



Full wwPDB EM Validation Report ⓘ

Apr 24, 2025 – 11:06 AM EDT

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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

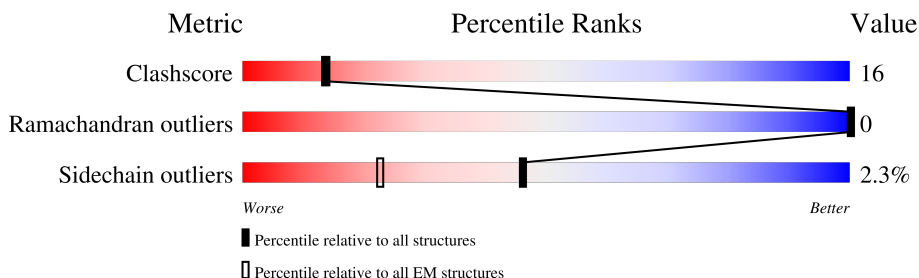
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	<div> <div>13%</div> <div>42%</div> <div>23%</div> <div>35%</div> </div>

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
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

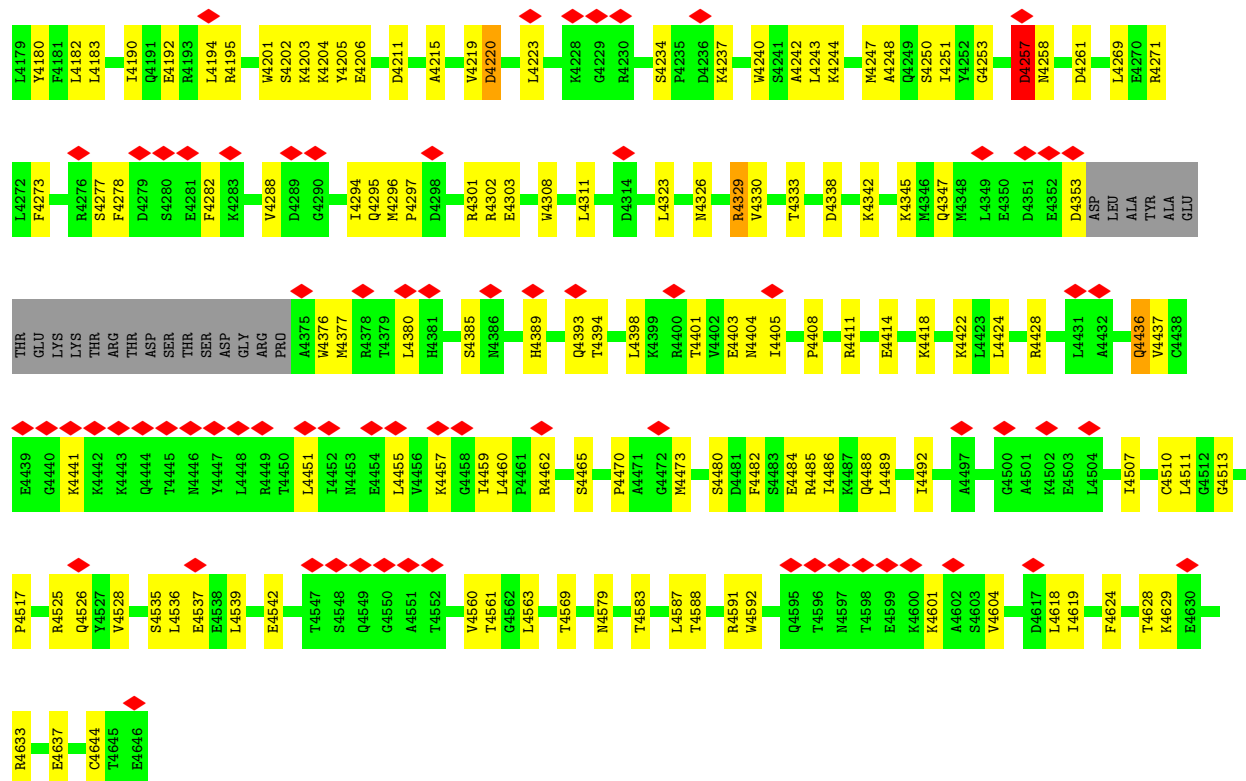
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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



E3100	F2992	T2882	M2779	Q2677	P2596	L2508	L2413	S2334	T2287	N2145	V2070	K1992
A3101	D2995	P2883	D2787	R2678	P2597	K2509	Q2414	L2335	L2286	V2146	P2071	T1993
L3102	E2996	E2888	G2598	V2679	G2598	M2510	T2415	P2336	L2288	P2147	F2072	S1994
V3106	S2997	L2889	H2791	I2683	T2602	R2511	Q2416	R2339	D2269	L2149	C2076	A1995
G3106	N2998	R2890	Y2792	R2684	M2603	E2513	R2417	R2340	P2270	E2152	C2077	P1996
K3107	D2891	D2892	S2795	V2687	F2606	L2514	D2418	R2341	N2271	E2164	D2077	I1997
L3000	V2893	V2894	R2796	Y2693	L2609	G2515	A2419	E2344	T2272	V2169	E2078	E2000
D3001	E2798	R2694	E2798	R2694	F2606	E2516	A2420	Q2346	R2273	Q2169	Q2079	L2001
F3004	W2802	Q2698	W2802	Q2698	D2614	L2518	W2423	D2347	E2274	Y2170	L2080	L2002
L3005	F2807	L2703	F2807	L2703	M2615	L2526	F2427	L2348	D2277	W2175	G2088	N2003
E3006	E2808	E2704	E2808	E2704	V2617	P2527	K2435	K2349	G2278	L2090	G2089	N2004
T3010	R2811	R2706	R2811	R2706	W2531	E2538	E2438	T2352	L2279	L2178	R2091	Q2005
L3012	E2814	T2715	E2814	T2715	D2536	E2538	H2439	L2353	F2280	E2181	A2092	F2010
V3017	L2816	Q2716	L2816	Q2716	Y2537	E2538	Q2442	A2354	T2281	C2186	L2093	A2013
G3023	V2818	T2716	V2818	T2716	D2537	E2538	E2444	W2363	R2291	L2190	L2093	N2019
D3024	E2819	T2717	E2819	T2717	Y2537	E2538	E2445	F2364	R2292	L2191	L2093	P2020
C3033	Q2820	D2717	Q2820	D2717	W2545	E2538	L2449	E2366	E2294	G2101	S2095	G2021
K3034	L2821	R2720	L2821	R2720	W2548	E2538	T2450	L2374	L2295	K2104	S2026	T19
E3040	L2822	R2726	L2822	R2726	W2568	E2538	T2451	P2375	L2296	R2107	S2027	ALA
G3041	W2825	R2726	W2825	R2726	V2569	E2538	L2452	P2376	K2297	L2108	N2027	GLY
L3042	A2829	Y2731	L3042	Y2731	P2570	E2538	R2453	R2377	Q2299	Q2109	N2027	ARG
M3043	E2837	P2732	M3043	P2732	Q2554	E2538	L2455	L2379	W2300	K2110	L2028	ARG
L3044	L2838	V2733	L3044	V2733	E2558	E2538	L2458	L2382	Q2299	R2113	L2029	N2031
D3045	E2839	Y2738	D3045	Y2738	P2560	E2538	F2459	R2383	F2302	E2116	L2032	L2031
E3048	E2840	L2744	E3048	L2744	K2561	E2538	L2462	S2384	D2304	R2117	L2032	K2033
W3053	E2841	T2745	W3053	T2745	V2568	E2538	H2463	L2385	G2305	H2218	E2117	F2036
F3054	W2845	Q2746	F3054	Q2746	V2569	E2538	Q2464	D2306	D2306	G2219	G2119	R2037
Q3057	E2849	I2747	Q3057	I2747	L2555	E2538	C2466	D2307	D2307	V2222	A2121	S2038
V3065	N2849	T2750	V3065	T2750	Q2566	E2538	Y2472	E2389	P2309	G2224	V2122	L2039
F3066	V2853	F2751	F3066	F2751	K2567	E2538	W2475	GLY	E2310	G2229	D2123	K2043
S3071	A2854	N2752	S3071	N2752	W2569	E2538	L2475	ASP	W2311	K2230	E2124	F2044
S3072	L2855	M2755	S3072	M2755	V2575	E2538	V2495	GLN	W2312	S2231	G2125	D2045
E3073	K2856	L2756	E3073	L2756	R2576	E2538	Q2482	ARG	E2313	W2232	E2126	R2046
G3074	H2857	R2757	G3074	R2757	F2662	E2538	L2483	ARG	L2315	A2233	I2127	Q2047
D3077	R2863	P2760	D3077	P2760	C2663	E2538	Y2493	ARG	L2319	W2234	A2128	L2048
R3078	E2864	R2763	R3078	R2763	D2664	E2538	L2494	LYS	D2320	R2235	E2129	L2049
T3081	R2869	A2766	T3081	A2766	E2665	E2538	V2495	GLY	L2321	L2237	N2130	A2050
F3086	Y2873	T2770	F3086	T2770	L2666	E2538	W2500	ASP	W2322	L2237	L2131	Q2051
F3094	S2874	E2775	F3094	E2775	L2668	E2538	T2498	GLY	K2323	L2238	F2132	W2052
D3096	K2879	Q2675	D3096	Q2675	L2685	E2538	W2584	GLY	L2324	L2244	E2135	N2053
W3097	D2880	G2675	W3097	D2672	P2590	E2538	S2503	GLY	L2325	G2249	Q2136	L2055
	Y2881	T2676		T2676	L2591	E2538	D2505	A2408	L2327	K2257	I2137	Q2057
											E2143	R2060
											T2144	L2065
												T2069

