



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 08:10 AM UTC

PDB ID : 9BN1 / pdb_00009bn1
EMDB ID : EMD-44718
Title : State-8 of motor domain from full-length human dynein-1 in apo condition
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

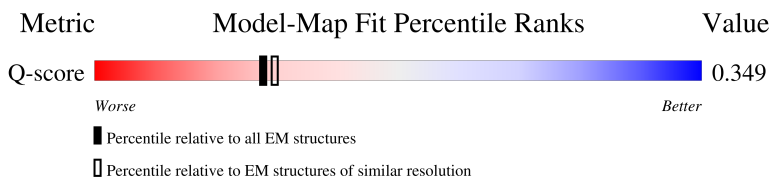
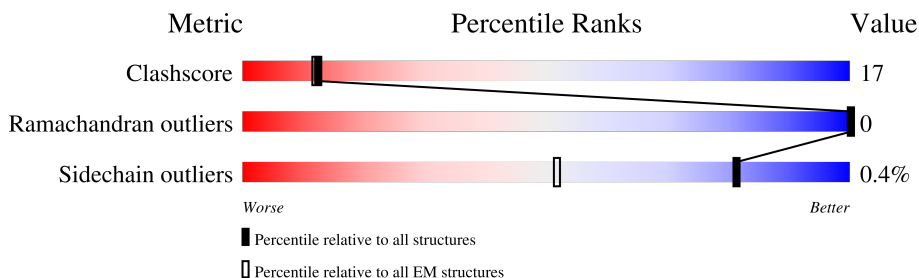
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

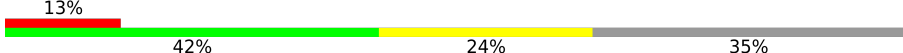
The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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

Mol	Chain	Length	Quality of chain
1	A	4646	

2 Entry composition [i](#)

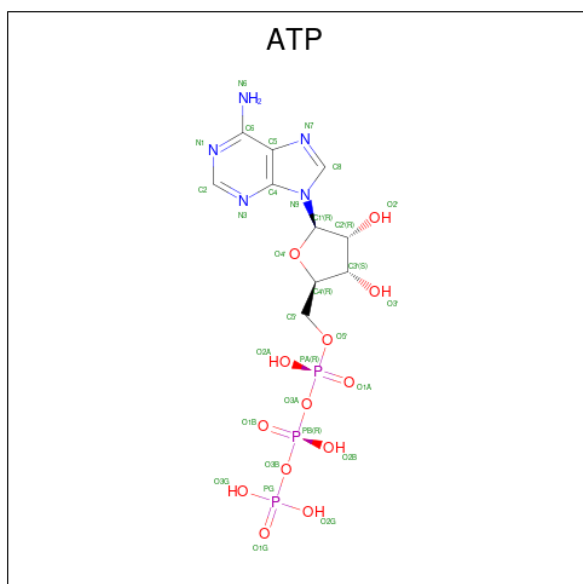
There are 4 unique types of molecules in this entry. The entry contains 24476 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

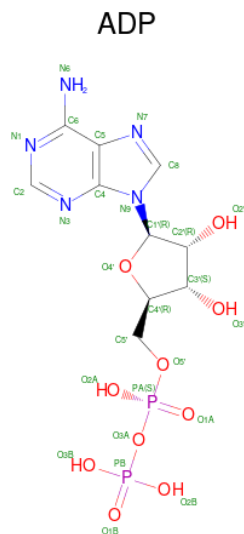
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3029	24390	15542	4208	4518	122	0	0

- Molecule 2 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
			Total	C	N	O	P	
2	A	1	31	10	5	13	3	0

- Molecule 3 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
3	A	1	Total 27	C 10	N 5	O 10	P 2	0
3	A	1	Total 27	C 10	N 5	O 10	P 2	0

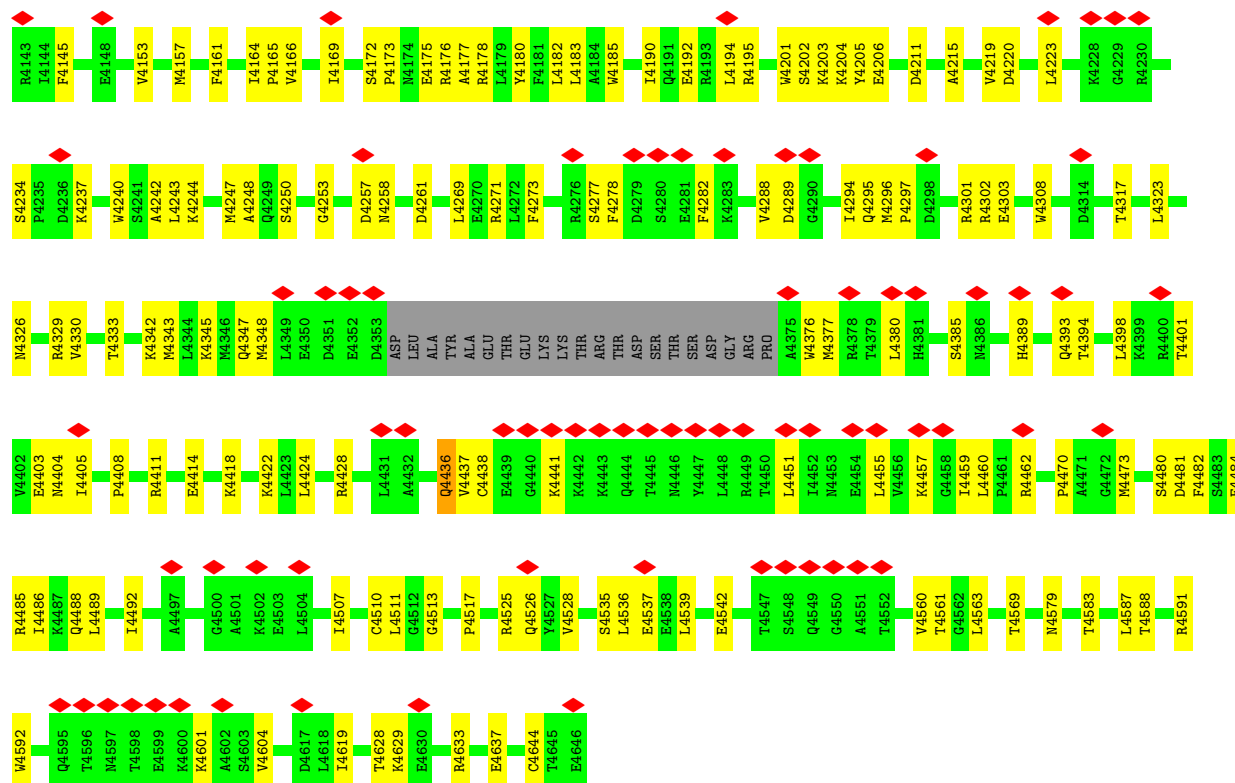
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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



Q3057	M2953	V2853	F2652	H2577	Q2482	ARG	K2323	V2236	E2133	Y2055	S1986
V3065	V2958	L2855	C2663	E2578	L2483	LYS	L2324	L2237	Q2134	S2056	N1987
F3066	R2757	L2755	E2664	A2579	E2484	GLY	L2325	L2238	E2135	Q2057	P1988
T3067	P2760	H2857	E2665	L2580	Q2485	LYS	L2326	L2244	L2136	R2060	N1989
N3068	R2763	R2863	L2667	Y2493	Y2493	ASP	L2327	G2249	L2137	L2085	Y1990
N3069	R2766	E2864	T2668	T2583	L2494	GLU	P2328	K2257	E2143	T2069	D1991
F3070	A2766	R2869	L2671	L2498	I2498	GLY	N2329	K2261	E2144	V2070	K1992
S3071	T2770	P2870	K2672	L2499	L2499	GLU	G2330	K2271	M2145	P2071	T1993
S3072	M2773	L2871	G2675	L2591	W2500	GLU	E2331	K2287	Y2146	F2072	S1994
G3073	E2775	S2874	Q2676	P2596	S2503	A2408	R2332	L2287	P2147	L2075	A1995
G3074	E2776	L2872	Q2677	G2597	G2504	A2409	R2333	L2288	L2148	C2076	P1996
N3078	E2777	S2877	E2678	G2598	L2505	L2413	L2334	L2289	L2149	D2077	I1997
T3081	E2779	S2879	V2679	L2599	S2506	Q2414	S2335	D2289	E2152	E2000	E2000
F3086	M2779	D2880	I2680	P2602	L2508	T2415	L2336	N2270	V2164	F2078	E2000
F3094	D2787	Y2881	L2683	M2603	K2509	Q2416	S2337	N2271	Q2169	Q2079	L2001
G3095	Y2792	L2882	R2684	F2606	M2510	R2418	L2338	N2272	Y2170	L2080	L2002
N3096	H2791	P2883	Q2698	L2609	R2511	A2419	P2339	N2273	M2175	F2088	N2003
N3097	Y2792	S2883	V2687	D2614	A2512	T2421	E2344	E2274	L2178	L2090	K2004
E3100	S2795	L2888	Y2688	M2615	E2513	L2422	Q2345	D2277	E2181	R2091	Q2005
A3101	P2796	R2889	R2694	L2616	L2514	M2423	Q2346	L2278	C2186	A2092	F2010
L3102	E2797	S2890	Q2698	V2617	E2517	F2427	D2347	L2279	Y2190	L2093	A2013
V3105	E2798	L2894	L2698	F2622	L2526	K2435	K2349	L2281	L2191	S2095	V2096
G3106	W2802	K2898	L2699	S2623	P2527	E2438	T2352	R2285	G2101	V2097	N2019
K3107	F2807	L2899	S2624	S2624	T2528	H2439	A2354	V2290	K2104	V2098	P2020
T3110	E2808	Y2900	E2629	E2629	N2531	Q2442	R2358	S2291	M2202	G2101	G2021
S3111	R2814	E2903	L2630	L2630	D2536	L2443	C2359	R2292	W2203	GLY	ALA
K3112	L2815	L2904	L2632	L2632	Y2537	E2444	W2363	G2293	K2206	ARG	ARG
N3113	P2715	D2905	K2633	K2633	E2538	L2449	F2364	L2294	K2207	S2026	S2026
L3114	T2716	L2906	T2634	T2634	L2450	T2450	F2365	L2295	Q2109	N2027	N2027
L3115	P2817	P2907	F2635	F2635	R2451	R2451	S2366	Q2296	K2110	L2028	L2028
E3116	V2818	V2907	D2636	D2636	L2452	L2452	E2366	K2297	R2113	D2030	D2030
K3117	L2818	L2908	L2636	L2636	R2453	R2453	M2373	Q2299	E2116	N2031	N2031
N3118	E2819	G2909	R2642	R2642	C2454	C2454	L2374	W2300	E2117	L2032	L2032
N3119	G2820	L2910	R2643	R2643	L2455	L2455	F2375	L2301	R2118	K2033	K2033
V3120	L2821	L2911	T2644	T2644	Q2554	Q2554	N2376	V2302	G2119	F2036	F2036
F3125	L2822	R2912	G2647	G2647	E2558	E2558	F2377	F2303	E2120	R2037	R2037
N3126	W2825	L2913	L2647	L2647	T2559	T2559	L2378	D2304	A2121	S2038	S2038
F3127	A2829	L2934	L2650	L2650	K2561	K2561	L2379	G2305	V2122	L2040	L2040
V3128	L2837	L2935	A2651	A2651	V2569	V2569	L2382	D2306	G2229	T2041	T2041
V3129	Y2738	L2936	P2652	P2652	T2570	T2570	R2383	V2307	E2124	T2042	T2042
N3130	Y2738	L2937	V2653	V2653	K2561	K2561	P2386	D2308	G2125	K2043	K2043
K3131	E2839	L2940	Q2654	Q2654	L2569	L2569	P2386	P2309	E2126	P2044	P2044
D3132	E2840	L2941	L2655	L2655	T2571	T2571	E2389	E2310	I2127	B2045	B2045
K3133	E2841	L2942	G2656	G2656	L2672	L2672	GLY	W2311	A2127	R2046	R2046
D3045	L2747	L2943	K2657	K2657	D2673	D2673	GLU	V2312	M2232	Q2047	Q2047
E3046	I2747	L2944	W2658	W2658	T2574	T2574	ASP	E2313	E2234	L2048	L2048
E3048	T2750	L2945	L2659	L2659	V2575	V2575	GLU	M2314	A2235	N2129	N2129
E3049	F2751	N2947	V2660	V2660	R2576	R2576	ALA	L2315	R2234	E2130	E2130
W3053	N2752	R2948	L2661	L2661			GLN	L2319	R2235	L2131	L2131
F3054							ARG	D2320		P2132	P2132
A3142								N2322			

F4077	M4078	Q4079	A4080	M4081	K4082	A4083	T4084	M4085	T4086	A4087	V4088	K4089	S4090	G4091	R4092	M4093	V4094	M4095	L4096	K4097	M4098	M4099	M4100	L4101	A4102	P4103	Q4104	W4105	L4106	M4107	Q4108	L4109	M4110	K4111	K4112	L4113	L4116	Q4117	P4118	H4119	A4120	C4121	F4122	R4123	L4124	M4127	M4128	E4129	K4133	V4134	L4138	L4139	R4140	A4141	G4142						
R3989	L3990	L3991	L3992	A4003	M4004	A4005	H4006	M4007	F4008	L4013	G4014	A4015	S4016	F4017	M4018	M4021	E4022	Q4023	P4024	L4025	D4026	L4027	L4028	H4029	I4030	E4034	M4038	L4042	D4050	A4051	S4052	G4053	H4054	D4057	L4058	A4059	A4060	E4061	M4063	I4066	T4067	S4068	I4071	G4072	S4073	A4074	E4075	G4076													
T3765	I3766	I3767	T3768	T3769	R3770	E3771	N3772	L3773	K3774	R3775	E3776	A3777	R3778	E3779	V3780	T3781	R3782	K3783	V3784	E3785	E3786	T3787	R3788	I3789	V3790	M3791	D3792	I3793	T3794	T3795	V3796	V3797	Q3800	Y3801	L3804	A3807	S3810	I3811	Y3812	T3813	M3814	M3815	K3819	Y3825	Q3826	T3827	S3828	L3829	Q3830	F3831	I3835	Y3836									
H3837	N3838	V3839	E3842	N3845	L3846	K3847	G3848	D3851	H3852	T3853	Q3854	R3855	L3856	I3859	T3860	K3861	D3862	V3866	R3870	V3871	A3872	R3873	G3874	M3875	D3879	R3880	I3881	T3882	F3883	A3884	M3885	L3886	L3887	A3888	R3889	K3890	K3891	L3892	K3893	T3900	Y3901	D3902	A3903	Q3906	H3907	R3910	G3911	N3912	E3913	A3980	I3983	G3984	Q3985	A3986	I3987	H3988					
I3914	V3915	L3916	S3917	A3918	G3919	S3920	T3921	P3922	R3923	I3924	Q3925	G3926	L3927	E3930	E3933	V3936	R3937	L3938	S3939	C3940	F3944	K3945	L3946	L3947	I3948	A3949	K3950	V3951	Q3952	A3953	D3954	E3955	Q3956	F3957	G3958	I3959	E3967	V3970	L3973	M3974	S3975	E3976	E3977	A3980	I3983	G3984	Q3985	A3986	I3987	H3988											
ALA	VAL	GLU	A3470	K3471	F3472	N3473	R3474	S3475	T3476	A3477	L3478	L3479	K3480	S3481	L3482	S3483	A3484	E3485	R3486	E3487	F3488	E3489	E3490	K3491	T3492	S3493	E3494	T3495	F3496	K3497	N3498	Q3499	I3503	A3504	G3505	L3509	S3510	A3511	I3514	A3517	G3518	Y3519	F3520	D3521	M3524	W3532	L3536	Q3537	N3540	I3541	Q3542										
LYS	ARG	GLU	GLY	LEU	ARG	ASN	ALA	LEU	GLN	LYS	LEU	GLU	ASP	ALA	ARG	LYS	MET	LYS	ASN	TYR	MET	VAL	PRO	ALA	ALA	TYR	ASN	LYS	ARG	ALA	CYS	LEU	TYR	LYS	ALA	GLY	GLU	TYR	PRO	MET	THR	VAL	LYS	ILE	ASN	ILE	TYR	ALA	ALA	ASP	GLU	LEU	ALA								
PHE	ILE	PRO	THR	ILE	VAL	ASN	PHE	SER	ALA	GLU	GLY	GLU	ILE	ARG	GLY	LYS	MET	LYS	ASN	TYR	MET	VAL	PRO	ALA	ALA	TYR	ASN	LYS	ARG	ALA	CYS	LEU	TYR	LYS	ALA	GLY	GLU	TYR	PRO	MET	THR	VAL	LYS	TRP	ASP	GLN	MET	SER	GLN	ILE	ALA	GLN	ARG	LYS	GLY	ASP	VAL	LEU	ASP	GLU	ASN



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50945	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.817	Depositor
Minimum map value	-0.311	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	333.312, 333.312, 333.312	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.302, 1.302, 1.302	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.18	0/24908	0.40	1/33751 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1862	ALA	CB-CA-C	-5.13	110.68	116.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1603	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	24390	0	24462	826	0
2	A	31	0	12	4	0
3	A	54	0	24	7	0
4	A	1	0	0	0	0
All	All	24476	0	24498	826	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 17.

