



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:32 PM UTC

PDB ID : 9BM7 / pdb_00009bm7
EMDB ID : EMD-44690
Title : State-7b of motor domain from full-length human dynein-1 in 5 mM ATP
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.58 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

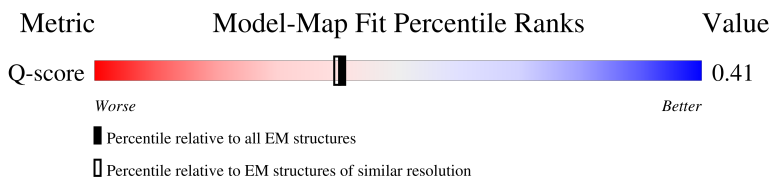
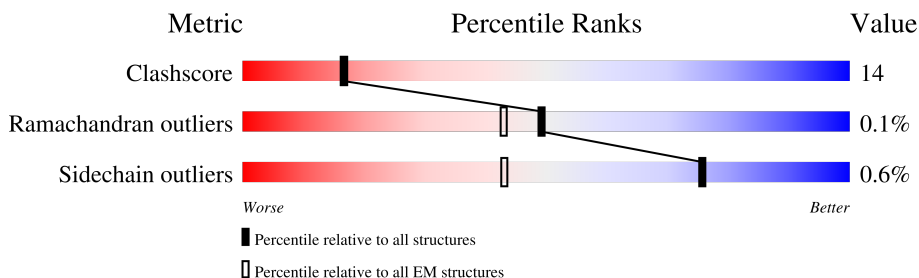
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.58 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	12629 (3.08 - 4.08)

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](#)

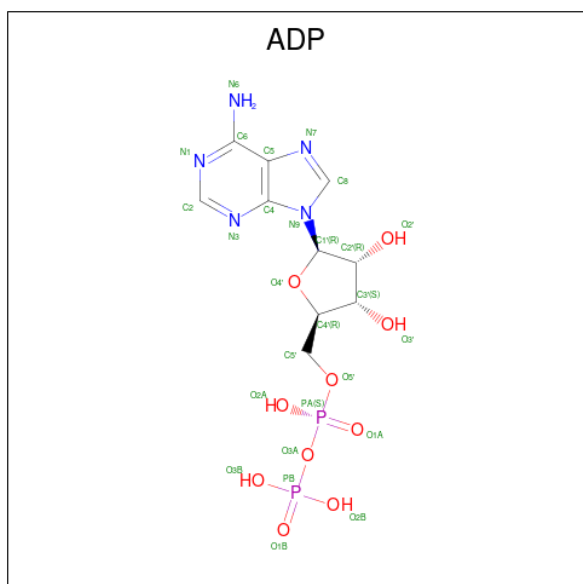
There are 3 unique types of molecules in this entry. The entry contains 21818 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	2703	21702	13828	3748	4016	110	0	0

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



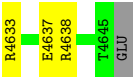
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0
2	A	1	27	10	5	10	2	0

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



I3208	D3045	K2966	R2863	V2774	I2866	A2583	L2446	F2343	E2248	GLY	ALA
K3209	E3048	Y2967	E2864	E2775	N2867	A2583	N2447	E2344	K2257	GLU	GLY
E3210	E3049	T2968	K2865	N2779	L2868	V2569	D2448	Q2346	E2133	SER	SER
T3211	E3049	D2971	A2866	S2780	D2870	L2572	R2451	D2347	Y2265		
V3212	L3050	F2972	M2867	F2784	Q2877	V2575	L2452	L2348	L2268		
Q3213	Y3051	D2973	S2868	T2785	I2880	V2575	R2453	R2358	L2136		
Q3214	K3052	E2974	R2869	Q2786	T2680	L2580	S2460	G2359	L2137		
V3215	T3055	D2975	P2870	Q2787	S2881	L2580	M2461	G2360	L2138		
E3216	S3056	L2976	L2872	D2787	F2882	T2583	Q2464	M2361	Q2139		
E3217	Q3057	R2977	T2788	T2788	I2883	E2587	A2465	V2362	E2143		
E3218	T2978	T2979	S2878	H2791	R2884	E2587	A2466	D2367	E2144		
L3219	V2979			Y2792	R2894	H2588	R2467	L2369	M2145		
R3220	R2982	S2983	L2882	Y2792	R2894	P2591	N2468	S2370	V2146		
ASP	S2983			R2797	D2697	L2591	M2473	T2371	K2148		
LEU	N2987			E2798	Q2888	P2591	N2473	D2372	L2161		
ARG	I2990			N2799	T2899	S2599	M2481	I2374	Y2170		
ILE	T3067			R2801	V2709	G2600	Q2485	I2385	L2048		
TLE	M3068			W2802	A2711	M2603	Q2491	P2386	L2049		
LYS	N3068			V2803	G2710	L2605	R2492	L2387	L2054		
SER	P3070			G2804	C2712	L2605	L2494	D2388	L2055		
GLN	D2995			G2805	P2713		Y2496	GLU	S2056		
GLU	E2996			I2806	N2714		L2497	GLY	L2065		
LEU	L3000			R2811	D2717		L2498	ASP	A2066		
VAL	D3001			L2812	R2720		L2499	ALA	N2067		
LYS	S3002			E2813	R2723		W2500	GLU	N2067		
ASN	E3006			T2814	F2727		S2501	ASP	L2191		
ASP	R3007			E2815	L2728		L2502	ALA	L2192		
ALA	N3008			L2816	R2729		L2514	ARG	D2195		
ALA	T3010			P2817	H2730		L2514	ARG	W2203		
ALA	L3011			L2822	V2731		L2517	LYS	V2207		
THR	A3013			I2822	P2732		L2518	LYS	Y2211		
S3082	N3009			G2820	V2733		V2524	ASP	Q2212		
P3083	T3016			E2828	S2743		P2628	GLU	I2213		
A3084	L3012			L2829	I2747		E2629	GLU	L2220		
L3085	A3013			E2830	N2752		P2632	GLY	M2221		
F3086	N3014			L2831	R2753		H2637	ALA	M2222		
N3087	G3015			R2832	A2754		Y2638	ALA	V2223		
R3088	E3016			E2833	M2755		L2641	ALA	S2226		
C3089	V3017			R2834	L2756		E2638	ALA	K2230		
V3090	L3020			D2835	R2757		E2538	ALA	S2231		
L3091	A3027			Q2834	L2762		S2542	ALA	M2232		
N3092	M3030			D2840	R2763		G2543	ALA	W2234		
W3093	C3033			E2841	T2764		W2545	ALA	R2235		
F3094	E3035			R2843	Y2765		W2548	ALA	L2241		
G3095	Q3038			R2844	T2770		E2556	ALA	E2242		
D3096	R3039			K2866	T2773		V2557	ALA	R2243		
W3097	E3040			H2867				ASP	L2244		
L3102	G3106			E2861				GLU			
V3105	K3107			E2862							
G3106	T3110										
G3106	M3113										
L3194											
E3195											
E3196											
Q3197											
Q3198											
H3200											
L3201											
M3202											
V3203											
G3204											
L3205											
R3206											
K3207											





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66008	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	0.552	Depositor
Minimum map value	-0.340	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	332.80002, 332.80002, 332.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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	0.20	0/22168	0.36	0/30054

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	21702	0	21742	610	0
2	A	54	0	24	7	0
3	A	62	0	24	11	0
All	All	21818	0	21790	610	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 14.

