Full wwPDB EM Validation Report (i)

Feb 13, 2024 – 05:35 AM EST

PDB ID	:	3J67
EMDB ID	:	EMD-5757
Title	:	Structural mechanism of the dynein powerstroke (post-powerstroke state)
Authors	:	Lin, J.; Okada, K.; Raytchev, M.; Smith, M.C.; Nicastro, D.
Deposited on	:	2013-12-22
Resolution	:	34.00 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 (i) 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 (i)) were used in the production of this report:

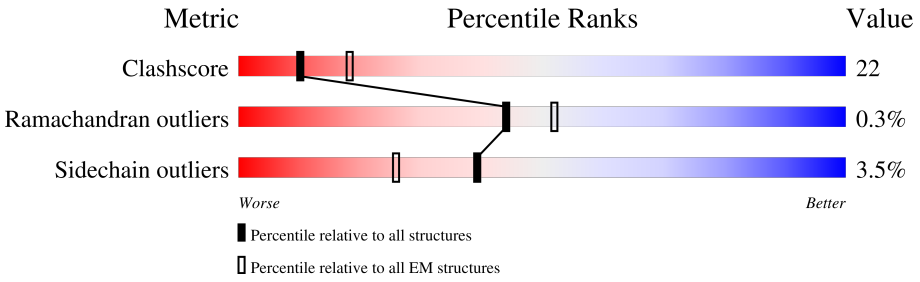
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

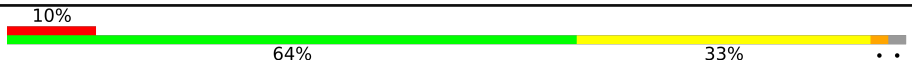
The reported resolution of this entry is 34.00 Å.

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	

2 Entry composition (i)

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.

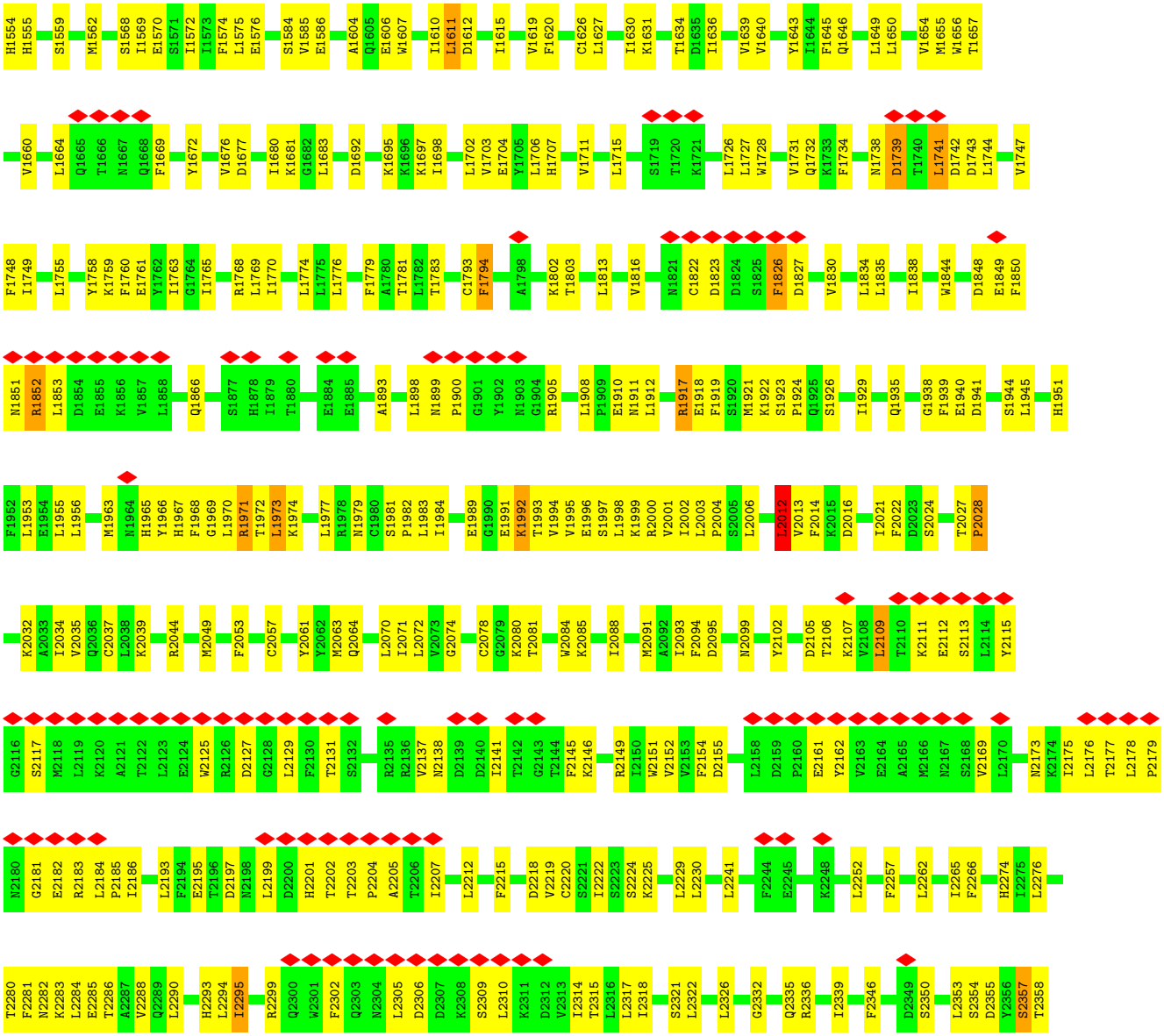
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2245	18105	11610	3004	3403	88	0	0