All (826) 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:1457:MET:HE1	1:A:3659:ARG:HA	1.41	1.03
1:A:2444:GLU:H	1:A:2510:MET:HE1	1.33	0.92
1:A:2667:ASN:HD22	1:A:2712:CYS:HB2	1.35	0.91
1:A:1550:ILE:HG23	1:A:1638:LEU:HD21	1.51	0.90
1:A:3206:ARG:HH12	1:A:3209:LYS:HD3	1.35	0.89
1:A:2232:MET:HE3	1:A:2232:MET:H	1.37	0.88
1:A:2307:VAL:HA	1:A:2311:TRP:HE1	1.42	0.83
1:A:2238:LEU:HD11	1:A:2249:GLY:HA3	1.63	0.80
1:A:4169:ILE:HD11	1:A:4177:ALA:HA	1.63	0.80
1:A:3207:LYS:HZ1	1:A:3753:LEU:HB3	1.47	0.78
1:A:1360:ARG:NH2	1:A:2902:GLU:OE1	2.17	0.76
1:A:3889:ARG:HH22	1:A:4347:GLN:HG3	1.51	0.76
1:A:1411:ARG:HA	1:A:1414:LYS:HE2	1.66	0.75
1:A:1462:PHE:HB2	1:A:3628:ARG:HD3	1.69	0.75
1:A:3212:VAL:HG22	1:A:3482:LEU:HD13	1.69	0.75
1:A:4377:MET:HE3	1:A:4438:CYS:HA	1.67	0.75
1:A:4539:LEU:HD12	1:A:4592:TRP:HB3	1.68	0.74
1:A:3659:ARG:HE	1:A:3661:LEU:HD21	1.49	0.74
1:A:1417:MET:HE1	1:A:1424:TRP:HB2	1.70	0.73
1:A:2304:ASP:OD1	1:A:2726:ARG:NH2	2.21	0.73
1:A:3662:ILE:HD11	1:A:3671:LEU:HD12	1.69	0.73
1:A:3481:SER:HB3	1:A:3770:LEU:HD22	1.69	0.72
1:A:2294:GLU:O	1:A:2299:GLN:NE2	2.22	0.72
1:A:3951:VAL:HA	1:A:3957:PHE:CE2	2.25	0.72
1:A:2874:SER:HB2	1:A:2920:LEU:HD11	1.70	0.71
1:A:3115:LEU:HG	1:A:3143:ILE:HG13	1.72	0.70
1:A:3488:ARG:HA	1:A:3491:LYS:HD3	1.73	0.70
1:A:3536:LEU:HB3	1:A:3541:ILE:HB	1.71	0.70
1:A:1530:ILE:HD11	1:A:1589:MET:HE1	1.74	0.70
1:A:2581:LEU:HD12	1:A:2591:LEU:HD21	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2856:LYS:HG3	1:A:2857:HIS:HD2	1.56	0.70
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.73	0.69
1:A:1963:LEU:HB3	1:A:1967:MET:HG3	1.75	0.69
1:A:3838:ASN:OD1	1:A:3870:ARG:NH2	2.25	0.69
1:A:2606:PHE:HE1	1:A:2617:VAL:HG11	1.57	0.69
1:A:3885:MET:HE1	1:A:4008:PHE:HD2	1.56	0.68
1:A:4085:ASN:O	1:A:4089:LYS:NZ	2.26	0.68
1:A:4234:SER:HB3	1:A:4237:LYS:HG2	1.76	0.68
1:A:2845:TRP:O	1:A:2849:ASN:ND2	2.24	0.68
1:A:4173:PRO:HD2	1:A:4223:LEU:HD21	1.75	0.68
1:A:4244:LYS:NZ	1:A:4273:PHE:O	2.24	0.68
1:A:3835:ILE:HD12	1:A:3870:ARG:HG3	1.75	0.67
1:A:2964:HIS:HA	1:A:3643:PRO:HG2	1.76	0.67
1:A:2096:VAL:HG12	1:A:2097:LEU:HD23	1.76	0.67
1:A:3532:TRP:O	1:A:3536:LEU:HD12	1.94	0.67
1:A:1835:SER:OG	1:A:1837:GLU:OE1	2.11	0.67
1:A:1964:GLU:HG2	1:A:1967:MET:HE3	1.77	0.67
1:A:2377:ASN:OD1	2:A:4701:ATP:O2'	2.12	0.67
1:A:1861:MET:HE1	1:A:1889:TYR:HB3	1.76	0.67
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.77	0.67
1:A:1420:LEU:HD13	1:A:1437:VAL:HG11	1.76	0.67
1:A:2053:MET:HE2	1:A:2097:LEU:HB2	1.76	0.66
1:A:2652:PRO:HB3	1:A:2659:LEU:HD12	1.77	0.66
1:A:4003:ALA:O	1:A:4006:HIS:HB3	1.95	0.66
1:A:1356:PRO:HB2	1:A:1401:ILE:HD13	1.77	0.66
1:A:2577:HIS:O	1:A:2581:LEU:HD22	1.96	0.66
1:A:4180:TYR:OH	1:A:4220:ASP:OD2	2.12	0.66
1:A:3475:SER:O	1:A:3479:LEU:HD22	1.96	0.66
1:A:3559:ARG:NH2	1:A:3737:GLU:OE1	2.28	0.66
1:A:2775:GLU:O	1:A:2779:MET:HG3	1.96	0.66
1:A:1478:VAL:HG11	1:A:1488:ARG:HE	1.61	0.66
1:A:3133:LEU:HD11	1:A:3141:GLU:HB3	1.76	0.66
1:A:3731:LEU:HD13	1:A:3734:LEU:HD22	1.77	0.65
1:A:3973:LEU:HD12	1:A:3992:LEU:HD11	1.78	0.65
1:A:3875:MET:HE1	1:A:3883:PHE:HB2	1.76	0.65
1:A:1598:GLN:NE2	1:A:1602:GLU:OE2	2.28	0.65
1:A:2210:LEU:O	1:A:2214:THR:HG23	1.97	0.65
1:A:3856:LEU:O	1:A:3860:THR:HG23	1.96	0.65
1:A:1941:MET:SD	1:A:1942:GLY:N	2.70	0.65
1:A:2970:GLU:N	1:A:2970:GLU:OE1	2.26	0.65
1:A:2382:LEU:HD22	1:A:2420:ALA:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3186:LEU:HD21	1:A:3510:SER:HB2	1.77	0.64
1:A:3537:GLN:HB3	1:A:3543:PHE:HE1	1.62	0.64
1:A:1551:PHE:HB3	1:A:1558:LYS:HZ3	1.61	0.64
1:A:2043:LYS:HE3	1:A:2044:PRO:HD2	1.79	0.64
1:A:4075:GLU:O	1:A:4079:GLN:NE2	2.27	0.64
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.79	0.64
1:A:1510:SER:HB2	1:A:3629:PHE:HB3	1.79	0.63
1:A:3115:LEU:HD23	1:A:3140:ARG:HD3	1.79	0.63
1:A:4157:MET:HE1	1:A:4185:TRP:HA	1.79	0.63
1:A:2414:GLN:NE2	1:A:2418:ASP:OD1	2.22	0.63
1:A:3146:SER:O	1:A:3150:VAL:HG23	1.98	0.63
1:A:3879:ASP:OD2	1:A:4342:LYS:NZ	2.30	0.63
1:A:3585:ARG:NH1	1:A:3694:SER:O	2.32	0.62
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.64	0.62
1:A:3167:ARG:NH1	1:A:3519:TYR:OH	2.32	0.62
1:A:4097:LYS:HA	1:A:4127:THR:HG23	1.81	0.62
1:A:2987:ASN:OD1	1:A:3057:GLN:NE2	2.32	0.62
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.81	0.62
1:A:2346:GLN:HB2	1:A:2726:ARG:HD2	1.81	0.62
1:A:2752:ASN:ND2	1:A:2766:ALA:O	2.32	0.62
1:A:3553:LEU:HB2	1:A:3578:ILE:HD13	1.82	0.62
1:A:4206:GLU:N	1:A:4206:GLU:OE1	2.33	0.62
1:A:2536:ASP:OD1	1:A:2576:ARG:NH1	2.33	0.62
1:A:4247:MET:HE3	1:A:4247:MET:HA	1.81	0.62
1:A:4248:ALA:HB2	1:A:4269:LEU:HD12	1.81	0.62
1:A:4042:LEU:HD23	1:A:4128:MET:HE1	1.82	0.62
1:A:2312:VAL:HA	1:A:2315:LEU:HD12	1.81	0.62
1:A:1351:TRP:HE3	1:A:1429:LEU:HB3	1.65	0.62
1:A:1460:GLU:HA	1:A:1463:LEU:HG	1.81	0.62
1:A:2088:PHE:CE2	1:A:2145:MET:HE2	2.34	0.61
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	1.82	0.61
1:A:3211:THR:O	1:A:3215:VAL:HG22	1.99	0.61
1:A:1965:GLU:OE1	1:A:1965:GLU:N	2.32	0.61
1:A:2210:LEU:HD22	1:A:2222:MET:HE1	1.83	0.61
1:A:2222:MET:HB2	1:A:2344:GLU:HA	1.82	0.61
1:A:2603:MET:HE1	3:A:4702:ADP:N6	2.15	0.61
1:A:4247:MET:HB2	1:A:4269:LEU:HD11	1.83	0.61
1:A:2715:PRO:HA	1:A:2720:ARG:HB3	1.83	0.61
1:A:3828:SER:HB2	1:A:4140:ARG:HG3	1.81	0.61
1:A:1408:LEU:HD21	1:A:1450:LEU:HD22	1.81	0.61
1:A:3158:ASN:ND2	1:A:3169:MET:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4013:LEU:HB3	1:A:4017:PHE:CD2	2.36	0.61
1:A:4401:THR:OG1	1:A:4404:ASN:ND2	2.33	0.61
1:A:2386:PRO:HG3	1:A:2413:LEU:HD22	1.83	0.61
1:A:3917:SER:HB2	1:A:3920:SER:HB3	1.82	0.60
1:A:1477:LEU:HD11	1:A:1582:VAL:HG12	1.83	0.60
1:A:1816:VAL:HG11	1:A:2052:VAL:HG12	1.83	0.60
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.82	0.60
1:A:2940:GLY:HA3	1:A:3174:ARG:HG3	1.83	0.60
1:A:1650:LEU:HD21	1:A:1698:ILE:HD11	1.83	0.60
1:A:1923:LEU:O	1:A:1925:ARG:NH1	2.34	0.60
1:A:1701:TRP:O	1:A:1705:VAL:HG23	2.01	0.60
1:A:3206:ARG:NH1	1:A:3209:LYS:HD3	2.13	0.60
1:A:2088:PHE:HE2	1:A:2145:MET:HE2	1.67	0.60
1:A:2889:LEU:HD21	1:A:2920:LEU:HD21	1.83	0.60
1:A:1880:VAL:HG21	1:A:2052:VAL:HG21	1.83	0.60
1:A:2665:GLU:HB3	1:A:2668:LEU:HB2	1.82	0.60
1:A:2581:LEU:HD12	1:A:2591:LEU:CD2	2.32	0.60
1:A:3892:LEU:HD11	1:A:3983:ILE:HG21	1.84	0.60
1:A:4403:GLU:OE2	1:A:4403:GLU:N	2.33	0.60
1:A:2558:GLU:HG2	1:A:2560:HIS:H	1.67	0.59
1:A:3791:MET:SD	1:A:3791:MET:N	2.74	0.59
1:A:2683:ILE:O	1:A:2687:VAL:HG12	2.02	0.59
1:A:3606:ASP:N	1:A:3606:ASP:OD1	2.33	0.59
1:A:1419:ARG:NH2	1:A:1448:ASP:OD2	2.35	0.59
1:A:3107:LYS:NZ	1:A:3140:ARG:HB3	2.17	0.59
1:A:2747:ILE:HD11	3:A:4702:ADP:C6	2.36	0.59
1:A:4393:GLN:HG2	1:A:4394:THR:HG22	1.84	0.59
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.84	0.59
1:A:4525:ARG:HG2	1:A:4536:LEU:HD22	1.82	0.59
1:A:1674:LEU:HB3	1:A:1685:MET:HE1	1.85	0.59
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.35	0.59
1:A:4482:PHE:O	1:A:4486:ILE:HG12	2.02	0.59
1:A:2444:GLU:N	1:A:2510:MET:HE1	2.11	0.59
1:A:4105:TRP:CE2	1:A:4109:LEU:HD21	2.38	0.59
1:A:2423:MET:HE1	1:A:2462:LEU:HD13	1.85	0.58
1:A:2943:LYS:N	3:A:4703:ADP:O1B	2.36	0.58
1:A:3933:GLU:OE1	1:A:3937:ARG:NH2	2.34	0.58
1:A:1812:ILE:O	1:A:1816:VAL:HG12	2.02	0.58
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.84	0.58
1:A:2598:GLY:HA3	1:A:2795:SER:HB2	1.84	0.58
1:A:3148:VAL:O	1:A:3152:GLN:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3101:ALA:O	1:A:3105:VAL:HG23	2.03	0.58
1:A:3882:THR:O	1:A:3886:LEU:HD22	2.04	0.58
1:A:4202:SER:OG	1:A:4261:ASP:OD2	2.21	0.58
1:A:2503:SER:HB3	1:A:2514:LEU:HD13	1.85	0.58
1:A:2527:PRO:HD3	1:A:2545:TRP:CE2	2.38	0.58
1:A:4511:LEU:HG	1:A:4560:VAL:HG11	1.84	0.58
1:A:1331:GLY:O	1:A:1335:GLU:HG2	2.04	0.58
1:A:1589:MET:SD	1:A:1589:MET:N	2.77	0.58
1:A:2677:GLN:HB2	1:A:2680:ILE:HG12	1.84	0.58
1:A:3739:GLN:O	1:A:3743:ARG:HG2	2.03	0.58
1:A:3692:LEU:O	1:A:3696:VAL:HG12	2.04	0.58
1:A:3885:MET:HE3	1:A:3885:MET:HA	1.86	0.58
1:A:3910:ARG:HH21	1:A:4348:MET:HE2	1.67	0.58
1:A:1738:TYR:HE2	1:A:1792:LEU:HD21	1.69	0.57
1:A:2202:MET:SD	1:A:2202:MET:N	2.77	0.57
1:A:2816:LEU:HD23	1:A:2821:LEU:HD22	1.86	0.57
1:A:2889:LEU:O	1:A:2893:VAL:HG12	2.04	0.57
1:A:4398:LEU:HD12	1:A:4414:GLU:HG2	1.85	0.57
1:A:4436:GLN:HG3	1:A:4441:LYS:HB3	1.85	0.57
1:A:1484:CYS:HB2	1:A:1579:MET:HG3	1.87	0.57
1:A:1695:HIS:HB3	1:A:1700:GLU:HG3	1.87	0.57
1:A:1891:THR:HG22	1:A:4250:SER:HA	1.87	0.57
1:A:2581:LEU:O	1:A:2585:LEU:HG	2.04	0.57
1:A:2654:GLN:NE2	1:A:2655:LEU:O	2.37	0.57
1:A:4103:PRO:HA	1:A:4106:LEU:HD12	1.86	0.57
1:A:3871:VAL:HG12	1:A:3875:MET:HE2	1.86	0.57
1:A:1452:VAL:O	1:A:1456:GLU:HG2	2.04	0.57
1:A:1530:ILE:HG23	1:A:1534:PHE:CE1	2.39	0.57
1:A:1731:THR:OG1	1:A:1732:SER:N	2.37	0.57
1:A:2210:LEU:HG	1:A:2237:LEU:HD23	1.87	0.57
1:A:2964:HIS:ND1	1:A:2965:ARG:O	2.37	0.57
1:A:3040:GLU:OE1	1:A:3053:TRP:NE1	2.38	0.57
1:A:2096:VAL:HG22	1:A:2144:THR:HG21	1.87	0.56
1:A:3514:ILE:HD11	1:A:3582:ARG:HB2	1.86	0.56
1:A:1342:GLN:O	1:A:1346:MET:HG3	2.05	0.56
1:A:1425:VAL:HB	1:A:1428:GLU:HB3	1.87	0.56
1:A:1644:SER:OG	1:A:1645:LYS:NZ	2.38	0.56
1:A:2048:LEU:O	1:A:2052:VAL:HG22	2.05	0.56
1:A:3110:THR:HB	1:A:3113:MET:HG3	1.87	0.56
1:A:2839:GLU:OE1	1:A:2841:GLU:HB3	2.05	0.56
1:A:2028:LEU:HD23	1:A:2033:LYS:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2526:LEU:HG	1:A:2527:PRO:HD2	1.87	0.56
1:A:2679:VAL:O	1:A:2683:ILE:HG13	2.06	0.56
1:A:3731:LEU:HG	1:A:3791:MET:HE1	1.87	0.56
1:A:4288:VAL:HG11	1:A:4294:ILE:HD11	1.87	0.56
1:A:1628:ARG:HG2	1:A:1657:MET:SD	2.46	0.56
1:A:2808:GLU:OE2	1:A:2811:ARG:NH2	2.38	0.56
1:A:2999:VAL:HG13	1:A:3005:LEU:HD21	1.88	0.56
1:A:1933:ASP:OD1	1:A:1933:ASP:N	2.36	0.55
1:A:2573:ASP:O	1:A:2577:HIS:ND1	2.33	0.55
