



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 01:10 AM UTC

PDB ID : 9BN3 / pdb_00009bn3
EMDB ID : EMD-44720
Title : The alpha registry-locked dynein motor domain mutant in 5mM ATP condition, class1
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

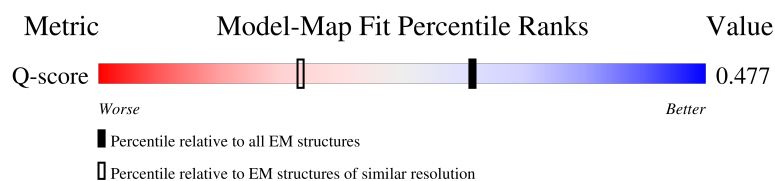
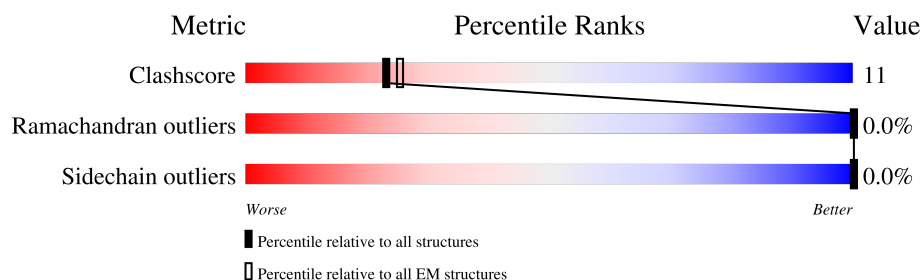
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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 3 unique types of molecules in this entry. The entry contains 23152 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2866	Total	C	N	O	S	0	0
			23040	14688	3978	4259	115		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2389	ASP	GLU	conflict	UNP Q14204

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



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

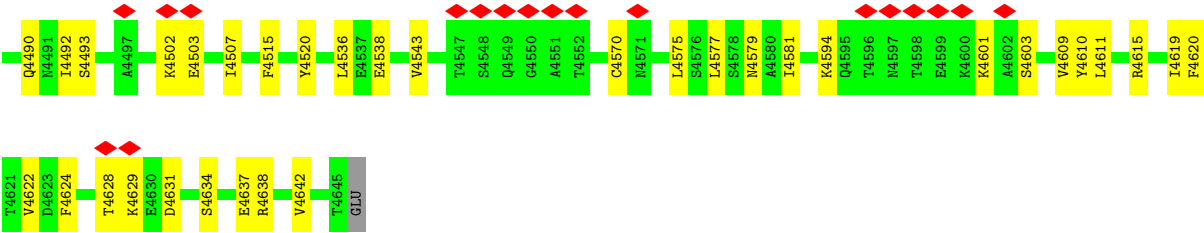
-
- The diagram illustrates the chemical structure of Adenosine Triphosphate (ATP). It consists of an adenine base (a purine ring system with an amino group at position 6) attached to a ribose sugar (a five-membered ring with hydroxyl groups at positions 2' and 3'). The ribose is linked to a chain of three phosphate groups (labeled alpha, beta, and gamma) via phosphodiester bonds. The alpha phosphate is directly attached to the 5' carbon of the ribose. The beta and gamma phosphates are linked in series. The structure is shown with stereochemistry, indicating the orientation of the hydroxyl groups and the phosphate chain. The atoms are labeled with their respective element symbols and positions (e.g., N1, N3, N7, N9, C2, C4, C5, C6, C1', C2', C3', C4', C5', O1, O2, O3, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100).



R1887	G1770	K1645	R1567	I1501	LYS	VAL	TRP	ARG	GLU	ALA	ASN	GLU	GLU	ASN	GLU	ASN	PHE
C1888	G1771	Q1651	F1568	N1502	ASN	ALA	GLU	PHE	LEU	TYR	SER	LEU	LEU	LEU	LEU	LEU	ASN
M1892	G1772	Q1659	Q1569	S1503	ALA	PHE	GLU	PHE	GLN	GLU	GLN	THR	THR	THR	THR	THR	GLN
R1899	G1773	A1659	S1572	V1504	VAL	VAL	LEU	PRO	ILE	VAL	MET	ASN	ASN	GLY	GLY	GLY	LYS
S1903	D1774	I1665	T1573	S1505	GLN	GLN	ASP	SER	SER	ASP	PRO	VAL	VAL	ASP	VAL	VAL	VAL
P1904	A1775	L1666	E1574	M1507	ASP	ASP	LEU	TRP	TRP	LEU	GLY	THR	THR	GLY	GLY	GLY	ASP
T1910	E1776	N1667	F1575	K1508	VAL	LEU	LEU	TYR	ARG	LEU	VAL	LEU	LEU	LEU	LEU	LEU	LEU
G1911	D1669	E1668	L1576	L1509	LEU	GLY	GLY	ILE	ILE	GLY	THR	THR	THR	THR	THR	THR	ILE
K1912	N1670	N1670	A1577	S1510	VAL	VAL	TRP	ASN	ASN	LEU	ALA	PRO	PRO	PRO	PRO	PRO	VAL
G1920	T1788	E1680	M1579	P1511	GLN	GLN	GLU	ILE	ILE	MET	SER	GLU	GLU	GLU	GLU	GLU	GLU
H1921	L1789	G1681	K1580	Y1512	GLY	GLY	GLU	GLU	GLU	LYS	GLU	ILE	ILE	ILE	ILE	ILE	GLY
Q1922	S1795	E1682	K1581	Y1513	GLU	GLU	ALA	ALA	ALA	ILE	SER	SER	SER	SER	SER	SER	LYS
F1926	Q1800	M1685	V1582	K1514	ALA	ALA	GLN	GLY	GLY	MET	LYS	VAL	VAL	VAL	VAL	VAL	ALA
V1927	R1804	I1692	K1583	V1515	LEU	VAL	TRP	ALA	ALA	VAL	LEU	ASP	THR	THR	THR	THR	LYS
L1928	R1805	T1693	K1584	F1516	GLU	ILE	LEU	PHE	PHE	ILE	GLU	GLU	GLU	GLU	GLU	GLU	VAL
D1933	K1806	E1694	S1585	E1517	PHE	GLU	ILE	ASP	ASP	THR	GLY	THR	THR	THR	THR	THR	ARG
E1934	L1807	E1694	P1586	E1518	LYS	GLN	GLY	ILE	ILE	GLY	VAL	VAL	VAL	VAL	VAL	VAL	LEU
F1938	K1808	K1697	L1587	D1519	K1463	GLU	GLU	ARG	ARG	SER	GLN	GLY	GLY	GLY	GLY	GLY	GLU
V1954	I1812	I1698	V1588	A1520	Q1465	GLU	GLU	THR	THR	GLU	MET	ASP	ALA	ALA	ALA	ALA	ARG
E1959	T1813	N1699	M1589	L1521	Q1466	ALA	LEU	PHE	LEU	ALA	GLY	VAL	VAL	VAL	VAL	VAL	LEU
R1962	T1814	E1700	D1590	S1522	R1467	LYS	GLY	ARG	ARG	GLY	ASP	THR	THR	THR	THR	THR	GLY
R1966	L1815	W1701	V1591	W1523	E1468	ASP	PRO	LEU	LEU	ILE	SER	GLY	GLY	GLY	GLY	GLY	ALA
A1970	L1818	L1702	L1592	E1524	V1469	THR	TRP	LYS	LYS	ALA	ALA	ASN	ASN	ASN	ASN	ASN	LYS
I1978	Q1818	M1709	N1593	D1525	W1470	HIS	VAL	ILE	ILE	ILE	ILE	LYS	LYS	LYS	LYS	LYS	THR
R1983	K1834	R1710	I1594	K1526	N1471	TRP	SER	ASP	ASP	TRP	VAL	VAL	VAL	VAL	VAL	VAL	LYS
E1984	T1711	T1712	Q1595	L1527	T1472	LYS	VAL	ARG	ARG	GLN	GLN	GLN	GLN	GLN	GLN	GLN	PHE
H1985	S1840	L1713	G1596	N1528	Y1473	GLN	GLU	GLY	GLY	GLN	GLN	GLN	GLN	GLN	GLN	GLN	LEU
S1986	Q1841	A1714	V1597	R1529	E1474	MET	PRO	CYS	CYS	ALA	ALA	VAL	VAL	VAL	VAL	VAL	VAL
H1987	M1842	K1715	Q1598	T1530	L1475	LYS	LEU	ALA	ALA	ASN	ASN	ARG	ARG	ARG	ARG	ARG	LEU
P1988	F1846	V1721	R1599	M1531	L1476	ARG	LEU	LYS	LYS	LEU	LEU	LEU	LEU	LEU	LEU	LEU	ASN
H1989	D1847	P1724	S1600	A1532	D1477	HIS	GLN	MET	MET	GLN	GLN	GLN	GLN	GLN	GLN	GLN	THR
Y1990	P1848	E1725	L1601	L1533	L1477	VAL	ASN	GLY	GLY	ASN	ASN	ASP	ASP	ASP	ASP	ASP	ALA
D1991	D1852	Q1855	E1602	F1534	Y1478	TRP	TRP	ILE	ILE	VAL	VAL	TRP	TRP	TRP	TRP	TRP	GLN
T1992	Q1860	T1731	R1603	D1535	Y1480	VAL	ASP	VAL	VAL	GLN	GLN	GLN	GLN	GLN	GLN	GLN	VAL
T1993	Q1861	T1733	A1605	I1538	Q1481	VAL	LEU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	SER
S1994	M1861	I1733	D1606	D1539	N1482	SER	LEU	THR	THR	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
A1995	K1865	D1734	K1610	Q1541	C1483	GLU	LEU	GLY	GLY	ALA	ALA	VAL	VAL	VAL	VAL	VAL	LEU
P1996	Y1868	T1737	K1613	R1542	R1485	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY
T1997	E1871	L1749	E1617	R1543	L1486	GLY	GLN	GLY	GLY	GLN	GLN	GLY	GLY	GLY	GLY	GLY	THR
T1998	Y1872	W1750	Y1618	W1544	I1487	ILE	ILE	SER	SER	PHE	PHE	GLY	GLY	GLY	GLY	GLY	GLY
L2001	E1877	V1751	L1619	G1549	R1488	TRP	ALA	GLU	GLU	ASP	ASP	LEU	LEU	LEU	LEU	LEU	ASN
L2002	Q1876	L1752	E1620	T1552	G1489	VAL	ARG	GLU	GLU	VAL	VAL	LEU	LEU	LEU	LEU	LEU	LYS
N2003	D1877	E1760	R1621	S1553	W1490	ASP	LEU	ARG	ARG	ARG	ARG	THR	THR	THR	THR	THR	THR
	K1878	T1764	F1626	S1554	D1491	GLN	GLN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
			P1627	A1555	D1492												
			R1628		L1493												
			E1635	K1558	F1494												
			D1636	H1559	N1495												
			L1637	L1560	V1497												
			G1642	L1561	K1498												
				P1562	F1499												
				V1563	K1499												
				E1564	H1500												
				T1565													
				Q1566													

ARG	P3137	K3050	K2966	D2862	L2759	Q2654	Q2424	V2345	E2242	K2007
ILE	S3138	Y3051	E2970	R2863	L2762	L2655	F2427	Q2346	R2243	M2018
LYS	R3139	K3052	E2971	E2864	A2766	V2660	T2428	Y2350	E2245	M2019
SER	R3140	K3053	D2971	K2865	K2766	L2661	S2429	A2351	G2246	PRO
GLN	E3141	F3054	L2976	A2866	T2770	F2662	N2430	T2352	G2247	GLY
LEU		F3055	L2977	M2867		C2663		L2353	V2248	TYR
GLU	V3144	I3059	V2979	S2868	M2773	D2664	L2437	A2354	K2261	ALA
VAL	S3145	V3065	L2980	R2869	V2774	E2665	H2439	V2356	Y2265	GLY
ASN	C3147	F3066	R2981	P2870		E2666	A2440	F2441	D2269	ASP
ALA	V3148	T3067		L2871	R2783	L2668	Q2442	F2442	P2270	SER
ALA	H3151	M3068	K2986	S2878	F2784	P2669	H2445	H2445	D2269	ASN
ASP	K3152	N3069	N2987	K2879	T2785	D2670	L2437	F2438	N2130	K2034
LYS	L3153	P3070	E2988	D2880	Q2786	M2671	A2440	V2356	P2132	L2035
LYS	L3154	S3071	K2989	D2885	V2802	K2673	L2437	A2354	R2273	F2036
LEU	H3155	S3072	D2995	Q2886		F2682	L2449	V2356	D2277	R2037
LYS	K3156	E3073	E2996	Q2887	L2806		T2450	V2356	F2280	Q2038
LYS	A3157	G3074	S2997	E2887		M2686	R2451	L2369	K2286	L2039
LYS	N3158	L3075	N2998	R2890	L2809	D2697	C2454	T2371	V2291	P2044
MET		K3076	V2999	R2890	L2810	D2697	S2457	I2374	R2292	D2045
VAL	K3163	K3077	L3000	K2894	L2810	D2697	L2458	N2377	R2292	R2046
ASP	R3164	R3078	D3001	K2898	T2815	V2701	L2462	N2377	V2291	F2059
GLN	M3169	A3079	F3004	E2903	L2816	K2702	L2462	N2377	R2292	L2065
GLN	T3172	A3080	K3005	E2903	P2817	L2703	R2467	L2382	G2293	A2066
GLU	T3172	T3081	L3005	E2904	V2818	E2704	R2467	L2382	L2295	L2067
LYS	Y3176	A3084	E3006	L2905	F2819	R2705	R2468	L2382	L2295	F2068
LYS		L3085	K3007	L2906	G2820	Q2707	V2469	L2382	Q2296	L2069
LYS	E3193	F3086	M3008	D2906	L2821	F2708	A2470	L2382	W2300	V2070
VAL	L3194	N3087	G3015	V2910	T2822	V2709	Q2471	L2382	D2306	ASP
MET	E3195	F3086	G3015	V2910	L2823	V2709	Y2472	L2382	V2307	L2075
GLN	K3197	N3087	F3021	N2913	L2824	V2709	Y2472	L2382	D2307	Q2079
GLU	Q3198	N3087	E3022	N2913	V2825	K2721	M2481	L2382	D2308	Y2086
ILE	Q3198	N3087	G3023	T2922	A2829	R2726	Q2485	L2382	F2310	L2090
GLN	H3200	G3095	D3024	D2923	L2830	P2731	Q2485	L2382	W2311	L2093
GLN	L3201	G3095	E3025	R2924	L2831	P2732	Q2485	L2382	V2312	L2097
LEU	N3202	A3101	Y3026	L2925	L2832	E2628	R2488	L2382	E2313	G2101
HIS	V3203			Q2928	F2833	E2629		L2382	L2210	L2093
LYS	G3204	V3105	L3029	Q2928	V2838	L2630	L2498	L2382	L2213	L2097
GLN	L3205	M3113	M3030	F2929	E2839	K2633	L2498	L2382	L2220	L2097
GLU	K3207	M3113	T3031	Q2929	D2840	T2634	W2500	L2382	M2221	G2101
VAL	K3207	M3113	T3031	Q2929	D2840	T2634	W2500	L2382	G2227	K2104
ILE	K3209	M3119	C3032	L2933	R2844	F2635	L2502	L2382	S2226	K2105
ASP	E3210	P3123	K3034	L2935	T2845	D2636	D2505	L2382	K2230	E2106
LYS	T3211	D3124	E3035	L2936	D2847	H2637	P2527	L2382	S2231	Q2109
GLN	V3212	Y3125	S2939	L2937	E2848	K2643	P2530	L2382	M2232	K2110
MET	Q3213	K3126	G3038	L2938	N2849	N2643	N2531	L2382	A2233	I2111
SER	D3213	P3127	Q3038	G2937	L2850	Q2646	L2532	L2382	L2234	K2112
VAL	Q3214	F3128	K3039	V2938	D2851	Q2647	P2533	L2382	R2235	K2113
LYS	V3215	V3129	Q3039	L2939	T2852	Q2647	P2533	L2382	K2236	E2114
GLU	V3215	Y3130	E3040	R2948	V2853	V2648	L2535	L2382	K2236	LYS
ASP	E3216	K3131	G3041	I2961	L2756	V2649	L2535	L2382	K2236	
ASP	E3217	K3131	L3042	K2962	R2757	V2649	L2535	L2382	K2236	
LYS	R3218	K3132	M3043	H2964	L2758	V2649	L2535	L2382	K2236	
LYS	R3219	L3133	L3044	H2964	L2758	V2649	L2535	L2382	K2236	
LYS	R3220	P3134	D3045	R2965	L2758	V2649	L2535	L2382	K2236	
ASP	Q3135	Q3135	S3046	R2965	L2758	V2649	L2535	L2382	K2236	
LEU	LEU	P3136	E3048	R2965	L2758	V2649	L2535	L2382	K2236	





