



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 02:21 AM UTC

PDB ID : 9BMU / pdb_00009bmu
EMDB ID : EMD-44711
Title : State-6 of motor domain from full-length human dynein-1 in 5 mM ADP
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.70 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

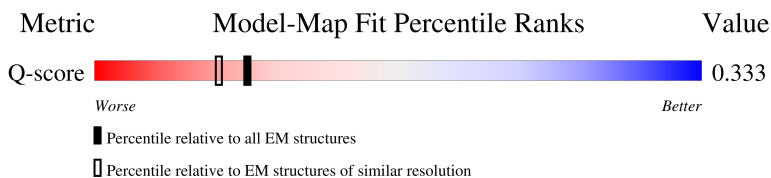
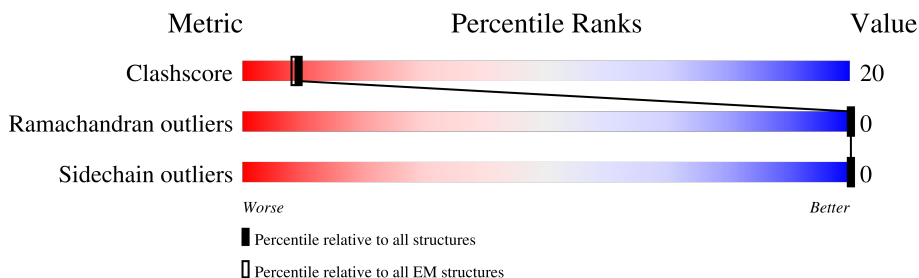
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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](#)

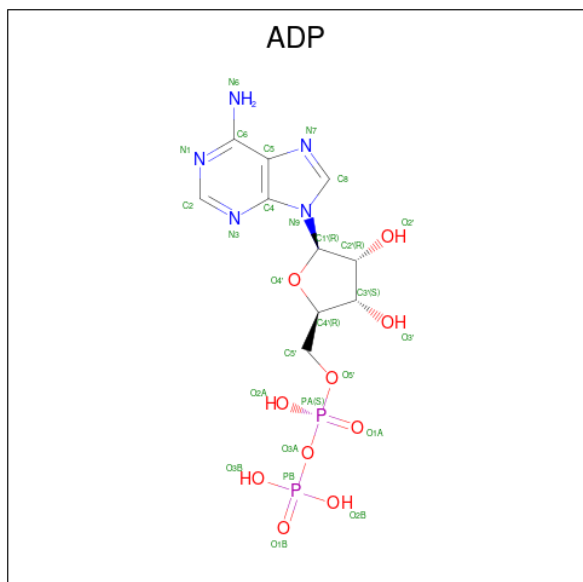
There are 3 unique types of molecules in this entry. The entry contains 21776 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	2698	21664	13799	3740	4014	111	0	0

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



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

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



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



GLY	L2993	E2904	I2822	V2734	K2651	H2577	K2491	P2411	R2340	G2266	E2180	N2067
LEU	M2994	L2905	R2823	Y2735	P2652	E2676	R2492	M2412	I2341	D2269	E2181	N2071
LYS	D2995	L2909	A2826	Y2736	V2653	L2581	L2493	Q2413	M2342	P2270	K2184	F2072
ASP	N2998	L2910	H2827	Y2737	Q2654	Y2682	L2494	E2344	F2343	N2271	V2185	F2074
ARG	V2999	V2910	A2827	Y2738	K2657	V2683	Y2495	V2345	K2184	R2272	E2188	L2075
ALA	L3000	L2912	R2831	P2739	K2658	V2684	Y2496	Q2346	V2344	R2273	D2195	K2074
THR	N2913	N2913	R2831	L2744	L2659	V2685	A2200	D2347	V2345	R2274	E2198	L2075
SER	S3002	E2914	D2835	Y2747	V2660	A2686	T2422	D2348	K2349	E2274	D2195	H2086
	G3003	V2915	R2837	Y2748	L2661	E2687	L2499	M2423	Y2350	R2275	E2198	H2085
	F3004	L2837	V2838	G2749	F2662	H2688	S2501	Q2424	A2351	T2276		
	L3005	V2838	V2838	T2750	T2666	K2689	L2502		T2352	D2277		
	E3006	E2839	F2751	F2751	N2667	L2590	S2503	F2427	L2352	L2278		
		D2840	L2668		G2504	L2591	G2504		V2356	L2279		
		E2841	P2669		D2506	L2592	D2506	G2431	V2357	T2280		
		E2842	L2756		S2507	L2593	L2432	T2432	S2357	T2281		
		R2843	R2757		D2670	L2594	T2434	V2433	R2358	H2282		
		D2847	R2763		M2671	G2595	K2435	K2435	G2359	V2283		
		I2850			T2676	P2596	K2436	A2436	G2360	L2208		
		D2851			Q2677		M2510	A2437	M2361	Q2209		
		L2852			T2678		R2511	L2437	V2362	R2284		
		V2853			K2678		A2512	E2438	W2363	R2285		
		K2943			V2679		E2513	I2446	L2369	I2287		
		T2944			I2680		E2516		S2370	I2288		
		T2945			F2682		T2517	L2449	M2373	R2292		
		L2946			I2683		T2518	T2450	L2374	E2294		
		S2947			R2684		I2521	L2452	R2295	Q2296		
		R2948			Q2685		V2524	G2454	K2297	R2298		
		F2949			K2686		P2525	L2455	L2362	W2300		
		V2950			E2688		L2526	G2456	R2382	G2229		
		M2953			H2689		P2527	S2457	R2383	I2301		
		L2956			Q2690		I2534	S2460	P2386	V2302		
		S2957			G2691		T2535	M2461	L2387	F2303		
		V2958			F2692		D2536	L2462	D2388	D2304		
		Q2960			L2702		E2538	H2463	E2389	P2309		
		I2961			L2703		W2548	Q2464	E2310	W2311		
		H2964			E2704		E2538	A2465	E2310	R2236		
		R2965			R2705		P2563	C2466	L2237	L2238		
		K2966			I2706		E2568	R2467	K2239	K2239		
		Y2967			Q2707		H2560	N2468	A2240	L2241		
		T2968			F2708		E2568	V2469	E2242	R2243		
		G2969			V2709		H2560	Y2472	R2320	R2243		
		E2970			C2712		A2563	N2473	D2321	L2244		
		L2976			K2721		A2563	P2480	L2325	E2245		
		V3064			K2722		V2568	Q2481	T2326	G2248		
		V3065			L2723		V2568	Q2482	L2327	E2248		
		L2980			R2726		V2569	E2483	P2328	G2249		
		R2981			F2727		T2570	Q2484	N2329	T2254		
		K2986			L2728		T2571	Q2485	G2330	D2255		
		L2897			R2729		L2572	L2486	E2331	E2259		
		K2898			H2730		D2573	E2487	R2332	L2157		
		V2899			H2731		T2574	R2488	E2333	L2163		
PRO	F2990	F2990	F2900	E2819	V2732	G2647	V2575	Y2489	ALA	Y2337		
SER	A2991	F2992	V2901		V2733	L2650	R2576		ALA			
SER												
GLU												



F4635	Y4636	E4637	R4638	V4642	T4645	GLU	P4324	M4325	N4326	A4327	E4328	M4339	M4343	L4344	K4345	M4346	Q4347	MET	LEU	GLU	ASP	GLU	ASP	GLU	ASP	ASP	LEU	ALA	TYR	ALA	GLU	THR	GLU	LYS	LYS	THR	THR	THR	ASP	SER	THR	SER	ASP	GLY	ARG	P4374	A4375	W4376	T4379	I4391	P4392	Q4393	E4394	L4398	K4399	R4400	T4401	V4402	I4405	R4411	F4412	F4413	I4507
R4508	V4509	F4515	R4525	Q4526	M4532	S4533	W4534	S4535	L4536	E4537	E4538	L4541	E4542	V4543	Q4549	L4553	D4554	A4555	C4556	S4557	L4565	K4574	L4577	S4578	L4585	R4591	V4592	V4593	K4594	V4604	V4605	T4606	L4607	P4608	V4609	L4618	V4622	D4623	F4624	E4625	K4629	R4633	S4634																				
E4414	K4418	L4423	R4428	Q4429	D4430	V4434	K4441	K4442	K4443	Q4444	T4445	M4446	Y4447	L4448	R4449	I4452	M4453	E4454	L4455	V4456	I4459	L4460	P4461	W4464	S4465	H4466	G4472	M4473	T4474	V4475	I4476	Q4477	W4478	V4479	F4482	S4483	E4484	R4485	I4486	K4487	Q4488	L4489	I4492	L4504	K4505	M4506	I4507																
A4241	A4242	L4243	K4244	A4248	Q4249	S4250	I4251	Y4252	F4260	D4261	Q4262	R4263	L4264	R4271	L4272	T4275	R4276	S4277	F4278	F4282	K4287	V4288	D4289	Q4290	H4291	K4292	D4293	M4296	P4297	I4300	R4301	R4302	E4303	E4304	F4305	V4306	Q4307	W4308	V4309	E4310	L4311	L4312	P4313	D4314	T4315	P4318	S4319	W4320	L4321														

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93339	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	0.603	Depositor
Minimum map value	-0.336	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	329.984, 329.984, 329.984	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0312, 1.0312, 1.0312	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP

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	0/22127	0.40	0/29993

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2229	GLY	Peptide

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	21664	0	21700	885	0
2	A	81	0	36	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	12	5	0
All	All	21776	0	21748	886	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 20.