P4103	H4029	D3946	R3870	I3789	S3729	V3644	L3567	R3488	GLN	L3175
C4104	I4030	L3947	R3870	V3790	D3730	L3645	P3568	W3489	LYS	H3175
W4105	E4034	L3948	R3873	M3791	L3731	P3646	A3569	E3490	ALA	L3186
M4107	E3950	G3874	G3874	K3792	L3732	P3647	D3570	K3491	ASN	E3189
Q4108	N4038	V3951	M3875	E3793	K3733	L3648	P3571	T3492	LYS	K3190
L4109		Q3952		V3794	L3734	N3650	L3572	S3493	LYS	R3191
E4110	L4042	Q3953	D3879	E3795	Q3735	R3651	C3573	E3494	VAL	
K4111	M4043	D3954	H3880	T3796	G3736	E3652	A3577	E3494	MET	E3196
K4112		E3955	I3881	V3797	V3653	V3654	I3578	F3496	LYS	Q3197
L4113		Q3956	T3882	Q3800	E3737	R3654	M3579	T3497	GLN	Q3198
L4116	A4051	F3957	Q3886	Q3800	F3738	R3655	L3580	T3498	GLY	M3199
Q4117	G4052	G3958	L3887	Y3801	Q3739	T3656	K3581	Q3499	ILE	H3200
P4118	G4053	I3959	L3887	L3804	L3740	G3658	R3582		GLY	L3201
H4119	H4054	I3959	A3888		R3741	G3658	P3583		GLN	L3202
A4120		E3967	R3889	A3807	L3742	R3659	R3584		ALA	V3203
C4121	D4057	V3970	K3890	S3810	Q3744	V3660	R3585		LYS	G3204
R4122	A4058	P3971	K3891	I3811	L3745	L3661	Y3586		GLN	L3205
R4123	A4060	L3972	L3892	F3812	E3746	I3662	P3587		GLY	K3206
L4124	L3973	L3973	F3893	F3813	K3747	L3663	L3588		VAL	R3207
T4127	W3974	W3974	T3900	T3814	E3748	L3664	D3591		ILE	I3208
M4128	Q4062	S3975	Y3901	M3815	S3748	G3665	P3592		THR	K3209
E4129	N4063	E3976	A3902	K3819	L3749	Q3667	G3594		ASP	E3210
		E3977	A3903		L3750	D3668	M3601		LYS	T3211
K4133	I4066	A3980	Q3906	Y3825	Q3751	L3671	Y3604		ALA	V3212
V4134	T4067	A3980	H3907	Q3826	A3752		K3605		LYS	D3213
L4138	I4071	T3983	R3910	S3827	L3753	L3677	D3606		ARG	Q3214
L4139	G4072	Q3984	G3811	L3828	K3754	F3676	R3607		GLY	V3215
R4140	S4073	Q3985	N3912	L3829	E3755	L3679	K3608		ASP	E3216
A4141	A4074	I3987	E3913	F3831	V3756	D3683	I3609		LYS	E3217
G4075	G4075	H3988	I3914	I3835	K3757	P3684	T3612		ASP	L3218
F4077	F4077	L3990	V3915	H3836	G3758	V3685	L3536		GLY	R3219
N4078	N4078	R3989	V3916	H3837	R3759	V3686	Q3537		ASN	K3220
Q4079	Q4079	L3991	S3917	N3838	I3760	E3687	I3541		PRO	D3221
A4080	A4080	L3992	A3918	V3839	L3761	D3691	F3543		ALA	LEU
D4081	D4081	D3999	G3919	E3842	D3762	L3692	R3544		THR	
K4082	K4082	A4003	S3920	E3842	D3763	C3693	I3547		ILE	ARG
A4083	A4083	M4004	T3921	N3845	D3764	S3694	A3548		VAL	LYS
N4085	N4085	A4005	P3922	L3846	T3765	R3695	R3549		GLN	SER
T4086	T4086	H4006	R3923	K3847	T3766	V3696	T3550		ALA	GLY
A4087	A4087	L4013	I3924	G3848	I3766	V3699	E3551		VAL	LEU
V4088	V4088	G4014	Q3925		I3767	V3703	Y3552		GLY	GLY
K4089	K4089	E4015	G3926	D3851	T3768	V3704	R3628		ILE	SER
S4090	S4090	S4016	L3927	H3852	T3769	T3704	F3629		LYS	VAL
G4091	G4091	F4017	E3930	Q3854	L3770	P3632	N3631		LYS	LYS
R4092	R4092	F4017	E3930	R3855	E3771	R3705	L3633		ASP	ALA
W4093	W4093	M4021	E3933	L3856	N3772	V3716	L3633		ALA	ALA
V4094	V4094	E4022	E3933		L3773	R3721	D3637		ASP	ALA
M4095	M4095	Q4023	V3936	I3859	K3774		V3638		LYS	ASN
E4175	E4175	P4024	R3937	T3860	R3775	V3724	E3639		ARG	LEU
R4176	R4176	L4025	L3938	K3861	E3776	D3725	D3642		GLY	VAL
A4177	A4098	D4026	S3939	D3862	A3777	E3726	P3643		LYS	LYS
R4178	N4098	L4027	C3940	V3866	A3778	R3728	S3565		VAL	VAL
	H4100	T4028	C3940		E3779	K3728	S3566		ASP	GLN
	L4101		F3944		V3780	T3781				
	A4102		K3945		T3781	K3782				
					K3783	V3784				
					E3785	E3786				
					T3787	D3788				



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 (\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 (\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, MG, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/24908	0.53	4/33751 (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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2002	LEU	CA-CB-CG	5.88	128.82	115.30
1	A	4257	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	1429	LEU	CA-CB-CG	5.20	127.25	115.30
1	A	3479	LEU	CA-CB-CG	5.10	127.03	115.30

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	767	0
2	A	31	0	12	2	0
3	A	54	0	24	5	0
4	A	1	0	0	0	0
All	All	24476	0	24498	767	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 16.

All (767) 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: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: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: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: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:2581:LEU:HD12	1:A:2591:LEU:HD21	1.74	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:2377:ASN:OD1	2:A:4701:ATP:O2'	2.12	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: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: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
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: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:2414:GLN:NE2	1:A:2418:ASP:OD1	2.22	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4248:ALA:HB2	1:A:4269:LEU:HD12	1.81	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: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:2222:MET:HB2	1:A:2344:GLU:HA	1.82	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:4105:TRP:CE2	1:A:4109:LEU:HD21	2.38	0.59
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
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: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:2568:VAL:HG13	1:A:2603:MET:HE3	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:1457:MET:CE	1:A:3659:ARG:HA	2.35	0.55
1:A:2190:TYR:O	1:A:2377:ASN:ND2	2.39	0.55
1:A:2232:MET:CE	1:A:2232:MET:H	2.18	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:1551:PHE:HB3	1:A:1558:LYS:HZ2	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3175:HIS:CE1	1:A:3585:ARG:HH12	2.25	0.55
1:A:1457:MET:HE3	1:A:3659:ARG:HG2	1.89	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1457:MET:HE3	1:A:3659:ARG:HA	1.91	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:3873:ARG:HH12	1:A:4021:MET:HA	1.73	0.53
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:4247:MET:HE2	1:A:4247:MET:HA	1.91	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
1:A:2538:GLU:HB2	1:A:2548:TRP:CE2	2.44	0.52
1:A:3851:ASP:HB3	1:A:3854:GLN:HB2	1.92	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:2795:SER:OG	1:A:2798:GLU:OE1	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:4510:CYS:SG	1:A:4561:THR:OG1	2.69	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
1:A:1810:HIS:NE2	1:A:1876:GLN:O	2.44	0.51
1:A:2444:GLU:H	1:A:2510:MET:CE	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4099:VAL:HG22	1:A:4128:MET:HB2	1.92	0.49
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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:3756:VAL:HB	1:A:3759:ARG:HB2	1.96	0.48
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:1551:PHE:HB3	1:A:1558:LYS:NZ	2.28	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: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: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:1576:LEU:HD22	1:A:1579:MET:HE2	1.95	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4194:LEU:HD12	1:A:4194:LEU:H	1.80	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
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: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: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: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:4377:MET:HE3	1:A:4437:VAL:HG12	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:3122:VAL:HG23	1:A:3126:MET:HE1	1.97	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: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:1769:MET:HE2	1:A:1774:ASP:O	2.16	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2855:LEU:HD11	1:A:2863:ARG:HE	1.81	0.45
1:A:3024:ASP:N	1:A:3024:ASP:OD1	2.50	0.45
1:A:1424:TRP:CH2	1:A:1434:ILE:HG22	2.52	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: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:2452:LEU:HD23	1:A:2452:LEU:HA	1.71	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4166:VAL:HA	1:A:4169:ILE:HG22	1.99	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:4042:LEU:HD23	1:A:4128:MET:HE1	1.99	0.44
1:A:4247:MET:HE3	1:A:4251:ILE:HB	1.98	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: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: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:2423:MET:HE1	1:A:2462:LEU:HD22	2.00	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: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: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
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:2667:ASN:ND2	1:A:2712:CYS:HB2	2.17	0.43
1:A:2916:LEU:HD23	1:A:2916:LEU:HA	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4178:ARG:O	1:A:4182:LEU:HG	2.19	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: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:3591:ASP:CG	1:A:3594:GLY:H	2.22	0.43
1:A:1697:LYS:O	1:A:1700:GLU:HG2	2.18	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3001:ASP:N	1:A:3001:ASP:OD1	2.53	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: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
1:A:2920:LEU:HD13	1:A:2920:LEU:HA	1.78	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:1457:MET:HE1	1:A:3659:ARG:HA	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1785:VAL:O	1:A:1789:LEU:HD13	2.20	0.42
1:A:2614:ASP:C	1:A:2657:LYS:HD2	2.41	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:4104:GLY:HA2	1:A:4107:MET:CE	2.50	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:2444:GLU:H	1:A:2510:MET:HE3	1.85	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: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:3540:ASN:O	1:A:3540:ASN:ND2	2.52	0.41
1:A:3639:GLU:HG3	1:A:3686:VAL:HG21	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1837:GLU:H	1:A:1837:GLU:CD	2.19	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:2444:GLU:O	1:A:2510:MET:HE1	2.20	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:2965:ARG:HD3	1:A:3642:ASP:CG	2.40	0.41
1:A:4257:ASP:OD1	1:A:4257:ASP:C	2.59	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:2458:LEU:HD12	1:A:2458:LEU:HA	1.87	0.41
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:3959:ILE:HD12	1:A:3959:ILE:H	1.86	0.41
1:A:4105:TRP:O	1:A:4109:LEU:HG	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3787:THR:OG1	1:A:3788:ASP:N	2.54	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: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:1887:ARG:HH12	1:A:4253:GLY:C	2.25	0.40
1:A:3819:LYS:HE2	1:A:3826:GLN:HE22	1.86	0.40
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:4628:THR:C	1:A:4629:LYS:HD2	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4104:GLY:HA2	1:A:4107:MET:HE2	2.03	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3019/4646 (65%)	2946 (98%)	73 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2696/4125 (65%)	2634 (98%)	62 (2%)	45	63