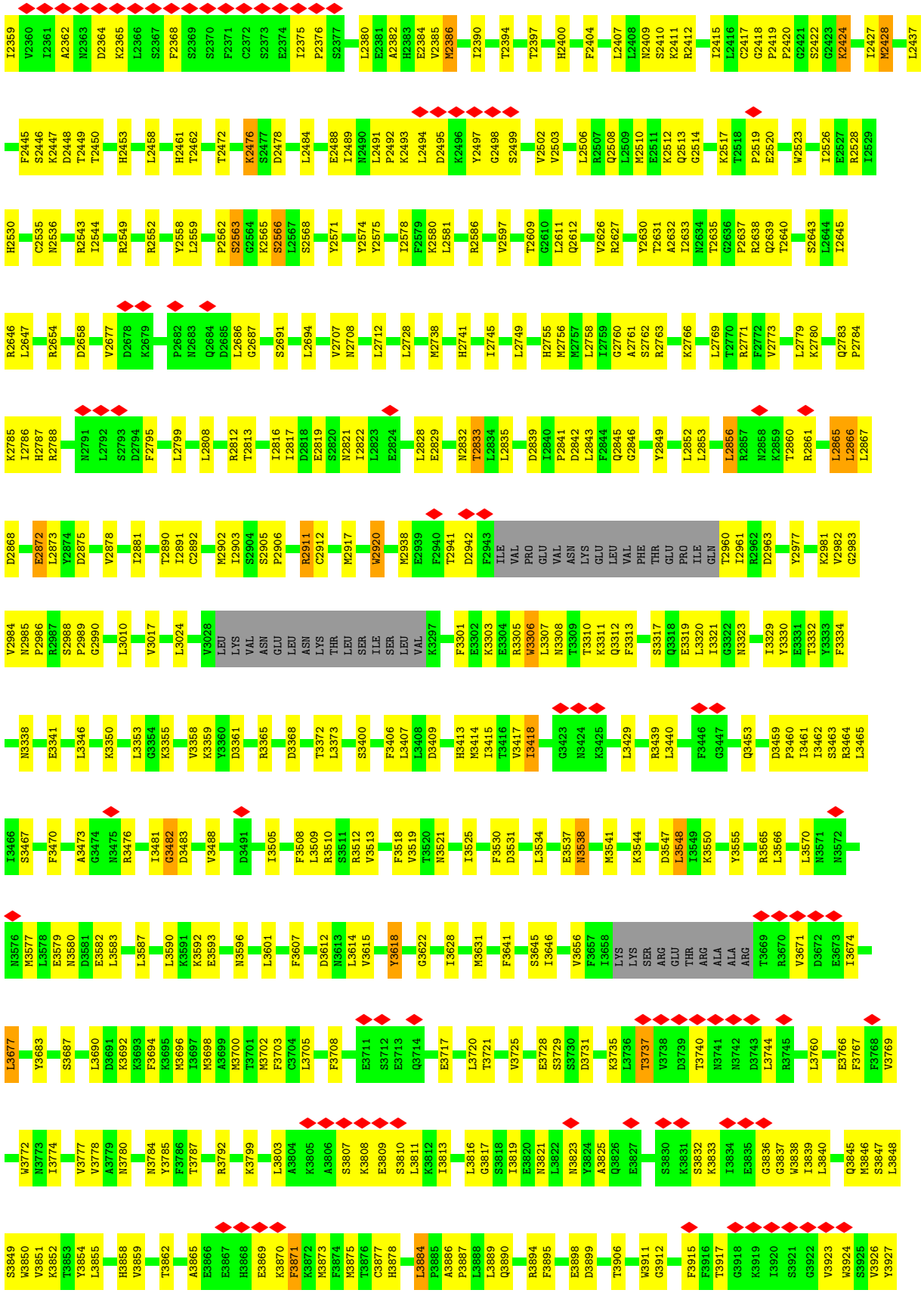
3 Residue-property plots (i)

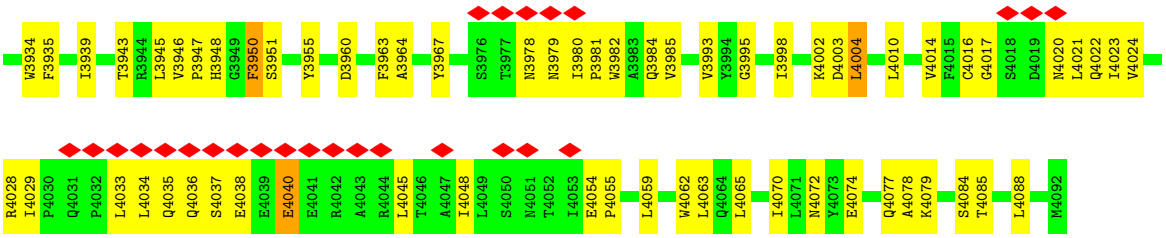
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

Chain A:




I2359 V2360 I2361 A2362 N2363 D2364 K2365 L2366 S2367 F2368 S2369 S2370 F2371 C2372 S2373 E2374 I2375 P2376 S2377 L2380 E2381 A2382 H2383 E2384 V2385 M2386 I2390 T2394 T2397 H2400 F2404 L2407 L2408 N2409 S2410 K2411 R2412 I2415 L2416 C2417 G2418 P2419 P2420 G2421 S2422 G2423 K2424 I2427 M2428 L2437
F2445 S2446 K2447 D2448 T2449 T2450 H2453 L2458 H2461 T2462 T2472 K2476 S2477 D2478 L2484 E2488 I2489 N2490 L2491 P2492 K2493 L2494 D2495 K2496 Y2497 G2498 S2499 V2502 V2503 L2506 R2507 Q2508 L2509 M2510 E2511 K2512 Q2513 G2514 K2517 T2518 P2519 E2520 W2523 I2526 E2527 R2528 I2529
H2530 C2535 N2536 R2543 I2544 R2549 R2552 Y2558 L2559 P2562 S2563 G2564 K2565 S2566 L2567 S2568 Y2571 Y2574 Y2575 I2578 F2579 K2580 L2581 R2586 V2597 T2609 G2610 L2611 Q2612 V2626 R2627 Y2630 T2631 A2632 I2633 N2634 T2635 G2636 P2637 R2638 Q2639 T2640 S2643 L2644 I2645
R2646 L2647 R2654 D2658 V2677 D2678 K2679 P2682 N2683 Q2684 D2685 L2686 G2687 S2691 L2694 V2707 N2708 L2712 L2728 M2738 H2741 I2745 L2749 H2755 M2756 M2757 L2758 I2759 G2760 A2761 S2762 R2763 K2766 L2769 T2770 R2771 F2772 V2773 L2779 K2780 Q2783 P2784
K2785 I2786 H2787 R2788 N2791 L2792 S2793 D2794 F2795 L2799 L2808 R2812 T2813 I2816 I2817 D2818 E2819 S2820 N2821 I2822 L2823 E2824 L2828 E2829 N2832 T2833 L2834 L2835 D2839 I2840 P2841 D2842 L2843 F2844 Q2845 G2846 Y2849 L2852 L2853 L2856 R2857 N2858 K2859 T2860 R2861 L2865 L2866 L2867
D2868 E2872 L2873 Y2874 D2875 V2878 I2881 T2890 I2891 C2892 M2902 I2903 S2904 S2905 P2906 R2911 C2912 M2917 W2920 M2938 E2939 F2940 T2941 D2942 F2943 ILE VAL PRO GLU VAL ASN LYS GLU LEU VAL PHE THR GLU PRO ILE GLN T2960 I2961 R2962 D2963 Y2977 K2981 V2982 G2983
V2984 N2985 P2986 R2987 S2988 P2989 G2990 L3010 V3017 L3024 V3028 LEU LYS VAL ASN GLU LEU ASN LYS THR LEU SER ILE SER LEU VAL K3297 F3301 E3302 K3303 E3304 R3305 W3306 L3307 N3308 T3309 T3310 K3311 Q3312 F3313 S3317 Q3318 E3319 L3320 I3321 G3322 N3323 I3329 Y3330 E3331 T3332 Y3333 F3334
N3338 E3341 L3346 K3350 L3353 G3354 K3355 V3358 K3359 Y3360 D3361 R3365 D3368 T3372 L3373 S3400 F3406 L3407 L3408 D3409 H3413 M3414 I3415 T3416 V3417 I3418 G3423 N3424 K3425 L3429 R3439 L3440 F3446 G3447 Q3453 D3459 P3460 I3461 I3462 S3463 R3464 L3465
I3466 S3467 F3470 A3473 G3474 N3475 R3476 I3481 G3482 D3483 V3488 D3491 I3505 F3508 L3509 R3510 S3511 R3512 V3513 F3518 V3519 T3520 N3521 I3525 F3530 D3531 L3534 E3537 N3538 M3541 K3544 D3547 L3548 I3549 K3550 Y3555 R3565 L3566 L3570 N3571 N3572
N3576 M3577 L3578 E3579 N3580 D3581 E3582 L3583 L3587 L3590 K3591 K3592 E3593 N3596 L3601 F3607 D3612 N3613 L3614 V3615 Y3618 G3622 I3628 M3631 F3641 S3645 I3646 V3656 F3657 I3658 LYS LYS SER ARG GLU THR ARG ALA ALA ARG T3669 R3670 V3671 D3672 E3673 I3674
L3677 Y3683 S3687 L3690 D3691 K3692 K3693 F3694 K3695 M3696 I3697 M3698 A3699 M3700 T3701 M3702 F3703 C3704 L3705 F3708 E3711 S3712 E3713 Q3714 E3717 L3720 T3721 V3725 E3728 S3729 S3730 D3731 K3735 L3736 T3737 V3738 D3739 T3740 N3741 N3742 D3743 L3744 R3745 L3760 E3766 F3767 F3768 V3769
W3772 N3773 I3774 V3777 V3778 A3779 N3780 N3784 Y3785 F3786 T3787 R3792 K3799 L3803 A3804 K3805 A3806 S3807 K3808 E3809 S3810 L3811 K3812 I3813 L3816 G3817 S3818 I3819 E3820 N3821 L3822 N3823 Y3824 A3825 Q3826 E3827 S3830 K3831 S3832 K3833 I3834 E3835 G3836 G3837 W3838 I3839 L3840 Q3845 M3846 S3847 L3848
S3849 W3850 V3851 K3852 T3853 Y3854 L3855 H3858 V3859 T3862 A3865 E3866 E3867 H3868 E3869 K3870 F3871 K3872 M3873 F3874 M3875 T3876 C3877 H3878 L3884 P3885 A3886 P3887 L3888 L3889 Q3890 R3894 F3895 E3898 D3899 T3906 W3911 G3912 F3915 F3916 T3917 G3918 K3919 I3920 S3921 G3922 V3923 W3924 S3925 V3926 Y3927