All (610) 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	0.96	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3660:VAL:HG22	1:A:3671:LEU:HD13	1.60	0.84
1:A:2437:LEU:HD22	1:A:2502:LEU:HD21	1.61	0.81
1:A:1882:THR:HB	1:A:1883:PRO:HD2	1.64	0.79
1:A:1812:ILE:HD13	1:A:2056:SER:HA	1.64	0.78
1:A:2302:VAL:HA	1:A:2342:MET:HB2	1.66	0.77
1:A:2221:MET:HB2	1:A:2361:MET:HB2	1.67	0.76
1:A:2910:VAL:HG11	1:A:3105:VAL:HG22	1.69	0.74
1:A:3114:ASP:HB3	1:A:3191:ARG:HH12	1.52	0.74
1:A:3888:ALA:HA	1:A:4013:LEU:HD11	1.69	0.74
1:A:1769:MET:HE3	1:A:1769:MET:HA	1.69	0.74
1:A:2934:LEU:HB3	1:A:3091:LEU:HA	1.70	0.73
1:A:3662:ILE:HG23	1:A:3671:LEU:HD11	1.71	0.72
1:A:2324:LEU:HD11	1:A:2332:ARG:HD3	1.70	0.72
1:A:2814:GLU:HG3	1:A:2815:THR:HG23	1.70	0.72
1:A:2446:ILE:HD11	1:A:2714:PRO:HB3	1.70	0.72
1:A:2925:ILE:HG21	1:A:2933:LEU:HD22	1.72	0.72
1:A:3009:ASN:HD21	1:A:3084:ALA:HB1	1.55	0.70
1:A:3961:LEU:O	1:A:3997:ARG:NH1	2.25	0.70
1:A:3115:LEU:O	1:A:3139:HIS:ND1	2.24	0.69
1:A:2419:ALA:O	1:A:2423:MET:HG2	1.92	0.69
1:A:4021:MET:HE3	1:A:4021:MET:HA	1.75	0.69
1:A:2220:LEU:HB2	1:A:2342:MET:HE1	1.75	0.69
1:A:1708:GLU:O	1:A:1712:THR:HG23	1.93	0.68
1:A:3141:GLU:N	1:A:3141:GLU:OE1	2.27	0.68
1:A:2996:GLU:OE2	1:A:3069:ASN:ND2	2.27	0.68
1:A:2213:ILE:HG22	1:A:2220:LEU:HD22	1.74	0.68
1:A:2974:GLU:OE1	1:A:2977:ARG:NH1	2.27	0.68
1:A:2481:MET:HE1	1:A:2485:GLN:HG2	1.76	0.68
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.76	0.67
1:A:1628:ARG:HB3	1:A:1657:MET:HB2	1.76	0.67
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.76	0.67
1:A:2464:GLN:NE2	1:A:2468:ASN:OD1	2.27	0.67
1:A:3967:GLU:N	1:A:3967:GLU:OE1	2.25	0.67
1:A:2223:VAL:HG21	1:A:2348:LEU:HD12	1.76	0.67
1:A:3134:PRO:HG2	1:A:3137:PRO:HA	1.77	0.67
1:A:3627:LEU:HD21	1:A:3662:ILE:HD11	1.77	0.66
1:A:3588:LEU:HB3	1:A:3696:VAL:HG11	1.78	0.66
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.28	0.66
1:A:2093:LEU:O	1:A:2097:LEU:HG	1.96	0.66
1:A:2943:LYS:NZ	2:A:4704:ADP:O2B	2.28	0.66
1:A:3592:PRO:HG3	1:A:3684:PRO:HG3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2054:LEU:HD21	1:A:2097:LEU:HD22	1.77	0.65
1:A:2464:GLN:OE1	1:A:2467:ARG:NH1	2.29	0.65
1:A:2987:ASN:OD1	1:A:3057:GLN:NE2	2.30	0.65
1:A:3557:ASP:OD1	1:A:3558:GLU:N	2.29	0.65
1:A:2963:VAL:HA	1:A:2967:TYR:HD1	1.61	0.65
1:A:4069:ILE:HD13	1:A:4080:ALA:HA	1.78	0.65
1:A:2065:LEU:HD12	1:A:2137:LEU:HD23	1.79	0.64
1:A:2983:SER:OG	1:A:3061:ASN:O	2.15	0.64
1:A:2819:GLU:HG3	1:A:2865:LYS:HZ2	1.63	0.64
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.79	0.64
1:A:3831:PHE:O	1:A:3835:ILE:HD12	1.98	0.64
1:A:2995:ASP:OD1	1:A:3067:THR:OG1	2.15	0.63
1:A:3828:SER:HB3	1:A:4140:ARG:HG3	1.80	0.63
1:A:2285:ARG:NH2	1:A:2331:GLU:OE1	2.32	0.63
1:A:3030:MET:HE3	1:A:3050:LEU:HD22	1.80	0.63
1:A:2133:GLU:HA	1:A:2136:ILE:HD12	1.79	0.62
1:A:2337:PRO:O	1:A:2340:ARG:NH1	2.32	0.62
1:A:2299:GLN:HB2	1:A:2339:VAL:HG22	1.81	0.62
1:A:1879:LEU:HG	2:A:4701:ADP:C6	2.35	0.62
1:A:2095:SER:O	1:A:2098:VAL:HG22	2.00	0.62
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.82	0.62
1:A:3576:ASN:ND2	1:A:3700:ASN:O	2.33	0.61
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.81	0.61
1:A:3618:ALA:HB1	1:A:3621:LYS:HE2	1.81	0.61
1:A:3948:ILE:O	1:A:3952:GLN:HG2	1.99	0.61
1:A:2467:ARG:NH2	1:A:2587:GLU:OE2	2.33	0.61
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.34	0.61
1:A:3923:ARG:HB2	1:A:3927:LEU:HD23	1.81	0.61
1:A:1911:GLY:HA2	1:A:1914:GLU:OE1	2.00	0.61
1:A:3017:VAL:HB	1:A:3020:LEU:HD23	1.82	0.61
1:A:4257:ASP:OD1	1:A:4258:ASN:N	2.34	0.61
1:A:1876:GLN:OE1	1:A:1921:HIS:NE2	2.33	0.60
1:A:2386:PRO:C	1:A:2388:ASP:H	2.09	0.60
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.81	0.60
1:A:1720:SER:O	1:A:1724:VAL:HG12	2.01	0.60
1:A:1796:VAL:O	1:A:1805:ARG:NH2	2.34	0.60
1:A:1808:LEU:O	1:A:1812:ILE:HG22	2.01	0.60
1:A:3006:GLU:O	1:A:3010:THR:HG23	2.02	0.60
1:A:3088:ARG:NH2	3:A:4703:ATP:O3G	2.34	0.60
1:A:3910:ARG:HB2	1:A:4344:LEU:HD11	1.84	0.60
1:A:3553:LEU:O	1:A:3582:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2694:ARG:NH2	1:A:2697:ASP:OD2	2.35	0.60
1:A:3659:ARG:HE	1:A:3670:ASP:HB2	1.65	0.59
1:A:1967:MET:O	1:A:1971:VAL:HG22	2.02	0.59
1:A:2221:MET:HE1	1:A:2343:PHE:CG	2.37	0.59
1:A:2922:ILE:HG22	1:A:2926:PHE:HE1	1.67	0.59
1:A:3653:VAL:HG13	1:A:3660:VAL:HG23	1.83	0.59
1:A:2297:LYS:O	1:A:2338:ASN:ND2	2.35	0.59
1:A:3066:PHE:HE1	1:A:3068:MET:HB2	1.66	0.59
1:A:4238:ILE:HD12	1:A:4238:ILE:H	1.67	0.59
1:A:4027:LEU:O	1:A:4031:VAL:HG22	2.02	0.59
1:A:4084:ILE:O	1:A:4088:VAL:HG12	2.02	0.59
1:A:4105:TRP:O	1:A:4109:LEU:HD12	2.02	0.59
1:A:4600:LYS:NZ	1:A:4604:VAL:O	2.35	0.59
1:A:1630:TYR:O	1:A:1943:ARG:NH1	2.35	0.59
1:A:4193:ARG:HH21	1:A:4200:GLY:HA2	1.67	0.59
1:A:2370:SER:H	1:A:2373:MET:HE2	1.66	0.59
1:A:4312:LEU:HD21	1:A:4320:TRP:HZ3	1.68	0.59
1:A:4088:VAL:HG22	1:A:4118:PRO:HD2	1.83	0.59
1:A:2542:SER:OG	1:A:2544:GLU:OE1	2.16	0.58
1:A:4109:LEU:O	1:A:4113:LEU:HG	2.03	0.58
1:A:3123:PRO:HG3	1:A:3540:ASN:HB2	1.84	0.58
1:A:2514:LEU:O	1:A:2518:ILE:HG12	2.02	0.58
1:A:2091:ARG:HH21	2:A:4701:ADP:H5'1	1.69	0.58
1:A:4271:ARG:NH1	1:A:4637:GLU:OE1	2.37	0.58
1:A:1628:ARG:NH1	1:A:1871:GLU:OE2	2.36	0.58
1:A:1810:HIS:NE2	1:A:1876:GLN:O	2.37	0.58
1:A:1636:ASP:O	1:A:1640:ILE:HG12	2.02	0.58
1:A:1686:PHE:HA	1:A:1712:THR:HG21	1.85	0.58
1:A:2897:LEU:HD21	1:A:2911:LEU:HB2	1.86	0.58
1:A:4201:TRP:O	1:A:4203:LYS:N	2.37	0.58
1:A:2498:ILE:HG23	1:A:2502:LEU:HD13	1.86	0.57
1:A:2839:GLU:N	1:A:2842:GLU:OE1	2.36	0.57
1:A:2223:VAL:HG22	1:A:2345:VAL:HG13	1.84	0.57
1:A:1908:ALA:HA	1:A:1912:LYS:HZ1	1.67	0.57
1:A:4437:VAL:HG21	1:A:4444:GLN:HB2	1.87	0.57
1:A:2037:ARG:NH2	1:A:4214:SER:OG	2.38	0.57
1:A:2321:ASP:O	1:A:2323:LYS:NZ	2.32	0.57
1:A:3921:THR:OG1	1:A:3923:ARG:NE	2.37	0.57
1:A:2569:VAL:HB	1:A:2747:ILE:HG13	1.87	0.57
1:A:3519:TYR:HA	1:A:3700:ASN:HB2	1.87	0.57
1:A:4172:SER:HB3	1:A:4173:PRO:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2557:VAL:O	1:A:2757:ARG:NH2	2.37	0.57
1:A:3488:ARG:NH1	1:A:3746:GLU:OE2	2.36	0.57
1:A:4454:GLU:N	1:A:4454:GLU:OE2	2.37	0.57
1:A:2320:ASP:HB3	1:A:2358:ARG:HD3	1.85	0.57
1:A:3654:ARG:HB2	1:A:3661:LEU:HB3	1.86	0.57
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.70	0.57
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.37	0.57
1:A:1745:TYR:O	1:A:1807:LYS:NZ	2.36	0.57
1:A:2887:GLU:N	1:A:2887:GLU:OE1	2.38	0.57
1:A:1899:ARG:HG3	1:A:1986:SER:HB3	1.85	0.56
1:A:2277:ASP:OD1	1:A:2277:ASP:N	2.38	0.56
1:A:2697:ASP:OD1	1:A:2697:ASP:N	2.38	0.56
1:A:3008:MET:O	1:A:3012:LEU:HG	2.05	0.56
1:A:2203:TRP:O	1:A:2207:VAL:HG23	2.05	0.56
1:A:3876:LEU:HD22	1:A:4146:VAL:HG11	1.87	0.56
1:A:1892:MET:HE2	1:A:1892:MET:HA	1.87	0.56
1:A:1623:ARG:HH21	1:A:1943:ARG:HD2	1.71	0.56
1:A:1632:VAL:O	1:A:1943:ARG:NH1	2.39	0.56
1:A:3602:ASN:HA	1:A:3605:LYS:HE3	1.86	0.56
1:A:2265:TYR:OH	1:A:2311:TRP:O	2.19	0.56
1:A:2495:VAL:HG21	1:A:2524:VAL:HG11	1.88	0.56
1:A:3916:LEU:HD12	1:A:3937:ARG:HD3	1.88	0.56
1:A:2925:ILE:HG12	1:A:2933:LEU:HD13	1.87	0.55
1:A:3113:MET:HB2	1:A:3115:LEU:HD13	1.89	0.55
1:A:3043:MET:SD	1:A:3043:MET:N	2.67	0.55
1:A:3506:ASP:OD1	1:A:3544:ARG:N	2.37	0.55
1:A:1687:LYS:HE3	1:A:1715:LYS:HE3	1.89	0.55
1:A:2307:VAL:HG12	1:A:2345:VAL:HG21	1.89	0.55
1:A:2992:PHE:HB3	1:A:3064:VAL:HA	1.88	0.55
1:A:3683:ASP:OD1	1:A:3685:THR:N	2.40	0.55
1:A:3734:LEU:HD21	1:A:3784:VAL:HG12	1.87	0.55
1:A:1819:ARG:HD2	1:A:1823:ARG:HH22	1.72	0.55
1:A:3821:ILE:HD12	1:A:3821:ILE:H	1.70	0.55
1:A:3938:LEU:HD11	1:A:3991:LEU:HB3	1.89	0.55
1:A:2935:LEU:HD23	1:A:3092:ASN:HB3	1.88	0.55
1:A:3133:LEU:HB3	1:A:3134:PRO:HD3	1.88	0.55
1:A:4025:LEU:HG	1:A:4027:LEU:HB3	1.88	0.54
1:A:4577:LEU:HD22	1:A:4638:ARG:HH21	1.72	0.54
1:A:1819:ARG:NE	1:A:1823:ARG:HH12	2.05	0.54
1:A:3607:ARG:HB2	1:A:3632:PRO:HG3	1.89	0.54
1:A:2866:ALA:O	1:A:2869:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4572:ASN:HB2	1:A:4574:LYS:HE2	1.89	0.54
1:A:2592:VAL:HB	1:A:2733:VAL:HG12	1.90	0.54
1:A:3115:LEU:H	1:A:3140:ARG:HH21	1.55	0.54
1:A:4095:MET:HB2	1:A:4125:PHE:HB2	1.90	0.54
1:A:1940:ALA:O	1:A:1944:ILE:HG12	2.08	0.54
1:A:4084:ILE:HG22	1:A:4094:VAL:HG11	1.90	0.54
1:A:1685:MET:HE2	1:A:1685:MET:HA	1.90	0.53
1:A:4037:PRO:HG3	1:A:4120:ALA:HA	1.90	0.53
1:A:3116:GLU:OE1	1:A:3140:ARG:NH2	2.42	0.53
1:A:4409:LEU:HD21	1:A:4558:PHE:HE2	1.73	0.53
1:A:4544:ASN:OD1	1:A:4573:ASN:ND2	2.41	0.53
1:A:3102:LEU:HD22	1:A:3176:TYR:CD1	2.42	0.53
1:A:4179:LEU:HD12	1:A:4223:LEU:HD11	1.90	0.53
1:A:2922:ILE:CG2	1:A:2926:PHE:HE1	2.22	0.53
1:A:3164:ARG:HH21	1:A:4375:ALA:HB2	1.74	0.53
1:A:3580:LEU:HD21	1:A:3699:VAL:HG11	1.90	0.53
1:A:4378:ARG:H	1:A:4378:ARG:HD2	1.74	0.53
1:A:2307:VAL:HA	1:A:2311:TRP:HE1	1.73	0.53
1:A:1724:VAL:HA	1:A:1727:PHE:HB2	1.90	0.53
1:A:2935:LEU:HD13	1:A:2943:LYS:HB2	1.91	0.53
1:A:2967:TYR:CE2	1:A:2971:ASP:HB2	2.44	0.53
1:A:4109:LEU:HA	1:A:4112:LYS:HB3	1.91	0.53
1:A:1882:THR:HG22	1:A:2048:LEU:HD23	1.91	0.52
1:A:3873:ARG:HD3	1:A:4021:MET:HE1	1.91	0.52
1:A:2191:LEU:HB3	3:A:4702:ATP:N6	2.25	0.52
1:A:4187:HIS:CD2	1:A:4212:LEU:HD12	2.44	0.52
1:A:2147:PRO:HB3	1:A:2362:VAL:HG22	1.92	0.52
1:A:2936:ILE:O	1:A:3094:PHE:N	2.42	0.52
1:A:3916:LEU:HB2	1:A:3937:ARG:HE	1.74	0.52
1:A:1940:ALA:O	1:A:1943:ARG:HG2	2.10	0.52
1:A:2492:ARG:HG2	1:A:2545:TRP:CE2	2.45	0.52
1:A:2801:ARG:NH2	1:A:3089:CYS:O	2.43	0.52
1:A:1762:VAL:O	1:A:1766:LEU:HG	2.09	0.52
1:A:1697:LYS:HB2	1:A:1700:GLU:HG2	1.92	0.51
1:A:1718:ALA:O	1:A:1722:THR:HG23	2.10	0.51
1:A:2982:ARG:HD2	1:A:2990:ILE:HD11	1.91	0.51
1:A:4489:LEU:HD11	1:A:4515:PHE:HE1	1.75	0.51
1:A:1649:LYS:O	1:A:1652:LYS:NZ	2.42	0.51
1:A:2473:ASN:OD1	1:A:2481:MET:N	2.39	0.51
1:A:2831:ARG:NH2	1:A:2921:ARG:HG3	2.25	0.51
1:A:2935:LEU:HD21	1:A:3092:ASN:HD22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3907:HIS:HA	1:A:3911:GLY:HA3	1.93	0.51
1:A:3909:LEU:HD21	1:A:4343:MET:HE3	1.92	0.51
1:A:2192:THR:H	3:A:4702:ATP:HN61	1.58	0.51
1:A:2819:GLU:HA	1:A:2865:LYS:HZ2	1.74	0.51
1:A:1778:LEU:HB3	1:A:1827:LYS:HZ2	1.75	0.51
1:A:3207:LYS:HZ3	1:A:3750:LEU:HA	1.76	0.51
1:A:3839:VAL:O	1:A:3843:ASN:ND2	2.39	0.51
1:A:1632:VAL:HG12	1:A:1656:LYS:HD3	1.93	0.51
1:A:3746:GLU:O	1:A:3750:LEU:HG	2.11	0.51
1:A:1782:LEU:HD12	1:A:1827:LYS:HE3	1.92	0.51
1:A:3471:LYS:HB3	1:A:3474:ARG:HG2	1.93	0.51
1:A:1800:GLN:HE21	1:A:1804:ARG:HD2	1.75	0.50
1:A:1939:GLN:H	1:A:1939:GLN:CD	2.18	0.50
1:A:4165:PRO:HD2	1:A:4168:ARG:HD3	1.93	0.50
1:A:1838:TRP:CZ2	1:A:1843:ARG:HG2	2.47	0.50
1:A:2802:TRP:O	1:A:2806:ILE:HG13	2.11	0.50
1:A:1634:ASP:N	1:A:1634:ASP:OD1	2.40	0.50
1:A:4106:LEU:HG	1:A:4138:LEU:HD23	1.93	0.50
1:A:4250:SER:OG	1:A:4251:ILE:N	2.43	0.50
1:A:2049:ILE:HG21	1:A:2090:LEU:HD11	1.92	0.50
1:A:2242:GLU:HG3	1:A:2248:GLU:HA	1.93	0.50
1:A:2665:GLU:HB3	1:A:2668:LEU:HD12	1.92	0.50
1:A:3167:ARG:NH2	1:A:3684:PRO:O	2.44	0.50
1:A:3928:THR:OG1	1:A:3931:GLN:OE1	2.28	0.50
1:A:1706:GLU:OE2	1:A:1710:ARG:NH2	2.45	0.50
1:A:2030:ASP:OD1	1:A:2030:ASP:N	2.42	0.50
1:A:2822:ILE:HB	1:A:2865:LYS:HE3	1.94	0.50
1:A:3034:LYS:HD3	1:A:3044:LEU:HD22	1.94	0.50
1:A:3087:ASN:O	1:A:3088:ARG:HG2	2.12	0.50
1:A:4157:MET:HA	1:A:4157:MET:HE2	1.94	0.50
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.46	0.50
1:A:2694:ARG:HH21	1:A:2699:THR:HG21	1.77	0.50
1:A:3751:GLN:HA	1:A:3754:ASN:HD21	1.77	0.50
1:A:2572:LEU:HA	1:A:2575:VAL:HG12	1.94	0.49
1:A:3720:GLU:OE2	1:A:3855:ARG:NH1	2.42	0.49
1:A:4065:GLN:HE21	1:A:4092:ARG:HB3	1.77	0.49
1:A:2600:GLY:N	3:A:4703:ATP:O1B	2.44	0.49
1:A:4388:LEU:HD21	1:A:4431:LEU:HB3	1.93	0.49
1:A:2090:LEU:O	1:A:2094:LYS:HG3	2.13	0.49
1:A:2635:PHE:HB3	1:A:2650:LEU:HD21	1.94	0.49
1:A:2638:TYR:HD2	1:A:2659:LEU:HD11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2787:ASP:OD1	1:A:2788:THR:N	2.45	0.49
1:A:3519:TYR:HB2	1:A:3698:PHE:HB3	1.95	0.49
1:A:1968:LEU:O	1:A:1972:SER:OG	2.24	0.49
1:A:2179:ARG:NH1	1:A:2195:ASP:OD1	2.45	0.49
1:A:2934:LEU:HD21	1:A:3086:PHE:HD1	1.78	0.49
1:A:2144:THR:C	1:A:2145:MET:HE2	2.37	0.49
1:A:2230:LYS:HB2	3:A:4702:ATP:O2B	2.12	0.49
1:A:2322:ASN:OD1	1:A:2324:LEU:HB3	2.12	0.49
1:A:4018:MET:SD	1:A:4018:MET:N	2.86	0.49
1:A:4407:ASP:OD1	1:A:4410:PHE:N	2.40	0.49
1:A:2563:ALA:HB3	1:A:2804:ARG:HG3	1.95	0.49
1:A:3873:ARG:HD2	1:A:4025:LEU:HD13	1.94	0.49
1:A:1759:SER:OG	1:A:1844:PHE:O	2.30	0.49
1:A:4410:PHE:O	1:A:4414:GLU:HG3	2.11	0.49
1:A:3001:ASP:OD1	1:A:3001:ASP:N	2.45	0.49
1:A:3201:LEU:HD12	1:A:3743:ARG:NH2	2.27	0.49
1:A:4600:LYS:HZ2	1:A:4604:VAL:HG23	1.77	0.49
1:A:1778:LEU:HB3	1:A:1827:LYS:NZ	2.28	0.48
1:A:2307:VAL:HG23	1:A:2312:VAL:HG11	1.94	0.48
1:A:4154:LYS:HB2	1:A:4312:LEU:HD23	1.95	0.48
1:A:2303:PHE:N	1:A:2342:MET:O	2.38	0.48
1:A:3489:TRP:NE1	1:A:3746:GLU:OE1	2.47	0.48
1:A:4105:TRP:CE2	1:A:4109:LEU:HD11	2.49	0.48
1:A:2861:ILE:HD12	1:A:2865:LYS:NZ	2.28	0.48
1:A:3489:TRP:HH2	1:A:3750:LEU:HD11	1.78	0.48
1:A:4013:LEU:HD23	1:A:4017:PHE:CZ	2.48	0.48
1:A:1683:GLU:OE1	1:A:1683:GLU:N	2.46	0.48
1:A:2637:HIS:CD2	1:A:2637:HIS:C	2.91	0.48
1:A:2865:LYS:H	1:A:2865:LYS:HD3	1.78	0.48
1:A:4176:ARG:NH1	1:A:4220:ASP:OD1	2.47	0.48
1:A:2342:MET:HE3	1:A:2342:MET:HA	1.96	0.48
1:A:2628:PRO:HB3	1:A:2682:PHE:CD2	2.49	0.48
1:A:3566:SER:OG	1:A:3602:ASN:OD1	2.21	0.48
1:A:3907:HIS:NE2	1:A:3938:LEU:HD22	2.28	0.48
1:A:4205:TYR:HE2	1:A:4256:VAL:HG22	1.78	0.48
1:A:2290:SER:HB3	1:A:2295:LEU:HD23	1.96	0.48
1:A:2764:THR:HG23	1:A:2765:TYR:HD2	1.78	0.48
1:A:2936:ILE:CD1	1:A:3068:MET:HB3	2.44	0.48
1:A:3207:LYS:HB3	1:A:3207:LYS:HE3	1.50	0.48
1:A:4432:ALA:O	1:A:4436:GLN:HG2	2.13	0.48
1:A:2878:SER:HB3	1:A:2882:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.96	0.48
1:A:3748:SER:O	1:A:3751:GLN:HG2	2.14	0.48
1:A:2922:ILE:O	1:A:2925:ILE:HG22	2.14	0.48
1:A:3027:ALA:HA	1:A:3030:MET:HG2	1.95	0.48
1:A:3779:GLU:OE2	1:A:3782:ARG:NH1	2.39	0.48
1:A:3492:THR:HG21	1:A:3743:ARG:NH1	2.29	0.47
1:A:1903:SER:O	1:A:1903:SER:OG	2.21	0.47
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.47	0.47
1:A:3835:ILE:HG23	1:A:3866:VAL:HG12	1.96	0.47
1:A:4042:LEU:HD13	1:A:4139:LEU:HD23	1.95	0.47
1:A:2308:ASP:OD1	1:A:2311:TRP:HD1	1.97	0.47
1:A:2496:TYR:CE1	1:A:2500:TRP:HD1	2.32	0.47
1:A:2797:ARG:NE	1:A:3087:ASN:OD1	2.43	0.47
1:A:2897:LEU:HD21	1:A:2911:LEU:HD12	1.96	0.47
1:A:2102:ASN:OD1	1:A:2105:ARG:NH2	2.37	0.47
1:A:2145:MET:O	1:A:2148:LYS:HG2	2.14	0.47
1:A:2666:ILE:HG22	1:A:2712:CYS:HB3	1.96	0.47