All (886) 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:3126:MET:HE3	1:A:3127:PRO:HD2	1.50	0.93
1:A:2603:MET:HE1	2:A:4703:ADP:C4	2.04	0.93
1:A:2688:GLU:HB2	1:A:2730:HIS:HE1	1.33	0.90
1:A:2619:GLY:HA2	1:A:2662:PHE:HB3	1.58	0.84
1:A:2473:ASN:HB2	1:A:2481:MET:HE1	1.60	0.83
1:A:2794:TYR:HE1	1:A:2836:ARG:HH21	1.30	0.80
1:A:2609:LEU:HD23	1:A:2660:VAL:HG21	1.65	0.78
1:A:4058:LEU:HA	1:A:4061:GLU:HG2	1.65	0.78
1:A:2995:ASP:OD1	1:A:3067:THR:OG1	2.02	0.78
1:A:2304:ASP:HA	1:A:2344:GLU:HB3	1.66	0.78
1:A:3154:LEU:HG	1:A:3516:TYR:HD2	1.49	0.78
1:A:3990:LEU:HD21	1:A:4008:PHE:HB2	1.65	0.77
1:A:1743:ASP:OD2	1:A:1804:ARG:NH2	2.17	0.77
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.67	0.77
1:A:2029:PRO:HG2	1:A:2032:LEU:HD12	1.66	0.76
1:A:3876:LEU:HD23	1:A:3878:GLN:H	1.51	0.75
1:A:2657:LYS:H	1:A:2705:ARG:HD2	1.51	0.75
1:A:2230:LYS:HE2	1:A:2344:GLU:HG3	1.68	0.75
1:A:2749:GLY:HA2	1:A:2770:THR:HG21	1.69	0.75
1:A:1888:CYS:HB2	1:A:2041:MET:HE1	1.69	0.74
1:A:2018:MET:HE2	1:A:2027:ASN:HA	1.70	0.74
1:A:3485:GLU:OE2	1:A:3489:TRP:NE1	2.16	0.74
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.68	0.74
1:A:4376:TRP:HA	1:A:4379:THR:HG22	1.69	0.74
1:A:3830:GLN:NE2	1:A:3834:ASP:OD2	2.21	0.74
1:A:2511:ARG:HH21	1:A:2735:TYR:HB3	1.53	0.73
1:A:1769:MET:HE3	1:A:1777:PRO:HD2	1.71	0.72
1:A:2584:TRP:CH2	1:A:2732:PRO:HB2	2.23	0.72
1:A:4106:LEU:HD23	1:A:4135:PRO:HD2	1.71	0.72
1:A:1816:VAL:HG13	1:A:1819:ARG:HH22	1.54	0.72
1:A:1631:PHE:HA	1:A:1944:ILE:HG22	1.70	0.72
1:A:2936:ILE:HG22	1:A:3068:MET:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2895:ALA:HA	1:A:2898:LYS:HE2	1.72	0.72
1:A:4271:ARG:HD3	1:A:4633:ARG:HD2	1.70	0.72
1:A:3907:HIS:HD2	1:A:3991:LEU:HD11	1.54	0.72
1:A:4574:LYS:NZ	1:A:4625:GLU:OE2	2.22	0.72
1:A:1951:VAL:HG13	1:A:1953:ALA:H	1.54	0.71
1:A:2273:ARG:NH2	1:A:2329:ASN:O	2.24	0.71
1:A:3154:LEU:HG	1:A:3516:TYR:CD2	2.25	0.71
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.72	0.71
1:A:2603:MET:HE1	2:A:4703:ADP:C5	2.25	0.70
1:A:3046:SER:OG	1:A:3049:GLU:OE1	2.09	0.70
1:A:2755:MET:HE1	1:A:2807:PHE:HA	1.72	0.70
1:A:3190:LYS:HB3	1:A:3503:ILE:HD11	1.72	0.70
1:A:3710:SER:O	1:A:3714:ASN:ND2	2.24	0.70
1:A:4400:ARG:HH21	1:A:4405:ILE:HG12	1.56	0.70
1:A:2680:ILE:HG12	1:A:2723:LEU:HD12	1.73	0.69
1:A:2831:ARG:HB3	1:A:2924:ARG:HH22	1.55	0.69
1:A:4154:LYS:HE3	1:A:4310:GLU:HA	1.73	0.69
1:A:3907:HIS:HE1	1:A:3937:ARG:HG3	1.57	0.69
1:A:1912:LYS:NZ	2:A:4701:ADP:O2B	2.26	0.69
1:A:2485:GLN:OE1	1:A:2488:ARG:NH1	2.26	0.69
1:A:2836:ARG:HG2	1:A:3091:LEU:HB3	1.73	0.69
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.25	0.68
1:A:3490:GLU:O	1:A:3493:SER:OG	2.09	0.68
1:A:1917:LYS:HG2	1:A:1927:VAL:HG21	1.74	0.68
1:A:3154:LEU:HB3	1:A:3171:ILE:HD13	1.75	0.68
1:A:2287:ILE:HA	1:A:2294:GLU:HG3	1.76	0.68
1:A:2220:LEU:HB2	1:A:2342:MET:HG3	1.76	0.68
1:A:3106:GLY:O	1:A:3110:THR:OG1	2.09	0.67
1:A:4393:GLN:OE1	1:A:4428:ARG:NH2	2.25	0.67
1:A:2213:ILE:HD11	1:A:2360:GLY:HA3	1.75	0.67
1:A:2054:LEU:HG	1:A:2097:LEU:HD22	1.76	0.67
1:A:2337:PRO:O	1:A:2340:ARG:NH1	2.27	0.67
1:A:4036:LYS:HG3	1:A:4038:ASN:H	1.60	0.67
1:A:2612:LEU:HB3	1:A:2615:MET:HE2	1.76	0.67
1:A:3971:PRO:HG2	1:A:3973:LEU:HD11	1.77	0.67
1:A:4301:ARG:NH1	1:A:4303:GLU:OE2	2.26	0.67
1:A:4525:ARG:HG2	1:A:4536:LEU:HD22	1.75	0.67
1:A:2457:SER:HB2	1:A:2732:PRO:HB3	1.77	0.67
1:A:1949:CYS:HA	1:A:2012:MET:HE3	1.74	0.67
1:A:2067:ASN:HB3	1:A:4537:GLU:HG2	1.77	0.67
1:A:4221:THR:HG23	1:A:4222:TRP:HD1	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2275:TRP:HE1	1:A:2285:ARG:NH2	1.93	0.67
1:A:3734:LEU:HD13	1:A:3783:LYS:HB3	1.77	0.67
1:A:1750:VAL:HG23	1:A:1811:LEU:HD21	1.76	0.66
1:A:2231:SER:OG	1:A:2344:GLU:OE2	2.12	0.66
1:A:3736:GLY:O	1:A:3740:LEU:N	2.27	0.66
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.76	0.66
1:A:2605:LEU:HD13	1:A:2662:PHE:HE2	1.60	0.66
1:A:2853:VAL:HA	1:A:2856:LYS:HG2	1.78	0.66
1:A:3727:LYS:O	1:A:3731:LEU:N	2.28	0.66
1:A:2245:GLU:OE1	1:A:2298:ARG:NH2	2.27	0.66
1:A:4248:ALA:O	1:A:4262:GLN:NE2	2.29	0.65
1:A:1961:ASN:ND2	1:A:2019:ASN:O	2.29	0.65
1:A:4194:LEU:HD21	1:A:4207:PHE:HD2	1.61	0.65
1:A:3950:LYS:NZ	1:A:3973:LEU:HG	2.12	0.65
1:A:2571:THR:H	1:A:2574:THR:HG22	1.61	0.65
1:A:2652:PRO:O	1:A:2705:ARG:NH2	2.29	0.65
1:A:4196:TYR:OH	1:A:4328:GLU:OE2	2.12	0.65
1:A:3892:LEU:HD12	1:A:3898:GLU:HG3	1.78	0.64
1:A:2747:ILE:HD11	2:A:4703:ADP:C6	2.33	0.64
1:A:4264:LEU:HD11	1:A:4637:GLU:HA	1.79	0.64
1:A:2536:ASP:OD1	1:A:2576:ARG:NH1	2.31	0.64
1:A:3057:GLN:HE22	1:A:3060:ARG:HH21	1.43	0.64
1:A:3567:LEU:HD12	1:A:3568:PRO:HD2	1.79	0.64
1:A:2660:VAL:HG12	1:A:2707:GLN:HG3	1.80	0.64
1:A:2269:ASP:HB2	1:A:2274:GLU:HG3	1.78	0.64
1:A:3553:LEU:O	1:A:3582:ARG:NH2	2.30	0.64
1:A:3989:ARG:HG3	1:A:4004:MET:HE2	1.81	0.63
1:A:1882:THR:HG23	1:A:2045:ASP:HB2	1.80	0.63
1:A:3885:MET:SD	1:A:4343:MET:HE1	2.39	0.63
1:A:3715:GLU:OE2	1:A:3718:LYS:NZ	2.31	0.63
1:A:4474:THR:H	1:A:4477:GLN:NE2	1.95	0.63
1:A:3981:THR:HG23	1:A:3984:GLY:H	1.64	0.63
1:A:2086:TYR:OH	1:A:2153:ASP:OD2	2.11	0.62
1:A:2527:PRO:HD2	1:A:2534:ILE:HD12	1.81	0.62
1:A:2831:ARG:HG3	1:A:2924:ARG:HH12	1.64	0.62
1:A:3654:ARG:HB2	1:A:3661:LEU:HB2	1.82	0.62
1:A:4043:MET:HE1	1:A:4125:PHE:HB3	1.81	0.62
1:A:1985:HIS:HA	1:A:1997:ILE:HG12	1.81	0.62
1:A:3974:TRP:HZ2	1:A:3985:GLN:HG2	1.64	0.62
1:A:4448:LEU:O	1:A:4452:ILE:HG12	1.99	0.62
1:A:1889:TYR:HD1	1:A:1919:LEU:HD13	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2073:PHE:HE2	1:A:2093:LEU:HA	1.65	0.62
1:A:3973:LEU:HB2	1:A:3992:LEU:HD11	1.80	0.62
1:A:4532:ASN:HB3	1:A:4534:TRP:CZ3	2.35	0.62
1:A:4034:GLU:O	1:A:4143:ARG:NH1	2.31	0.61
1:A:2284:LEU:HD22	1:A:2325:LEU:HD13	1.81	0.61
1:A:2605:LEU:HD11	1:A:2709:VAL:HG11	1.81	0.61
1:A:2934:LEU:HB3	1:A:3091:LEU:HA	1.80	0.61
1:A:3100:GLU:HA	1:A:3130:TYR:HE1	1.65	0.61
1:A:3194:LEU:HD11	1:A:3499:GLN:OE1	2.00	0.61
1:A:1908:ALA:HA	1:A:1912:LYS:HZ1	1.65	0.61
1:A:3588:LEU:HD11	1:A:3638:VAL:HG11	1.83	0.61
1:A:4312:LEU:HD12	1:A:4313:PRO:HD2	1.81	0.61
1:A:1708:GLU:O	1:A:1712:THR:HG23	2.00	0.61
1:A:1882:THR:HA	1:A:2048:LEU:HD23	1.83	0.61
1:A:2464:GLN:NE2	1:A:2468:ASN:OD1	2.34	0.61
1:A:2822:ILE:HD11	1:A:2858:PHE:CE2	2.36	0.61
1:A:3893:LYS:HZ3	1:A:3900:THR:HA	1.65	0.61
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	1.83	0.61
1:A:2729:ARG:HG3	1:A:2730:HIS:HD2	1.66	0.61
1:A:1938:PHE:HB2	1:A:1967:MET:HE1	1.83	0.60
1:A:4176:ARG:NH1	1:A:4220:ASP:OD1	2.33	0.60
1:A:2134:GLN:HG2	1:A:2168:VAL:HG21	1.83	0.60
1:A:4190:ILE:HG23	1:A:4201:TRP:HZ2	1.66	0.60
1:A:1654:PHE:HE1	1:A:1702:LEU:HD11	1.66	0.60
1:A:1882:THR:HG22	1:A:1884:LEU:H	1.66	0.60
1:A:2223:VAL:HG21	1:A:2348:LEU:HD11	1.84	0.60
1:A:4192:GLU:OE1	1:A:4195:ARG:NH1	2.35	0.60
1:A:3044:LEU:HD22	1:A:3049:GLU:HG3	1.84	0.60
1:A:3067:THR:O	1:A:3068:MET:HE2	2.02	0.60
1:A:1796:VAL:HG22	1:A:1808:LEU:HB3	1.84	0.60
1:A:2037:ARG:HH22	1:A:4250:SER:HG	1.48	0.60
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.84	0.60
1:A:3500:MET:O	1:A:3503:ILE:HG22	2.01	0.60
1:A:1626:PHE:HE1	1:A:1706:GLU:HG3	1.67	0.60
1:A:1891:THR:HG21	1:A:2039:LEU:HD21	1.84	0.60
1:A:3646:ASN:OD1	1:A:3650:ASN:ND2	2.35	0.59
1:A:3909:LEU:HB3	1:A:4344:LEU:HD13	1.83	0.59
1:A:3993:ILE:HD11	1:A:4000:ARG:HB2	1.83	0.59
1:A:2588:HIS:HA	1:A:2707:GLN:OE1	2.02	0.59
1:A:2901:TYR:OH	1:A:2909:LEU:N	2.34	0.59
1:A:3558:GLU:OE2	1:A:3562:TRP:NE1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3849:VAL:O	1:A:3855:ARG:NH1	2.36	0.59
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.84	0.59
1:A:3010:THR:HG23	1:A:3017:VAL:HG22	1.84	0.59
1:A:1755:GLN:NE2	1:A:1814:GLU:OE2	2.34	0.59
1:A:2037:ARG:NH2	1:A:4250:SER:OG	2.30	0.58
1:A:2327:LEU:HD12	1:A:2331:GLU:HB3	1.85	0.58
1:A:2484:GLU:OE2	1:A:2488:ARG:NH2	2.36	0.58
1:A:2112:LYS:HD2	1:A:2113:ARG:HH12	1.69	0.58
1:A:2863:ARG:O	1:A:2863:ARG:NH1	2.29	0.58
1:A:3877:HIS:HA	1:A:3880:HIS:CE1	2.38	0.58
1:A:2592:VAL:HG13	1:A:2733:VAL:HG23	1.85	0.58
1:A:3872:ALA:HB1	1:A:3880:HIS:CD2	2.38	0.58
1:A:4629:LYS:HD2	1:A:4629:LYS:O	2.03	0.58
1:A:2275:TRP:HZ2	1:A:2281:THR:HG21	1.68	0.58
1:A:4443:LYS:HD3	1:A:4444:GLN:H	1.67	0.58
1:A:2203:TRP:CH2	1:A:2236:VAL:HG11	2.39	0.58
1:A:3046:SER:HG	1:A:3049:GLU:CD	2.11	0.58
1:A:3826:GLN:HB3	1:A:4140:ARG:HD3	1.84	0.58
1:A:3993:ILE:HD13	1:A:4004:MET:HB2	1.84	0.58
1:A:1880:VAL:HG21	1:A:2049:ILE:HA	1.86	0.58
1:A:2205:GLU:O	1:A:2209:GLN:HG3	2.03	0.58
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.84	0.58
1:A:1930:PHE:CD2	1:A:1941:MET:HE1	2.39	0.58
1:A:2452:LEU:HD22	1:A:2729:ARG:HD2	1.84	0.58
1:A:3985:GLN:O	1:A:3989:ARG:HG2	2.04	0.57
1:A:2840:ASP:O	1:A:2843:ARG:HG2	2.03	0.57
1:A:3132:LYS:HE3	1:A:3132:LYS:HA	1.86	0.57
1:A:3785:GLU:O	1:A:3789:ILE:HG13	2.04	0.57
1:A:3884:ALA:HB1	1:A:4009:VAL:HG21	1.85	0.57
1:A:3909:LEU:HD11	1:A:4343:MET:HG2	1.86	0.57
1:A:2813:LEU:HD21	1:A:2816:LEU:HG	1.87	0.57
1:A:2934:LEU:HD23	1:A:3091:LEU:HD12	1.86	0.57
1:A:4171:LYS:HG3	1:A:4172:SER:H	1.69	0.57
1:A:2179:ARG:HD3	1:A:2208:LEU:HD11	1.87	0.57
1:A:2469:VAL:HG13	1:A:2481:MET:HE2	1.86	0.57
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.38	0.57
1:A:2635:PHE:HE2	1:A:2706:ILE:HD13	1.70	0.57
1:A:2944:THR:OG1	1:A:2948:ARG:NH2	2.38	0.57
1:A:4423:LEU:HD13	1:A:4466:HIS:HD2	1.69	0.57
1:A:1748:GLN:HG3	1:A:1749:LEU:HD22	1.86	0.57
1:A:2275:TRP:HB2	1:A:2329:ASN:HD22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3950:LYS:O	1:A:3954:ASP:N	2.31	0.57
1:A:1884:LEU:HD13	1:A:2044:PRO:HA	1.86	0.56
1:A:1840:SER:OG	1:A:1841:GLN:OE1	2.20	0.56
1:A:2814:GLU:OE1	1:A:2814:GLU:N	2.38	0.56
1:A:1889:TYR:CD1	1:A:1919:LEU:HD13	2.40	0.56
1:A:2480:PRO:O	1:A:2482:GLN:NE2	2.37	0.56
1:A:2943:LYS:HG2	1:A:3094:PHE:CD2	2.40	0.56
1:A:3204:GLY:HA2	1:A:3207:LYS:HE2	1.88	0.56
1:A:3066:PHE:CE1	1:A:3068:MET:HE3	2.41	0.56
1:A:2639:CYS:HA	1:A:2652:PRO:HA	1.87	0.56
1:A:3948:ILE:HA	1:A:3951:VAL:HG12	1.87	0.56
1:A:4538:GLU:OE1	1:A:4594:LYS:NZ	2.29	0.56
1:A:3654:ARG:N	1:A:3661:LEU:O	2.39	0.56
1:A:2211:TYR:O	1:A:2214:THR:OG1	2.20	0.56
1:A:2369:LEU:HD11	1:A:2374:ILE:HD11	1.87	0.56
1:A:2623:SER:N	1:A:2626:THR:OG1	2.39	0.56
1:A:3628:ARG:HH21	1:A:3670:ASP:HB2	1.71	0.56
1:A:1985:HIS:HB2	1:A:1997:ILE:HG21	1.87	0.56
1:A:2195:ASP:N	1:A:2198:GLU:OE1	2.38	0.56
1:A:2266:GLY:HA3	1:A:2275:TRP:CH2	2.41	0.56
1:A:3520:PHE:HB3	1:A:3524:MET:HB2	1.88	0.56
1:A:2091:ARG:HB2	2:A:4701:ADP:O3'	2.06	0.56
1:A:2388:ASP:OD1	1:A:2389:GLU:N	2.39	0.56
1:A:2744:LEU:HA	1:A:2747:ILE:HG22	1.88	0.56
1:A:2826:ALA:HA	1:A:2850:ILE:HD11	1.88	0.56
1:A:3133:LEU:HD11	1:A:3141:GLU:HB3	1.86	0.56
1:A:4534:TRP:CG	1:A:4594:LYS:HZ3	2.24	0.56
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.38	0.55
1:A:2620:LEU:N	1:A:2662:PHE:O	2.40	0.55
1:A:2864:GLU:OE2	1:A:2864:GLU:N	2.38	0.55
1:A:4010:SER:HB2	1:A:4015:GLU:HA	1.88	0.55
1:A:3088:ARG:NH2	2:A:4703:ADP:O3B	2.38	0.55
1:A:2688:GLU:HB2	1:A:2730:HIS:CE1	2.26	0.55
1:A:3570:ASP:OD1	1:A:3571:ASP:N	2.39	0.55
1:A:3874:GLY:HA3	1:A:4144:ILE:HG13	1.89	0.55
1:A:3907:HIS:CD2	1:A:3991:LEU:HD11	2.40	0.55
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	1.88	0.55
1:A:4577:LEU:HG	1:A:4635:PHE:CE2	2.41	0.55
1:A:2536:ASP:HA	1:A:2576:ARG:HH11	1.72	0.55
1:A:2464:GLN:HG2	1:A:2583:THR:HA	1.89	0.55
1:A:4485:ARG:O	1:A:4488:GLN:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2452:LEU:HD22	1:A:2729:ARG:HB2	1.88	0.55
1:A:4205:TYR:OH	1:A:4261:ASP:OD2	2.17	0.55
1:A:4483:SER:C	1:A:4487:LYS:HZ3	2.15	0.55
1:A:1628:ARG:HG3	1:A:1657:MET:HE3	1.89	0.55
1:A:2811:ARG:HB3	1:A:2812:PRO:HD3	1.88	0.55
1:A:4129:GLU:OE2	1:A:4131:ASN:ND2	2.40	0.55
1:A:1706:GLU:O	1:A:1710:ARG:HG3	2.07	0.54
1:A:2755:MET:CE	1:A:2807:PHE:HA	2.36	0.54
1:A:2964:HIS:NE2	1:A:2966:LYS:HB3	2.22	0.54
1:A:3161:LEU:HB3	1:A:3168:THR:HG22	1.89	0.54
1:A:3790:VAL:HG13	1:A:3794:VAL:HB	1.88	0.54
1:A:2288:ILE:HD12	1:A:2333:LEU:HD23	1.89	0.54
1:A:2992:PHE:HD2	1:A:3064:VAL:HG23	1.72	0.54
1:A:4318:PRO:HB2	1:A:4325:ASN:HA	1.89	0.54
1:A:4301:ARG:O	1:A:4304:GLU:HG2	2.07	0.54
1:A:2581:LEU:HD13	1:A:2591:LEU:HD21	1.90	0.54
1:A:2615:MET:HG3	1:A:2658:TRP:HB2	1.89	0.54
1:A:2797:ARG:HH21	1:A:3087:ASN:ND2	2.06	0.54
1:A:2876:TRP:CH2	1:A:2953:MET:HG2	2.43	0.54
1:A:2943:LYS:HA	1:A:3094:PHE:HE2	1.73	0.54
1:A:3639:GLU:HG2	1:A:3686:VAL:HG21	1.90	0.54
1:A:2202:MET:SD	1:A:2202:MET:N	2.80	0.54
1:A:2507:ARG:HG2	1:A:2510:MET:HE1	1.89	0.54
1:A:2038:SER:C	1:A:2039:LEU:HD22	2.33	0.54
1:A:2148:LYS:HE2	1:A:2361:MET:HB3	1.90	0.54
1:A:3723:ASP:OD1	1:A:3724:VAL:N	2.40	0.54
1:A:4107:MET:O	1:A:4111:LYS:HG2	2.07	0.54
1:A:2609:LEU:HG	1:A:2612:LEU:HD12	1.90	0.54
1:A:3872:ALA:HB1	1:A:3880:HIS:HD2	1.72	0.54
1:A:2509:LYS:O	1:A:2513:GLU:HG3	2.08	0.54
1:A:3606:ASP:OD1	1:A:3607:ARG:N	2.41	0.54
1:A:4036:LYS:HZ1	1:A:4038:ASN:HB2	1.73	0.54
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.89	0.53
1:A:1748:GLN:HE22	1:A:1872:TYR:HA	1.73	0.53
1:A:2628:PRO:HB3	1:A:2682:PHE:CD2	2.43	0.53
1:A:2726:ARG:NH2	3:A:4702:ATP:O3G	2.38	0.53
1:A:1879:LEU:HD22	2:A:4701:ADP:C6	2.43	0.53
1:A:1892:MET:N	1:A:1892:MET:HE2	2.22	0.53
1:A:3030:MET:HE1	1:A:3051:TYR:HD1	1.73	0.53
1:A:3974:TRP:NE1	1:A:3976:GLU:OE2	2.40	0.53
1:A:4095:MET:HG3	1:A:4097:LYS:NZ	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4605:VAL:N	1:A:4624:PHE:O	2.25	0.53
1:A:2594:CYS:HA	1:A:2712:CYS:O	2.09	0.53
1:A:2882:ILE:HD12	1:A:2883:PRO:HD2	1.90	0.53
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.90	0.53
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.91	0.53
1:A:1677:SER:OG	1:A:1678:SER:N	2.42	0.53
1:A:2948:ARG:HG3	1:A:2958:VAL:HG21	1.91	0.53
1:A:2347:ASP:OD1	1:A:2348:LEU:N	2.40	0.53
1:A:2568:VAL:HG21	1:A:2607:SER:HB2	1.91	0.53
1:A:4190:ILE:HG23	1:A:4201:TRP:CZ2	2.43	0.53
1:A:4446:ASN:OD1	1:A:4447:TYR:N	2.41	0.53
1:A:2275:TRP:HE1	1:A:2285:ARG:HH21	1.55	0.53
1:A:3193:GLU:O	1:A:3196:GLU:HG3	2.09	0.53
1:A:2453:ARG:HB2	1:A:2729:ARG:HA	1.90	0.53
1:A:2615:MET:HG3	1:A:2658:TRP:O	2.08	0.53