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1397	ASN
1	A	1398	MET
1	A	1409	LYS
1	A	1447	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1559	HIS
1	A	1767	SER
1	A	1820	ASP
1	A	1983	ARG
1	A	1990	TYR
1	A	2232	MET
1	A	2303	PHE
1	A	2377	ASN
1	A	2384	SER
1	A	2551	LYS
1	A	2584	TRP
1	A	2720	ARG
1	A	2880	ASP
1	A	2881	TYR
1	A	2953	MET
1	A	2983	SER
1	A	2986	LYS
1	A	2992	PHE
1	A	3006	GLU
1	A	3043	MET
1	A	3044	LEU
1	A	3077	ASP
1	A	3113	MET
1	A	3120	TYR
1	A	3125	TYR
1	A	3196	GLU
1	A	3198	GLN
1	A	3207	LYS
1	A	3524	MET
1	A	3540	ASN
1	A	3572	LEU
1	A	3606	ASP
1	A	3607	ARG
1	A	3619	PHE
1	A	3651	ARG
1	A	3655	ARG
1	A	3838	ASN
1	A	3910	ARG
1	A	3957	PHE
1	A	3972	TYR
1	A	3999	ASP
1	A	4043	MET

Continued on next page...

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Mol	Chain	Res	Type
1	A	4054	HIS
1	A	4078	ASN
1	A	4127	THR
1	A	4156	ASN
1	A	4161	PHE
1	A	4171	LYS
1	A	4220	ASP
1	A	4257	ASP
1	A	4311	LEU
1	A	4329	ARG
1	A	4338	ASP
1	A	4353	ASP
1	A	4436	GLN
1	A	4465	SER
1	A	4618	LEU
1	A	4624	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2057	GLN
1	A	2130	ASN
1	A	2299	GLN
1	A	2707	GLN
1	A	2752	ASN
1	A	2857	HIS
1	A	4404	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	4702	-	24,29,29	0.86	0	29,45,45	1.27	2 (6%)
2	ATP	A	4701	4	28,33,33	0.88	1 (3%)	34,52,52	0.65	1 (2%)
3	ADP	A	4703	-	24,29,29	0.85	0	29,45,45	1.19	2 (6%)

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	4702	-	-	0/12/32/32	0/3/3/3
2	ATP	A	4701	4	-	4/18/38/38	0/3/3/3
3	ADP	A	4703	-	-	3/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4701	ATP	PA-O3A	-2.70	1.56	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4702	ADP	N3-C2-N1	-3.75	123.58	128.67
3	A	4703	ADP	N3-C2-N1	-3.64	123.73	128.67
3	A	4703	ADP	C4-C5-N7	-2.56	106.63	109.34
3	A	4702	ADP	C4-C5-N7	-2.32	106.88	109.34
2	A	4701	ATP	C5-C6-N6	2.28	123.78	120.31

There are no chirality outliers.

All (7) torsion outliers are listed below:

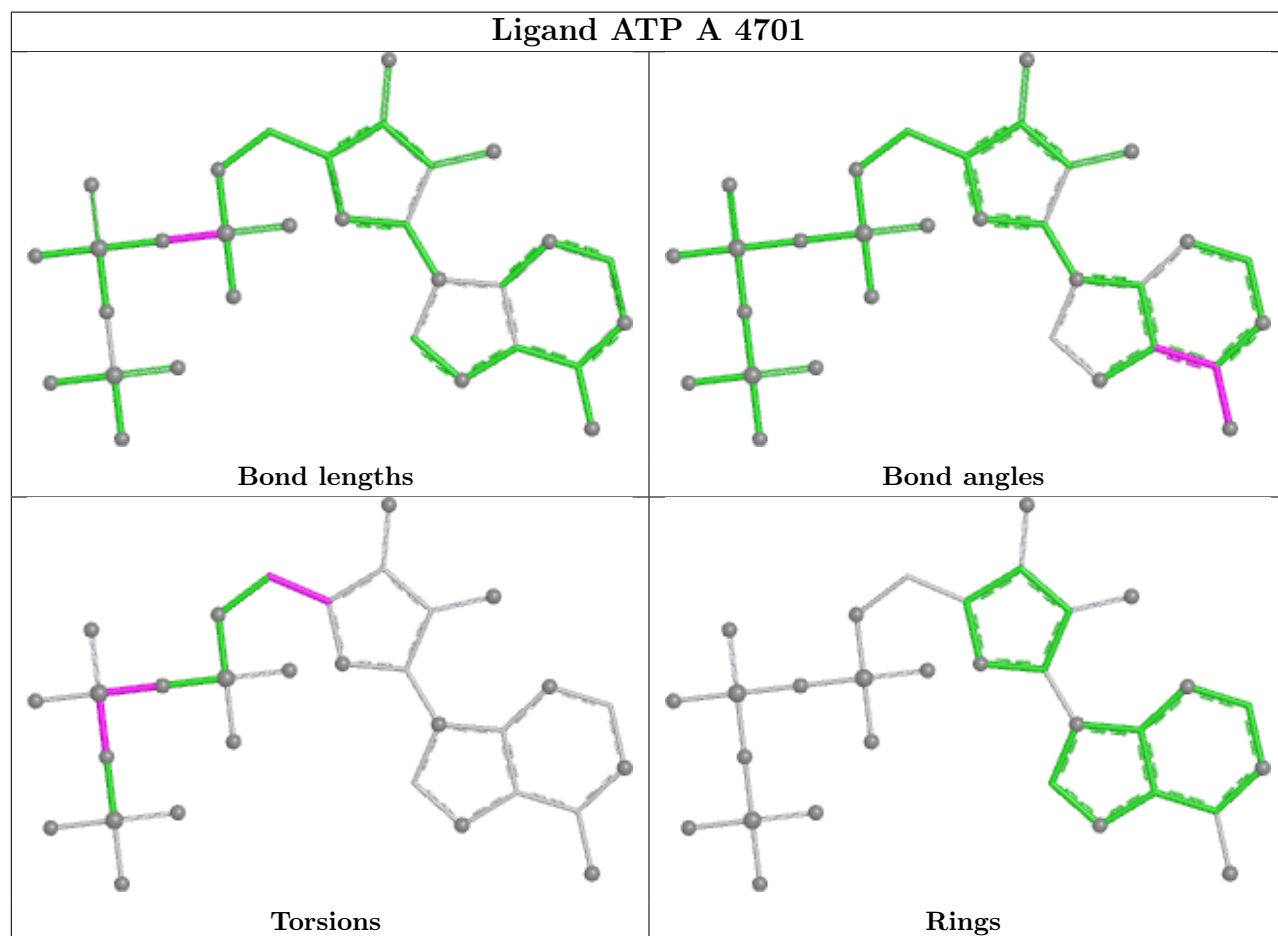
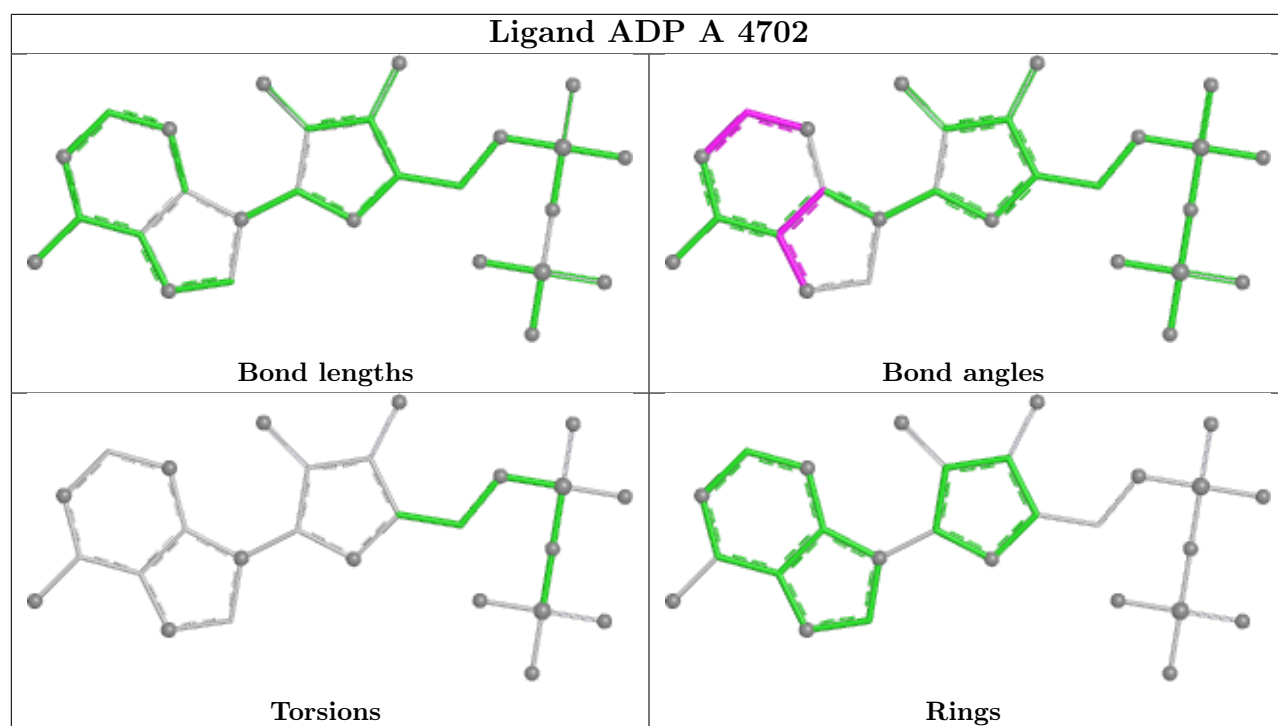
Mol	Chain	Res	Type	Atoms
2	A	4701	ATP	O4'-C4'-C5'-O5'
2	A	4701	ATP	C3'-C4'-C5'-O5'
3	A	4703	ADP	C5'-O5'-PA-O1A
2	A	4701	ATP	PG-O3B-PB-O2B
2	A	4701	ATP	PA-O3A-PB-O1B
3	A	4703	ADP	C3'-C4'-C5'-O5'
3	A	4703	ADP	O4'-C4'-C5'-O5'