1:A:2755:MET:HG2	1:A:2756:LEU:HD23	1.96	0.47
1:A:3818:LEU:HD12	1:A:3821:ILE:HD13	1.96	0.47
1:A:4485:ARG:NH1	1:A:4513:GLY:O	2.48	0.47
1:A:2045:ASP:O	1:A:2049:ILE:HG12	2.15	0.47
1:A:2094:LYS:HA	1:A:2097:LEU:HD12	1.97	0.47
1:A:2752:ASN:OD1	1:A:2770:THR:OG1	2.20	0.47
1:A:2755:MET:HE1	1:A:2806:ILE:HG22	1.97	0.47
1:A:3043:MET:HG2	1:A:3045:ASP:OD1	2.15	0.47
1:A:3174:ARG:HE	2:A:4704:ADP:H5'1	1.80	0.47
1:A:3194:LEU:HD21	1:A:3500:MET:HB2	1.97	0.47
1:A:3581:LYS:HD3	1:A:3581:LYS:HA	1.67	0.47
1:A:3664:LEU:HD12	1:A:3664:LEU:HA	1.80	0.47
1:A:3747:LYS:HD3	1:A:3750:LEU:HD12	1.97	0.47
1:A:3902:ASP:OD1	1:A:3902:ASP:N	2.48	0.47
1:A:3985:GLN:HE21	1:A:3989:ARG:NH2	2.13	0.47
1:A:2068:LYS:NZ	1:A:4537:GLU:OE1	2.30	0.47
1:A:2764:THR:HG23	1:A:2765:TYR:CD2	2.49	0.47
1:A:3002:SER:O	1:A:3006:GLU:HG3	2.15	0.47
1:A:4381:HIS:CE1	1:A:4435:VAL:HG13	2.49	0.47
1:A:1914:GLU:OE2	1:A:1914:GLU:N	2.48	0.46
1:A:3110:THR:HA	1:A:3113:MET:HE3	1.96	0.46
1:A:2139:GLN:HG3	1:A:2170:TYR:HE1	1.80	0.46
1:A:2915:VAL:HG13	1:A:2946:LEU:HD11	1.97	0.46
1:A:2641:TYR:CE2	1:A:2694:ARG:HD3	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3745:LEU:HB3	1:A:3773:LEU:HD21	1.98	0.46
1:A:2374:ILE:HD13	3:A:4702:ATP:H1'	1.98	0.46
1:A:2798:GLU:OE1	1:A:2801:ARG:NH2	2.49	0.46
1:A:2856:LYS:HG2	1:A:2857:HIS:HD2	1.81	0.46
1:A:4399:LYS:HB3	1:A:4414:GLU:HG2	1.96	0.46
1:A:4595:GLN:OE1	1:A:4597:ASN:N	2.48	0.46
1:A:2324:LEU:HD12	1:A:2325:LEU:N	2.31	0.46
1:A:3158:ASN:ND2	1:A:3169:MET:O	2.38	0.46
1:A:3207:LYS:HD3	1:A:3754:ASN:HB3	1.97	0.46
1:A:4239:PRO:HB2	1:A:4242:ALA:HB3	1.98	0.46
1:A:4565:LEU:HB2	1:A:4585:LEU:HD21	1.97	0.46
1:A:3870:ARG:NH2	1:A:4034:GLU:HB3	2.30	0.46
1:A:4179:LEU:HD11	1:A:4238:ILE:HG21	1.96	0.46
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.97	0.46
1:A:2556:GLU:OE2	1:A:2753:ARG:NH2	2.46	0.46
1:A:3756:VAL:HG23	1:A:3758:GLY:H	1.79	0.46
1:A:4097:LYS:HA	1:A:4127:THR:HG22	1.98	0.46
1:A:4274:THR:HG23	1:A:4276:ARG:H	1.81	0.46
1:A:4451:LEU:HD12	1:A:4451:LEU:HA	1.70	0.46
1:A:4511:LEU:HD12	1:A:4517:PRO:HB3	1.97	0.46
1:A:2148:LYS:HB2	1:A:2361:MET:SD	2.56	0.46
1:A:2612:LEU:HB2	1:A:2615:MET:HG2	1.98	0.46
1:A:2835:ASP:OD1	1:A:2835:ASP:C	2.59	0.46
1:A:3016:GLU:HB3	1:A:3055:THR:HG22	1.98	0.46
1:A:3175:HIS:HD2	1:A:3585:ARG:NH2	2.13	0.46
1:A:1903:SER:HA	1:A:2016:ILE:O	2.15	0.46
1:A:2775:GLU:O	1:A:2779:MET:HG3	2.16	0.46
1:A:4601:LYS:HE2	1:A:4603:SER:OG	2.16	0.46
1:A:1912:LYS:HG2	1:A:2041:MET:SD	2.56	0.46
1:A:4186:PHE:O	1:A:4190:ILE:HG23	2.15	0.46
1:A:1747:ALA:HB2	1:A:1807:LYS:HG2	1.96	0.45
1:A:2231:SER:HA	1:A:2234:TRP:NE1	2.32	0.45
1:A:2387:LEU:HD13	1:A:2387:LEU:HA	1.71	0.45
1:A:2599:SER:N	3:A:4703:ATP:O1B	2.48	0.45
1:A:2138:ILE:HG23	1:A:2161:LEU:HD13	1.97	0.45
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.15	0.45
1:A:2637:HIS:HD2	1:A:2637:HIS:O	1.99	0.45
1:A:3683:ASP:OD1	1:A:3683:ASP:C	2.59	0.45
1:A:3832:PHE:HA	1:A:3835:ILE:CD1	2.46	0.45
1:A:2030:ASP:HA	1:A:2033:LYS:HG2	1.99	0.45
1:A:3870:ARG:HH22	1:A:4034:GLU:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1904:PRO:O	1:A:1912:LYS:HD2	2.17	0.45
1:A:1947:GLY:O	1:A:1951:VAL:HG12	2.17	0.45
1:A:2192:THR:N	3:A:4702:ATP:HN61	2.14	0.45
1:A:3513:PHE:HZ	1:A:3575:GLU:HB3	1.81	0.45
1:A:3704:THR:H	1:A:3707:SER:HB3	1.81	0.45
1:A:3751:GLN:HA	1:A:3754:ASN:ND2	2.32	0.45
1:A:4445:THR:OG1	1:A:4446:ASN:N	2.49	0.45
1:A:2411:PRO:O	1:A:2415:ILE:HG12	2.16	0.45
1:A:3513:PHE:CD1	1:A:3513:PHE:C	2.95	0.45
1:A:1694:GLU:HG2	1:A:1695:HIS:ND1	2.31	0.45
1:A:2485:GLN:HE21	1:A:2542:SER:HA	1.82	0.45
1:A:2665:GLU:N	1:A:2711:ALA:O	2.41	0.45
1:A:2283:VAL:O	1:A:2287:ILE:HG12	2.17	0.45
1:A:2500:TRP:CE2	1:A:2535:ILE:HD11	2.52	0.45
1:A:1914:GLU:OE1	2:A:4701:ADP:H8	2.00	0.45
1:A:2290:SER:HA	1:A:2294:GLU:HB2	1.98	0.45
1:A:3586:TYR:O	1:A:3696:VAL:HG13	2.17	0.45
1:A:3608:LYS:HB2	1:A:3608:LYS:HE3	1.62	0.45
1:A:4258:ASN:N	1:A:4258:ASN:OD1	2.49	0.45
1:A:2603:MET:HE3	1:A:2603:MET:HB3	1.72	0.45
1:A:2975:ASP:O	1:A:2979:VAL:HG12	2.16	0.45
1:A:3113:MET:O	1:A:3140:ARG:NH2	2.50	0.45
1:A:3718:LYS:HB2	1:A:3718:LYS:HE2	1.63	0.45
1:A:3729:SER:OG	1:A:3733:LYS:NZ	2.49	0.45
1:A:3929:VAL:O	1:A:3933:GLU:HG2	2.17	0.45
1:A:2221:MET:CE	1:A:2343:PHE:HB2	2.48	0.44
1:A:2865:LYS:HD3	1:A:2865:LYS:N	2.32	0.44
1:A:3814:THR:O	1:A:4346:MET:HE1	2.17	0.44
1:A:1992:LYS:HA	1:A:1992:LYS:HD2	1.82	0.44
1:A:2819:GLU:HA	1:A:2865:LYS:NZ	2.32	0.44
1:A:2956:LEU:H	1:A:2956:LEU:HD12	1.82	0.44
1:A:3601:MET:HE2	1:A:3601:MET:HA	2.00	0.44
1:A:4090:SER:OG	1:A:4092:ARG:NH2	2.50	0.44
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.51	0.44
1:A:2605:LEU:HD23	1:A:2662:PHE:CE1	2.52	0.44
1:A:2717:ASP:OD2	1:A:2720:ARG:NH1	2.49	0.44
1:A:4033:THR:OG1	1:A:4034:GLU:OE2	2.35	0.44
1:A:4251:ILE:HB	1:A:4252:TYR:H	1.68	0.44
1:A:1742:ILE:HG22	1:A:1750:VAL:HG21	1.99	0.44
1:A:3107:LYS:HE2	1:A:3107:LYS:HB2	1.70	0.44
1:A:1747:ALA:O	1:A:1750:VAL:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2784:PHE:O	1:A:2792:TYR:HB3	2.17	0.44
1:A:4078:ASN:O	1:A:4082:LYS:HG2	2.17	0.44
1:A:1941:MET:HA	1:A:1944:ILE:CG1	2.47	0.44
1:A:1985:HIS:HA	1:A:1997:ILE:HG13	1.98	0.44
1:A:3856:LEU:HA	1:A:3859:ILE:HG22	2.00	0.44
1:A:4344:LEU:HD23	1:A:4344:LEU:HA	1.81	0.44
1:A:2628:PRO:O	1:A:2632:LEU:HD22	2.18	0.44
1:A:2831:ARG:HD2	1:A:2831:ARG:N	2.31	0.44
1:A:3066:PHE:CE1	1:A:3068:MET:HB2	2.51	0.44
1:A:3957:PHE:HZ	1:A:3996:PHE:CE1	2.36	0.44
1:A:1711:VAL:O	1:A:1715:LYS:HG3	2.18	0.44
1:A:2453:ARG:HD3	1:A:2728:LEU:O	2.17	0.44
1:A:2872:LEU:HD22	1:A:2920:LEU:HD12	1.99	0.44
1:A:4096:LEU:HB2	1:A:4126:LEU:HD23	1.99	0.44
1:A:4605:VAL:HG12	1:A:4632:PRO:HB3	2.00	0.44
1:A:2178:LEU:HG	1:A:2182:LEU:HD23	2.00	0.43
1:A:2609:LEU:HD13	1:A:2617:VAL:HG13	2.00	0.43
1:A:2919:VAL:HG13	1:A:2950:VAL:HG22	2.00	0.43
1:A:4088:VAL:CG2	1:A:4118:PRO:HD2	2.48	0.43
1:A:2773:MET:HG3	1:A:2802:TRP:CZ3	2.53	0.43
1:A:2786:GLN:HE22	1:A:3083:PRO:HG3	1.82	0.43
1:A:3588:LEU:HD21	1:A:3698:PHE:CE2	2.53	0.43
1:A:3705:ARG:HA	1:A:3813:PHE:HE2	1.82	0.43
1:A:4179:LEU:HD23	1:A:4179:LEU:HA	1.78	0.43
1:A:2677:GLN:HB2	1:A:2680:ILE:HB	2.00	0.43
1:A:3140:ARG:HE	1:A:3140:ARG:HB2	1.69	0.43
1:A:4107:MET:HE1	1:A:4137:ASN:HB2	1.99	0.43
1:A:4158:LEU:HD12	1:A:4158:LEU:HA	1.86	0.43
1:A:1651:GLN:HA	1:A:1654:PHE:HB2	2.00	0.43
1:A:1709:MET:O	1:A:1713:LEU:HD23	2.19	0.43
1:A:2271:ASN:OD1	1:A:2272:THR:HG23	2.19	0.43
1:A:3207:LYS:NZ	1:A:3750:LEU:HA	2.33	0.43
1:A:2232:MET:HA	1:A:2235:ARG:HB2	2.00	0.43
1:A:3200:HIS:HB3	1:A:3747:LYS:HE3	2.00	0.43
1:A:4038:ASN:ND2	1:A:4117:GLN:OE1	2.46	0.43
1:A:4108:GLN:HA	1:A:4111:LYS:HD2	2.00	0.43
1:A:2935:LEU:HD23	1:A:2935:LEU:HA	1.68	0.43
1:A:4394:THR:HA	1:A:4424:LEU:HD21	2.00	0.43
1:A:4631:ASP:OD2	1:A:4633:ARG:NE	2.41	0.43
1:A:1707:LYS:HE3	1:A:1707:LYS:HB2	1.67	0.43
1:A:1941:MET:HG3	1:A:1944:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2221:MET:HE3	1:A:2359:CYS:SG	2.59	0.43
1:A:3570:ASP:OD1	1:A:3571:ASP:N	2.52	0.43
1:A:1884:LEU:HD21	1:A:2041:MET:HB2	1.99	0.43
1:A:1931:ASN:OD1	1:A:1932:CYS:N	2.52	0.43
1:A:2410:SER:N	1:A:2411:PRO:HD2	2.34	0.43
1:A:1999:CYS:SG	1:A:2001:LEU:HD23	2.59	0.43
1:A:2085:HIS:HB2	1:A:2361:MET:CE	2.49	0.43
1:A:2211:TYR:CE1	1:A:2241:LEU:HD21	2.54	0.43
1:A:2221:MET:HE1	1:A:2343:PHE:HB2	2.01	0.43
1:A:2605:LEU:HD11	1:A:2709:VAL:HG11	2.01	0.43
1:A:2811:ARG:HD2	1:A:2812:PRO:HD3	2.01	0.43
1:A:2863:ARG:HB3	1:A:2866:ALA:HB3	2.01	0.43
1:A:2933:LEU:HB3	1:A:3065:VAL:HG23	2.00	0.43
1:A:3585:ARG:HB2	1:A:3697:THR:HG23	1.99	0.43
1:A:2326:THR:HA	1:A:2332:ARG:HE	1.83	0.42
1:A:3115:LEU:H	1:A:3140:ARG:NH2	2.16	0.42
1:A:3626:ALA:HA	1:A:3631:ASN:HB2	2.01	0.42
1:A:3661:LEU:HG	1:A:3668:ASP:OD1	2.18	0.42
1:A:2460:SER:HB2	1:A:2589:LYS:HE3	2.01	0.42
1:A:3030:MET:HE3	1:A:3030:MET:HA	1.99	0.42
1:A:3030:MET:CE	1:A:3050:LEU:HD22	2.48	0.42
1:A:3055:THR:O	1:A:3059:ILE:HG23	2.19	0.42
1:A:3169:MET:SD	1:A:3169:MET:N	2.92	0.42
1:A:2371:THR:HG22	1:A:2451:ARG:HD2	2.00	0.42
1:A:2717:ASP:OD2	1:A:2720:ARG:HD3	2.19	0.42
1:A:1938:PHE:HB2	1:A:1967:MET:HE1	2.00	0.42
1:A:2095:SER:O	1:A:2096:VAL:C	2.62	0.42
1:A:2799:MET:HE3	1:A:2799:MET:HB3	1.92	0.42
1:A:2841:GLU:HA	1:A:2844:ARG:HG2	2.00	0.42
1:A:2905:LEU:HD12	1:A:2905:LEU:HA	1.91	0.42
1:A:3169:MET:HB3	1:A:3693:CYS:SG	2.59	0.42
1:A:3793:GLU:O	1:A:3797:VAL:HG23	2.18	0.42
1:A:1957:PHE:O	1:A:2017:THR:HB	2.18	0.42
1:A:2589:LYS:HE2	1:A:2589:LYS:HB2	1.80	0.42
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.54	0.42
1:A:3033:CYS:HB2	1:A:3050:LEU:HD21	2.02	0.42
1:A:3600:ILE:HD12	1:A:3600:ILE:HA	1.95	0.42
1:A:3851:ASP:O	1:A:3855:ARG:HG3	2.19	0.42
1:A:4084:ILE:HG13	1:A:4085:ASN:N	2.34	0.42
1:A:2226:SER:HA	3:A:4702:ATP:O3G	2.19	0.42
1:A:2743:SER:O	1:A:2747:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2143:GLU:OE2	1:A:2212:GLN:NE2	2.50	0.42
1:A:2614:ASP:OD1	1:A:2614:ASP:N	2.31	0.42
1:A:2900:PHE:CE2	1:A:2949:PHE:HB2	2.55	0.42
1:A:2963:VAL:HA	1:A:2967:TYR:CD1	2.47	0.42
1:A:3620:ARG:O	1:A:3623:LEU:HG	2.20	0.42
1:A:1825:LEU:HD23	1:A:1825:LEU:HA	1.88	0.42
1:A:1854:LEU:O	1:A:1867:ASN:ND2	2.44	0.42
1:A:2232:MET:HE3	1:A:2232:MET:HB2	1.76	0.42
1:A:2257:LYS:HA	1:A:2257:LYS:HD2	1.94	0.42
1:A:4233:ILE:HD12	1:A:4234:SER:H	1.85	0.42
1:A:1704:LEU:HD13	1:A:1704:LEU:HA	1.88	0.42
1:A:1785:VAL:HG13	1:A:1815:LEU:HD12	2.01	0.42
1:A:2385:ILE:HD13	1:A:2385:ILE:HA	1.88	0.42
1:A:2811:ARG:HB3	1:A:2812:PRO:HD2	2.01	0.42
1:A:1966:ARG:H	1:A:1966:ARG:HG3	1.67	0.41
1:A:3489:TRP:CZ2	1:A:3746:GLU:HB3	2.54	0.41
1:A:4248:ALA:O	1:A:4253:GLY:HA3	2.20	0.41
1:A:1713:LEU:HD13	1:A:1749:LEU:HD21	2.01	0.41
1:A:3639:GLU:H	1:A:3639:GLU:CD	2.26	0.41
1:A:4388:LEU:HD22	1:A:4428:ARG:CZ	2.49	0.41
1:A:1657:MET:N	1:A:1657:MET:SD	2.85	0.41
1:A:1713:LEU:CD1	1:A:1749:LEU:HD21	2.50	0.41
1:A:1789:LEU:CD2	1:A:1815:LEU:HB3	2.50	0.41
1:A:1882:THR:H	1:A:1885:THR:HB	1.85	0.41
1:A:2901:TYR:CD1	1:A:2908:PRO:HA	2.55	0.41
1:A:4631:ASP:OD2	1:A:4633:ARG:HB2	2.20	0.41
1:A:1714:ALA:HB2	1:A:1853:VAL:HG23	2.03	0.41
1:A:1756:ILE:HD11	1:A:1857:LEU:HD13	2.03	0.41
1:A:2221:MET:HE2	1:A:2221:MET:HA	2.03	0.41
1:A:4203:LYS:HB2	1:A:4205:TYR:HE1	1.84	0.41
1:A:1687:LYS:HB2	1:A:1687:LYS:HE2	1.83	0.41
1:A:1797:LEU:HD23	1:A:1797:LEU:HA	1.87	0.41
1:A:2329:ASN:OD1	1:A:2330:GLY:N	2.53	0.41
1:A:2532:ILE:HD13	1:A:2532:ILE:HA	1.91	0.41
1:A:2827:HIS:O	1:A:2831:ARG:HG2	2.19	0.41
1:A:3763:ASP:O	1:A:3767:ILE:HG12	2.20	0.41
1:A:1665:ILE:HD11	1:A:1677:SER:HB3	2.02	0.41
1:A:1963:LEU:HD23	1:A:1963:LEU:HA	1.81	0.41
1:A:1998:THR:HB	1:A:2005:GLN:HG2	2.03	0.41
1:A:2054:LEU:CD2	1:A:2097:LEU:HD22	2.46	0.41
1:A:2517:TYR:HD2	1:A:2518:ILE:HD13	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2933:LEU:HD12	1:A:2933:LEU:HA	1.79	0.41
1:A:3162:ALA:HA	1:A:3166:GLY:HA2	2.03	0.41
1:A:4071:ILE:HG22	1:A:4071:ILE:O	2.20	0.41
1:A:4243:LEU:HD23	1:A:4243:LEU:HA	1.78	0.41
1:A:1664:ILE:HG22	1:A:1676:ILE:HG22	2.01	0.41
1:A:1936:PHE:CE1	1:A:1963:LEU:HD21	2.56	0.41
1:A:2627:THR:OG1	1:A:2629:GLU:HG2	2.21	0.41
1:A:3205:LEU:HD23	1:A:3205:LEU:HA	1.82	0.41
1:A:4139:LEU:HD23	1:A:4139:LEU:HA	1.81	0.41
1:A:1638:LEU:HD23	1:A:1641:ILE:HD11	2.02	0.41
1:A:2222:MET:HE3	1:A:2222:MET:HB2	1.96	0.41
1:A:2992:PHE:HB3	1:A:3064:VAL:HG13	2.02	0.41
1:A:3035:GLU:O	1:A:3038:GLN:HG2	2.21	0.41
1:A:3203:VAL:HA	1:A:3206:ARG:HE	1.85	0.41
1:A:3969:THR:O	1:A:3969:THR:OG1	2.31	0.41
1:A:4100:HIS:ND1	1:A:4128:MET:HB2	2.36	0.41
1:A:4149:PRO:HA	1:A:4150:PRO:HD3	1.94	0.41
1:A:2268:LEU:HD12	1:A:2268:LEU:HA	1.92	0.41
1:A:2371:THR:HG22	1:A:2451:ARG:HH11	1.86	0.41
1:A:2600:GLY:HA2	3:A:4703:ATP:H5'1	2.03	0.41
1:A:2609:LEU:HA	1:A:2609:LEU:HD23	1.86	0.41
1:A:2684:ARG:NH2	3:A:4702:ATP:O1G	2.54	0.41
1:A:2723:LEU:HD13	1:A:2727:PHE:CE2	2.56	0.41
1:A:2791:HIS:HA	1:A:3086:PHE:CD2	2.56	0.41
1:A:2893:VAL:HG13	1:A:2911:LEU:HD11	2.02	0.41
1:A:2922:ILE:HA	1:A:2925:ILE:HG22	2.03	0.41
1:A:3128:VAL:HG21	1:A:3149:PHE:HB2	2.03	0.41
1:A:3489:TRP:CH2	1:A:3750:LEU:HD21	2.56	0.41
1:A:3588:LEU:HA	1:A:3679:LEU:HB2	2.02	0.41
1:A:3692:LEU:HD12	1:A:3692:LEU:O	2.21	0.41
1:A:3840:LEU:HA	1:A:3840:LEU:HD23	1.76	0.41
1:A:3936:VAL:O	1:A:3939:SER:OG	2.36	0.41
1:A:4436:GLN:HB2	1:A:4442:LYS:HD2	2.03	0.41
1:A:2091:ARG:NH2	2:A:4701:ADP:H5'1	2.34	0.41
1:A:2284:LEU:HD12	1:A:2284:LEU:HA	1.85	0.41
1:A:2369:LEU:HA	1:A:2373:MET:CE	2.51	0.41
1:A:2762:LEU:HD13	1:A:2821:LEU:HD22	2.01	0.41
1:A:3052:LYS:HE3	1:A:3052:LYS:HB2	1.85	0.41
1:A:3923:ARG:HD2	1:A:3948:ILE:HD12	2.02	0.41
1:A:4233:ILE:HD11	1:A:4237:LYS:CB	2.51	0.41
1:A:2327:LEU:HD12	1:A:2327:LEU:HA	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.56	0.40
1:A:2834:GLN:NE2	1:A:2843:ARG:HB3	2.36	0.40
1:A:3780:VAL:O	1:A:3784:VAL:HG13	2.21	0.40
1:A:3832:PHE:HA	1:A:3835:ILE:HD12	2.03	0.40
1:A:3873:ARG:HD3	1:A:3873:ARG:HA	1.95	0.40
1:A:4615:ARG:H	1:A:4615:ARG:HG2	1.69	0.40
1:A:1884:LEU:HD11	1:A:2041:MET:HA	2.03	0.40
1:A:1905:PHE:CZ	1:A:2040:ALA:HB2	2.56	0.40
1:A:2049:ILE:HD12	2:A:4701:ADP:N1	2.36	0.40
1:A:2426:TYR:OH	1:A:2491:GLN:OE1	2.12	0.40
1:A:2500:TRP:CE2	1:A:2580:LEU:HD11	2.57	0.40
1:A:3207:LYS:O	1:A:3211:THR:HG23	2.21	0.40
1:A:3908:PHE:HE2	1:A:4343:MET:HE1	1.85	0.40
1:A:3912:ASN:O	1:A:3937:ARG:NH1	2.54	0.40
1:A:2453:ARG:HB2	1:A:2729:ARG:HA	2.04	0.40
1:A:2620:LEU:HD23	1:A:2620:LEU:HA	1.72	0.40
1:A:2967:TYR:HD2	1:A:2968:THR:N	2.19	0.40
1:A:2976:LEU:HD23	1:A:2976:LEU:HA	1.85	0.40
1:A:3570:ASP:HB3	1:A:3573:CYS:SG	2.61	0.40
1:A:3570:ASP:OD2	1:A:3572:LEU:HB3	2.22	0.40
1:A:3747:LYS:HD3	1:A:3747:LYS:HA	1.98	0.40
1:A:3991:LEU:HD23	1:A:3991:LEU:HA	1.95	0.40
1:A:4269:LEU:HD23	1:A:4269:LEU:HA	1.84	0.40
1:A:4442:LYS:HE3	1:A:4442:LYS:HB2	1.78	0.40
1:A:1907:PRO:HD2	1:A:2042:THR:HA	2.04	0.40
1:A:2323:LYS:HE2	1:A:2323:LYS:HB2	1.80	0.40
1:A:3126:MET:SD	1:A:3126:MET:N	2.94	0.40
1:A:3484:ALA:O	1:A:3487:GLU:HG2	2.21	0.40
1:A:3875:MET:HE3	1:A:3879:ASP:HB2	2.02	0.40
1:A:4067:THR:O	1:A:4069:ILE:HG13	2.22	0.40
1:A:4168:ARG:NH2	1:A:4220:ASP:OD2	2.55	0.40
1:A:1656:LYS:HE2	1:A:1656:LYS:HB3	1.84	0.40
1:A:2869:ARG:HB2	1:A:2870:PRO:HD3	2.02	0.40
1:A:3551:GLU:OE2	1:A:3551:GLU:N	2.33	0.40
1:A:3586:TYR:HA	1:A:3587:PRO:HD3	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2689/4646 (58%)	2606 (97%)	80 (3%)	3 (0%)	48 79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4172	SER
1	A	4251	ILE
1	A	2387	LEU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2401/4125 (58%)	2387 (99%)	14 (1%)	78 79