1:A:2640:GLU:HG2	1:A:2653:VAL:HG22	1.91	0.53
1:A:3950:LYS:HZ2	1:A:3973:LEU:HG	1.74	0.53
1:A:4405:ILE:O	1:A:4411:ARG:NH1	2.39	0.53
1:A:4461:PRO:HG2	1:A:4464:TRP:CE3	2.44	0.53
1:A:4489:LEU:HA	1:A:4492:ILE:HG12	1.91	0.53
1:A:1905:PHE:HE1	1:A:2038:SER:HB3	1.74	0.52
1:A:2234:TRP:CE2	1:A:2302:VAL:HG21	2.44	0.52
1:A:3949:ALA:O	1:A:3952:GLN:NE2	2.42	0.52
1:A:4071:ILE:HG21	1:A:4099:VAL:HA	1.91	0.52
1:A:2300:TRP:CG	1:A:2342:MET:HE1	2.44	0.52
1:A:3986:ALA:O	1:A:3990:LEU:HD23	2.09	0.52
1:A:1961:ASN:HD21	1:A:2019:ASN:HB3	1.75	0.52
1:A:2584:TRP:HE3	1:A:2591:LEU:HD22	1.73	0.52
1:A:3147:CYS:O	1:A:3150:VAL:HG12	2.09	0.52
1:A:4475:VAL:O	1:A:4479:VAL:HG23	2.09	0.52
1:A:2768:PRO:HB2	1:A:2858:PHE:HE1	1.74	0.52
1:A:2819:GLU:HA	1:A:2861:ILE:HD11	1.90	0.52
1:A:3751:GLN:O	1:A:3755:GLU:HG2	2.09	0.52
1:A:4098:ASN:HB2	1:A:4100:HIS:CE1	2.44	0.52
1:A:1766:LEU:HD22	1:A:1778:LEU:HD11	1.90	0.52
1:A:2969:GLY:HA2	1:A:3004:PHE:HE2	1.75	0.52
1:A:1816:VAL:HA	1:A:1819:ARG:NH1	2.25	0.52
1:A:2747:ILE:HG23	1:A:2748:TYR:CD2	2.45	0.52
1:A:2422:ILE:HG23	1:A:2487:GLU:HG2	1.92	0.52
1:A:1884:LEU:HD21	1:A:2041:MET:SD	2.50	0.52
1:A:2511:ARG:HD3	1:A:2535:ILE:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3585:ARG:NH1	1:A:3694:SER:O	2.42	0.52
1:A:4156:ASN:ND2	1:A:4188:ALA:HA	2.25	0.52
1:A:4402:VAL:HA	1:A:4405:ILE:HD12	1.91	0.52
1:A:2837:LEU:O	1:A:2843:ARG:NH2	2.43	0.52
1:A:2486:LEU:O	1:A:2490:ILE:HG12	2.10	0.52
1:A:1672:VAL:HA	1:A:1691:SER:HA	1.91	0.51
1:A:1698:ILE:HD12	1:A:1701:TRP:NE1	2.24	0.51
1:A:1713:LEU:HD22	1:A:1749:LEU:HD21	1.92	0.51
1:A:2437:LEU:HD22	1:A:2455:LEU:HD21	1.90	0.51
1:A:2492:ARG:HH22	1:A:2525:PRO:HB2	1.75	0.51
1:A:2684:ARG:HD2	1:A:2726:ARG:HB3	1.92	0.51
1:A:3544:ARG:NH1	1:A:3546:ASP:OD1	2.43	0.51
1:A:2835:ASP:OD1	1:A:2921:ARG:NH1	2.44	0.51
1:A:2874:SER:HB3	1:A:2884:VAL:HG21	1.92	0.51
1:A:2900:PHE:O	1:A:2904:GLU:N	2.43	0.51
1:A:3990:LEU:HD22	1:A:4004:MET:HG3	1.92	0.51
1:A:4452:ILE:O	1:A:4456:VAL:HG23	2.10	0.51
1:A:3649:LEU:HD12	1:A:3695:ARG:HH21	1.75	0.51
1:A:4251:ILE:HG22	1:A:4252:TYR:CD2	2.45	0.51
1:A:4489:LEU:HD11	1:A:4515:PHE:HE1	1.75	0.51
1:A:1666:LEU:HG	1:A:1673:VAL:HA	1.92	0.51
1:A:2472:TYR:HD2	1:A:2481:MET:HE3	1.75	0.51
1:A:2481:MET:SD	1:A:2481:MET:N	2.83	0.51
1:A:3115:LEU:HD13	1:A:3143:ILE:HD13	1.92	0.51
1:A:4088:VAL:HG23	1:A:4118:PRO:HA	1.93	0.51
1:A:4098:ASN:HB2	1:A:4100:HIS:HE1	1.75	0.51
1:A:1905:PHE:CE1	1:A:2038:SER:HB3	2.46	0.51
1:A:2222:MET:HE1	1:A:2342:MET:HB3	1.92	0.51
1:A:2311:TRP:H	1:A:2311:TRP:CD1	2.28	0.51
1:A:4002:LEU:O	1:A:4006:HIS:ND1	2.43	0.51
1:A:4066:ILE:HD11	1:A:4095:MET:HB2	1.93	0.51
1:A:4240:TRP:CD1	1:A:4275:THR:HG1	2.29	0.51
1:A:1736:ASN:O	1:A:1740:THR:HG23	2.11	0.51
1:A:2595:GLY:HA2	1:A:2735:TYR:CE1	2.46	0.51
1:A:2614:ASP:C	1:A:2657:LYS:HD2	2.36	0.51
1:A:3888:ALA:HA	1:A:4013:LEU:HD21	1.93	0.51
1:A:4186:PHE:O	1:A:4189:ILE:HG22	2.10	0.51
1:A:1633:GLY:O	1:A:1637:LEU:N	2.41	0.51
1:A:3700:ASN:HD22	1:A:3702:THR:HG22	1.75	0.51
1:A:3716:VAL:HB	1:A:3836:TYR:OH	2.10	0.51
1:A:2423:MET:HG3	1:A:2427:PHE:HE2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2093:LEU:O	1:A:2097:LEU:HG	2.10	0.51
1:A:1662:SER:HB2	1:A:1679:ARG:HD3	1.92	0.51
1:A:1632:VAL:O	1:A:1943:ARG:NH1	2.44	0.50
1:A:2787:ASP:OD1	1:A:2788:THR:N	2.44	0.50
1:A:2935:LEU:HD13	1:A:2943:LYS:HB3	1.93	0.50
1:A:3603:GLU:HG2	1:A:3604:TYR:CD1	2.46	0.50
1:A:2785:THR:OG1	1:A:2787:ASP:OD1	2.24	0.50
1:A:2935:LEU:HB2	1:A:3067:THR:HG22	1.92	0.50
1:A:3607:ARG:HG3	1:A:3632:PRO:HG3	1.93	0.50
1:A:4154:LYS:HB2	1:A:4312:LEU:HD23	1.92	0.50
1:A:2277:ASP:HB3	1:A:2285:ARG:HH22	1.76	0.50
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.47	0.50
1:A:2670:ASP:HA	1:A:2721:LYS:HE3	1.92	0.50
1:A:3045:ASP:OD1	1:A:3046:SER:N	2.42	0.50
1:A:3495:THR:HG23	1:A:3496:PHE:HD1	1.76	0.50
1:A:3576:ASN:ND2	1:A:3700:ASN:O	2.45	0.50
1:A:3017:VAL:HB	1:A:3020:LEU:HG	1.93	0.50
1:A:3544:ARG:NH2	1:A:3546:ASP:OD2	2.44	0.50
1:A:3818:LEU:HD22	1:A:4346:MET:SD	2.51	0.50
1:A:4075:GLU:O	1:A:4079:GLN:HG2	2.12	0.50
1:A:1778:LEU:HB3	1:A:1826:ILE:HD11	1.94	0.50
1:A:3810:SER:HB3	1:A:3890:ILE:HD12	1.94	0.50
1:A:4109:LEU:HD12	1:A:4112:LYS:HD3	1.93	0.50
1:A:4321:LEU:HD23	1:A:4321:LEU:H	1.77	0.50
1:A:2600:GLY:O	1:A:2604:THR:OG1	2.21	0.50
1:A:3742:LEU:HD12	1:A:3776:GLU:HB3	1.94	0.50
1:A:3950:LYS:HE3	1:A:3973:LEU:HA	1.94	0.50
1:A:4095:MET:HG3	1:A:4097:LYS:HZ1	1.77	0.50
1:A:3207:LYS:HZ3	1:A:3754:ASN:HB3	1.77	0.49
1:A:3586:TYR:O	1:A:3696:VAL:HG13	2.11	0.49
1:A:2210:LEU:O	1:A:2214:THR:HG23	2.11	0.49
1:A:2461:MET:HG3	1:A:2584:TRP:HE1	1.77	0.49
1:A:2909:LEU:HA	2:A:4704:ADP:C2	2.47	0.49
1:A:3021:PHE:CE2	1:A:3029:LEU:HB2	2.48	0.49
1:A:3213:ASP:O	1:A:3216:GLU:HG2	2.12	0.49
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.94	0.49
1:A:1880:VAL:HG21	1:A:2049:ILE:HG12	1.95	0.49
1:A:2964:HIS:HA	1:A:3643:PRO:HB2	1.94	0.49
1:A:3733:LYS:C	1:A:3736:GLY:H	2.21	0.49
1:A:4042:LEU:HD23	1:A:4126:LEU:HB2	1.94	0.49
1:A:4277:SER:HA	1:A:4282:PHE:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4423:LEU:HD13	1:A:4466:HIS:CD2	2.45	0.49
1:A:2609:LEU:HB3	1:A:2617:VAL:HG22	1.95	0.49
1:A:2912:PHE:CZ	1:A:2915:VAL:HG23	2.48	0.49
1:A:2757:ARG:HA	1:A:2763:ARG:HH11	1.76	0.49
1:A:4306:VAL:O	1:A:4309:VAL:HG12	2.12	0.49
1:A:4430:ASP:O	1:A:4434:VAL:HG23	2.12	0.49
1:A:2075:LEU:HD22	1:A:4526:GLN:OE1	2.13	0.49
1:A:2667:ASN:HB3	1:A:2723:LEU:HD21	1.95	0.49
1:A:2890:ARG:NH1	1:A:2911:LEU:O	2.43	0.49
1:A:2946:LEU:O	1:A:2950:VAL:HG23	2.12	0.49
1:A:4110:GLU:HG3	1:A:4137:ASN:OD1	2.12	0.49
1:A:1886:ASP:OD1	1:A:1886:ASP:N	2.44	0.49
1:A:1896:LEU:HD21	1:A:2013:ALA:HB2	1.94	0.49
1:A:2280:PHE:CE1	1:A:2301:ILE:HG21	2.48	0.49
1:A:2897:LEU:CD1	1:A:2911:LEU:HD21	2.42	0.49
1:A:4398:LEU:HD12	1:A:4414:GLU:HA	1.94	0.49
1:A:1665:ILE:O	1:A:1674:LEU:N	2.39	0.49
1:A:2935:LEU:HD23	1:A:3092:ASN:OD1	2.13	0.49
1:A:2912:PHE:CE2	1:A:2914:GLU:HB2	2.48	0.49
1:A:3893:LYS:NZ	1:A:3900:THR:HA	2.27	0.49
1:A:4052:SER:O	1:A:4055:VAL:HG12	2.13	0.49
1:A:4300:ILE:N	1:A:4304:GLU:OE2	2.33	0.49
1:A:2813:LEU:CD2	1:A:2816:LEU:HG	2.41	0.49
1:A:3660:VAL:HG13	1:A:3671:LEU:HB3	1.94	0.48
1:A:3870:ARG:NH2	1:A:4034:GLU:HB2	2.27	0.48
1:A:1644:SER:OG	1:A:1645:LYS:NZ	2.41	0.48
1:A:2685:GLN:HE21	1:A:2692:PHE:HA	1.78	0.48
1:A:2773:MET:HG3	1:A:2802:TRP:CZ3	2.48	0.48
1:A:2886:GLN:OE1	1:A:2886:GLN:N	2.36	0.48
1:A:1900:LEU:HB2	1:A:2035:LEU:O	2.13	0.48
1:A:2228:SER:O	1:A:2369:LEU:HB2	2.14	0.48
1:A:2571:THR:H	1:A:2574:THR:CG2	2.25	0.48
1:A:3149:PHE:O	1:A:3153:THR:HG23	2.14	0.48
1:A:3187:PHE:CE1	1:A:3191:ARG:HG3	2.49	0.48
1:A:3598:GLU:OE2	1:A:3598:GLU:N	2.28	0.48
1:A:3784:VAL:O	1:A:3787:THR:OG1	2.26	0.48
1:A:4099:VAL:HG22	1:A:4128:MET:HB3	1.96	0.48
1:A:2723:LEU:HB2	1:A:2728:LEU:HD11	1.95	0.48
1:A:3744:GLN:O	1:A:3747:LYS:HG3	2.12	0.48
1:A:3817:SER:O	1:A:3820:GLN:HG2	2.12	0.48
1:A:3839:VAL:HG12	1:A:3840:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1766:LEU:HD21	1:A:1778:LEU:HD21	1.95	0.48
1:A:1825:LEU:HD11	1:A:1838:TRP:CE3	2.49	0.48
1:A:1979:GLN:HB3	1:A:2035:LEU:HD13	1.96	0.48
1:A:3730:ASP:O	1:A:3734:LEU:N	2.43	0.48
1:A:3730:ASP:O	1:A:3734:LEU:HG	2.14	0.48
1:A:4260:PHE:HE2	1:A:4618:LEU:HD11	1.79	0.48
1:A:4482:PHE:O	1:A:4486:ILE:HG12	2.14	0.48
1:A:2548:TRP:CE2	1:A:2576:ARG:HG2	2.49	0.48
1:A:2558:GLU:CD	1:A:2560:HIS:H	2.22	0.48
1:A:2622:PHE:HD2	1:A:2666:ILE:HA	1.79	0.48
1:A:3596:ALA:HB2	1:A:3701:PHE:CD1	2.49	0.48
1:A:1633:GLY:HA2	1:A:1943:ARG:NH2	2.28	0.48
1:A:2912:PHE:HE2	1:A:2914:GLU:HB2	1.78	0.48
1:A:2934:LEU:HD12	1:A:3066:PHE:O	2.13	0.48
1:A:3544:ARG:HH11	1:A:3547:ILE:HB	1.77	0.48
1:A:4318:PRO:HB3	1:A:4327:ALA:HB3	1.96	0.48
1:A:3046:SER:N	1:A:3049:GLU:OE2	2.47	0.48
1:A:3133:LEU:HD12	1:A:3134:PRO:HD2	1.96	0.48
1:A:3909:LEU:HD21	1:A:4343:MET:HB3	1.94	0.48
1:A:4097:LYS:HA	1:A:4127:THR:CG2	2.44	0.48
1:A:1914:GLU:OE2	2:A:4701:ADP:H3'	2.14	0.47
1:A:2352:THR:O	1:A:2356:VAL:HG23	2.13	0.47
1:A:2373:MET:HE1	3:A:4702:ATP:C4	2.50	0.47
1:A:2936:ILE:HD11	1:A:3091:LEU:HD21	1.95	0.47
1:A:2726:ARG:HH21	3:A:4702:ATP:PG	2.37	0.47
1:A:3635:VAL:HB	1:A:3679:LEU:HD23	1.97	0.47
1:A:2461:MET:CG	1:A:2584:TRP:HE1	2.28	0.47
1:A:1937:ASP:OD2	1:A:1940:ALA:HB3	2.14	0.47
1:A:2050:ALA:O	1:A:2054:LEU:HB2	2.15	0.47
1:A:3021:PHE:CD2	1:A:3025:GLU:HG3	2.50	0.47
1:A:4232:ASN:OD1	1:A:4233:ILE:N	2.47	0.47
1:A:1698:ILE:HD12	1:A:1701:TRP:HE1	1.79	0.47
1:A:1975:VAL:HA	1:A:1978:ILE:HG22	1.96	0.47
1:A:3012:LEU:HD11	1:A:3064:VAL:HG11	1.96	0.47
1:A:3214:GLN:O	1:A:3218:LEU:HG	2.14	0.47
1:A:3624:GLU:O	1:A:3628:ARG:HG2	2.15	0.47
1:A:3819:LYS:HE3	1:A:3826:GLN:OE1	2.15	0.47
1:A:1850:GLN:HE21	1:A:1855:GLN:HE21	1.62	0.47
1:A:2412:MET:O	1:A:2415:ILE:HG22	2.15	0.47
1:A:3491:LYS:HA	1:A:3494:GLU:OE1	2.15	0.47
1:A:4181:PHE:HE2	1:A:4296:MET:HE1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2038:SER:O	1:A:2039:LEU:HD22	2.15	0.47
1:A:2511:ARG:NH2	1:A:2735:TYR:HB3	2.26	0.47
1:A:2910:VAL:HG22	2:A:4704:ADP:N1	2.29	0.47
1:A:3833:LEU:O	1:A:3837:HIS:ND1	2.38	0.47
1:A:4179:LEU:HD23	1:A:4179:LEU:HA	1.76	0.47
1:A:4556:CYS:O	1:A:4591:ARG:HA	2.13	0.47
1:A:1665:ILE:N	1:A:1675:GLY:O	2.34	0.47
1:A:1809:GLU:OE2	1:A:2057:GLN:NE2	2.46	0.47
1:A:2369:LEU:HD21	1:A:2374:ILE:CG1	2.44	0.47
1:A:2968:THR:HG23	1:A:2970:GLU:HG3	1.96	0.47
1:A:3517:ALA:HA	1:A:3520:PHE:HD2	1.80	0.47
1:A:3544:ARG:O	1:A:3547:ILE:HG22	2.15	0.47
1:A:3950:LYS:HA	1:A:3953:ALA:HB3	1.96	0.47
1:A:4303:GLU:O	1:A:4306:VAL:HB	2.15	0.47
1:A:1940:ALA:O	1:A:1944:ILE:HG12	2.15	0.47
1:A:2185:VAL:HG13	1:A:2239:LYS:HD2	1.96	0.47
1:A:3576:ASN:HB3	1:A:3701:PHE:CE2	2.49	0.47
1:A:3796:THR:O	1:A:3799:GLN:HG3	2.15	0.47
1:A:3907:HIS:CE1	1:A:3937:ARG:HG3	2.46	0.47
1:A:1683:GLU:HG3	1:A:1685:MET:HE3	1.96	0.47
1:A:2230:LYS:HZ2	1:A:2345:VAL:C	2.23	0.47
1:A:2412:MET:HA	1:A:2415:ILE:HG22	1.97	0.47
1:A:2781:GLN:OE1	1:A:2794:TYR:HB2	2.14	0.47
1:A:2138:ILE:HD12	1:A:2168:VAL:HG22	1.96	0.46
1:A:3886:LEU:HD22	1:A:4343:MET:HE2	1.97	0.46
1:A:4525:ARG:HD3	1:A:4592:TRP:CH2	2.49	0.46
1:A:1949:CYS:HA	1:A:2012:MET:CE	2.42	0.46
1:A:1964:GLU:OE2	1:A:1964:GLU:N	2.33	0.46
1:A:2934:LEU:N	1:A:3090:VAL:O	2.41	0.46
1:A:3591:ASP:OD1	1:A:3591:ASP:N	2.48	0.46
1:A:3733:LYS:HA	1:A:3736:GLY:HA3	1.98	0.46
1:A:4318:PRO:HG3	1:A:4328:GLU:HG2	1.97	0.46
1:A:4485:ARG:O	1:A:4489:LEU:HG	2.16	0.46
1:A:1626:PHE:CZ	1:A:1628:ARG:HB3	2.51	0.46
1:A:1891:THR:CG2	1:A:2039:LEU:HD21	2.45	0.46
1:A:3935:VAL:HG22	1:A:3996:PHE:HE1	1.80	0.46
1:A:3945:LYS:HE3	1:A:3945:LYS:HB3	1.82	0.46
1:A:3993:ILE:HG21	1:A:4004:MET:HG2	1.98	0.46
1:A:2981:ARG:NH2	1:A:3025:GLU:OE2	2.48	0.46
1:A:3620:ARG:NH1	1:A:3644:VAL:HG11	2.30	0.46
1:A:4086:THR:O	1:A:4090:SER:OG	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4554:ASP:N	1:A:4557:SER:OG	2.48	0.46
1:A:3121:ILE:O	1:A:3540:ASN:ND2	2.46	0.46
1:A:3653:VAL:HG12	1:A:3662:ILE:HD11	1.98	0.46
1:A:2223:VAL:O	1:A:2363:TRP:HA	2.15	0.46
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.49	0.46
1:A:2869:ARG:O	1:A:2871:ILE:HD12	2.15	0.46
1:A:4411:ARG:O	1:A:4414:GLU:HG3	2.16	0.46
1:A:3034:LYS:HE3	1:A:3038:GLN:NE2	2.31	0.46
1:A:3167:ARG:CZ	1:A:3685:THR:HA	2.46	0.46
1:A:4260:PHE:CE2	1:A:4608:PRO:HB3	2.51	0.46
1:A:2943:LYS:HG2	1:A:3094:PHE:HD2	1.78	0.46
1:A:3204:GLY:O	1:A:3207:LYS:HG2	2.15	0.46
1:A:3653:VAL:HA	1:A:3662:ILE:HG12	1.98	0.46
1:A:2085:HIS:HB3	1:A:2348:LEU:HD12	1.98	0.46
1:A:2142:CYS:O	1:A:2146:VAL:HB	2.15	0.46
1:A:2596:PRO:HB2	1:A:2738:TYR:CZ	2.50	0.46
1:A:2747:ILE:HD11	2:A:4703:ADP:C5	2.51	0.46
1:A:2827:HIS:NE2	1:A:2881:TYR:OH	2.46	0.46
1:A:2873:TYR:CE2	1:A:2883:PRO:HD3	2.51	0.46
1:A:3017:VAL:HG12	1:A:3019:GLY:H	1.80	0.46
1:A:3113:MET:HG2	1:A:3115:LEU:HG	1.98	0.46
1:A:3807:ALA:O	1:A:3811:ILE:HD12	2.16	0.46
1:A:4190:ILE:HD12	1:A:4201:TRP:CZ2	2.51	0.46
1:A:2075:LEU:HD11	1:A:4536:LEU:HD12	1.98	0.46
1:A:2623:SER:HA	1:A:2668:LEU:HD23	1.97	0.46
1:A:3790:VAL:HG22	1:A:3794:VAL:HG21	1.97	0.46
1:A:4260:PHE:CD2	1:A:4608:PRO:HB3	2.50	0.46
1:A:4606:THR:OG1	1:A:4623:ASP:OD2	2.27	0.46
1:A:1912:LYS:HG2	1:A:2041:MET:HG3	1.98	0.45
1:A:2873:TYR:HB3	1:A:2881:TYR:CZ	2.51	0.45
1:A:3797:VAL:O	1:A:3800:GLN:HG2	2.16	0.45
1:A:1816:VAL:HG22	1:A:1819:ARG:HH12	1.82	0.45
1:A:2577:HIS:CE1	1:A:2736:VAL:HG22	2.51	0.45
1:A:2680:ILE:HD12	1:A:2680:ILE:HA	1.80	0.45
1:A:3175:HIS:CE1	1:A:3585:ARG:HH12	2.33	0.45
1:A:2382:LEU:HD12	1:A:2463:HIS:CE1	2.51	0.45
1:A:2969:GLY:HA2	1:A:3004:PHE:CE2	2.51	0.45
1:A:3627:LEU:HD13	1:A:3669:ILE:HG21	1.99	0.45
1:A:4543:VAL:HG21	1:A:4622:VAL:HB	1.97	0.45
1:A:1838:TRP:CZ2	1:A:1843:ARG:HG2	2.51	0.45
1:A:2230:LYS:HE2	1:A:2344:GLU:CG	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2446:ILE:N	1:A:2505:ASP:OD2	2.50	0.45
1:A:2449:LEU:HD12	1:A:2453:ARG:NH2	2.32	0.45
1:A:2654:GLN:N	1:A:2654:GLN:OE1	2.50	0.45
1:A:4036:LYS:HD2	1:A:4037:PRO:HD2	1.98	0.45
1:A:4050:ASP:N	1:A:4050:ASP:OD1	2.49	0.45
1:A:4196:TYR:O	1:A:4200:GLY:N	2.36	0.45
1:A:3168:THR:O	1:A:3169:MET:HE2	2.16	0.45
1:A:4221:THR:HG23	1:A:4222:TRP:CD1	2.46	0.45
1:A:2960:GLN:HB3	1:A:2993:ILE:HG13	1.98	0.45
1:A:3586:TYR:HA	1:A:3587:PRO:HD3	1.82	0.45
1:A:4009:VAL:HG13	1:A:4018:MET:HE1	1.97	0.45
1:A:4454:GLU:HG3	1:A:4459:ILE:HG23	1.99	0.45
1:A:1738:TYR:HE1	1:A:1741:TRP:HZ3	1.64	0.45
1:A:2370:SER:HB3	1:A:2373:MET:HB2	1.99	0.45
1:A:2496:TYR:CE1	1:A:2500:TRP:HD1	2.34	0.45
1:A:3191:ARG:CZ	1:A:3500:MET:HE1	2.47	0.45
1:A:4532:ASN:HB3	1:A:4534:TRP:HZ3	1.79	0.45
1:A:1877:ASP:OD2	1:A:1878:LYS:N	2.50	0.45
1:A:2149:LEU:HD11	1:A:2157:LEU:HD22	1.99	0.45
1:A:2255:ASP:HA	1:A:2304:ASP:O	2.16	0.45
1:A:2275:TRP:CZ2	1:A:2277:ASP:HA	2.52	0.45
1:A:4303:GLU:O	1:A:4307:GLN:OE1	2.34	0.45
1:A:4312:LEU:HD12	1:A:4313:PRO:CD	2.46	0.45
1:A:2152:GLU:O	1:A:2155:PRO:HD2	2.16	0.45
1:A:2219:GLY:HA2	1:A:2341:ILE:O	2.17	0.45
1:A:2219:GLY:HA3	1:A:2319:LEU:HD22	1.99	0.45
1:A:3021:PHE:CE2	1:A:3025:GLU:HG3	2.52	0.45
1:A:3951:VAL:HG23	1:A:3957:PHE:CD2	2.52	0.45
1:A:4182:LEU:HD11	1:A:4272:LEU:HB3	1.99	0.45