1:A:3654:ARG:HH22	1:A:3663:THR:H	1.54	0.55
1:A:2127:ILE:O	1:A:2131:LEU:HG	2.06	0.55
1:A:3483:SER:O	1:A:3487:GLU:HG2	2.06	0.55
1:A:2190:TYR:O	1:A:2377:ASN:ND2	2.39	0.55
1:A:1974:GLN:O	1:A:1978:ILE:HG12	2.06	0.55
1:A:2126:GLU:O	1:A:2130:ASN:ND2	2.40	0.55
1:A:2375:PHE:HE2	1:A:2455:LEU:HD11	1.72	0.55
1:A:4169:ILE:HG21	1:A:4302:ARG:HD3	1.89	0.55
1:A:2147:PRO:HG3	1:A:2209:GLN:HB3	1.89	0.55
1:A:2910:VAL:HG11	1:A:3105:VAL:HG22	1.89	0.55
1:A:3175:HIS:CE1	1:A:3585:ARG:HH12	2.25	0.55
1:A:2373:MET:HE3	2:A:4701:ATP:N3	2.21	0.55
1:A:3130:TYR:CZ	1:A:3132:LYS:HB3	2.42	0.55
1:A:1362:ASN:OD1	1:A:1363:LEU:N	2.38	0.55
1:A:1397:ASN:O	1:A:1401:ILE:HG12	2.07	0.55
1:A:2143:GLU:OE2	1:A:2170:TYR:OH	2.25	0.55
1:A:3126:MET:HG3	1:A:3128:VAL:HG23	1.88	0.55
1:A:3191:ARG:HG2	1:A:3503:ILE:HD13	1.89	0.55
1:A:4542:GLU:HB2	1:A:4591:ARG:HG2	1.89	0.55
1:A:2510:MET:HA	1:A:2513:GLU:HG2	1.89	0.55
1:A:3586:TYR:O	1:A:3696:VAL:HG23	2.06	0.55
1:A:2684:ARG:HH22	1:A:2726:ARG:HH21	1.55	0.54
1:A:2995:ASP:OD1	1:A:2996:GLU:N	2.34	0.54
1:A:4108:GLN:HA	1:A:4111:LYS:HD2	1.89	0.54
1:A:2229:GLY:N	2:A:4701:ATP:O1A	2.37	0.54
1:A:2277:ASP:OD1	1:A:2285:ARG:NH2	2.33	0.54
1:A:2961:ILE:HD11	1:A:2998:ASN:HD22	1.72	0.54
1:A:4023:GLN:HG2	1:A:4024:PRO:HD2	1.89	0.54
1:A:4088:VAL:HG23	1:A:4118:PRO:HA	1.89	0.54
1:A:2994:MET:HE2	1:A:3066:PHE:HE1	1.72	0.54
1:A:3807:ALA:O	1:A:3811:ILE:HG12	2.07	0.54
1:A:1466:ILE:HD12	1:A:1500:HIS:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2499:LEU:HD21	1:A:2518:ILE:HG21	1.89	0.54
1:A:2935:LEU:HD22	1:A:3094:PHE:HE1	1.73	0.54
1:A:4088:VAL:HG21	1:A:4116:LEU:HD11	1.89	0.54
1:A:2644:THR:OG1	1:A:2647:GLY:O	2.23	0.54
1:A:3505:GLY:O	1:A:3509:LEU:HD23	2.08	0.54
1:A:2224:GLY:O	1:A:2230:LYS:NZ	2.40	0.54
1:A:2366:GLU:OE2	1:A:2451:ARG:NH2	2.41	0.54
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.41	0.54
1:A:4408:PRO:O	1:A:4411:ARG:HG2	2.08	0.54
1:A:4042:LEU:HD21	1:A:4138:LEU:HG	1.89	0.54
1:A:2609:LEU:HD22	1:A:2615:MET:HG3	1.89	0.53
1:A:2664:ASP:OD1	1:A:2665:GLU:HG2	2.07	0.53
1:A:2873:TYR:CE2	1:A:2883:PRO:HD3	2.43	0.53
1:A:4051:ALA:HA	1:A:4054:HIS:CE1	2.43	0.53
1:A:4240:TRP:HB3	1:A:4244:LYS:NZ	2.23	0.53
1:A:2175:MET:HB3	1:A:2178:LEU:HD13	1.89	0.53
1:A:2299:GLN:O	1:A:2339:VAL:HA	2.07	0.53
1:A:2602:THR:HG22	1:A:2662:PHE:HZ	1.73	0.53
1:A:2614:ASP:O	1:A:2615:MET:HE2	2.07	0.53
1:A:4082:LYS:O	1:A:4086:THR:HG23	2.08	0.53
1:A:2175:MET:SD	1:A:2175:MET:N	2.82	0.53
1:A:3100:GLU:HG2	1:A:3130:TYR:HE1	1.74	0.53
1:A:3592:PRO:HB3	1:A:3684:PRO:HD3	1.90	0.53
1:A:2757:ARG:HG3	1:A:2763:ARG:HH22	1.74	0.53
1:A:2030:ASP:HA	1:A:2033:LYS:HB2	1.89	0.53
1:A:2438:GLU:O	1:A:2442:GLN:HG2	2.08	0.53
1:A:2585:LEU:HB3	1:A:2707:GLN:HE22	1.73	0.53
1:A:1858:SER:HB3	1:A:1865:LYS:HE2	1.91	0.53
1:A:3133:LEU:HD12	1:A:3134:PRO:HD2	1.90	0.53
1:A:2124:GLU:HA	1:A:2127:ILE:HD12	1.90	0.53
1:A:2603:MET:HE1	3:A:4702:ADP:C6	2.43	0.53
1:A:3873:ARG:HH12	1:A:4021:MET:HA	1.73	0.53
1:A:2994:MET:HE2	1:A:3066:PHE:CE1	2.44	0.52
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.92	0.52
1:A:3654:ARG:CZ	1:A:3663:THR:HG23	2.38	0.52
1:A:1792:LEU:O	1:A:1796:VAL:HG12	2.08	0.52
1:A:1961:ASN:ND2	1:A:2019:ASN:O	2.43	0.52
1:A:2257:LYS:O	1:A:2678:ARG:NE	2.39	0.52
1:A:4459:ILE:HG22	1:A:4462:ARG:HH12	1.73	0.52
1:A:4535:SER:OG	1:A:4537:GLU:OE1	2.27	0.52
1:A:2307:VAL:HG13	1:A:2312:VAL:HG11	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2538:GLU:HB2	1:A:2548:TRP:CE2	2.44	0.52
1:A:2671:MET:HE2	1:A:2721:LYS:HG2	1.92	0.52
1:A:3851:ASP:HB3	1:A:3854:GLN:HB2	1.92	0.52
1:A:3989:ARG:O	1:A:4004:MET:HE1	2.10	0.52
1:A:2795:SER:OG	1:A:2798:GLU:OE1	2.21	0.52
1:A:3645:LEU:HD12	1:A:3648:VAL:HB	1.92	0.52
1:A:2503:SER:HB2	1:A:2511:ARG:HG2	1.91	0.52
1:A:1971:VAL:HA	1:A:1974:GLN:OE1	2.09	0.52
1:A:2445:HIS:NE2	1:A:2449:LEU:HD22	2.25	0.52
1:A:2515:GLY:O	1:A:2518:ILE:HG22	2.10	0.52
1:A:3789:ILE:HD12	1:A:3792:GLN:NE2	2.23	0.52
1:A:4080:ALA:O	1:A:4084:ILE:HG12	2.10	0.52
1:A:1410:ASP:O	1:A:1414:LYS:HG3	2.09	0.52
1:A:1530:ILE:HG23	1:A:1534:PHE:HE1	1.74	0.52
1:A:1667:ASN:HB2	1:A:1672:VAL:HG22	1.92	0.52
1:A:4108:GLN:O	1:A:4112:LYS:HG2	2.08	0.51
1:A:4561:THR:HG22	1:A:4587:LEU:HD23	1.92	0.51
1:A:1397:ASN:O	1:A:1397:ASN:ND2	2.37	0.51
1:A:2629:GLU:O	1:A:2633:LYS:HG2	2.10	0.51
1:A:3219:ARG:HD3	1:A:3479:LEU:HD21	1.92	0.51
1:A:3954:ASP:HB3	1:A:3957:PHE:CD2	2.45	0.51
1:A:1802:PRO:O	1:A:1806:ARG:HG2	2.11	0.51
1:A:3703:VAL:HG21	1:A:3829:LEU:HD22	1.93	0.51
1:A:1626:PHE:HB3	1:A:1629:PHE:CD2	2.45	0.51
1:A:1698:ILE:HA	1:A:1701:TRP:NE1	2.25	0.51
1:A:1938:PHE:HA	1:A:1941:MET:HG3	1.92	0.51
1:A:2893:VAL:HG11	1:A:2916:LEU:HD21	1.93	0.51
1:A:3208:ILE:O	1:A:3212:VAL:HG23	2.10	0.51
1:A:4569:THR:HG22	1:A:4583:THR:HG21	1.92	0.51
1:A:2134:GLN:O	1:A:2138:ILE:HG22	2.10	0.51
1:A:2666:ILE:HG22	1:A:2712:CYS:HB3	1.93	0.51
1:A:3886:LEU:O	1:A:3890:ILE:HG12	2.11	0.51
1:A:1769:MET:HE2	1:A:1774:ASP:O	2.11	0.51
1:A:1944:ILE:O	1:A:1948:LEU:HG	2.11	0.51
1:A:3139:HIS:O	1:A:3143:ILE:HG12	2.10	0.51
1:A:4488:GLN:O	1:A:4492:ILE:HG12	2.11	0.51
1:A:1961:ASN:ND2	1:A:2019:ASN:H	2.09	0.51
1:A:2660:VAL:HA	1:A:2707:GLN:O	2.10	0.51
1:A:3544:ARG:HB2	1:A:3547:ILE:HD11	1.92	0.51
1:A:1546:TYR:O	1:A:1550:ILE:HG12	2.11	0.51
1:A:1752:LEU:O	1:A:1756:ILE:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1810:HIS:NE2	1:A:1876:GLN:O	2.44	0.51
1:A:1817:HIS:O	1:A:1821:VAL:HG12	2.10	0.51
1:A:2791:HIS:HB3	1:A:3086:PHE:HE1	1.76	0.51
1:A:2028:LEU:HD23	1:A:2033:LYS:HG3	1.91	0.50
1:A:2057:GLN:NE2	1:A:2098:VAL:HA	2.27	0.50
1:A:2937:GLY:HA2	1:A:3095:GLY:HA2	1.92	0.50
1:A:1473:TYR:OH	1:A:1492:ASP:OD2	2.24	0.50
1:A:1816:VAL:HG11	1:A:2052:VAL:CG1	2.41	0.50
1:A:1850:GLN:HB2	1:A:1856:GLN:HG2	1.92	0.50
1:A:2290:SER:HA	1:A:2294:GLU:HG2	1.92	0.50
1:A:2569:VAL:HB	1:A:2747:ILE:HG13	1.94	0.50
1:A:3140:ARG:O	1:A:3144:VAL:HG13	2.11	0.50
1:A:1521:LEU:HD13	1:A:1524:GLU:OE1	2.10	0.50
1:A:1747:ALA:HB2	1:A:1807:LYS:HG2	1.92	0.50
1:A:1562:PRO:O	1:A:1564:GLU:N	2.42	0.50
1:A:1650:LEU:HA	1:A:1653:HIS:HD2	1.75	0.50
1:A:2888:GLU:OE1	1:A:2888:GLU:N	2.42	0.50
1:A:1836:PHE:CD2	1:A:4242:ALA:HA	2.47	0.50
1:A:2818:VAL:O	1:A:2822:ILE:HG12	2.11	0.50
1:A:3544:ARG:HH11	1:A:3544:ARG:HG3	1.76	0.50
1:A:3580:LEU:HD21	1:A:3699:VAL:HG11	1.93	0.50
1:A:4288:VAL:HG21	1:A:4294:ILE:HG12	1.94	0.50
1:A:2373:MET:HE3	2:A:4701:ATP:C4	2.47	0.50
1:A:2513:GLU:O	1:A:2516:GLU:HG3	2.11	0.50
1:A:2050:ALA:O	1:A:2054:LEU:HG	2.11	0.50
1:A:2319:LEU:HB3	1:A:2358:ARG:HB3	1.93	0.50
1:A:4424:LEU:HD12	1:A:4486:ILE:HG21	1.93	0.50
1:A:2310:GLU:N	1:A:2310:GLU:OE2	2.44	0.50
1:A:2635:PHE:HB3	1:A:2650:LEU:HD21	1.94	0.50
1:A:4164:ILE:HD12	1:A:4165:PRO:HD2	1.93	0.50
1:A:2455:LEU:HD12	1:A:2459:PHE:CZ	2.47	0.49
1:A:2880:ASP:HB2	1:A:2882:ILE:HD11	1.94	0.49
1:A:3491:LYS:O	1:A:3495:THR:HG23	2.11	0.49
1:A:4385:SER:O	1:A:4389:HIS:ND1	2.45	0.49
1:A:4485:ARG:NH1	1:A:4513:GLY:O	2.46	0.49
1:A:1687:LYS:HG3	1:A:1715:LYS:HE3	1.94	0.49
1:A:2323:LYS:HB3	1:A:2335:LEU:HB3	1.94	0.49
1:A:4480:SER:O	1:A:4484:GLU:HG2	2.12	0.49
1:A:2278:GLY:N	1:A:2281:THR:OG1	2.45	0.49
1:A:2373:MET:HE2	1:A:2374:ILE:N	2.26	0.49
1:A:4099:VAL:HG22	1:A:4128:MET:HB2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1457:MET:HA	1:A:1460:GLU:HG3	1.94	0.49
1:A:1891:THR:HG21	1:A:2039:LEU:HD13	1.94	0.49
1:A:2053:MET:HB3	1:A:2097:LEU:HD12	1.93	0.49
1:A:3811:ILE:O	1:A:3815:MET:HG3	2.13	0.49
1:A:3881:ILE:HD13	1:A:4018:MET:HE1	1.93	0.49
1:A:1500:HIS:O	1:A:1504:VAL:HG12	2.13	0.49
1:A:1544:TRP:HE1	1:A:1572:SER:HA	1.77	0.49
1:A:1794:ASP:OD2	1:A:2060:ARG:NH1	2.45	0.49
1:A:2041:MET:HE3	1:A:2042:THR:H	1.78	0.49
1:A:1537:TRP:CE3	1:A:1601:LEU:HD11	2.47	0.49
1:A:3486:ARG:O	1:A:3490:GLU:HG2	2.12	0.49
1:A:4082:LYS:HD3	1:A:4082:LYS:N	2.28	0.49
1:A:1398:MET:SD	1:A:1399:LEU:N	2.85	0.49
1:A:2109:GLN:HB3	1:A:2113:ARG:NH2	2.28	0.49
1:A:3588:LEU:HB2	1:A:3696:VAL:HG21	1.94	0.49
1:A:3622:ASN:O	1:A:3625:SER:OG	2.25	0.49
1:A:3967:GLU:HB2	1:A:4004:MET:HB2	1.95	0.49
1:A:4297:PRO:HB3	1:A:4308:TRP:CD1	2.48	0.49
1:A:2028:LEU:HD21	1:A:2036:PHE:HB2	1.94	0.49
1:A:2332:ARG:HH21	1:A:2334:SER:HB3	1.77	0.49
1:A:3478:LEU:O	1:A:3482:LEU:HG	2.13	0.49
1:A:3989:ARG:C	1:A:4004:MET:HE1	2.37	0.49
1:A:4073:SER:OG	1:A:4075:GLU:OE1	2.30	0.49
1:A:4563:LEU:HD23	1:A:4644:CYS:HA	1.94	0.49
1:A:3517:ALA:HA	1:A:3520:PHE:HD1	1.78	0.49
1:A:3891:LYS:HD3	1:A:4013:LEU:HD23	1.95	0.49
1:A:1667:ASN:HD22	1:A:1672:VAL:HG22	1.77	0.49
1:A:1720:SER:O	1:A:1724:VAL:HG23	2.13	0.49
1:A:3986:ALA:HA	1:A:3989:ARG:HE	1.78	0.49
1:A:4257:ASP:OD1	1:A:4258:ASN:N	2.46	0.49
1:A:4377:MET:HE1	1:A:4437:VAL:HG12	1.95	0.49
1:A:1947:GLY:O	1:A:1951:VAL:HG22	2.13	0.48
1:A:2049:ILE:HG21	1:A:2090:LEU:HD11	1.95	0.48
1:A:4510:CYS:SG	1:A:4561:THR:OG1	2.69	0.48
1:A:1676:ILE:HG12	1:A:1684:VAL:HB	1.95	0.48
1:A:2071:PRO:O	1:A:2075:LEU:HG	2.12	0.48
1:A:2297:LYS:HB2	1:A:2299:GLN:HE21	1.78	0.48
1:A:2363:TRP:HE1	1:A:2365:SER:HB3	1.76	0.48
1:A:2481:MET:HE2	1:A:2481:MET:HA	1.95	0.48
1:A:2773:MET:HE2	1:A:2802:TRP:CG	2.47	0.48
1:A:3756:VAL:HB	1:A:3759:ARG:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3801:TYR:HD2	1:A:3856:LEU:HD13	1.78	0.48
1:A:3973:LEU:HD12	1:A:3992:LEU:CD1	2.43	0.48
1:A:4042:LEU:HD13	1:A:4142:GLY:HA3	1.94	0.48
1:A:1495:ASN:O	1:A:1499:GLU:HG2	2.12	0.48
1:A:2094:LYS:O	1:A:2098:VAL:HG12	2.13	0.48
1:A:3737:GLU:O	1:A:3741:ARG:HG2	2.13	0.48
1:A:2590:PRO:HG2	1:A:2687:VAL:HG21	1.95	0.48
1:A:1928:LEU:HB3	1:A:1930:PHE:CE1	2.47	0.48
1:A:2752:ASN:HD22	1:A:2770:THR:HB	1.77	0.48
1:A:3197:GLN:HB3	1:A:3496:PHE:CE2	2.48	0.48
1:A:2419:ALA:O	1:A:2423:MET:HG2	2.14	0.48
1:A:2934:LEU:HD12	1:A:2935:LEU:N	2.28	0.48
1:A:3204:GLY:O	1:A:3208:ILE:HG12	2.13	0.48