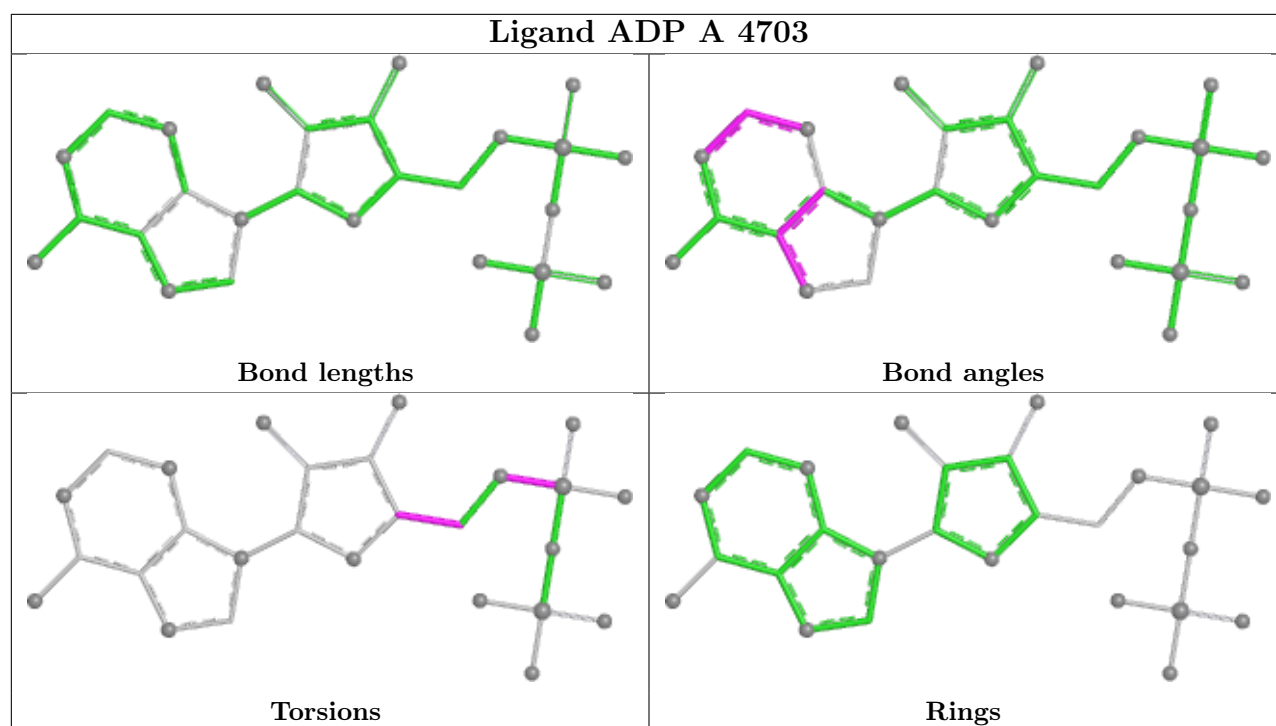
There are no ring outliers.

3 monomers are involved in 7 short contacts:

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

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

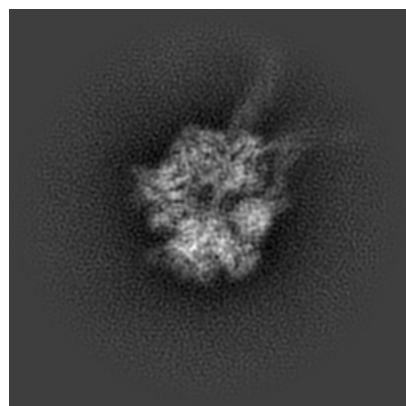
6 Map visualisation [i](#)

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

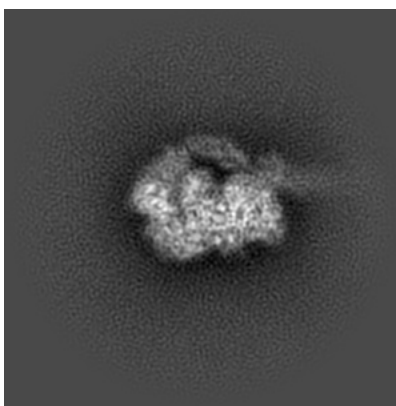
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

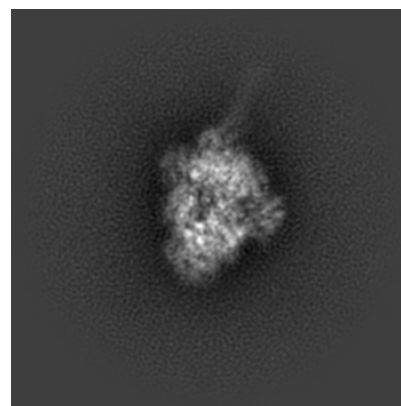
6.1.1 Primary map



X

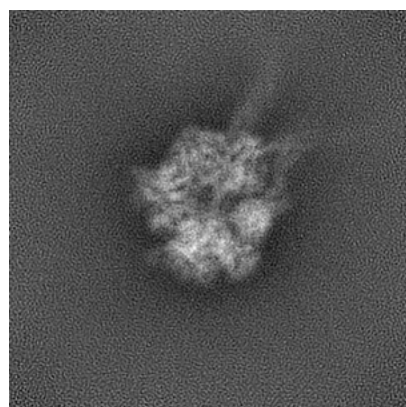


Y

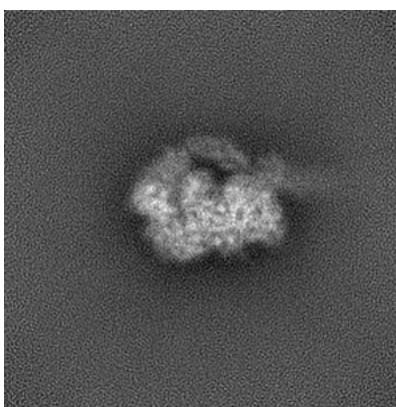


Z

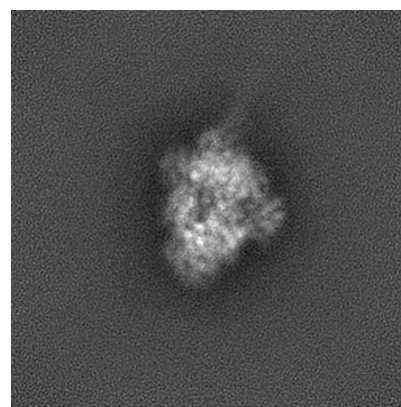
6.1.2 Raw map



X



Y

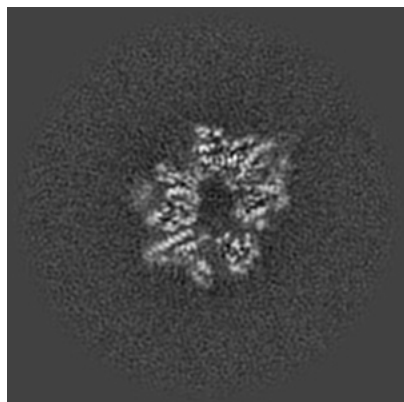


Z

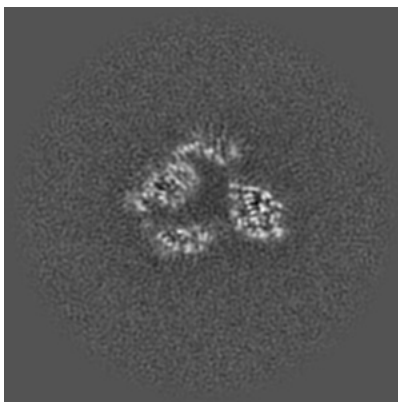
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