1:A:4414:GLU:O	1:A:4418:LYS:HG2	2.17	0.45
1:A:4578:SER:O	1:A:4638:ARG:NH2	2.50	0.45
1:A:1821:VAL:HG21	1:A:1841:GLN:HG3	1.99	0.45
1:A:1886:ASP:HA	1:A:1889:TYR:HB2	1.98	0.45
1:A:2138:ILE:HD11	1:A:2168:VAL:HG13	1.99	0.45
1:A:2538:GLU:HB3	1:A:2548:TRP:NE1	2.32	0.45
1:A:3819:LYS:HA	1:A:3825:TYR:O	2.16	0.45
1:A:4110:GLU:HA	1:A:4113:LEU:HG	1.99	0.45
1:A:1659:ALA:HB1	1:A:1873:LEU:HD13	1.99	0.44
1:A:2105:ARG:HA	1:A:2108:ILE:HG12	1.98	0.44
1:A:2237:LEU:HG	1:A:2300:TRP:HH2	1.82	0.44
1:A:2609:LEU:HA	1:A:2612:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2691:GLY:HA2	1:A:2703:LEU:HD23	1.98	0.44
1:A:2777:TYR:HB2	1:A:2799:MET:HE1	1.99	0.44
1:A:3950:LYS:HZ1	1:A:3973:LEU:HG	1.82	0.44
1:A:2223:VAL:HG22	1:A:2348:LEU:HD21	1.99	0.44
1:A:2435:LYS:O	1:A:2438:GLU:HG3	2.16	0.44
1:A:2608:ALA:O	1:A:2612:LEU:HG	2.17	0.44
1:A:3006:GLU:OE1	1:A:3009:ASN:ND2	2.49	0.44
1:A:3789:ILE:O	1:A:3793:GLU:HG3	2.17	0.44
1:A:3825:TYR:CE1	1:A:3875:MET:HA	2.52	0.44
1:A:3870:ARG:HH22	1:A:4034:GLU:HB2	1.82	0.44
1:A:1852:ASP:HB3	1:A:1855:GLN:NE2	2.32	0.44
1:A:2553:PRO:HD2	1:A:2570:PRO:HB2	1.99	0.44
1:A:3882:THR:HG22	1:A:4339:MET:SD	2.57	0.44
1:A:2238:LEU:HB2	1:A:2300:TRP:CZ3	2.52	0.44
1:A:2427:PHE:CE1	1:A:2433:VAL:HG21	2.53	0.44
1:A:2464:GLN:CB	1:A:2583:THR:HG23	2.48	0.44
1:A:2677:GLN:HB2	1:A:2680:ILE:HG22	1.99	0.44
1:A:3999:ASP:OD1	1:A:4000:ARG:N	2.50	0.44
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.81	0.44
1:A:4604:VAL:HA	1:A:4625:GLU:HA	1.98	0.44
1:A:1938:PHE:CB	1:A:1967:MET:HE1	2.48	0.44
1:A:2427:PHE:CD1	1:A:2433:VAL:HG21	2.52	0.44
1:A:2666:ILE:O	1:A:2669:PRO:HD2	2.17	0.44
1:A:2729:ARG:HG3	1:A:2730:HIS:CD2	2.48	0.44
1:A:2755:MET:SD	1:A:2807:PHE:HD1	2.40	0.44
1:A:2852:THR:C	1:A:2856:LYS:HZ2	2.25	0.44
1:A:3783:LYS:HA	1:A:3783:LYS:HD3	1.66	0.44
1:A:4293:ASP:OD1	1:A:4293:ASP:N	2.50	0.44
1:A:4565:LEU:HD13	1:A:4585:LEU:HD21	1.98	0.44
1:A:2563:ALA:HA	1:A:2751:PHE:CE2	2.53	0.44
1:A:2688:GLU:HG3	1:A:2689:HIS:ND1	2.32	0.44
1:A:3154:LEU:HB3	1:A:3171:ILE:CD1	2.46	0.44
1:A:3214:GLN:O	1:A:3217:GLU:HG3	2.17	0.44
1:A:3544:ARG:NH1	1:A:3547:ILE:HB	2.33	0.44
1:A:1928:LEU:HD23	1:A:1948:LEU:HD21	2.00	0.44
1:A:2103:VAL:O	1:A:2106:GLU:HG3	2.17	0.44
1:A:2460:SER:HB2	1:A:2589:LYS:NZ	2.33	0.44
1:A:2857:HIS:C	1:A:2858:PHE:HD1	2.25	0.44
1:A:3512:ALA:O	1:A:3516:TYR:HB2	2.17	0.44
1:A:3846:LEU:HD22	1:A:3855:ARG:NH1	2.32	0.44
1:A:1713:LEU:CD2	1:A:1749:LEU:HD21	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2624:SER:HB2	1:A:2670:ASP:OD2	2.18	0.44
1:A:3653:VAL:O	1:A:3654:ARG:NE	2.49	0.44
1:A:3704:THR:HG23	1:A:3707:SER:H	1.82	0.44
1:A:4577:LEU:HD22	1:A:4638:ARG:NE	2.33	0.44
1:A:2304:ASP:OD1	1:A:2726:ARG:NH2	2.50	0.44
1:A:2316:ASN:O	1:A:2358:ARG:NH1	2.50	0.44
1:A:2980:LEU:HD21	1:A:3011:LEU:HD11	1.99	0.44
1:A:3628:ARG:HH12	1:A:3669:ILE:HG23	1.83	0.44
1:A:4173:PRO:HG2	1:A:4176:ARG:HE	1.83	0.44
1:A:4297:PRO:HG3	1:A:4308:TRP:CG	2.53	0.44
1:A:2231:SER:HB2	3:A:4702:ATP:O2A	2.18	0.43
1:A:2296:GLN:OE1	1:A:2296:GLN:N	2.47	0.43
1:A:2726:ARG:O	1:A:2729:ARG:HG2	2.16	0.43
1:A:2838:VAL:HA	1:A:3093:TRP:CD2	2.53	0.43
1:A:4346:MET:HA	1:A:4346:MET:HE2	2.00	0.43
1:A:1633:GLY:HA2	1:A:1943:ARG:CZ	2.48	0.43
1:A:1872:TYR:CZ	1:A:1874:GLY:HA2	2.53	0.43
1:A:1888:CYS:O	1:A:1892:MET:HG2	2.17	0.43
1:A:2203:TRP:HH2	1:A:2236:VAL:HG11	1.79	0.43
1:A:2309:PRO:HD3	1:A:2350:TYR:O	2.18	0.43
1:A:2453:ARG:NH1	1:A:2733:VAL:HG12	2.33	0.43
1:A:4541:LEU:HB3	1:A:4592:TRP:CZ3	2.52	0.43
1:A:2104:LYS:HB2	1:A:2136:ILE:HD13	1.99	0.43
1:A:2494:LEU:O	1:A:2498:ILE:HG13	2.18	0.43
1:A:4507:ILE:HG23	1:A:4509:VAL:HG13	2.00	0.43
1:A:2831:ARG:HH21	1:A:2921:ARG:HH21	1.65	0.43
1:A:3098:SER:OG	1:A:3099:THR:N	2.52	0.43
1:A:4324:PRO:HD3	1:A:4638:ARG:HG2	2.01	0.43
1:A:1667:ASN:OD1	1:A:1667:ASN:N	2.50	0.43
1:A:1716:LEU:HG	1:A:1745:TYR:HD1	1.82	0.43
1:A:1745:TYR:O	1:A:1807:LYS:HE2	2.18	0.43
1:A:1945:PHE:HZ	1:A:1978:ILE:HG21	1.83	0.43
1:A:2377:ASN:C	1:A:2377:ASN:HD22	2.26	0.43
1:A:3851:ASP:O	1:A:3855:ARG:HG3	2.19	0.43
1:A:3914:ILE:HB	1:A:3937:ARG:HD2	2.00	0.43
1:A:3947:LEU:HD11	1:A:3973:LEU:HD23	2.00	0.43
1:A:3960:TRP:HZ3	1:A:3996:PHE:HD2	1.66	0.43
1:A:4036:LYS:HZ2	1:A:4038:ASN:H	1.65	0.43
1:A:4055:VAL:HG11	1:A:4095:MET:HE2	2.00	0.43
1:A:4110:GLU:HB3	1:A:4111:LYS:NZ	2.34	0.43
1:A:3057:GLN:NE2	1:A:3060:ARG:HH21	2.11	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3638:VAL:HG12	1:A:3681:THR:HB	2.00	0.43
1:A:1701:TRP:O	1:A:1705:VAL:HG23	2.18	0.43
1:A:1850:GLN:HE21	1:A:1855:GLN:NE2	2.17	0.43
1:A:2135:GLU:HG2	1:A:2168:VAL:HG23	2.00	0.43
1:A:2603:MET:HA	1:A:2606:PHE:HB2	2.01	0.43
1:A:2957:SER:O	1:A:2991:ALA:N	2.48	0.43
1:A:3614:PHE:CE2	1:A:3641:TYR:HA	2.54	0.43
1:A:4097:LYS:HA	1:A:4127:THR:HG22	2.01	0.43
1:A:4194:LEU:HD22	1:A:4201:TRP:NE1	2.33	0.43
1:A:4287:LYS:HE3	1:A:4287:LYS:HB2	1.66	0.43
1:A:4577:LEU:HD23	1:A:4577:LEU:HA	1.87	0.43
1:A:1826:ILE:O	1:A:1829:LYS:HD2	2.19	0.43
1:A:2135:GLU:HG2	1:A:2168:VAL:CG2	2.49	0.43
1:A:4413:PHE:HD2	1:A:4504:LEU:HD21	1.83	0.43
1:A:2071:PRO:O	1:A:2075:LEU:HG	2.18	0.43
1:A:2460:SER:HB2	1:A:2589:LYS:HZ2	1.84	0.43
1:A:2512:ALA:O	1:A:2516:GLU:HG3	2.18	0.43
1:A:3730:ASP:C	1:A:3733:LYS:H	2.27	0.43
1:A:3756:VAL:O	1:A:3759:ARG:HG2	2.18	0.43
1:A:1816:VAL:HA	1:A:1819:ARG:HH12	1.84	0.43
1:A:2650:LEU:HD22	1:A:2692:PHE:HE2	1.84	0.43
1:A:2685:GLN:NE2	1:A:2692:PHE:HA	2.34	0.43
1:A:4485:ARG:HA	1:A:4488:GLN:OE1	2.18	0.43
1:A:2373:MET:SD	3:A:4702:ATP:C2	3.11	0.42
1:A:2778:THR:O	1:A:2782:GLU:OE1	2.36	0.42
1:A:3100:GLU:HA	1:A:3130:TYR:CE1	2.51	0.42
1:A:2679:VAL:O	1:A:2683:ILE:HD12	2.18	0.42
1:A:3973:LEU:HD13	1:A:3992:LEU:HD13	2.01	0.42
1:A:4189:ILE:HG13	1:A:4321:LEU:HB2	2.00	0.42
1:A:2823:ARG:HG3	1:A:2873:TYR:HE1	1.84	0.42
1:A:2856:LYS:HG3	1:A:2857:HIS:ND1	2.34	0.42
1:A:3506:ASP:OD1	1:A:3543:PHE:HB2	2.19	0.42
1:A:3554:SER:OG	1:A:3559:ARG:NH1	2.48	0.42
1:A:3636:GLN:HA	1:A:3680:SER:OG	2.19	0.42
1:A:3957:PHE:CZ	1:A:3961:LEU:HD13	2.54	0.42
1:A:3966:PRO:HG3	1:A:3997:ARG:NH1	2.34	0.42
1:A:1861:MET:HE2	1:A:1890:LEU:HB2	2.01	0.42
1:A:2768:PRO:HB2	1:A:2858:PHE:CE1	2.54	0.42
1:A:3487:GLU:O	1:A:3491:LYS:HG2	2.18	0.42
1:A:3544:ARG:NH1	1:A:3544:ARG:HB3	2.33	0.42
1:A:2375:PHE:CD2	1:A:2427:PHE:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2386:PRO:HG3	1:A:2413:LEU:HD13	2.02	0.42
1:A:1880:VAL:CG2	1:A:2049:ILE:HG12	2.50	0.42
1:A:2074:LYS:HA	1:A:2074:LYS:HD2	1.81	0.42
1:A:2154:ILE:HB	1:A:2155:PRO:HD3	2.01	0.42
1:A:2614:ASP:HA	1:A:2657:LYS:NZ	2.33	0.42
1:A:2735:TYR:CE2	1:A:2737:ASP:HB3	2.55	0.42
1:A:2837:LEU:HD13	1:A:2842:GLU:HB3	2.02	0.42
1:A:3612:THR:O	1:A:3635:VAL:HA	2.19	0.42
1:A:3641:TYR:CD2	1:A:3692:LEU:HD21	2.55	0.42
1:A:4107:MET:HE3	1:A:4107:MET:HB3	1.95	0.42
1:A:1910:THR:N	2:A:4701:ADP:O2B	2.51	0.42
1:A:2420:ALA:HA	1:A:2423:MET:HG2	2.02	0.42
1:A:2507:ARG:O	1:A:2511:ARG:HG3	2.19	0.42
1:A:3191:ARG:NH1	1:A:3500:MET:HE1	2.35	0.42
1:A:4241:SER:HA	1:A:4244:LYS:HE3	2.00	0.42
1:A:1802:PRO:O	1:A:1805:ARG:HB3	2.19	0.42
1:A:2220:LEU:HD12	1:A:2342:MET:HG3	2.00	0.42
1:A:2595:GLY:HA3	1:A:2736:VAL:O	2.20	0.42
1:A:2748:TYR:CZ	1:A:2799:MET:HB3	2.55	0.42
1:A:4017:PHE:HB3	1:A:4018:MET:HE2	2.02	0.42
1:A:1923:LEU:HD12	1:A:1954:TRP:CH2	2.55	0.42
1:A:1965:GLU:OE1	1:A:1965:GLU:N	2.52	0.42
1:A:2242:GLU:HG3	1:A:2248:GLU:HA	2.01	0.42
1:A:2831:ARG:HD3	1:A:2921:ARG:HG2	2.02	0.42
1:A:2960:GLN:HA	1:A:2993:ILE:O	2.19	0.42
1:A:3895:THR:HB	1:A:3898:GLU:OE2	2.19	0.42
1:A:4296:MET:HE2	1:A:4296:MET:HA	2.01	0.42
1:A:1818:GLN:HA	1:A:1821:VAL:HG12	2.01	0.42
1:A:1946:VAL:HG22	1:A:1950:GLN:HE22	1.85	0.42
1:A:2157:LEU:HD12	1:A:2157:LEU:HA	1.83	0.42
1:A:2254:ILE:HG23	1:A:2279:LEU:HD23	2.01	0.42
1:A:2789:GLN:OE1	1:A:2790:PRO:HD2	2.20	0.42
1:A:2910:VAL:HG21	1:A:3105:VAL:HG22	2.02	0.42
1:A:2929:PRO:O	1:A:2930:GLN:HG3	2.20	0.42
1:A:3563:GLN:OE1	1:A:3567:LEU:HD23	2.19	0.42
1:A:3781:THR:O	1:A:3785:GLU:HG2	2.19	0.42
1:A:3907:HIS:CG	1:A:3941:LEU:HD11	2.55	0.42
1:A:4313:PRO:HB2	1:A:4315:THR:HG22	2.01	0.42
1:A:1628:ARG:O	1:A:1631:PHE:HD2	2.03	0.41
1:A:1843:ARG:NH2	1:A:1860:GLN:HG2	2.35	0.41
1:A:2387:LEU:HD22	1:A:2467:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2465:ALA:HB2	1:A:2493:TYR:CE1	2.55	0.41
1:A:2739:PRO:HD2	1:A:2796:PRO:HG3	2.02	0.41
1:A:2964:HIS:CD2	1:A:2966:LYS:HB3	2.55	0.41
1:A:3731:LEU:HD12	1:A:3790:VAL:HG21	2.02	0.41
1:A:4178:ARG:NH1	1:A:4278:PHE:HA	2.34	0.41
1:A:2932:HIS:ND1	1:A:3064:VAL:HG12	2.35	0.41
1:A:3109:PHE:HB3	1:A:3180:ILE:HG21	2.02	0.41
1:A:3495:THR:HG23	1:A:3496:PHE:CD1	2.55	0.41
1:A:3888:ALA:O	1:A:4012:ASN:ND2	2.52	0.41
1:A:4507:ILE:HD12	1:A:4507:ILE:HA	1.92	0.41
2:A:4703:ADP:N3	2:A:4703:ADP:H2'	2.35	0.41
1:A:2518:ILE:HA	1:A:2521:ILE:HG12	2.01	0.41
1:A:3005:LEU:HD23	1:A:3009:ASN:HD21	1.86	0.41
1:A:3814:THR:O	1:A:3818:LEU:HD23	2.20	0.41
1:A:4069:ILE:O	1:A:4096:LEU:HA	2.21	0.41
1:A:1632:VAL:HG12	1:A:1656:LYS:HD2	2.01	0.41
1:A:2671:MET:SD	1:A:2677:GLN:HG3	2.61	0.41
1:A:2959:TYR:N	1:A:2991:ALA:O	2.53	0.41
1:A:3101:ALA:O	1:A:3105:VAL:HG23	2.19	0.41
1:A:3649:LEU:HB2	1:A:3695:ARG:HE	1.86	0.41
1:A:3824:LEU:HA	1:A:4139:LEU:HD13	2.03	0.41
1:A:3931:GLN:O	1:A:3935:VAL:HG23	2.20	0.41
1:A:4027:LEU:HD22	1:A:4058:LEU:HD22	2.02	0.41
1:A:4288:VAL:HB	1:A:4320:TRP:CD1	2.54	0.41
1:A:4391:ILE:HD11	1:A:4479:VAL:HG13	2.01	0.41
1:A:2316:ASN:HB2	1:A:2358:ARG:CZ	2.51	0.41
1:A:2584:TRP:HB3	1:A:2591:LEU:HD23	2.02	0.41
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.54	0.41
1:A:3164:ARG:HH21	1:A:4374:PRO:N	2.18	0.41
1:A:3208:ILE:O	1:A:3212:VAL:HG23	2.20	0.41
1:A:4222:TRP:CZ3	1:A:4242:ALA:HB1	2.56	0.41
1:A:4264:LEU:HD12	1:A:4264:LEU:HA	1.82	0.41
1:A:1801:PRO:HA	1:A:1802:PRO:HD3	1.96	0.41
1:A:2431:GLY:O	1:A:2435:LYS:HE2	2.21	0.41
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.55	0.41
1:A:3014:ASN:ND2	1:A:3016:GLU:OE2	2.54	0.41
1:A:3683:ASP:HB3	1:A:3686:VAL:HB	2.01	0.41
1:A:3893:LYS:HD2	1:A:3893:LYS:HA	1.79	0.41
1:A:4038:ASN:HA	1:A:4118:PRO:HG3	2.02	0.41
1:A:4131:ASN:OD1	1:A:4134:VAL:HG23	2.21	0.41
1:A:2677:GLN:O	1:A:2680:ILE:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3518:GLY:HA3	1:A:3579:MET:HE1	2.03	0.41
1:A:3865:GLN:HE22	1:A:4017:PHE:HA	1.85	0.41
1:A:3881:ILE:HD13	1:A:4006:HIS:CD2	2.55	0.41
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	2.02	0.41
1:A:1637:LEU:O	1:A:1641:ILE:HG12	2.21	0.41
1:A:1691:SER:OG	1:A:1694:GLU:OE1	2.36	0.41
1:A:1755:GLN:HG2	1:A:1814:GLU:OE2	2.21	0.41
1:A:1792:LEU:HD22	1:A:1808:LEU:HD22	2.03	0.41
1:A:1914:GLU:CD	2:A:4701:ADP:H3'	2.45	0.41
1:A:1975:VAL:O	1:A:1978:ILE:HG22	2.21	0.41
1:A:2211:TYR:O	1:A:2215:GLN:HG2	2.20	0.41
1:A:2578:GLU:OE2	1:A:2608:ALA:HA	2.21	0.41
1:A:4187:HIS:ND1	1:A:4212:LEU:HD13	2.35	0.41
1:A:4455:LEU:HD21	1:A:4464:TRP:CH2	2.56	0.41
1:A:4607:LEU:HB2	1:A:4622:VAL:HG23	2.02	0.41
1:A:1682:GLU:HB2	1:A:1803:LEU:HD21	2.03	0.41
1:A:1782:LEU:O	1:A:1786:GLU:HG2	2.21	0.41
1:A:1797:LEU:HD21	1:A:2128:ALA:HB2	2.03	0.41
1:A:2383:ARG:NH2	1:A:2424:GLN:OE1	2.48	0.41
1:A:2605:LEU:HD11	1:A:2709:VAL:CG1	2.50	0.41
1:A:2703:LEU:HD12	1:A:2706:ILE:HD12	2.03	0.41
1:A:2827:HIS:O	1:A:2831:ARG:HG2	2.20	0.41
1:A:2838:VAL:HG12	1:A:3093:TRP:CD1	2.55	0.41
1:A:3503:ILE:HG13	1:A:3552:TYR:OH	2.20	0.41
1:A:3733:LYS:HA	1:A:3733:LYS:HD3	1.87	0.41
1:A:3786:GLU:O	1:A:3790:VAL:HG23	2.21	0.41
1:A:3824:LEU:HD11	1:A:4044:CYS:SG	2.60	0.41
1:A:3898:GLU:OE1	1:A:3898:GLU:N	2.41	0.41
1:A:4543:VAL:HG11	1:A:4624:PHE:CZ	2.56	0.41
1:A:4607:LEU:HD23	1:A:4607:LEU:HA	1.87	0.41
1:A:1904:PRO:HA	1:A:2039:LEU:HB2	2.03	0.41
1:A:2259:ILE:HG12	1:A:2263:HIS:HB2	2.03	0.41
1:A:2628:PRO:HG3	1:A:2679:VAL:HA	2.02	0.41
1:A:2956:LEU:CD2	1:A:2989:LYS:HB3	2.51	0.41
1:A:4194:LEU:HD21	1:A:4207:PHE:CD2	2.48	0.41
1:A:1746:GLN:O	1:A:1750:VAL:HG22	2.20	0.40
1:A:1916:VAL:HG11	1:A:1956:CYS:HB2	2.03	0.40
1:A:2492:ARG:NH2	1:A:2525:PRO:HB2	2.35	0.40
1:A:2504:GLY:O	1:A:2735:TYR:N	2.54	0.40
1:A:2616:GLU:O	1:A:2660:VAL:HG22	2.20	0.40
1:A:3913:GLU:OE1	1:A:3913:GLU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4194:LEU:HD22	1:A:4201:TRP:HE1	1.86	0.40
1:A:1735:PRO:O	1:A:1739:ILE:HD12	2.21	0.40
1:A:2114:GLU:O	1:A:2118:ARG:HG2	2.21	0.40
1:A:2687:VAL:HG13	1:A:2730:HIS:ND1	2.36	0.40
1:A:2847:ASP:HA	1:A:2850:ILE:HG22	2.02	0.40
1:A:3044:LEU:HB3	1:A:3049:GLU:CG	2.51	0.40
1:A:4109:LEU:O	1:A:4112:LYS:HG2	2.21	0.40
1:A:4318:PRO:HA	1:A:4321:LEU:CD2	2.51	0.40
1:A:2114:GLU:OE2	1:A:2118:ARG:NH2	2.46	0.40
1:A:2238:LEU:HD11	1:A:2249:GLY:HA3	2.03	0.40
1:A:2269:ASP:CB	1:A:2274:GLU:HG3	2.47	0.40
1:A:2282:HIS:O	1:A:2286:LYS:HG2	2.21	0.40
1:A:2778:THR:O	1:A:2781:GLN:HB2	2.20	0.40
1:A:2976:LEU:HD23	1:A:2976:LEU:HA	1.89	0.40
1:A:3207:LYS:O	1:A:3211:THR:HG23	2.21	0.40
1:A:3690:PRO:HA	1:A:3693:CYS:SG	2.61	0.40
1:A:4553:LEU:HD23	1:A:4553:LEU:H	1.86	0.40
1:A:1904:PRO:O	1:A:1912:LYS:HD2	2.21	0.40
1:A:1940:ALA:HA	1:A:1943:ARG:HG2	2.03	0.40
1:A:2113:ARG:HA	1:A:2113:ARG:NE	2.37	0.40
1:A:2184:LYS:HE3	1:A:2243:ARG:HH12	1.85	0.40
1:A:2511:ARG:HD3	1:A:2535:ILE:CD1	2.51	0.40
1:A:2793:ILE:O	1:A:2793:ILE:HG13	2.21	0.40
1:A:3821:ILE:HG22	1:A:4345:LYS:HD2	2.03	0.40
1:A:3916:LEU:HD11	1:A:3937:ARG:HE	1.87	0.40
1:A:3973:LEU:HD22	1:A:3992:LEU:HD22	2.03	0.40
1:A:4180:TYR:O	1:A:4183:LEU:HG	2.20	0.40
1:A:4239:PRO:HB2	1:A:4242:ALA:HB3	2.04	0.40
1:A:1882:THR:HG22	1:A:1884:LEU:N	2.33	0.40
1:A:1886:ASP:HA	1:A:1889:TYR:HD2	1.87	0.40
1:A:2241:LEU:HB3	1:A:2298:ARG:NH2	2.36	0.40
1:A:2603:MET:HG3	1:A:2604:THR:N	2.37	0.40
1:A:2680:ILE:HD11	1:A:2727:PHE:CZ	2.57	0.40
1:A:3734:LEU:HB3	1:A:3783:LYS:HB3	2.04	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	2684/4646 (58%)	2592 (97%)	92 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2397/4125 (58%)	2397 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1651	GLN
1	A	1790	ASN
1	A	1817	HIS
1	A	1850	GLN
1	A	1863	ASN
1	A	2003	ASN
1	A	2212	GLN
1	A	2215	GLN
1	A	2491	GLN
1	A	2730	HIS
1	A	2791	HIS