W3934
F3935
I3939
T3943
R3944
L3945
V3946
P3947
H3948
G3949
F3950
S3951
Y3955
D3960
F3963
A3964
Y3967
S3976
T3977
N3978
N3979
I3980
P3981
W3982
A3983
Q3984
V3985
V3993
Y3994
G3995
I3998
K4002
D4003
L4004
L4010
V4014
F4015
C4016
G4017
S4018
D4019
M4020
L4021
Q4022
I4023
V4024
R4028
I4029
P4030
Q4031
P4032
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S4037
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N4051
T4052
I4053
E4054
P4055
L4059
W4062
L4063
Q4064
L4065
I4070
L4071
N4072
Y4073
E4074
Q4077
A4078
K4079
S4084
T4085
L4088
M4092

4 Experimental information (i)

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 ($e^-/Å^2$)	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	152.188	Depositor
Minimum voxel value	98.743	Depositor
Average voxel value	122.468	Depositor
Voxel value standard deviation	7.227	Depositor
Recommended contour level	126.3	Depositor
Tomogram size (Å)	492.8, 354.816, 492.8	wwPDB
Tomogram dimensions	50, 36, 50	wwPDB
Tomogram angles (°)	90.0, 90.0, 90.0	wwPDB
Grid spacing (Å)	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	0.59	1/18472 (0.0%)	0.82	12/24968 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2872	GLU	CG-CD	7.51	1.63	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1741	LEU	CB-CG-CD1	8.43	125.33	111.00
1	A	1973	LEU	CB-CG-CD1	-7.36	98.48	111.00
1	A	2872	GLU	OE1-CD-OE2	-7.28	114.56	123.30
1	A	2866	LEU	CA-CB-CG	6.14	129.43	115.30
1	A	1769	LEU	CA-CB-CG	6.05	129.21	115.30
1	A	2866	LEU	CB-CG-CD1	6.04	121.28	111.00
1	A	2012	LEU	CA-CB-CG	5.82	128.68	115.30
1	A	3577	MET	CG-SD-CE	5.71	109.34	100.20
1	A	1611	LEU	CB-CG-CD2	-5.42	101.79	111.00
1	A	1776	LEU	CB-CG-CD1	-5.27	102.04	111.00
1	A	1769	LEU	CB-CG-CD1	5.25	119.92	111.00
1	A	1917	ARG	NE-CZ-NH2	-5.09	117.75	120.30