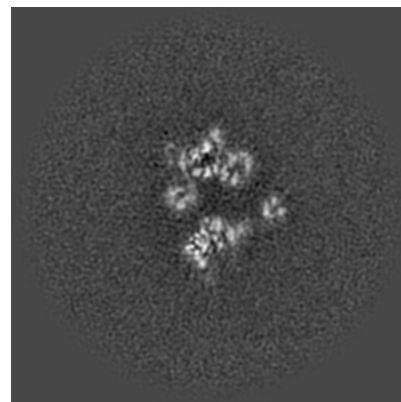
6.2.1 Primary map



X Index: 128

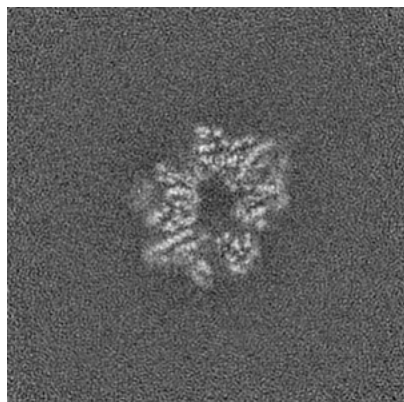


Y Index: 128



Z Index: 128

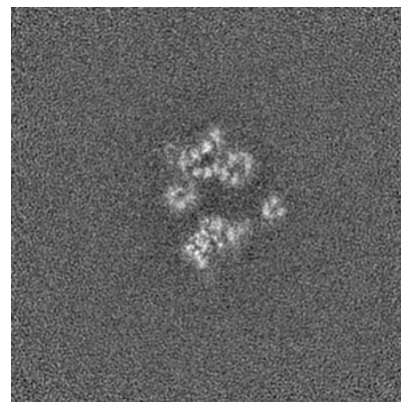
6.2.2 Raw map



X Index: 128



Y Index: 128

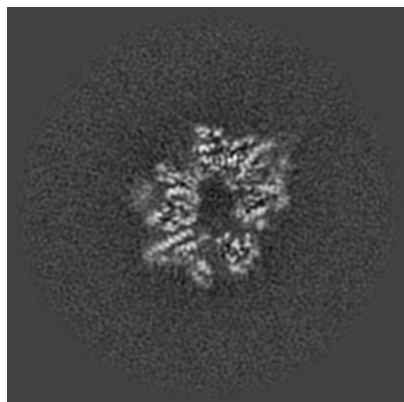


Z Index: 128

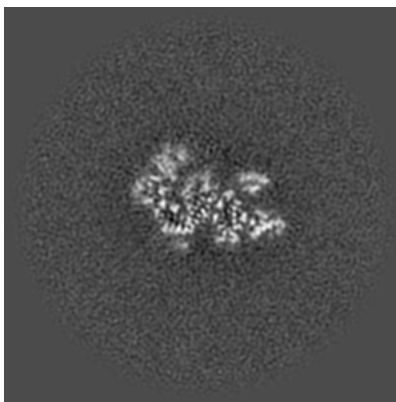
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

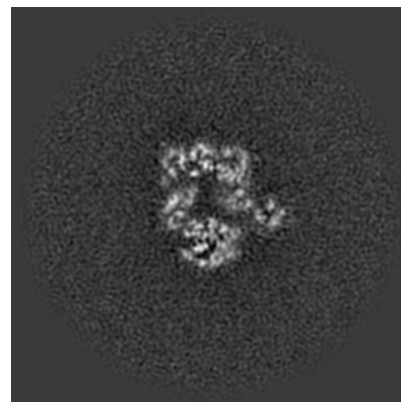
6.3.1 Primary map



X Index: 128

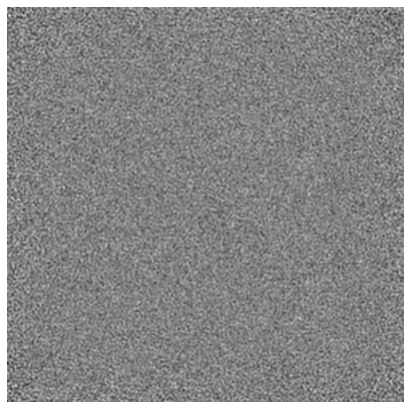


Y Index: 111

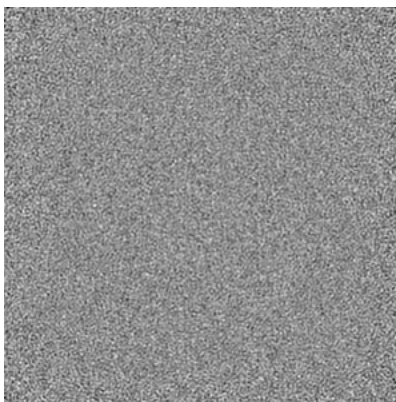


Z Index: 119

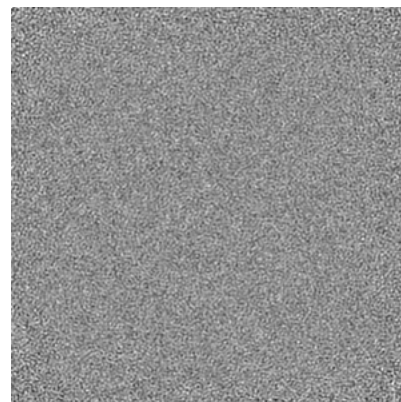
6.3.2 Raw map



X Index: 0



Y Index: 0

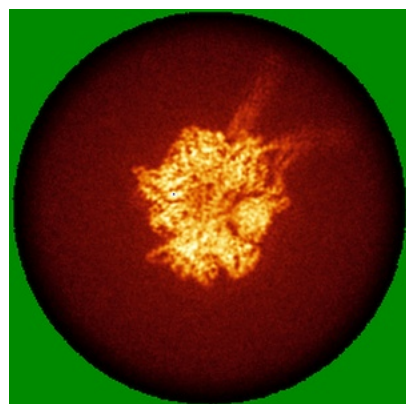


Z Index: 0

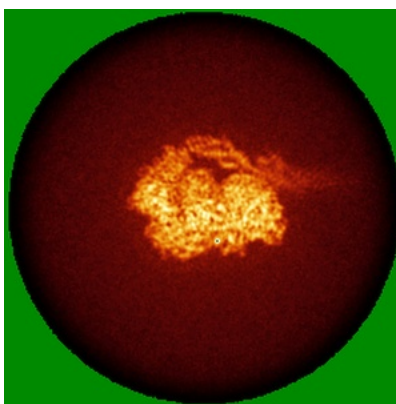
The images above show the largest variance slices of the map in three orthogonal directions.

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

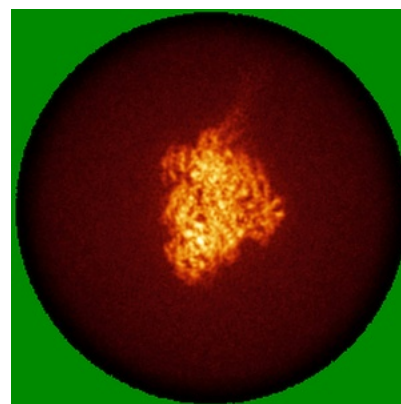
6.4.1 Primary map



X

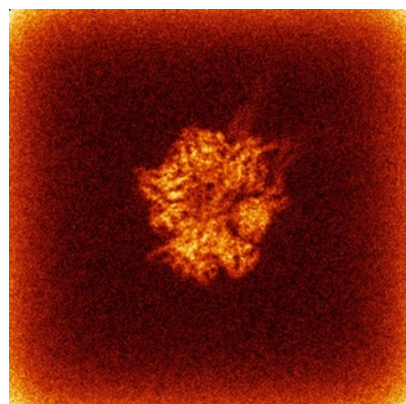


Y

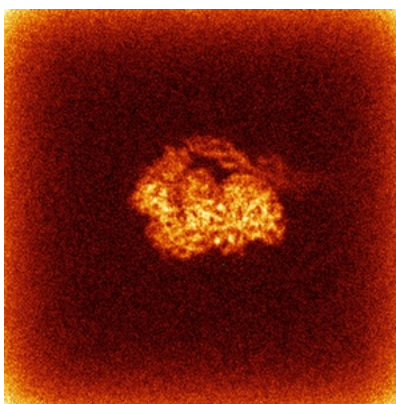


Z

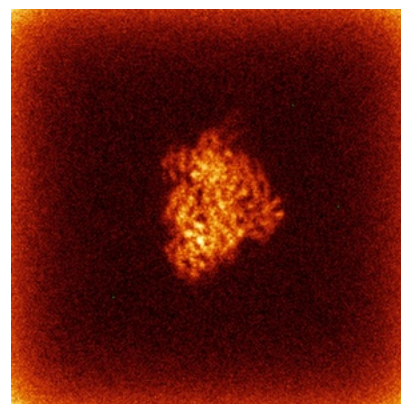
6.4.2 Raw map



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.