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Mol	Chain	Res	Type
1	A	3057	GLN
1	A	3158	ASN
1	A	3650	ASN
1	A	3667	GLN
1	A	3700	ASN
1	A	3714	ASN
1	A	3772	ASN
1	A	3792	GLN
1	A	3820	GLN
1	A	3852	HIS
1	A	3907	HIS
1	A	4191	GLN
1	A	4291	HIS
1	A	4466	HIS

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
3	ATP	A	4702	-	32,33,33	0.75	2 (6%)	48,52,52	0.37	0
2	ADP	A	4704	-	28,29,29	1.36	5 (17%)	43,45,45	1.80	9 (20%)
2	ADP	A	4701	-	28,29,29	1.36	4 (14%)	43,45,45	1.92	10 (23%)
2	ADP	A	4703	-	28,29,29	1.41	4 (14%)	43,45,45	1.96	8 (18%)

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
3	ATP	A	4702	-	-	5/22/38/38	0/3/3/3
2	ADP	A	4704	-	-	5/16/32/32	0/3/3/3
2	ADP	A	4701	-	-	5/16/32/32	0/3/3/3
2	ADP	A	4703	-	-	7/16/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4703	ADP	C5-C4	4.79	1.47	1.39
2	A	4701	ADP	C5-C4	4.53	1.47	1.39
2	A	4704	ADP	C5-C4	4.36	1.46	1.39
3	A	4702	ATP	PA-O3A	-2.72	1.56	1.59
3	A	4702	ATP	PB-O3B	-2.64	1.56	1.59
2	A	4703	ADP	C5-C6	2.59	1.48	1.41
2	A	4704	ADP	C5-C6	2.58	1.48	1.41
2	A	4703	ADP	C5-N7	-2.57	1.34	1.39
2	A	4701	ADP	C5-N7	-2.54	1.34	1.39
2	A	4701	ADP	C5-C6	2.46	1.47	1.41
2	A	4704	ADP	C5-N7	-2.36	1.34	1.39
2	A	4704	ADP	C8-N7	2.36	1.36	1.31
2	A	4704	ADP	C4-N9	-2.22	1.33	1.37
2	A	4703	ADP	C8-N7	2.16	1.35	1.31
2	A	4701	ADP	C8-N7	2.15	1.35	1.31

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	C5-C4-N3	-6.42	117.87	126.72
2	A	4701	ADP	C5-C4-N3	-6.41	117.89	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4704	ADP	C5-C4-N3	-5.43	119.24	126.72
2	A	4703	ADP	N3-C4-N9	5.16	135.94	127.17
2	A	4701	ADP	N3-C4-N9	5.12	135.87	127.17
2	A	4704	ADP	N3-C4-N9	4.21	134.32	127.17
2	A	4703	ADP	C2-N3-C4	3.81	121.15	111.83
2	A	4701	ADP	C2-N3-C4	3.77	121.03	111.83
2	A	4703	ADP	C3'-C2'-C1'	3.66	108.38	101.46
2	A	4704	ADP	C2-N3-C4	3.57	120.55	111.83
2	A	4704	ADP	C4-C5-N7	-3.55	106.52	110.58
2	A	4703	ADP	C4-C5-N7	-3.43	106.66	110.58
2	A	4701	ADP	C4-C5-N7	-3.34	106.77	110.58
2	A	4704	ADP	N3-C2-N1	-3.25	123.66	128.58
2	A	4701	ADP	N3-C2-N1	-2.95	124.12	128.58
2	A	4704	ADP	C4-N9-C8	2.93	108.82	105.74
2	A	4703	ADP	N3-C2-N1	-2.81	124.32	128.58
2	A	4703	ADP	C5-N7-C8	2.56	107.47	103.45
2	A	4704	ADP	C5-N7-C8	2.54	107.44	103.45
2	A	4703	ADP	C4-N9-C8	2.52	108.38	105.74
2	A	4701	ADP	C5-N7-C8	2.44	107.28	103.45
2	A	4701	ADP	C4-N9-C8	2.34	108.19	105.74
2	A	4701	ADP	C2'-C3'-C4'	2.31	107.07	102.61
2	A	4701	ADP	C3'-C2'-C1'	2.30	105.82	101.46
2	A	4704	ADP	C6-C5-N7	2.25	136.42	132.09
2	A	4704	ADP	N9-C8-N7	-2.23	110.77	113.94
2	A	4701	ADP	O3B-PB-O2B	2.06	115.55	107.80

There are no chirality outliers.

