



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 06:41 AM UTC

PDB ID : 3J68 / pdb_00003j68
EMDB ID : EMD-5758
Title : Structural mechanism of the dynein powerstroke (pre-powerstroke state)
Authors : Lin, J.; Okada, K.; Raytchev, M.; Smith, M.C.; Nicastro, D.
Deposited on : 2013-12-23
Resolution : 30.00 Å (reported)
Based on initial model : 4AKI

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
MolProbity : 4-5-2 with Phenix2.0
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

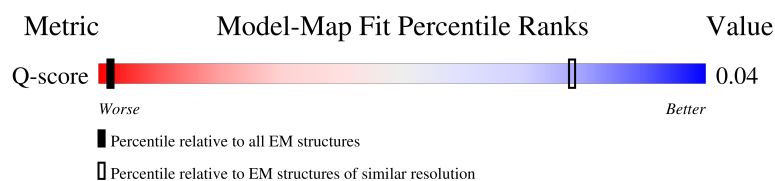
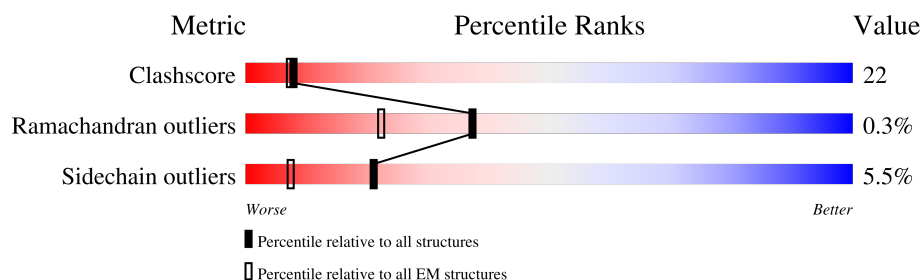
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 30.00 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	9 (30.00 - 30.30)

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	2286	 61% 34%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18105 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.

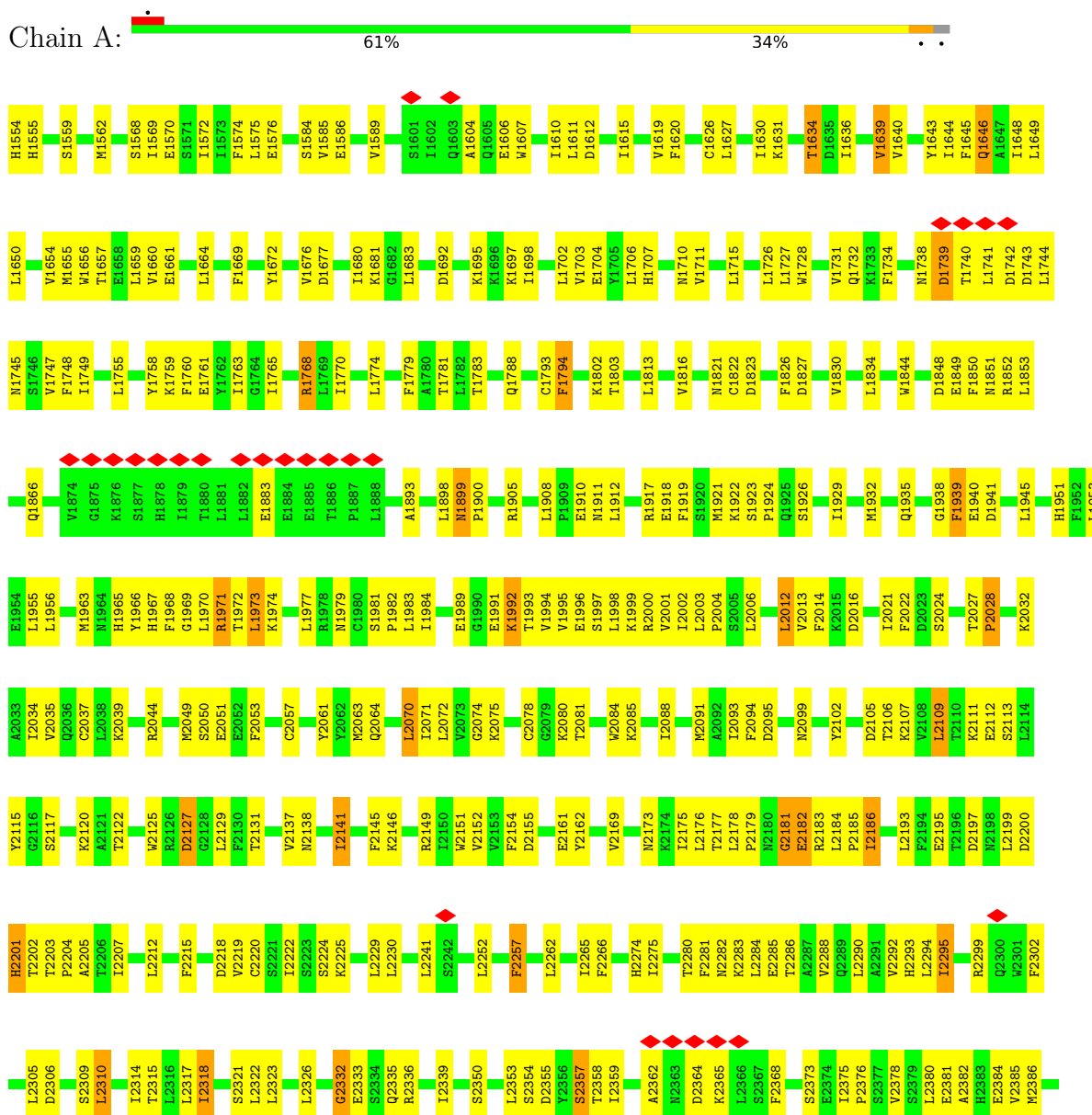
- Molecule 1 is a protein called Dynein motor domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2245	18105	11610	3004	3403	88	0	0

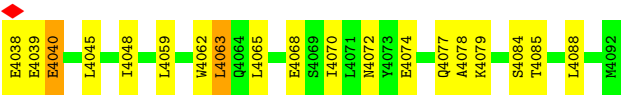
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Dynein motor domain



H3948	G3949	F3950	S3951	Y3955	E3969	K3970	F3971	F3972	F3973	S3976	T3977	K3978	N3979	P3980	P3981	K3982	K3983	Q3984	V3985	T3992	V3993	T3994	G3995	T3998	K4002	K4003	L4004	L4010	V4014	F4015	C4016	G4017	S4018	P4019	N4020	L4021	Q4022	I4023	V4024	R4028	I4029	P4030	Q4031	P4032	L4033	L4034	Q4035	S4037																																																																																	
T3862	A3865	E3869	K3870	F3871	F3872	M3873	F3874	M3875	T3876	C3877	H3878	L3880	A3881	K3882	L3883	L3884	L3885	L3886	L3887	L3888	L3889	L3890	L3891	L3892	L3893	L3894	L3895	L3896	L3897	L3898	L3899	L3900	L3901	L3902	L3903	L3904	L3905	L3906	L3907	L3908	L3909	L3910	L3911	L3912	L3913	L3914	L3915	L3916	L3917	L3918	L3919	L3920	L3921	L3922	L3923	L3924	L3925	L3926	L3927	L3928	L3929	L3930	L3931	L3932	L3933	L3934	L3935	L3936	L3937	L3938	L3939	L3940	L3941	L3942	L3943	L3944	L3945	L3946	L3947																																																		
V3777	V3778	N3779	N3780	N3781	N3782	N3783	N3784	N3785	N3786	N3787	N3788	N3789	N3790	N3791	N3792	N3793	N3794	N3795	N3796	N3797	N3798	N3799	N3800	N3801	N3802	N3803	N3804	N3805	N3806	N3807	N3808	N3809	N3810	N3811	N3812	N3813	N3814	N3815	N3816	N3817	N3818	N3819	N3820	N3821	N3822	N3823	N3824	N3825	N3826	N3827	N3828	N3829	N3830	N3831	N3832	N3833	N3834	N3835	N3836	N3837	N3838	N3839	N3840	N3841	N3842	N3843	N3844	N3845	N3846	N3847	N3848	N3849	N3850	N3851	N3852	N3853	N3854	N3855	N3856	N3857																																																	
D3581	E3582	L3583	M3584	L3585	L3586	L3587	L3588	L3589	K3590	L3591	L3592	E3593	N3594	L3595	L3596	L3597	L3598	L3599	L3600	E3601	E3602	E3603	E3604	E3605	E3606	E3607	E3608	E3609	E3610	E3611	E3612	E3613	E3614	E3615	E3616	E3617	E3618	E3619	E3620	E3621	E3622	E3623	E3624	E3625	E3626	E3627	E3628	E3629	E3630	E3631	E3632	E3633	E3634	E3635	E3636	E3637	E3638	E3639	E3640	E3641	E3642	E3643	E3644	E3645	E3646	E3647	E3648	E3649	E3650	E3651	E3652	E3653	E3654	E3655	E3656	E3657	E3658	E3659	E3660	E3661	E3662	E3663	E3664	E3665	E3666	E3667	E3668	E3669	E3670	E3671	E3672	E3673	E3674																																				
L3677	V3682	Y3683	F3686	S3687	L3689	D3690	L3691	L3692	L3693	L3694	L3695	L3696	L3697	L3698	L3699	L3700	L3701	L3702	L3703	L3704	L3705	L3706	L3707	L3708	E3717	L3720	T3721	L3725	E3728	S3729	D3731	K3735	L3736	L3737	T3740	L3744	L3760	E3766	F3767	F3768	V3769	W3772	H3773	L3774	L3775	L3776	L3777	L3778	L3779	L3780	L3781	L3782	L3783	L3784	L3785	L3786	L3787	L3788	L3789	L3790	L3791	L3792	L3793	L3794	L3795	L3796	L3797	L3798	L3799	L3800	L3801	L3802	L3803	L3804	L3805	L3806	L3807	L3808	L3809	L3810	L3811	L3812	L3813	L3814	L3815	L3816	L3817	L3818	L3819	L3820	L3821	L3822	L3823	L3824	L3825	L3826	L3827	L3828	L3829	L3830	L3831	L3832	L3833	L3834	L3835	L3836	L3837	L3838	L3839	L3840	L3841	L3842	L3843	L3844	L3845	L3846	L3847	L3848	L3849	L3850	L3851	L3852	L3853	L3854	L3855	L3856	L3857	L3858	L3859
T3862	A3865	E3869	K3870	F3871	F3872	M3873	F3874	M3875	T3876	C3877	H3878	L3880	A3881	K3882	L3883	L3884	L3885	L3886	L3887	L3888	L3889	L3890	L3891	L3892	L3893	L3894	L3895	L3896	L3897	L3898	L3899	L3900	L3901	L3902	L3903	L3904	L3905	L3906	L3907	L3908	L3909	L3910	L3911	L3912	L3913	L3914	L3915	L3916	L3917	L3918	L3919	L3920	L3921	L3922	L3923	L3924	L3925	L3926	L3927	L3928	L3929	L3930	L3931	L3932	L3933	L3934	L3935	L3936	L3937	L3938	L3939	L3940	L3941	L3942	L3943	L3944	L3945	L3946	L3947																																																		
H3948	G3949	F3950	S3951	Y3955	E3969	K3970	F3971	F3972	F3973	S3976	T3977	K3978	N3979	P3980	P3981	K3982	K3983	Q3984	V3985	T3992	V3993	T3994	G3995	T3998	K4002	K4003	L4004	L4010	V4014	F4015	C4016	G4017	S4018	P4019	N4020	L4021	Q4022	I4023	V4024	R4028	I4029	P4030	Q4031	P4032	L4033	L4034	Q4035	S4037																																																																																	
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F2795	L2799	L2808	S2811	R2812	T2813	L2816	L2817	E2818	E2819	N2821	L2822	L2828	E2829	N2832	T2833	L2834	L2835	D2839	L2840	P2841	D2842	L2843	F2844	Q2845	Q2846	Y2849	L2852	L2853	L2856	R2857	N2858	K2859	T2860	R2861	S2862	L2863	G2864	L2865	L2866	L2867	L2868	E2872	L2873	V2878																																																																																					
L2881	F2889	I2891	M2902	L2903	S2904	S2905	P2906	R2911	C2912	W2916	M2917	W2920	M2932	I2936	P2937	M2938	T2941	D2942	F2943	I2944	VAL	PRO	GLU	VAL	ASN	L3307	L3308	L3309	T3310	K3311	Q3312	Q3313	S3317	G3318	E3319	L3320	L3321	G3322	N3323	T3329	Y3330	Y3331	I3341	I3342	S3343	R3344	L3345	L3346	L3347	L3348	L3349	K3350	Y3355	L3359	R3365	L3366	L3370	E3379	N3380																																																																						
R2987	S2988	P2989	G2990	L2993	L3010	V3017	L3024	F3028	LEU	VAL	ASN	GLU	LEU	ASN	THR	LEU	ILE	SER	LEU	VAL	K3297	K3303	E3304	R3305	W3306	L3307	N3308	T3309	K3310	K3311	Q3312	F3313	S3317	G3318	E3319	L3320	L3321	G3322	N3323	T3329	Y3330	Y3331	I3341	I3342	S3343	R3344	L3345	L3346	L3347	L3348	L3349	K3350	Y3355	L3359	R3365	L3366	L3370	E3379	N3380																																																																						
E3341	L3346	K3350	L3353	V3358	K3359	D3361	R3365	D3368	V3371	T3372	L3373	L3380	S3400	Q3401	D3402	F3406	L3407	L3408	D3409	F3410	S3411	H3413	M3414	I3415	I3418	K3425	L3429	R3439	L3440	Q3453	E3456	D3459	P3460	I3461	I3462	S3463	R3464	L3465	I3466	S3467																																																																																									
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D3581	E3582	L3583	M3584	L3585	L3586	L3587	L3588	L3589	K3590	L3591	L3592	E3593	N3594	L3595	L3596	L3597	L3598	L3599	L3600	E3601	E3602	E3603	E3604	E3605	E3606	E3607	E3608	E3609	E3610	E3611	E3612	E3613	E3614	E3615	E3616	E3617	E3618	E3619	E3620	E3621	E3622	E3623	E3624	E3625	E3626	E3627	E3628	E3629	E3630	E3631	E3632	E3633	E3634	E3635	E3636	E3637	E3638	E3639	E3640	E3641	E3642	E3643	E3644	E3645	E3646	E3647	E3648	E3649	E3650	E3651	E3652	E3653	E3654	E3655	E3656	E3657	E3658	E3659	E3660	E3661	E3662	E3663	E3664	E3665	E3666	E3667	E3668	E3669	E3670	E3671	E3672	E3673	E3674																																				
L3677	V3682	Y3683	F3686	S3687	L3689	D3690	L3691	L3692	L3693	L3694	L3695	L3696	L3697	L3698	L3699	L3700	L3701	L3702	L3703	L3704	L3705	L3706	L3707	L3708	E3717	L3720	T3721	L3725	E3728	S3729	D3731	K3735	L3736	L3737	T3740	L3744	L3760	E3766	F3767	F3768	V3769	W3772	H3773	L3774	L3775	L3776	L3777	L3778	L3779	L3780	L3781	L3782	L3783	L3784	L3785	L3786	L3787	L3788	L3789	L3790	L3791	L3792	L3793	L3794	L3795	L3796	L3797	L3798	L3799	L3800	L3801	L3802	L3803	L3804	L3805	L3806	L3807	L3808	L3809	L3810	L3811	L3812	L3813	L3814	L3815	L3816	L3817	L3818	L3819	L3820	L3821	L3822	L3823	L3824	L3825	L3826	L3827	L3828	L3829	L3830	L3831	L3832	L3833	L3834	L3835	L3836	L3837	L3838	L3839	L3840	L3841	L3842	L3843	L3844	L3845	L3846	L3847	L3848	L3849	L3850	L3851	L3852	L3853	L3854	L3855	L3856	L3857	L3858	L3859
T3862	A3865	E3869	K3870	F3871	F3872	M3873	F3874	M3875	T3876	C3877	H3878	L3880	A3881	K3882	L3883	L3884	L3885	L3886	L3887	L3888	L3889	L3890	L3891	L3892	L3893	L3894	L3895	L3896	L3897	L3898	L3899	L3900	L3901	L3902	L3903	L3904	L3905	L3906	L3907	L3908	L3909	L3910	L3911	L3912	L3913	L3914	L3915	L3916	L3917	L3918	L3919	L3920	L3921	L3922	L3923	L3924	L3925	L3926	L3927	L3928	L3929	L3930	L3931	L3932	L3933	L3934	L3935	L3936	L3937	L3938	L3939	L3940	L3941	L3942	L3943	L3944	L3945	L3946	L3947																																																		
H3948	G3949	F3950	S3951	Y3955	E3969	K3970	F3971	F3972	F3973	S3976	T3977	K3978	N3979	P3980	P3981	K3982	K3983	Q3984	V3985	T3992	V3993	T3994	G3995	T3998	K4002	K4003	L4004	L4010	V4014	F4015	C4016	G4017	S4018	P4019	N4020	L4021	Q4022	I4023	V4024	R4028	I4029	P4030	Q4031	P4032	L4033	L4034	Q4035	S4037																																																																																	
L2484	E2488	L2489	N2490	L2491	P2492	K2493	L2494	L2495	K2496	L2497	L2498	N2499	S2510	K2511	R2512	G2513	G2514	L2506	R2507	Q2508	L2509	M2510	E2511	G2512	Q2513	G2514	K2517	L2518	L2519	E2520	W2523	L2526	R2527	R2528	L2529	H2530	G2535	N2536	P2537	R2543	L2544	M2545	M2546	R2549	R2552	Y2558	S2559	L2562	S2563	G2564																																																																															
K2565	S2566	L2567	S2568	Y2571	Y2574	Y2575	K2576	L2577	L2578	L2579	K2580	R2586	E2590	Y2597	G2609	G2610	T2611	Q2612	V2626	T2627	Y2630	T2631	A2632	G2636	P2637	R2638	Q2639	T2640	S2643	L2644	L2645	P2646	L2647	R2654	D2658	Y2661	E2665	Y2677	Q2678	P2682	N2683	Q2684																																																																																							
L2432	L2437	Y2440	F2445	S2446	K2447	D2448	T2449	T2450	H2453	L2458	T2462	T2472	K2476	S2477	D2478	L2479	N2481	L2484	E2488	L2491	P2492	K2493	L2494	L2495	K2496	L2497	L2498	N2499	S2510	K2511	R2512	G2513	G2514	L2506	R2507	Q2508	L2509	M2510	E2511	G2512	Q2513	G2514	K2517	L2518	L2519																																																																																				