1:A:3490:GLU:O	1:A:3494:GLU:HG2	2.14	0.48
1:A:3724:VAL:HG13	1:A:3793:GLU:OE2	2.13	0.48
1:A:3856:LEU:O	1:A:3859:ILE:HG22	2.13	0.48
1:A:1332:VAL:HG23	1:A:1377:LEU:HB3	1.95	0.48
1:A:1798:MET:SD	1:A:1799:GLU:N	2.87	0.48
1:A:1738:TYR:CE2	1:A:1792:LEU:HD21	2.48	0.48
1:A:1898:ALA:O	1:A:1983:ARG:NH1	2.47	0.48
1:A:3591:ASP:CG	1:A:3594:GLY:H	2.22	0.48
1:A:3885:MET:HE1	1:A:4008:PHE:CD2	2.45	0.48
1:A:4192:GLU:OE1	1:A:4195:ARG:NH1	2.45	0.48
1:A:4492:ILE:HG22	1:A:4507:ILE:HG12	1.95	0.48
1:A:1460:GLU:HB3	1:A:1516:PHE:CE1	2.49	0.48
1:A:1661:VAL:HG22	1:A:1676:ILE:HD12	1.95	0.48
1:A:1909:GLY:O	1:A:2043:LYS:NZ	2.47	0.48
1:A:2461:MET:HE1	1:A:2500:TRP:HB3	1.94	0.48
1:A:2942:GLY:O	1:A:2946:LEU:HD22	2.14	0.48
1:A:3588:LEU:HD13	1:A:3679:LEU:HB3	1.96	0.48
1:A:3810:SER:HB3	1:A:3890:ILE:HD12	1.94	0.48
1:A:2703:LEU:HD12	1:A:2706:ILE:HD13	1.96	0.47
1:A:1444:ALA:HA	1:A:1447:LYS:HE2	1.95	0.47
1:A:2232:MET:H	1:A:2232:MET:CE	2.18	0.47
1:A:4194:LEU:HD12	1:A:4194:LEU:H	1.80	0.47
1:A:1397:ASN:HD22	1:A:1397:ASN:C	2.15	0.47
1:A:2418:ASP:O	1:A:2422:ILE:HG12	2.14	0.47
1:A:2614:ASP:OD1	1:A:2614:ASP:N	2.47	0.47
1:A:1711:VAL:HG12	1:A:1715:LYS:HE2	1.96	0.47
1:A:2303:PHE:CD2	1:A:2341:ILE:HD11	2.49	0.47
1:A:4093:TRP:CD1	1:A:4123:ARG:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2000:GLU:HG2	1:A:2005:GLN:HE22	1.78	0.47
1:A:3189:GLU:OE1	1:A:3582:ARG:NH2	2.47	0.47
1:A:3769:THR:O	1:A:3773:LEU:HD12	2.14	0.47
1:A:1551:PHE:HB3	1:A:1558:LYS:NZ	2.28	0.47
1:A:2500:TRP:CD2	1:A:2580:LEU:HD11	2.49	0.47
1:A:2969:GLY:HA2	1:A:3004:PHE:HE1	1.78	0.47
1:A:2998:ASN:OD1	1:A:2998:ASN:N	2.45	0.47
1:A:3012:LEU:HD11	1:A:3066:PHE:HE2	1.79	0.47
1:A:4016:SER:O	1:A:4016:SER:OG	2.30	0.47
1:A:4405:ILE:O	1:A:4411:ARG:NH2	2.48	0.47
1:A:1504:VAL:HA	1:A:1507:MET:HE2	1.95	0.47
1:A:2080:LEU:HD13	1:A:2149:LEU:HD11	1.97	0.47
1:A:2308:ASP:OD1	1:A:2311:TRP:HD1	1.97	0.47
1:A:4271:ARG:HG2	1:A:4633:ARG:NH1	2.30	0.47
1:A:2329:ASN:OD1	1:A:2330:GLY:N	2.47	0.47
1:A:4563:LEU:HD12	1:A:4588:THR:HG21	1.97	0.47
1:A:2614:ASP:C	1:A:2657:LYS:HD2	2.41	0.47
1:A:2905:LEU:HD12	1:A:2906:ASP:N	2.30	0.47
1:A:3866:VAL:O	1:A:3870:ARG:HG2	2.15	0.47
1:A:3923:ARG:HD3	1:A:3924:ILE:N	2.30	0.47
1:A:1350:PRO:O	1:A:1354:VAL:HG13	2.15	0.46
1:A:1426:VAL:HA	1:A:1429:LEU:HD13	1.96	0.46
1:A:1691:SER:O	1:A:1695:HIS:ND1	2.31	0.46
1:A:1751:VAL:O	1:A:1755:GLN:HG3	2.16	0.46
1:A:2798:GLU:OE1	1:A:2798:GLU:N	2.41	0.46
1:A:4301:ARG:NH1	1:A:4303:GLU:OE1	2.48	0.46
1:A:2218:HIS:HA	1:A:2340:ARG:HH11	1.79	0.46
1:A:2108:ILE:HG12	1:A:2131:LEU:HD11	1.97	0.46
1:A:2127:ILE:HA	1:A:2130:ASN:HD21	1.80	0.46
1:A:2881:TYR:HE1	1:A:2927:ARG:HH22	1.63	0.46
1:A:3537:GLN:HB3	1:A:3543:PHE:CE1	2.46	0.46
1:A:3716:VAL:HG23	1:A:3836:TYR:OH	2.15	0.46
1:A:1332:VAL:HB	1:A:1377:LEU:HD22	1.96	0.46
1:A:1867:ASN:O	1:A:1925:ARG:NH2	2.28	0.46
1:A:2203:TRP:CH2	1:A:2236:VAL:HG11	2.50	0.46
1:A:2495:VAL:O	1:A:2498:ILE:HG13	2.16	0.46
1:A:3566:SER:O	1:A:3566:SER:OG	2.34	0.46
1:A:1551:PHE:CE2	1:A:1565:THR:HA	2.51	0.46
1:A:2145:MET:O	1:A:2149:LEU:HD23	2.15	0.46
1:A:2301:ILE:O	1:A:2341:ILE:HD12	2.15	0.46
1:A:3624:GLU:HB3	1:A:3628:ARG:HH22	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4088:VAL:O	1:A:4119:HIS:N	2.48	0.46
1:A:4414:GLU:O	1:A:4418:LYS:HG2	2.16	0.46
1:A:1822:THR:O	1:A:1826:ILE:HG13	2.15	0.46
1:A:1867:ASN:OD1	1:A:1867:ASN:N	2.49	0.46
1:A:2505:ASP:HB3	1:A:2733:VAL:HG23	1.98	0.46
1:A:3114:ASP:HB2	1:A:3191:ARG:HH12	1.81	0.46
1:A:3476:THR:HA	1:A:3479:LEU:HD23	1.97	0.46
1:A:3947:LEU:HD23	1:A:3948:ILE:HD12	1.96	0.46
1:A:1766:LEU:HD11	1:A:1830:ILE:HG22	1.97	0.46
1:A:2207:VAL:O	1:A:2210:LEU:HB3	2.16	0.46
1:A:2760:PRO:HA	1:A:2763:ARG:HD3	1.96	0.46
1:A:3107:LYS:HZ1	1:A:3140:ARG:HB3	1.79	0.46
1:A:3604:TYR:HA	1:A:3607:ARG:HH21	1.81	0.46
1:A:3985:GLN:O	1:A:3989:ARG:HG3	2.15	0.46
1:A:1837:GLU:H	1:A:1837:GLU:CD	2.19	0.46
1:A:2953:MET:O	1:A:2953:MET:HE3	2.15	0.46
1:A:3659:ARG:HE	1:A:3661:LEU:CD2	2.24	0.46
1:A:4457:LYS:HB2	1:A:4459:ILE:HG12	1.97	0.46
1:A:2948:ARG:HG2	1:A:2958:VAL:HG21	1.98	0.46
1:A:3646:ASN:OD1	1:A:3695:ARG:NH1	2.49	0.46
1:A:4330:VAL:O	1:A:4333:THR:OG1	2.22	0.46
1:A:4451:LEU:HD23	1:A:4455:LEU:HD23	1.97	0.45
1:A:1449:VAL:HG23	1:A:1450:LEU:HD23	1.99	0.45
1:A:1864:ALA:HB1	1:A:1866:PHE:CZ	2.51	0.45
1:A:2965:ARG:HD3	1:A:3642:ASP:CG	2.40	0.45
1:A:2979:VAL:HG21	1:A:2992:PHE:HE2	1.80	0.45
1:A:3753:LEU:O	1:A:3756:VAL:HG22	2.16	0.45
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.51	0.45
1:A:2472:TYR:CD1	1:A:2541:ILE:HG21	2.51	0.45
1:A:3100:GLU:HG2	1:A:3130:TYR:CE1	2.51	0.45
1:A:4104:GLY:HA2	1:A:4107:MET:HE3	1.98	0.45
1:A:4215:ALA:O	1:A:4219:VAL:HG12	2.15	0.45
1:A:4302:ARG:NH2	1:A:4303:GLU:HG3	2.31	0.45
1:A:4633:ARG:O	1:A:4637:GLU:HG3	2.17	0.45
1:A:1443:GLU:O	1:A:1447:LYS:HG3	2.17	0.45
1:A:3568:PRO:HB2	1:A:3570:ASP:OD2	2.17	0.45
1:A:4460:LEU:O	1:A:4462:ARG:NH1	2.47	0.45
1:A:1417:MET:SD	1:A:1422:VAL:HG23	2.56	0.45
1:A:1872:TYR:CZ	1:A:1874:GLY:HA2	2.51	0.45
1:A:2229:GLY:HA2	1:A:2232:MET:HE1	1.98	0.45
1:A:2855:LEU:HD11	1:A:2863:ARG:HE	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1424:TRP:CH2	1:A:1434:ILE:HG22	2.52	0.45
1:A:1887:ARG:HH12	1:A:4253:GLY:C	2.25	0.45
1:A:2077:ASP:HA	1:A:2088:PHE:HD1	1.82	0.45
1:A:2152:GLU:OE1	1:A:2152:GLU:N	2.43	0.45
1:A:2642:ARG:HH12	1:A:2651:ALA:HB3	1.81	0.45
1:A:3705:ARG:HA	1:A:3813:PHE:HE2	1.82	0.45
1:A:4628:THR:C	1:A:4629:LYS:HD2	2.41	0.45
1:A:1581:LYS:O	1:A:1584:LYS:NZ	2.44	0.45
1:A:4071:ILE:HD11	1:A:4096:LEU:HD22	1.98	0.45
1:A:1649:LYS:HE3	1:A:1649:LYS:HB3	1.85	0.45
1:A:2031:ASN:OD1	1:A:2031:ASN:N	2.47	0.45
1:A:2623:SER:OG	1:A:3081:THR:O	2.21	0.45
1:A:2654:GLN:OE1	1:A:2657:LYS:HB2	2.16	0.45
1:A:3691:ASP:O	1:A:3695:ARG:HG3	2.17	0.45
1:A:4203:LYS:NZ	1:A:4205:TYR:OH	2.49	0.45
1:A:4489:LEU:HD13	1:A:4492:ILE:HD11	1.99	0.45
1:A:2057:GLN:NE2	1:A:2101:GLY:HA3	2.32	0.45
1:A:2107:ARG:HD2	1:A:2110:LYS:NZ	2.31	0.45
1:A:2269:ASP:HB3	1:A:2274:GLU:HB2	1.99	0.45
1:A:2694:ARG:O	1:A:2698:GLN:N	2.42	0.45
1:A:2705:ARG:H	1:A:2706:ILE:HD12	1.81	0.45
1:A:1446:VAL:O	1:A:1450:LEU:HG	2.17	0.45
1:A:1461:GLU:HA	1:A:1464:LYS:HD3	1.99	0.45
1:A:1486:LEU:HD23	1:A:1486:LEU:HA	1.81	0.45
1:A:1673:VAL:HG12	1:A:1686:PHE:HE1	1.81	0.45
1:A:1857:LEU:HD23	1:A:1857:LEU:HA	1.83	0.45
1:A:1860:GLN:HG2	1:A:1865:LYS:HD3	1.99	0.45
1:A:1979:GLN:HG3	1:A:2036:PHE:CE1	2.52	0.45
1:A:2219:GLY:HA2	1:A:2341:ILE:O	2.16	0.45
1:A:2755:MET:HG3	1:A:2807:PHE:HB2	1.98	0.45
1:A:4105:TRP:CZ2	1:A:4109:LEU:HD21	2.51	0.45
1:A:3107:LYS:O	1:A:3107:LYS:HD3	2.17	0.44
1:A:3132:LYS:HE2	1:A:3132:LYS:HB2	1.64	0.44
1:A:3557:ASP:OD1	1:A:3558:GLU:HG3	2.16	0.44
1:A:4172:SER:O	1:A:4176:ARG:NH1	2.49	0.44
1:A:1425:VAL:O	1:A:1428:GLU:N	2.44	0.44
1:A:2261:LYS:NZ	1:A:2310:GLU:O	2.51	0.44
1:A:2452:LEU:HD23	1:A:2452:LEU:HA	1.71	0.44
1:A:2481:MET:HE1	1:A:2485:GLN:OE1	2.17	0.44
1:A:2571:THR:HG23	1:A:2574:THR:H	1.83	0.44
1:A:2717:ASP:O	1:A:2720:ARG:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2849:ASN:O	1:A:2853:VAL:HG12	2.17	0.44
1:A:2891:ASP:O	1:A:2894:LYS:HG2	2.18	0.44
1:A:3044:LEU:HB3	1:A:3049:GLU:CD	2.43	0.44
1:A:4166:VAL:HA	1:A:4169:ILE:HG22	1.99	0.44
1:A:4257:ASP:OD1	1:A:4257:ASP:C	2.59	0.44
1:A:1392:GLY:HA2	1:A:1395:LYS:HE3	1.99	0.44
1:A:1445:ILE:O	1:A:1449:VAL:HG13	2.18	0.44
1:A:2308:ASP:HB2	1:A:2674:TYR:CD2	2.52	0.44
1:A:2792:TYR:CZ	1:A:2837:LEU:HD23	2.52	0.44
1:A:4027:LEU:HG	1:A:4058:LEU:HD22	1.99	0.44
1:A:2107:ARG:HA	1:A:2110:LYS:HG2	1.99	0.44
1:A:2439:HIS:O	1:A:2443:LEU:HG	2.17	0.44
1:A:3482:LEU:HD12	1:A:3483:SER:N	2.32	0.44
1:A:3750:LEU:O	1:A:3754:ASN:ND2	2.50	0.44
1:A:3831:PHE:O	1:A:3835:ILE:HG12	2.17	0.44
1:A:3835:ILE:HG23	1:A:3866:VAL:HG12	1.98	0.44
1:A:3944:PHE:O	1:A:3947:LEU:HD22	2.18	0.44
1:A:1529:ARG:O	1:A:1533:LEU:HD23	2.18	0.44
1:A:2527:PRO:HG3	1:A:2545:TRP:CG	2.52	0.44
1:A:3097:TRP:CZ3	1:A:3105:VAL:HG21	2.53	0.44
1:A:4025:LEU:HD23	1:A:4027:LEU:HB2	1.99	0.44
1:A:1392:GLY:HA2	1:A:1395:LYS:HG2	1.99	0.44
1:A:3524:MET:HE2	1:A:3524:MET:HA	1.99	0.44
1:A:2047:GLN:O	1:A:2051:GLN:HG3	2.18	0.44
1:A:1551:PHE:HE2	1:A:1565:THR:HA	1.83	0.44
1:A:2037:ARG:HH22	1:A:4211:ASP:HA	1.83	0.44
1:A:2133:GLU:H	1:A:2133:GLU:CD	2.26	0.44
1:A:3768:THR:O	1:A:3771:GLU:HG2	2.17	0.44
1:A:3776:GLU:O	1:A:3779:GLU:HG3	2.18	0.44
1:A:4470:PRO:HD2	1:A:4473:MET:SD	2.58	0.44
1:A:3757:LYS:HA	1:A:3757:LYS:HD2	1.84	0.44
1:A:4087:ALA:HA	1:A:4090:SER:OG	2.18	0.44
1:A:1456:GLU:CD	1:A:1512:TYR:HB3	2.42	0.43
1:A:3760:ILE:HD12	1:A:3766:ILE:HG21	1.99	0.43
1:A:3921:THR:HA	1:A:3936:VAL:HG21	2.00	0.43
1:A:3970:VAL:HG13	1:A:3992:LEU:HD22	1.99	0.43
1:A:1424:TRP:NE1	1:A:1433:GLN:HB3	2.32	0.43
1:A:2423:MET:HE1	1:A:2462:LEU:HD22	2.01	0.43
1:A:3219:ARG:HH11	1:A:3479:LEU:HD23	1.83	0.43
1:A:3733:LYS:HB2	1:A:3737:GLU:HB2	2.00	0.43
1:A:3787:THR:O	1:A:3790:VAL:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4113:LEU:HD11	1:A:4124:LEU:HD23	2.00	0.43
1:A:4536:LEU:HD23	1:A:4536:LEU:HA	1.81	0.43
1:A:1765:ALA:O	1:A:1769:MET:HG3	2.18	0.43
1:A:2041:MET:HE3	1:A:2041:MET:HA	2.00	0.43
1:A:2667:ASN:ND2	1:A:2712:CYS:HB2	2.17	0.43
1:A:2871:ILE:C	1:A:2872:LEU:HD23	2.43	0.43
1:A:2916:LEU:HD23	1:A:2916:LEU:HA	1.87	0.43
1:A:4178:ARG:O	1:A:4182:LEU:HG	2.19	0.43
1:A:4215:ALA:HB2	1:A:4247:MET:HE1	2.00	0.43
1:A:1363:LEU:HD11	1:A:1435:TRP:CZ2	2.53	0.43
1:A:1571:ILE:HG23	1:A:1604:LEU:HD22	2.01	0.43
1:A:2482:GLN:OE1	1:A:2483:ILE:N	2.51	0.43
1:A:2672:ASP:N	1:A:2676:THR:O	2.37	0.43
1:A:3511:ALA:O	1:A:3514:ILE:HG22	2.19	0.43
1:A:3731:LEU:CG	1:A:3791:MET:HE1	2.48	0.43
1:A:3983:ILE:O	1:A:3987:ILE:HG13	2.18	0.43
1:A:2238:LEU:HB2	1:A:2300:TRP:CZ3	2.53	0.43