All (22) torsion outliers are listed below:

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

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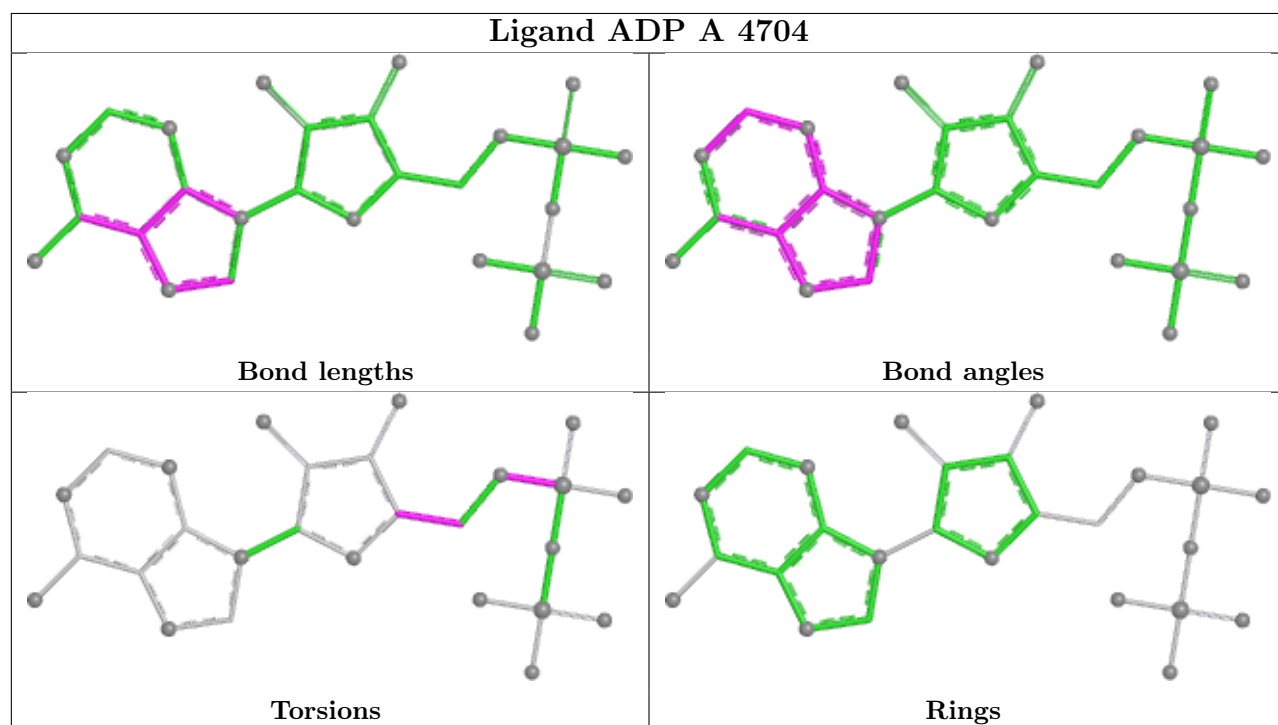
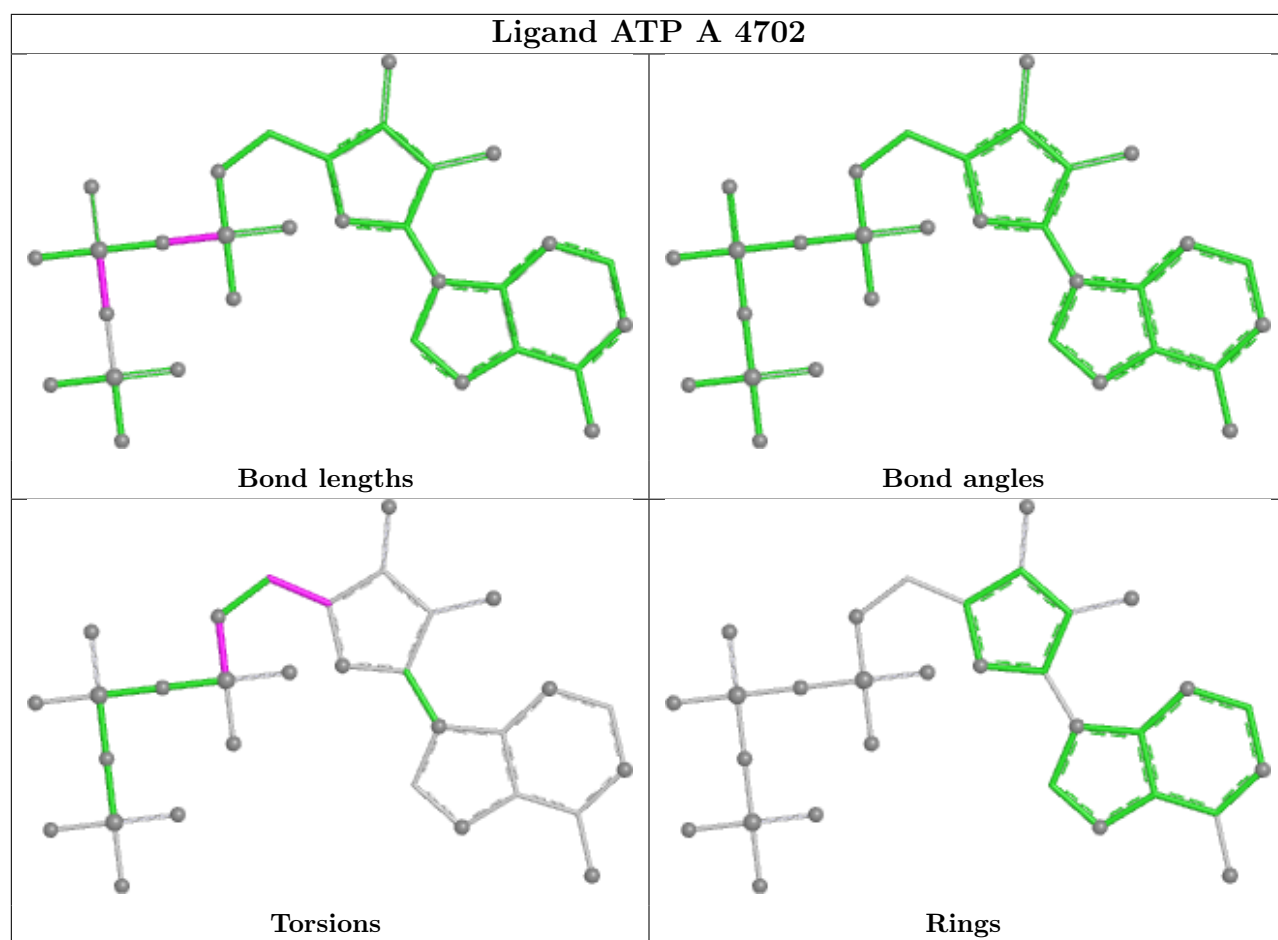
Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	O4'-C4'-C5'-O5'
2	A	4704	ADP	C3'-C4'-C5'-O5'
2	A	4703	ADP	C3'-C4'-C5'-O5'
2	A	4701	ADP	C3'-C4'-C5'-O5'
2	A	4701	ADP	C5'-O5'-PA-O1A
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	C5'-O5'-PA-O3A
2	A	4703	ADP	C2'-C1'-N9-C8
2	A	4703	ADP	C4'-C5'-O5'-PA
2	A	4703	ADP	C2'-C1'-N9-C4

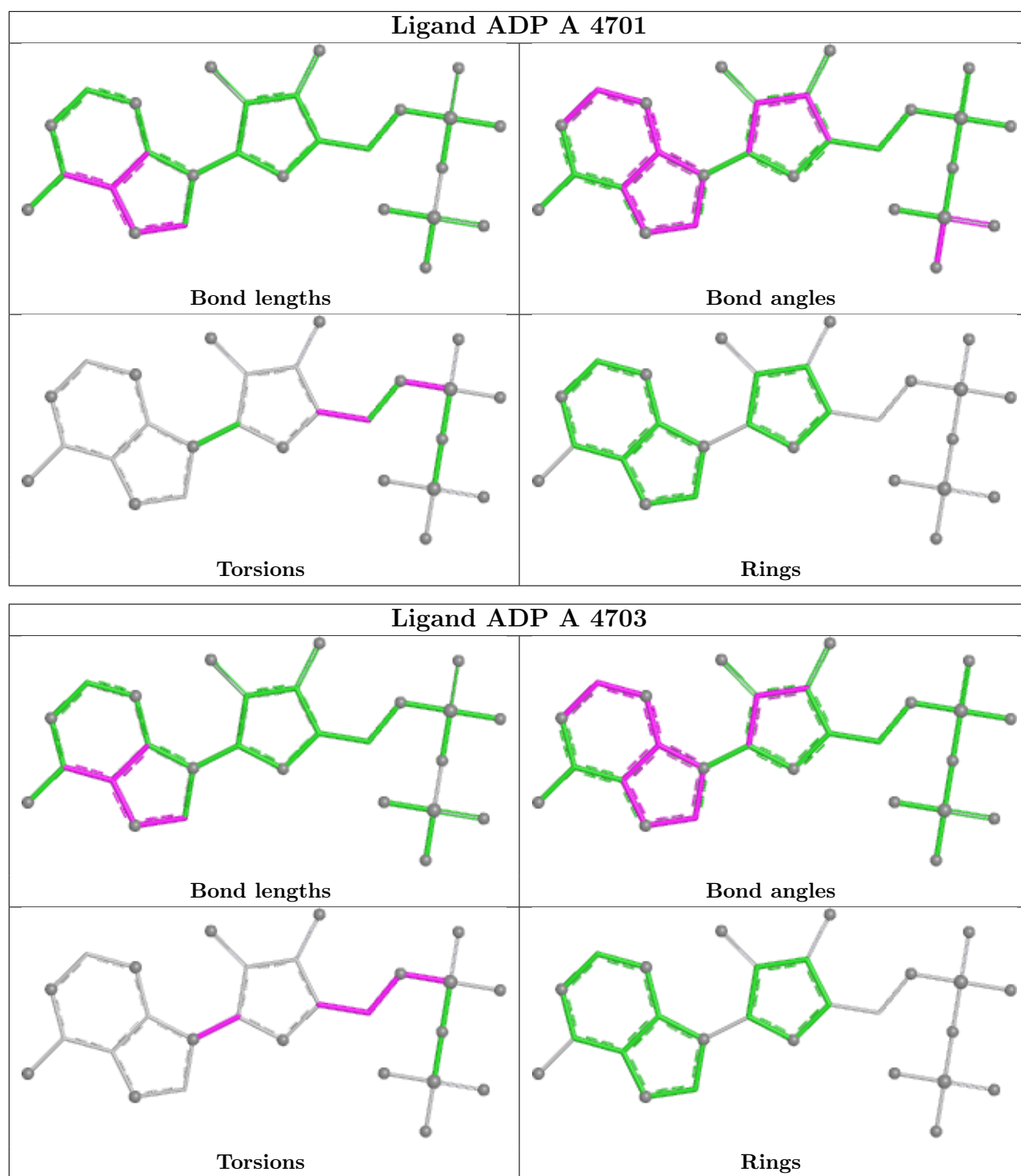
There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4702	ATP	5	0
2	A	4704	ADP	2	0
2	A	4701	ADP	6	0
2	A	4703	ADP	6	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

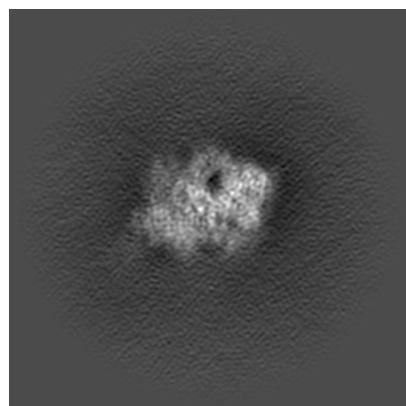
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44711. These allow visual inspection of the internal detail of the map and identification of artifacts.

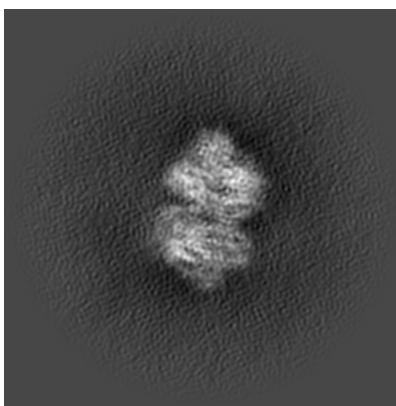
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

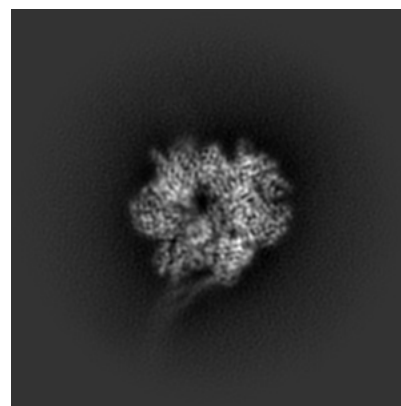
6.1.1 Primary map



X

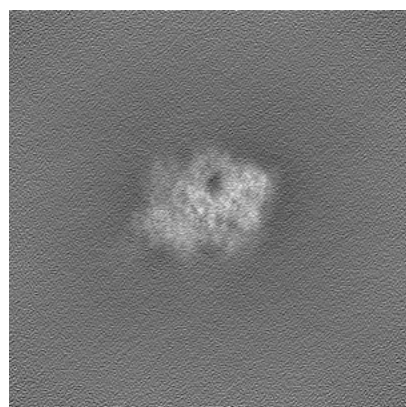


Y

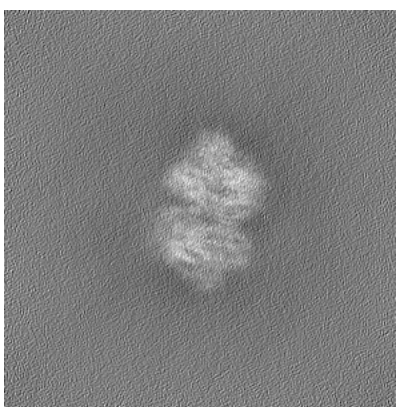


Z

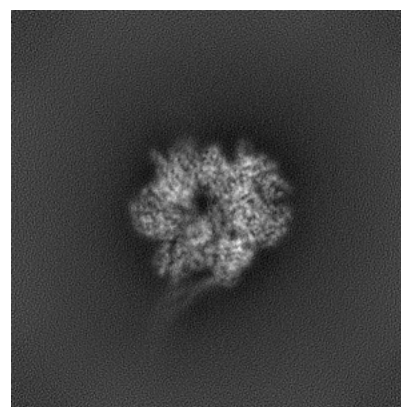
6.1.2 Raw map



X



Y

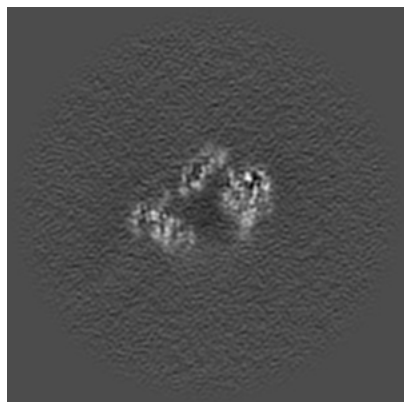


Z

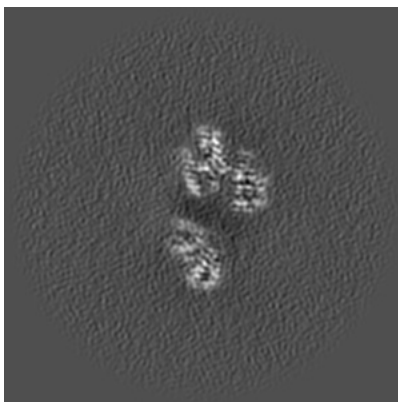
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

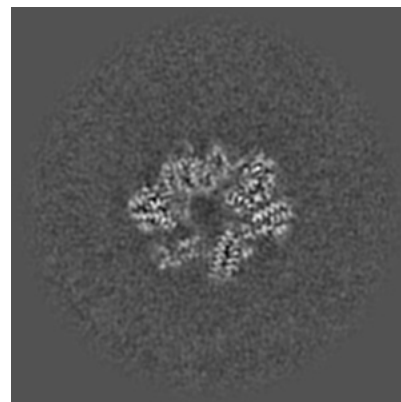
6.2.1 Primary map



X Index: 160

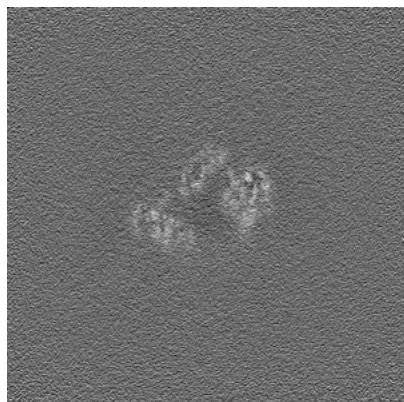


Y Index: 160

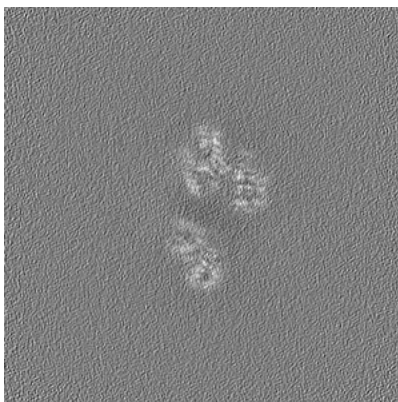


Z Index: 160

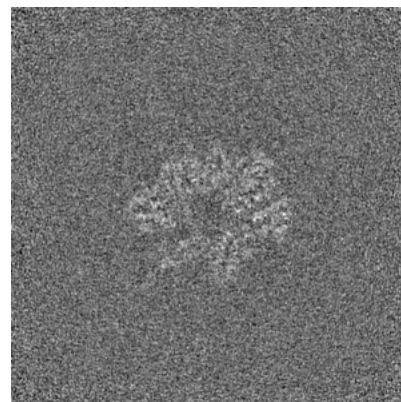
6.2.2 Raw map



X Index: 160



Y Index: 160

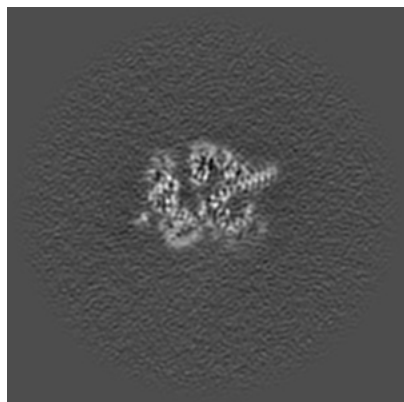


Z Index: 160

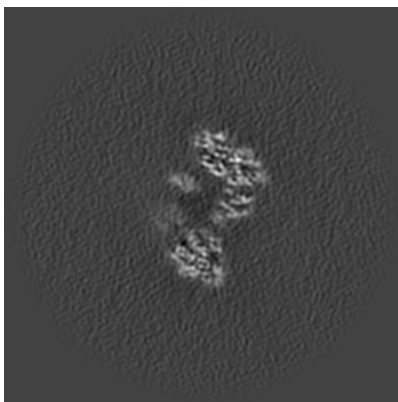
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