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	18105	0	18146	780	0
All	All	18105	0	18146	780	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 (780) 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	1.20
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:1992:LYS:HG3	1:A:2024:SER:HB2	1.17	1.13
1:A:3525:ILE:HD11	1:A:3646:ILE:HG22	1.25	1.13
1:A:2141:ILE:HD12	1:A:2146:LYS:HE2	1.20	1.13
1:A:2707:VAL:HB	1:A:2712:LEU:HD11	1.19	1.11
1:A:3777:VAL:HG11	1:A:3895:PHE:HE1	1.07	1.10
1:A:2380:LEU:HD13	1:A:2390:ILE:HD11	1.34	1.08
1:A:2111:LYS:HD3	1:A:2161:GLU:HG3	1.18	1.08
1:A:2107:LYS:HE3	1:A:2495:ASP:OD2	1.51	1.08
1:A:3024:LEU:HD11	1:A:3303:LYS:HG3	1.31	1.08
1:A:3530:PHE:CD1	1:A:3618:TYR:HD2	1.71	1.08
1:A:1645:PHE:HB3	1:A:1765:ILE:HG22	1.34	1.07
1:A:2380:LEU:HD22	1:A:2384:GLU:OE1	1.54	1.07
1:A:2494:LEU:HD13	1:A:2498:GLY:CA	1.85	1.07
1:A:3303:LYS:HA	1:A:3306:TRP:CD1	1.90	1.07
1:A:2920:TRP:HB2	1:A:2989:PRO:HG3	1.06	1.06
1:A:2488:GLU:HB3	1:A:2491:LEU:HD12	1.36	1.05
1:A:1992:LYS:CG	1:A:2024:SER:HB2	1.86	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1823:ASP:HB2	1:A:1852:ARG:O	1.56	1.05
1:A:2494:LEU:CD1	1:A:2498:GLY:HA2	1.85	1.05
1:A:1645:PHE:HB3	1:A:1765:ILE:CG2	1.86	1.04
1:A:2988:SER:HB3	1:A:2989:PRO:HD2	1.04	1.04
1:A:2707:VAL:CB	1:A:2712:LEU:HD11	1.89	1.03
1:A:1983:LEU:HD22	1:A:1997:SER:OG	1.58	1.02
1:A:2988:SER:HB3	1:A:2989:PRO:CD	1.90	1.02
1:A:2386:MET:HB2	1:A:2627:ARG:HD3	1.42	1.01
1:A:2448:ASP:HB2	1:A:2829:GLU:OE2	1.59	1.00
1:A:1822:CYS:HB2	1:A:1853:LEU:HD21	1.43	1.00
1:A:2476:LYS:CD	1:A:2476:LYS:H	1.74	1.00
1:A:3777:VAL:CG1	1:A:3895:PHE:HE1	1.74	0.99
1:A:3534:LEU:HD12	1:A:3618:TYR:HE2	1.24	0.98
1:A:2380:LEU:CD1	1:A:2390:ILE:HD11	1.93	0.98
1:A:1620:PHE:CD1	1:A:1760:PHE:CZ	2.50	0.98
1:A:3534:LEU:CD1	1:A:3618:TYR:CE2	2.45	0.98
1:A:3303:LYS:O	1:A:3306:TRP:HD1	1.43	0.98
1:A:3777:VAL:HG11	1:A:3895:PHE:CE1	1.97	0.97
1:A:3406:PHE:HB2	1:A:3513:VAL:CG1	1.94	0.97
1:A:1802:LYS:HG2	1:A:1921:MET:HG3	1.47	0.96
1:A:2476:LYS:H	1:A:2476:LYS:HD3	1.26	0.95
1:A:2064:GLN:OE1	1:A:2091:MET:HE1	1.66	0.95
1:A:1970:LEU:HD13	1:A:1974:LYS:HE3	1.46	0.94
1:A:3024:LEU:CD1	1:A:3303:LYS:HG3	1.96	0.94
1:A:3534:LEU:HD12	1:A:3618:TYR:CE2	2.01	0.94
1:A:2787:HIS:HA	1:A:3460:PRO:HD2	1.49	0.94
1:A:2988:SER:CB	1:A:2989:PRO:HD2	1.97	0.94
1:A:2386:MET:CB	1:A:2627:ARG:HD3	1.95	0.94
1:A:3460:PRO:O	1:A:3463:SER:HB2	1.67	0.94
1:A:4065:LEU:HD11	1:A:4070:ILE:HD11	1.48	0.94
1:A:1645:PHE:CB	1:A:1765:ILE:HG22	1.96	0.93
1:A:3509:LEU:CD1	1:A:3513:VAL:HG21	1.98	0.93
1:A:3530:PHE:CD1	1:A:3618:TYR:CD2	2.56	0.93
1:A:1620:PHE:HD1	1:A:1760:PHE:HZ	1.07	0.93
1:A:4033:LEU:HD11	1:A:4035:GLN:HB2	1.47	0.92
1:A:2563:SER:HB3	1:A:2566:SER:H	1.35	0.92
1:A:2111:LYS:HD3	1:A:2161:GLU:CG	2.00	0.91
1:A:2400:HIS:CD2	1:A:2559:LEU:HD13	2.06	0.91
1:A:2137:VAL:O	1:A:2141:ILE:HG23	1.69	0.91
1:A:2400:HIS:NE2	1:A:2559:LEU:HD13	1.86	0.90
1:A:3737:THR:HB	1:A:3740:THR:OG1	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1992:LYS:HE2	1:A:2024:SER:O	1.71	0.90
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:2787:HIS:HA	1:A:3460:PRO:CD	2.03	0.89
1:A:2446:SER:H	1:A:2449:THR:CG2	1.86	0.89
1:A:4033:LEU:HD13	1:A:4035:GLN:HB2	1.54	0.88
1:A:3946:VAL:HG12	1:A:3950:PHE:O	1.72	0.88
1:A:2446:SER:H	1:A:2449:THR:HG23	1.39	0.88
1:A:1726:LEU:HD12	1:A:3984:GLN:HB3	1.55	0.88
1:A:2787:HIS:HA	1:A:3460:PRO:CG	2.02	0.88
1:A:1866:GLN:OE1	1:A:1911:ASN:HB2	1.73	0.88
1:A:1924:PRO:HB2	1:A:1929:ILE:HD11	1.56	0.88
1:A:1562:MET:HB3	1:A:1569:ILE:HD11	1.55	0.87
1:A:2064:GLN:NE2	1:A:2091:MET:SD	2.47	0.87
1:A:2920:TRP:HB2	1:A:2989:PRO:CG	1.99	0.87
1:A:3303:LYS:O	1:A:3306:TRP:CD1	2.28	0.86
1:A:3534:LEU:HD13	1:A:3618:TYR:HE2	1.39	0.86
1:A:1649:LEU:HD11	1:A:1704:GLU:HG3	1.57	0.86
1:A:2787:HIS:HA	1:A:3460:PRO:HG2	1.56	0.85
1:A:2112:GLU:HB3	1:A:2117:SER:HB2	1.57	0.85