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	433112	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.677	Depositor
Minimum map value	-1.892	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	412.488, 412.488, 412.488	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1458, 1.1458, 1.1458	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: ADP, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.15	1/23533 (0.0%)	0.36	4/31898 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3587	PRO	CG-CD	-5.96	1.30	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3587	PRO	N-CD-CG	-10.98	86.73	103.20
1	A	3587	PRO	CA-CB-CG	-8.66	88.05	104.50
1	A	3587	PRO	N-CA-CB	-6.07	98.07	103.35
1	A	3587	PRO	CA-N-CD	-5.47	104.34	112.00

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	23040	0	23108	513	0
2	A	81	0	36	0	0
3	A	31	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	23152	0	23156	513	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 (513) 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	1.26	0.79
1:A:4043:MET:HB2	1:A:4127:THR:HA	1.63	0.79
1:A:1511:PRO:HG3	1:A:3628:ARG:HE	1.47	0.78
1:A:3209:LYS:HG3	1:A:3486:ARG:HH21	1.48	0.78
1:A:3137:PRO:HB3	1:A:3141:GLU:HB2	1.66	0.77
1:A:3113:MET:O	1:A:3140:ARG:NH2	2.18	0.76
1:A:1814:GLU:HG2	1:A:1878:LYS:HE2	1.67	0.76
1:A:2261:LYS:HE3	1:A:2311:TRP:HB3	1.68	0.75
1:A:3942:PRO:HA	1:A:3945:LYS:HE3	1.69	0.75
1:A:1582:VAL:HG23	1:A:1591:VAL:HG11	1.69	0.74
1:A:2822:ILE:HD11	1:A:2854:ALA:HB1	1.70	0.73
1:A:3730:ASP:OD1	1:A:3733:LYS:NZ	2.21	0.73
1:A:3158:ASN:ND2	1:A:3169:MET:O	2.20	0.73
1:A:4326:ASN:HD21	1:A:4581:ILE:HG23	1.53	0.73
1:A:3839:VAL:O	1:A:3843:ASN:ND2	2.23	0.71
1:A:2500:TRP:HZ2	1:A:2576:ARG:HD3	1.55	0.71
1:A:3826:GLN:HB3	1:A:4140:ARG:HD2	1.73	0.71
1:A:3585:ARG:HB2	1:A:3697:THR:HG23	1.72	0.70
1:A:2294:GLU:O	1:A:2338:ASN:ND2	2.25	0.70
1:A:2467:ARG:O	1:A:2471:GLN:NE2	2.25	0.70
1:A:3602:ASN:HA	1:A:3605:LYS:HE3	1.74	0.70
1:A:1751:VAL:HG13	1:A:1814:GLU:HG3	1.71	0.70
1:A:2829:ALA:O	1:A:2833:PHE:HB2	1.91	0.69
1:A:2640:GLU:HG2	1:A:2653:VAL:HG22	1.74	0.69
1:A:2138:ILE:HD12	1:A:2161:LEU:HD22	1.74	0.69
1:A:2354:ALA:HB1	1:A:2358:ARG:HH21	1.57	0.69
1:A:1978:ILE:HD11	1:A:2001:LEU:HD11	1.76	0.68
1:A:1709:MET:HE3	1:A:1871:GLU:HA	1.75	0.68
1:A:1588:VAL:HG13	1:A:1589:MET:HE3	1.76	0.67
1:A:2625:ALA:HB3	1:A:3006:GLU:HG3	1.76	0.67
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.75	0.67
1:A:4176:ARG:NH1	1:A:4220:ASP:OD1	2.28	0.67
1:A:2885:ASP:OD2	1:A:2886:GLN:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2485:GLN:OE1	1:A:2488:ARG:NH2	2.27	0.66
1:A:4037:PRO:HG2	1:A:4117:GLN:HE21	1.61	0.66
1:A:1795:SER:O	1:A:1800:GLN:NE2	2.28	0.66
1:A:4324:PRO:HD3	1:A:4638:ARG:HG3	1.78	0.65
1:A:3912:ASN:O	1:A:3937:ARG:NH1	2.30	0.65
1:A:4033:THR:OG1	1:A:4034:GLU:OE1	2.15	0.65
1:A:2867:MET:SD	1:A:2868:SER:N	2.69	0.64
1:A:3194:LEU:HD13	1:A:3503:ILE:HD11	1.79	0.64
1:A:1808:LEU:O	1:A:1812:ILE:HD12	1.98	0.64
1:A:4065:GLN:HE21	1:A:4092:ARG:HD3	1.62	0.64
1:A:4448:LEU:O	1:A:4452:ILE:HG12	1.98	0.64
1:A:3736:GLY:O	1:A:3740:LEU:N	2.31	0.64
1:A:1711:VAL:O	1:A:1715:LYS:HG2	1.98	0.64
1:A:2937:GLY:HA3	1:A:3094:PHE:HB2	1.80	0.63
1:A:3004:PHE:O	1:A:3008:MET:HG2	1.98	0.63
1:A:3691:ASP:HB2	1:A:3695:ARG:HH12	1.65	0.62
1:A:2068:LYS:NZ	1:A:2164:VAL:O	2.32	0.62
1:A:2356:VAL:HG23	1:A:2361:MET:HE1	1.80	0.62
1:A:3875:MET:HE1	1:A:3883:PHE:HB2	1.82	0.62
1:A:2759:ILE:HD12	1:A:2762:LEU:HD12	1.82	0.62
1:A:3854:GLN:O	1:A:3858:ILE:HG13	2.00	0.61
1:A:3877:HIS:HA	1:A:3880:HIS:CD2	2.35	0.61
1:A:4577:LEU:HD22	1:A:4638:ARG:HD2	1.81	0.61
1:A:3561:ARG:NH1	1:A:3603:GLU:OE2	2.33	0.61
1:A:2505:ASP:HB3	1:A:2733:VAL:HG23	1.81	0.61
1:A:1752:LEU:HD11	1:A:1868:TYR:CZ	2.36	0.61
1:A:2413:LEU:O	1:A:2417:ARG:HG3	2.01	0.61
1:A:1659:ALA:HB2	1:A:1926:PHE:HD1	1.64	0.60
1:A:2704:GLU:HG3	1:A:2705:ARG:HG3	1.84	0.60
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.84	0.60
1:A:2265:TYR:OH	1:A:2311:TRP:O	2.19	0.60
1:A:2930:GLN:OE1	1:A:2930:GLN:N	2.27	0.60
1:A:3508:LEU:HD23	1:A:3536:LEU:HD21	1.81	0.60
1:A:3923:ARG:HH12	1:A:3952:GLN:HB2	1.67	0.60
1:A:2663:CYS:HB2	1:A:2710:GLY:HA2	1.84	0.60
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.84	0.60
1:A:3826:GLN:HB2	1:A:4139:LEU:HB3	1.85	0.59
1:A:2270:PRO:HA	1:A:2273:ARG:HH21	1.67	0.59
1:A:1760:GLU:O	1:A:1764:THR:HG23	2.02	0.59
1:A:3215:VAL:HG11	1:A:3478:LEU:HD11	1.83	0.59
1:A:4040:PRO:HB3	1:A:4124:LEU:HD22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4172:SER:HB2	1:A:4173:PRO:HD2	1.84	0.59
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.84	0.58
1:A:1587:LEU:HB3	1:A:1590:ASP:HB2	1.85	0.58
1:A:3849:VAL:HG12	1:A:3855:ARG:HG3	1.85	0.58
1:A:2622:PHE:CD1	1:A:2626:THR:HG21	2.38	0.58
1:A:1734:ASP:HB3	1:A:1737:THR:HG22	1.84	0.58
1:A:3981:THR:HG23	1:A:3984:GLY:H	1.67	0.58
1:A:2280:PHE:HE1	1:A:2315:LEU:HD21	1.68	0.58
1:A:2179:ARG:HE	1:A:2208:LEU:HD11	1.69	0.58
1:A:3972:TYR:HE1	1:A:3989:ARG:HH21	1.51	0.58
1:A:1910:THR:HG23	1:A:2044:PRO:HD3	1.85	0.57
1:A:1852:ASP:OD2	1:A:1855:GLN:NE2	2.31	0.57
1:A:1887:ARG:HD3	1:A:2039:LEU:HD11	1.85	0.57
1:A:3909:LEU:HB3	1:A:4344:LEU:HD13	1.86	0.57
1:A:1561:LEU:HD23	1:A:1564:GLU:HG3	1.87	0.57
1:A:3873:ARG:HD2	1:A:4025:LEU:HD13	1.87	0.57
1:A:4201:TRP:HZ3	1:A:4207:PHE:HE1	1.52	0.57
1:A:2773:MET:HG3	1:A:2825:TRP:HE1	1.68	0.57
1:A:2890:ARG:HG2	1:A:2894:LYS:HE2	1.87	0.57
1:A:2933:LEU:HD12	1:A:3065:VAL:HG22	1.87	0.57
1:A:4445:THR:HG22	1:A:4448:LEU:HD23	1.86	0.57
1:A:2210:LEU:HG	1:A:2220:LEU:HD21	1.87	0.57
1:A:2533:PRO:HB2	1:A:2535:ILE:HG22	1.87	0.57
1:A:2623:SER:HA	1:A:2668:LEU:HD23	1.87	0.57
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	1.86	0.57
1:A:2961:ILE:HB	1:A:2998:ASN:HD21	1.68	0.57
1:A:4176:ARG:HH12	1:A:4220:ASP:HA	1.68	0.57
1:A:2851:ASP:OD1	1:A:2865:LYS:NZ	2.38	0.56
1:A:4106:LEU:HD23	1:A:4135:PRO:HD2	1.87	0.56
1:A:3126:MET:HE1	1:A:3538:GLN:HG2	1.87	0.56
1:A:1511:PRO:HG2	1:A:3670:ASP:HB3	1.86	0.56
1:A:1814:GLU:OE2	1:A:1878:LYS:NZ	2.29	0.56
1:A:4399:LYS:NZ	1:A:4493:SER:OG	2.38	0.56
1:A:4453:ASN:O	1:A:4457:LYS:NZ	2.38	0.56
1:A:2292:ARG:H	1:A:2292:ARG:HH11	1.53	0.56
1:A:3208:ILE:HB	1:A:3486:ARG:HH22	1.71	0.56
1:A:4172:SER:OG	1:A:4176:ARG:NE	2.28	0.56
1:A:2280:PHE:CE1	1:A:2315:LEU:HD21	2.41	0.55
1:A:2826:ALA:HA	1:A:2850:ILE:HD11	1.88	0.55
1:A:2423:MET:HE2	1:A:2427:PHE:HE2	1.71	0.55
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2665:GLU:HB3	1:A:2668:LEU:HB2	1.88	0.55
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.89	0.55
1:A:1846:PHE:CE2	1:A:1848:PRO:HG3	2.41	0.55
1:A:2308:ASP:HB3	1:A:2311:TRP:NE1	2.21	0.55
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.41	0.55
1:A:2320:ASP:HB3	1:A:2358:ARG:HD3	1.87	0.55
1:A:2622:PHE:HD1	1:A:2626:THR:HG21	1.72	0.55
1:A:2849:ASN:HA	1:A:2852:THR:HG22	1.87	0.55
1:A:2065:LEU:HD11	1:A:2133:GLU:HB3	1.88	0.55
1:A:3734:LEU:HD21	1:A:3783:LYS:HB3	1.89	0.54
1:A:4069:ILE:HD13	1:A:4080:ALA:HA	1.89	0.54
1:A:2925:ILE:HG21	1:A:2933:LEU:HG	1.87	0.54
1:A:3033:CYS:HB2	1:A:3053:TRP:HZ3	1.72	0.54
1:A:2922:ILE:HG23	1:A:2933:LEU:HD11	1.89	0.54
1:A:1626:PHE:CE1	1:A:1628:ARG:HB2	2.42	0.54
1:A:3126:MET:SD	1:A:3539:ALA:HB2	2.48	0.54
1:A:2457:SER:HB3	1:A:2732:PRO:HB3	1.88	0.54
1:A:3691:ASP:O	1:A:3695:ARG:NH1	2.40	0.54
1:A:3567:LEU:HB2	1:A:3599:PHE:CE1	2.42	0.54
1:A:4227:ALA:HB2	1:A:4233:ILE:HD13	1.89	0.54
1:A:3207:LYS:HE3	1:A:3753:LEU:HB3	1.90	0.54
1:A:4247:MET:HG2	1:A:4251:ILE:HD11	1.90	0.54
1:A:3614:PHE:HE2	1:A:3638:VAL:HG12	1.73	0.53
1:A:3724:VAL:HA	1:A:3727:LYS:HG2	1.89	0.53
1:A:4169:ILE:HG21	1:A:4302:ARG:HE	1.73	0.53
1:A:1463:LEU:HB2	1:A:1507:MET:HE1	1.90	0.53
1:A:2441:PHE:HA	1:A:2449:LEU:HD23	1.90	0.53
1:A:3502:THR:OG1	1:A:3544:ARG:N	2.42	0.53
1:A:3034:LYS:O	1:A:3038:GLN:HG2	2.09	0.53
1:A:3148:VAL:O	1:A:3152:GLN:HG2	2.08	0.53
1:A:3055:THR:O	1:A:3059:ILE:HG12	2.08	0.53
1:A:3638:VAL:HG11	1:A:3679:LEU:HB3	1.91	0.53
1:A:3730:ASP:HA	1:A:3733:LYS:HZ2	1.73	0.53
1:A:4201:TRP:CZ3	1:A:4207:PHE:HE1	2.26	0.53
1:A:2630:LEU:HA	1:A:2633:LYS:NZ	2.23	0.53
1:A:1806:ARG:NH2	1:A:1876:GLN:O	2.42	0.53
1:A:2113:ARG:O	1:A:2113:ARG:HG3	2.08	0.53
1:A:2221:MET:HG3	1:A:2343:PHE:HB2	1.91	0.53
1:A:3731:LEU:HD11	1:A:3790:VAL:HG12	1.90	0.53
1:A:2648:VAL:HG12	1:A:2701:VAL:HG23	1.90	0.53
1:A:3499:GLN:O	1:A:3503:ILE:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4201:TRP:HE1	1:A:4264:LEU:HD23	1.74	0.53
1:A:1618:TYR:HA	1:A:1621:ARG:HG2	1.91	0.52
1:A:2423:MET:HE1	1:A:2462:LEU:HD13	1.90	0.52