4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	Not provided	
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	6000	Depositor
Maximum defocus (nm)	8000	Depositor
Magnification	13500	Depositor
Image detector	GENERIC GATAN (2k x 2k)	Depositor
Maximum voxel value	160.067	Depositor
Minimum voxel value	96.788	Depositor
Average voxel value	123.910	Depositor
Voxel value standard deviation	7.732	Depositor
Recommended contour level	127	Depositor
Tomogram size ($\text{\AA}$)	492.8, 354.816, 492.8	wwPDB
Tomogram dimensions	50, 36, 50	wwPDB
Tomogram angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Grid spacing ($\text{\AA}$)	9.856, 9.856, 9.856	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.79	4/18472 (0.0%)	1.18	57/24968 (0.2%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2872	GLU	CA-CB	6.05	1.62	1.53
1	A	3980	ILE	CA-C	5.41	1.58	1.52
1	A	2867	LEU	C-N	5.31	1.40	1.33
1	A	2867	LEU	C-O	5.22	1.30	1.24

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2127	ASP	N-CA-C	11.22	123.07	111.07
1	A	2333	GLU	N-CA-C	-8.58	102.01	111.36
1	A	2938	MET	N-CA-C	8.06	121.16	110.53
1	A	2182	GLU	N-CA-C	8.05	120.35	108.60
1	A	2752	VAL	CB-CA-C	-7.50	102.36	111.97
1	A	2181	GLY	N-CA-C	7.44	121.54	113.58
1	A	2537	PRO	CA-C-N	-7.26	113.42	120.83
1	A	2537	PRO	C-N-CA	-7.26	113.42	120.83
1	A	1939	PHE	N-CA-C	7.05	118.62	111.07
1	A	2479	ILE	N-CA-C	6.91	117.06	110.42
1	A	2942	ASP	N-CA-C	6.88	118.78	111.28
1	A	3900	ILE	CB-CA-C	-6.86	102.89	110.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3459	ASP	CA-C-N	6.56	126.80	119.32
1	A	3459	ASP	C-N-CA	6.56	126.80	119.32
1	A	3461	ILE	N-CA-C	6.41	117.16	110.62
1	A	3809	GLU	CB-CA-C	-6.37	109.22	116.54
1	A	1794	PHE	N-CA-C	6.34	118.75	108.41
1	A	2481	ASN	N-CA-C	6.18	119.19	110.23
1	A	2916	TRP	N-CA-C	6.02	118.22	108.41
1	A	1740	THR	N-CA-C	5.99	118.06	109.14
1	A	2257	PHE	N-CA-C	5.93	118.19	108.52
1	A	2332	GLY	N-CA-C	-5.83	106.67	114.25
1	A	3981	PRO	CA-C-N	5.82	130.00	120.63
1	A	3981	PRO	C-N-CA	5.82	130.00	120.63
1	A	2373	SER	N-CA-C	5.80	119.85	111.56
1	A	3980	ILE	N-CA-C	5.79	121.40	108.88
1	A	2590	GLU	CA-C-N	-5.79	113.71	119.56
1	A	2590	GLU	C-N-CA	-5.79	113.71	119.56
1	A	2872	GLU	CB-CG-CD	5.71	122.30	112.60
1	A	2752	VAL	N-CA-CB	5.59	117.09	110.55
1	A	2840	ILE	CA-C-N	5.55	125.64	119.32
1	A	2840	ILE	C-N-CA	5.55	125.64	119.32
1	A	3402	ASP	N-CA-C	-5.38	106.71	113.28
1	A	2867	LEU	CA-C-O	-5.38	114.40	120.32
1	A	4039	GLU	CA-C-N	5.37	127.47	120.28
1	A	4039	GLU	C-N-CA	5.37	127.47	120.28
1	A	2120	LYS	N-CA-C	5.35	117.80	111.33
1	A	2988	SER	CA-C-N	5.34	126.52	119.84
1	A	2988	SER	C-N-CA	5.34	126.52	119.84
1	A	2378	VAL	N-CA-C	5.27	115.90	108.36
1	A	3413	HIS	N-CA-C	-5.27	106.69	113.23
1	A	2201	HIS	N-CA-C	5.25	117.08	111.36
1	A	2761	ALA	CB-CA-C	-5.24	110.11	117.23
1	A	2811	SER	N-CA-C	5.23	118.12	111.69
1	A	1899	ASN	CA-C-N	-5.22	114.97	120.66
1	A	1899	ASN	C-N-CA	-5.22	114.97	120.66
1	A	2564	GLY	N-CA-C	-5.15	108.61	115.40
1	A	2905	SER	CA-C-N	5.14	124.31	118.97
1	A	2905	SER	C-N-CA	5.14	124.31	118.97
1	A	2418	GLY	CA-C-N	5.12	125.65	120.38
1	A	2418	GLY	C-N-CA	5.12	125.65	120.38
1	A	1883	GLU	N-CA-C	5.10	118.24	111.30
1	A	3707	LYS	N-CA-C	5.09	118.59	112.38
1	A	3982	TRP	N-CA-C	5.06	118.92	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4063	LEU	N-CA-C	-5.06	101.51	109.25
1	A	1821	ASN	N-CA-CB	5.01	117.97	109.94
1	A	4015	PHE	N-CA-C	5.00	119.22	111.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1739	ASP	Peptide

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	18105	0	18146	811	0
All	All	18105	0	18146	811	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 22.