1:A:2494:LEU:HD13	1:A:2498:GLY:HA2	0.94	0.85
1:A:2141:ILE:CD1	1:A:2146:LYS:HE2	2.06	0.85
1:A:1940:GLU:HB2	1:A:1989:GLU:O	1.77	0.84
1:A:3024:LEU:HD11	1:A:3303:LYS:CG	2.07	0.84
1:A:3656:VAL:HG13	1:A:3677:LEU:HB3	1.59	0.84
1:A:2131:THR:HG22	1:A:2176:LEU:HD21	1.59	0.84
1:A:2106:THR:OG1	1:A:2154:PHE:HB3	1.78	0.84
1:A:2274:HIS:HE1	1:A:2326:LEU:O	1.61	0.84
1:A:2766:LYS:HE2	1:A:2890:THR:HB	1.58	0.84
1:A:2336:ARG:HD3	1:A:2355:ASP:OD2	1.77	0.84
1:A:2745:ILE:HG23	1:A:2756:MET:HE1	1.57	0.83
1:A:1649:LEU:CD1	1:A:1704:GLU:HG3	2.08	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:2920:TRP:CB	1:A:2989:PRO:HG3	2.01	0.82
1:A:2111:LYS:NZ	1:A:2161:GLU:HG2	1.94	0.82
1:A:2755:HIS:HB2	1:A:2911:ARG:O	1.79	0.82
1:A:1604:ALA:HA	1:A:1607:TRP:NE1	1.95	0.81
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:3923:VAL:HG23	1:A:4038:GLU:HA	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3645:SER:HB3	1:A:3890:GLN:HE21	1.45	0.81
1:A:3303:LYS:C	1:A:3306:TRP:HD1	1.84	0.80
1:A:3799:LYS:O	1:A:3803:LEU:HG	1.82	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:2332:GLY:HA2	1:A:2335:GLN:HB2	1.62	0.80
1:A:2476:LYS:NZ	1:A:2528:ARG:HD2	1.97	0.80
1:A:2064:GLN:OE1	1:A:2091:MET:CE	2.29	0.80
1:A:4033:LEU:CD1	1:A:4035:GLN:CB	2.60	0.79
1:A:3303:LYS:CA	1:A:3306:TRP:CD1	2.66	0.79
1:A:3530:PHE:HD1	1:A:3618:TYR:HD2	1.31	0.79
1:A:1604:ALA:HA	1:A:1607:TRP:CD1	2.18	0.78
1:A:1956:LEU:HB3	1:A:1968:PHE:CE2	2.18	0.78
1:A:1970:LEU:HD12	1:A:1971:ARG:N	1.99	0.78
1:A:3509:LEU:HD12	1:A:3513:VAL:CG2	2.13	0.78
1:A:2181:GLY:O	1:A:2182:GLU:HG3	1.83	0.78
1:A:2707:VAL:CG1	1:A:2712:LEU:CD1	2.61	0.77
1:A:2064:GLN:OE1	1:A:2151:TRP:HH2	1.67	0.77
1:A:2476:LYS:HG2	1:A:2478:ASP:O	1.85	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:2107:LYS:HE2	1:A:2499:SER:HB3	1.67	0.76
1:A:3534:LEU:HD11	1:A:3614:LEU:HD23	1.67	0.76
1:A:3816:LEU:HD23	1:A:3847:SER:OG	1.86	0.76
1:A:1939:PHE:HD2	1:A:1940:GLU:O	1.67	0.76
1:A:3525:ILE:CD1	1:A:3646:ILE:HG22	2.13	0.76
1:A:2563:SER:HB2	1:A:2566:SER:OG	1.86	0.75
1:A:1620:PHE:CD1	1:A:1760:PHE:HZ	1.96	0.75
1:A:3939:ILE:HG13	1:A:4010:LEU:CD2	2.16	0.75
1:A:2745:ILE:HG23	1:A:2756:MET:CE	2.17	0.75
1:A:3946:VAL:CG1	1:A:3950:PHE:O	2.34	0.75
1:A:2411:LYS:HG2	1:A:2530:HIS:HE1	1.51	0.74
1:A:1569:ILE:HA	1:A:1584:SER:HA	1.70	0.74
1:A:2176:LEU:O	1:A:2183:ARG:HA	1.88	0.73
1:A:3406:PHE:HB2	1:A:3513:VAL:HG11	1.69	0.73
1:A:3406:PHE:HB2	1:A:3513:VAL:HG12	1.69	0.73
1:A:1744:LEU:HA	1:A:1760:PHE:CE2	2.23	0.73
1:A:2707:VAL:CG1	1:A:2712:LEU:HD11	2.18	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	0.73
1:A:1956:LEU:HB3	1:A:1968:PHE:HE2	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2112:GLU:HB3	1:A:2117:SER:CB	2.19	0.73
1:A:3871:PHE:CZ	1:A:3873:MET:HB2	2.22	0.73
1:A:2707:VAL:HB	1:A:2712:LEU:CD1	2.09	0.73
1:A:1822:CYS:SG	1:A:1850:PHE:HA	2.29	0.72
1:A:1940:GLU:HG3	1:A:1941:ASP:H	1.52	0.72
1:A:1645:PHE:CB	1:A:1765:ILE:CG2	2.61	0.72
1:A:1849:GLU:HG2	1:A:1899:ASN:HD22	1.53	0.72
1:A:1983:LEU:HD21	1:A:2000:ARG:HD2	1.69	0.72
1:A:3566:LEU:HA	1:A:3583:LEU:CD2	2.18	0.72
1:A:2787:HIS:CA	1:A:3460:PRO:HD2	2.20	0.72
1:A:2111:LYS:HZ2	1:A:2161:GLU:HG2	1.51	0.72
1:A:3618:TYR:N	1:A:3618:TYR:CD1	2.54	0.71
1:A:3303:LYS:CA	1:A:3306:TRP:HD1	2.02	0.71
1:A:3525:ILE:HD11	1:A:3646:ILE:CG2	2.15	0.71
1:A:3774:ILE:O	1:A:3778:VAL:HG23	1.91	0.71
1:A:3777:VAL:CG1	1:A:3895:PHE:CE1	2.63	0.71
1:A:3530:PHE:HD1	1:A:3618:TYR:CD2	2.04	0.70
1:A:3792:ARG:HB2	1:A:3955:TYR:CD1	2.26	0.70
1:A:1774:LEU:HD21	1:A:1922:LYS:O	1.91	0.70
1:A:2175:ILE:HG12	1:A:2183:ARG:HB3	1.74	0.70
1:A:2960:THR:HB	1:A:2963:ASP:HB2	1.73	0.70
1:A:3645:SER:HB3	1:A:3890:GLN:NE2	2.06	0.70
1:A:1612:ASP:HA	1:A:1615:ILE:CD1	2.21	0.70
1:A:3871:PHE:HZ	1:A:3873:MET:HB2	1.56	0.70
1:A:2125:TRP:CZ2	1:A:2178:LEU:HD13	2.28	0.69
1:A:2514:GLY:O	1:A:2523:TRP:CH2	2.45	0.69
1:A:3305:ARG:O	1:A:3307:LEU:N	2.24	0.69