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1739	ILE
1	A	1748	GLN
1	A	1914	GLU
1	A	2133	GLU
1	A	2220	LEU
1	A	2367	ASP
1	A	2387	LEU
1	A	2388	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2452	LEU
1	A	2614	ASP
1	A	2780	SER
1	A	3623	LEU
1	A	4315	THR
1	A	4454	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1800	GLN
1	A	1922	GLN
1	A	1974	GLN
1	A	2637	HIS
1	A	2689	HIS
1	A	2707	GLN
1	A	2725	HIS
1	A	3009	ASN
1	A	3631	ASN
1	A	3636	GLN
1	A	3754	ASN
1	A	3772	ASN
1	A	3838	ASN
1	A	3994	GLN
1	A	4012	ASN
1	A	4065	GLN
1	A	4174	ASN
1	A	4326	ASN
1	A	4389	HIS
1	A	4477	GLN
1	A	4526	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 [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	4701	-	28,29,29	0.47	0	43,45,45	0.56	0
2	ADP	A	4704	-	28,29,29	1.38	5 (17%)	43,45,45	1.81	9 (20%)
3	ATP	A	4703	-	32,33,33	0.49	0	48,52,52	0.32	0
3	ATP	A	4702	-	32,33,33	0.55	0	48,52,52	0.60	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	-	-	3/16/32/32	0/3/3/3
2	ADP	A	4704	-	-	5/16/32/32	0/3/3/3
3	ATP	A	4703	-	-	4/22/38/38	0/3/3/3
3	ATP	A	4702	-	-	6/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4704	ADP	C5-C4	4.45	1.47	1.39
2	A	4704	ADP	C5-C6	2.58	1.48	1.41
2	A	4704	ADP	C5-N7	-2.49	1.34	1.39
2	A	4704	ADP	C8-N7	2.28	1.36	1.31
2	A	4704	ADP	C4-N9	-2.08	1.33	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4704	ADP	C5-C4-N3	-5.69	118.88	126.72
2	A	4704	ADP	N3-C4-N9	4.39	134.63	127.17
2	A	4704	ADP	C2-N3-C4	3.60	120.63	111.83
2	A	4704	ADP	C4-C5-N7	-3.56	106.51	110.58
2	A	4704	ADP	N3-C2-N1	-3.10	123.88	128.58
2	A	4704	ADP	C4-N9-C8	2.59	108.46	105.74
2	A	4704	ADP	C5-N7-C8	2.53	107.43	103.45
2	A	4704	ADP	C3'-C2'-C1'	2.20	105.63	101.46
2	A	4704	ADP	C6-C5-N7	2.10	136.14	132.09