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.44	0.52
1:A:1959:GLU:HB3	1:A:1962:ARG:HG3	1.90	0.52
1:A:3723:ASP:O	1:A:3726:GLU:HG3	2.10	0.52
1:A:3729:SER:O	1:A:3733:LYS:HG3	2.09	0.52
1:A:2232:MET:HE2	1:A:2232:MET:HA	1.92	0.52
1:A:3741:ARG:HH12	1:A:3776:GLU:HG2	1.75	0.52
1:A:3559:ARG:O	1:A:3563:GLN:HG2	2.08	0.52
1:A:2963:VAL:HG11	1:A:2998:ASN:HA	1.92	0.52
1:A:2944:THR:O	1:A:2948:ARG:HG3	2.10	0.52
1:A:2382:LEU:O	1:A:2416:GLN:NE2	2.39	0.52
1:A:3818:LEU:HD23	1:A:4346:MET:HE2	1.91	0.52
1:A:4247:MET:O	1:A:4252:TYR:HB2	2.10	0.52
1:A:2910:VAL:HG21	1:A:3105:VAL:HG22	1.92	0.51
1:A:4492:ILE:HG12	1:A:4507:ILE:HD13	1.91	0.51
1:A:4070:ALA:HA	1:A:4097:LYS:HB2	1.92	0.51
1:A:2079:GLN:HG2	1:A:2160:LEU:HD21	1.91	0.51
1:A:2581:LEU:HD13	1:A:2605:LEU:HD12	1.92	0.51
1:A:4188:ALA:O	1:A:4192:GLU:HG2	2.10	0.51
1:A:1659:ALA:HB2	1:A:1926:PHE:CD1	2.43	0.51
1:A:1666:LEU:HB3	1:A:1670:ASN:HA	1.92	0.51
1:A:3556:ALA:HB2	1:A:3737:GLU:OE1	2.11	0.51
1:A:4306:VAL:O	1:A:4310:GLU:HG3	2.11	0.51
1:A:2635:PHE:HB3	1:A:2650:LEU:HD11	1.91	0.51
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	1.90	0.51
1:A:2346:GLN:HB2	1:A:2726:ARG:HD2	1.92	0.51
1:A:3838:ASN:HA	1:A:3842:GLU:CD	2.36	0.51
1:A:2383:ARG:NH2	1:A:2424:GLN:OE1	2.43	0.51
1:A:1599:ARG:O	1:A:1602:GLU:HG3	2.10	0.51
1:A:2823:ARG:HE	1:A:2871:ILE:HG23	1.75	0.51
1:A:4201:TRP:HZ3	1:A:4207:PHE:CE1	2.29	0.51
1:A:2818:VAL:O	1:A:2822:ILE:HG22	2.11	0.51
1:A:3649:LEU:HB3	1:A:3695:ARG:HB3	1.93	0.51
1:A:1533:LEU:HD11	1:A:1597:VAL:HG12	1.93	0.51
1:A:2354:ALA:HB1	1:A:2358:ARG:NH2	2.25	0.51
1:A:3704:THR:H	1:A:3707:SER:HB3	1.76	0.50
1:A:4168:ARG:NH1	1:A:4220:ASP:OD2	2.41	0.50
1:A:3487:GLU:O	1:A:3490:GLU:HG3	2.11	0.50
1:A:3488:ARG:HH12	1:A:3773:LEU:HD22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1619:LEU:HG	1:A:1637:LEU:HD23	1.94	0.50
1:A:2071:PRO:O	1:A:2075:LEU:HG	2.12	0.50
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.93	0.50
1:A:3690:PRO:HA	1:A:3693:CYS:HB2	1.94	0.50
1:A:1698:ILE:HA	1:A:1701:TRP:CD1	2.47	0.49
1:A:1933:ASP:OD1	1:A:1934:GLU:N	2.43	0.49
1:A:3128:VAL:HG22	1:A:3145:ASN:OD1	2.12	0.49
1:A:1904:PRO:HB2	1:A:1912:LYS:HB3	1.94	0.49
1:A:2308:ASP:HB3	1:A:2311:TRP:CD1	2.47	0.49
1:A:1899:ARG:HB3	1:A:1983:ARG:HA	1.95	0.49
1:A:2862:ASP:OD1	1:A:2863:ARG:N	2.45	0.49
1:A:2935:LEU:HD23	1:A:3092:ASN:HB2	1.94	0.49
1:A:3193:GLU:O	1:A:3196:GLU:HG3	2.12	0.49
1:A:1680:GLU:CD	1:A:1680:GLU:H	2.20	0.49
1:A:2868:SER:OG	1:A:2870:PRO:HD2	2.12	0.49
1:A:3923:ARG:NH1	1:A:3952:GLN:HB2	2.28	0.49
1:A:2527:PRO:HD3	1:A:2545:TRP:CD2	2.48	0.49
1:A:2756:LEU:HD12	1:A:2766:ALA:HB2	1.94	0.49
1:A:4486:ILE:O	1:A:4490:GLN:HG3	2.12	0.49
1:A:1926:PHE:CE2	1:A:1928:LEU:HD11	2.47	0.49
1:A:2759:ILE:HG13	1:A:2759:ILE:O	2.13	0.49
1:A:3030:MET:HE1	1:A:3051:TYR:HB2	1.94	0.49
1:A:4474:THR:HG22	1:A:4476:ILE:H	1.78	0.49
1:A:1888:CYS:HA	1:A:2039:LEU:HD22	1.95	0.49
1:A:2188:GLU:OE2	1:A:2243:ARG:NH2	2.46	0.49
1:A:2327:LEU:HD12	1:A:2331:GLU:HB3	1.95	0.49
1:A:2838:VAL:HG13	1:A:3093:TRP:CZ2	2.47	0.49
1:A:3628:ARG:HD3	1:A:3628:ARG:O	2.12	0.49
1:A:2457:SER:OG	1:A:2501:SER:HB2	2.13	0.49
1:A:2671:MET:HB2	1:A:2721:LYS:HG2	1.95	0.49
1:A:3133:LEU:N	1:A:3134:PRO:HD3	2.27	0.49
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.95	0.49
1:A:4140:ARG:HG3	1:A:4140:ARG:HH11	1.78	0.49
1:A:1927:VAL:HG22	1:A:1954:TRP:HB2	1.95	0.49
1:A:2134:GLN:O	1:A:2138:ILE:HG12	2.13	0.49
1:A:3724:VAL:HG21	1:A:3797:VAL:HG11	1.93	0.49
1:A:4046:VAL:HG21	1:A:4148:GLU:HG2	1.93	0.49
1:A:1698:ILE:HA	1:A:1701:TRP:NE1	2.28	0.48
1:A:4481:ASP:OD1	1:A:4482:PHE:N	2.46	0.48
1:A:2269:ASP:OD1	1:A:2269:ASP:N	2.46	0.48
1:A:2617:VAL:HG13	1:A:2660:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3628:ARG:HD3	1:A:3628:ARG:C	2.38	0.48
1:A:3587:PRO:O	1:A:3587:PRO:HG2	2.12	0.48
1:A:3931:GLN:O	1:A:3935:VAL:HG23	2.13	0.48
1:A:4175:GLU:HG3	1:A:4278:PHE:CE2	2.48	0.48
1:A:1711:VAL:HG13	1:A:1715:LYS:HE3	1.95	0.48
1:A:2449:LEU:HD11	1:A:2454:CYS:SG	2.53	0.48
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.95	0.48
1:A:2831:ARG:HA	1:A:2831:ARG:NE	2.28	0.48
1:A:2849:ASN:O	1:A:2853:VAL:HG22	2.13	0.48
1:A:4445:THR:H	1:A:4448:LEU:HB2	1.79	0.48
1:A:2660:VAL:HG12	1:A:2707:GLN:HB3	1.94	0.48
1:A:2740:GLY:N	1:A:2743:SER:OG	2.47	0.48
1:A:3591:ASP:HB3	1:A:3701:PHE:HB2	1.94	0.48
1:A:2104:LYS:NZ	1:A:2133:GLU:OE2	2.47	0.48
1:A:2785:THR:OG1	1:A:2787:ASP:OD1	2.27	0.48
1:A:2809:ALA:HB1	1:A:2824:ILE:HD13	1.96	0.48
1:A:3151:HIS:CE1	1:A:3176:TYR:HB2	2.48	0.48
1:A:3642:ASP:OD2	1:A:3644:VAL:HG12	2.14	0.48
1:A:1665:ILE:HG13	1:A:1685:MET:HE1	1.96	0.47
1:A:2309:PRO:HD3	1:A:2350:TYR:O	2.13	0.47
1:A:4100:HIS:HB3	1:A:4128:MET:HB2	1.96	0.47
1:A:1721:VAL:O	1:A:1725:GLU:HG2	2.15	0.47
1:A:2340:ARG:HG2	1:A:2340:ARG:HH11	1.78	0.47
1:A:2472:TYR:CE2	1:A:2481:MET:HB3	2.50	0.47
1:A:3801:TYR:CD1	1:A:3856:LEU:HD13	2.49	0.47
1:A:4095:MET:HE2	1:A:4097:LYS:HE2	1.95	0.47
1:A:4178:ARG:HD2	1:A:4278:PHE:CE2	2.49	0.47
1:A:2365:SER:O	1:A:2368:VAL:HG22	2.14	0.47
1:A:3034:LYS:NZ	1:A:3035:GLU:OE2	2.46	0.47
1:A:2309:PRO:HG3	1:A:2352:THR:HG23	1.96	0.47
1:A:3555:ASN:HB2	1:A:3558:GLU:OE1	2.15	0.47
1:A:2999:VAL:HG11	1:A:3078:ARG:HH12	1.78	0.47
1:A:3144:VAL:O	1:A:3148:VAL:HG23	2.14	0.47
1:A:1938:PHE:HZ	1:A:1970:ALA:HB3	1.79	0.47
1:A:2609:LEU:HD22	1:A:2660:VAL:HG21	1.97	0.47
1:A:3872:ALA:HB1	1:A:3880:HIS:ND1	2.30	0.47
1:A:4575:LEU:HG	1:A:4624:PHE:HB3	1.97	0.47
1:A:1575:PHE:HD1	1:A:1604:LEU:HD21	1.80	0.47
1:A:2423:MET:CE	1:A:2462:LEU:HD13	2.45	0.47
1:A:2654:GLN:O	1:A:2705:ARG:NH2	2.48	0.47
1:A:2939:SER:O	1:A:3172:THR:HB	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4157:MET:HE1	1:A:4181:PHE:CE1	2.50	0.47
1:A:4416:GLU:OE2	1:A:4515:PHE:N	2.31	0.47
1:A:1682:GLU:OE1	1:A:1872:TYR:OH	2.27	0.47
1:A:2059:PHE:HE1	1:A:2101:GLY:HA2	1.80	0.47
1:A:2308:ASP:HB3	1:A:2311:TRP:HE1	1.80	0.47
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.15	0.47
1:A:2686:MET:SD	1:A:2703:LEU:HD11	2.55	0.47
1:A:2935:LEU:HD22	1:A:3094:PHE:CE1	2.50	0.47
1:A:3872:ALA:O	1:A:3880:HIS:HE1	1.98	0.47
1:A:1463:LEU:HD21	1:A:1519:ASP:HB3	1.97	0.47
1:A:4296:MET:SD	1:A:4297:PRO:HD2	2.55	0.47
1:A:4538:GLU:HB3	1:A:4594:LYS:HE2	1.96	0.47
1:A:1520:ALA:O	1:A:1524:GLU:N	2.47	0.46
1:A:3152:GLN:O	1:A:3156:GLN:HG2	2.14	0.46
1:A:2132:PRO:HB2	1:A:2135:GLU:OE1	2.15	0.46
1:A:2306:ASP:HA	1:A:2345:VAL:HG23	1.97	0.46
1:A:4175:GLU:HG3	1:A:4278:PHE:HE2	1.81	0.46
1:A:2890:ARG:NH2	1:A:2913:ASN:OD1	2.44	0.46
1:A:3197:GLN:HG3	1:A:3496:PHE:CE2	2.50	0.46
1:A:4266:ASN:O	1:A:4270:GLU:HG3	2.15	0.46
1:A:1804:ARG:O	1:A:1808:LEU:HD23	2.16	0.46
1:A:1998:THR:HG22	1:A:2007:LYS:HA	1.98	0.46
1:A:2034:LYS:HG3	1:A:2035:LEU:HG	1.97	0.46
1:A:2179:ARG:NH1	1:A:2195:ASP:OD1	2.49	0.46
1:A:2624:SER:HA	1:A:2669:PRO:HA	1.98	0.46
1:A:3739:GLN:O	1:A:3743:ARG:HG2	2.16	0.46
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.81	0.46
1:A:2226:SER:OG	3:A:4702:ATP:O1G	2.26	0.46
1:A:2937:GLY:C	1:A:3070:PRO:HD3	2.41	0.46
1:A:4201:TRP:NE1	1:A:4264:LEU:HD23	2.30	0.46
1:A:1503:SER:O	1:A:1507:MET:HG3	2.16	0.46
1:A:2138:ILE:HD11	1:A:2165:PHE:CG	2.51	0.46
1:A:2577:HIS:O	1:A:2581:LEU:HG	2.15	0.46
1:A:3659:ARG:HG3	1:A:3661:LEU:HG	1.96	0.46
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.98	0.46
1:A:2152:GLU:OE2	1:A:2152:GLU:N	2.42	0.45
1:A:4570:CYS:HB3	1:A:4575:LEU:HD23	1.98	0.45
1:A:2650:LEU:HD22	1:A:2703:LEU:HD22	1.98	0.45
1:A:4136:VAL:O	1:A:4140:ARG:HG2	2.17	0.45
1:A:3909:LEU:HD21	1:A:4343:MET:HE3	1.98	0.45
1:A:1699:ASN:OD1	1:A:1700:GLU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3084:ALA:HA	1:A:3087:ASN:HB3	1.99	0.45
1:A:2209:GLN:O	1:A:2213:ILE:HG12	2.16	0.45
1:A:1789:LEU:HD13	1:A:1815:LEU:HB3	1.99	0.45
1:A:2037:ARG:HH21	1:A:4251:ILE:HA	1.81	0.45
1:A:2890:ARG:O	1:A:2894:LYS:HG3	2.15	0.45
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.50	0.45
1:A:2309:PRO:HA	1:A:2312:VAL:HG22	1.99	0.45
1:A:3204:GLY:HA2	1:A:3750:LEU:HD21	1.99	0.45
1:A:1501:ILE:HA	1:A:1504:VAL:HG22	1.98	0.45
1:A:1579:MET:HA	1:A:1582:VAL:HG12	1.99	0.45
1:A:2469:VAL:HG13	1:A:2481:MET:SD	2.57	0.45
1:A:2242:GLU:HG3	1:A:2248:GLU:HA	1.99	0.45
1:A:4611:LEU:HD23	1:A:4611:LEU:H	1.82	0.45
1:A:1561:LEU:HD11	1:A:1618:TYR:CG	2.52	0.44
1:A:1713:LEU:HD13	1:A:1749:LEU:HD11	1.99	0.44
1:A:2994:MET:HE2	1:A:2994:MET:HB3	1.82	0.44
1:A:3715:GLU:OE2	1:A:3841:TYR:OH	2.29	0.44
1:A:4502:LYS:HE2	1:A:4502:LYS:HB2	1.69	0.44
1:A:2445:HIS:NE2	1:A:2449:LEU:HD22	2.32	0.44
1:A:3590:ILE:HB	1:A:3700:ASN:HA	2.00	0.44