1:A:4033:LEU:HD13	1:A:4035:GLN:CB	2.21	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:2003:LEU:HA	1:A:2006:LEU:HD12	1.74	0.69
1:A:1970:LEU:HD13	1:A:1974:LYS:CE	2.20	0.68
1:A:2386:MET:HB3	1:A:2627:ARG:HD3	1.75	0.68
1:A:1967:HIS:C	1:A:1968:PHE:HD1	1.97	0.68
1:A:3848:LEU:HD21	1:A:3852:LYS:HE3	1.75	0.68
1:A:1646:GLN:NE2	1:A:1758:TYR:OH	2.26	0.68
1:A:3785:TYR:HE2	1:A:3859:VAL:HG22	1.57	0.68
1:A:3979:ASN:O	1:A:3981:PRO:HD2	1.92	0.68
1:A:1995:VAL:HG21	1:A:2024:SER:HB3	1.74	0.68
1:A:3509:LEU:HD12	1:A:3513:VAL:HG21	1.75	0.68
1:A:2294:LEU:HB3	1:A:2317:LEU:HD22	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3509:LEU:CD1	1:A:3513:VAL:CG2	2.68	0.68
1:A:3837:GLY:O	1:A:3871:PHE:HD1	1.77	0.68
1:A:2285:GLU:HB2	1:A:2412:ARG:NH2	2.08	0.68
1:A:2293:HIS:CE1	1:A:2409:ASN:HB3	2.29	0.68
1:A:3850:TRP:NE1	1:A:3854:TYR:HB3	2.08	0.68
1:A:2252:LEU:HD21	1:A:2310:LEU:HD23	1.76	0.68
1:A:3566:LEU:HA	1:A:3583:LEU:HD21	1.76	0.68
1:A:2745:ILE:HG12	1:A:2756:MET:HE3	1.76	0.68
1:A:3509:LEU:HD11	1:A:3513:VAL:HG21	1.76	0.67
1:A:1983:LEU:HB3	1:A:1993:THR:HG23	1.75	0.67
1:A:2107:LYS:CE	1:A:2495:ASP:OD2	2.37	0.67
1:A:2419:PRO:O	1:A:2424:LYS:HE3	1.93	0.67
1:A:2080:LYS:HG2	1:A:2215:PHE:CE1	2.30	0.67
1:A:1698:ILE:O	1:A:1702:LEU:HG	1.94	0.67
1:A:2305:LEU:HD11	1:A:2368:PHE:CG	2.29	0.67
1:A:1744:LEU:HA	1:A:1760:PHE:CD2	2.29	0.67
1:A:2476:LYS:HZ1	1:A:2528:ARG:HD2	1.59	0.67
1:A:2293:HIS:NE2	1:A:2409:ASN:HB3	2.09	0.67
1:A:2493:LYS:HG3	1:A:2494:LEU:H	1.60	0.67
1:A:1630:ILE:HA	1:A:1634:THR:HG22	1.75	0.67
1:A:3998:ILE:HG21	1:A:4004:LEU:HG	1.77	0.66
1:A:3935:PHE:HB2	1:A:4014:VAL:HG11	1.76	0.66
1:A:1822:CYS:SG	1:A:1849:GLU:O	2.53	0.66
1:A:3473:ALA:HB3	1:A:3476:ARG:O	1.96	0.66
1:A:1626:CYS:SG	1:A:1639:VAL:HG11	2.35	0.66
1:A:1703:VAL:HG13	1:A:1770:ILE:HD13	1.78	0.66
1:A:2631:THR:O	1:A:2635:THR:HG22	1.96	0.66
1:A:3979:ASN:C	1:A:3981:PRO:HD2	2.16	0.66
1:A:2141:ILE:HD12	1:A:2146:LYS:CE	2.12	0.66
1:A:2220:CYS:SG	1:A:2224:SER:HB2	2.36	0.65
1:A:2495:ASP:O	1:A:2498:GLY:N	2.30	0.65
1:A:1645:PHE:CG	1:A:1765:ILE:HG22	2.32	0.65
1:A:2707:VAL:CG1	1:A:2712:LEU:HD12	2.26	0.65
1:A:3819:ILE:O	1:A:3823:ASN:HB2	1.96	0.65
1:A:2448:ASP:HB2	1:A:2829:GLU:CD	2.17	0.65
1:A:3566:LEU:CD1	1:A:3570:LEU:HD11	2.26	0.65
1:A:2290:LEU:HD13	1:A:2407:LEU:HD23	1.79	0.65
1:A:2382:ALA:O	1:A:2385:VAL:HG12	1.96	0.65
1:A:3566:LEU:O	1:A:3570:LEU:HG	1.97	0.65
1:A:1706:LEU:CD2	1:A:1935:GLN:HG2	2.27	0.65
1:A:2842:ASP:O	1:A:2845:GLN:HG2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2512:LYS:O	1:A:2513:GLN:HB2	1.97	0.65
1:A:2514:GLY:HA3	1:A:2523:TRP:CZ2	2.32	0.65
1:A:2095:ASP:CG	1:A:2149:ARG:NH2	2.50	0.64
1:A:2779:LEU:HD23	1:A:2812:ARG:O	1.98	0.64
1:A:3459:ASP:OD2	1:A:3461:ILE:HG12	1.97	0.64
1:A:3618:TYR:N	1:A:3618:TYR:HD1	1.94	0.64
1:A:3998:ILE:CG2	1:A:4004:LEU:HG	2.27	0.64
1:A:1826:PHE:HE1	1:A:1853:LEU:HD22	1.62	0.64
1:A:2285:GLU:HB2	1:A:2412:ARG:HH22	1.62	0.64
1:A:3566:LEU:HD13	1:A:3570:LEU:CD1	2.27	0.64
1:A:1612:ASP:HA	1:A:1615:ILE:HD11	1.78	0.64
1:A:1938:GLY:O	1:A:1989:GLU:HB3	1.98	0.64
1:A:2728:LEU:HD12	1:A:2771:ARG:CZ	2.27	0.64
1:A:2315:THR:HG21	1:A:2350:SER:HB3	1.80	0.64
1:A:3010:LEU:HD21	1:A:3317:SER:HB3	1.79	0.64
1:A:3737:THR:OG1	1:A:3740:THR:HB	1.98	0.63
1:A:1953:LEU:CD1	1:A:1973:LEU:HB3	2.27	0.63
1:A:3303:LYS:HD2	1:A:3306:TRP:CD1	2.33	0.63
1:A:1970:LEU:CD1	1:A:1974:LYS:HE3	2.24	0.63
1:A:1738:ASN:O	1:A:1739:ASP:OD1	2.16	0.63
1:A:3641:PHE:HA	1:A:3889:LEU:HD21	1.81	0.63
1:A:1995:VAL:HG22	1:A:2022:PHE:CE2	2.33	0.63
1:A:2222:ILE:HG23	1:A:2284:LEU:HD11	1.79	0.63
1:A:1827:ASP:HB3	1:A:1830:VAL:HG12	1.81	0.63
1:A:2563:SER:CB	1:A:2566:SER:OG	2.47	0.63
1:A:1991:GLU:O	1:A:1995:VAL:HG23	1.99	0.62
1:A:3785:TYR:CE2	1:A:3859:VAL:HG22	2.33	0.62
1:A:2282:ASN:HB3	1:A:2552:ARG:HG3	1.82	0.62
1:A:3792:ARG:HB2	1:A:3955:TYR:CE1	2.34	0.62
1:A:1748:PHE:CD2	1:A:1755:LEU:HD22	2.34	0.62