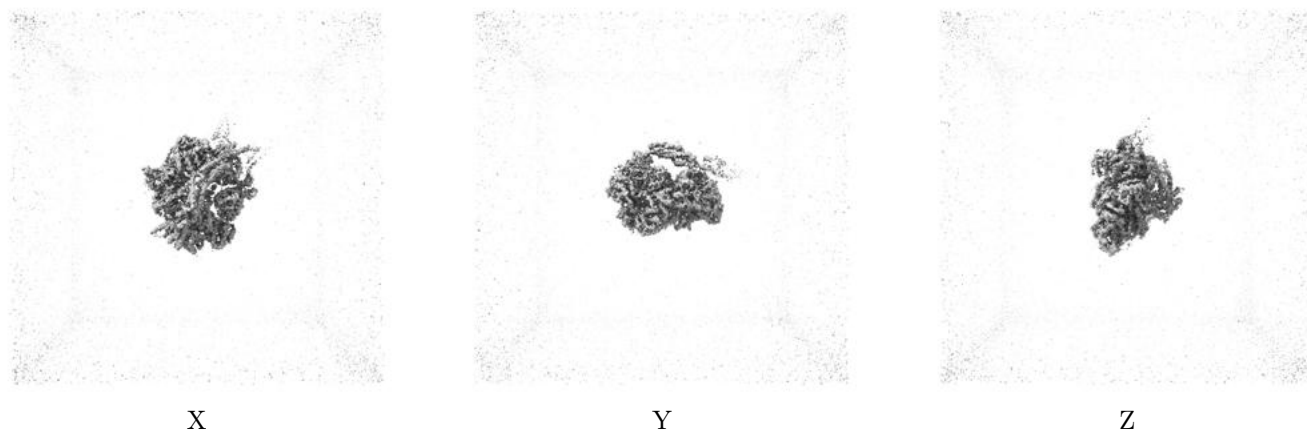
6.5 Orthogonal surface views [i](#)

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.

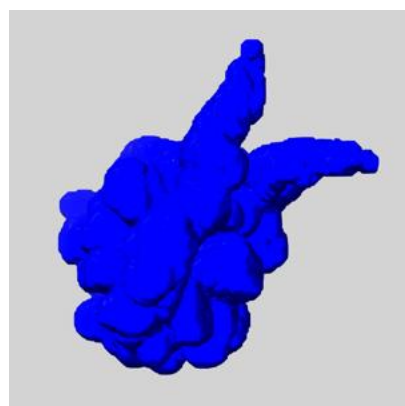
6.6 Mask visualisation [i](#)

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

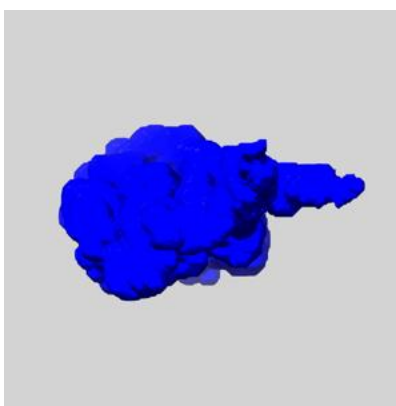
A mask typically either:

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

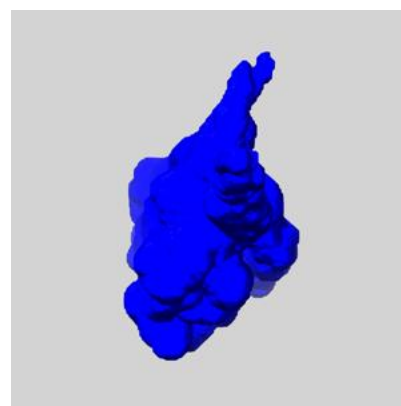
6.6.1 emd_44718_msk_1.map [i](#)