1:A:3612:THR:O	1:A:3635:VAL:HA	2.16	0.44
1:A:4154:LYS:HE3	1:A:4310:GLU:HA	1.98	0.44
1:A:1860:GLN:HG2	1:A:1865:LYS:HG2	2.00	0.44
1:A:2371:THR:HG22	1:A:2451:ARG:HD2	1.99	0.44
1:A:3976:GLU:HB3	1:A:3979:PRO:HD2	1.99	0.44
1:A:4185:TRP:CD1	1:A:4284:LEU:HD12	2.53	0.44
1:A:1697:LYS:HD2	1:A:1698:ILE:H	1.82	0.44
1:A:1888:CYS:O	1:A:1892:MET:HG2	2.18	0.44
1:A:2046:ARG:HG2	1:A:2090:LEU:HD13	2.00	0.44
1:A:2086:TYR:OH	1:A:2153:ASP:OD2	2.24	0.44
1:A:2663:CYS:N	1:A:2709:VAL:O	2.47	0.44
1:A:2770:THR:O	1:A:2774:VAL:HG23	2.18	0.44
1:A:4326:ASN:O	1:A:4330:VAL:HG23	2.18	0.44
1:A:1613:LYS:O	1:A:1617:GLU:HG2	2.18	0.44
1:A:2245:GLU:HB2	1:A:2247:VAL:HG12	2.00	0.44
1:A:2454:CYS:HB3	1:A:2502:LEU:HD12	1.98	0.44
1:A:3015:GLY:HA3	1:A:3059:ILE:HD11	2.00	0.44
1:A:4117:GLN:OE1	1:A:4117:GLN:N	2.50	0.44
1:A:1651:GLN:N	1:A:1651:GLN:OE1	2.49	0.44
1:A:2593:LEU:HD23	1:A:2734:VAL:HB	1.99	0.44
1:A:1920:GLY:HA3	1:A:1927:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2106:GLU:OE1	1:A:2109:GLN:NE2	2.50	0.43
1:A:4503:GLU:O	1:A:4507:ILE:HG13	2.17	0.43
1:A:2569:VAL:HG21	1:A:2747:ILE:HA	2.01	0.43
1:A:2845:TRP:CE2	1:A:2849:ASN:ND2	2.87	0.43
1:A:2374:ILE:HA	3:A:4702:ATP:H8	1.83	0.43
1:A:2806:ILE:O	1:A:2810:LEU:HG	2.18	0.43
1:A:3724:VAL:HG11	1:A:3797:VAL:HG21	2.01	0.43
1:A:3811:ILE:HD11	1:A:3864:PHE:CE1	2.53	0.43
1:A:4099:VAL:HG11	1:A:4126:LEU:HB3	2.01	0.43
1:A:4113:LEU:HD23	1:A:4113:LEU:HA	1.86	0.43
1:A:2831:ARG:HG3	1:A:2924:ARG:NH1	2.33	0.43
1:A:3609:ILE:HD11	1:A:3634:LEU:HB2	2.01	0.43
1:A:2458:LEU:O	1:A:2462:LEU:HG	2.19	0.43
1:A:2749:GLY:O	1:A:2753:ARG:HG3	2.18	0.43
1:A:3555:ASN:O	1:A:3559:ARG:HG3	2.19	0.43
1:A:3633:LEU:HB3	1:A:3677:ILE:HD12	2.01	0.43
1:A:3638:VAL:HG22	1:A:3681:THR:HB	2.01	0.43
1:A:1903:SER:N	1:A:2037:ARG:O	2.48	0.43
1:A:2354:ALA:O	1:A:2358:ARG:HB2	2.18	0.43
1:A:2596:PRO:HB2	1:A:2738:TYR:CE1	2.53	0.43
1:A:3620:ARG:HE	1:A:3620:ARG:HB3	1.56	0.43
1:A:3721:ARG:HG2	1:A:3852:HIS:CE1	2.53	0.43
1:A:4196:TYR:O	1:A:4200:GLY:N	2.51	0.43
1:A:4473:MET:HB2	1:A:4477:GLN:OE1	2.19	0.43
1:A:3157:ALA:HB1	1:A:3524:MET:HE2	2.01	0.43
1:A:3812:TYR:CZ	1:A:3829:LEU:HD13	2.54	0.43
1:A:3877:HIS:O	1:A:3877:HIS:ND1	2.49	0.43
1:A:4601:LYS:HE2	1:A:4603:SER:HB3	2.01	0.43
1:A:2075:LEU:HD11	1:A:4536:LEU:HD13	2.01	0.43
1:A:2981:ARG:NH1	1:A:3032:GLN:OE1	2.50	0.43
1:A:2995:ASP:OD2	1:A:2998:ASN:HB2	2.19	0.43
1:A:3562:TRP:CZ2	1:A:3581:LYS:HD2	2.54	0.43
1:A:4172:SER:CB	1:A:4176:ARG:HH21	2.32	0.43
1:A:3204:GLY:C	1:A:3489:TRP:HZ3	2.27	0.42
1:A:4333:THR:O	1:A:4337:VAL:HG23	2.19	0.42
1:A:1588:VAL:HA	1:A:1591:VAL:HG22	2.01	0.42
1:A:3745:LEU:HD12	1:A:3745:LEU:HA	1.88	0.42
1:A:4003:ALA:O	1:A:4007:MET:HG3	2.19	0.42
1:A:1544:TRP:HE1	1:A:1572:SER:HA	1.84	0.42
1:A:1635:GLU:OE1	1:A:1635:GLU:N	2.33	0.42
1:A:3029:LEU:HD11	1:A:3054:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3803:PRO:HA	1:A:3806:THR:HG22	2.01	0.42
1:A:3844:PRO:HA	1:A:3847:LYS:HE3	2.00	0.42
1:A:4004:MET:HE3	1:A:4007:MET:HB2	2.01	0.42
1:A:4543:VAL:HG21	1:A:4622:VAL:HG23	2.01	0.42
1:A:1504:VAL:HA	1:A:1507:MET:HE2	2.01	0.42
1:A:1554:SER:OG	1:A:1642:GLY:HA3	2.18	0.42
1:A:3892:LEU:HD13	1:A:3983:ILE:HG21	2.00	0.42
1:A:2410:SER:HB3	1:A:2411:PRO:HD3	2.01	0.42
1:A:3885:MET:HE3	1:A:3885:MET:HB2	1.81	0.42
1:A:4044:CYS:SG	1:A:4144:ILE:HG23	2.59	0.42
1:A:2668:LEU:HD13	1:A:2720:ARG:HH12	1.85	0.42
1:A:3005:LEU:HD21	1:A:3078:ARG:NH1	2.35	0.42
1:A:3146:SER:OG	1:A:3508:LEU:HD21	2.19	0.42
1:A:4179:LEU:HD11	1:A:4238:ILE:HD12	2.01	0.42
1:A:4189:ILE:HD13	1:A:4321:LEU:HD23	2.01	0.42
1:A:2227:GLY:O	1:A:2369:LEU:HD23	2.20	0.42
1:A:2852:THR:HA	1:A:2855:LEU:HG	2.01	0.42
1:A:2965:ARG:NH2	1:A:3640:SER:O	2.53	0.42
1:A:3562:TRP:HB3	1:A:3567:LEU:HD22	2.02	0.42
1:A:1692:ILE:HG23	1:A:1701:TRP:CD1	2.55	0.42
1:A:2592:VAL:HB	1:A:2733:VAL:HG12	2.02	0.42
1:A:2783:ARG:HD3	1:A:2845:TRP:CE2	2.54	0.42
1:A:2820:GLY:O	1:A:2824:ILE:HG13	2.20	0.42
1:A:2935:LEU:N	1:A:3066:PHE:O	2.45	0.42
1:A:3139:HIS:NE2	1:A:3541:ILE:HG23	2.34	0.42
1:A:3512:ALA:O	1:A:3516:TYR:HB2	2.19	0.42
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	2.02	0.42
1:A:2277:ASP:OD1	1:A:2277:ASP:N	2.52	0.42
1:A:2300:TRP:CD1	1:A:2340:ARG:HB2	2.55	0.42
1:A:2961:ILE:HB	1:A:2998:ASN:ND2	2.34	0.42
1:A:3740:LEU:O	1:A:3744:GLN:HG2	2.20	0.42
1:A:3997:ARG:HH21	1:A:4000:ARG:HD3	1.85	0.42
1:A:2627:THR:OG1	1:A:2629:GLU:HG2	2.20	0.42
1:A:3604:TYR:HD1	1:A:3607:ARG:HD3	1.85	0.42
1:A:4634:SER:HA	1:A:4637:GLU:HG2	2.01	0.42
1:A:1492:ASP:OD1	1:A:1492:ASP:N	2.50	0.41
1:A:1814:GLU:O	1:A:1818:GLN:HG3	2.20	0.41
1:A:2457:SER:HB2	1:A:2584:TRP:CZ2	2.55	0.41
1:A:2628:PRO:HB3	1:A:2682:PHE:CD2	2.55	0.41
1:A:2635:PHE:HE1	1:A:2661:LEU:HD11	1.85	0.41
1:A:3154:LEU:HA	1:A:3154:LEU:HD12	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4339:MET:HE2	1:A:4339:MET:HB3	1.98	0.41
1:A:3030:MET:HA	1:A:3033:CYS:SG	2.60	0.41
1:A:3966:PRO:CD	1:A:4000:ARG:HG3	2.50	0.41
1:A:2179:ARG:NH2	1:A:2205:GLU:OE2	2.53	0.41
1:A:2633:LYS:NZ	1:A:2633:LYS:HB2	2.36	0.41
1:A:2851:ASP:OD2	1:A:2869:ARG:NH1	2.52	0.41
1:A:3196:GLU:HA	1:A:3199:MET:HG3	2.02	0.41
1:A:3611:ARG:NH2	1:A:3636:GLN:OE1	2.53	0.41
1:A:2847:ASP:O	1:A:2850:ILE:HG22	2.21	0.41
1:A:3835:ILE:HG12	1:A:3870:ARG:HD2	2.02	0.41
1:A:4178:ARG:HD2	1:A:4278:PHE:CD2	2.55	0.41
1:A:4631:ASP:OD1	1:A:4631:ASP:N	2.53	0.41
1:A:1840:SER:O	1:A:1861:MET:HE3	2.20	0.41
1:A:2230:LYS:HG2	1:A:2364:PHE:CD1	2.56	0.41
1:A:2925:ILE:O	1:A:2928:GLN:HG2	2.20	0.41
1:A:2935:LEU:O	1:A:3067:THR:HA	2.20	0.41
1:A:2936:ILE:HG12	1:A:3068:MET:HB3	2.03	0.41
1:A:3101:ALA:O	1:A:3105:VAL:HG23	2.20	0.41
1:A:3818:LEU:HD23	1:A:3818:LEU:HA	1.93	0.41
1:A:3821:ILE:HD13	1:A:4345:LYS:HD3	2.03	0.41
1:A:3932:ALA:O	1:A:3936:VAL:HG23	2.21	0.41
1:A:4342:LYS:O	1:A:4345:LYS:HG2	2.20	0.41
1:A:1834:LYS:HA	1:A:1834:LYS:HD2	1.90	0.41
1:A:2235:ARG:O	1:A:2239:LYS:HG2	2.20	0.41
1:A:2505:ASP:HA	1:A:2735:TYR:HB2	2.02	0.41
1:A:2976:LEU:HA	1:A:2979:VAL:HG12	2.02	0.41
1:A:3085:LEU:HD23	1:A:3085:LEU:HA	1.92	0.41
1:A:4628:THR:HG23	1:A:4629:LYS:HG3	2.02	0.41
1:A:1806:ARG:HE	1:A:1875:VAL:HG11	1.86	0.41
1:A:1985:HIS:ND1	1:A:1997:ILE:HD12	2.35	0.41
1:A:2377:ASN:C	1:A:2377:ASN:HD22	2.28	0.41
1:A:2498:ILE:HG23	1:A:2502:LEU:HD22	2.03	0.41
1:A:2668:LEU:HD13	1:A:2720:ARG:NH1	2.36	0.41
1:A:3743:ARG:HA	1:A:3743:ARG:HD3	1.93	0.41
1:A:3764:ASP:HA	1:A:3767:ILE:HB	2.02	0.41
1:A:3959:ILE:HD12	1:A:3959:ILE:H	1.85	0.41
1:A:4431:LEU:O	1:A:4435:VAL:HG23	2.20	0.41
1:A:2111:ILE:CD1	1:A:2131:LEU:HD21	2.51	0.41
1:A:3015:GLY:HA3	1:A:3059:ILE:CD1	2.51	0.41
1:A:3127:PRO:HG2	1:A:3130:TYR:CD1	2.55	0.41
1:A:3133:LEU:HD23	1:A:3141:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3606:ASP:OD1	1:A:3607:ARG:HG3	2.20	0.41
1:A:3873:ARG:HA	1:A:3873:ARG:HD3	1.76	0.41
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	2.03	0.41
1:A:4629:LYS:HE2	1:A:4629:LYS:HB2	1.90	0.41
1:A:3791:MET:HA	1:A:3794:VAL:HB	2.03	0.41
1:A:3871:VAL:HG12	1:A:3875:MET:SD	2.61	0.41
1:A:4204:LYS:HE2	1:A:4204:LYS:HB2	1.97	0.41
1:A:2605:LEU:HD11	1:A:2709:VAL:HG11	2.02	0.40
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.57	0.40
1:A:4610:TYR:CZ	1:A:4615:ARG:HB3	2.56	0.40
1:A:2093:LEU:O	1:A:2097:LEU:HG	2.21	0.40
1:A:2500:TRP:CZ2	1:A:2576:ARG:HD3	2.45	0.40
1:A:3664:LEU:HB3	1:A:3669:ILE:HD13	2.02	0.40
1:A:1783:SER:O	1:A:1787:VAL:HG23	2.22	0.40
1:A:2439:HIS:O	1:A:2442:GLN:HG2	2.22	0.40
1:A:3154:LEU:HD22	1:A:3516:TYR:CD1	2.56	0.40
1:A:3205:LEU:HG	1:A:3489:TRP:HE3	1.86	0.40
1:A:4111:LYS:HD3	1:A:4111:LYS:HA	1.81	0.40
1:A:4481:ASP:O	1:A:4485:ARG:HG3	2.22	0.40
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.86	0.40
1:A:1702:LEU:HA	1:A:1702:LEU:HD23	1.89	0.40
1:A:2018:MET:SD	1:A:2028:LEU:HB3	2.62	0.40
1:A:2527:PRO:HD3	1:A:2545:TRP:CE2	2.56	0.40
1:A:4336:GLY:O	1:A:4340:ILE:HG12	2.21	0.40
1:A:1842:MET:SD	1:A:1922:GLN:HG2	2.61	0.40
1:A:1912:LYS:HB2	1:A:1912:LYS:HE2	1.92	0.40
1:A:2231:SER:HA	1:A:2234:TRP:NE1	2.36	0.40
1:A:2880:ASP:OD2	1:A:2880:ASP:N	2.44	0.40
1:A:4058:LEU:O	1:A:4061:GLU:HG3	2.21	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	2854/4646 (61%)	2750 (96%)	103 (4%)	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	2548/4125 (62%)	2547 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4029	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1598	GLN
1	A	1755	GLN
1	A	1863	ASN
1	A	1894	GLN
1	A	1922	GLN
1	A	2005	GLN
1	A	2031	ASN
1	A	2134	GLN
1	A	2139	GLN
1	A	2187	GLN
1	A	2217	ASN
1	A	2439	HIS
1	A	2442	GLN
1	A	2471	GLN

