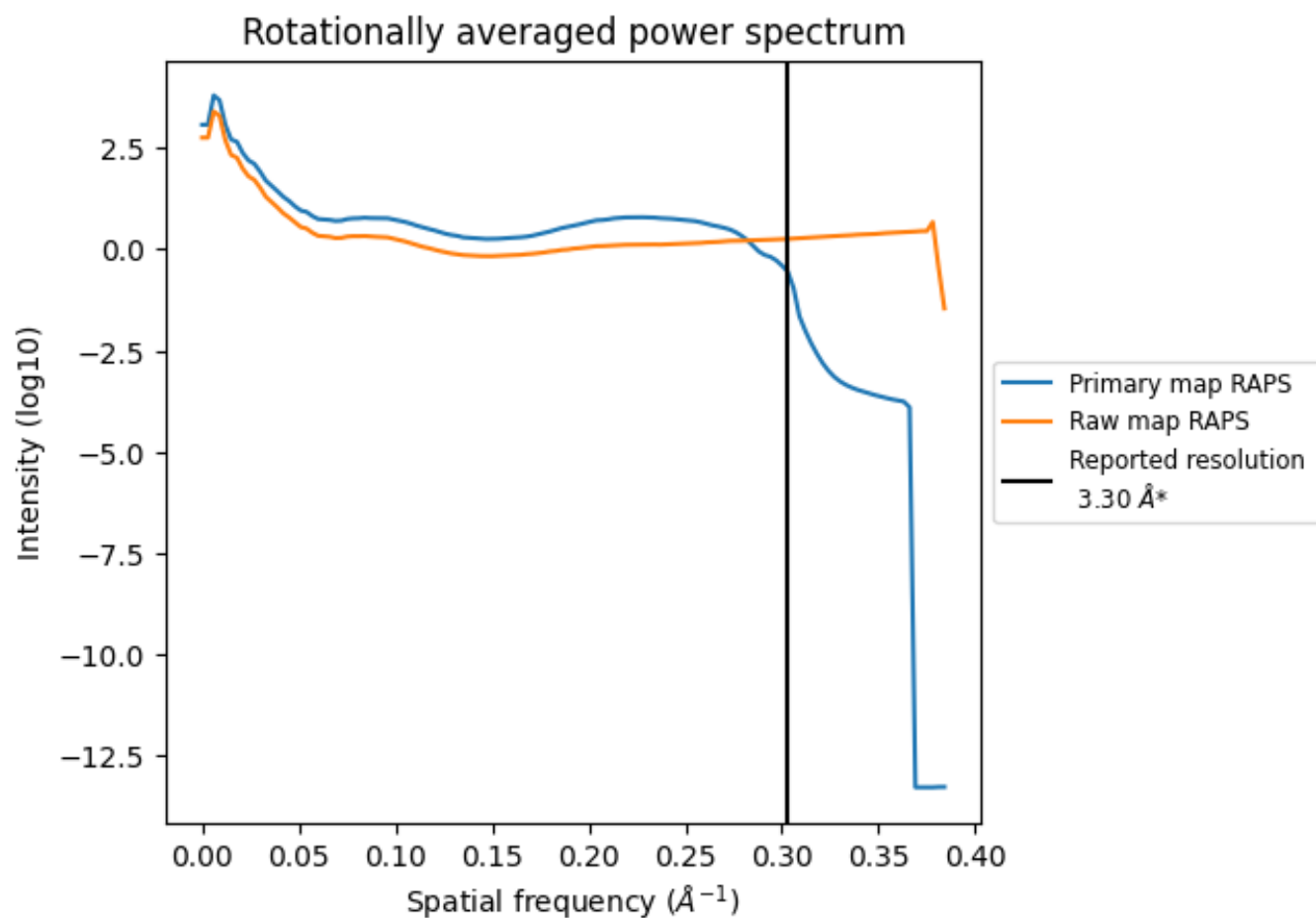
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 128 nm³; this corresponds to an approximate mass of 116 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 ⓘ