There are no chirality outliers.

All (18) torsion outliers are listed below:

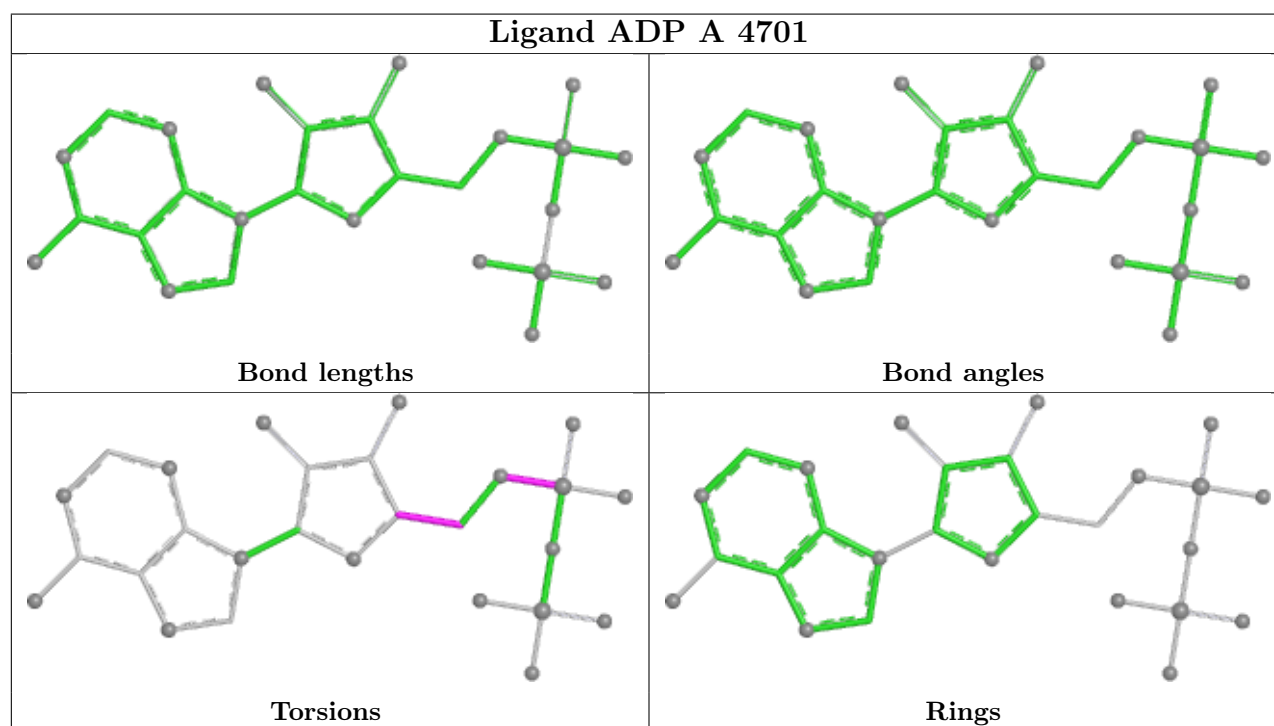
Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A
3	A	4702	ATP	C5'-O5'-PA-O2A
3	A	4702	ATP	C5'-O5'-PA-O3A
3	A	4703	ATP	C5'-O5'-PA-O3A
3	A	4703	ATP	O4'-C4'-C5'-O5'
3	A	4703	ATP	PA-O3A-PB-O1B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

There are no ring outliers.

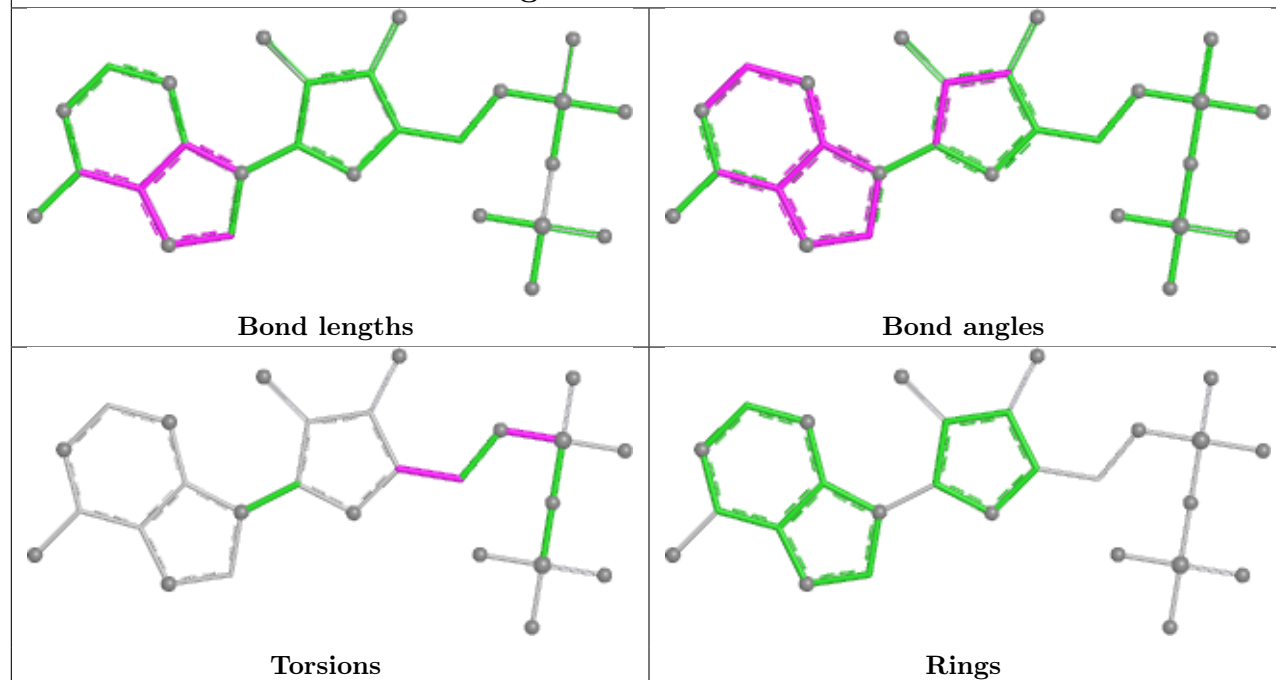
4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	5	0
2	A	4704	ADP	2	0
3	A	4703	ATP	4	0
3	A	4702	ATP	7	0

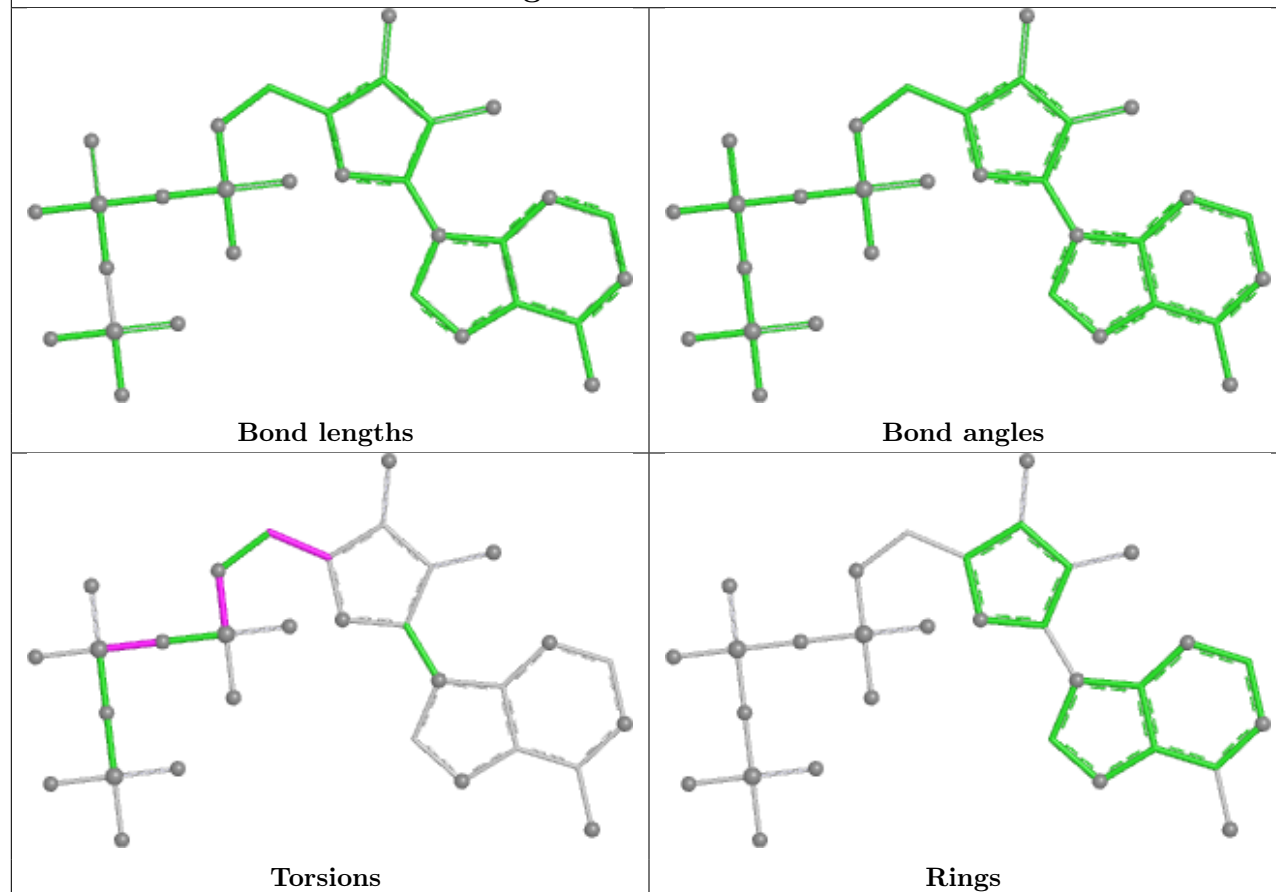
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