All (811) 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:1620:PHE:HD1	1:A:1760:PHE:CZ	1.58	1.22
1:A:4033:LEU:CD1	1:A:4035:GLN:HB2	1.76	1.16
1:A:3534:LEU:CD1	1:A:3618:TYR:HE2	1.59	1.15
1:A:3777:VAL:HG11	1:A:3895:PHE:HE1	1.06	1.15
1:A:2111:LYS:HD3	1:A:2161:GLU:HG3	1.18	1.14
1:A:3525:ILE:HD11	1:A:3646:ILE:HG22	1.25	1.12
1:A:3024:LEU:HD11	1:A:3303:LYS:HG3	1.31	1.12
1:A:1645:PHE:HB3	1:A:1765:ILE:HG22	1.34	1.09
1:A:2107:LYS:HE3	1:A:2495:ASP:OD2	1.51	1.09
1:A:2141:ILE:HD12	1:A:2146:LYS:HE2	1.20	1.09
1:A:2488:GLU:HB3	1:A:2491:LEU:HD12	1.36	1.08
1:A:2707:VAL:HB	1:A:2712:LEU:HD11	1.19	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1992:LYS:HG3	1:A:2024:SER:HB2	1.17	1.07
1:A:2380:LEU:HD13	1:A:2390:ILE:HD11	1.34	1.06
1:A:3303:LYS:HA	1:A:3306:TRP:CD1	1.89	1.06
1:A:3530:PHE:CD1	1:A:3618:TYR:HD2	1.71	1.06
1:A:2380:LEU:HD22	1:A:2384:GLU:OE1	1.55	1.06
1:A:1645:PHE:HB3	1:A:1765:ILE:CG2	1.87	1.05
1:A:2494:LEU:CD1	1:A:2498:GLY:HA2	1.86	1.05
1:A:2494:LEU:HD13	1:A:2498:GLY:CA	1.85	1.05
1:A:1823:ASP:HB2	1:A:1852:ARG:O	1.56	1.04
1:A:2988:SER:HB3	1:A:2989:PRO:HD2	1.04	1.04
1:A:2064:GLN:OE1	1:A:2091:MET:HE1	1.58	1.03
1:A:1983:LEU:HD22	1:A:1997:SER:OG	1.58	1.03
1:A:2707:VAL:CB	1:A:2712:LEU:HD11	1.89	1.03
1:A:1992:LYS:CG	1:A:2024:SER:HB2	1.86	1.03
1:A:2920:TRP:HB2	1:A:2989:PRO:HG3	1.06	1.02
1:A:2988:SER:HB3	1:A:2989:PRO:CD	1.90	1.02
1:A:3777:VAL:CG1	1:A:3895:PHE:HE1	1.74	1.01
1:A:2448:ASP:HB2	1:A:2829:GLU:OE2	1.59	1.01
1:A:2386:MET:HB2	1:A:2627:ARG:HD3	1.42	1.00
1:A:3534:LEU:HD12	1:A:3618:TYR:HE2	1.24	1.00
1:A:1620:PHE:CD1	1:A:1760:PHE:CZ	2.50	1.00
1:A:1822:CYS:HB2	1:A:1853:LEU:HD21	1.43	0.99
1:A:3303:LYS:O	1:A:3306:TRP:HD1	1.43	0.99
1:A:3534:LEU:CD1	1:A:3618:TYR:CE2	2.45	0.99
1:A:2380:LEU:CD1	1:A:2390:ILE:HD11	1.93	0.98
1:A:1970:LEU:HD13	1:A:1974:LYS:HE3	1.45	0.98
1:A:3777:VAL:HG11	1:A:3895:PHE:CE1	1.97	0.98
1:A:2476:LYS:H	1:A:2476:LYS:HD3	1.26	0.97
1:A:2476:LYS:H	1:A:2476:LYS:CD	1.74	0.97
1:A:4033:LEU:HD11	1:A:4035:GLN:HB2	1.47	0.97
1:A:2386:MET:CB	1:A:2627:ARG:HD3	1.95	0.96
1:A:3534:LEU:HD12	1:A:3618:TYR:CE2	2.01	0.96
1:A:3406:PHE:HB2	1:A:3513:VAL:CG1	1.94	0.96
1:A:2988:SER:CB	1:A:2989:PRO:HD2	1.97	0.95
1:A:4065:LEU:HD11	1:A:4070:ILE:HD11	1.48	0.95
1:A:1645:PHE:CB	1:A:1765:ILE:HG22	1.96	0.95
1:A:3024:LEU:CD1	1:A:3303:LYS:HG3	1.96	0.95
1:A:1802:LYS:HG2	1:A:1921:MET:HG3	1.47	0.94
1:A:3509:LEU:CD1	1:A:3513:VAL:HG21	1.98	0.94
1:A:2787:HIS:HA	1:A:3460:PRO:HD2	1.49	0.94
1:A:2137:VAL:O	1:A:2141:ILE:HG23	1.69	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3530:PHE:CD1	1:A:3618:TYR:CD2	2.56	0.93
1:A:3460:PRO:O	1:A:3463:SER:HB2	1.67	0.92
1:A:2563:SER:HB3	1:A:2566:SER:H	1.35	0.92
1:A:3737:THR:HB	1:A:3740:THR:OG1	1.70	0.92
1:A:1992:LYS:HE2	1:A:2024:SER:O	1.71	0.91
1:A:2494:LEU:HD13	1:A:2498:GLY:HA2	0.94	0.91
1:A:1620:PHE:HD1	1:A:1760:PHE:HZ	1.07	0.91
1:A:2400:HIS:NE2	1:A:2559:LEU:HD13	1.86	0.91
1:A:2111:LYS:HD3	1:A:2161:GLU:CG	2.00	0.90
1:A:2920:TRP:HB2	1:A:2989:PRO:CG	1.99	0.90
1:A:2400:HIS:CD2	1:A:2559:LEU:HD13	2.06	0.90
1:A:3946:VAL:HG12	1:A:3950:PHE:O	1.72	0.90
1:A:2787:HIS:HA	1:A:3460:PRO:CG	2.02	0.89
1:A:2745:ILE:HG23	1:A:2756:MET:HE1	1.53	0.89
1:A:1939:PHE:CD2	1:A:1940:GLU:O	2.26	0.89
1:A:1823:ASP:CB	1:A:1852:ARG:O	2.20	0.89
1:A:4033:LEU:HD13	1:A:4035:GLN:HB2	1.54	0.89
1:A:1726:LEU:HD12	1:A:3984:GLN:HB3	1.55	0.88
1:A:2787:HIS:HA	1:A:3460:PRO:CD	2.03	0.88
1:A:2064:GLN:NE2	1:A:2091:MET:SD	2.47	0.88
1:A:3534:LEU:HD13	1:A:3618:TYR:HE2	1.38	0.88
1:A:1866:GLN:OE1	1:A:1911:ASN:HB2	1.74	0.87
1:A:2787:HIS:HA	1:A:3460:PRO:HG2	1.56	0.87
1:A:2112:GLU:HB3	1:A:2117:SER:HB2	1.57	0.87
1:A:1924:PRO:HB2	1:A:1929:ILE:HD11	1.55	0.87
1:A:3303:LYS:O	1:A:3306:TRP:CD1	2.28	0.87
1:A:1562:MET:HB3	1:A:1569:ILE:HD11	1.55	0.86
1:A:1649:LEU:HD11	1:A:1704:GLU:HG3	1.56	0.86
1:A:2446:SER:H	1:A:2449:THR:CG2	1.86	0.86
1:A:2766:LYS:HE2	1:A:2890:THR:HB	1.58	0.85
1:A:2446:SER:H	1:A:2449:THR:HG23	1.39	0.85
1:A:3303:LYS:C	1:A:3306:TRP:HD1	1.84	0.85
1:A:2920:TRP:CB	1:A:2989:PRO:HG3	2.01	0.85
1:A:1649:LEU:CD1	1:A:1704:GLU:HG3	2.07	0.84
1:A:2336:ARG:HD3	1:A:2355:ASP:OD2	1.77	0.84
1:A:3024:LEU:HD11	1:A:3303:LYS:CG	2.07	0.84
1:A:2141:ILE:CD1	1:A:2146:LYS:HE2	2.06	0.84
1:A:1940:GLU:HB2	1:A:1989:GLU:O	1.77	0.84
1:A:2476:LYS:HZ1	1:A:2528:ARG:HD2	1.43	0.83
1:A:3656:VAL:HG13	1:A:3677:LEU:HB3	1.59	0.83
1:A:2755:HIS:HB2	1:A:2911:ARG:O	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2274:HIS:HE1	1:A:2326:LEU:O	1.61	0.83
1:A:2106:THR:OG1	1:A:2154:PHE:HB3	1.78	0.83
1:A:2428:MET:HE2	1:A:2432:LEU:HD12	1.61	0.83
1:A:2131:THR:HG22	1:A:2176:LEU:HD21	1.59	0.83
1:A:2488:GLU:HB3	1:A:2491:LEU:CD1	2.08	0.82
1:A:2488:GLU:CB	1:A:2491:LEU:HD12	2.09	0.82
1:A:3923:VAL:HG23	1:A:4038:GLU:HA	1.62	0.82
1:A:1849:GLU:HG2	1:A:1899:ASN:ND2	1.95	0.81
1:A:3303:LYS:HA	1:A:3306:TRP:NE1	1.95	0.81
1:A:3645:SER:HB3	1:A:3890:GLN:HE21	1.45	0.81
1:A:2332:GLY:HA2	1:A:2335:GLN:HB2	1.62	0.81
1:A:2111:LYS:NZ	1:A:2161:GLU:HG2	1.94	0.81
1:A:1620:PHE:CD1	1:A:1760:PHE:HZ	1.96	0.80
1:A:1604:ALA:HA	1:A:1607:TRP:NE1	1.95	0.80
1:A:1630:ILE:HG22	1:A:1655:MET:SD	2.21	0.80
1:A:2362:ALA:HB3	1:A:2365:LYS:O	1.81	0.80
1:A:4033:LEU:CD1	1:A:4035:GLN:CB	2.60	0.80
1:A:3799:LYS:O	1:A:3803:LEU:HG	1.82	0.79
1:A:2476:LYS:NZ	1:A:2528:ARG:HD2	1.97	0.79
1:A:1970:LEU:HD12	1:A:1971:ARG:N	1.98	0.79
1:A:2064:GLN:OE1	1:A:2091:MET:CE	2.29	0.78
1:A:1604:ALA:HA	1:A:1607:TRP:CD1	2.18	0.78
1:A:2181:GLY:O	1:A:2182:GLU:HG3	1.83	0.78
1:A:3509:LEU:HD12	1:A:3513:VAL:CG2	2.13	0.78
1:A:1956:LEU:HB3	1:A:1968:PHE:CE2	2.18	0.78
1:A:2707:VAL:HB	1:A:2712:LEU:CD1	2.09	0.78
1:A:2707:VAL:CG1	1:A:2712:LEU:CD1	2.61	0.78
1:A:2476:LYS:HG2	1:A:2478:ASP:O	1.84	0.77
1:A:3303:LYS:CA	1:A:3306:TRP:CD1	2.66	0.77
1:A:1645:PHE:CB	1:A:1765:ILE:CG2	2.61	0.77
1:A:3534:LEU:HD11	1:A:3614:LEU:HD23	1.67	0.77
1:A:1939:PHE:HD2	1:A:1940:GLU:O	1.67	0.76
1:A:2032:LYS:O	1:A:2035:VAL:HG12	1.85	0.76
1:A:3460:PRO:O	1:A:3463:SER:CB	2.32	0.76
1:A:2563:SER:HB2	1:A:2566:SER:OG	1.86	0.75
1:A:3406:PHE:HB2	1:A:3513:VAL:HG12	1.69	0.75
1:A:3816:LEU:HD23	1:A:3847:SER:OG	1.86	0.75
1:A:3946:VAL:CG1	1:A:3950:PHE:O	2.34	0.75
1:A:2064:GLN:OE1	1:A:2151:TRP:HH2	1.67	0.75
1:A:3406:PHE:HB2	1:A:3513:VAL:HG11	1.69	0.75
1:A:3777:VAL:CG1	1:A:3895:PHE:CE1	2.63	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1983:LEU:HD21	1:A:2000:ARG:HD2	1.69	0.74
1:A:3618:TYR:N	1:A:3618:TYR:CD1	2.54	0.74
1:A:3871:PHE:CZ	1:A:3873:MET:HB2	2.22	0.74
1:A:3939:ILE:HG13	1:A:4010:LEU:CD2	2.16	0.74
1:A:3530:PHE:HD1	1:A:3618:TYR:HD2	1.31	0.74
1:A:2411:LYS:HG2	1:A:2530:HIS:HE1	1.51	0.74
1:A:2176:LEU:O	1:A:2183:ARG:HA	1.88	0.74
1:A:2107:LYS:HE2	1:A:2499:SER:HB3	1.67	0.74
1:A:1744:LEU:HA	1:A:1760:PHE:CE2	2.23	0.74
1:A:2745:ILE:HG23	1:A:2756:MET:CE	2.17	0.73
1:A:1569:ILE:HA	1:A:1584:SER:HA	1.70	0.73
1:A:1940:GLU:HG3	1:A:1941:ASP:H	1.52	0.73
1:A:3303:LYS:CA	1:A:3306:TRP:HD1	2.02	0.73
1:A:3566:LEU:HA	1:A:3583:LEU:CD2	2.18	0.73
1:A:3303:LYS:HA	1:A:3306:TRP:HD1	1.53	0.73
1:A:2707:VAL:CG1	1:A:2712:LEU:HD11	2.18	0.73
1:A:3525:ILE:CD1	1:A:3646:ILE:HG22	2.13	0.73
1:A:1967:HIS:C	1:A:1968:PHE:HD1	1.97	0.73
1:A:3534:LEU:HD13	1:A:3618:TYR:CE2	2.19	0.73
1:A:2201:HIS:CE1	1:A:2497:TYR:HA	2.24	0.72
1:A:1822:CYS:SG	1:A:1850:PHE:HA	2.29	0.72
1:A:2112:GLU:HB3	1:A:2117:SER:CB	2.19	0.72
1:A:3509:LEU:CD1	1:A:3513:VAL:CG2	2.68	0.72
1:A:2787:HIS:CA	1:A:3460:PRO:HD2	2.20	0.71
1:A:1849:GLU:HG2	1:A:1899:ASN:HD22	1.53	0.71
1:A:3979:ASN:C	1:A:3981:PRO:HD2	2.16	0.71
1:A:1970:LEU:HD13	1:A:1974:LYS:CE	2.20	0.71
1:A:1612:ASP:HA	1:A:1615:ILE:CD1	2.21	0.71
1:A:3792:ARG:HB2	1:A:3955:TYR:CD1	2.26	0.71
1:A:1956:LEU:HB3	1:A:1968:PHE:HE2	1.53	0.71
1:A:2960:THR:HB	1:A:2963:ASP:HB2	1.73	0.71
1:A:1774:LEU:HD21	1:A:1922:LYS:O	1.91	0.70
1:A:2141:ILE:HD12	1:A:2146:LYS:CE	2.11	0.70
1:A:3305:ARG:O	1:A:3307:LEU:N	2.24	0.70
1:A:2003:LEU:HA	1:A:2006:LEU:HD12	1.74	0.70
1:A:3530:PHE:HD1	1:A:3618:TYR:CD2	2.04	0.70
1:A:3774:ILE:O	1:A:3778:VAL:HG23	1.91	0.70
1:A:3645:SER:HB3	1:A:3890:GLN:NE2	2.06	0.70
1:A:1995:VAL:HG21	1:A:2024:SER:HB3	1.74	0.70
1:A:4033:LEU:HD13	1:A:4035:GLN:CB	2.21	0.70
1:A:2175:ILE:HG12	1:A:2183:ARG:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2294:LEU:HB3	1:A:2317:LEU:HD22	1.74	0.69
1:A:2095:ASP:CG	1:A:2149:ARG:NH2	2.50	0.69
1:A:2448:ASP:HB2	1:A:2829:GLU:CD	2.17	0.69
1:A:3631:MET:HE1	1:A:3698:MET:HG3	1.74	0.69
1:A:3979:ASN:O	1:A:3981:PRO:HD2	1.92	0.69
1:A:2514:GLY:O	1:A:2523:TRP:CH2	2.45	0.69
1:A:3871:PHE:HZ	1:A:3873:MET:HB2	1.56	0.69
1:A:2203:THR:HG22	1:A:2205:ALA:H	1.56	0.69
1:A:3330:TYR:OH	1:A:3346:LEU:HD22	1.92	0.69
1:A:2125:TRP:CZ2	1:A:2178:LEU:HD13	2.27	0.69
1:A:1646:GLN:NE2	1:A:1758:TYR:OH	2.26	0.68
1:A:1983:LEU:HB3	1:A:1993:THR:HG23	1.75	0.68
1:A:3935:PHE:HB2	1:A:4014:VAL:HG11	1.75	0.68
1:A:1630:ILE:HA	1:A:1634:THR:HG22	1.75	0.68
1:A:3850:TRP:NE1	1:A:3854:TYR:HB3	2.08	0.68
1:A:2419:PRO:O	1:A:2424:LYS:HE3	1.93	0.68
1:A:2305:LEU:HD11	1:A:2368:PHE:CG	2.29	0.68
1:A:2293:HIS:CE1	1:A:2409:ASN:HB3	2.29	0.68
1:A:3509:LEU:HD12	1:A:3513:VAL:HG21	1.75	0.68
1:A:3785:TYR:HE2	1:A:3859:VAL:HG22	1.57	0.68
1:A:2285:GLU:HB2	1:A:2412:ARG:NH2	2.08	0.68
1:A:2252:LEU:HD21	1:A:2310:LEU:HD23	1.76	0.67
1:A:2111:LYS:HZ2	1:A:2161:GLU:HG2	1.58	0.67
1:A:1744:LEU:HA	1:A:1760:PHE:CD2	2.29	0.67
1:A:3566:LEU:HA	1:A:3583:LEU:HD21	1.76	0.67