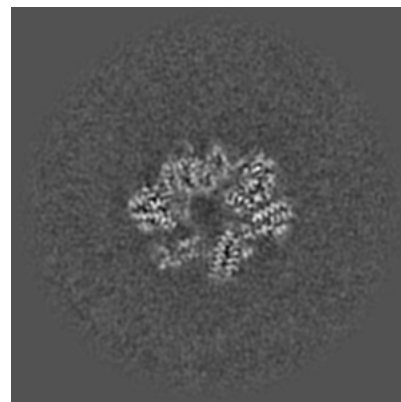
6.3.1 Primary map



X Index: 182

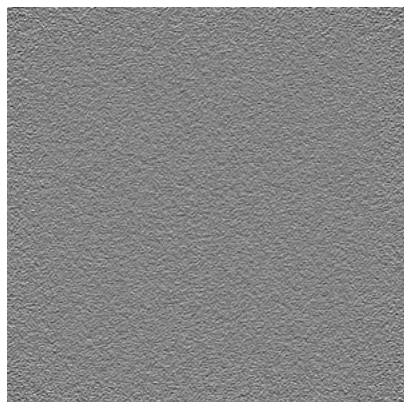


Y Index: 150

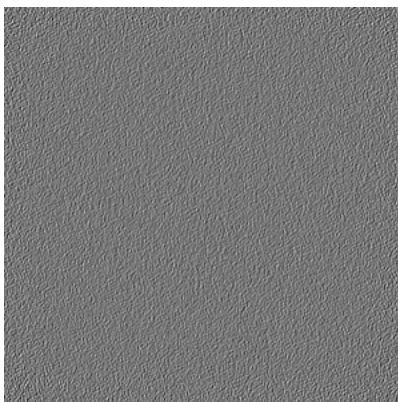


Z Index: 160

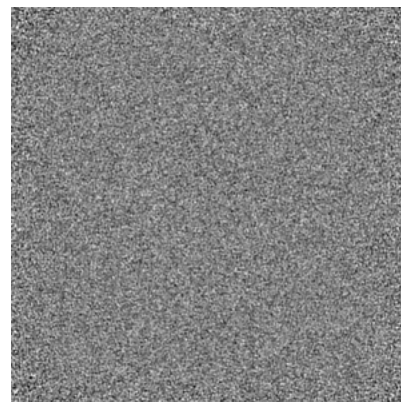
6.3.2 Raw map



X Index: 0



Y Index: 0

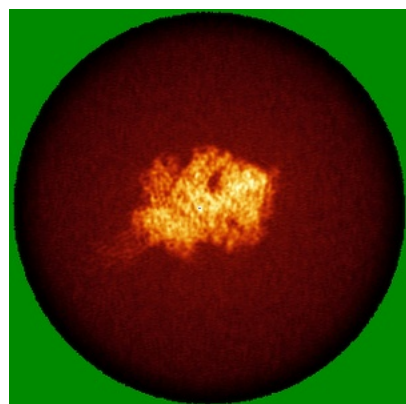


Z Index: 0

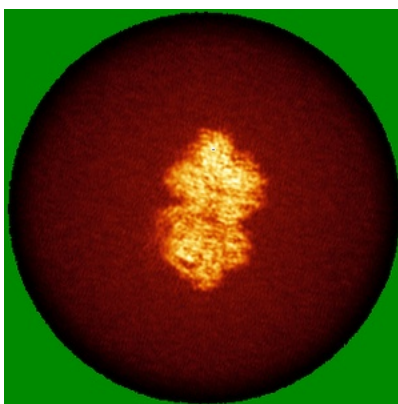
The images above show the largest variance slices of the map in three orthogonal directions.

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

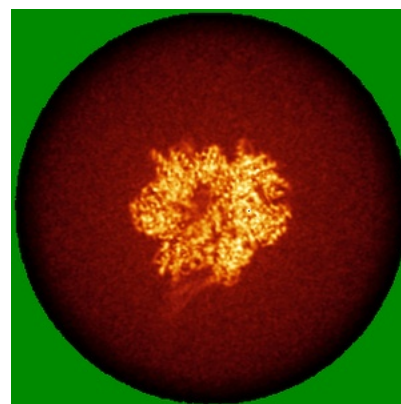
6.4.1 Primary map



X

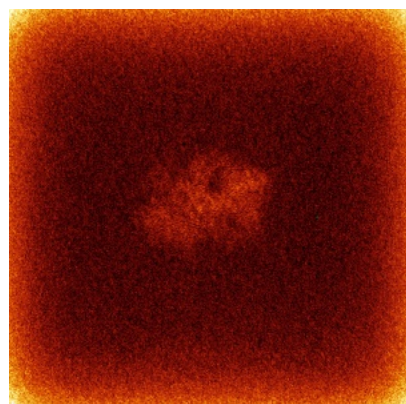


Y

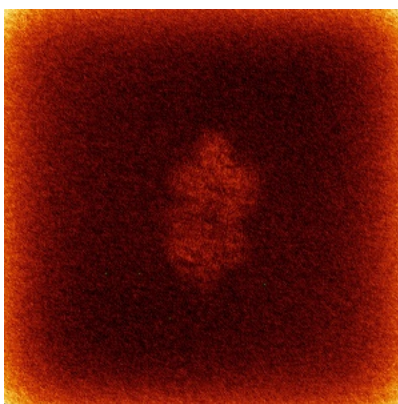


Z

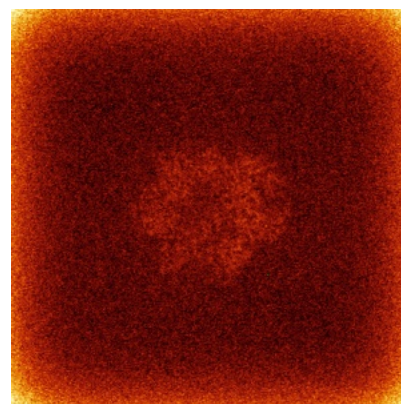
6.4.2 Raw map



X



Y

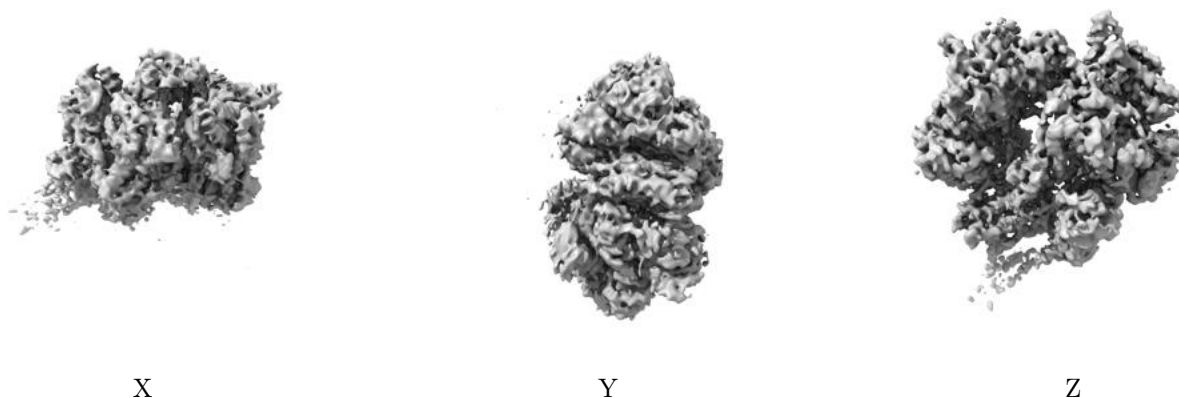


Z

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.

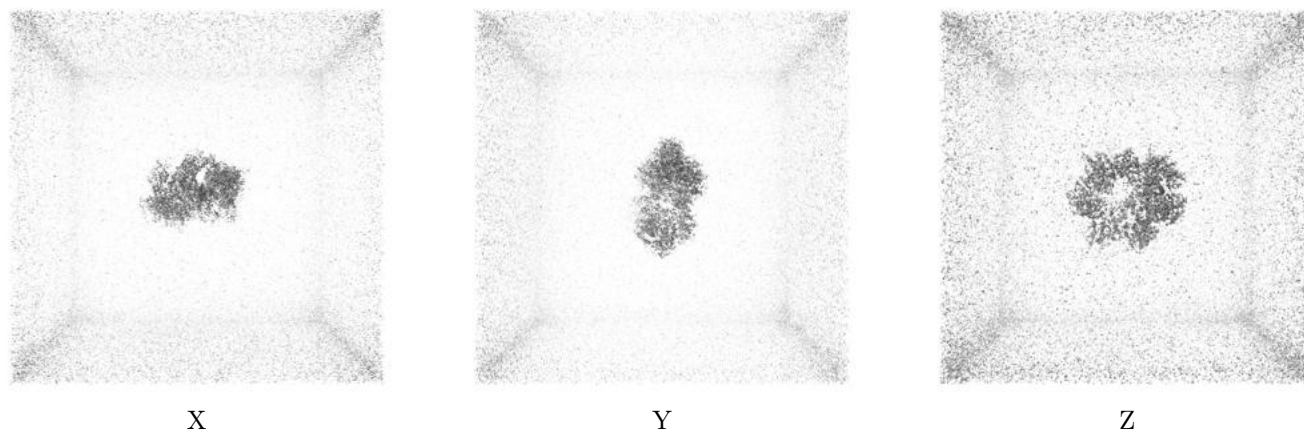
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

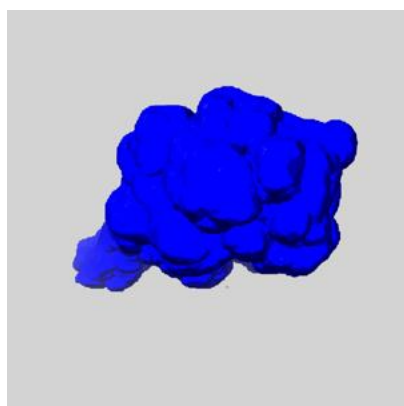
6.6 Mask visualisation [i](#)

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

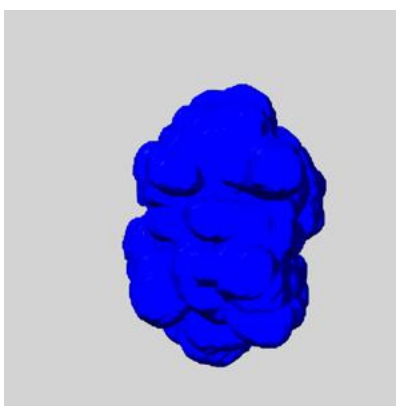
A mask typically either:

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

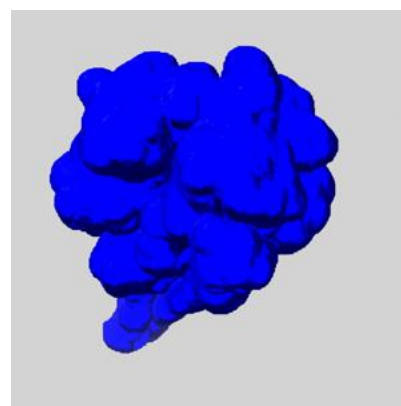
6.6.1 emd_44711_msk_1.map [i](#)



X



Y

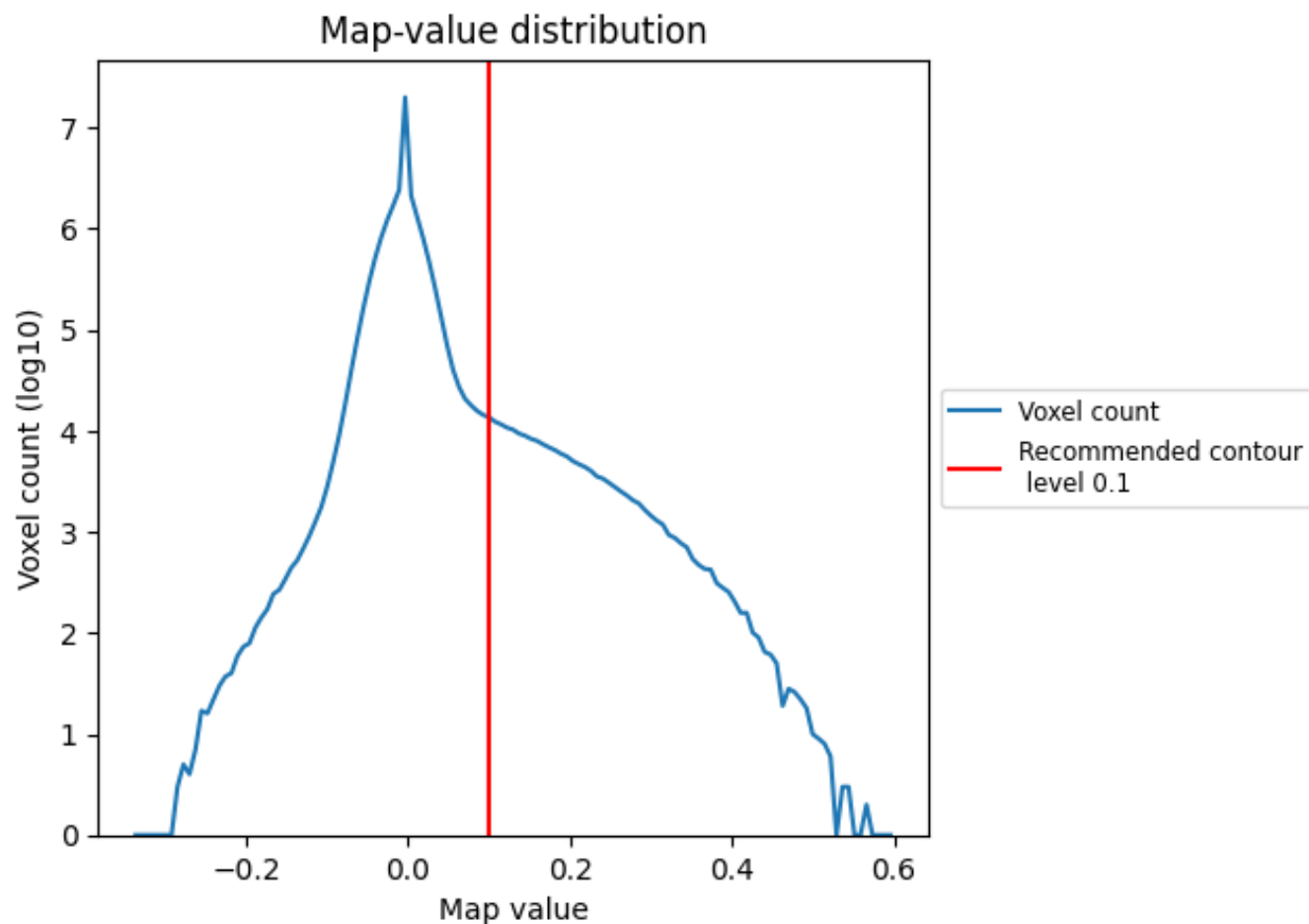


Z

7 Map analysis [i](#)

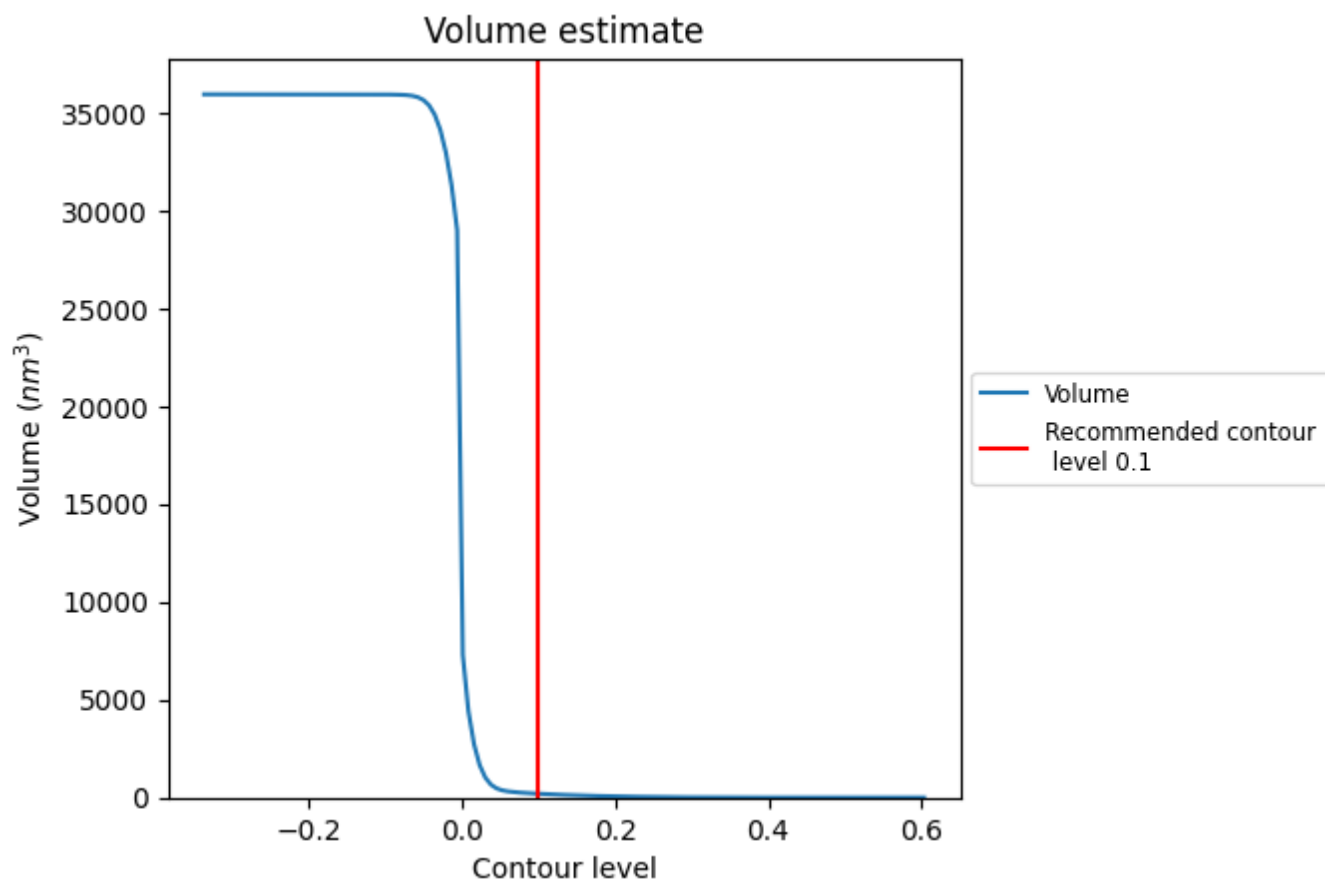
This section contains the results of statistical analysis of the map.