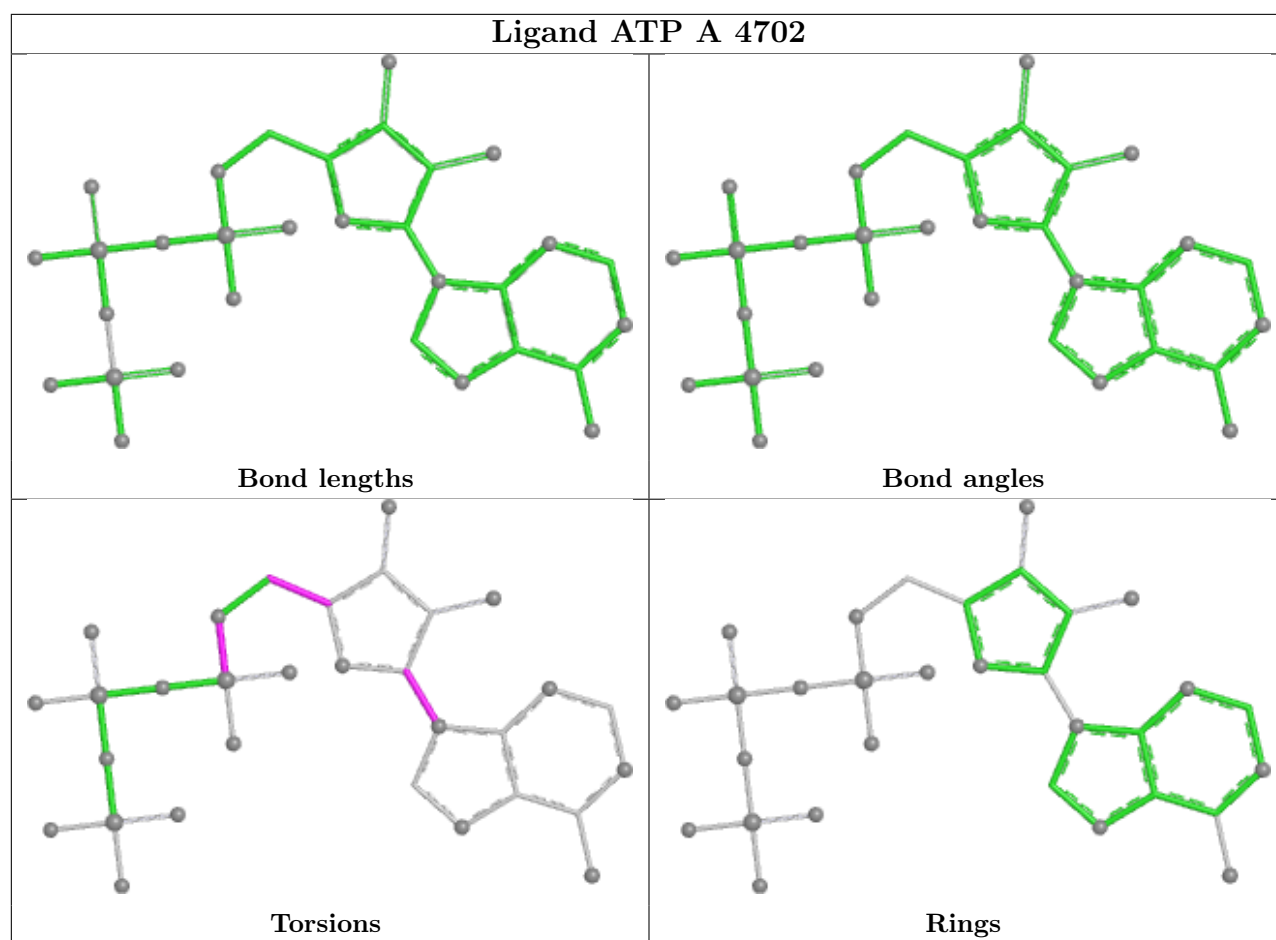


Ligand ADP A 4704



Ligand ATP A 4703





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.

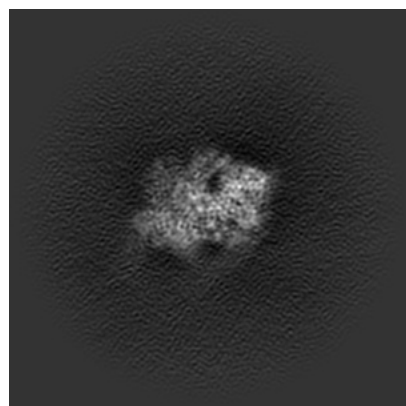
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44690. These allow visual inspection of the internal detail of the map and identification of artifacts.

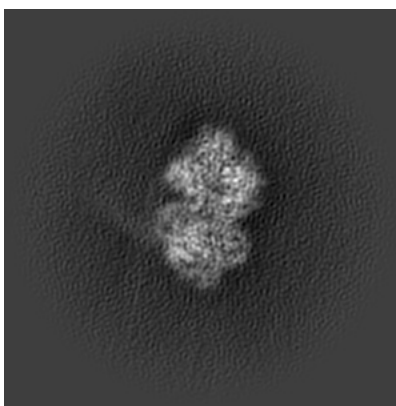
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

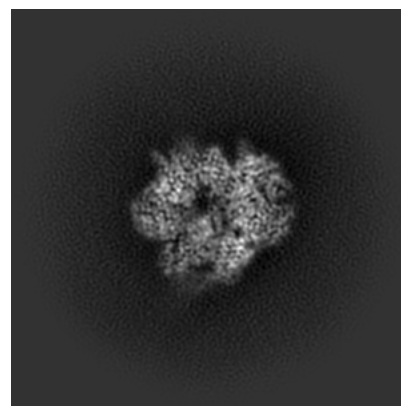
6.1.1 Primary map



X

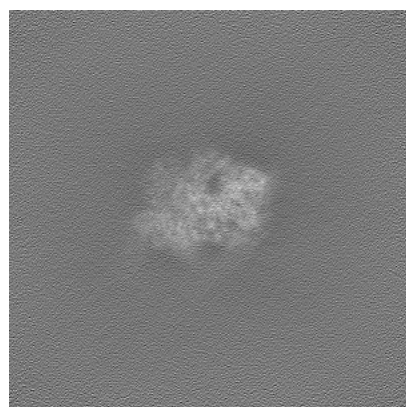


Y

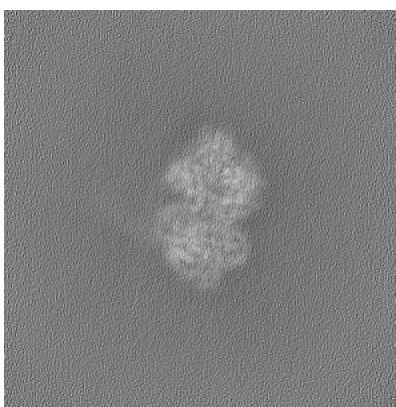


Z

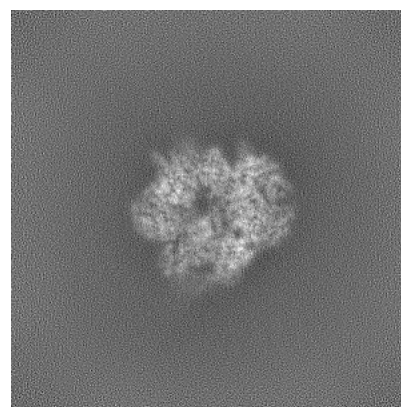
6.1.2 Raw map



X



Y

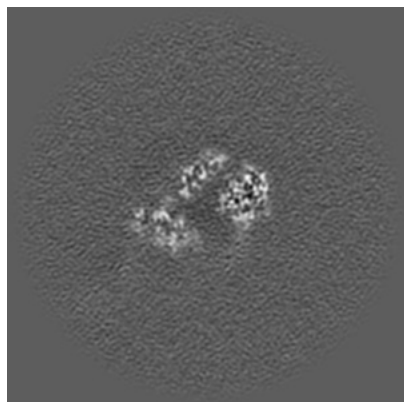


Z

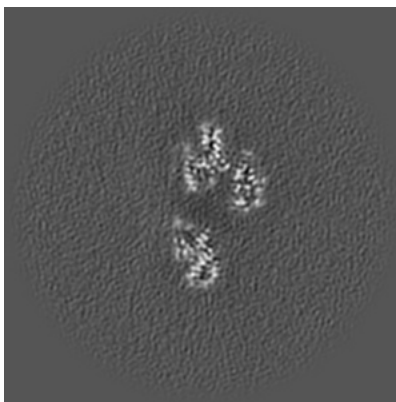
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

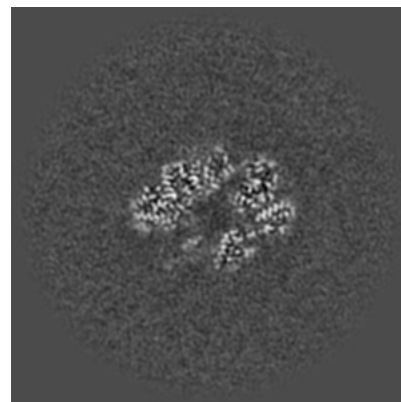
6.2.1 Primary map



X Index: 200

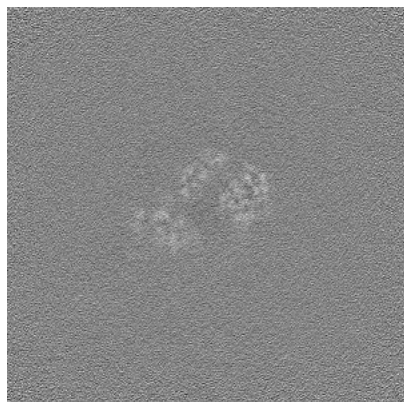


Y Index: 200

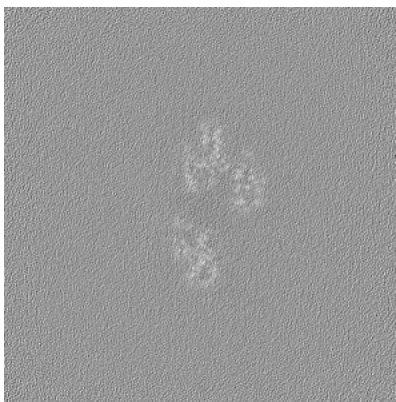


Z Index: 200

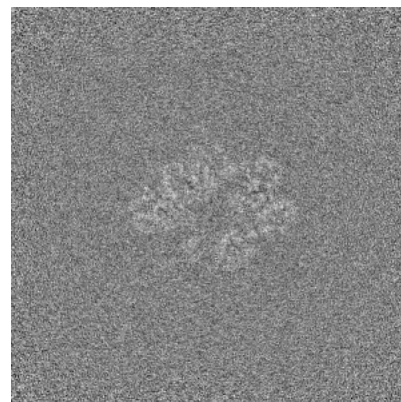
6.2.2 Raw map



X Index: 200



Y Index: 200

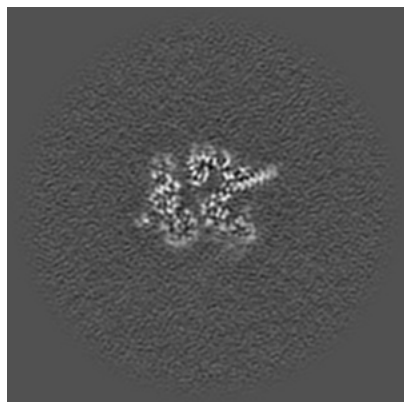


Z Index: 200

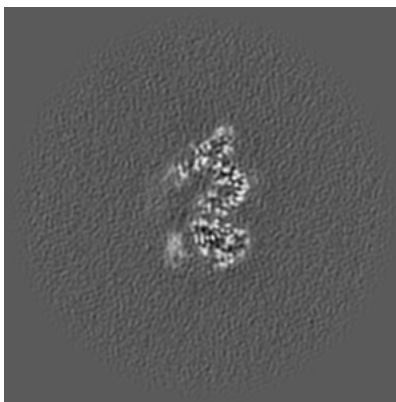
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

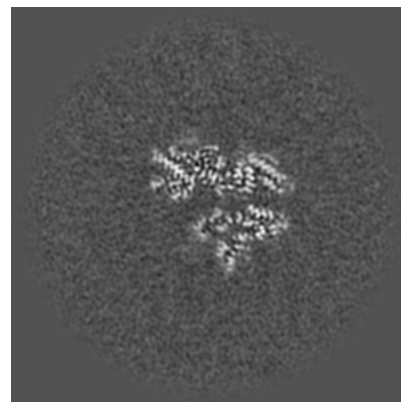
6.3.1 Primary map



X Index: 229

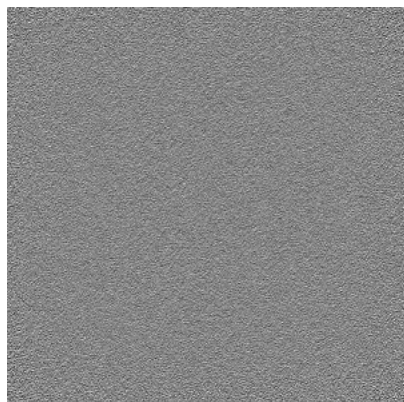


Y Index: 224

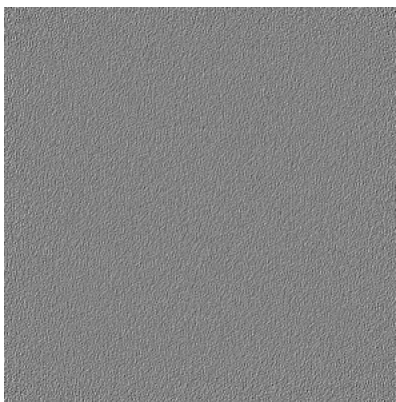


Z Index: 222

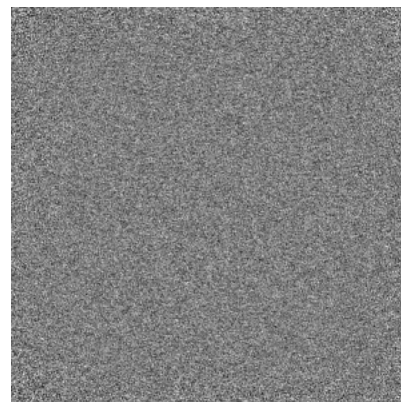
6.3.2 Raw map



X Index: 0



Y Index: 0

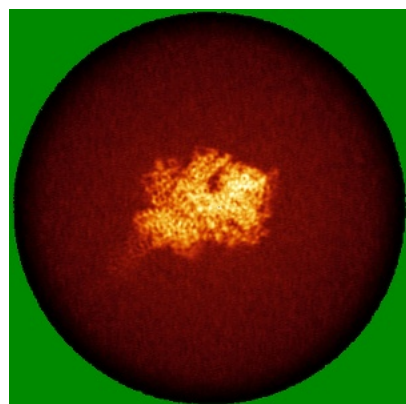


Z Index: 0

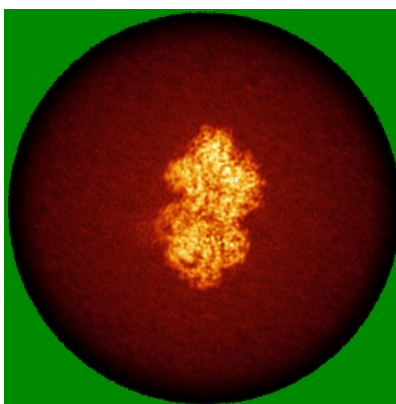
The images above show the largest variance slices of the map in three orthogonal directions.