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Mol	Chain	Res	Type
1	A	2689	HIS
1	A	2730	HIS
1	A	3182	HIS
1	A	3200	HIS
1	A	3214	GLN
1	A	3499	GLN
1	A	3542	GLN
1	A	3584	ASN
1	A	3772	ASN
1	A	3843	ASN
1	A	3880	HIS
1	A	3906	GLN
1	A	4065	GLN
1	A	4326	ASN

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
2	ADP	A	4703	-	28,29,29	1.41	4 (14%)	43,45,45	1.81	9 (20%)
3	ATP	A	4702	-	32,33,33	0.34	0	48,52,52	0.31	0
2	ADP	A	4704	-	28,29,29	1.39	4 (14%)	43,45,45	1.82	10 (23%)
2	ADP	A	4701	-	28,29,29	1.40	4 (14%)	43,45,45	1.84	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	4703	-	-	3/16/32/32	0/3/3/3
3	ATP	A	4702	-	-	5/22/38/38	0/3/3/3
2	ADP	A	4704	-	-	3/16/32/32	0/3/3/3
2	ADP	A	4701	-	-	3/16/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4703	ADP	C5-C4	4.67	1.47	1.39
2	A	4701	ADP	C5-C4	4.61	1.47	1.39
2	A	4704	ADP	C5-C4	4.60	1.47	1.39
2	A	4701	ADP	C5-C6	2.71	1.48	1.41
2	A	4703	ADP	C5-C6	2.62	1.48	1.41
2	A	4704	ADP	C5-C6	2.59	1.48	1.41
2	A	4704	ADP	C5-N7	-2.34	1.34	1.39
2	A	4703	ADP	C5-N7	-2.33	1.34	1.39
2	A	4704	ADP	C8-N7	2.32	1.36	1.31
2	A	4701	ADP	C5-N7	-2.29	1.34	1.39
2	A	4701	ADP	C8-N7	2.28	1.36	1.31
2	A	4703	ADP	C8-N7	2.24	1.36	1.31

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	ADP	C5-C4-N3	-5.69	118.89	126.72
2	A	4704	ADP	C5-C4-N3	-5.65	118.94	126.72
2	A	4703	ADP	C5-C4-N3	-5.64	118.95	126.72
2	A	4703	ADP	N3-C4-N9	4.51	134.84	127.17
2	A	4704	ADP	N3-C4-N9	4.48	134.79	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	ADP	N3-C4-N9	4.47	134.76	127.17
2	A	4701	ADP	C2-N3-C4	3.68	120.83	111.83
2	A	4704	ADP	C2-N3-C4	3.65	120.76	111.83
2	A	4701	ADP	C4-C5-N7	-3.63	106.43	110.58
2	A	4703	ADP	C2-N3-C4	3.62	120.67	111.83
2	A	4704	ADP	C4-C5-N7	-3.45	106.63	110.58
2	A	4704	ADP	N3-C2-N1	-3.38	123.47	128.58
2	A	4701	ADP	N3-C2-N1	-3.31	123.56	128.58
2	A	4703	ADP	C4-C5-N7	-3.29	106.83	110.58
2	A	4703	ADP	N3-C2-N1	-3.24	123.68	128.58
2	A	4701	ADP	C4-N9-C8	2.78	108.66	105.74
2	A	4704	ADP	C4-N9-C8	2.70	108.57	105.74
2	A	4701	ADP	C5-N7-C8	2.66	107.63	103.45
2	A	4703	ADP	C4-N9-C8	2.62	108.49	105.74
2	A	4704	ADP	C5-N7-C8	2.52	107.42	103.45
2	A	4703	ADP	C5-N7-C8	2.41	107.24	103.45
2	A	4701	ADP	C6-C5-N7	2.28	136.49	132.09
2	A	4704	ADP	C6-C5-N7	2.16	136.26	132.09
2	A	4701	ADP	N9-C8-N7	-2.12	110.93	113.94
2	A	4704	ADP	C3'-C2'-C1'	2.09	105.42	101.46
2	A	4703	ADP	C3'-C2'-C1'	2.05	105.34	101.46
2	A	4704	ADP	C2-N1-C6	2.04	122.08	118.73
2	A	4703	ADP	C6-C5-N7	2.01	135.97	132.09

There are no chirality outliers.

All (14) torsion outliers are listed below:

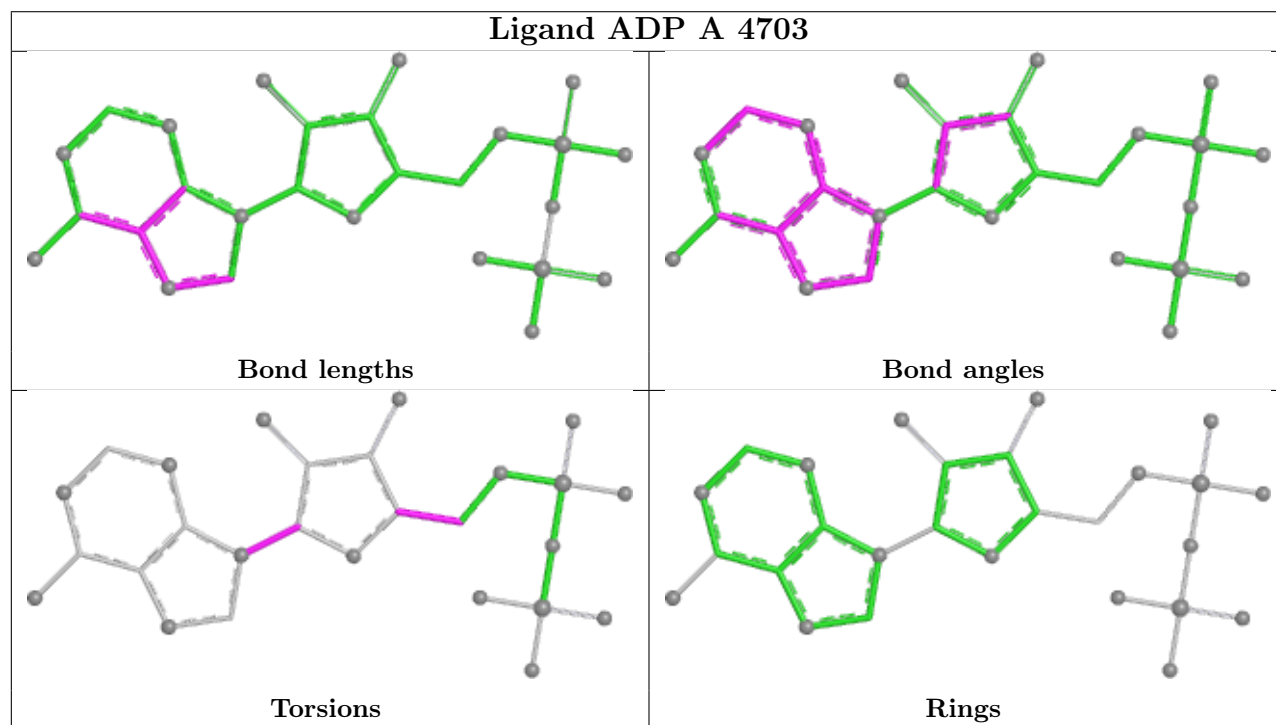
Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O1A
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4704	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C5'-O5'-PA-O2A
3	A	4702	ATP	C5'-O5'-PA-O3A
2	A	4704	ADP	C3'-C4'-C5'-O5'
2	A	4703	ADP	O4'-C1'-N9-C8
2	A	4703	ADP	O4'-C1'-N9-C4
3	A	4702	ATP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'
2	A	4703	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	PA-O3A-PB-O2B

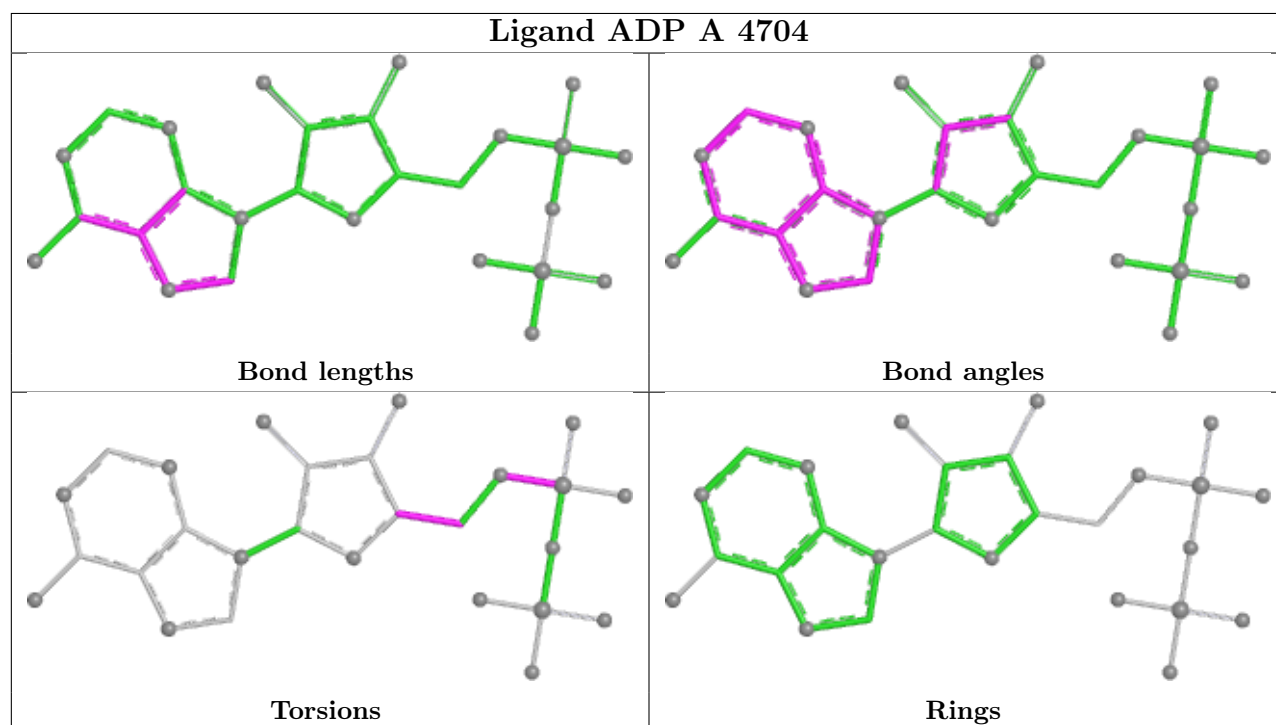
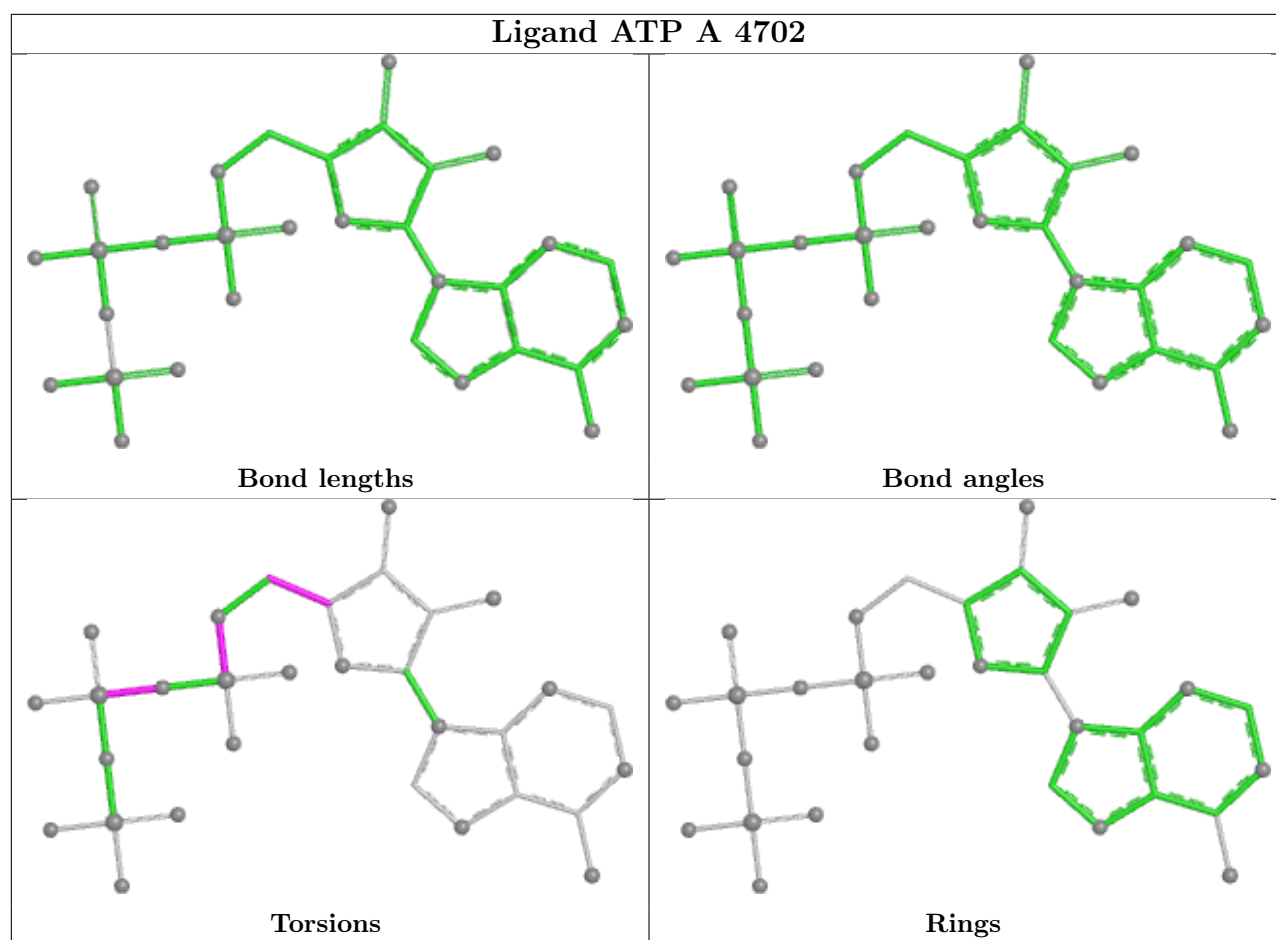
There are no ring outliers.