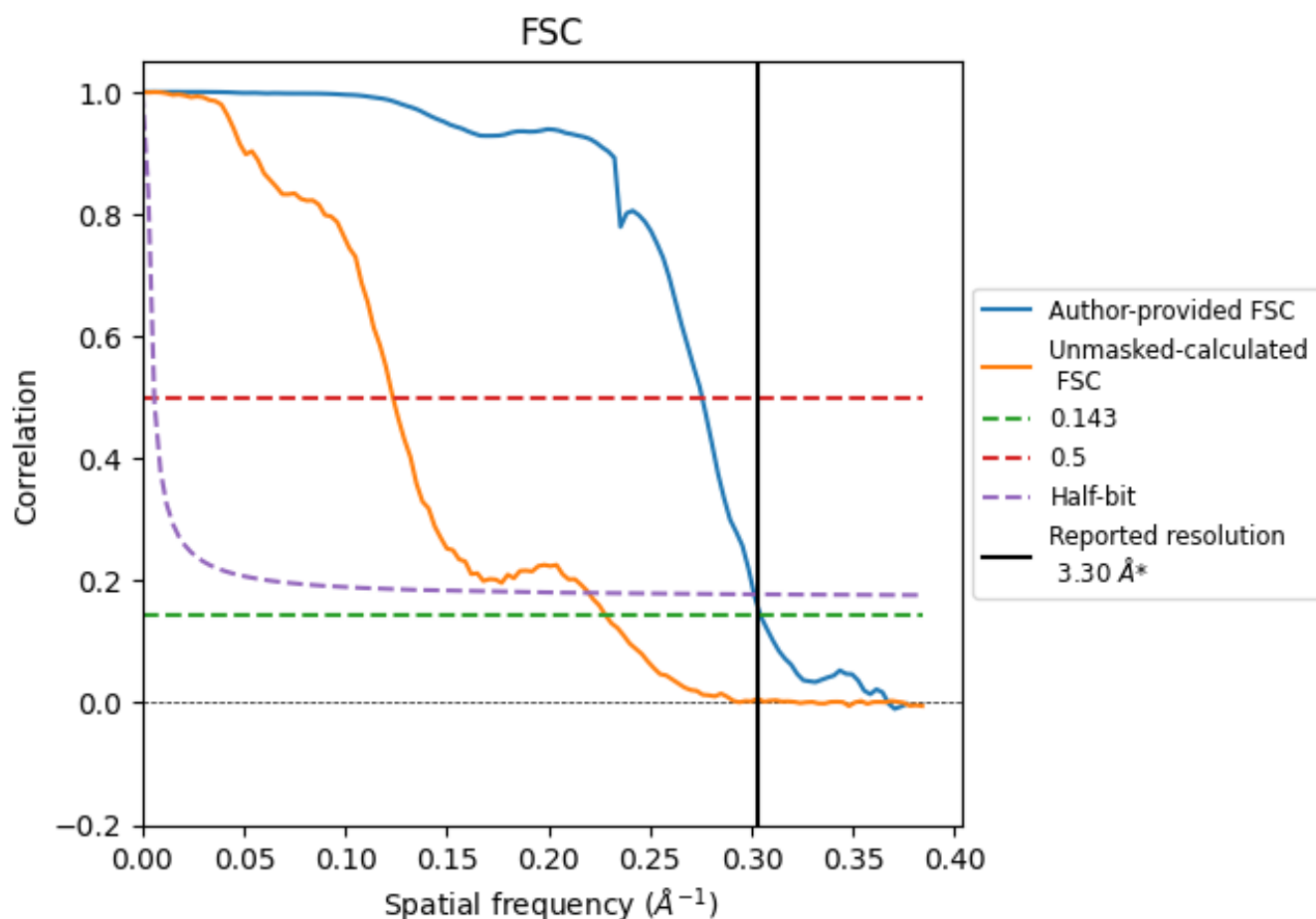


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

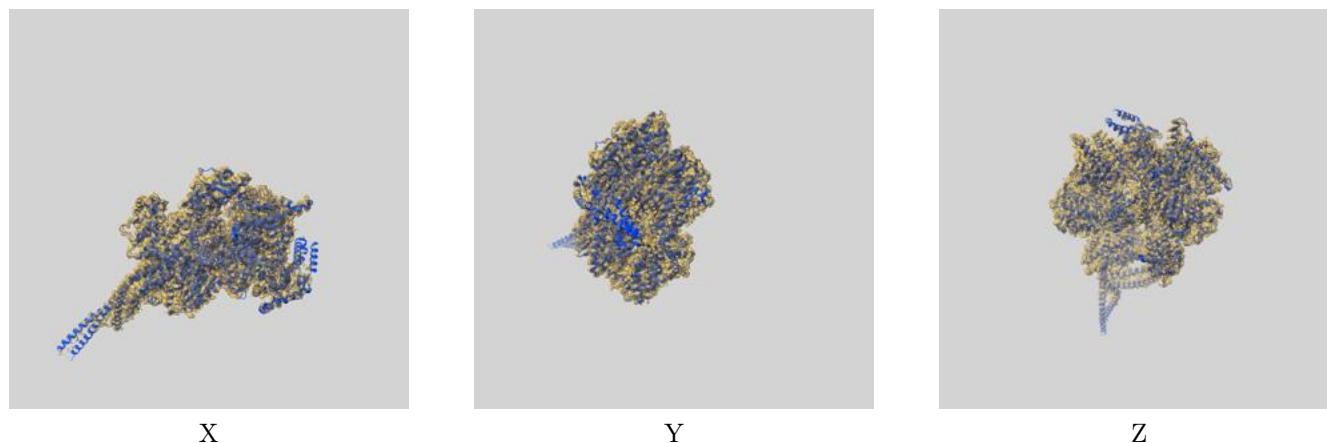
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.63	3.32
Unmasked-calculated*	4.38	8.10	4.55

*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 4.38 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