1:A:2792:TYR:OH	1:A:2838:VAL:HG22	2.18	0.43
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.54	0.43
1:A:3102:LEU:HB3	1:A:3148:VAL:HG22	2.01	0.43
1:A:3167:ARG:CZ	1:A:3685:THR:HA	2.48	0.43
1:A:3557:ASP:OD1	1:A:3558:GLU:N	2.51	0.43
1:A:1697:LYS:O	1:A:1700:GLU:HG2	2.18	0.43
1:A:1967:MET:HE2	1:A:1967:MET:HB3	1.89	0.43
1:A:3544:ARG:HB2	1:A:3547:ILE:CD1	2.49	0.43
1:A:2606:PHE:CE1	1:A:2617:VAL:HG11	2.45	0.43
1:A:2622:PHE:CZ	1:A:2631:LEU:HD11	2.53	0.43
1:A:2651:ALA:HB1	1:A:2705:ARG:HH21	1.83	0.43
1:A:3129:VAL:HG11	1:A:3149:PHE:HD1	1.84	0.43
1:A:3612:THR:HB	1:A:3633:LEU:HD21	2.00	0.43
1:A:4190:ILE:HG22	1:A:4201:TRP:HZ2	1.84	0.43
1:A:4204:LYS:HE2	1:A:4204:LYS:HB2	1.89	0.43
1:A:1679:ARG:H	1:A:1679:ARG:HG3	1.69	0.43
1:A:2374:ILE:HD13	1:A:2374:ILE:HA	1.91	0.43
1:A:3721:ARG:HB3	1:A:3724:VAL:HG23	2.00	0.43
1:A:3903:ALA:HA	1:A:3906:GLN:NE2	2.33	0.43
1:A:4277:SER:HA	1:A:4282:PHE:CG	2.54	0.43
1:A:2237:LEU:HD12	1:A:2237:LEU:O	2.19	0.43
1:A:2992:PHE:O	1:A:3065:VAL:N	2.44	0.43
1:A:3012:LEU:HD11	1:A:3066:PHE:CE2	2.53	0.43
1:A:3174:ARG:NH1	1:A:3650:ASN:OD1	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3583:PHE:CD2	1:A:3587:PRO:HD3	2.54	0.43
1:A:3731:LEU:HA	1:A:3734:LEU:HB2	2.00	0.43
1:A:4206:GLU:H	1:A:4206:GLU:CD	2.26	0.43
1:A:4240:TRP:HB3	1:A:4244:LYS:HZ3	1.83	0.43
1:A:4376:TRP:O	1:A:4380:LEU:HG	2.18	0.43
1:A:1789:LEU:CD1	1:A:1815:LEU:HB3	2.49	0.43
1:A:2093:LEU:O	1:A:2097:LEU:HG	2.19	0.43
1:A:2616:GLU:HB2	1:A:2657:LYS:HE3	2.01	0.43
1:A:3073:GLU:OE2	1:A:3074:GLY:N	2.52	0.43
1:A:3644:VAL:O	1:A:3647:PRO:HD2	2.19	0.43
1:A:3793:GLU:O	1:A:3797:VAL:HG23	2.19	0.43
1:A:4401:THR:OG1	1:A:4403:GLU:OE2	2.21	0.43
1:A:2673:LYS:HB2	1:A:2674:TYR:CE1	2.54	0.42
1:A:3169:MET:SD	1:A:3169:MET:N	2.91	0.42
1:A:4095:MET:O	1:A:4096:LEU:HD23	2.19	0.42
1:A:4528:VAL:HG21	1:A:4592:TRP:HB2	2.01	0.42
1:A:4601:LYS:HB2	1:A:4604:VAL:HG13	2.01	0.42
1:A:1554:SER:O	1:A:1557:ILE:HG22	2.19	0.42
1:A:1667:ASN:OD1	1:A:1668:GLU:N	2.50	0.42
1:A:1718:ALA:O	1:A:1721:VAL:HG12	2.20	0.42
1:A:2104:LYS:HA	1:A:2136:ILE:HD13	2.01	0.42
1:A:3948:ILE:HD12	1:A:3948:ILE:H	1.84	0.42
1:A:1695:HIS:HB2	1:A:1701:TRP:HB3	2.00	0.42
1:A:1351:TRP:O	1:A:1354:VAL:HG22	2.19	0.42
1:A:2352:THR:HG23	1:A:2354:ALA:H	1.84	0.42
1:A:2609:LEU:HD13	1:A:2617:VAL:HG22	2.01	0.42
1:A:2943:LYS:HG2	1:A:3094:PHE:CE2	2.55	0.42
1:A:3024:ASP:OD1	1:A:3024:ASP:N	2.50	0.42
1:A:3619:PHE:CZ	1:A:3623:LEU:HD12	2.53	0.42
1:A:1467:ARG:HA	1:A:1523:TRP:CZ2	2.55	0.42
1:A:1533:LEU:HD11	1:A:1597:VAL:HG13	2.01	0.42
1:A:1789:LEU:HD11	1:A:1815:LEU:HB3	2.01	0.42
1:A:1878:LYS:HE3	1:A:1878:LYS:HB3	1.88	0.42
1:A:2186:CYS:HB3	1:A:2191:LEU:O	2.19	0.42
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.55	0.42
1:A:2684:ARG:NH2	1:A:2726:ARG:HH21	2.16	0.42
1:A:2910:VAL:HG12	3:A:4703:ADP:N1	2.35	0.42
1:A:2603:MET:SD	3:A:4702:ADP:C5	3.13	0.42
1:A:2880:ASP:OD2	1:A:2880:ASP:N	2.52	0.42
1:A:3544:ARG:HG3	1:A:3544:ARG:NH1	2.33	0.42
1:A:4077:PHE:HD1	1:A:4105:TRP:CE3	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2475:ASN:OD1	1:A:2475:ASN:C	2.62	0.42
1:A:2920:LEU:HD13	1:A:2920:LEU:HA	1.78	0.42
1:A:3001:ASP:OD1	1:A:3001:ASP:N	2.53	0.42
1:A:3888:ALA:O	1:A:3892:LEU:HD23	2.19	0.42
1:A:4111:LYS:HB2	1:A:4112:LYS:NZ	2.34	0.42
1:A:4153:VAL:HG22	1:A:4192:GLU:HG3	2.01	0.42
1:A:4183:LEU:HD22	1:A:4273:PHE:HZ	1.85	0.42
1:A:1344:ASP:O	1:A:1347:LYS:HG2	2.20	0.42
1:A:2435:LYS:HA	1:A:2438:GLU:HG3	2.02	0.42
1:A:2744:LEU:HA	1:A:2747:ILE:HG22	2.02	0.42
1:A:3207:LYS:HZ1	1:A:3753:LEU:CB	2.26	0.42
1:A:3730:ASP:HA	1:A:3733:LYS:HG2	2.02	0.42
1:A:4086:THR:HA	1:A:4089:LYS:NZ	2.34	0.42
1:A:4134:VAL:HG13	1:A:4139:LEU:HD11	2.01	0.42
1:A:4175:GLU:HG3	1:A:4278:PHE:HE2	1.85	0.42
1:A:4289:ASP:OD1	1:A:4317:THR:OG1	2.31	0.42
1:A:1785:VAL:O	1:A:1789:LEU:HD13	2.20	0.42
1:A:4025:LEU:HD21	1:A:4027:LEU:HD13	2.00	0.42
1:A:4323:LEU:HD12	1:A:4323:LEU:H	1.85	0.42
1:A:4329:ARG:O	1:A:4333:THR:HG23	2.20	0.42
1:A:2379:LEU:O	1:A:2383:ARG:HG3	2.20	0.42
1:A:3131:ASP:OD1	1:A:3132:LYS:N	2.52	0.42
1:A:3839:VAL:HG23	1:A:3862:ASP:HB3	2.00	0.42
1:A:4105:TRP:HA	1:A:4108:GLN:HG2	2.02	0.42
1:A:1509:LEU:HB3	1:A:3631:ASN:HD21	1.84	0.41
1:A:2458:LEU:O	1:A:2462:LEU:HG	2.20	0.41
1:A:2508:LEU:HB2	1:A:2509:LYS:NZ	2.36	0.41
1:A:2575:VAL:HA	1:A:2578:GLU:OE1	2.20	0.41
1:A:2755:MET:HE2	1:A:2755:MET:HB3	1.88	0.41
1:A:3480:LYS:HD2	1:A:3480:LYS:HA	1.85	0.41
1:A:4295:GLN:OE1	1:A:4296:MET:N	2.52	0.41
1:A:1686:PHE:HB3	1:A:1708:GLU:OE2	2.20	0.41
1:A:3633:LEU:O	1:A:3677:ILE:HD12	2.21	0.41
1:A:3655:ARG:HA	1:A:3659:ARG:O	2.20	0.41
1:A:3797:VAL:O	1:A:3800:GLN:HB3	2.20	0.41
1:A:1692:ILE:H	1:A:1692:ILE:HD12	1.85	0.41
1:A:1743:ASP:OD1	1:A:1804:ARG:NE	2.53	0.41
1:A:2048:LEU:HD23	1:A:2048:LEU:HA	1.87	0.41
1:A:2072:PHE:HB2	1:A:2164:VAL:HG21	2.02	0.41
1:A:2898:LYS:HD3	1:A:2898:LYS:C	2.44	0.41
1:A:3540:ASN:O	1:A:3540:ASN:ND2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3639:GLU:HG3	1:A:3686:VAL:HG21	2.02	0.41
1:A:1628:ARG:HH12	1:A:1706:GLU:CD	2.29	0.41
1:A:2020:PRO:HA	1:A:2026:SER:HA	2.02	0.41
1:A:3759:ARG:NH1	1:A:3763:ASP:OD2	2.54	0.41
1:A:2113:ARG:HA	1:A:2116:GLU:HG2	2.03	0.41
1:A:2169:GLN:OE1	1:A:2169:GLN:N	2.53	0.41
1:A:2279:LEU:HD21	1:A:2693:TYR:CD2	2.56	0.41
1:A:2579:ALA:O	1:A:2583:THR:HG23	2.20	0.41
1:A:3211:THR:HG21	1:A:3753:LEU:HD11	2.02	0.41
1:A:3825:TYR:OH	1:A:3879:ASP:OD1	2.21	0.41
1:A:3907:HIS:NE2	1:A:3938:LEU:HA	2.35	0.41
1:A:4517:PRO:HG2	1:A:4619:ILE:HD12	2.03	0.41
1:A:1645:LYS:HA	1:A:1645:LYS:HD3	1.91	0.41
1:A:1661:VAL:HG13	1:A:1676:ILE:HD12	2.02	0.41
1:A:2065:LEU:HD21	1:A:2134:GLN:HG2	2.02	0.41
1:A:2616:GLU:O	1:A:2660:VAL:HG22	2.20	0.41
1:A:2797:ARG:HA	3:A:4702:ADP:H4'	2.03	0.41
1:A:3677:ILE:HD12	1:A:3677:ILE:HA	1.85	0.41
1:A:4038:ASN:OD1	1:A:4038:ASN:N	2.52	0.41
1:A:4104:GLY:HA2	1:A:4107:MET:CE	2.50	0.41
1:A:4526:GLN:HG2	1:A:4536:LEU:HD11	2.02	0.41
1:A:1711:VAL:O	1:A:1715:LYS:HG3	2.20	0.41
1:A:1978:ILE:O	1:A:1982:LEU:HD22	2.20	0.41
1:A:2075:LEU:HD11	1:A:4536:LEU:HD12	2.02	0.41
1:A:2335:LEU:HD23	1:A:2336:PRO:O	2.21	0.41
1:A:2561:LYS:HE2	1:A:2561:LYS:HB2	1.98	0.41
1:A:3601:MET:HA	1:A:3609:ILE:HD13	2.02	0.41
1:A:3654:ARG:NH1	1:A:3663:THR:HG23	2.36	0.41
1:A:4297:PRO:HB3	1:A:4308:TRP:CG	2.55	0.41
1:A:4345:LYS:HB3	1:A:4345:LYS:HE2	1.76	0.41
1:A:1548:GLU:HG2	1:A:1568:PHE:HZ	1.85	0.41
1:A:1692:ILE:HG23	1:A:1701:TRP:CD1	2.55	0.41
1:A:2443:LEU:HB3	1:A:2510:MET:CE	2.51	0.41
1:A:2528:THR:O	1:A:2528:THR:OG1	2.36	0.41
1:A:1484:CYS:CB	1:A:1579:MET:HE2	2.51	0.41
1:A:1507:MET:HE2	1:A:1507:MET:HB3	1.95	0.41
1:A:1702:LEU:HD23	1:A:1702:LEU:HA	1.87	0.41
1:A:1809:GLU:HG2	1:A:2056:SER:HB2	2.02	0.41
1:A:2113:ARG:HA	1:A:2116:GLU:CD	2.46	0.41
1:A:2458:LEU:HD12	1:A:2458:LEU:HA	1.87	0.41
1:A:2580:LEU:O	1:A:2583:THR:OG1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2596:PRO:HB2	1:A:2738:TYR:CE1	2.55	0.41
1:A:2624:SER:OG	1:A:3081:THR:HA	2.20	0.41
1:A:2746:GLN:O	1:A:2750:THR:HG22	2.21	0.41
1:A:2825:TRP:HH2	1:A:2853:VAL:HG13	1.86	0.41
1:A:2864:GLU:OE1	1:A:2864:GLU:N	2.37	0.41
1:A:3106:GLY:O	1:A:3110:THR:HG23	2.21	0.41
1:A:3509:LEU:HD21	1:A:3536:LEU:HD13	2.02	0.41
1:A:3716:VAL:HG21	1:A:3804:LEU:HD23	2.02	0.41
1:A:3729:SER:O	1:A:3733:LYS:HE3	2.20	0.41
1:A:3885:MET:HB3	1:A:4343:MET:HE2	2.03	0.41
1:A:3959:ILE:HD12	1:A:3959:ILE:H	1.86	0.41
1:A:4018:MET:HE2	1:A:4018:MET:HB3	1.87	0.41
1:A:4105:TRP:O	1:A:4109:LEU:HG	2.20	0.41
1:A:4393:GLN:CD	1:A:4393:GLN:H	2.29	0.41
1:A:4393:GLN:HA	1:A:4428:ARG:HH12	1.85	0.41
1:A:1655:LYS:HE3	1:A:1655:LYS:HB3	1.81	0.41
1:A:1697:LYS:HB2	1:A:1700:GLU:HG2	2.03	0.41
1:A:1698:ILE:HA	1:A:1701:TRP:CD1	2.56	0.41
1:A:1914:GLU:H	1:A:1914:GLU:HG3	1.70	0.41
1:A:1923:LEU:HD12	1:A:1954:TRP:CH2	2.56	0.41
1:A:1923:LEU:HD23	1:A:1923:LEU:HA	1.86	0.41
1:A:2069:ILE:HD11	1:A:2137:LEU:HD21	2.02	0.41
1:A:2206:LYS:HD3	1:A:2206:LYS:HA	1.78	0.41
1:A:2374:ILE:HG21	1:A:2455:LEU:HG	2.02	0.41
1:A:3656:THR:O	1:A:3659:ARG:HB2	2.21	0.41
1:A:1509:LEU:HB3	1:A:3631:ASN:ND2	2.35	0.40
1:A:1626:PHE:CE2	1:A:1628:ARG:HB3	2.56	0.40
1:A:1954:TRP:CD2	1:A:2013:ALA:HB3	2.56	0.40
1:A:2001:LEU:HA	1:A:2001:LEU:HD12	1.73	0.40
1:A:2984:GLY:HA3	1:A:3054:PHE:CE2	2.56	0.40
1:A:3548:ALA:H	1:A:3735:GLN:HE22	1.69	0.40
1:A:3627:LEU:HD11	1:A:3648:VAL:HG22	2.02	0.40
1:A:1623:ARG:HB3	1:A:1630:TYR:CZ	2.56	0.40
1:A:1627:PRO:HB2	1:A:1951:VAL:HG12	2.04	0.40
1:A:2937:GLY:HA3	1:A:2943:LYS:HD3	2.03	0.40
1:A:3010:THR:HB	1:A:3017:VAL:HG12	2.03	0.40
1:A:3068:MET:HE2	1:A:3068:MET:HB3	1.82	0.40
1:A:3556:ALA:O	1:A:3560:LEU:HG	2.21	0.40
1:A:3825:TYR:CE1	1:A:3875:MET:HG2	2.55	0.40
1:A:4408:PRO:HA	1:A:4411:ARG:NE	2.36	0.40
1:A:3819:LYS:HE2	1:A:3826:GLN:HE22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4066:ILE:HD11	1:A:4095:MET:HB2	2.02	0.40
1:A:4118:PRO:HB3	1:A:4122:PHE:CD2	2.56	0.40
1:A:4481:ASP:CG	1:A:4485:ARG:HE	2.29	0.40
1:A:1676:ILE:HD11	1:A:1872:TYR:CD2	2.56	0.40
1:A:1940:ALA:O	1:A:1944:ILE:HG13	2.21	0.40
1:A:2449:LEU:HA	1:A:2453:ARG:NH2	2.37	0.40
1:A:2463:HIS:HA	1:A:2466:CYS:SG	2.62	0.40
1:A:2937:GLY:C	1:A:3070:PRO:HD3	2.46	0.40
1:A:3107:LYS:HZ2	1:A:3140:ARG:HB3	1.84	0.40
1:A:3117:LYS:HG3	1:A:3119:ASN:OD1	2.21	0.40
1:A:3551:GLU:OE2	1:A:3735:GLN:NE2	2.44	0.40
1:A:3880:HIS:ND1	1:A:4021:MET:HG3	2.36	0.40
1:A:4418:LYS:O	1:A:4422:LYS:HG2	2.22	0.40
1:A:1504:VAL:O	1:A:1508:LYS:HG3	2.21	0.40
1:A:1521:LEU:HA	1:A:1524:GLU:OE1	2.22	0.40
1:A:2382:LEU:O	1:A:2416:GLN:NE2	2.54	0.40
1:A:4243:LEU:O	1:A:4247:MET:HG2	2.22	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	3019/4646 (65%)	2946 (98%)	73 (2%)	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	2696/4125 (65%)	2686 (100%)	10 (0%)	84 83