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.

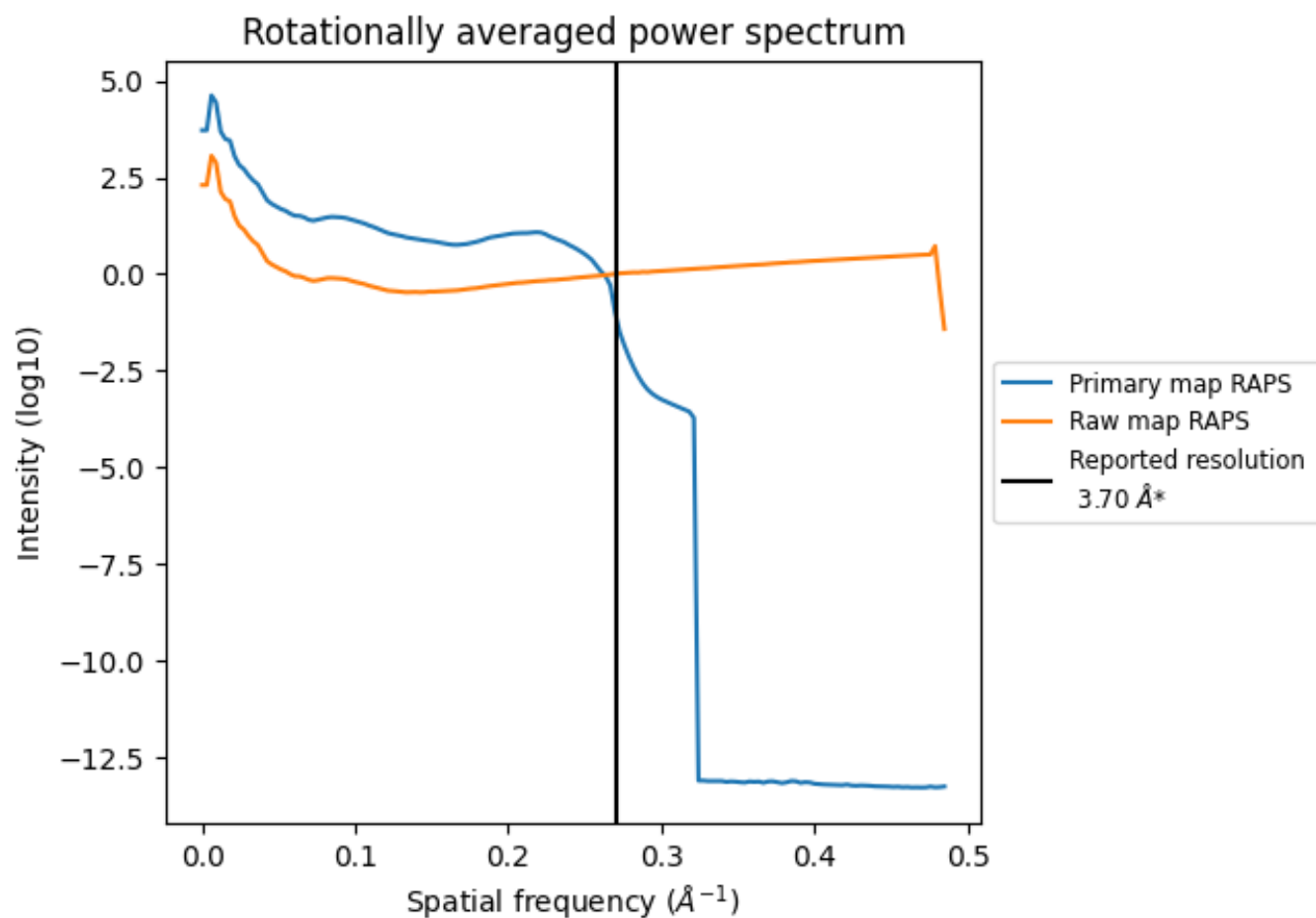
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 195 nm³; this corresponds to an approximate mass of 176 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 ⓘ

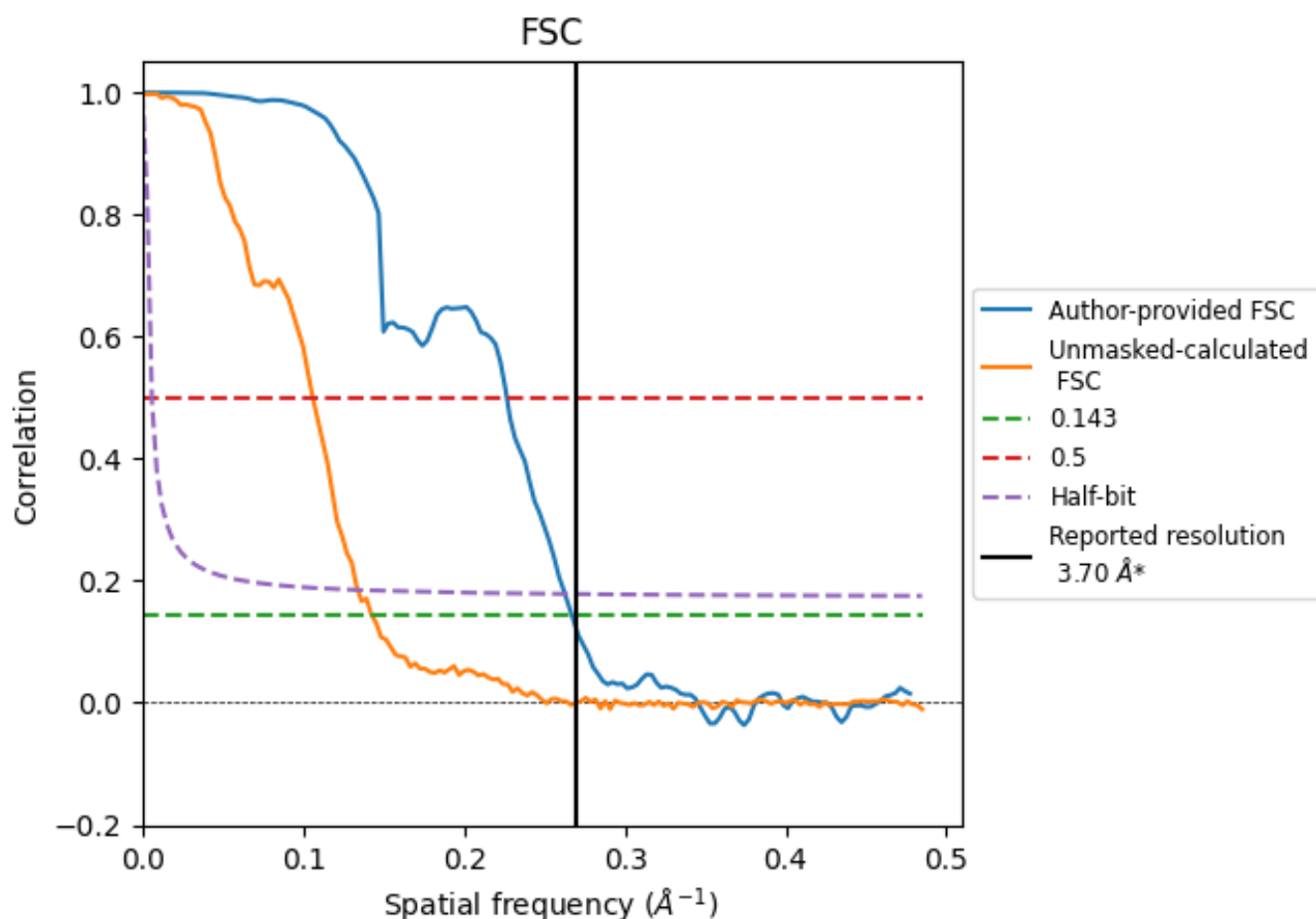


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

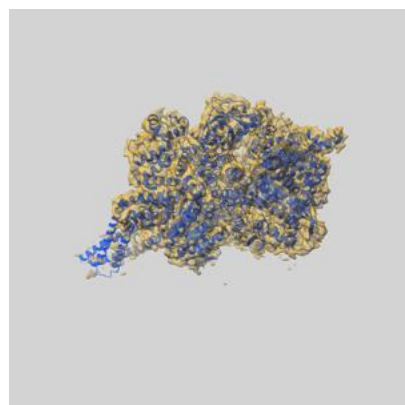
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.74	4.41	3.81
Unmasked-calculated*	7.00	9.43	7.46

*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 7.00 differs from the reported value 3.7 by more than 10 %

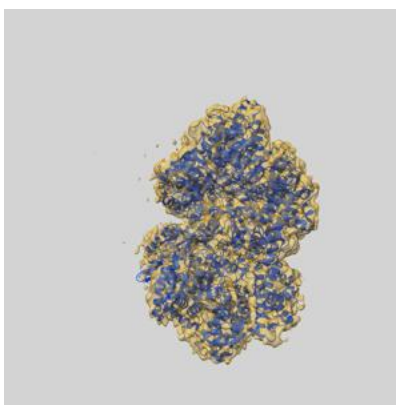
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44711 and PDB model 9BMU. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

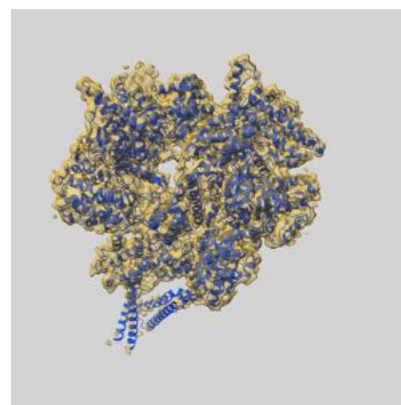
9.1 Map-model overlay [i](#)



X



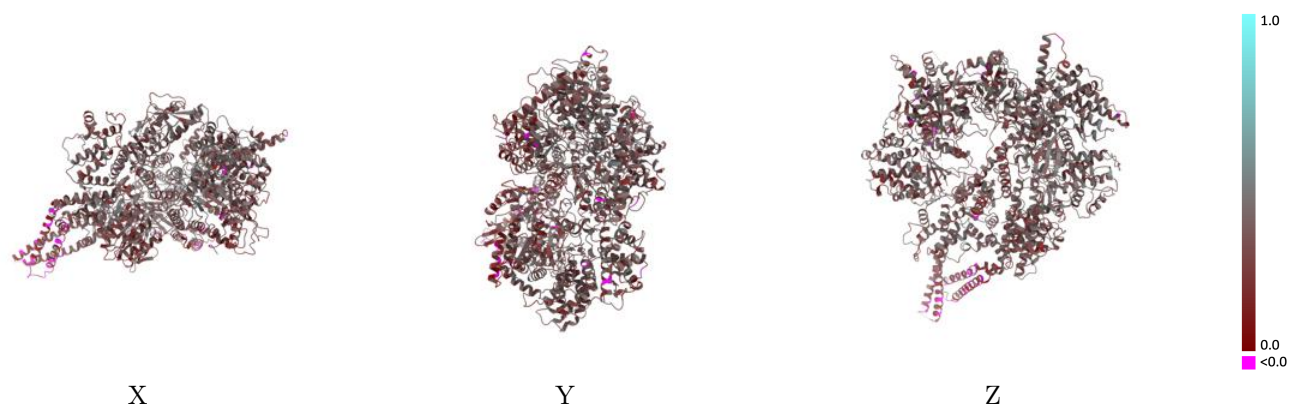
Y



Z

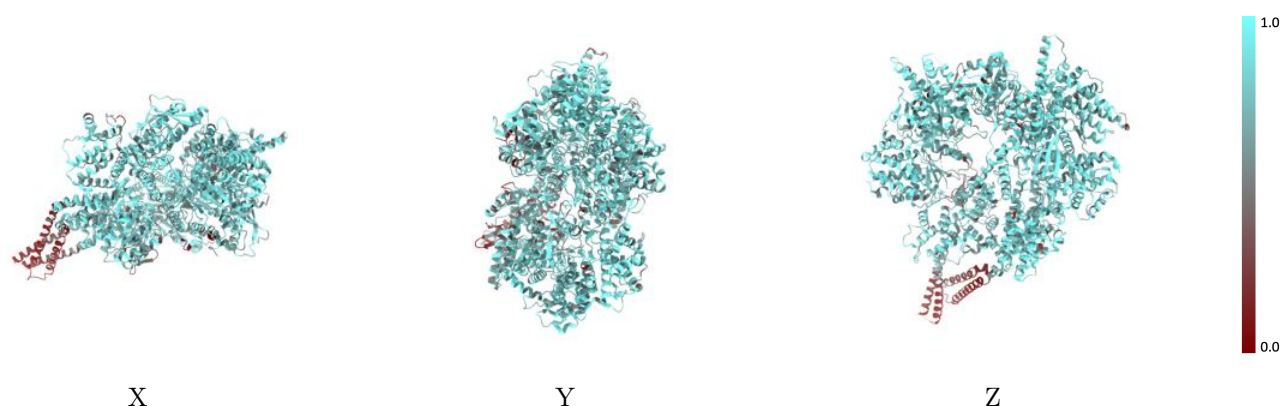
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



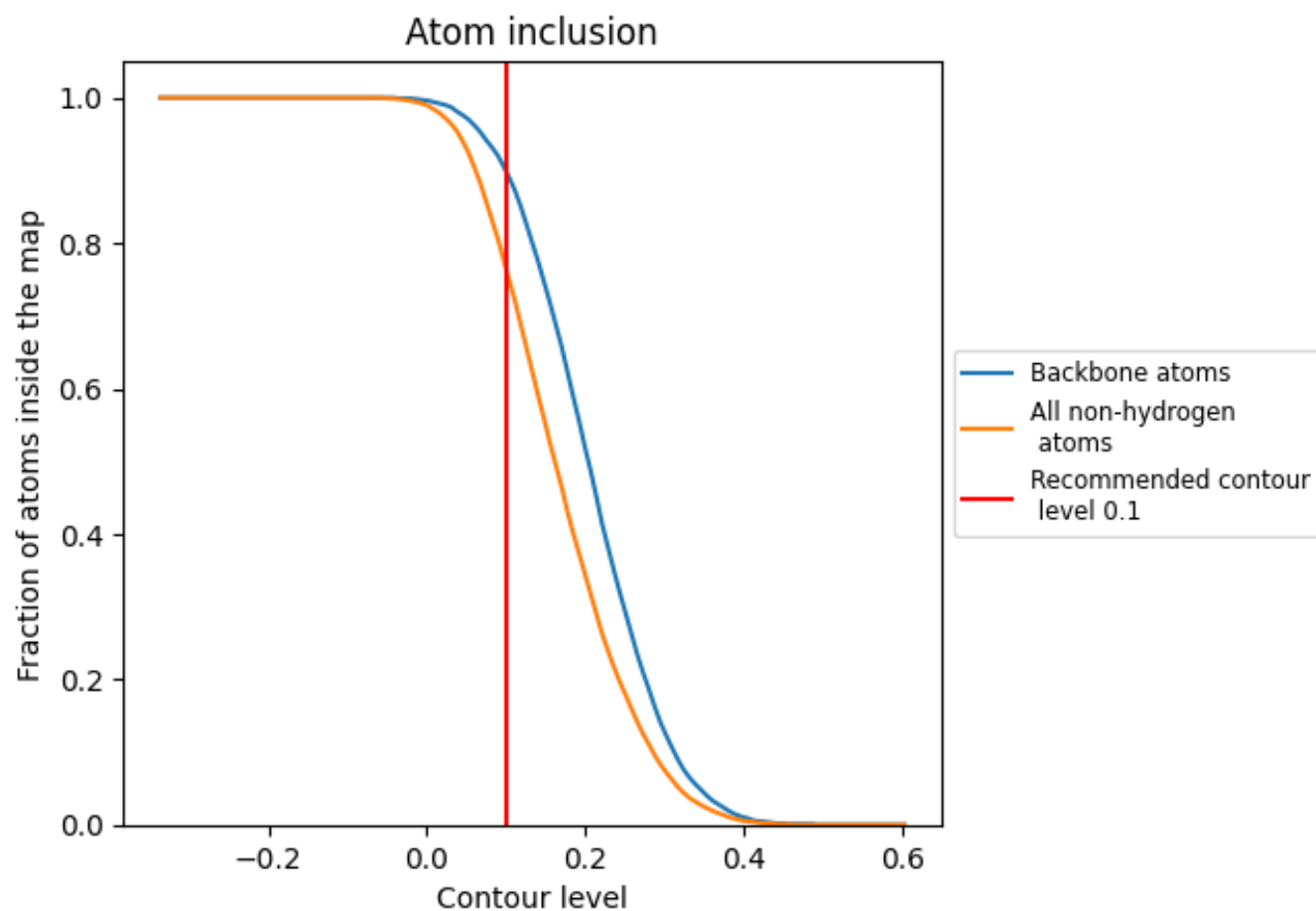
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 76% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7650	0.3330
A	0.7650	0.3330