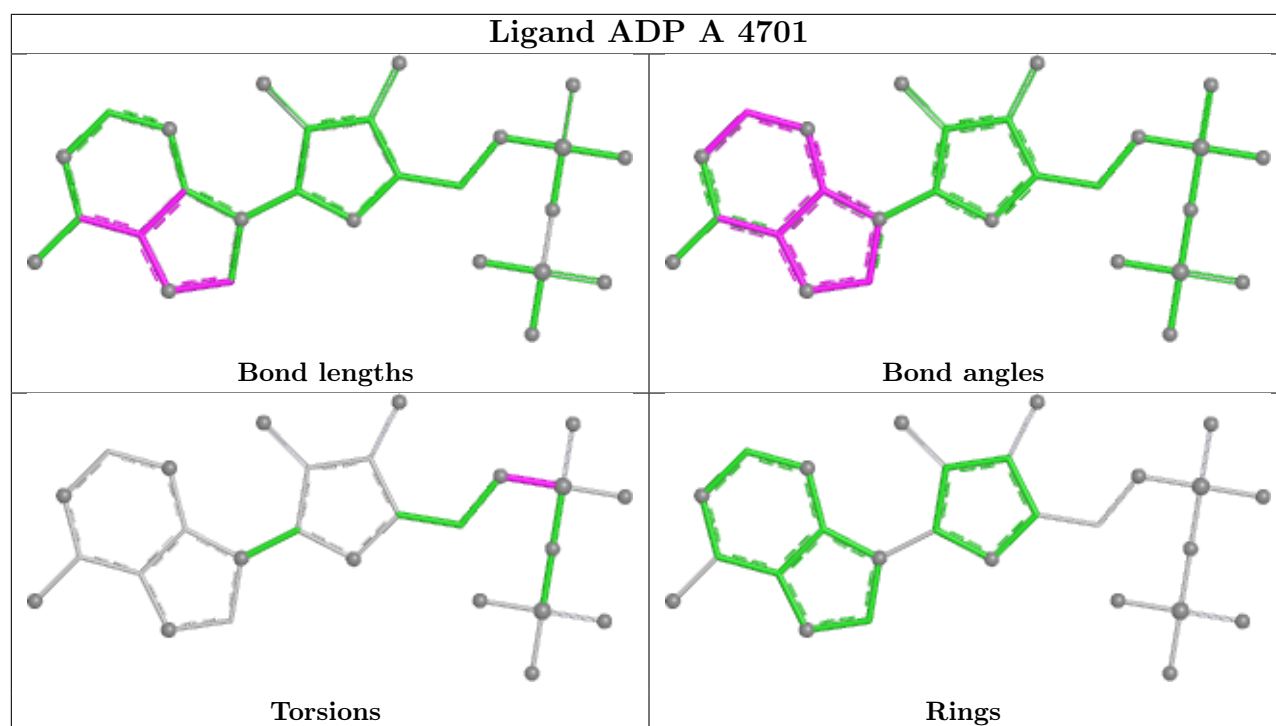
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4702	ATP	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.

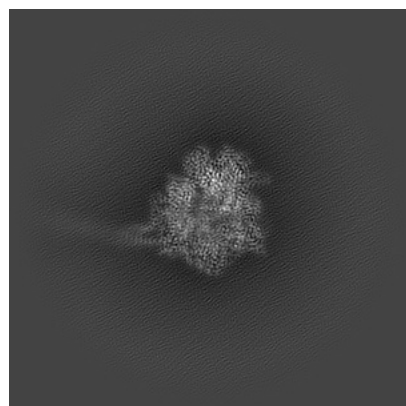
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44720. These allow visual inspection of the internal detail of the map and identification of artifacts.

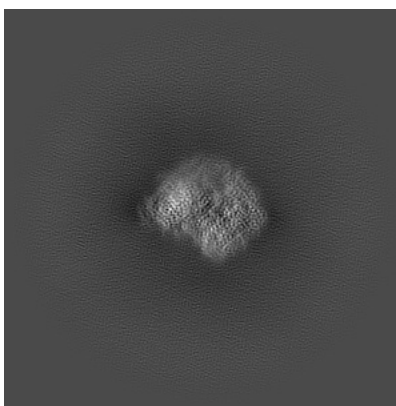
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

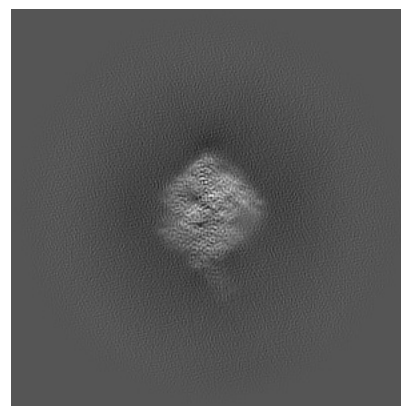
6.1.1 Primary map



X

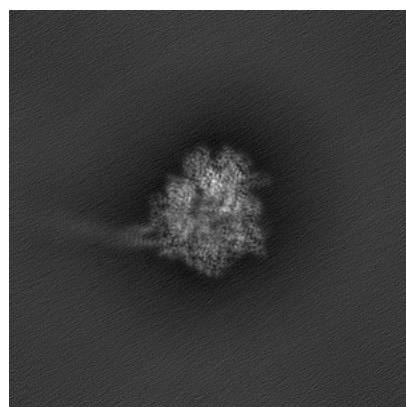


Y

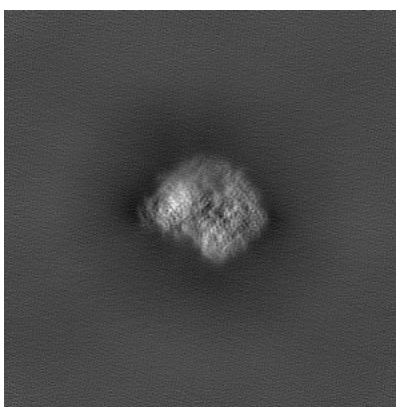


Z

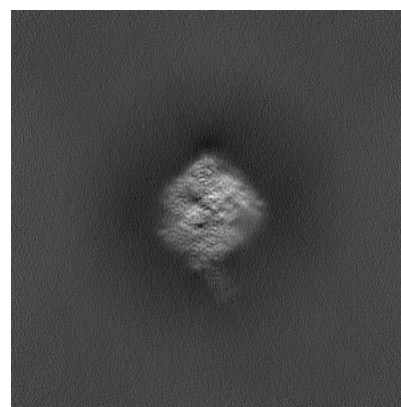
6.1.2 Raw map



X



Y

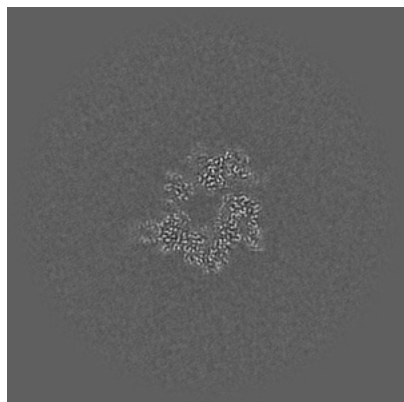


Z

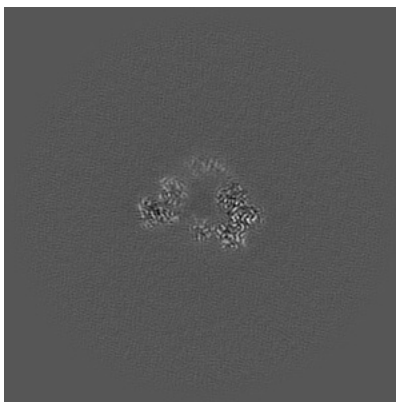
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

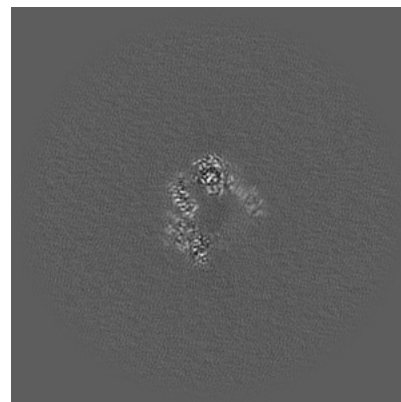
6.2.1 Primary map



X Index: 180

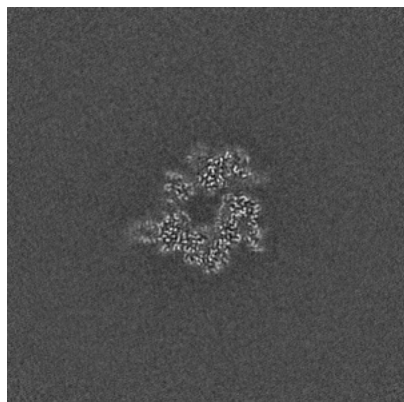


Y Index: 180

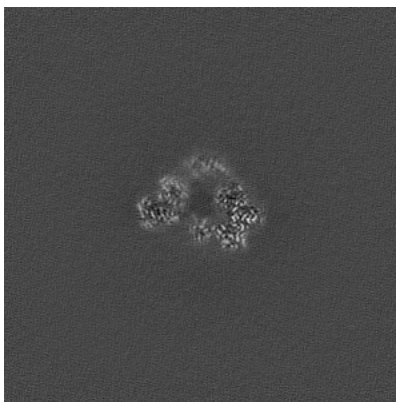


Z Index: 180

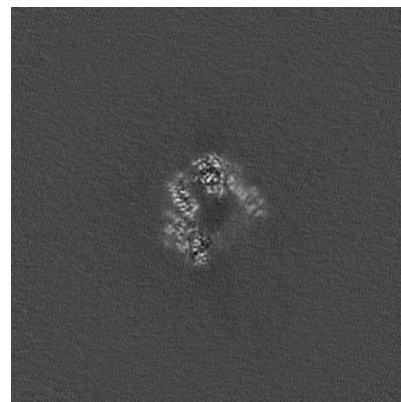
6.2.2 Raw map



X Index: 180



Y Index: 180

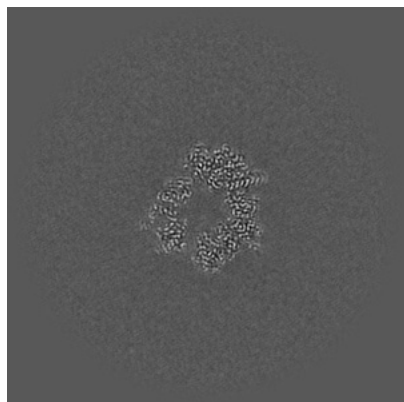


Z Index: 180

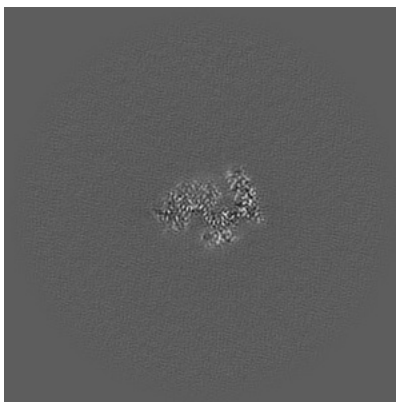
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

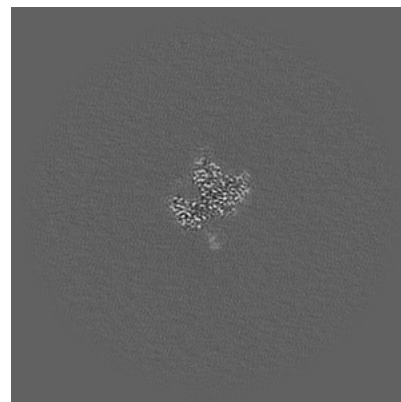
6.3.1 Primary map



X Index: 174

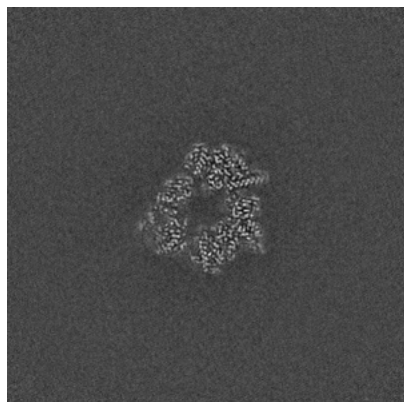


Y Index: 202

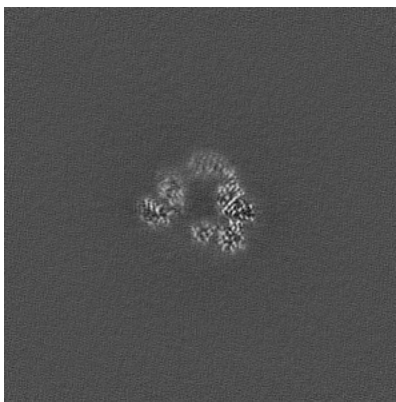


Z Index: 209

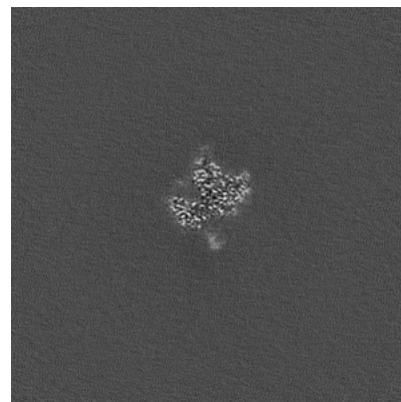
6.3.2 Raw map



X Index: 175



Y Index: 183

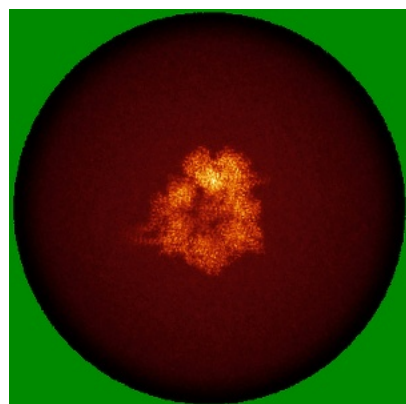


Z Index: 209

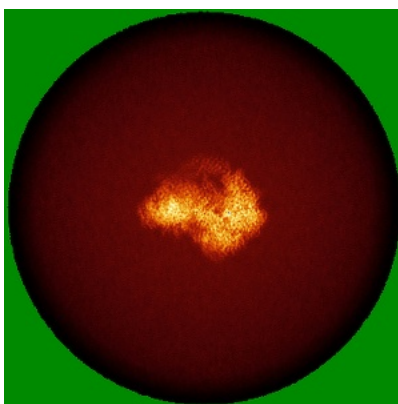
The images above show the largest variance slices of the map in three orthogonal directions.