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

Mol	Chain	Res	Type
1	A	1637	LEU
1	A	2359	CYS
1	A	2374	ILE
1	A	2787	ASP
1	A	3572	LEU
1	A	3676	VAL
1	A	3957	PHE
1	A	4127	THR
1	A	4161	PHE
1	A	4436	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1454	GLN
1	A	1790	ASN
1	A	2005	GLN
1	A	2057	GLN
1	A	2109	GLN
1	A	2130	ASN
1	A	2299	GLN
1	A	2689	HIS
1	A	2707	GLN
1	A	2752	ASN
1	A	2834	GLN
1	A	2857	HIS
1	A	2930	GLN
1	A	2954	ASN
1	A	2960	GLN
1	A	3061	ASN
1	A	3198	GLN
1	A	3555	ASN
1	A	3584	ASN
1	A	3667	GLN

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Mol	Chain	Res	Type
1	A	3792	GLN
1	A	3845	ASN
1	A	4262	GLN
1	A	4266	ASN
1	A	4526	GLN
1	A	4612	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	A	4703	-	28,29,29	1.38	4 (14%)	43,45,45	1.82	9 (20%)
2	ATP	A	4701	4	32,33,33	0.63	1 (3%)	48,52,52	0.39	0
3	ADP	A	4702	-	28,29,29	1.36	4 (14%)	43,45,45	1.87	10 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4703	ADP	C5-C4	4.61	1.47	1.39
3	A	4702	ADP	C5-C4	4.44	1.47	1.39
2	A	4701	ATP	PA-O3A	-2.70	1.56	1.59
3	A	4702	ADP	C5-C6	2.62	1.48	1.41
3	A	4703	ADP	C5-C6	2.62	1.48	1.41
3	A	4703	ADP	C5-N7	-2.37	1.34	1.39
3	A	4702	ADP	C5-N7	-2.35	1.34	1.39
3	A	4703	ADP	C8-N7	2.28	1.36	1.31
3	A	4702	ADP	C8-N7	2.27	1.36	1.31

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4702	ADP	C5-C4-N3	-5.93	118.55	126.72
3	A	4703	ADP	C5-C4-N3	-5.77	118.77	126.72
3	A	4702	ADP	N3-C4-N9	4.77	135.28	127.17
3	A	4703	ADP	N3-C4-N9	4.58	134.95	127.17
3	A	4702	ADP	C2-N3-C4	3.83	121.19	111.83
3	A	4703	ADP	C2-N3-C4	3.66	120.77	111.83
3	A	4703	ADP	C4-C5-N7	-3.45	106.63	110.58
3	A	4702	ADP	N3-C2-N1	-3.31	123.58	128.58
3	A	4702	ADP	C4-C5-N7	-3.24	106.88	110.58
3	A	4703	ADP	N3-C2-N1	-3.20	123.73	128.58
3	A	4702	ADP	C4-N9-C8	2.74	108.62	105.74
3	A	4703	ADP	C4-N9-C8	2.66	108.53	105.74
3	A	4703	ADP	C5-N7-C8	2.53	107.43	103.45
3	A	4702	ADP	C5-N7-C8	2.47	107.33	103.45
3	A	4703	ADP	C3'-C2'-C1'	2.35	105.91	101.46
3	A	4703	ADP	C6-C5-N7	2.08	136.11	132.09
3	A	4702	ADP	N9-C8-N7	-2.07	111.00	113.94
3	A	4702	ADP	C3'-C2'-C1'	2.04	105.32	101.46
3	A	4702	ADP	C6-C5-N7	2.04	136.02	132.09

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4701	ATP	O4'-C4'-C5'-O5'
2	A	4701	ATP	C3'-C4'-C5'-O5'
3	A	4703	ADP	C5'-O5'-PA-O1A
2	A	4701	ATP	PG-O3B-PB-O2B
2	A	4701	ATP	PA-O3A-PB-O1B
3	A	4703	ADP	C3'-C4'-C5'-O5'
3	A	4703	ADP	O4'-C4'-C5'-O5'

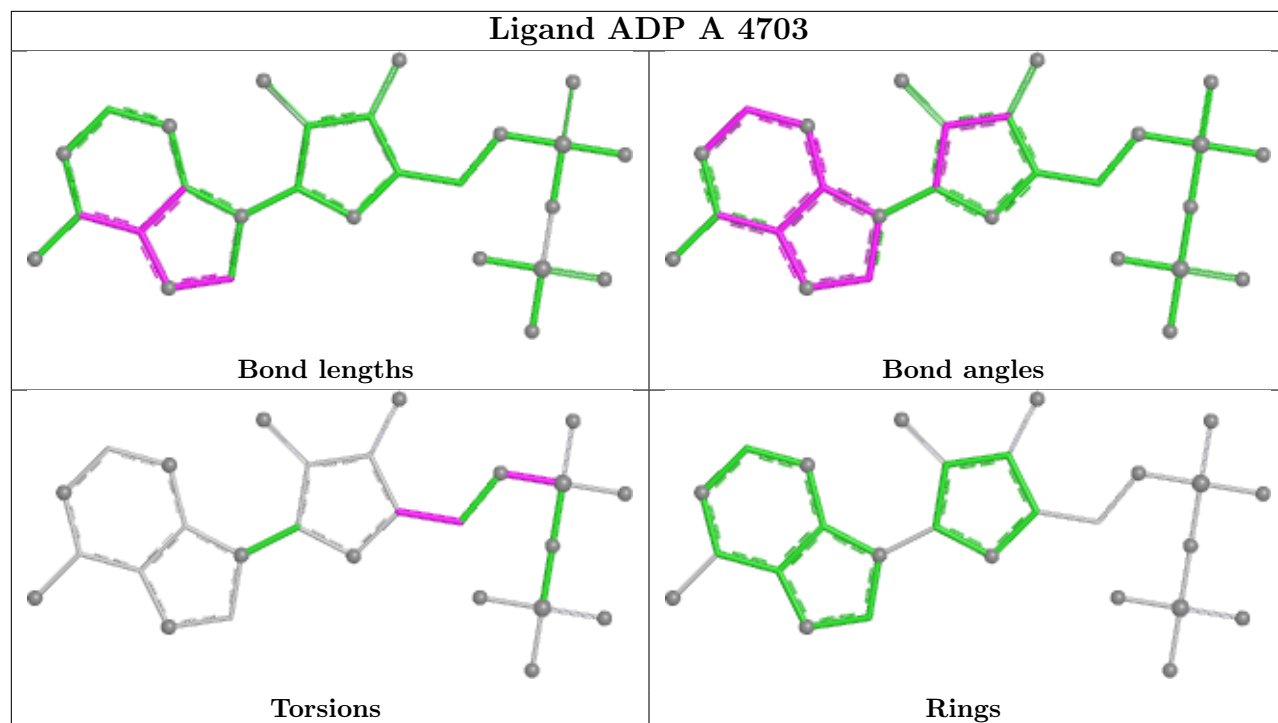
There are no ring outliers.

3 monomers are involved in 11 short contacts:

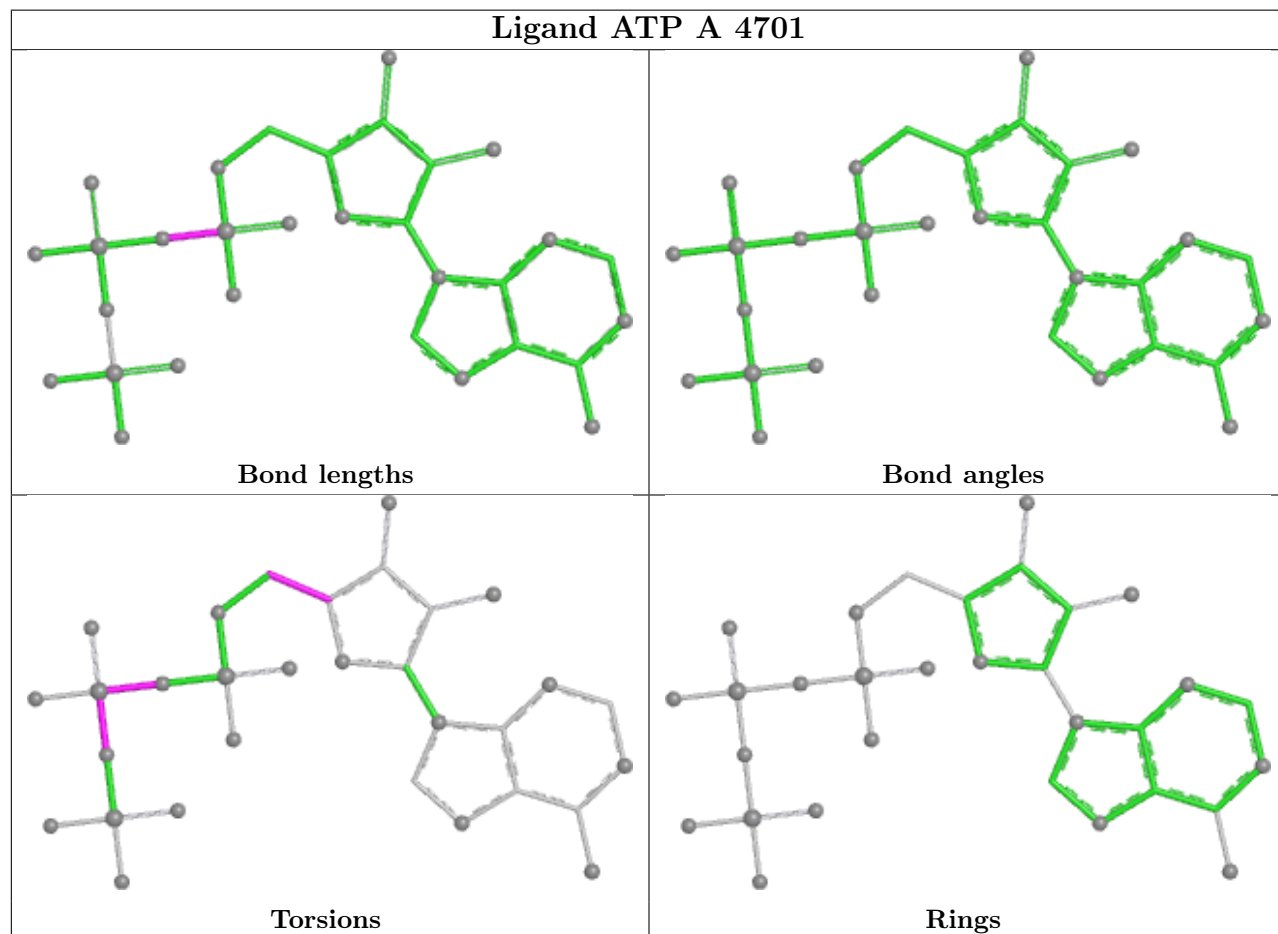
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4703	ADP	2	0
2	A	4701	ATP	4	0
3	A	4702	ADP	5	0

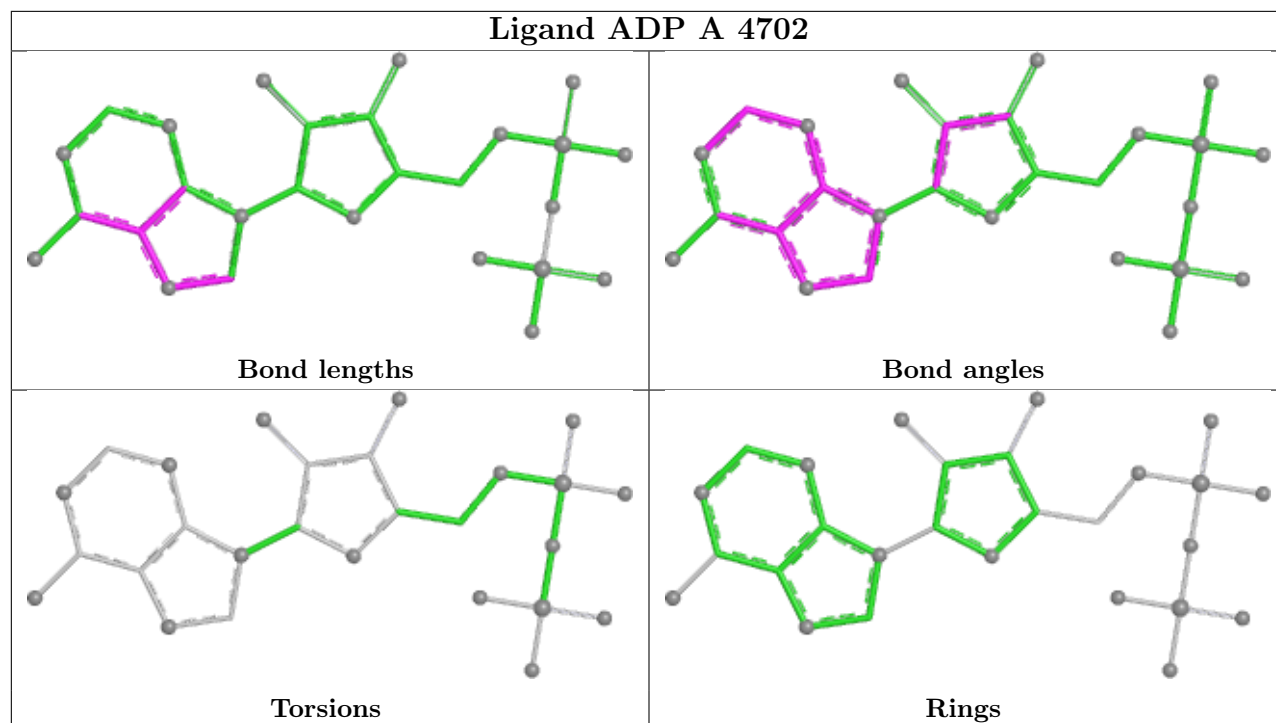
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 4703



Ligand ATP A 4701





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.

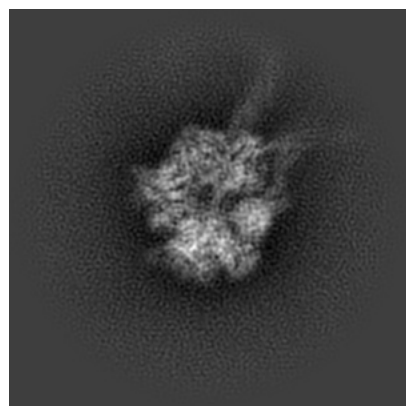
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44718. These allow visual inspection of the internal detail of the map and identification of artifacts.

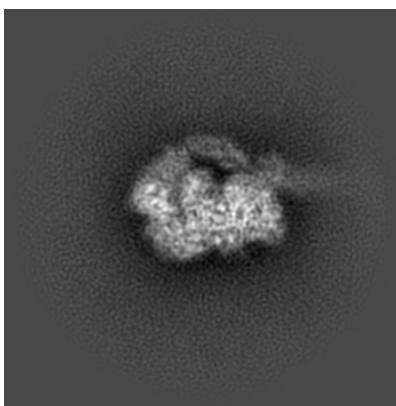
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

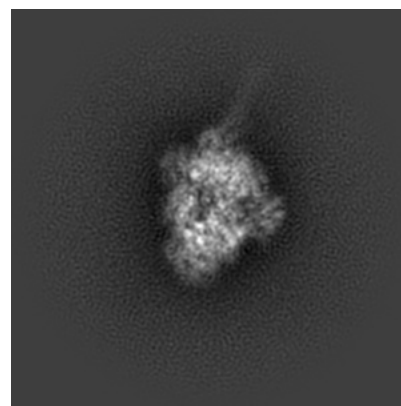
6.1.1 Primary map



X

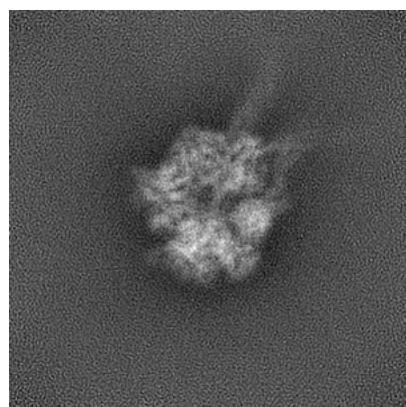


Y

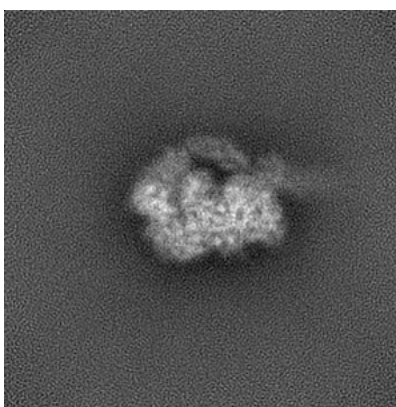


Z

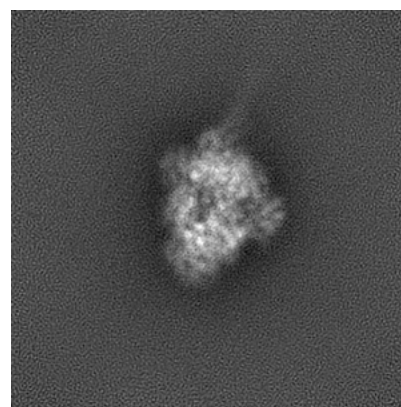
6.1.2 Raw map



X



Y

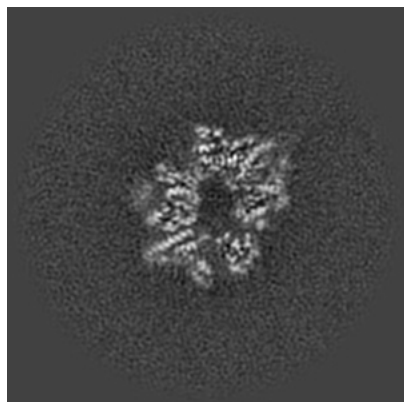


Z

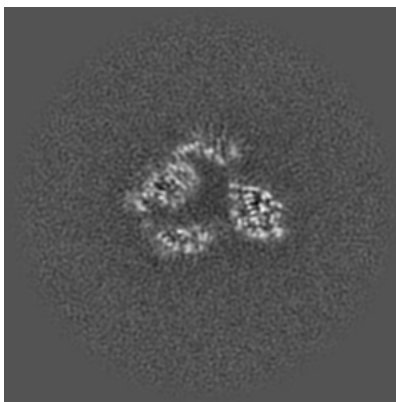
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