1:A:2293:HIS:NE2	1:A:2409:ASN:HB3	2.09	0.67
1:A:1698:ILE:O	1:A:1702:LEU:HG	1.94	0.67
1:A:2386:MET:HB3	1:A:2627:ARG:HD3	1.75	0.67
1:A:3848:LEU:HD21	1:A:3852:LYS:HE3	1.75	0.67
1:A:1626:CYS:SG	1:A:1639:VAL:HG11	2.35	0.67
1:A:3837:GLY:O	1:A:3871:PHE:HD1	1.77	0.67
1:A:1822:CYS:SG	1:A:1849:GLU:O	2.53	0.66
1:A:2493:LYS:HG3	1:A:2494:LEU:H	1.60	0.66
1:A:3473:ALA:HB3	1:A:3476:ARG:O	1.96	0.66
1:A:2707:VAL:CG1	1:A:2712:LEU:HD12	2.26	0.66
1:A:2107:LYS:CE	1:A:2495:ASP:OD2	2.37	0.66
1:A:2220:CYS:SG	1:A:2224:SER:HB2	2.36	0.66
1:A:2631:THR:O	1:A:2635:THR:HG22	1.96	0.66
1:A:2080:LYS:HG2	1:A:2215:PHE:CE1	2.30	0.66
1:A:1992:LYS:HG3	1:A:2024:SER:CB	2.11	0.65
1:A:2514:GLY:HA3	1:A:2523:TRP:CZ2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3566:LEU:CD1	1:A:3570:LEU:HD11	2.26	0.65
1:A:3566:LEU:O	1:A:3570:LEU:HG	1.97	0.65
1:A:2745:ILE:CG2	1:A:2756:MET:HE1	2.22	0.65
1:A:3948:HIS:NE2	1:A:4072:ASN:CG	2.55	0.65
1:A:3566:LEU:HD13	1:A:3570:LEU:CD1	2.27	0.65
1:A:3998:ILE:HG21	1:A:4004:LEU:HG	1.77	0.65
1:A:1706:LEU:CD2	1:A:1935:GLN:HG2	2.27	0.65
1:A:2382:ALA:O	1:A:2385:VAL:HG12	1.96	0.65
1:A:3819:ILE:O	1:A:3823:ASN:HB2	1.97	0.65
1:A:1703:VAL:HG13	1:A:1770:ILE:HD13	1.78	0.64
1:A:1953:LEU:CD1	1:A:1973:LEU:HB3	2.27	0.64
1:A:3459:ASP:OD2	1:A:3461:ILE:HG12	1.97	0.64
1:A:3998:ILE:CG2	1:A:4004:LEU:HG	2.27	0.64
1:A:2495:ASP:O	1:A:2498:GLY:N	2.30	0.64
1:A:2728:LEU:HD12	1:A:2771:ARG:CZ	2.27	0.64
1:A:3010:LEU:HD21	1:A:3317:SER:HB3	1.79	0.64
1:A:2222:ILE:HG23	1:A:2284:LEU:HD11	1.80	0.64
1:A:3303:LYS:HD2	1:A:3306:TRP:CD1	2.33	0.64
1:A:1826:PHE:HE1	1:A:1853:LEU:HD22	1.62	0.64
1:A:2779:LEU:HD23	1:A:2812:ARG:O	1.97	0.64
1:A:1970:LEU:CD1	1:A:1974:LYS:HE3	2.24	0.64
1:A:3509:LEU:HD11	1:A:3513:VAL:HG21	1.76	0.64
1:A:2290:LEU:HD13	1:A:2407:LEU:HD23	1.79	0.64
1:A:3737:THR:OG1	1:A:3740:THR:HB	1.98	0.63
1:A:1562:MET:CB	1:A:1569:ILE:HD11	2.29	0.63
1:A:3618:TYR:N	1:A:3618:TYR:HD1	1.94	0.63
1:A:1645:PHE:CG	1:A:1765:ILE:HG22	2.32	0.63
1:A:1827:ASP:HB3	1:A:1830:VAL:HG12	1.81	0.63
1:A:1938:GLY:O	1:A:1989:GLU:HB3	1.98	0.63
1:A:1612:ASP:HA	1:A:1615:ILE:HD11	1.78	0.63
1:A:3792:ARG:HB2	1:A:3955:TYR:CE1	2.33	0.63
1:A:1967:HIS:O	1:A:1968:PHE:HD1	1.82	0.63
1:A:2285:GLU:HB2	1:A:2412:ARG:HH22	1.63	0.63
1:A:2842:ASP:O	1:A:2845:GLN:HG2	1.97	0.63
1:A:2536:ASN:HB2	1:A:2543:ARG:HE	1.64	0.63
1:A:1748:PHE:CD2	1:A:1755:LEU:HD22	2.34	0.62
1:A:2512:LYS:O	1:A:2513:GLN:HB2	1.97	0.62
1:A:3409:ASP:HB3	1:A:3518:PHE:HB2	1.81	0.62
1:A:1738:ASN:O	1:A:1739:ASP:OD1	2.16	0.62
1:A:1995:VAL:HG22	1:A:2022:PHE:CE2	2.33	0.62
1:A:1991:GLU:O	1:A:1995:VAL:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2315:THR:HG21	1:A:2350:SER:HB3	1.80	0.62
1:A:2151:TRP:HE3	1:A:2193:LEU:HD11	1.64	0.62
1:A:2632:ALA:HB3	1:A:2647:LEU:HD21	1.80	0.62
1:A:3525:ILE:HD11	1:A:3646:ILE:CG2	2.15	0.62
1:A:1996:GLU:O	1:A:2000:ARG:HG3	2.00	0.62
1:A:3785:TYR:CE2	1:A:3859:VAL:HG22	2.33	0.62
1:A:3912:GLY:O	1:A:3915:PHE:CE2	2.53	0.62
1:A:2282:ASN:HB3	1:A:2552:ARG:HG3	1.82	0.61
1:A:2745:ILE:HG12	1:A:2756:MET:HE1	1.82	0.61
1:A:3641:PHE:HA	1:A:3889:LEU:HD21	1.81	0.61
1:A:1983:LEU:HD21	1:A:2000:ARG:CD	2.31	0.61
1:A:3307:LEU:HA	1:A:3310:THR:HB	1.81	0.61
1:A:3330:TYR:CE2	1:A:3346:LEU:HD13	2.36	0.61
1:A:1969:GLY:O	1:A:1972:THR:HB	2.01	0.61
1:A:3530:PHE:CE1	1:A:3618:TYR:CD2	2.88	0.61
1:A:3700:MET:HB3	1:A:4085:THR:HG21	1.81	0.61
1:A:1826:PHE:CE1	1:A:1853:LEU:HD22	2.35	0.61
1:A:1692:ASP:O	1:A:1695:LYS:HB3	2.00	0.61
1:A:3583:LEU:O	1:A:3587:LEU:HG	2.00	0.61
1:A:1574:PHE:HB3	1:A:1576:GLU:H	1.65	0.60
1:A:2677:VAL:HG11	1:A:2686:LEU:HD21	1.83	0.60
1:A:1900:PRO:HB3	1:A:1905:ARG:HA	1.83	0.60
1:A:2293:HIS:CE1	1:A:2409:ASN:CB	2.84	0.60
1:A:2563:SER:CB	1:A:2566:SER:OG	2.47	0.60
1:A:2785:LYS:HD3	1:A:3482:GLY:O	2.01	0.60
1:A:3817:GLY:H	1:A:3821:ASN:HB2	1.66	0.60
1:A:1630:ILE:CG2	1:A:1655:MET:SD	2.89	0.60
1:A:2394:THR:H	1:A:2397:THR:HB	1.64	0.60
1:A:3886:ALA:N	1:A:3887:PRO:HD2	2.17	0.60
1:A:1656:TRP:O	1:A:1660:VAL:HG12	2.01	0.60
1:A:3303:LYS:C	1:A:3306:TRP:CD1	2.74	0.60
1:A:1851:ASN:HD21	1:A:1899:ASN:HB2	1.66	0.60
1:A:3541:MET:HA	1:A:3544:LYS:HG2	1.83	0.60
1:A:2064:GLN:CD	1:A:2091:MET:CE	2.75	0.60
1:A:2514:GLY:C	1:A:2523:TRP:CH2	2.80	0.60
1:A:4065:LEU:HD11	1:A:4070:ILE:CD1	2.29	0.60
1:A:1620:PHE:HA	1:A:1760:PHE:CE1	2.37	0.60
1:A:2427:ILE:HD12	1:A:2559:LEU:CD2	2.31	0.60
1:A:2489:ILE:HG22	1:A:2535:CYS:HB3	1.84	0.60
1:A:2640:THR:HG23	1:A:2643:SER:H	1.66	0.60
1:A:1984:ILE:HG21	1:A:1989:GLU:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2181:GLY:C	1:A:2182:GLU:HG3	2.27	0.60
1:A:2155:ASP:OD1	1:A:2549:ARG:NH2	2.35	0.59
1:A:2728:LEU:HD12	1:A:2771:ARG:NH2	2.17	0.59
1:A:3429:LEU:HD21	1:A:3439:ARG:HB3	1.83	0.59
1:A:2339:ILE:HG23	1:A:2353:LEU:HB3	1.83	0.59
1:A:1726:LEU:CD1	1:A:3984:GLN:HB3	2.30	0.59
1:A:2081:THR:O	1:A:2085:LYS:HB2	2.02	0.59
1:A:2490:ASN:HB3	1:A:2546:MET:HE2	1.84	0.59
1:A:3851:VAL:HG13	1:A:3855:LEU:HD23	1.85	0.59
1:A:2380:LEU:HD11	1:A:2390:ILE:HD11	1.83	0.59
1:A:2354:SER:OG	1:A:2357:SER:HB2	2.02	0.59
1:A:1940:GLU:HG3	1:A:1941:ASP:N	2.18	0.58
1:A:2064:GLN:OE1	1:A:2151:TRP:CH2	2.55	0.58
1:A:2941:THR:HG22	1:A:2942:ASP:H	1.66	0.58
1:A:3555:TYR:HE1	1:A:3593:GLU:HG2	1.68	0.58
1:A:3592:LYS:O	1:A:3596:ASN:HB2	2.03	0.58
1:A:4021:LEU:HD23	1:A:4023:ILE:HG13	1.85	0.58
1:A:2784:PRO:HG2	1:A:2817:ILE:HD13	1.84	0.58
1:A:3618:TYR:O	1:A:3622:GLY:N	2.34	0.58
1:A:2034:ILE:HD12	1:A:2061:TYR:CZ	2.38	0.58
1:A:2386:MET:CB	1:A:2627:ARG:CD	2.77	0.58
1:A:2755:HIS:NE2	1:A:2835:LEU:HG	2.17	0.58
1:A:2241:LEU:HD13	1:A:2299:ARG:HH11	1.68	0.58
1:A:2257:PHE:HD1	1:A:2262:LEU:HD11	1.69	0.58
1:A:2336:ARG:CD	1:A:2355:ASP:OD2	2.50	0.58
1:A:3810:SER:O	1:A:3838:TRP:HB2	2.03	0.58
1:A:3537:GLU:OE1	1:A:3618:TYR:OH	2.21	0.58
1:A:3737:THR:HB	1:A:3740:THR:CB	2.33	0.58
1:A:3945:LEU:O	1:A:3948:HIS:O	2.21	0.58
1:A:1559:SER:HB3	1:A:1572:ILE:HG22	1.86	0.58
1:A:2488:GLU:CD	1:A:2491:LEU:HD11	2.29	0.58
1:A:3839:ILE:HG23	1:A:3873:MET:HG3	1.86	0.58
1:A:4033:LEU:HD12	1:A:4035:GLN:N	2.18	0.58
1:A:2201:HIS:NE2	1:A:2497:TYR:O	2.37	0.57
1:A:2332:GLY:HA2	1:A:2335:GLN:CB	2.31	0.57
1:A:3519:VAL:HG13	1:A:3521:ASN:ND2	2.19	0.57
1:A:2446:SER:H	1:A:2449:THR:HG21	1.67	0.57
1:A:1706:LEU:HD21	1:A:1935:GLN:HG2	1.86	0.57
1:A:1779:PHE:O	1:A:1783:THR:HG22	2.03	0.57
1:A:1911:ASN:OD1	1:A:1912:LEU:N	2.38	0.57
1:A:2095:ASP:CG	1:A:2149:ARG:HH22	2.11	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2071:ILE:HB	1:A:2212:LEU:HD12	1.85	0.57
1:A:4024:VAL:HG11	1:A:4062:TRP:CD2	2.38	0.57
1:A:2938:MET:SD	1:A:3321:ILE:HG21	2.45	0.57
1:A:1781:THR:HG21	1:A:1919:PHE:CD1	2.39	0.57
1:A:1965:HIS:HD2	1:A:2212:LEU:CD2	2.18	0.57
1:A:1970:LEU:HD12	1:A:1970:LEU:C	2.28	0.57
1:A:2846:GLY:O	1:A:2849:TYR:HB3	2.04	0.57
1:A:2437:LEU:H	1:A:2437:LEU:HD12	1.69	0.57
1:A:4017:GLY:HA3	1:A:4021:LEU:HD12	1.87	0.57
1:A:1704:GLU:OE2	1:A:1768:ARG:NH1	2.37	0.57
1:A:1710:ASN:HB2	1:A:1932:MET:HE1	1.87	0.57
1:A:2127:ASP:O	1:A:2131:THR:OG1	2.23	0.57
1:A:3912:GLY:O	1:A:3915:PHE:CZ	2.57	0.57
1:A:1822:CYS:SG	1:A:1849:GLU:C	2.88	0.57
1:A:2476:LYS:CD	1:A:2476:LYS:N	2.52	0.57
1:A:2808:LEU:HD21	1:A:2856:LEU:HD12	1.86	0.57
1:A:1620:PHE:CZ	1:A:1743:ASP:HB3	2.40	0.56
1:A:1995:VAL:HG22	1:A:2022:PHE:CD2	2.40	0.56
1:A:2419:PRO:O	1:A:2424:LYS:CE	2.52	0.56
1:A:2787:HIS:CA	1:A:3460:PRO:HG2	2.32	0.56
1:A:3939:ILE:HG13	1:A:4010:LEU:HD22	1.86	0.56
1:A:1619:VAL:HG12	1:A:1760:PHE:HD1	1.70	0.56
1:A:4023:ILE:HD12	1:A:4029:ILE:HD11	1.87	0.56
1:A:2627:ARG:NH1	1:A:2630:TYR:CE2	2.74	0.56
1:A:1983:LEU:HB3	1:A:1993:THR:CG2	2.36	0.56
1:A:2111:LYS:CD	1:A:2161:GLU:HG3	2.13	0.56
1:A:1940:GLU:CB	1:A:1989:GLU:O	2.51	0.56
1:A:2868:ASP:HB2	1:A:2872:GLU:OE1	2.06	0.56
1:A:4037:SER:HB3	1:A:4040:GLU:HB3	1.87	0.56
1:A:2111:LYS:HZ3	1:A:2161:GLU:HG2	1.69	0.56
1:A:2131:THR:HG22	1:A:2176:LEU:CD2	2.34	0.56
1:A:2410:SER:O	1:A:2411:LYS:HB2	2.06	0.56
1:A:2220:CYS:SG	1:A:2224:SER:CB	2.94	0.55
1:A:2386:MET:HB3	1:A:2627:ARG:CD	2.36	0.55
1:A:2115:TYR:OH	1:A:2162:TYR:O	2.23	0.55
1:A:2151:TRP:CE3	1:A:2193:LEU:HD11	2.41	0.55
1:A:3538:ASN:HB3	1:A:3541:MET:HG2	1.87	0.55
1:A:1823:ASP:HB2	1:A:1853:LEU:HD23	1.88	0.55
1:A:1852:ARG:O	1:A:1852:ARG:HG3	2.06	0.55
1:A:1939:PHE:O	1:A:1940:GLU:HB3	2.05	0.55
1:A:4022:GLN:O	1:A:4022:GLN:HG2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2305:LEU:HD11	1:A:2368:PHE:CD1	2.41	0.55
1:A:3303:LYS:HA	1:A:3306:TRP:HE1	1.67	0.55
1:A:2002:ILE:HG22	1:A:2006:LEU:HD11	1.88	0.55
1:A:3440:LEU:HD23	1:A:3462:ILE:HD12	1.88	0.55
1:A:3979:ASN:C	1:A:3981:PRO:CD	2.80	0.55
1:A:2400:HIS:NE2	1:A:2559:LEU:CD1	2.67	0.55
1:A:2788:ARG:HG3	1:A:3459:ASP:HA	1.89	0.55
1:A:2707:VAL:CB	1:A:2712:LEU:CD1	2.72	0.55
1:A:2476:LYS:HD3	1:A:2476:LYS:N	2.09	0.54
1:A:3683:TYR:O	1:A:3687:SER:HB2	2.07	0.54
1:A:2932:MET:HE1	1:A:2993:ILE:HG23	1.90	0.54
1:A:3817:GLY:H	1:A:3821:ASN:CB	2.21	0.54
1:A:2786:ILE:O	1:A:3460:PRO:HB2	2.07	0.54
1:A:3631:MET:CE	1:A:3698:MET:HG3	2.36	0.54
1:A:4059:LEU:HA	1:A:4063:LEU:HD13	1.89	0.54
1:A:2002:ILE:HB	1:A:2014:PHE:CE2	2.42	0.54
1:A:2707:VAL:HG12	1:A:2712:LEU:HD12	1.89	0.54
1:A:2141:ILE:HG22	1:A:2145:PHE:HB2	1.90	0.54
1:A:2230:LEU:HD23	1:A:2288:VAL:HG13	1.90	0.54
1:A:3877:CYS:SG	1:A:3884:LEU:CD2	2.96	0.54
1:A:2707:VAL:HG12	1:A:2712:LEU:CD1	2.37	0.54
1:A:2201:HIS:CE1	1:A:2497:TYR:CA	2.91	0.54
1:A:2462:THR:HG22	1:A:2476:LYS:HA	1.90	0.54
1:A:3481:ILE:O	1:A:3483:ASP:N	2.36	0.54