1:A:2536:ASN:HB2	1:A:2543:ARG:HE	1.64	0.62
1:A:3307:LEU:HA	1:A:3310:THR:HB	1.81	0.62
1:A:3583:LEU:O	1:A:3587:LEU:HG	2.00	0.62
1:A:1562:MET:CB	1:A:1569:ILE:HD11	2.29	0.62
1:A:1967:HIS:O	1:A:1968:PHE:HD1	1.82	0.62
1:A:1992:LYS:HG3	1:A:2024:SER:CB	2.11	0.62
1:A:2632:ALA:HB3	1:A:2647:LEU:HD21	1.80	0.62
1:A:1996:GLU:O	1:A:2000:ARG:HG3	2.00	0.62
1:A:2386:MET:CB	1:A:2627:ARG:CD	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1826:PHE:CE1	1:A:1853:LEU:HD22	2.35	0.61
1:A:2394:THR:H	1:A:2397:THR:HB	1.64	0.61
1:A:3912:GLY:O	1:A:3915:PHE:CE2	2.53	0.61
1:A:3409:ASP:HB3	1:A:3518:PHE:HB2	1.81	0.61
1:A:3700:MET:HB3	1:A:4085:THR:HG21	1.81	0.61
1:A:3330:TYR:CE2	1:A:3346:LEU:HD13	2.36	0.61
1:A:1726:LEU:CD1	1:A:3984:GLN:HB3	2.30	0.61
1:A:1574:PHE:HB3	1:A:1576:GLU:H	1.65	0.61
1:A:1692:ASP:O	1:A:1695:LYS:HB3	2.00	0.61
1:A:1851:ASN:HD21	1:A:1899:ASN:HB2	1.66	0.60
1:A:1630:ILE:CG2	1:A:1655:MET:SD	2.89	0.60
1:A:2151:TRP:HE3	1:A:2193:LEU:HD11	1.64	0.60
1:A:2677:VAL:HG11	1:A:2686:LEU:HD21	1.83	0.60
1:A:2427:ILE:HD12	1:A:2559:LEU:CD2	2.31	0.60
1:A:1900:PRO:HB3	1:A:1905:ARG:HA	1.83	0.60
1:A:2332:GLY:HA2	1:A:2335:GLN:CB	2.31	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:1620:PHE:HA	1:A:1760:PHE:CE1	2.37	0.60
1:A:1983:LEU:HD21	1:A:2000:ARG:CD	2.31	0.60
1:A:3886:ALA:N	1:A:3887:PRO:HD2	2.16	0.60
1:A:1656:TRP:O	1:A:1660:VAL:HG12	2.01	0.60
1:A:2640:THR:HG23	1:A:2643:SER:H	1.66	0.60
1:A:2755:HIS:NE2	1:A:2835:LEU:HG	2.17	0.60
1:A:2293:HIS:CE1	1:A:2409:ASN:CB	2.84	0.60
1:A:2941:THR:HG22	1:A:2942:ASP:H	1.67	0.60
1:A:4065:LEU:HD11	1:A:4070:ILE:CD1	2.28	0.59
1:A:3618:TYR:O	1:A:3622:GLY:N	2.34	0.59
1:A:2380:LEU:HD11	1:A:2390:ILE:HD11	1.83	0.59
1:A:2728:LEU:HD12	1:A:2771:ARG:NH2	2.17	0.59
1:A:3303:LYS:HA	1:A:3306:TRP:HE1	1.67	0.59
1:A:3429:LEU:HD21	1:A:3439:ARG:HB3	1.83	0.59
1:A:3948:HIS:NE2	1:A:4072:ASN:CG	2.55	0.59
1:A:2476:LYS:CD	1:A:2476:LYS:N	2.52	0.59
1:A:1940:GLU:HG3	1:A:1941:ASP:N	2.18	0.59
1:A:2071:ILE:HB	1:A:2212:LEU:HD12	1.85	0.59
1:A:2034:ILE:HD12	1:A:2061:TYR:CZ	2.38	0.59
1:A:2155:ASP:OD1	1:A:2549:ARG:NH2	2.35	0.58
1:A:2339:ILE:HG23	1:A:2353:LEU:HB3	1.83	0.58
1:A:3541:MET:HA	1:A:3544:LYS:HG2	1.83	0.58
1:A:3737:THR:HB	1:A:3740:THR:CB	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4024:VAL:HG11	1:A:4062:TRP:CD2	2.38	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:2489:ILE:HG22	1:A:2535:CYS:HB3	1.84	0.58
1:A:2081:THR:O	1:A:2085:LYS:HB2	2.02	0.58
1:A:3945:LEU:O	1:A:3948:HIS:O	2.21	0.58
1:A:2476:LYS:HD3	1:A:2476:LYS:N	2.09	0.58
1:A:4033:LEU:HD12	1:A:4035:GLN:N	2.18	0.58
1:A:1559:SER:HB3	1:A:1572:ILE:HG22	1.86	0.58
1:A:1779:PHE:O	1:A:1783:THR:HG22	2.03	0.58
1:A:3555:TYR:HE1	1:A:3593:GLU:HG2	1.68	0.58
1:A:3810:SER:O	1:A:3838:TRP:HB2	2.03	0.58
1:A:1984:ILE:HG21	1:A:1989:GLU:HG3	1.84	0.58
1:A:2201:HIS:NE2	1:A:2497:TYR:O	2.37	0.58
1:A:2419:PRO:O	1:A:2424:LYS:CE	2.52	0.58
1:A:3592:LYS:O	1:A:3596:ASN:HB2	2.03	0.58
1:A:2446:SER:H	1:A:2449:THR:HG21	1.67	0.58
1:A:2354:SER:OG	1:A:2357:SER:HB2	2.02	0.58
1:A:2437:LEU:H	1:A:2437:LEU:HD12	1.69	0.58
1:A:2787:HIS:CA	1:A:3460:PRO:HG2	2.32	0.58
1:A:3851:VAL:HG13	1:A:3855:LEU:HD23	1.84	0.58
1:A:4021:LEU:HD23	1:A:4023:ILE:HG13	1.85	0.58
1:A:3537:GLU:OE1	1:A:3618:TYR:OH	2.21	0.58
1:A:2476:LYS:HZ2	1:A:2528:ARG:HD2	1.68	0.57
1:A:3519:VAL:HG13	1:A:3521:ASN:ND2	2.19	0.57
1:A:2380:LEU:HD13	1:A:2390:ILE:CD1	2.23	0.57
1:A:2808:LEU:HD21	1:A:2856:LEU:HD12	1.86	0.57
1:A:2938:MET:SD	1:A:3321:ILE:HG21	2.45	0.57
1:A:3912:GLY:O	1:A:3915:PHE:CZ	2.57	0.57
1:A:1704:GLU:OE2	1:A:1768:ARG:NH1	2.37	0.57
1:A:2131:THR:HG22	1:A:2176:LEU:CD2	2.34	0.57
1:A:2784:PRO:HG2	1:A:2817:ILE:HD13	1.84	0.57
1:A:2846:GLY:O	1:A:2849:TYR:HB3	2.04	0.57
1:A:2111:LYS:CD	1:A:2161:GLU:HG3	2.13	0.57
1:A:2336:ARG:CD	1:A:2355:ASP:OD2	2.51	0.57
1:A:1781:THR:HG21	1:A:1919:PHE:CD1	2.39	0.57