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

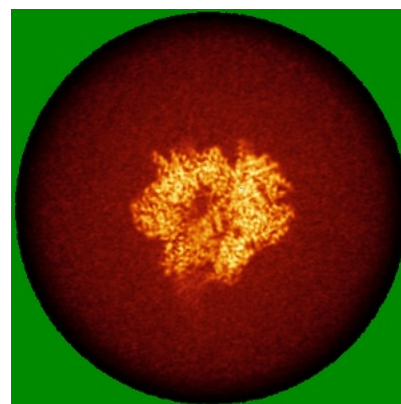
6.4.1 Primary map



X

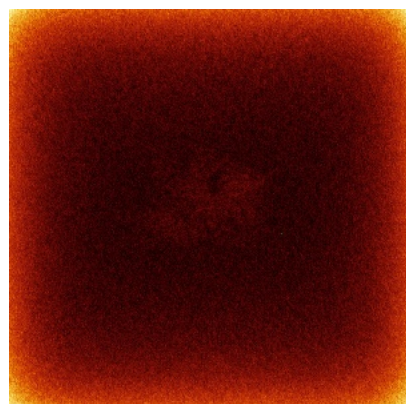


Y

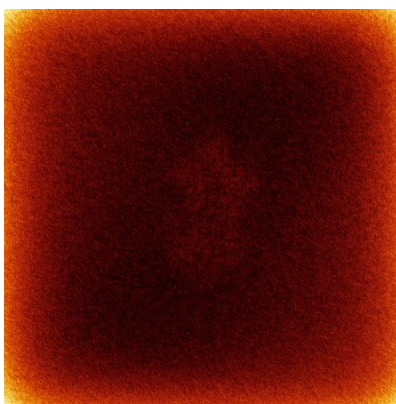


Z

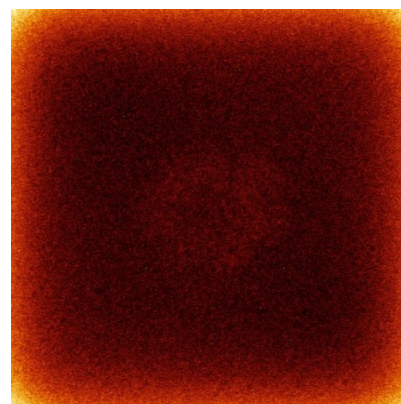
6.4.2 Raw map



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.

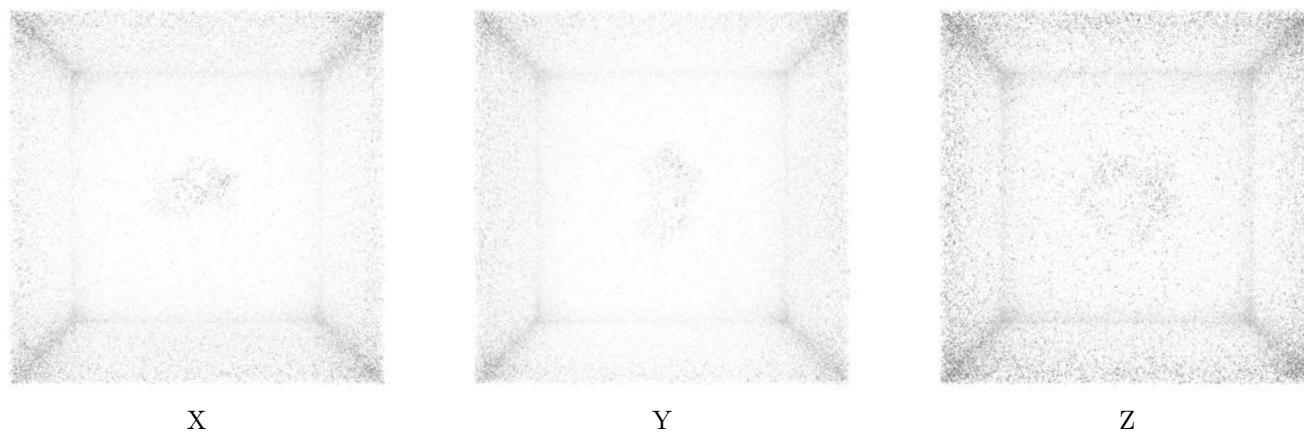
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. 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.

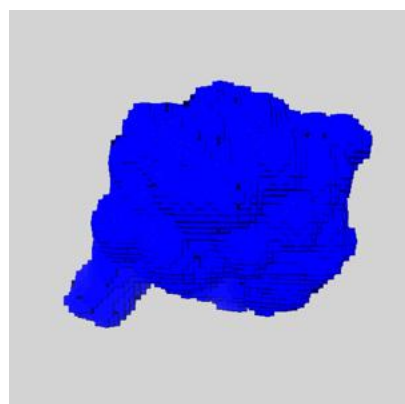
6.6 Mask visualisation [i](#)

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

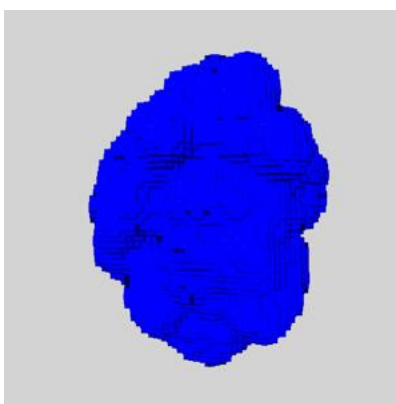
A mask typically either:

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

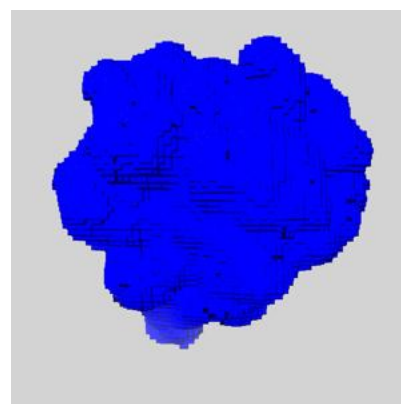
6.6.1 emd_44690_msk_1.map [i](#)



X



Y

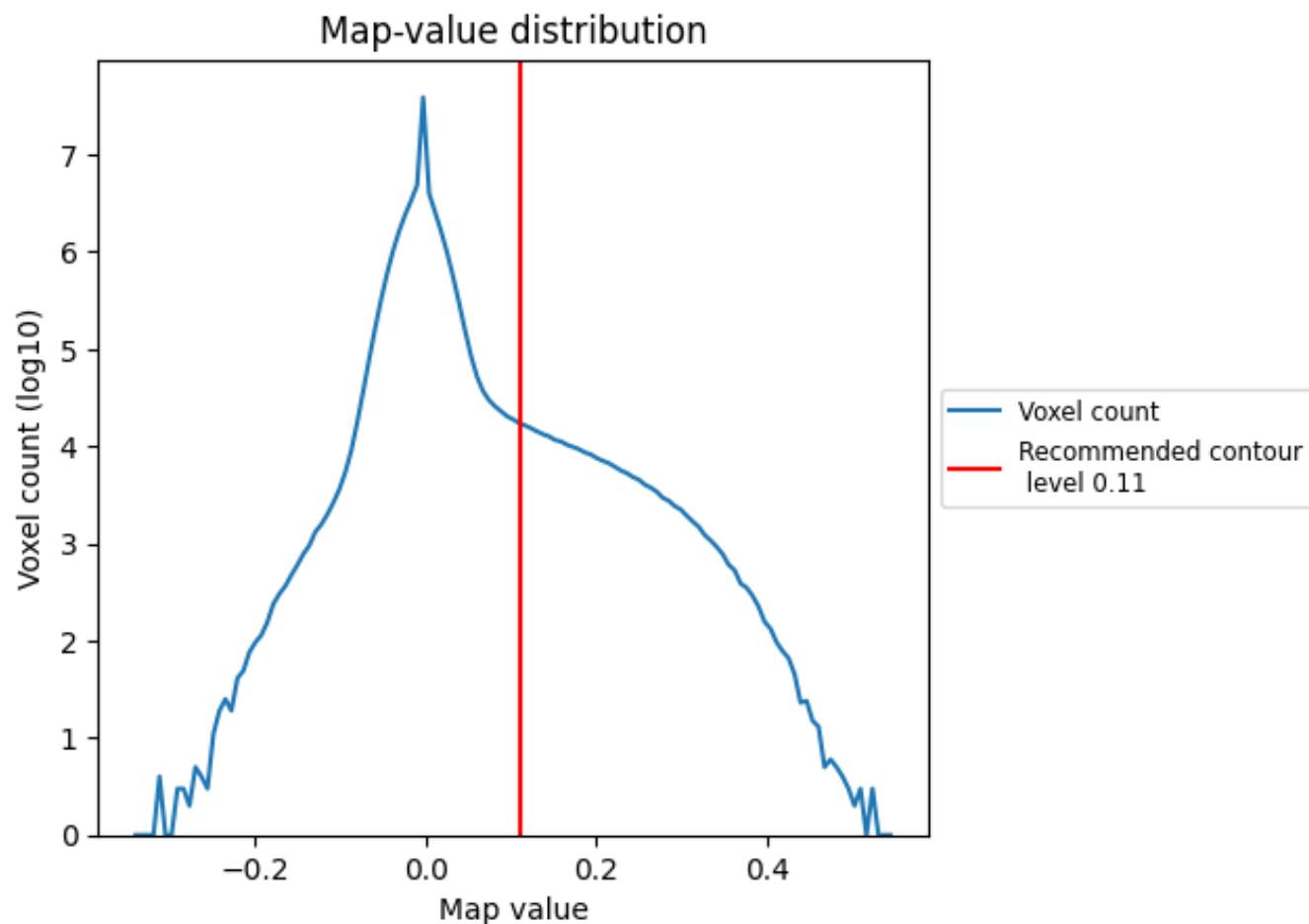


Z

7 Map analysis [i](#)

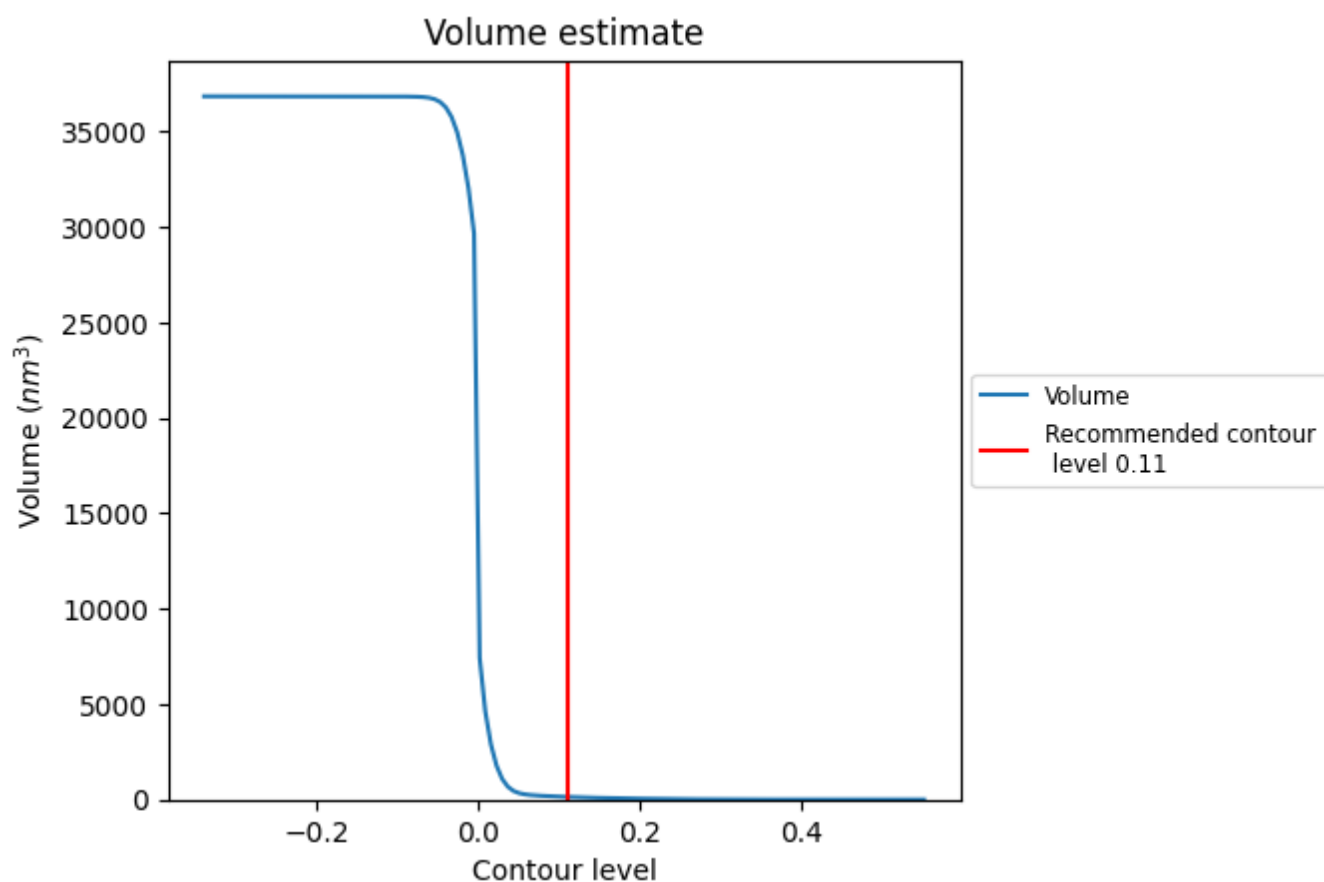
This section contains the results of statistical analysis of the map.

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.