1:A:3509:LEU:HD12	1:A:3513:VAL:HG23	1.88	0.54
1:A:4065:LEU:C	1:A:4065:LEU:HD12	2.33	0.54
1:A:2173:ASN:HB3	1:A:2175:ILE:HG22	1.90	0.54
1:A:3440:LEU:CD2	1:A:3462:ILE:HD12	2.38	0.54
1:A:2787:HIS:HB3	1:A:3461:ILE:HG23	1.91	0.53
1:A:2336:ARG:HG2	1:A:2355:ASP:OD1	2.08	0.53
1:A:2450:THR:H	1:A:2453:HIS:CE1	2.27	0.53
1:A:3645:SER:CB	1:A:3890:GLN:HE21	2.19	0.53
1:A:2786:ILE:HG12	1:A:2821:ASN:HA	1.90	0.53
1:A:1645:PHE:CZ	1:A:1649:LEU:HD22	2.43	0.53
1:A:2339:ILE:HG12	1:A:2353:LEU:HD23	1.90	0.53
1:A:2788:ARG:HB2	1:A:3459:ASP:HB3	1.91	0.53
1:A:2305:LEU:CD1	1:A:2368:PHE:CD1	2.91	0.53
1:A:3612:ASP:O	1:A:3615:VAL:HG22	2.09	0.53
1:A:3995:GLY:HA2	1:A:3998:ILE:HD13	1.91	0.53
1:A:1627:LEU:HD11	1:A:1631:LYS:HE3	1.89	0.53
1:A:3946:VAL:HA	1:A:3947:PRO:C	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3566:LEU:CA	1:A:3583:LEU:HD21	2.37	0.53
1:A:3656:VAL:CG1	1:A:3677:LEU:HB3	2.36	0.53
1:A:1981:SER:HB3	1:A:1982:PRO:HD3	1.91	0.53
1:A:2063:MET:HB3	1:A:2070:LEU:HD11	1.90	0.53
1:A:1749:ILE:HD13	1:A:1813:LEU:HD22	1.92	0.52
1:A:2833:THR:HG21	1:A:2841:PRO:HD2	1.91	0.52
1:A:3946:VAL:HB	1:A:3947:PRO:HA	1.91	0.52
1:A:1979:ASN:O	1:A:1983:LEU:HD13	2.09	0.52
1:A:2419:PRO:O	1:A:2424:LYS:NZ	2.42	0.52
1:A:2795:PHE:CE2	1:A:2799:LEU:HD11	2.44	0.52
1:A:3692:LYS:HE3	1:A:3898:GLU:HB3	1.91	0.52
1:A:3703:PHE:CE1	1:A:3766:GLU:HG2	2.43	0.52
1:A:2578:ILE:HG21	1:A:2630:TYR:HB2	1.91	0.52
1:A:3877:CYS:SG	1:A:3884:LEU:HD22	2.50	0.52
1:A:2285:GLU:CB	1:A:2412:ARG:NH2	2.73	0.52
1:A:1620:PHE:HA	1:A:1760:PHE:HE1	1.74	0.52
1:A:1939:PHE:HD1	1:A:1939:PHE:H	1.57	0.52
1:A:1926:SER:HA	1:A:1929:ILE:HD13	1.92	0.52
1:A:2177:THR:HG22	1:A:2183:ARG:HG2	1.91	0.52
1:A:2380:LEU:HD13	1:A:2390:ILE:CD1	2.23	0.52
1:A:1645:PHE:HB2	1:A:1697:LYS:HG3	1.91	0.52
1:A:1849:GLU:CG	1:A:1899:ASN:HD22	2.22	0.52
1:A:1963:MET:HB3	1:A:1966:TYR:CD2	2.45	0.52
1:A:2290:LEU:HD23	1:A:2321:SER:HA	1.91	0.52
1:A:4034:LEU:HD23	1:A:4034:LEU:O	2.10	0.52
1:A:1645:PHE:HZ	1:A:1768:ARG:HD2	1.75	0.52
1:A:2012:LEU:HD13	1:A:2016:ASP:OD2	2.10	0.52
1:A:3017:VAL:HG21	1:A:3313:PHE:CE2	2.44	0.52
1:A:4021:LEU:HD23	1:A:4023:ILE:CG1	2.39	0.52
1:A:2302:PHE:HA	1:A:2310:LEU:HD11	1.92	0.51
1:A:3323:ASN:HD21	1:A:3361:ASP:H	1.58	0.51
1:A:3547:ASP:HA	1:A:3550:LYS:HB3	1.91	0.51
1:A:3951:SER:HB2	1:A:4002:LYS:HD2	1.91	0.51
1:A:2106:THR:HG1	1:A:2154:PHE:HB3	1.71	0.51
1:A:2494:LEU:HD12	1:A:2494:LEU:O	2.10	0.51
1:A:2780:LYS:HD3	1:A:2813:THR:HG22	1.93	0.51
1:A:3934:TRP:CB	1:A:4023:ILE:HD13	2.41	0.51
1:A:1606:GLU:O	1:A:1610:ILE:HG12	2.11	0.51
1:A:1803:THR:HG21	1:A:1848:ASP:OD1	2.10	0.51
1:A:2645:ILE:CD1	1:A:2686:LEU:HG	2.40	0.51
1:A:3911:TRP:HH2	1:A:3926:VAL:CG1	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2637:PRO:O	1:A:2639:GLN:NE2	2.44	0.51
1:A:1650:LEU:HD11	1:A:1747:VAL:HG11	1.92	0.51
1:A:1604:ALA:HA	1:A:1607:TRP:HE1	1.72	0.51
1:A:1706:LEU:HD22	1:A:1935:GLN:HG2	1.93	0.51
1:A:2295:ILE:HG12	1:A:2314:ILE:HD12	1.93	0.51
1:A:2427:ILE:HD12	1:A:2559:LEU:HD22	1.92	0.51
1:A:1677:ASP:HA	1:A:1680:ILE:HD12	1.92	0.51
1:A:1849:GLU:CG	1:A:1899:ASN:ND2	2.70	0.51
1:A:2084:TRP:HE3	1:A:2088:ILE:HD12	1.76	0.51
1:A:1917:ARG:HD2	1:A:3963:PHE:CE2	2.46	0.51
1:A:3645:SER:CB	1:A:3890:GLN:NE2	2.74	0.51
1:A:3737:THR:OG1	1:A:3740:THR:CB	2.59	0.51
1:A:4065:LEU:HD12	1:A:4065:LEU:O	2.10	0.51
1:A:3848:LEU:HD12	1:A:3884:LEU:HD12	1.93	0.51
1:A:2034:ILE:CD1	1:A:2061:TYR:CZ	2.95	0.50
1:A:2112:GLU:CB	1:A:2117:SER:HB2	2.35	0.50
1:A:1707:HIS:O	1:A:1711:VAL:HG23	2.10	0.50
1:A:3566:LEU:HD11	1:A:3570:LEU:HD11	1.92	0.50
1:A:3839:ILE:CG2	1:A:3873:MET:HG3	2.41	0.50
1:A:3737:THR:CB	1:A:3740:THR:CB	2.89	0.50
1:A:2385:VAL:HG23	1:A:2574:TYR:HD1	1.77	0.50
1:A:3854:TYR:O	1:A:3858:HIS:HB2	2.10	0.50
1:A:2109:LEU:HD13	1:A:2129:LEU:HD23	1.94	0.50
1:A:1803:THR:HG21	1:A:1848:ASP:CG	2.37	0.50
1:A:1748:PHE:HD2	1:A:1755:LEU:HD22	1.77	0.50
1:A:2745:ILE:CG1	1:A:2756:MET:HE1	2.42	0.49
1:A:2960:THR:HG22	1:A:2961:ILE:N	2.28	0.49
1:A:3845:GLN:OE1	1:A:3878:HIS:HB2	2.11	0.49
1:A:1570:GLU:HB2	1:A:1585:VAL:HA	1.93	0.49
1:A:1657:THR:HG21	1:A:1734:PHE:O	2.12	0.49
1:A:1748:PHE:CE2	1:A:1755:LEU:HD22	2.47	0.49
1:A:2102:TYR:HB2	1:A:2152:VAL:HG22	1.93	0.49
1:A:2984:VAL:C	1:A:2986:PRO:HD3	2.37	0.49
1:A:2064:GLN:NE2	1:A:2091:MET:CE	2.76	0.49
1:A:2448:ASP:CB	1:A:2829:GLU:OE2	2.47	0.49
1:A:3692:LYS:HE3	1:A:3898:GLU:O	2.13	0.49
1:A:3787:THR:HG22	1:A:3875:MET:HB2	1.93	0.49
1:A:3855:LEU:HD12	1:A:3859:VAL:HG23	1.93	0.49
1:A:3869:GLU:O	1:A:3870:LYS:C	2.56	0.49
1:A:1664:LEU:HD23	1:A:1669:PHE:HZ	1.77	0.49
1:A:2563:SER:CB	1:A:2566:SER:H	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2982:VAL:HG12	1:A:2983:GLY:N	2.27	0.49
1:A:3350:LYS:HA	1:A:3353:LEU:HD12	1.94	0.49
1:A:3725:VAL:HG22	1:A:3731:ASP:HA	1.93	0.49
1:A:2034:ILE:CD1	1:A:2061:TYR:CE2	2.95	0.49
1:A:2074:GLY:O	1:A:2197:ASP:HA	2.13	0.49
1:A:2645:ILE:HD11	1:A:2686:LEU:HG	1.94	0.49
1:A:2762:SER:O	1:A:2763:ARG:HB2	2.12	0.49
1:A:1911:ASN:OD1	1:A:1912:LEU:HG	2.13	0.49
1:A:2002:ILE:HB	1:A:2014:PHE:HE2	1.78	0.49
1:A:2514:GLY:CA	1:A:2523:TRP:CZ2	2.96	0.49
1:A:2839:ASP:O	1:A:2841:PRO:HD3	2.12	0.49
1:A:3978:ASN:O	1:A:3981:PRO:CD	2.60	0.49
1:A:2364:ASP:O	1:A:2365:LYS:HG2	2.13	0.49
1:A:3671:VAL:O	1:A:3674:ILE:HG22	2.13	0.49
1:A:3373:LEU:O	1:A:3373:LEU:HD23	2.13	0.48
1:A:3889:LEU:HG	1:A:3894:ARG:HD3	1.95	0.48
1:A:1626:CYS:SG	1:A:1639:VAL:CG1	3.01	0.48
1:A:2169:VAL:HG13	1:A:2186:ILE:HG12	1.94	0.48
1:A:2354:SER:OG	1:A:2357:SER:CB	2.61	0.48
1:A:1802:LYS:HA	1:A:1921:MET:HE2	1.95	0.48
1:A:1967:HIS:NE2	1:A:2204:PRO:HB3	2.28	0.48
1:A:1983:LEU:HD21	1:A:2000:ARG:NE	2.28	0.48
1:A:2137:VAL:O	1:A:2141:ILE:CG2	2.50	0.48
1:A:2745:ILE:CB	1:A:2756:MET:HE1	2.44	0.48
1:A:3911:TRP:HH2	1:A:3926:VAL:HG12	1.77	0.48
1:A:1645:PHE:CD2	1:A:1765:ILE:HG22	2.48	0.48
1:A:2654:ARG:HH22	1:A:2691:SER:HB2	1.77	0.48
1:A:3566:LEU:HD13	1:A:3570:LEU:HD12	1.95	0.48
1:A:1626:CYS:HB2	1:A:1643:TYR:CD2	2.48	0.48
1:A:1849:GLU:OE2	1:A:1899:ASN:ND2	2.47	0.48
1:A:3414:MET:HE3	1:A:3518:PHE:CD1	2.48	0.48
1:A:3461:ILE:C	1:A:3463:SER:N	2.70	0.48
1:A:3541:MET:HB2	1:A:3607:PHE:HE1	1.78	0.48
1:A:2860:THR:HG22	1:A:2865:LEU:O	2.13	0.48
1:A:3737:THR:CB	1:A:3740:THR:HB	2.44	0.48
1:A:4033:LEU:HD12	1:A:4036:GLN:H	1.78	0.48
1:A:1731:VAL:HG12	1:A:1732:GLN:N	2.28	0.48
1:A:2828:LEU:HD13	1:A:2902:MET:SD	2.53	0.48
1:A:3703:PHE:HE1	1:A:3766:GLU:HG2	1.79	0.48
1:A:4034:LEU:HD23	1:A:4034:LEU:C	2.38	0.48
1:A:1794:PHE:HD1	1:A:1802:LYS:HB3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2084:TRP:CZ3	1:A:2085:LYS:HG3	2.49	0.48
1:A:3353:LEU:HD23	1:A:3358:VAL:HG11	1.95	0.48
1:A:1826:PHE:CE1	1:A:1853:LEU:CD2	2.96	0.48
1:A:2476:LYS:H	1:A:2476:LYS:HD2	1.72	0.48
1:A:2580:LYS:HG2	1:A:2586:ARG:HH22	1.79	0.47
1:A:2358:THR:HG22	1:A:2359:ILE:N	2.29	0.47
1:A:2741:HIS:O	1:A:2745:ILE:HG13	2.15	0.47
1:A:4084:SER:O	1:A:4088:LEU:HG	2.14	0.47
1:A:3721:THR:O	1:A:3725:VAL:HG23	2.14	0.47
1:A:2445:PHE:HA	1:A:2449:THR:HG21	1.96	0.47
1:A:2446:SER:N	1:A:2449:THR:HG23	2.19	0.47
1:A:3461:ILE:C	1:A:3463:SER:H	2.22	0.47
1:A:1844:TRP:CD1	1:A:1893:ALA:HB3	2.50	0.47
1:A:2125:TRP:CZ2	1:A:2178:LEU:CD1	2.97	0.47
1:A:3415:ILE:HD13	1:A:3453:GLN:HG3	1.97	0.47
1:A:3462:ILE:O	1:A:3465:LEU:N	2.45	0.47
1:A:3459:ASP:OD2	1:A:3461:ILE:CG1	2.61	0.47
1:A:3690:LEU:HD23	1:A:3694:PHE:HB3	1.96	0.47
1:A:3924:TRP:O	1:A:3927:TYR:HB3	2.15	0.47
1:A:2563:SER:C	1:A:2565:LYS:H	2.23	0.47
1:A:3612:ASP:O	1:A:3615:VAL:CG2	2.63	0.47
1:A:4033:LEU:HD12	1:A:4033:LEU:C	2.39	0.47
1:A:3592:LYS:O	1:A:3596:ASN:N	2.48	0.47
1:A:1554:HIS:O	1:A:1555:HIS:HB2	2.15	0.46
1:A:1636:ILE:O	1:A:1640:VAL:HG23	2.15	0.46
1:A:1683:LEU:HB3	1:A:1702:LEU:HD21	1.96	0.46
1:A:2105:ASP:OD2	1:A:2508:GLN:HB2	2.15	0.46
1:A:2318:ILE:O	1:A:2322:LEU:HB2	2.16	0.46
1:A:3934:TRP:HB3	1:A:4023:ILE:HD13	1.97	0.46
1:A:3877:CYS:SG	1:A:3884:LEU:HD21	2.55	0.46
1:A:1683:LEU:HD22	1:A:1698:ILE:HG23	1.96	0.46
1:A:3967:TYR:HE2	1:A:3985:VAL:HA	1.80	0.46
1:A:1681:LYS:HE2	1:A:1939:PHE:CE1	2.50	0.46
1:A:2878:VAL:HA	1:A:2881:ILE:HD12	1.97	0.46
1:A:2112:GLU:HB3	1:A:2117:SER:OG	2.16	0.46
1:A:2204:PRO:HA	1:A:2207:ILE:HD12	1.97	0.46
1:A:2199:LEU:O	1:A:2201:HIS:N	2.49	0.46
1:A:2424:LYS:H	1:A:2424:LYS:HG3	1.52	0.46
1:A:3848:LEU:O	1:A:3849:SER:C	2.59	0.46
1:A:2627:ARG:NH1	1:A:2630:TYR:CD2	2.84	0.46
1:A:2571:TYR:HA	1:A:2574:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2654:ARG:NH1	1:A:2658:ASP:OD1	2.49	0.46
1:A:1660:VAL:HG13	1:A:1728:TRP:CH2	2.51	0.46
1:A:2476:LYS:HZ2	1:A:2528:ARG:HB2	1.81	0.46
1:A:3508:PHE:O	1:A:3512:ARG:HG2	2.16	0.46
1:A:3570:LEU:HD23	1:A:3580:ASN:CG	2.41	0.46
1:A:3807:SER:O	1:A:3808:LYS:HB2	2.16	0.46
1:A:2286:THR:HA	1:A:2412:ARG:NE	2.31	0.45
1:A:2835:LEU:HD23	1:A:2911:ARG:HB2	1.97	0.45
1:A:3760:LEU:HD21	1:A:4078:ALA:HA	1.98	0.45
1:A:1586:GLU:HG3	1:A:1765:ILE:H	1.81	0.45
1:A:3330:TYR:CE1	1:A:3334:PHE:CD2	3.05	0.45
1:A:3612:ASP:C	1:A:3615:VAL:HG22	2.41	0.45
1:A:3821:ASN:O	1:A:3825:ALA:HB2	2.17	0.45
1:A:3995:GLY:HA2	1:A:3998:ILE:CD1	2.46	0.45
1:A:2358:THR:CG2	1:A:2359:ILE:N	2.80	0.45
1:A:2458:LEU:HG	1:A:2484:LEU:HD21	1.99	0.45
1:A:2707:VAL:HG11	1:A:2712:LEU:CD1	2.45	0.45
1:A:2099:ASN:HA	1:A:2149:ARG:O	2.17	0.45
1:A:2494:LEU:HB2	1:A:2499:SER:N	2.32	0.45
1:A:3470:PHE:CE1	1:A:3488:VAL:HG21	2.52	0.45
1:A:1951:HIS:O	1:A:1955:LEU:HB2	2.17	0.45
1:A:1967:HIS:C	1:A:1968:PHE:CD1	2.85	0.45
1:A:2037:CYS:SG	1:A:2094:PHE:HB2	2.57	0.45