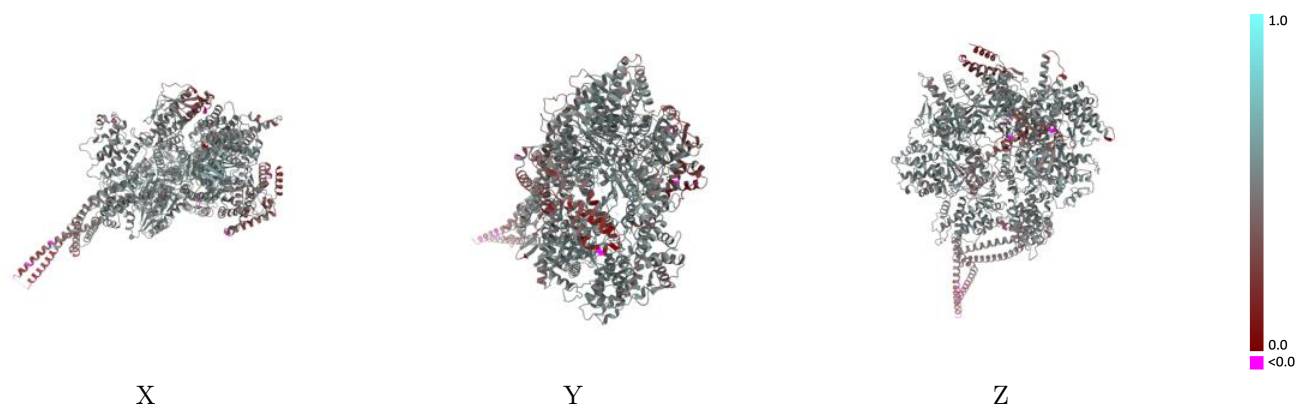
This section contains information regarding the fit between EMDB map EMD-44702 and PDB model 9BML. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



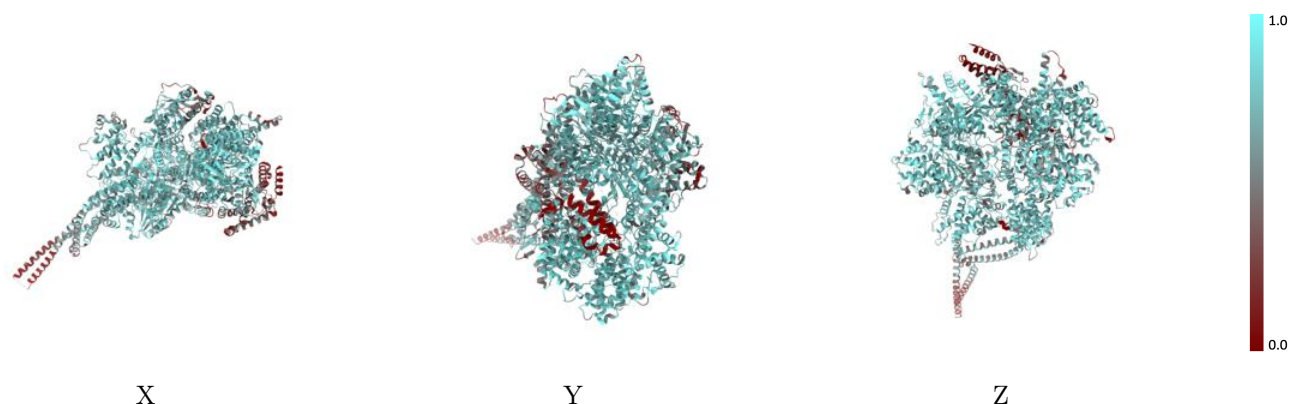
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