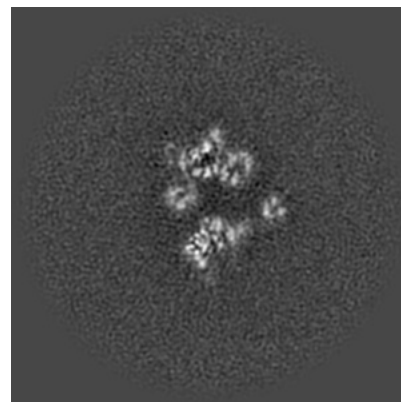
6.2.1 Primary map



X Index: 128

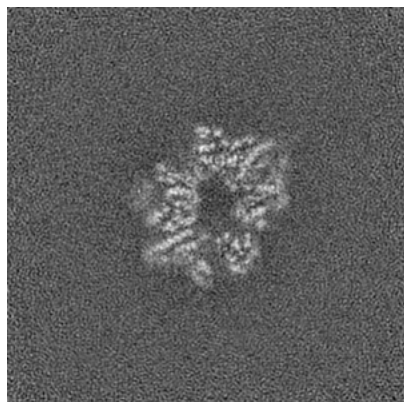


Y Index: 128

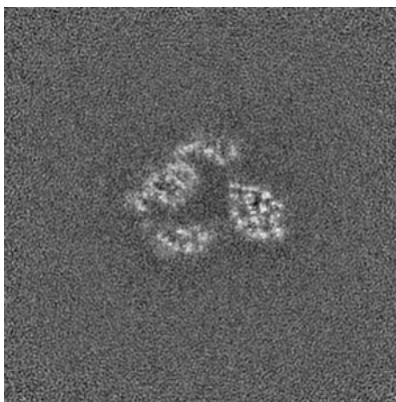


Z Index: 128

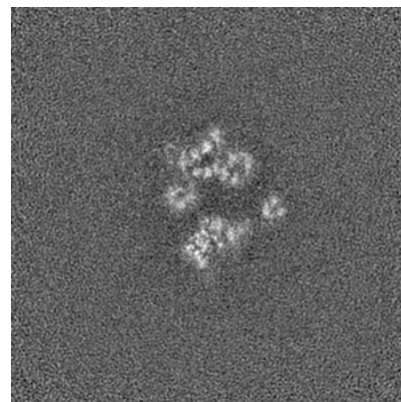
6.2.2 Raw map



X Index: 128



Y Index: 128

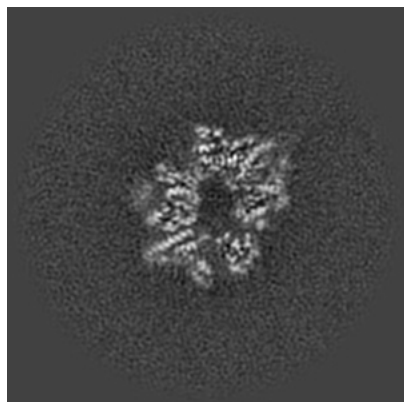


Z Index: 128

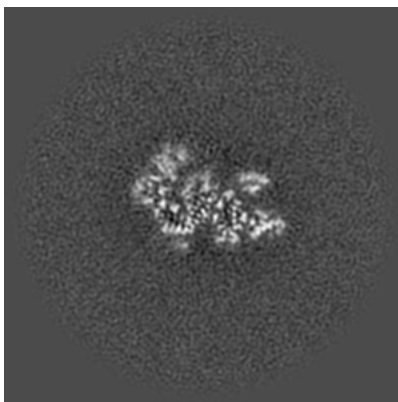
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

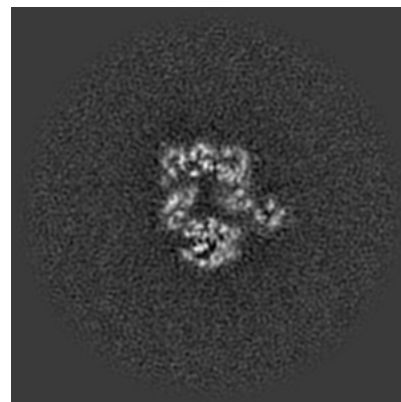
6.3.1 Primary map



X Index: 128

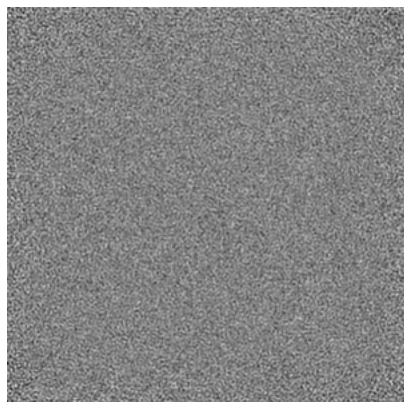


Y Index: 111

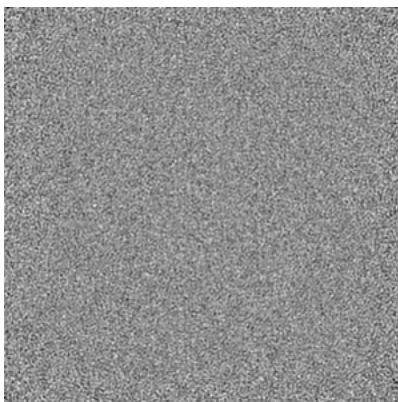


Z Index: 119

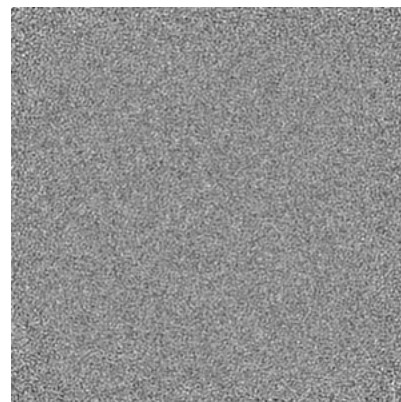
6.3.2 Raw map



X Index: 0



Y Index: 0

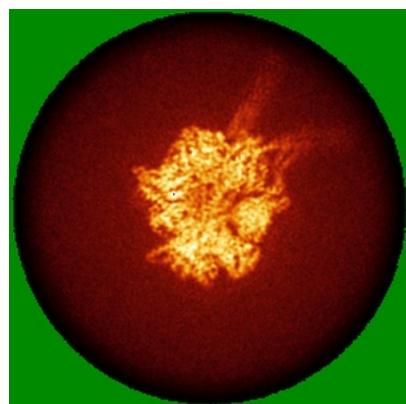


Z Index: 0

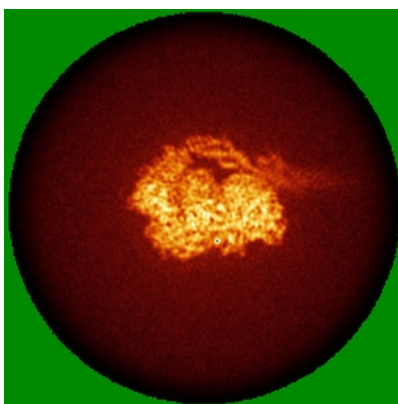
The images above show the largest variance slices of the map in three orthogonal directions.

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

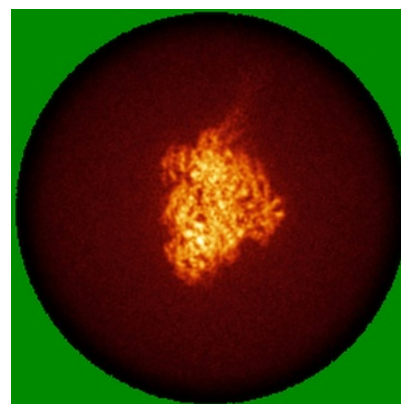
6.4.1 Primary map



X

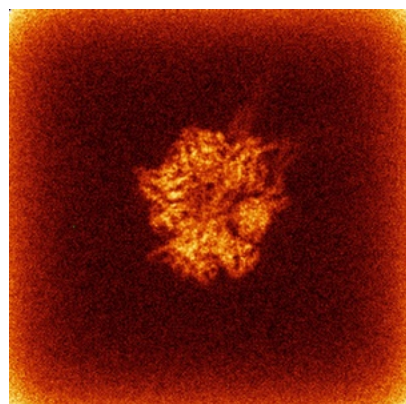


Y

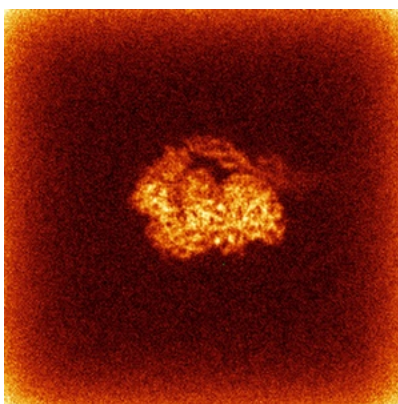


Z

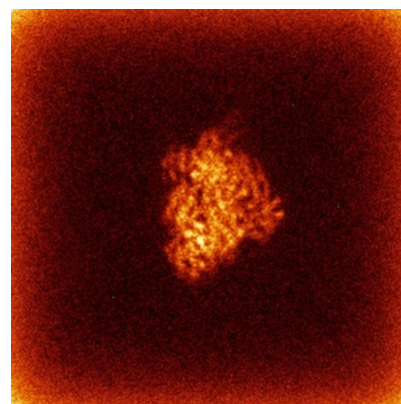
6.4.2 Raw map



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.

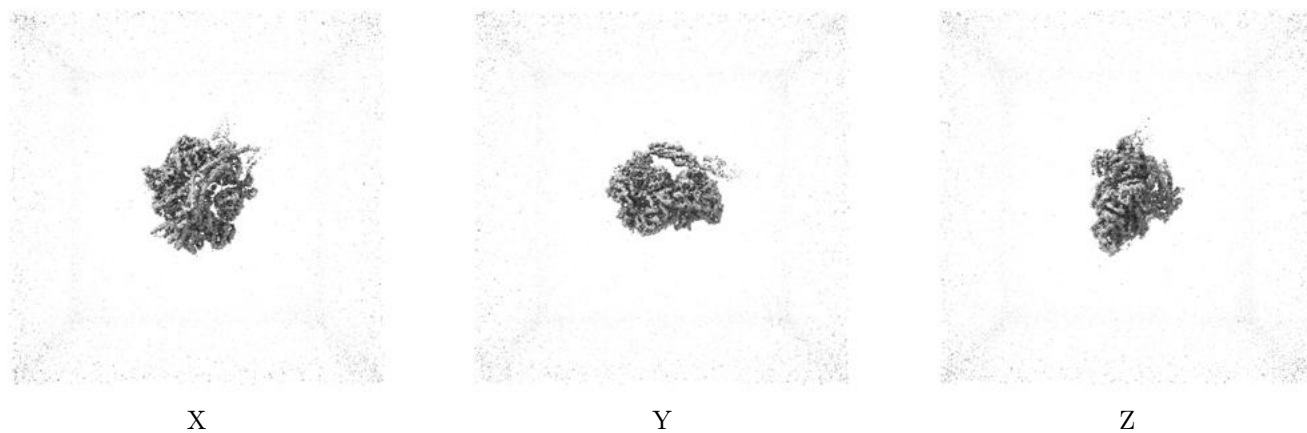
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

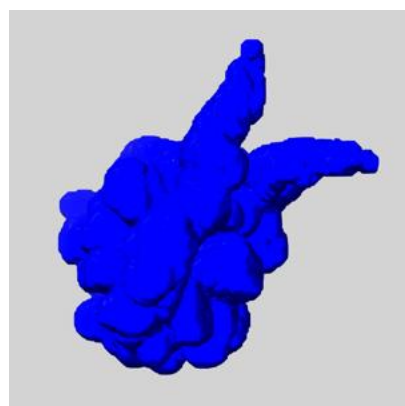
6.6 Mask visualisation [i](#)

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

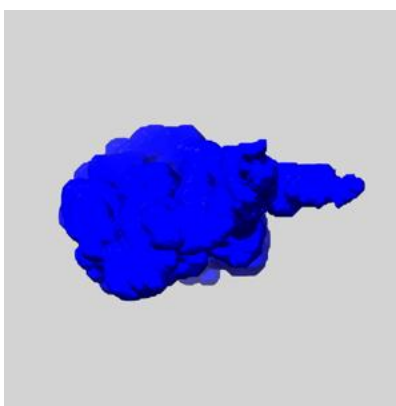
A mask typically either:

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

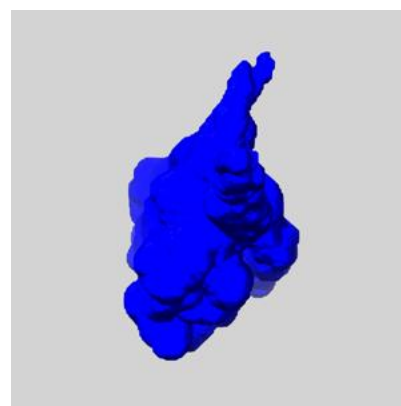
6.6.1 emd_44718_msk_1.map [i](#)



X



Y

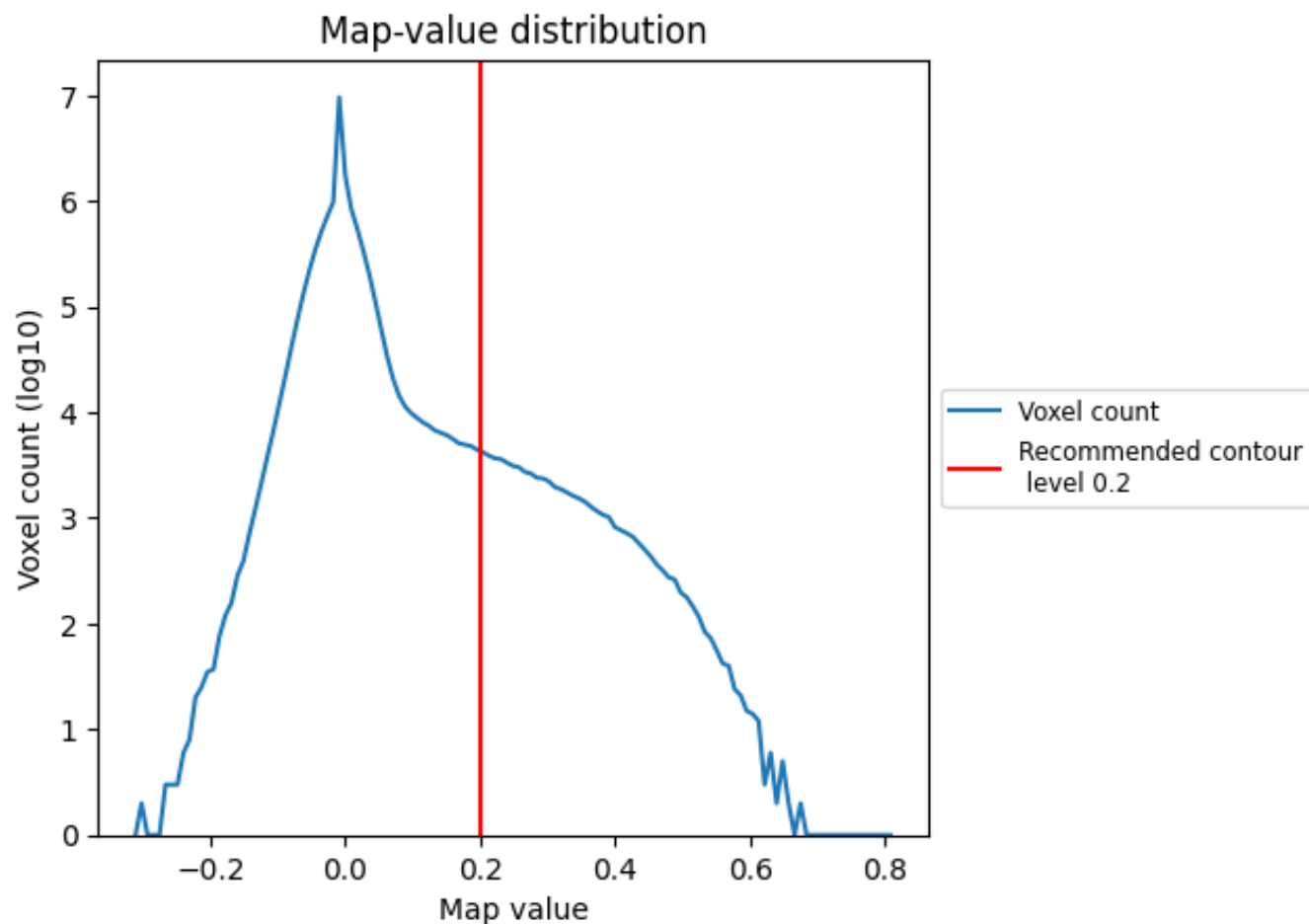


Z

7 Map analysis [i](#)

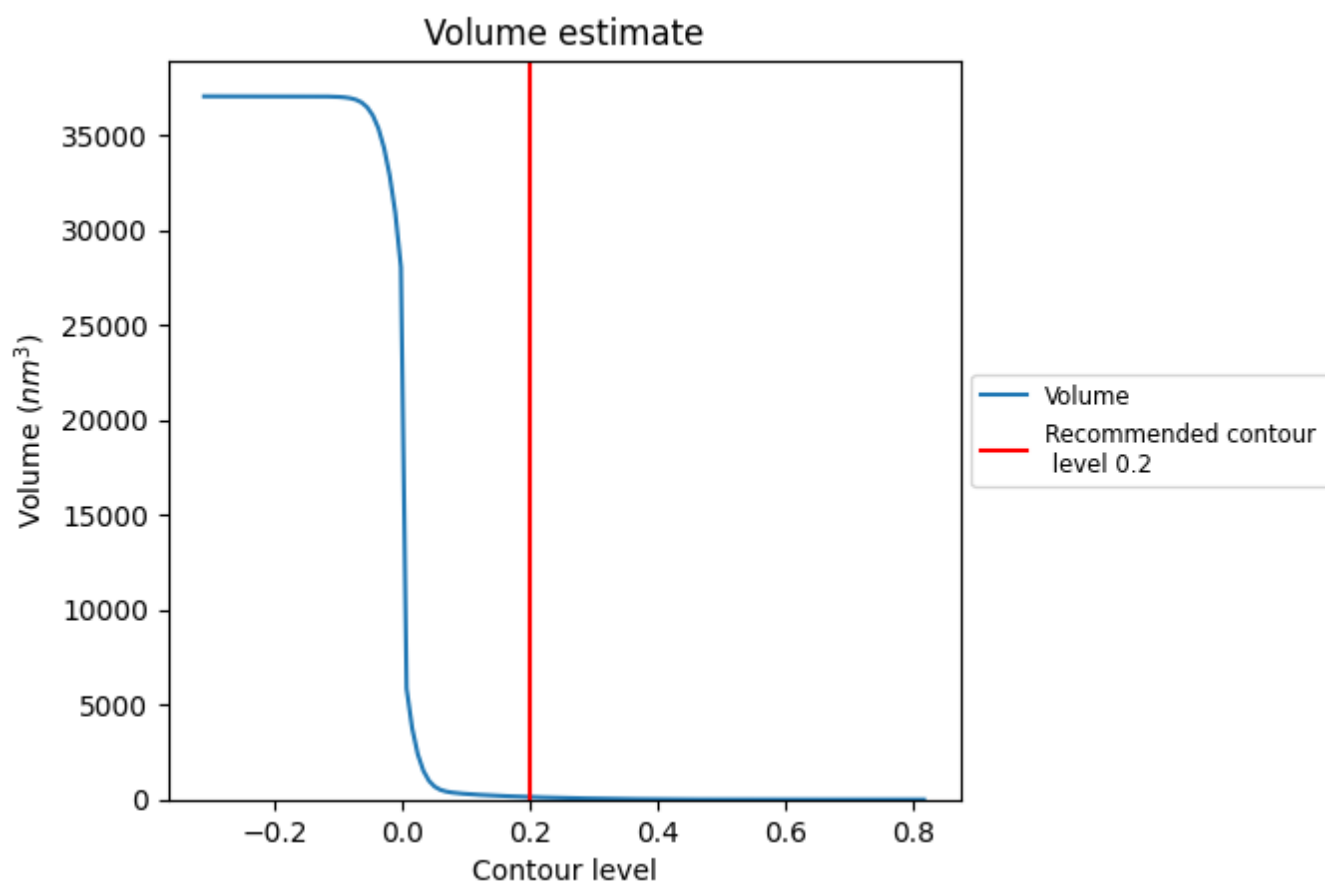
This section contains the results of statistical analysis of the map.