1:A:2175:ILE:HG13	1:A:2184:LEU:C	2.42	0.45
1:A:2417:CYS:O	1:A:2558:TYR:HA	2.17	0.45
1:A:1910:GLU:HB2	1:A:3846:MET:HA	1.98	0.45
1:A:2262:LEU:HA	1:A:2265:ILE:HD12	1.98	0.45
1:A:1945:LEU:HD13	1:A:1994:VAL:HG21	1.98	0.44
1:A:2274:HIS:CE1	1:A:2326:LEU:O	2.54	0.44
1:A:2766:LYS:CE	1:A:2890:THR:HB	2.39	0.44
1:A:3308:ASN:O	1:A:3312:GLN:HB2	2.17	0.44
1:A:1611:LEU:O	1:A:1615:ILE:HG23	2.17	0.44
1:A:1759:LYS:HE3	1:A:1761:GLU:OE2	2.17	0.44
1:A:1822:CYS:HB2	1:A:1853:LEU:CD2	2.31	0.44
1:A:1973:LEU:O	1:A:1977:LEU:HG	2.18	0.44
1:A:2749:LEU:HD12	1:A:2773:VAL:HG12	1.99	0.44
1:A:3319:GLU:HA	1:A:3359:LYS:O	2.17	0.44
1:A:3330:TYR:CD1	1:A:3334:PHE:CD2	3.05	0.44
1:A:2354:SER:H	1:A:2357:SER:HB2	1.83	0.44
1:A:2411:LYS:HG2	1:A:2530:HIS:CE1	2.41	0.44
1:A:3702:MET:HB3	1:A:3767:PHE:HZ	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3924:TRP:CD1	1:A:3924:TRP:C	2.95	0.44
1:A:1681:LYS:HE2	1:A:1939:PHE:CZ	2.53	0.44
1:A:2336:ARG:HG2	1:A:2355:ASP:CG	2.41	0.44
1:A:3566:LEU:HD23	1:A:3587:LEU:HD11	1.99	0.44
1:A:2027:THR:HA	1:A:2028:PRO:HD3	1.48	0.44
1:A:1995:VAL:HG22	1:A:2022:PHE:HE2	1.80	0.44
1:A:2155:ASP:OD1	1:A:2195:GLU:HG3	2.17	0.44
1:A:2386:MET:HB3	1:A:2627:ARG:NE	2.32	0.44
1:A:2646:ARG:NH1	1:A:2687:GLY:H	2.15	0.44
1:A:3939:ILE:HG13	1:A:4010:LEU:HD23	1.98	0.44
1:A:1620:PHE:CA	1:A:1760:PHE:CE1	3.01	0.44
1:A:1793:CYS:SG	1:A:1918:GLU:HG2	2.57	0.44
1:A:1826:PHE:O	1:A:1826:PHE:CG	2.70	0.44
1:A:1968:PHE:CD1	1:A:1968:PHE:N	2.84	0.44
1:A:2385:VAL:HG23	1:A:2574:TYR:CD1	2.53	0.44
1:A:2738:MET:HE3	1:A:2769:LEU:HD11	1.98	0.44
1:A:2783:GLN:HG2	1:A:2816:ILE:HB	1.99	0.44
1:A:3566:LEU:HD13	1:A:3570:LEU:HD11	1.86	0.44
1:A:2422:SER:H	1:A:2424:LYS:HZ1	1.65	0.44
1:A:2760:GLY:O	1:A:2761:ALA:HB3	2.18	0.44
1:A:2861:ARG:HD2	1:A:2866:LEU:HD13	2.00	0.44
1:A:1660:VAL:CG1	1:A:1728:TRP:CH2	3.01	0.44
1:A:2021:ILE:HG22	1:A:2022:PHE:HD1	1.82	0.44
1:A:2575:TYR:HD1	1:A:2578:ILE:HD11	1.83	0.44
1:A:3010:LEU:HD22	1:A:3320:LEU:HD12	1.99	0.44
1:A:3854:TYR:CD1	1:A:3854:TYR:C	2.96	0.44
1:A:3964:ALA:HB2	1:A:3993:VAL:HG11	1.99	0.44
1:A:1559:SER:CB	1:A:1572:ILE:HG22	2.47	0.43
1:A:2197:ASP:HB3	1:A:2549:ARG:HD2	1.99	0.43
1:A:1926:SER:HA	1:A:1929:ILE:CD1	2.48	0.43
1:A:2061:TYR:O	1:A:2064:GLN:HG2	2.17	0.43
1:A:2178:LEU:HB2	1:A:2182:GLU:H	1.83	0.43
1:A:3411:SER:O	1:A:3413:HIS:N	2.47	0.43
1:A:3566:LEU:HA	1:A:3583:LEU:HD23	2.00	0.43
1:A:1655:MET:HE3	1:A:1659:LEU:HD12	2.01	0.43
1:A:1953:LEU:HD11	1:A:1973:LEU:HB3	1.98	0.43
1:A:2404:PHE:CZ	1:A:2428:MET:HG2	2.53	0.43
1:A:3767:PHE:HB3	1:A:3769:VAL:HG23	2.00	0.43
1:A:4033:LEU:HD13	1:A:4035:GLN:CG	2.49	0.43
1:A:2517:LYS:NZ	1:A:2520:GLU:OE1	2.48	0.43
1:A:3509:LEU:CG	1:A:3513:VAL:HG21	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1646:GLN:OE1	1:A:1763:ILE:HG12	2.18	0.43
1:A:2266:PHE:HD1	1:A:2326:LEU:HD21	1.83	0.43
1:A:2375:ILE:HG22	1:A:2376:PRO:O	2.18	0.43
1:A:3338:ASN:H	1:A:3341:GLU:HB2	1.82	0.43
1:A:4033:LEU:CD1	1:A:4035:GLN:N	2.82	0.43
1:A:1611:LEU:O	1:A:1615:ILE:HG12	2.19	0.43
1:A:1655:MET:HE3	1:A:1659:LEU:CD1	2.49	0.43
1:A:3407:LEU:HD23	1:A:3518:PHE:CE2	2.53	0.43
1:A:2578:ILE:CG2	1:A:2630:TYR:HB2	2.49	0.43
1:A:4074:GLU:HA	1:A:4077:GLN:HE21	1.84	0.43
1:A:1741:LEU:O	1:A:1742:ASP:HB2	2.19	0.43
1:A:2738:MET:HG2	1:A:2769:LEU:HD21	2.00	0.43
1:A:2280:THR:HA	1:A:2283:LYS:HD2	1.99	0.43
1:A:2982:VAL:CG1	1:A:2983:GLY:N	2.82	0.43
1:A:3307:LEU:O	1:A:3311:LYS:N	2.27	0.43
1:A:3979:ASN:O	1:A:3981:PRO:CD	2.64	0.43
1:A:1998:LEU:CD1	1:A:2022:PHE:HZ	2.32	0.42
1:A:2072:LEU:HD11	1:A:2193:LEU:HD23	2.01	0.42
1:A:1830:VAL:O	1:A:1834:LEU:HG	2.19	0.42
1:A:2707:VAL:HG11	1:A:2712:LEU:HD12	2.00	0.42
1:A:1568:SER:HB2	1:A:1816:VAL:HG21	2.01	0.42
1:A:1991:GLU:O	1:A:1994:VAL:HB	2.19	0.42
1:A:2229:LEU:HD11	1:A:2285:GLU:HG3	2.02	0.42
1:A:2447:LYS:HE3	1:A:2493:LYS:HD3	2.00	0.42
1:A:2493:LYS:HG3	1:A:2494:LEU:N	2.33	0.42
1:A:2510:MET:O	1:A:2513:GLN:NE2	2.52	0.42
1:A:2512:LYS:O	1:A:2513:GLN:CB	2.66	0.42
1:A:1650:LEU:O	1:A:1654:VAL:HG23	2.19	0.42
1:A:2141:ILE:CG2	1:A:2145:PHE:HB2	2.49	0.42
1:A:2503:VAL:HA	1:A:2506:LEU:HD12	2.01	0.42
1:A:1710:ASN:CB	1:A:1932:MET:HE1	2.50	0.42
1:A:2050:SER:O	1:A:2051:GLU:C	2.62	0.42
1:A:2609:THR:HA	1:A:2612:GLN:O	2.20	0.42
1:A:3024:LEU:HD13	1:A:3303:LYS:HG3	1.92	0.42
1:A:3544:LYS:O	1:A:3548:LEU:HB2	2.19	0.42
1:A:3728:GLU:CG	1:A:4079:LYS:HE2	2.49	0.42
1:A:1992:LYS:HG2	1:A:2024:SER:HB2	1.92	0.42
1:A:2109:LEU:CD1	1:A:2129:LEU:HD23	2.49	0.42
1:A:2225:LYS:HD2	1:A:2281:PHE:CZ	2.55	0.42
1:A:2413:GLY:HA3	1:A:2510:MET:HE3	2.00	0.42
1:A:2640:THR:O	1:A:2643:SER:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3414:MET:O	1:A:3418:ILE:HG12	2.19	0.42
1:A:3785:TYR:CE2	1:A:3859:VAL:HG13	2.54	0.42
1:A:3816:LEU:HD23	1:A:3847:SER:HG	1.83	0.42
1:A:2199:LEU:O	1:A:2200:ASP:C	2.62	0.42
1:A:2786:ILE:HD12	1:A:3460:PRO:CG	2.50	0.42
1:A:3628:ILE:HG13	1:A:3705:LEU:HD23	2.00	0.42
1:A:3696:MET:SD	1:A:3760:LEU:HD23	2.59	0.42
1:A:1727:LEU:O	1:A:1731:VAL:HG23	2.20	0.42
1:A:1898:LEU:HD11	1:A:1908:LEU:CD2	2.50	0.42
1:A:3784:ASN:ND2	1:A:3865:ALA:O	2.52	0.42
1:A:3810:SER:HB3	1:A:3837:GLY:HA2	2.01	0.42
1:A:1702:LEU:HA	1:A:1702:LEU:HD23	1.86	0.42
1:A:1939:PHE:CD1	1:A:1939:PHE:N	2.87	0.42
1:A:1970:LEU:CD1	1:A:1970:LEU:C	2.92	0.42
1:A:2012:LEU:HD12	1:A:2013:VAL:N	2.35	0.42
1:A:2390:ILE:H	1:A:2426:MET:HE1	1.85	0.42
1:A:2494:LEU:HD12	1:A:2494:LEU:C	2.45	0.42
1:A:4045:LEU:O	1:A:4048:ILE:HG22	2.19	0.42
1:A:1569:ILE:HD12	1:A:1569:ILE:C	2.44	0.42
1:A:1672:TYR:O	1:A:1676:VAL:HG23	2.19	0.42
1:A:1781:THR:HG21	1:A:1919:PHE:CE1	2.55	0.42
1:A:2428:MET:HE1	1:A:2440:VAL:HG13	2.01	0.42
1:A:2568:SER:HA	1:A:2597:VAL:HG21	2.02	0.42
1:A:3505:ILE:O	1:A:3510:ARG:NH1	2.53	0.42
1:A:2492:PRO:CB	1:A:2502:VAL:HG11	2.49	0.41
1:A:2829:GLU:HA	1:A:2832:ASN:HD22	1.84	0.41
1:A:3464:ARG:O	1:A:3467:SER:O	2.38	0.41
1:A:3579:GLU:O	1:A:3582:GLU:N	2.43	0.41
1:A:1706:LEU:HD21	1:A:1935:GLN:CG	2.48	0.41
1:A:1992:LYS:CG	1:A:2024:SER:CB	2.78	0.41
1:A:2095:ASP:OD1	1:A:2149:ARG:NH2	2.53	0.41
1:A:2178:LEU:HB3	1:A:2179:PRO:HD2	2.01	0.41
1:A:2758:LEU:HD22	1:A:2917:MET:SD	2.60	0.41
1:A:3785:TYR:CD1	1:A:3785:TYR:N	2.87	0.41
1:A:1742:ASP:HB3	1:A:1745:ASN:HD22	1.86	0.41
1:A:1929:ILE:H	1:A:1929:ILE:HD12	1.86	0.41
1:A:1965:HIS:HD2	1:A:2212:LEU:HD23	1.85	0.41
1:A:2111:LYS:CD	1:A:2161:GLU:CG	2.84	0.41
1:A:2904:SER:O	1:A:2905:SER:C	2.61	0.41
1:A:3833:LYS:NZ	1:A:3862:THR:HG21	2.35	0.41
1:A:1575:LEU:O	1:A:1576:GLU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1966:TYR:CZ	1:A:2006:LEU:HD23	2.55	0.41
1:A:2001:VAL:O	1:A:2004:PRO:HD2	2.20	0.41
1:A:2053:PHE:HB2	1:A:2219:VAL:HB	2.02	0.41
1:A:2708:ASN:O	1:A:2712:LEU:HD13	2.20	0.41
1:A:2755:HIS:HB3	1:A:2912:CYS:SG	2.60	0.41
1:A:3365:ARG:HD2	1:A:3368:ASP:OD2	2.19	0.41
1:A:4033:LEU:HD12	1:A:4035:GLN:H	1.84	0.41
1:A:2420:PRO:HD3	1:A:2536:ASN:HD21	1.85	0.41
1:A:2760:GLY:HA3	1:A:2766:LYS:HD3	2.01	0.41
1:A:2819:GLU:HB3	1:A:2891:ILE:HG22	2.03	0.41
1:A:2860:THR:HG21	1:A:2867:LEU:HD12	2.02	0.41
1:A:3304:GLU:C	1:A:3306:TRP:H	2.29	0.41
1:A:3671:VAL:HA	1:A:3674:ILE:HG22	2.03	0.41
1:A:4022:GLN:O	1:A:4023:ILE:C	2.63	0.41
1:A:2306:ASP:HB2	1:A:2309:SER:HB3	2.02	0.41
1:A:2762:SER:O	1:A:2763:ARG:CB	2.68	0.41
1:A:3832:SER:O	1:A:3836:GLY:N	2.45	0.41
1:A:3846:MET:HG3	1:A:3847:SER:N	2.35	0.41
1:A:4033:LEU:CD1	1:A:4035:GLN:H	2.34	0.41
1:A:2225:LYS:HG2	1:A:2229:LEU:HD12	2.02	0.41
1:A:2786:ILE:HD12	1:A:3460:PRO:HG2	2.03	0.41
1:A:2891:ILE:HD11	1:A:2903:ILE:HD11	2.03	0.41
1:A:3947:PRO:O	1:A:3948:HIS:C	2.59	0.41
1:A:2044:ARG:HH21	1:A:2093:ILE:HD11	1.85	0.41
1:A:2099:ASN:HD22	1:A:2151:TRP:HE1	1.68	0.41
1:A:2852:LEU:HG	1:A:2856:LEU:HD13	2.03	0.41
1:A:3544:LYS:HE3	1:A:3607:PHE:CD1	2.55	0.41
1:A:3590:LEU:HD12	1:A:3593:GLU:HB2	2.02	0.41
1:A:1823:ASP:HB3	1:A:1852:ARG:O	2.16	0.41
1:A:2034:ILE:HD12	1:A:2061:TYR:CE2	2.55	0.41
1:A:2039:LYS:HG2	1:A:2049:MET:HG3	2.03	0.41
1:A:2138:ASN:ND2	1:A:2185:PRO:O	2.52	0.41
1:A:2141:ILE:HG22	1:A:2145:PHE:CB	2.51	0.41
1:A:3534:LEU:HD12	1:A:3618:TYR:CZ	2.52	0.41
1:A:4020:ASN:ND2	1:A:4028:ARG:HD3	2.35	0.41
1:A:2905:SER:HA	1:A:2906:PRO:HD2	1.85	0.41
1:A:3772:TRP:HZ3	1:A:3780:ASN:HD22	1.68	0.41
1:A:3809:GLU:HB3	1:A:3810:SER:H	1.54	0.41
1:A:2064:GLN:CD	1:A:2091:MET:SD	3.04	0.40
1:A:2985:ASN:N	1:A:2986:PRO:CD	2.84	0.40
1:A:3330:TYR:CZ	1:A:3346:LEU:HD13	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1822:CYS:SG	1:A:1850:PHE:CA	3.04	0.40
1:A:2489:ILE:HD11	1:A:2506:LEU:HD13	2.02	0.40
1:A:2661:VAL:HG12	1:A:2916:TRP:CE2	2.57	0.40
1:A:2977:TYR:HD1	1:A:2981:LYS:HG3	1.86	0.40
1:A:3708:PHE:CZ	1:A:3720:LEU:HD21	2.57	0.40
1:A:1715:LEU:HG	1:A:1727:LEU:HD22	2.02	0.40
1:A:2034:ILE:HG13	1:A:2061:TYR:CE2	2.57	0.40
1:A:2088:ILE:HG12	1:A:2151:TRP:CZ2	2.55	0.40
1:A:2488:GLU:CG	1:A:2491:LEU:HD12	2.51	0.40
1:A:1612:ASP:C	1:A:1615:ILE:HG12	2.46	0.40
1:A:1965:HIS:HD2	1:A:2212:LEU:HD21	1.85	0.40
1:A:2109:LEU:HB3	1:A:2113:SER:HB2	2.03	0.40
1:A:2332:GLY:HA2	1:A:2335:GLN:CG	2.51	0.40
1:A:2889:PHE:CE1	1:A:2902:MET:HE1	2.56	0.40
1:A:3682:VAL:HG13	1:A:3686:PHE:HD2	1.87	0.40
1:A:3737:THR:CB	1:A:3740:THR:OG1	2.56	0.40
1:A:3886:ALA:N	1:A:3887:PRO:CD	2.84	0.40
1:A:3978:ASN:O	1:A:3981:PRO:HD3	2.20	0.40
1:A:1744:LEU:HD22	1:A:1760:PHE:CD2	2.56	0.40
1:A:1968:PHE:HD1	1:A:1968:PHE:N	2.20	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	2237/2286 (98%)	2137 (96%)	93 (4%)	7 (0%)	36 72