X



Y

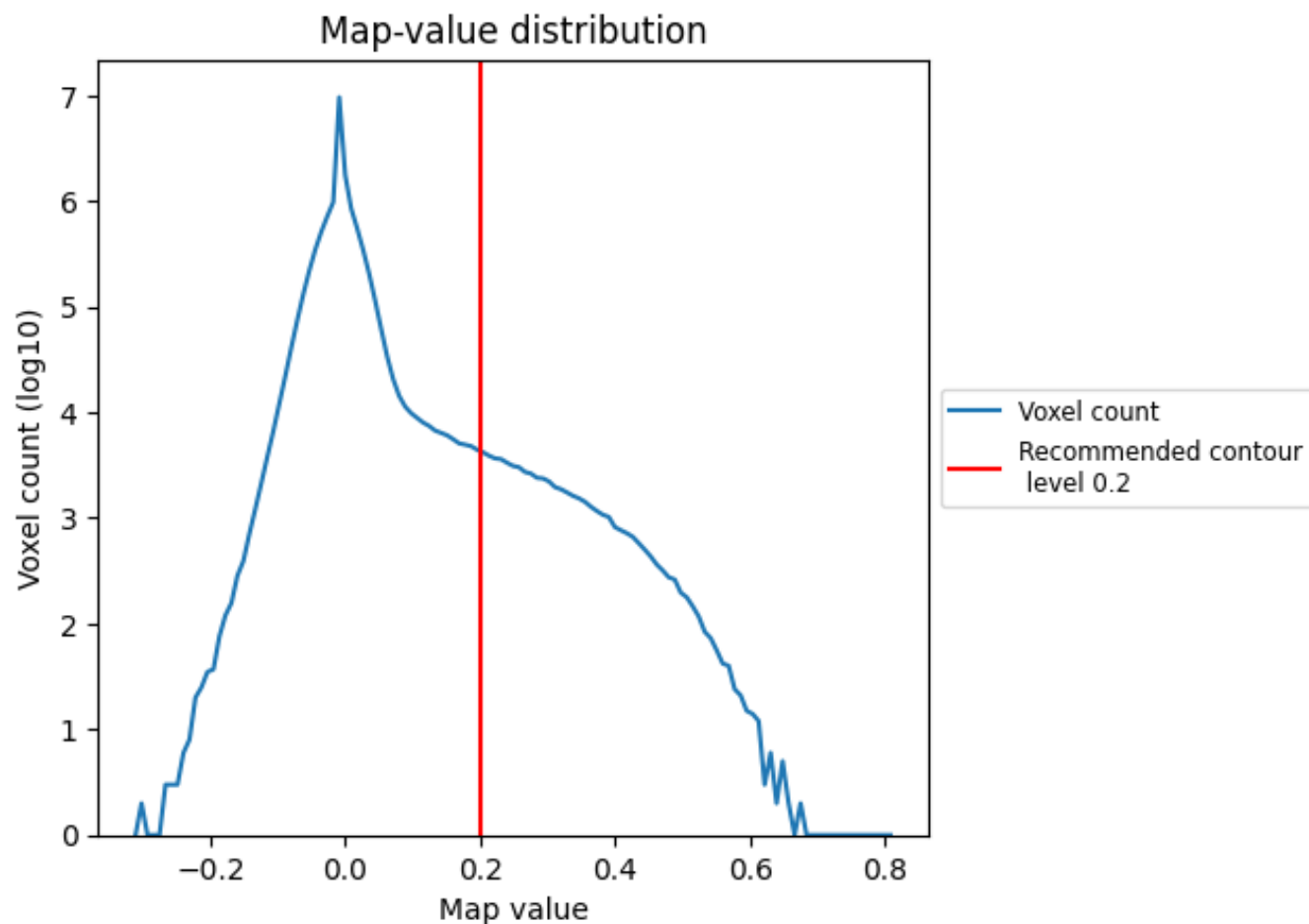


Z

7 Map analysis [i](#)

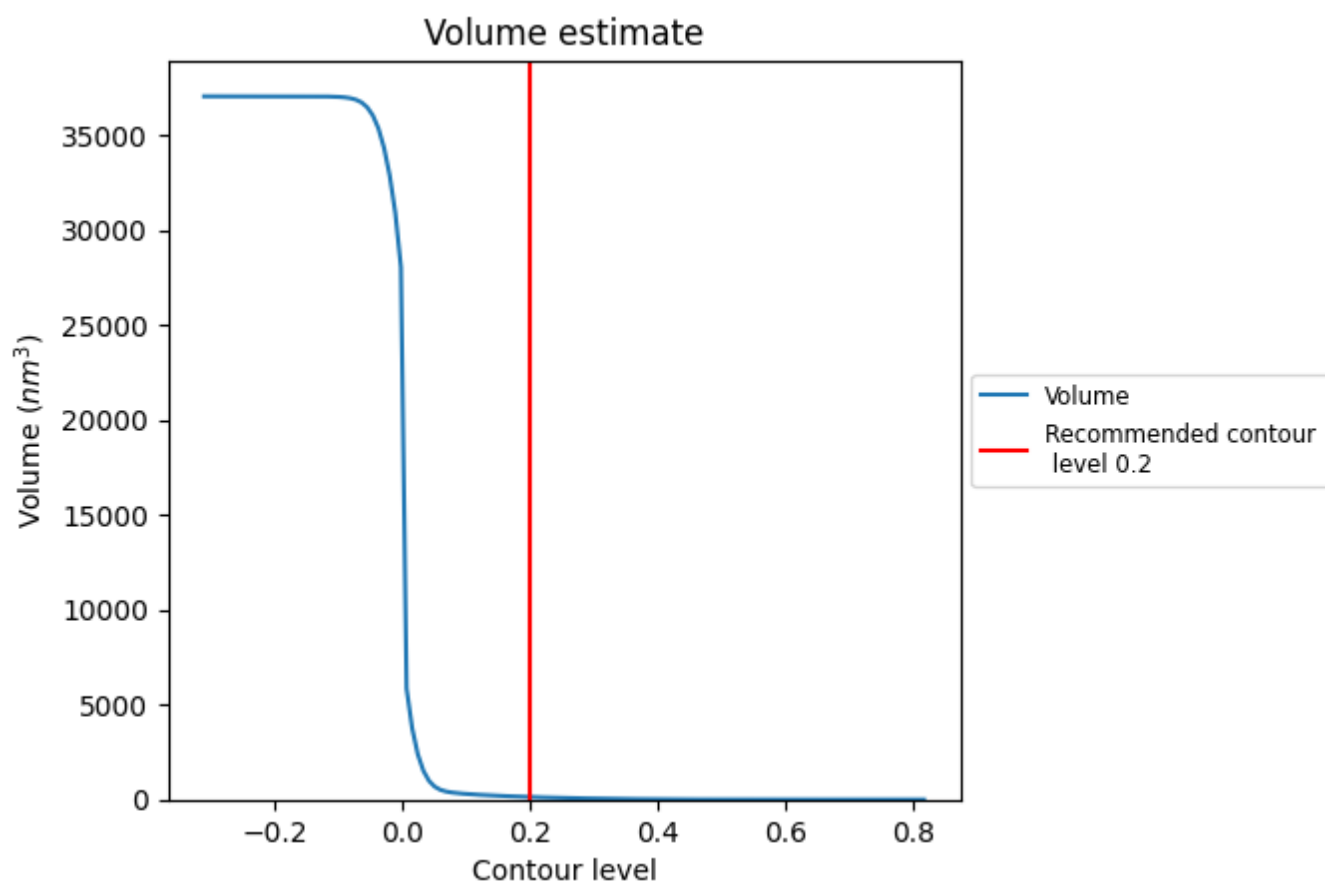
This section contains the results of statistical analysis of the map.

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.

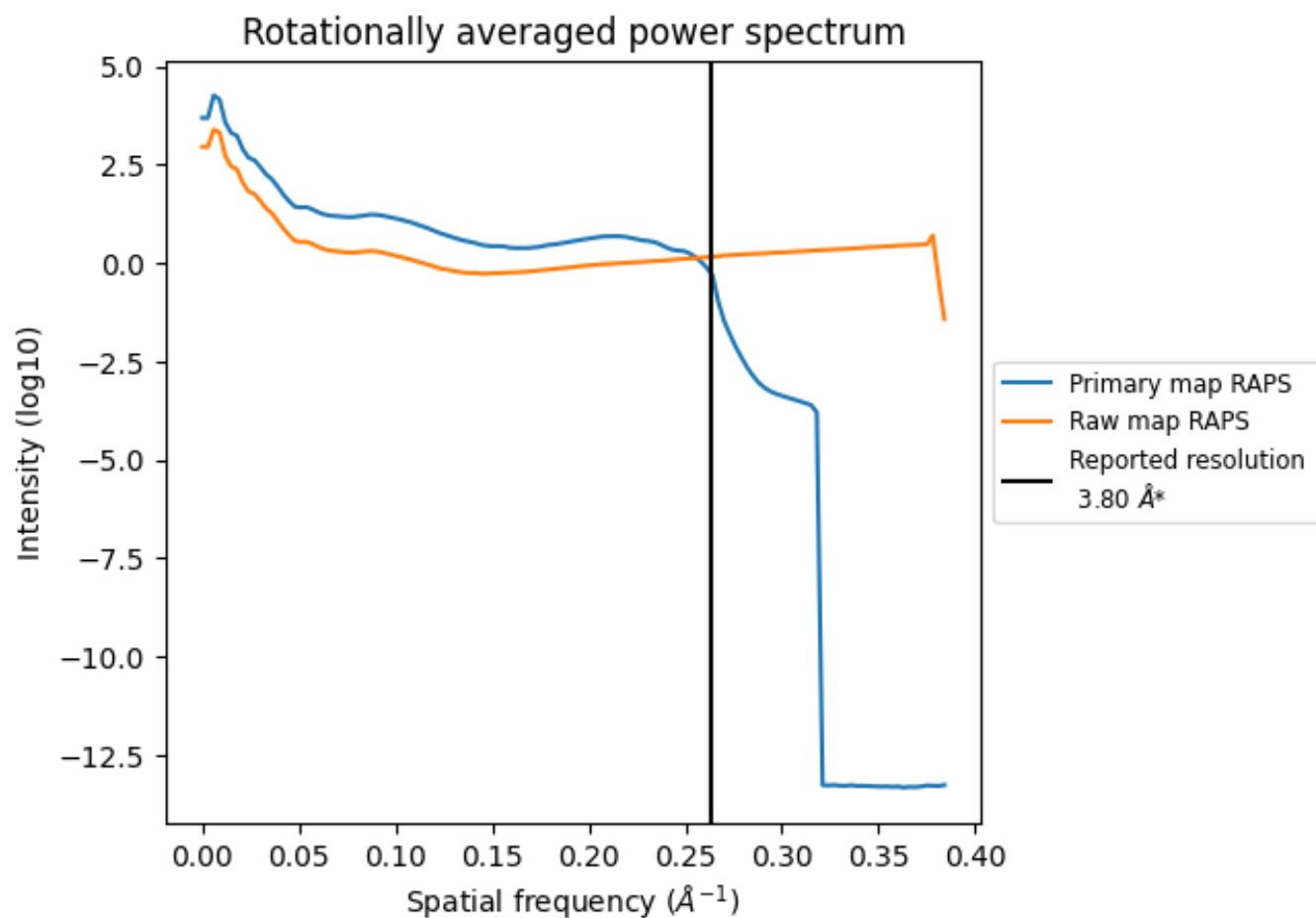
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 134 nm³; 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 ⓘ

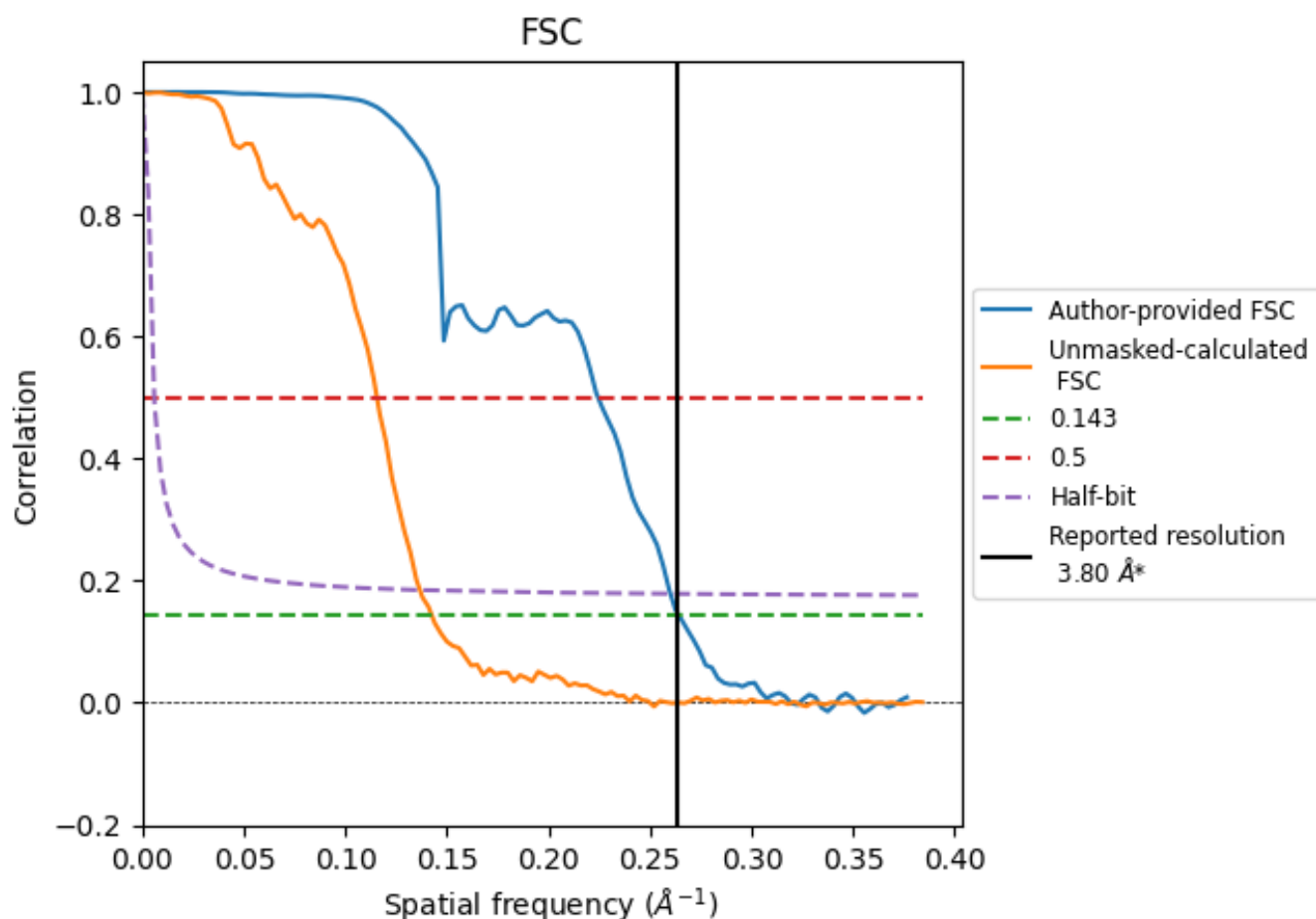


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

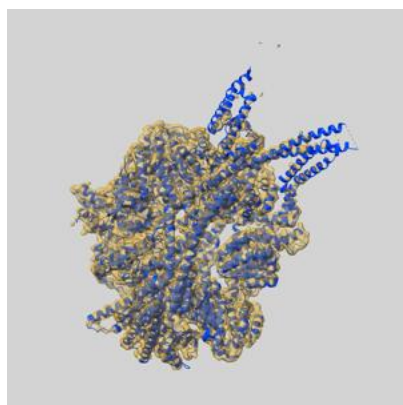
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.78	4.46	3.84
Unmasked-calculated*	7.01	8.65	7.31