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.

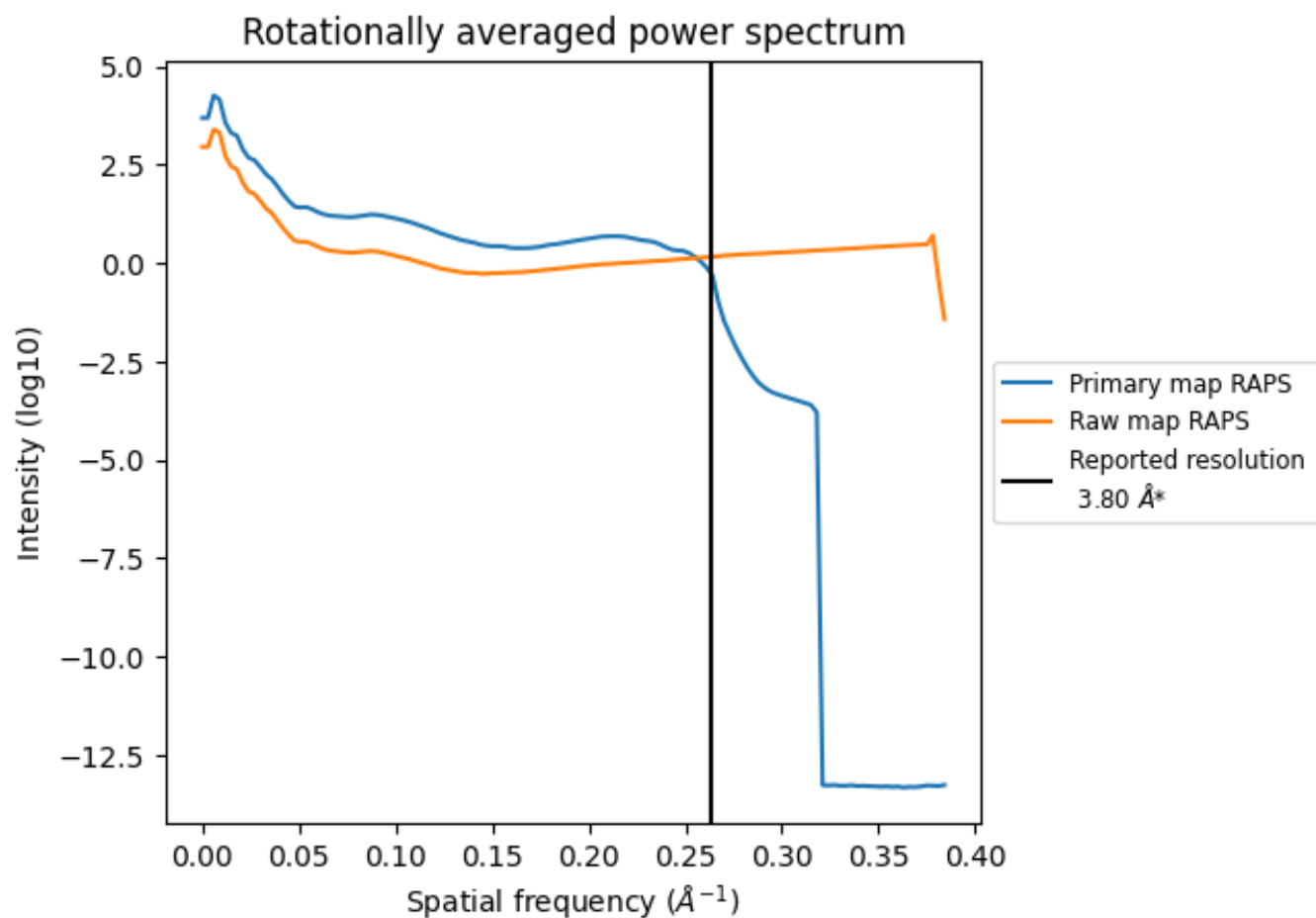
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 134 nm^3 ; this corresponds to an approximate mass of 121 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 ⓘ

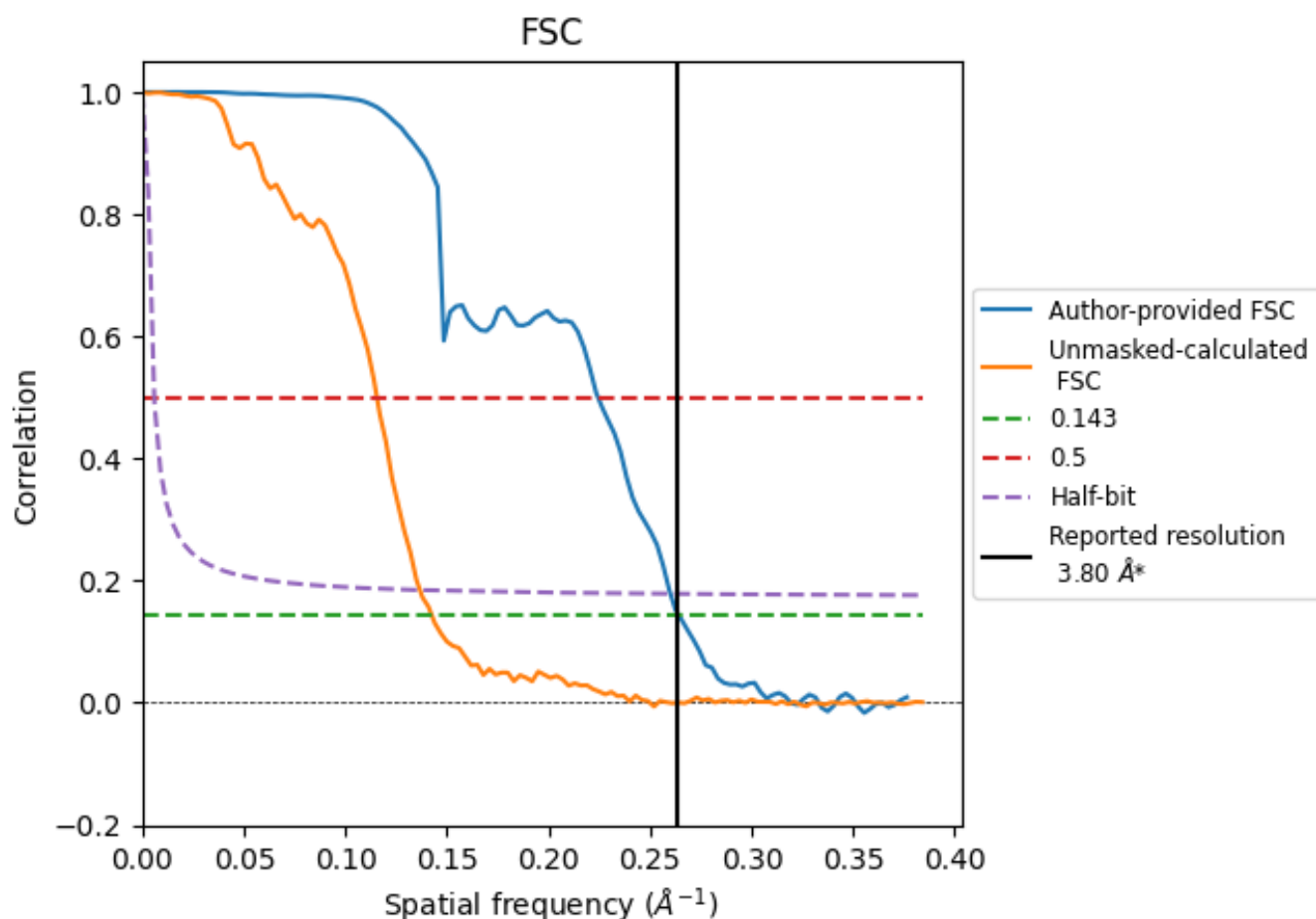


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 $0.263 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

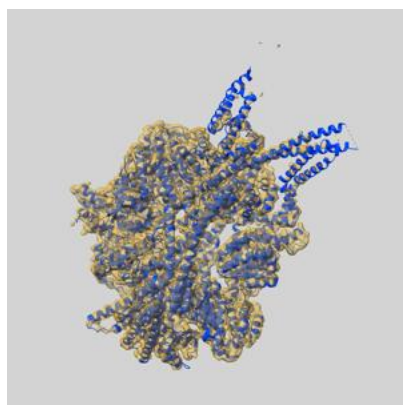
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.78	4.46	3.84
Unmasked-calculated*	7.01	8.65	7.31

*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 7.01 differs from the reported value 3.8 by more than 10 %

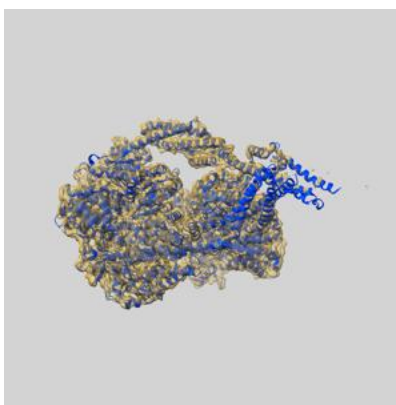
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44718 and PDB model 9BN1. Per-residue inclusion information can be found in section [3](#) on page [5](#).

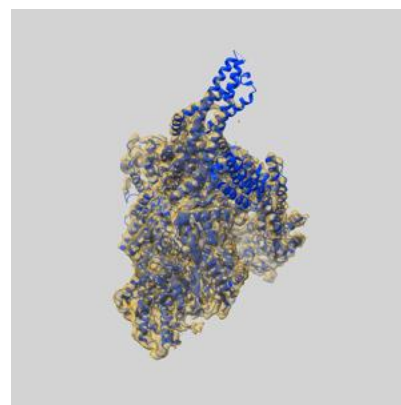
9.1 Map-model overlay [i](#)



X



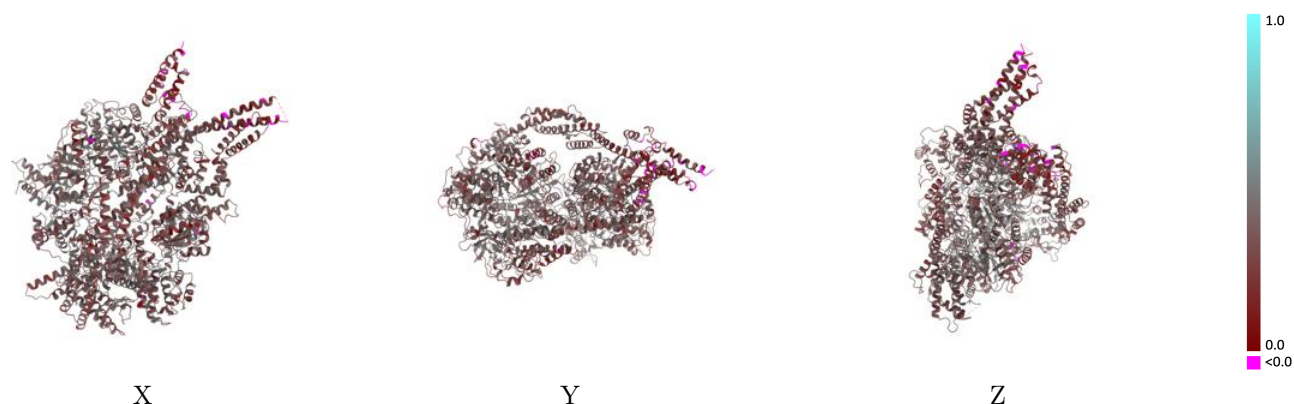
Y



Z

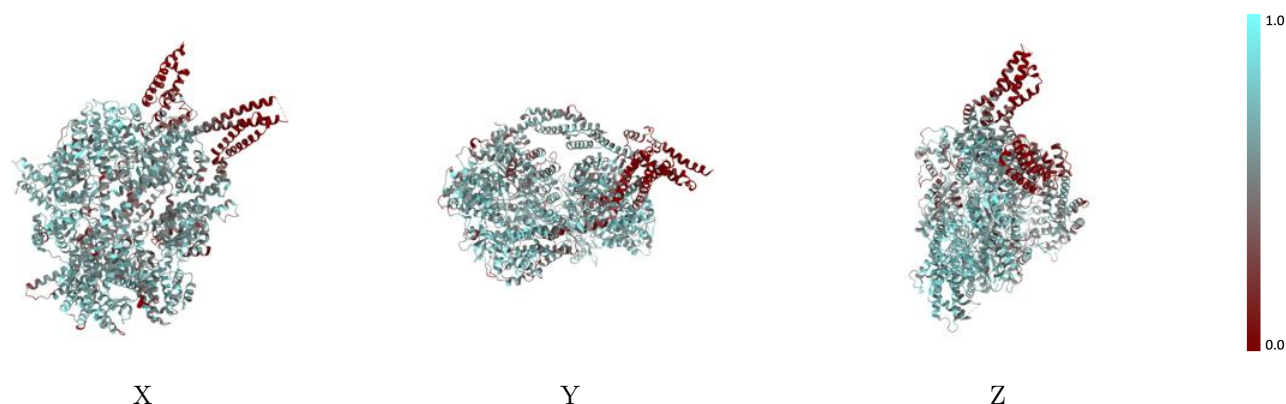
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



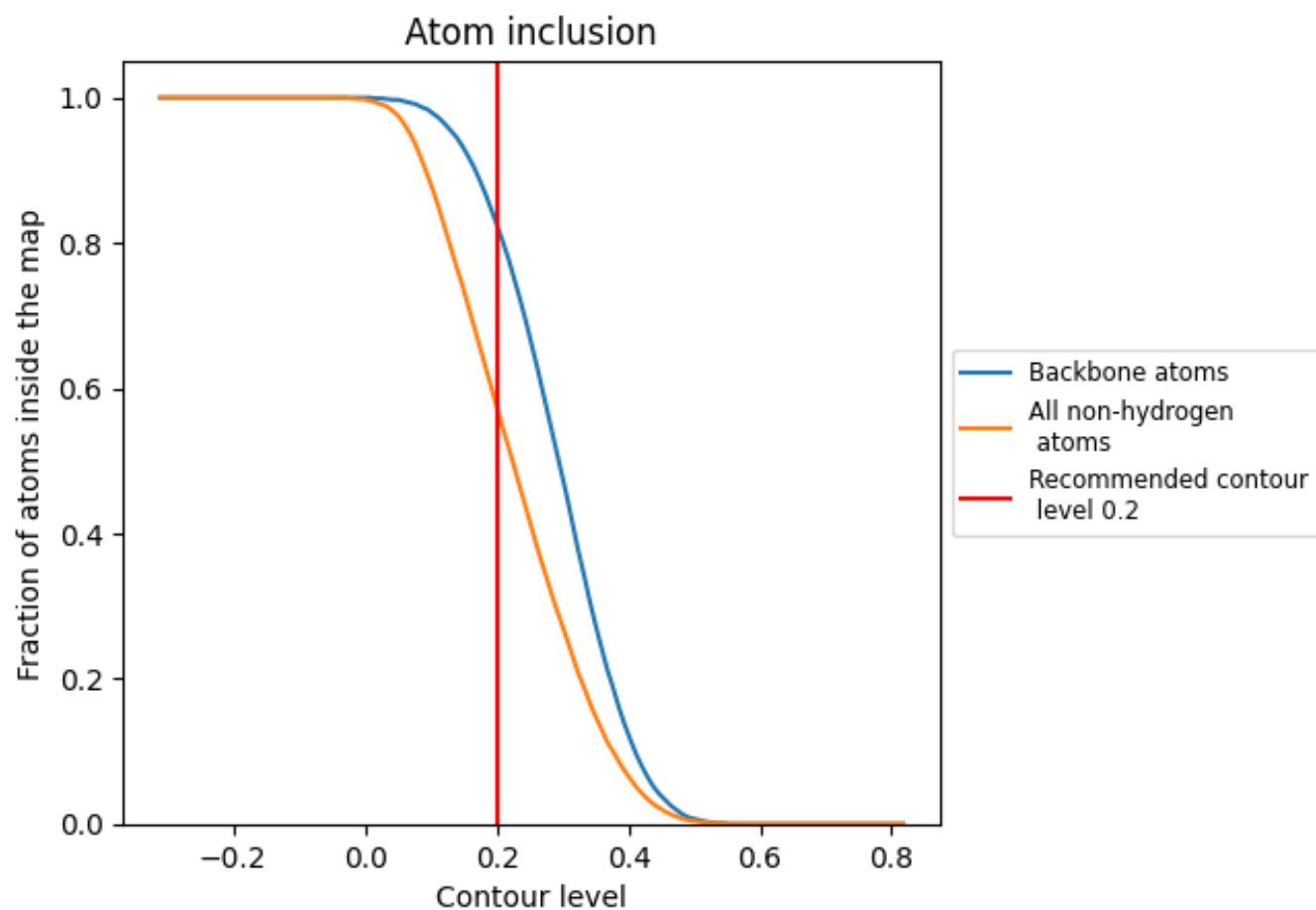
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	0.5750	0.3490
A	0.5750	0.3490