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2990	GLY

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Mol	Chain	Res	Type
1	A	3306	TRP
1	A	3482	GLY
1	A	2519	PRO
1	A	3980	ILE
1	A	2562	PRO
1	A	2028	PRO

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	2039/2078 (98%)	1927 (94%)	112 (6%)	19	41

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1589	VAL
1	A	1634	THR
1	A	1639	VAL
1	A	1644	ILE
1	A	1646	GLN
1	A	1648	ILE
1	A	1661	GLU
1	A	1768	ARG
1	A	1788	GLN
1	A	1923	SER
1	A	1971	ARG
1	A	1973	LEU
1	A	1992	LYS
1	A	1999	LYS
1	A	2012	LEU
1	A	2057	CYS
1	A	2070	LEU
1	A	2075	LYS
1	A	2078	CYS
1	A	2109	LEU

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Mol	Chain	Res	Type
1	A	2122	THR
1	A	2141	ILE
1	A	2186	ILE
1	A	2202	THR
1	A	2218	ASP
1	A	2275	ILE
1	A	2292	VAL
1	A	2295	ILE
1	A	2310	LEU
1	A	2318	ILE
1	A	2323	LEU
1	A	2357	SER
1	A	2381	GLU
1	A	2395	ILE
1	A	2397	THR
1	A	2424	LYS
1	A	2458	LEU
1	A	2472	THR
1	A	2476	LYS
1	A	2526	ILE
1	A	2544	ILE
1	A	2566	SER
1	A	2576	LYS
1	A	2611	LEU
1	A	2626	VAL
1	A	2638	ARG
1	A	2665	GLU
1	A	2689	ILE
1	A	2694	LEU
1	A	2700	LEU
1	A	2742	ILE
1	A	2751	GLN
1	A	2753	GLN
1	A	2764	THR
1	A	2822	ILE
1	A	2833	THR
1	A	2843	LEU
1	A	2853	LEU
1	A	2856	LEU
1	A	2865	LEU
1	A	2873	LEU
1	A	2911	ARG

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Mol	Chain	Res	Type
1	A	2936	ILE
1	A	2967	ASN
1	A	3329	ILE
1	A	3332	THR
1	A	3371	VAL
1	A	3372	THR
1	A	3380	LEU
1	A	3400	SER
1	A	3415	ILE
1	A	3418	ILE
1	A	3425	LYS
1	A	3456	GLU
1	A	3485	GLU
1	A	3534	LEU
1	A	3536	GLU
1	A	3538	ASN
1	A	3548	LEU
1	A	3559	LEU
1	A	3565	ARG
1	A	3584	MET
1	A	3601	LEU
1	A	3605	GLU
1	A	3618	TYR
1	A	3634	LYS
1	A	3646	ILE
1	A	3677	LEU
1	A	3717	GLU
1	A	3729	SER
1	A	3735	LYS
1	A	3737	THR
1	A	3744	LEU
1	A	3811	LEU
1	A	3823	ASN
1	A	3839	ILE
1	A	3844	ILE
1	A	3862	THR
1	A	3876	THR
1	A	3884	LEU
1	A	3906	THR
1	A	3917	THR
1	A	3943	THR
1	A	3976	SER

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Mol	Chain	Res	Type
1	A	3980	ILE
1	A	3982	TRP
1	A	3992	ILE
1	A	4004	LEU
1	A	4016	CYS
1	A	4021	LEU
1	A	4040	GLU
1	A	4068	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1622	GLN
1	A	1646	GLN
1	A	1714	GLN
1	A	1717	ASN
1	A	1736	GLN
1	A	1745	ASN
1	A	1851	ASN
1	A	1870	ASN
1	A	1873	GLN
1	A	1899	ASN
1	A	1951	HIS
1	A	1965	HIS
1	A	1979	ASN
1	A	2099	ASN
1	A	2231	ASN
1	A	2239	ASN
1	A	2270	ASN
1	A	2274	HIS
1	A	2282	ASN
1	A	2293	HIS
1	A	2335	GLN
1	A	2340	GLN
1	A	2383	HIS
1	A	2409	ASN
1	A	2429	ASN
1	A	2459	HIS
1	A	2500	GLN
1	A	2513	GLN
1	A	2530	HIS
1	A	2536	ASN