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

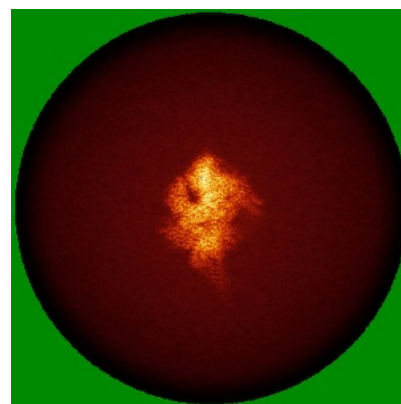
6.4.1 Primary map



X

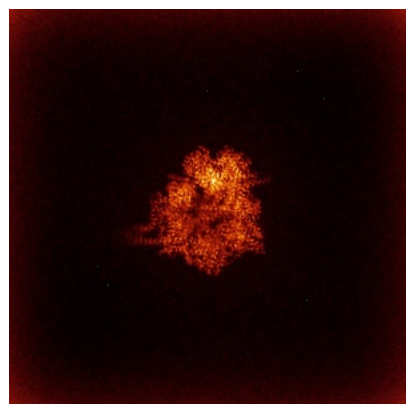


Y

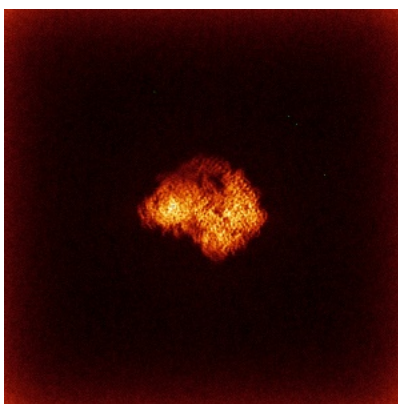


Z

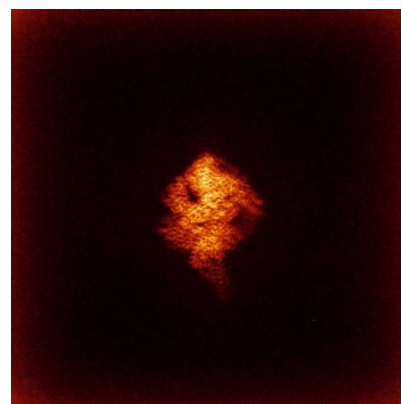
6.4.2 Raw map



X



Y

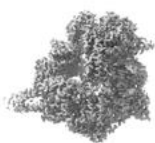


Z

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



X



Y



Z

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.

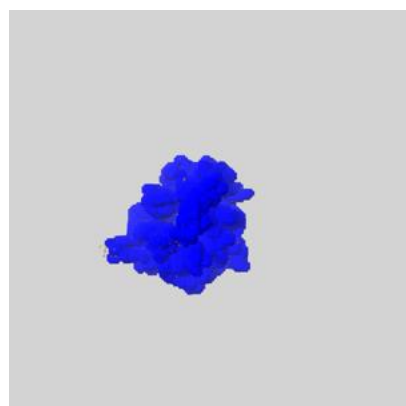
6.6 Mask visualisation [i](#)

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

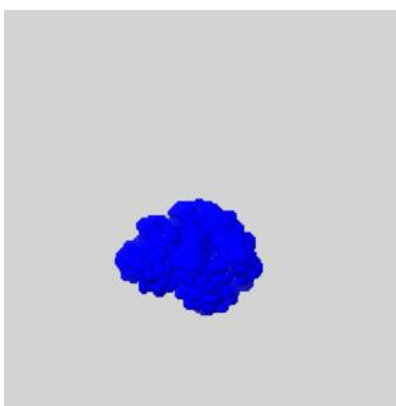
A mask typically either:

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

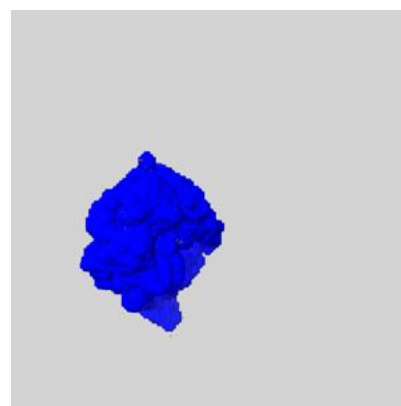
6.6.1 emd_44720_msk_1.map [i](#)



X



Y

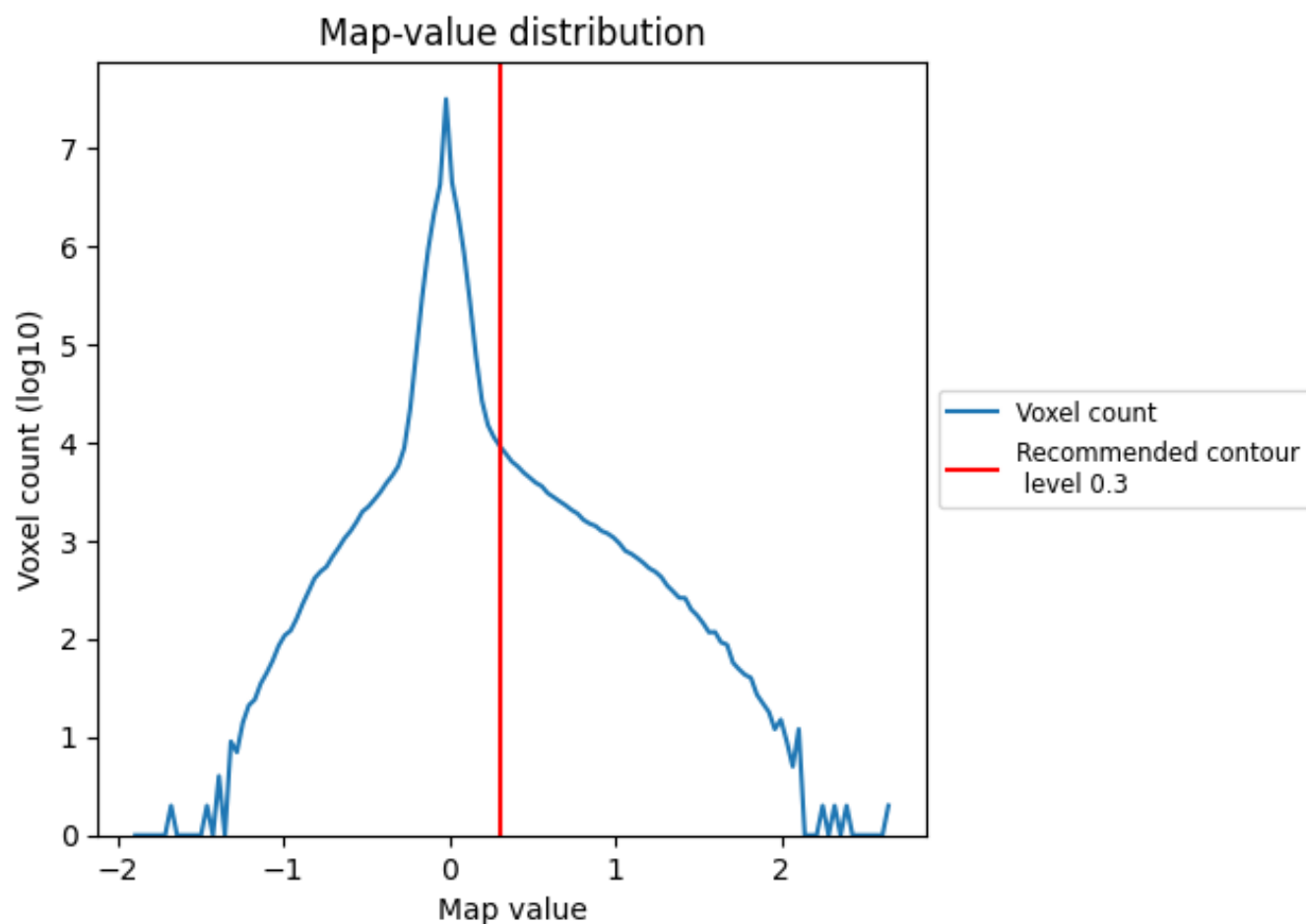


Z

7 Map analysis [i](#)

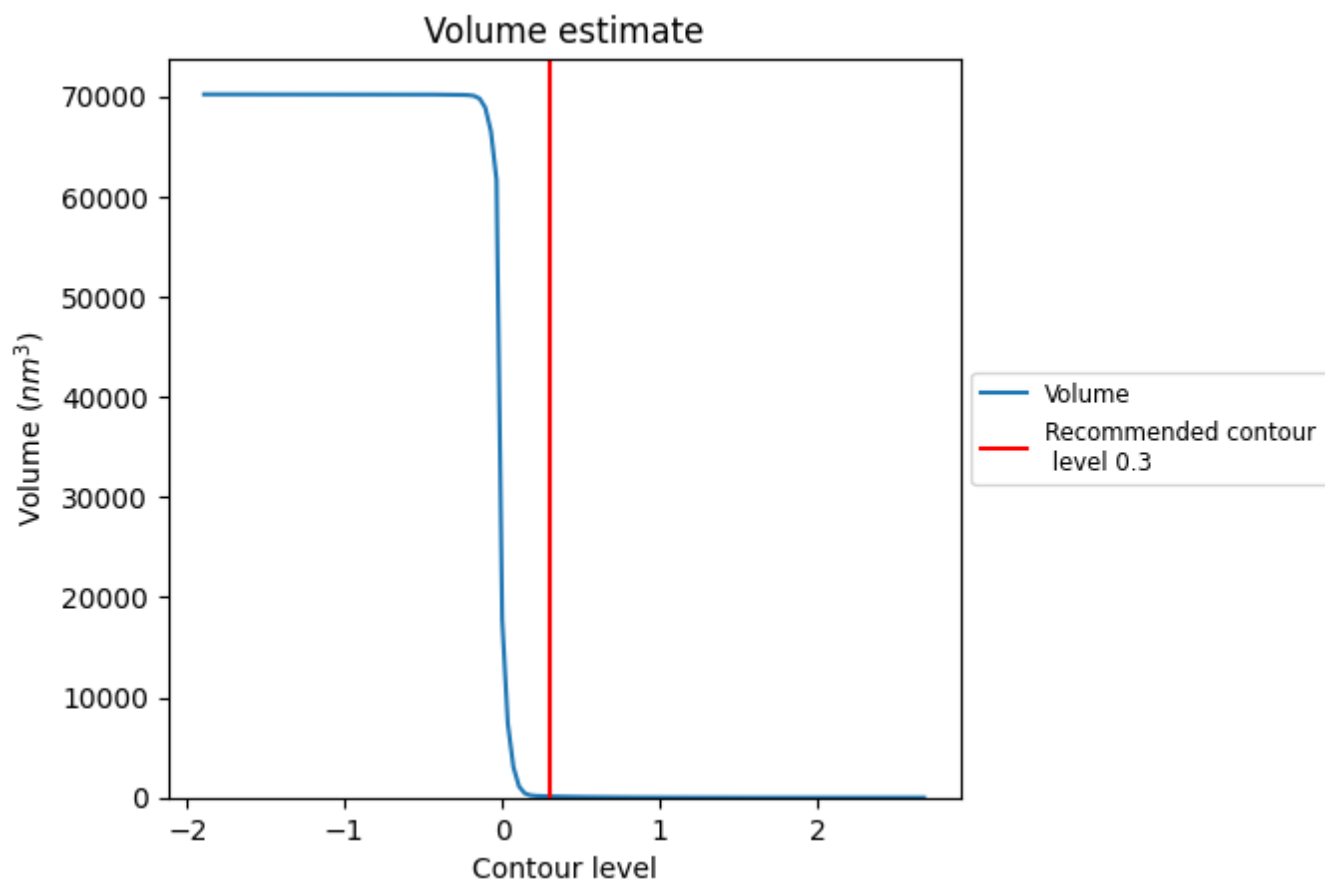
This section contains the results of statistical analysis of the map.

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.