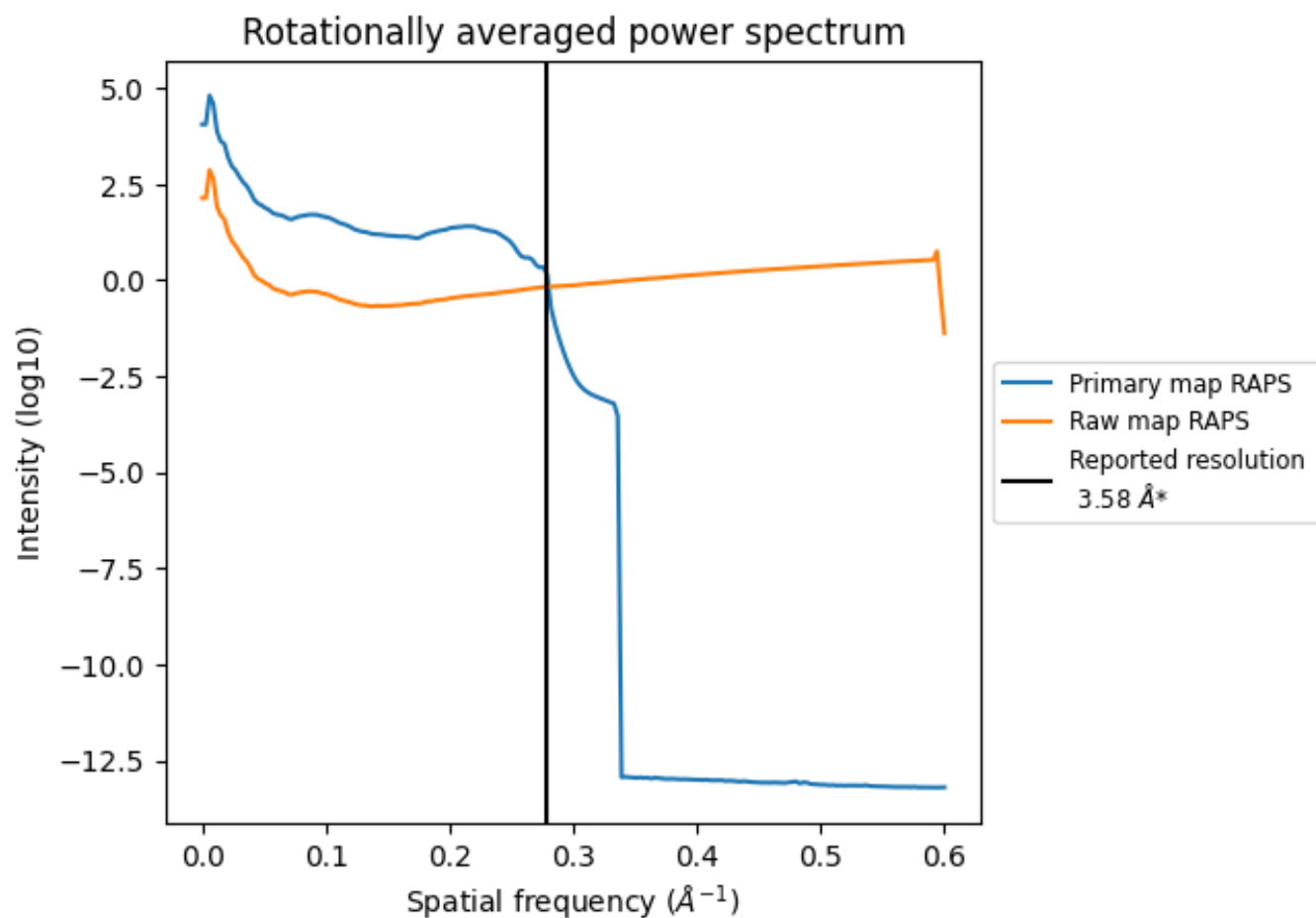
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 138 nm³; this corresponds to an approximate mass of 124 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 ⓘ

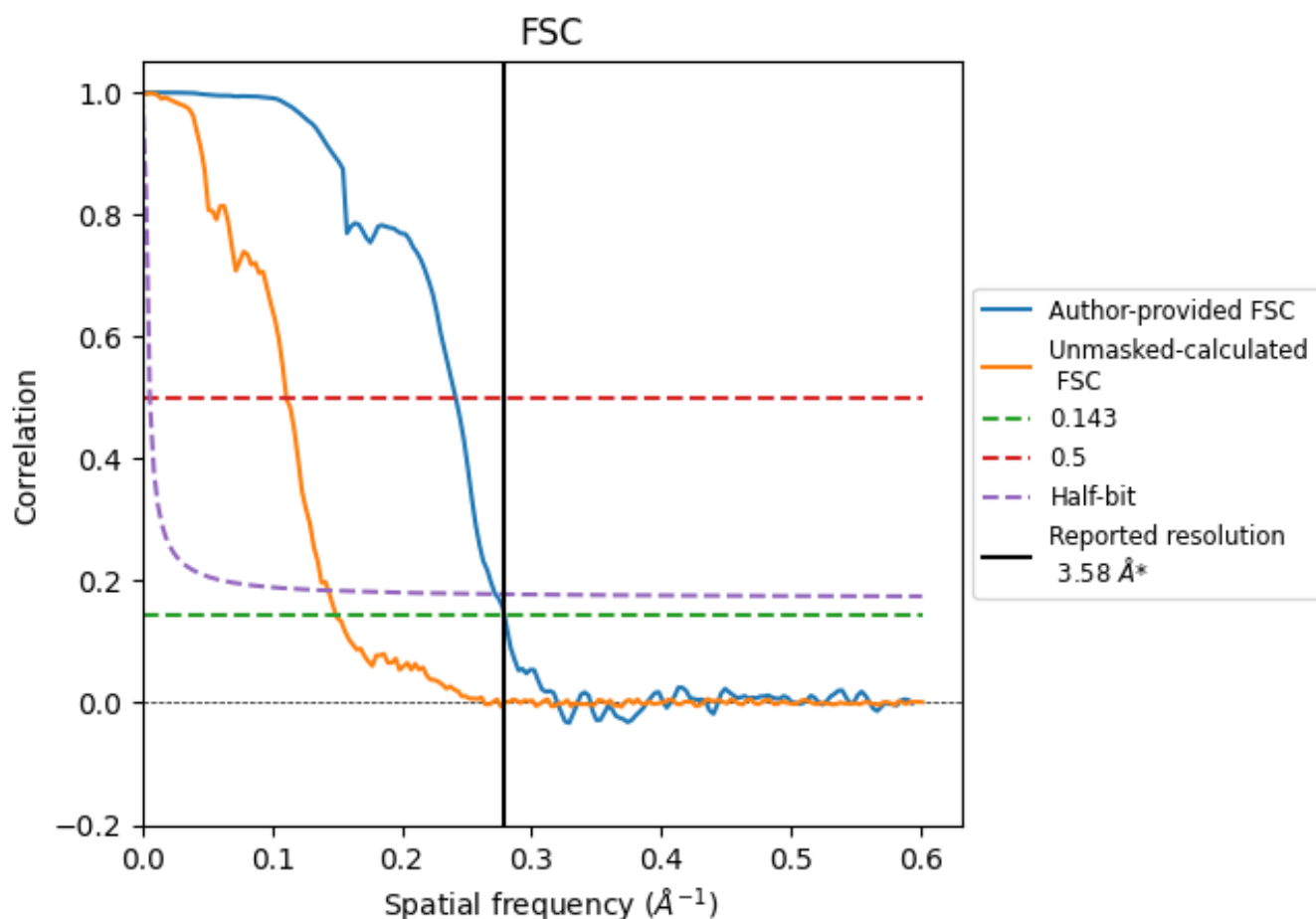


*Reported resolution corresponds to spatial frequency of 0.279 $\text{\AA}^{-1}$

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 0.279 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

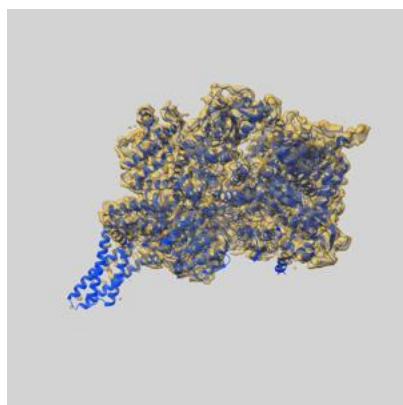
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.58	-	-
Author-provided FSC curve	3.58	4.14	3.68
Unmasked-calculated*	6.68	9.01	6.97

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.68 differs from the reported value 3.58 by more than 10 %

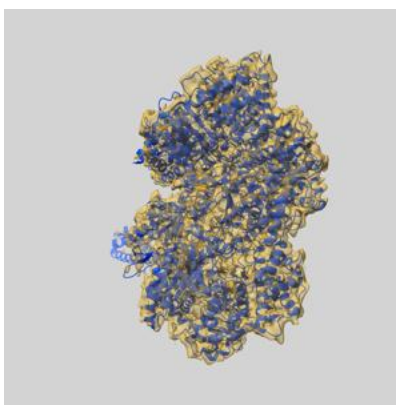
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44690 and PDB model 9BM7. Per-residue inclusion information can be found in section [3](#) on page [5](#).

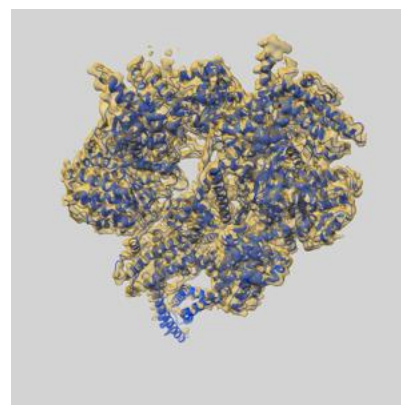
9.1 Map-model overlay [i](#)



X



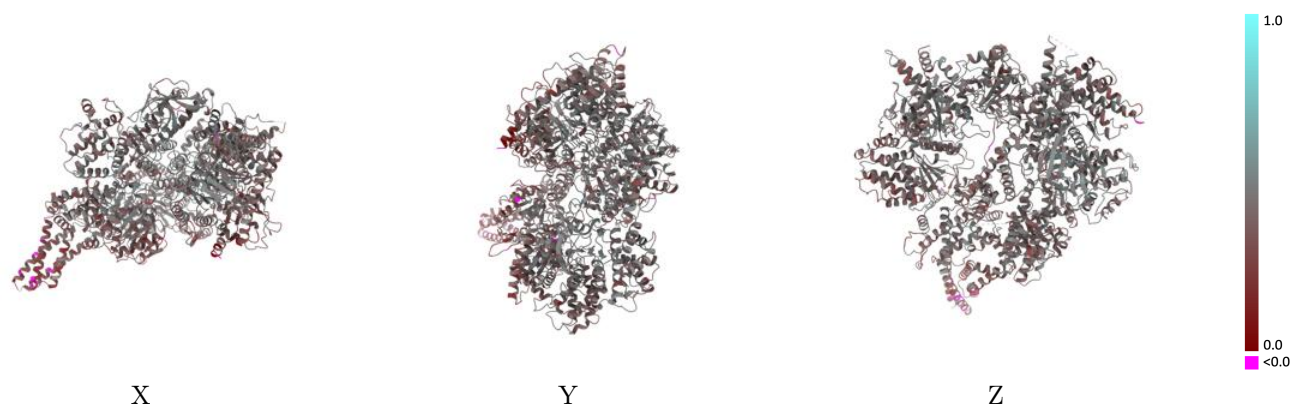
Y



Z

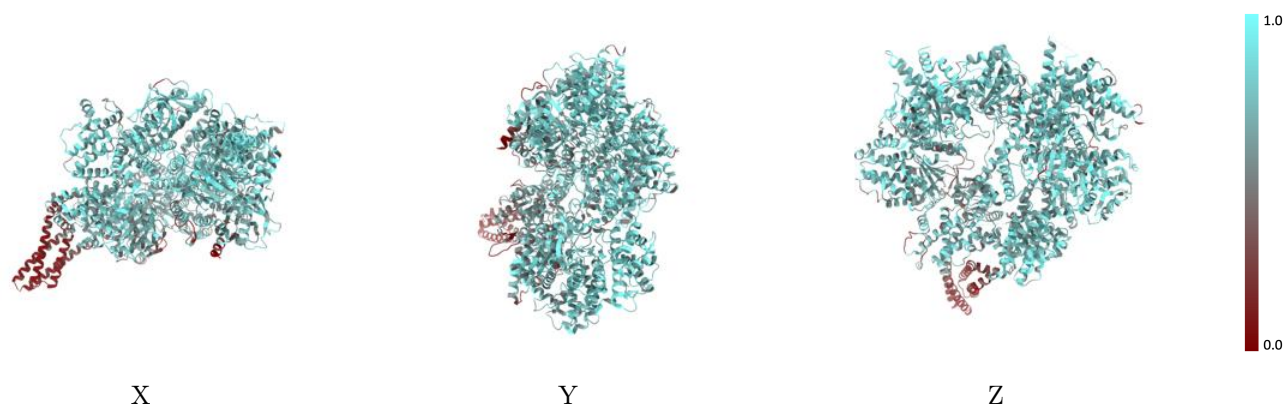
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



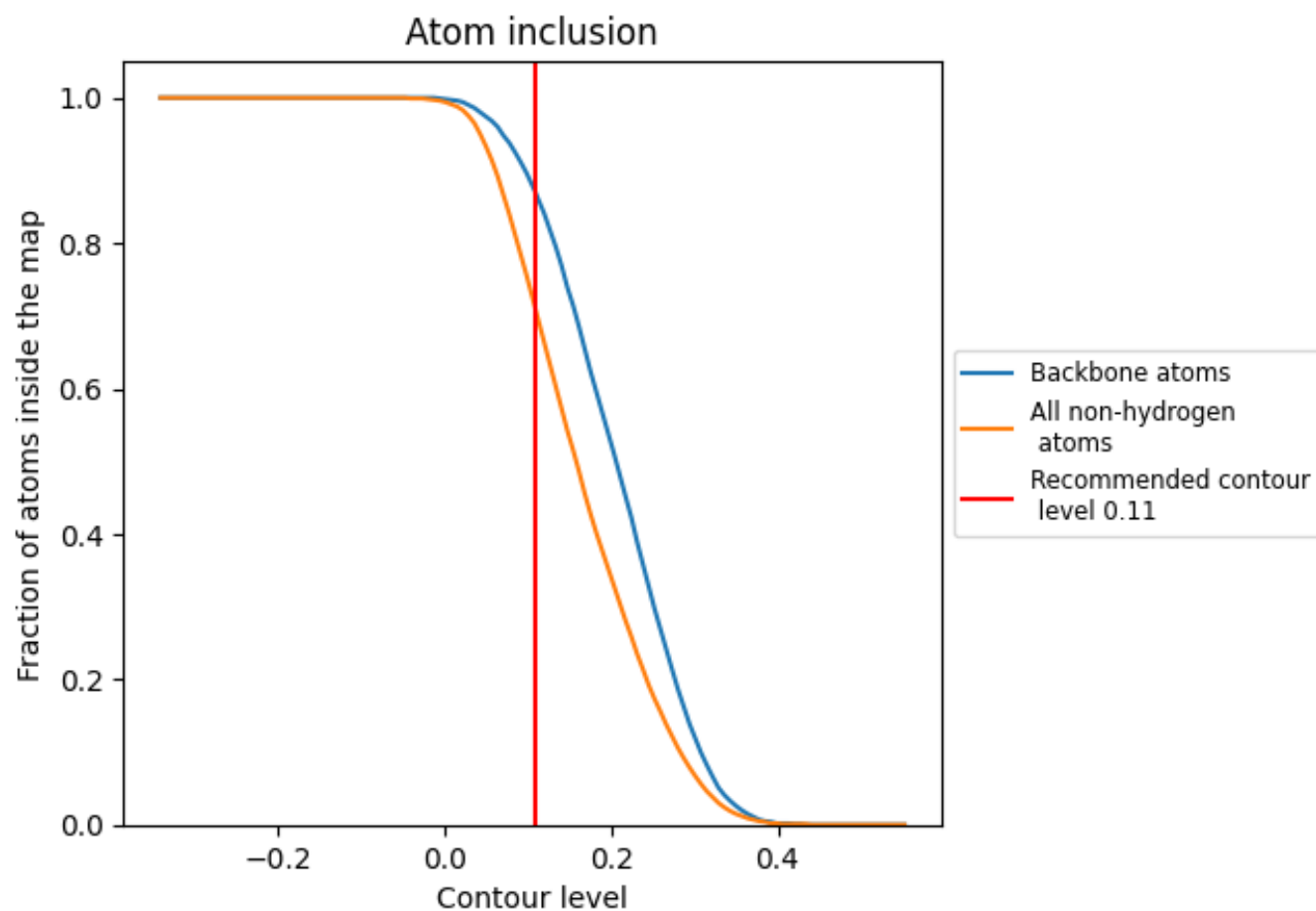
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 71% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7080	0.4100
A	0.7080	0.4100