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Mol	Chain	Res	Type
1	A	2601	ASN
1	A	2634	ASN
1	A	2683	ASN
1	A	2688	ASN
1	A	2708	ASN
1	A	2777	ASN
1	A	3025	ASN
1	A	3323	ASN
1	A	3336	HIS
1	A	3363	ASN
1	A	3475	ASN
1	A	3497	HIS
1	A	3521	ASN
1	A	3542	GLN
1	A	3576	ASN
1	A	3588	ASN
1	A	3637	GLN
1	A	3890	GLN
1	A	3962	GLN
1	A	4020	ASN
1	A	4036	GLN
1	A	4077	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 Tomogram visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5758. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



X



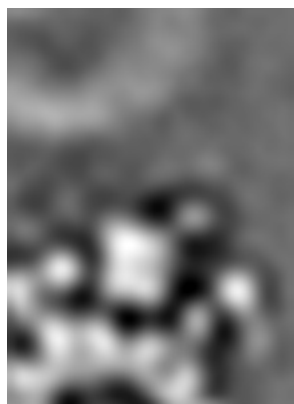
Y



Z

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

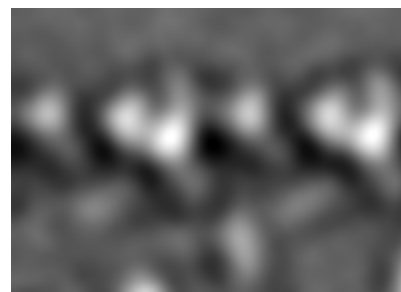
6.2 Central slices [i](#)



X Index: 25



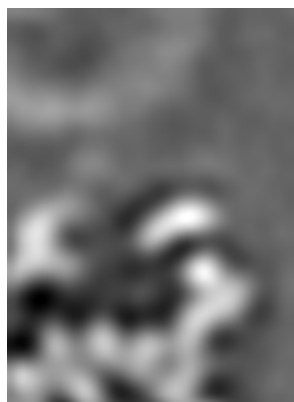
Y Index: 18



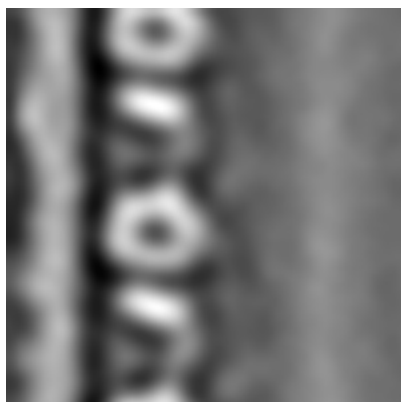
Z Index: 25

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

6.3 Largest variance slices [i](#)



X Index: 29



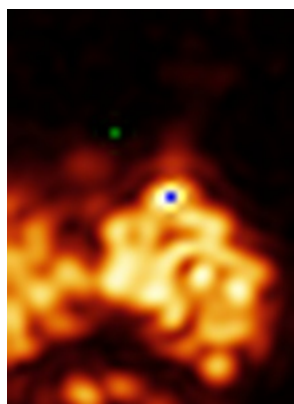
Y Index: 15



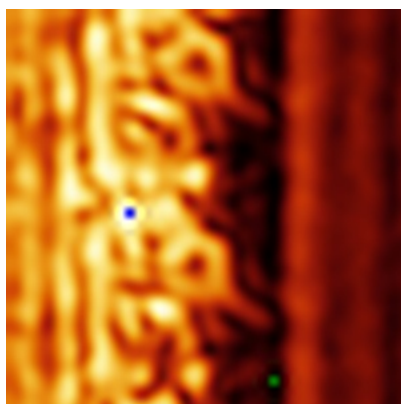
Z Index: 11

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

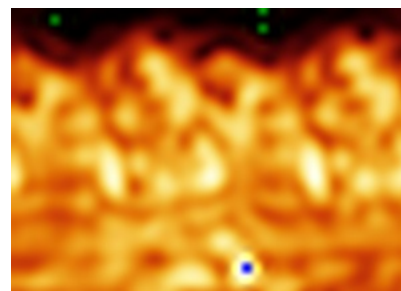
6.4 Orthogonal standard-deviation projections (False-color) [i](#)



X



Y



Z

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

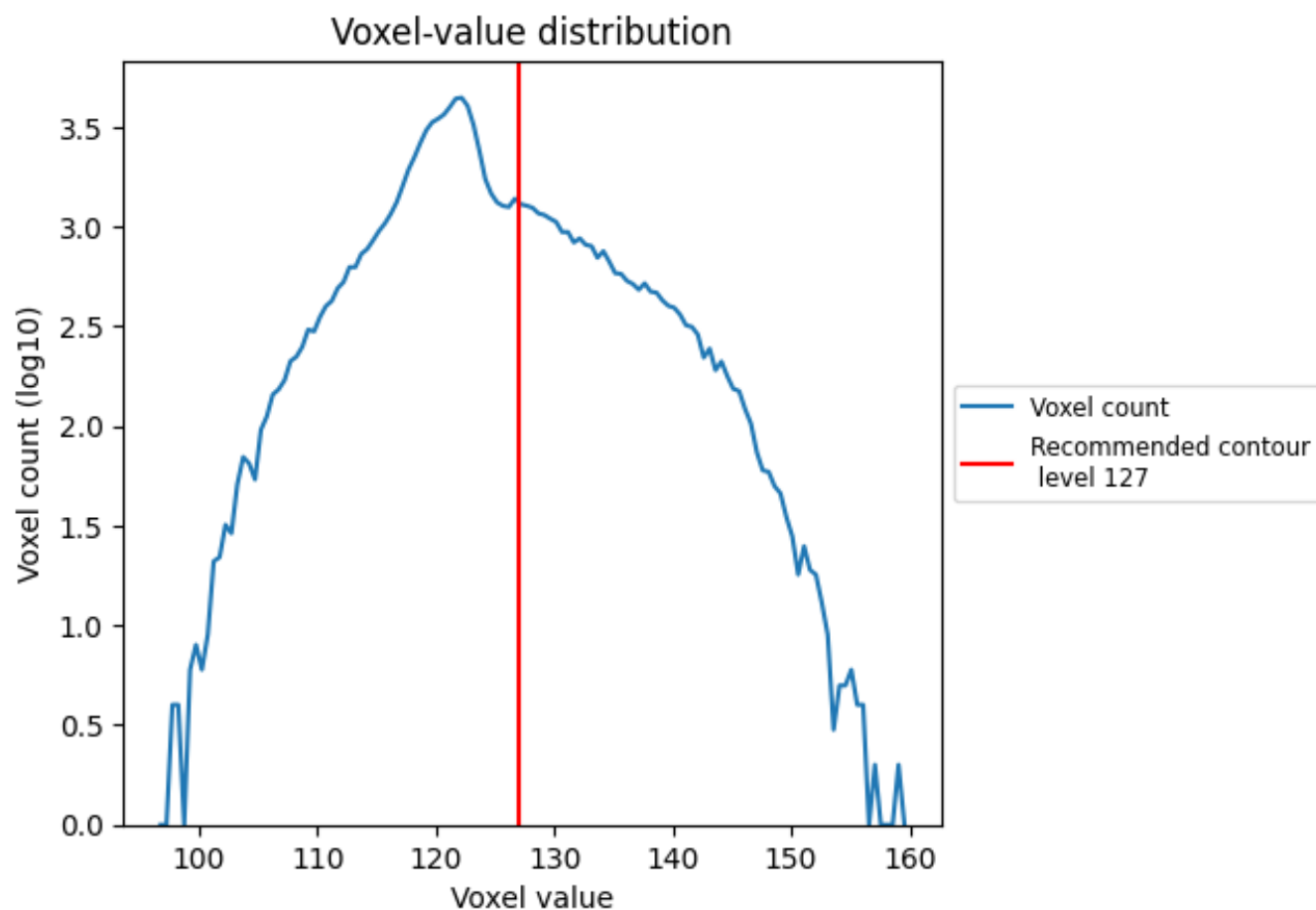
6.5 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Tomogram analysis [i](#)

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

7.1 Voxel-value distribution [i](#)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

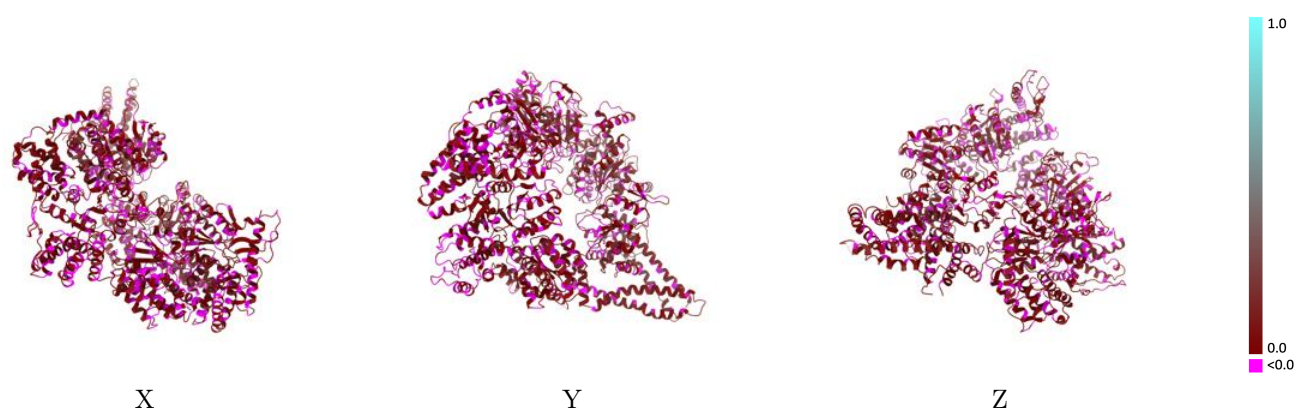
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5758 and PDB model 3J68. Per-residue inclusion information can be found in section 3 on page 4.

8.1 Map-model overlay [i](#)

This section was not generated.

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

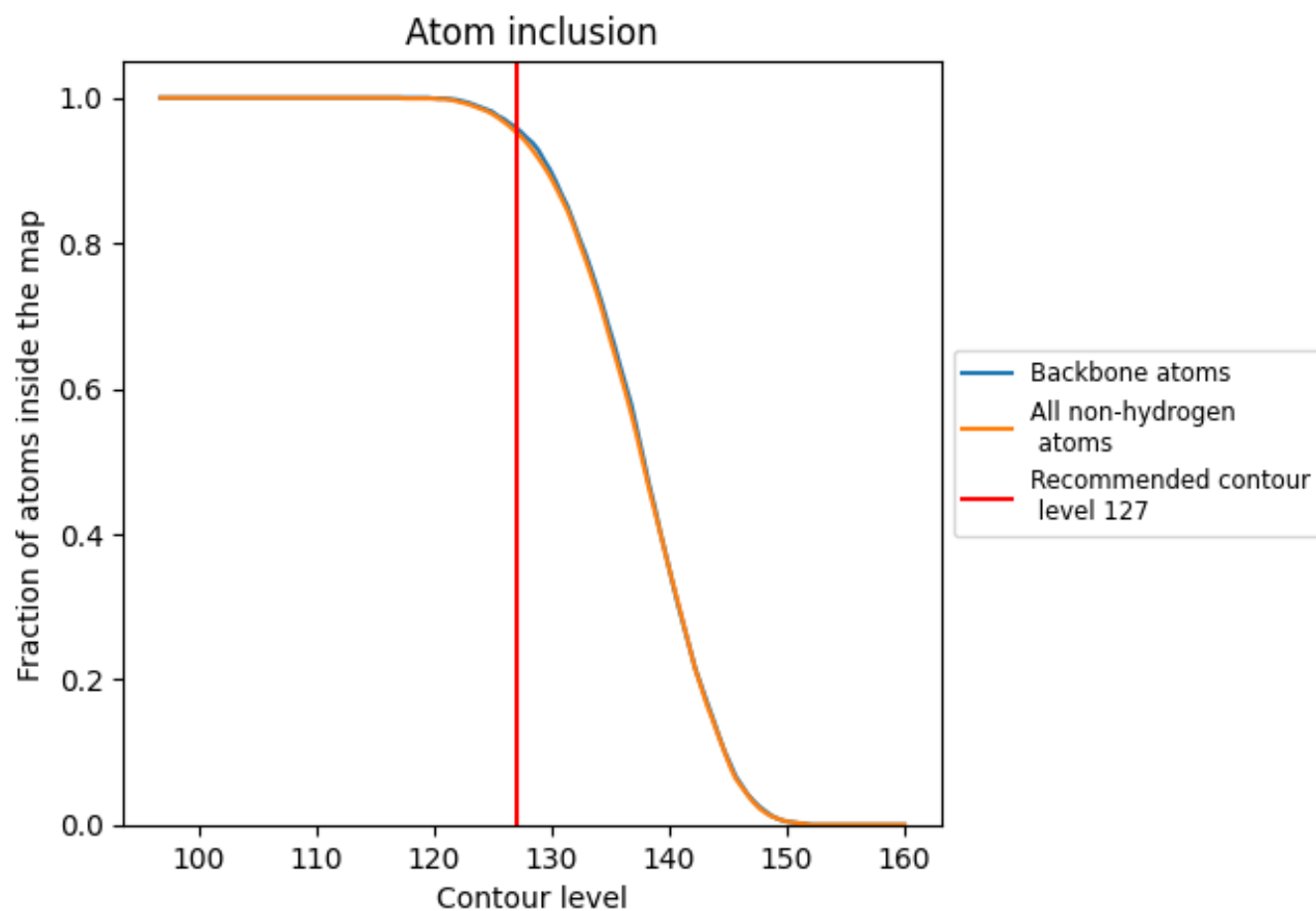


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

8.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (127) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9530	0.0400
A	0.9530	0.0400