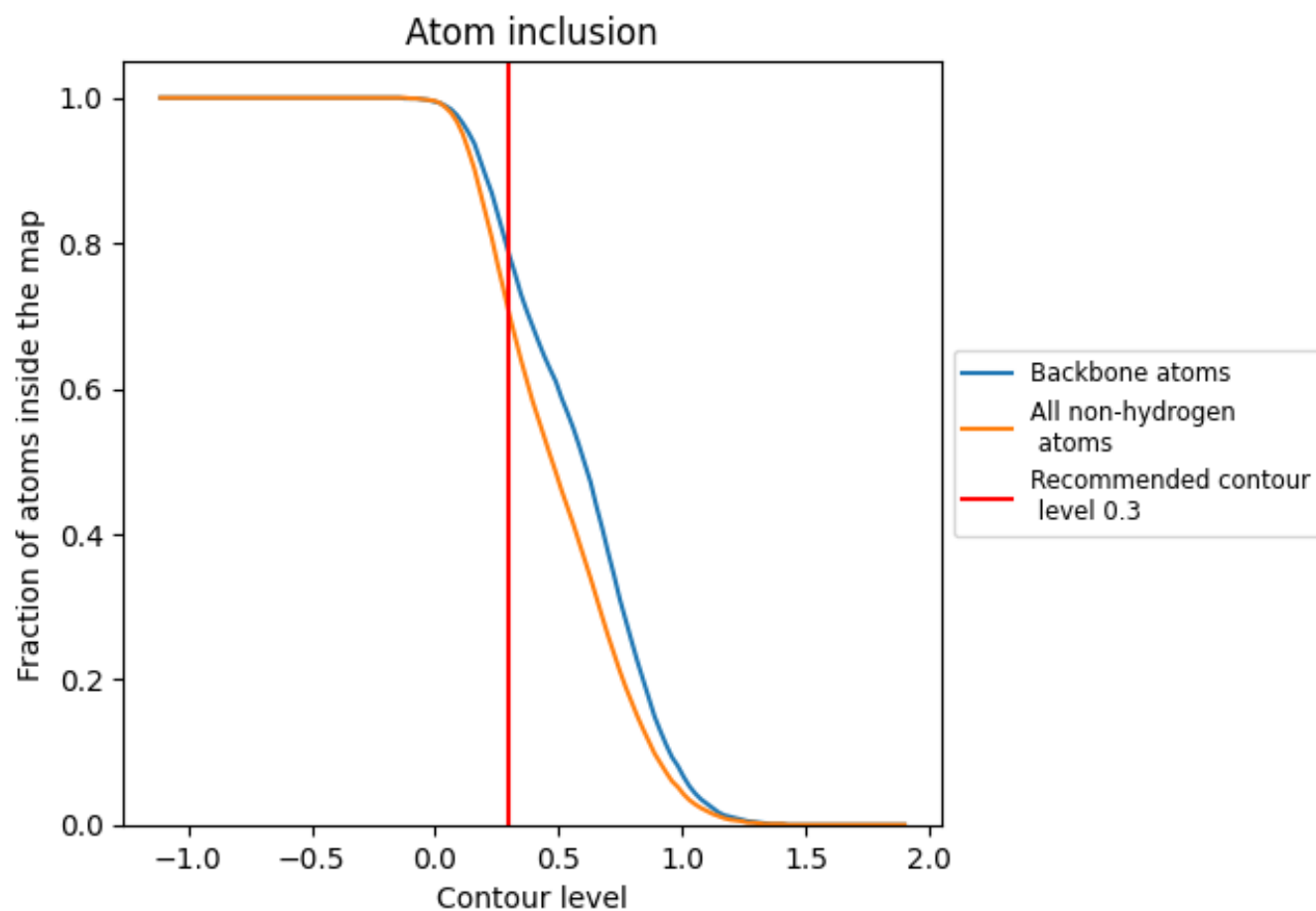
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 70% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7020	0.4800
A	0.7020	0.4800