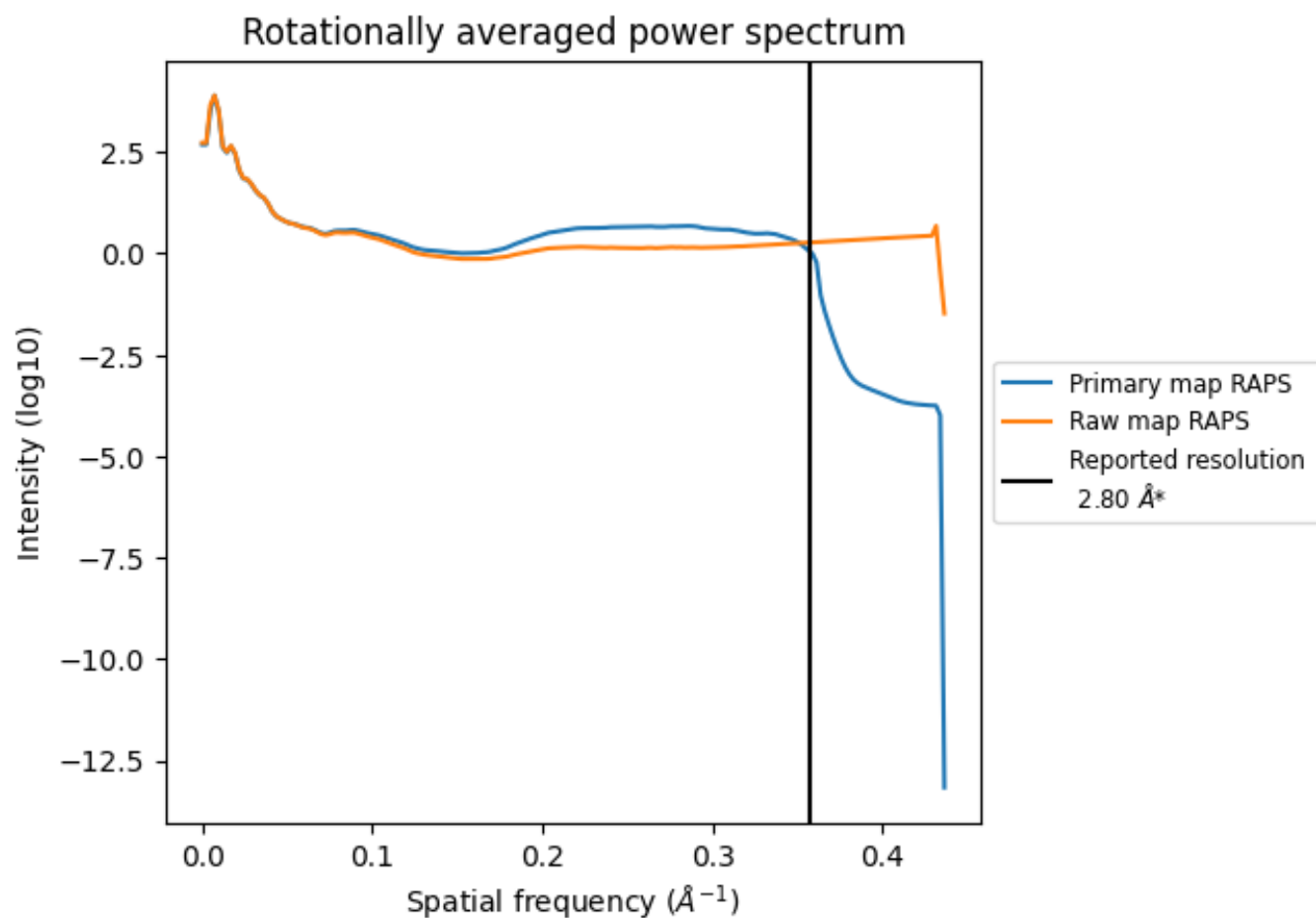
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm³; this corresponds to an approximate mass of 104 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 ⓘ

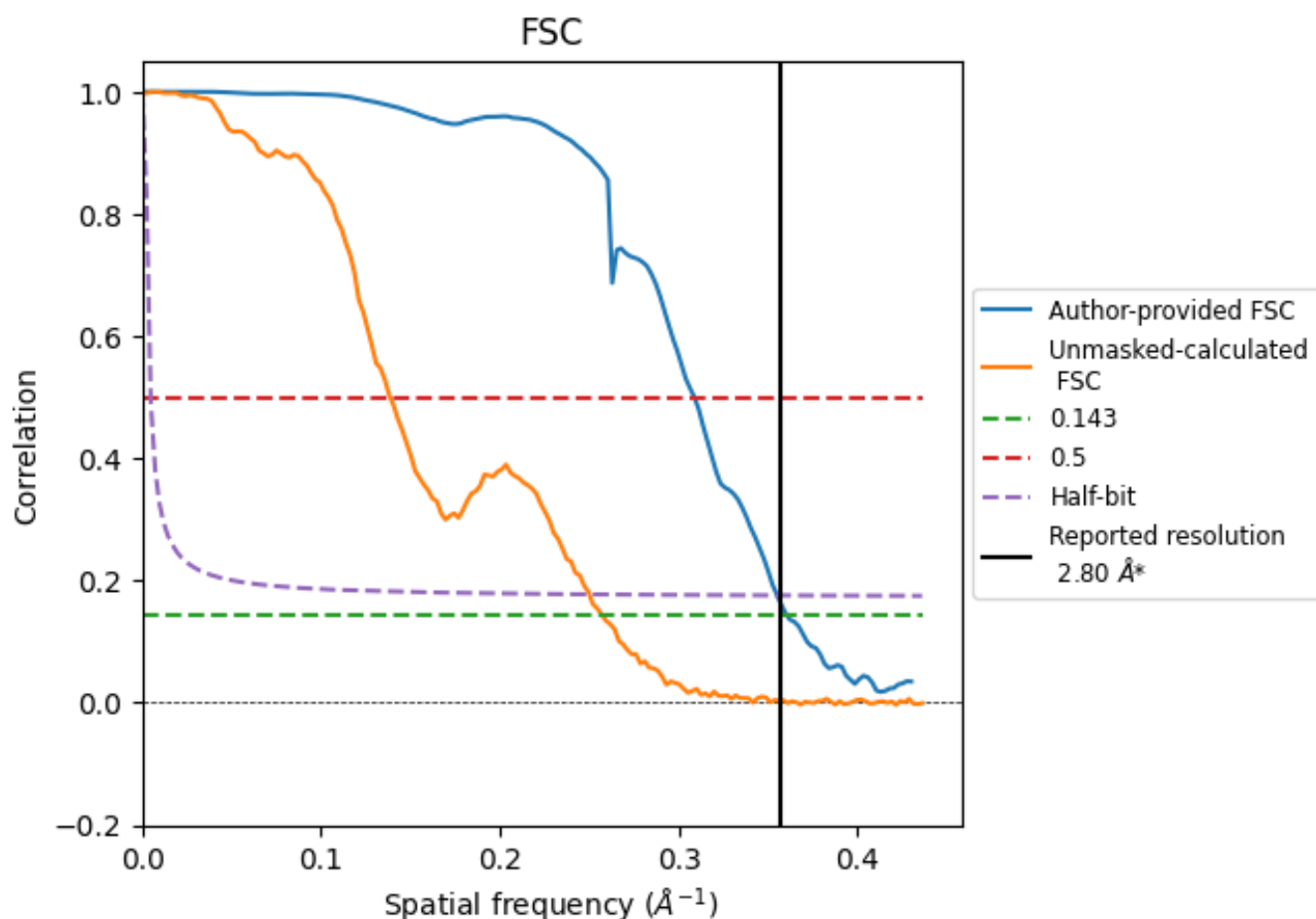


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

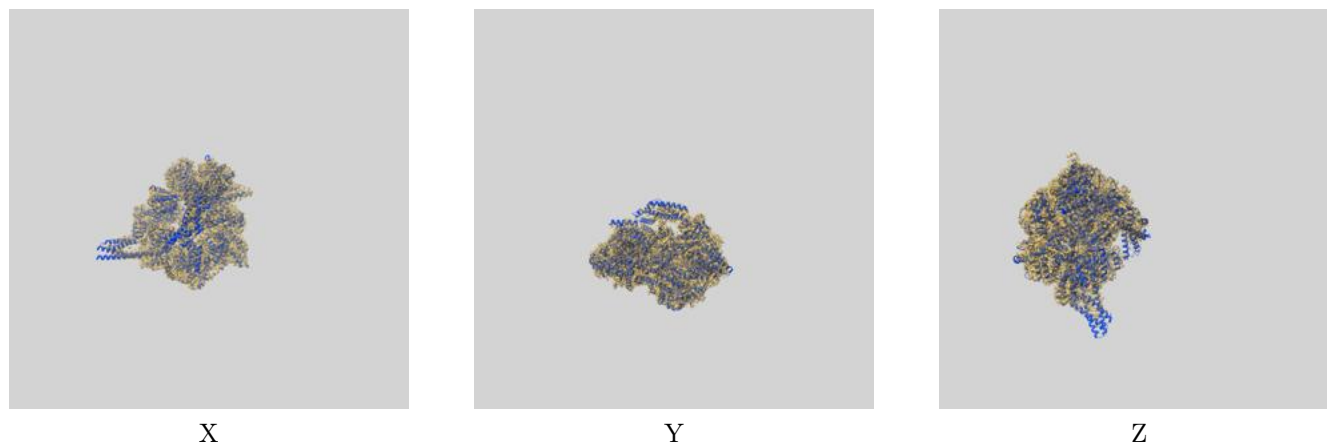
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.77	3.24	2.81
Unmasked-calculated*	3.89	7.21	4.00

*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 3.89 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

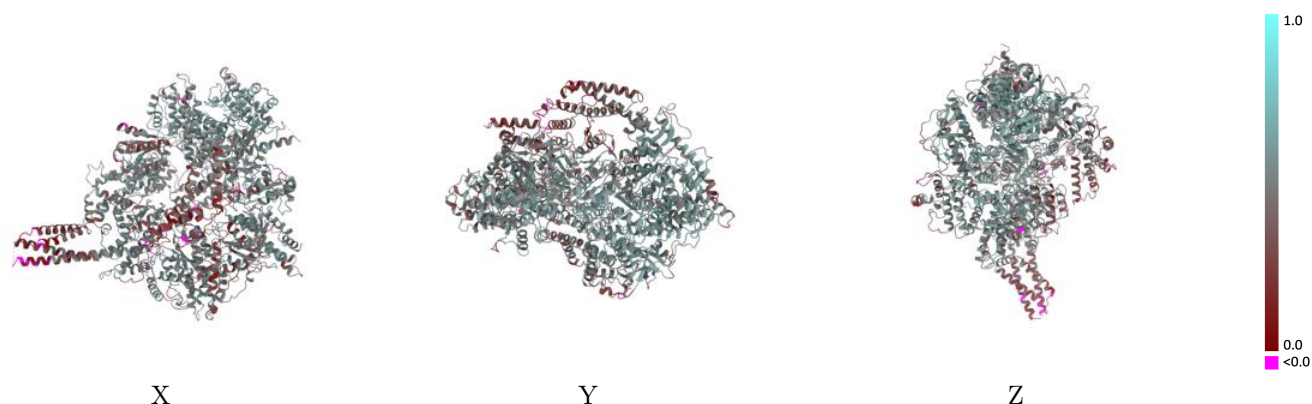
This section contains information regarding the fit between EMDB map EMD-44720 and PDB model 9BN3. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



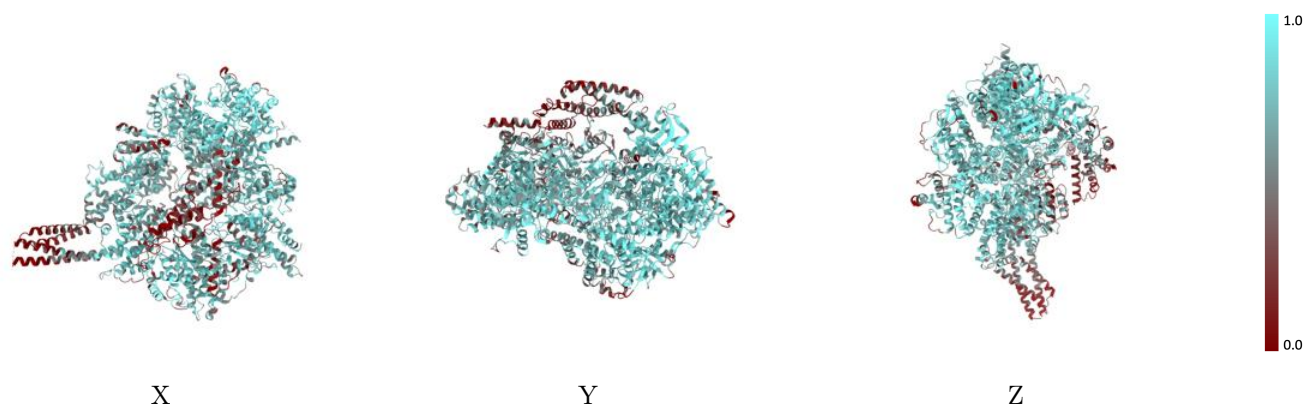
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



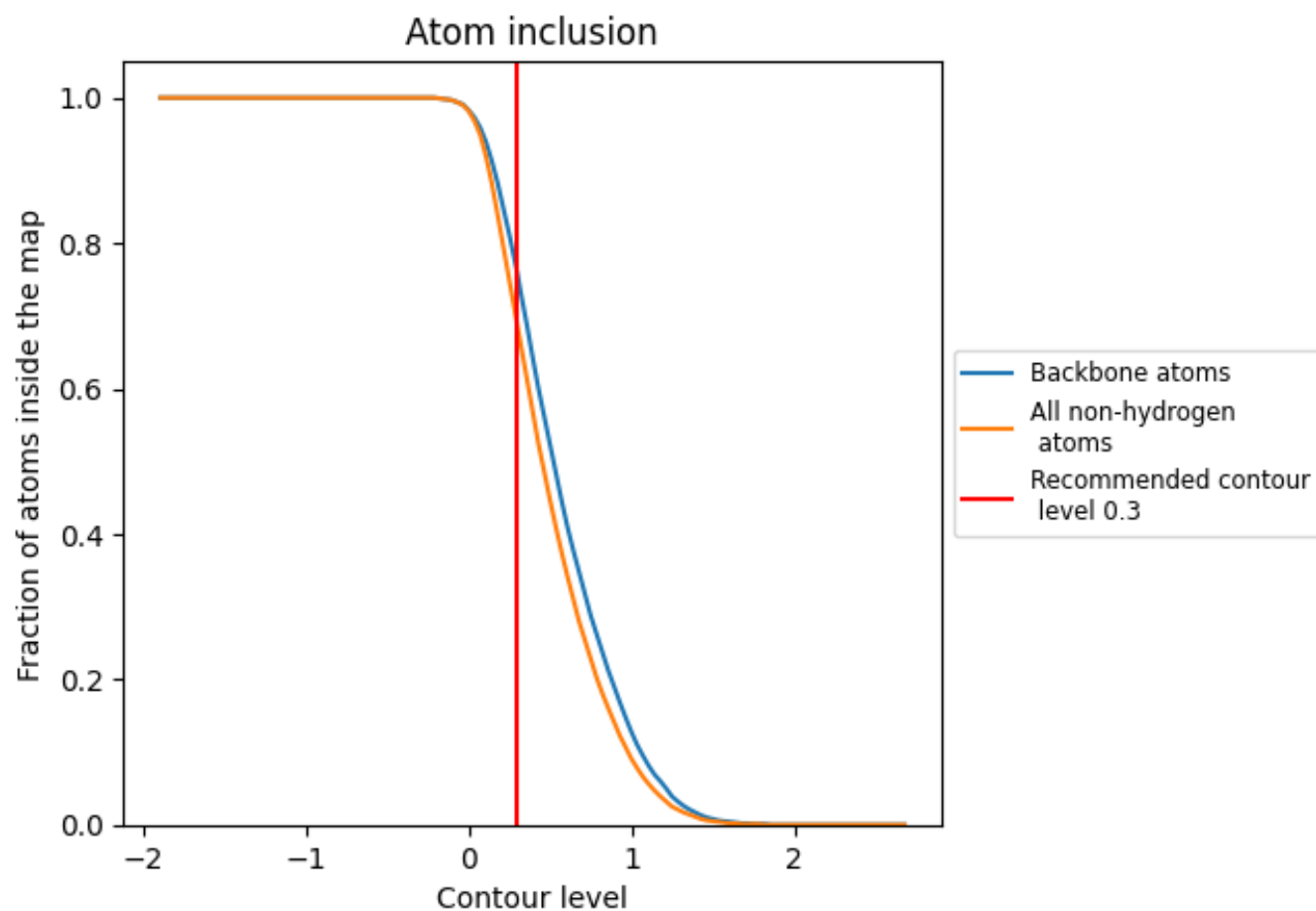
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 76% of all backbone atoms, 69% 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	0.6880	0.4770
A	0.6880	0.4770