*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 %

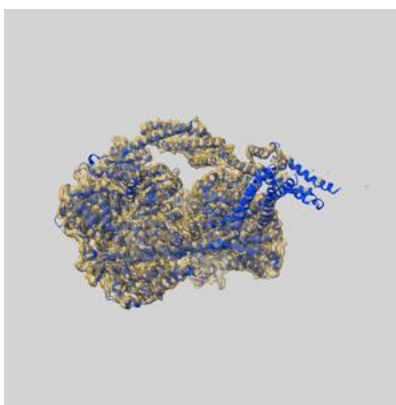
9 Map-model fit [i](#)

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](#).

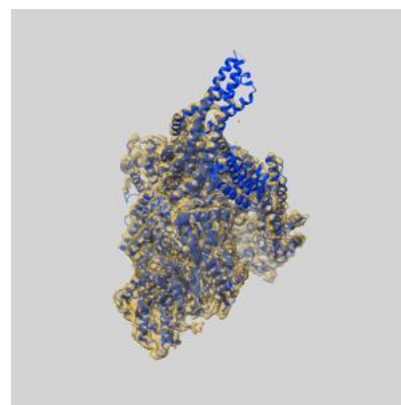
9.1 Map-model overlay [i](#)



X



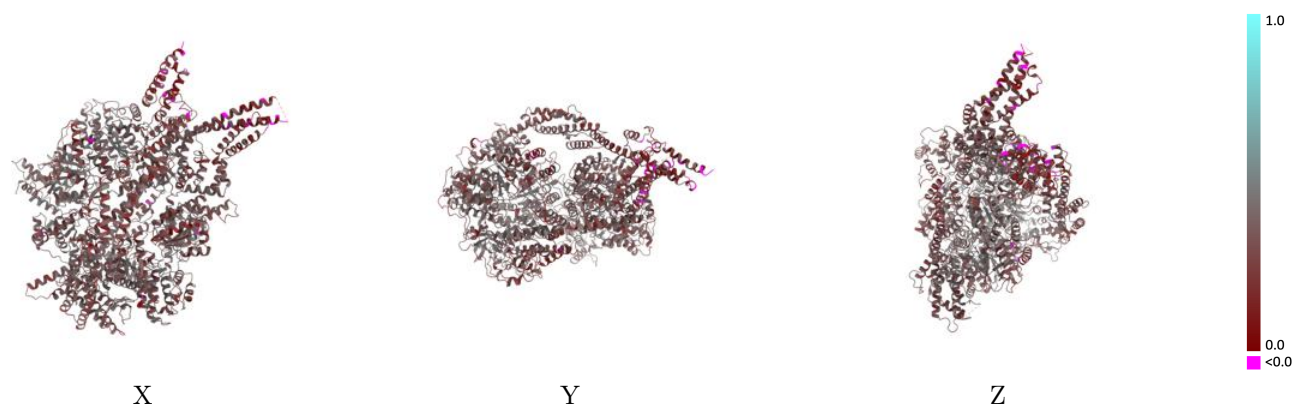
Y



Z

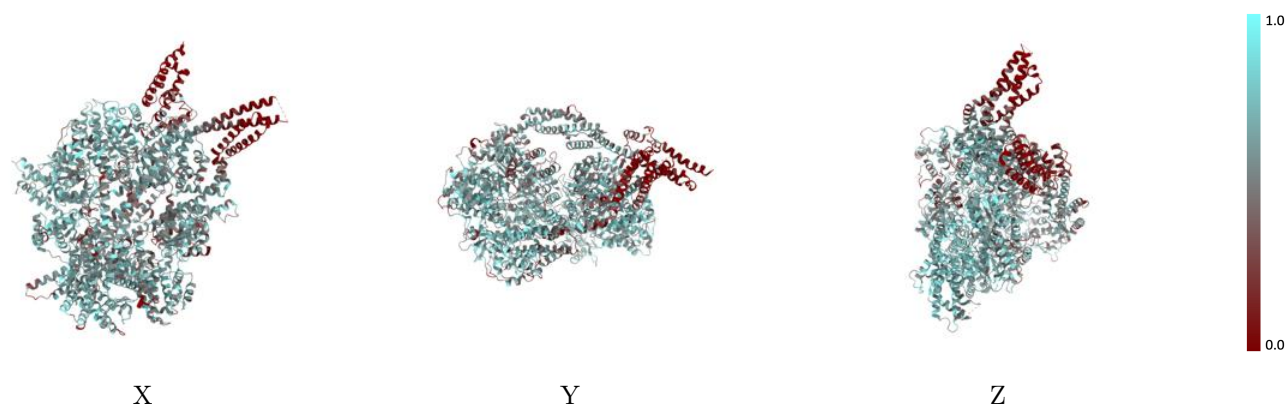
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



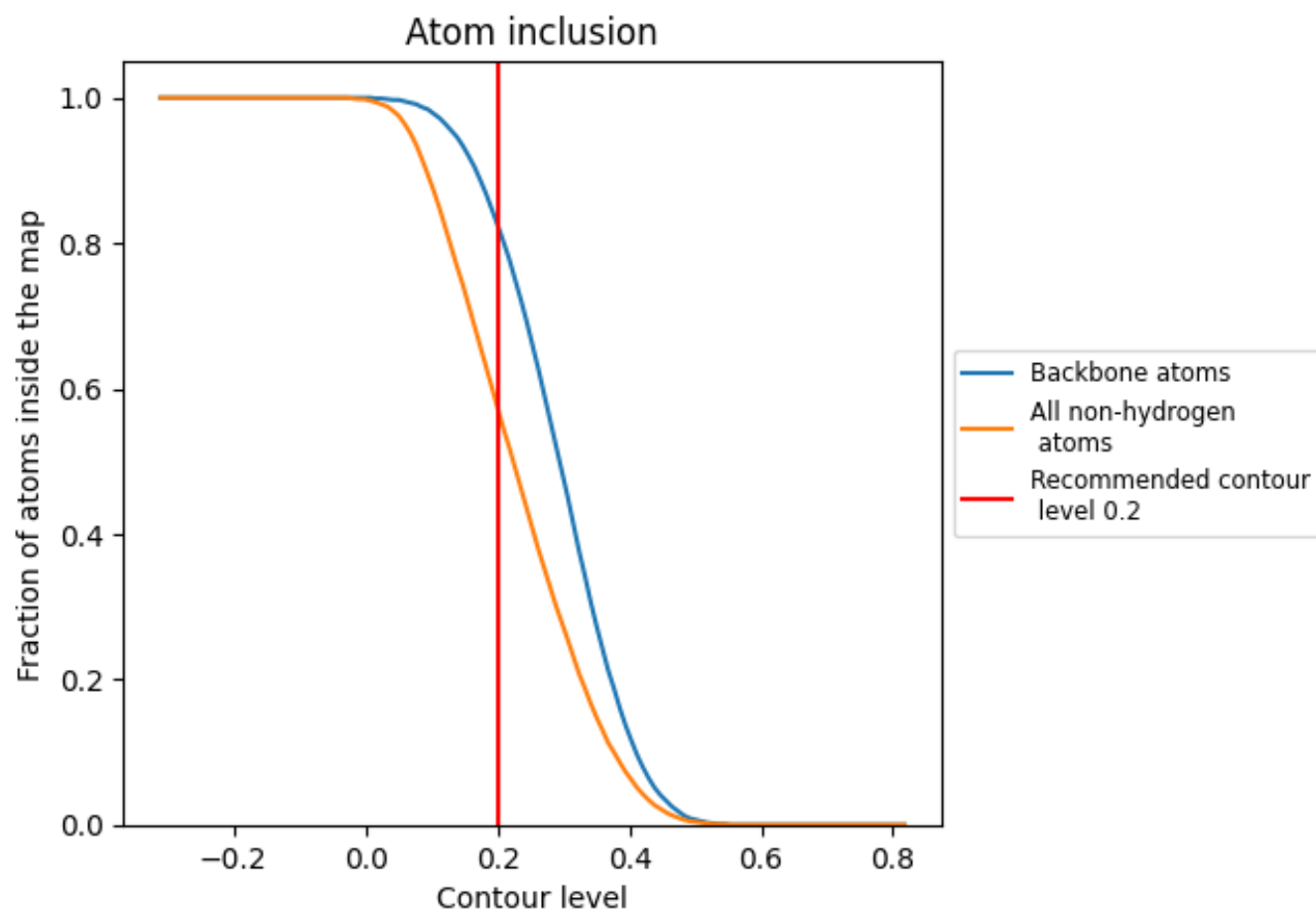
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div></div> 0.5750	<div></div> 0.3490
A	<div></div> 0.5750	<div></div> 0.3490