1:A:4037:SER:HB3	1:A:4040:GLU:HB3	1.87	0.57
1:A:1939:PHE:O	1:A:1940:GLU:HB3	2.05	0.57
1:A:1706:LEU:HD21	1:A:1935:GLN:HG2	1.86	0.57
1:A:3939:ILE:HG13	1:A:4010:LEU:HD22	1.86	0.57
1:A:4017:GLY:HA3	1:A:4021:LEU:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1911:ASN:OD1	1:A:1912:LEU:N	2.38	0.57
1:A:4022:GLN:O	1:A:4022:GLN:HG2	2.05	0.57
1:A:1619:VAL:HG12	1:A:1760:PHE:HD1	1.70	0.56
1:A:1965:HIS:HD2	1:A:2212:LEU:CD2	2.18	0.56
1:A:3631:MET:CE	1:A:3698:MET:HG3	2.36	0.56
1:A:1940:GLU:CB	1:A:1989:GLU:O	2.51	0.56
1:A:2627:ARG:NH1	1:A:2630:TYR:CE2	2.74	0.56
1:A:3538:ASN:HB3	1:A:3541:MET:HG2	1.87	0.56
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:2127:ASP:O	1:A:2131:THR:OG1	2.23	0.56
1:A:2137:VAL:O	1:A:2141:ILE:CG2	2.50	0.56
1:A:2868:ASP:HB2	1:A:2872:GLU:OE1	2.06	0.56
1:A:3839:ILE:HG23	1:A:3873:MET:HG3	1.86	0.56
1:A:1852:ARG:O	1:A:1852:ARG:HG3	2.06	0.56
1:A:2220:CYS:SG	1:A:2224:SER:CB	2.94	0.56
1:A:2305:LEU:HD11	1:A:2368:PHE:CD1	2.41	0.55
1:A:2514:GLY:C	1:A:2523:TRP:CH2	2.80	0.55
1:A:2386:MET:HB3	1:A:2627:ARG:CD	2.36	0.55
1:A:2707:VAL:HG12	1:A:2712:LEU:CD1	2.37	0.55
1:A:2106:THR:HG1	1:A:2154:PHE:HB3	1.71	0.55
1:A:3440:LEU:HD23	1:A:3462:ILE:HD12	1.88	0.55
1:A:2151:TRP:CE3	1:A:2193:LEU:HD11	2.41	0.55
1:A:2786:ILE:O	1:A:3460:PRO:HB2	2.07	0.55
1:A:1627:LEU:HD11	1:A:1631:LYS:HE3	1.89	0.55
1:A:1983:LEU:HB3	1:A:1993:THR:CG2	2.36	0.55
1:A:2410:SER:O	1:A:2411:LYS:HB2	2.06	0.55
1:A:3683:TYR:O	1:A:3687:SER:HB2	2.07	0.55
1:A:2788:ARG:HG3	1:A:3459:ASP:HA	1.89	0.55
1:A:2064:GLN:CD	1:A:2091:MET:CE	2.75	0.54
1:A:2707:VAL:HG12	1:A:2712:LEU:HD12	1.89	0.54
1:A:1823:ASP:HB2	1:A:1853:LEU:HD23	1.88	0.54
1:A:2002:ILE:HB	1:A:2014:PHE:CE2	2.42	0.54
1:A:2563:SER:CB	1:A:2566:SER:H	2.15	0.54
1:A:3877:CYS:SG	1:A:3884:LEU:CD2	2.96	0.54
1:A:2181:GLY:C	1:A:2182:GLU:HG3	2.27	0.54
1:A:4023:ILE:HD12	1:A:4029:ILE:HD11	1.87	0.54
1:A:4059:LEU:HA	1:A:4063:LEU:HD13	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:2064:GLN:OE1	1:A:2151:TRP:CH2	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2707:VAL:CB	1:A:2712:LEU:CD1	2.72	0.54
1:A:1849:GLU:CG	1:A:1899:ASN:ND2	2.70	0.54
1:A:1970:LEU:HD12	1:A:1970:LEU:C	2.28	0.54
1:A:1645:PHE:CZ	1:A:1649:LEU:HD22	2.43	0.54
1:A:2063:MET:HB3	1:A:2070:LEU:HD11	1.90	0.54
1:A:2305:LEU:CD1	1:A:2368:PHE:CD1	2.91	0.54
1:A:2002:ILE:HG22	1:A:2006:LEU:HD11	1.88	0.54
1:A:3566:LEU:HD13	1:A:3570:LEU:HD11	1.86	0.54
1:A:3703:PHE:CE1	1:A:3766:GLU:HG2	2.43	0.54
1:A:3509:LEU:HD12	1:A:3513:VAL:HG23	1.88	0.54
1:A:2336:ARG:HG2	1:A:2355:ASP:OD1	2.08	0.53
1:A:3440:LEU:CD2	1:A:3462:ILE:HD12	2.38	0.53
1:A:3817:GLY:H	1:A:3821:ASN:CB	2.21	0.53
1:A:2173:ASN:HB3	1:A:2175:ILE:HG22	1.90	0.53
1:A:3566:LEU:CA	1:A:3583:LEU:HD21	2.37	0.53
1:A:3612:ASP:O	1:A:3615:VAL:HG22	2.08	0.53
1:A:2786:ILE:HG12	1:A:2821:ASN:HA	1.90	0.53
1:A:2833:THR:HG21	1:A:2841:PRO:HD2	1.91	0.53
1:A:3547:ASP:HA	1:A:3550:LYS:HB3	1.91	0.53
1:A:2787:HIS:HB3	1:A:3461:ILE:HG23	1.91	0.53
1:A:3481:ILE:O	1:A:3483:ASP:N	2.36	0.53
1:A:1981:SER:HB3	1:A:1982:PRO:HD3	1.91	0.53
1:A:2450:THR:H	1:A:2453:HIS:CE1	2.27	0.53
1:A:1979:ASN:O	1:A:1983:LEU:HD13	2.09	0.53
1:A:2095:ASP:CG	1:A:2149:ARG:HH22	2.11	0.53
1:A:3656:VAL:CG1	1:A:3677:LEU:HB3	2.36	0.53
1:A:2201:HIS:CE1	1:A:2497:TYR:CA	2.91	0.53
1:A:2419:PRO:O	1:A:2424:LYS:NZ	2.42	0.52
1:A:1604:ALA:HA	1:A:1607:TRP:HE1	1.72	0.52
1:A:3946:VAL:HB	1:A:3947:PRO:HA	1.91	0.52
1:A:2788:ARG:HB2	1:A:3459:ASP:HB3	1.91	0.52
1:A:2795:PHE:CE2	1:A:2799:LEU:HD11	2.44	0.52
1:A:2012:LEU:HD13	1:A:2016:ASP:OD2	2.10	0.52
1:A:2339:ILE:HG12	1:A:2353:LEU:HD23	1.91	0.52
1:A:2488:GLU:CD	1:A:2491:LEU:HD11	2.29	0.52
1:A:1620:PHE:HA	1:A:1760:PHE:HE1	1.74	0.52
1:A:1822:CYS:SG	1:A:1849:GLU:C	2.88	0.52
1:A:2285:GLU:CB	1:A:2412:ARG:NH2	2.73	0.52
1:A:2462:THR:HG22	1:A:2476:LYS:HA	1.90	0.52
1:A:3017:VAL:HG21	1:A:3313:PHE:CE2	2.44	0.52
1:A:3692:LYS:HE3	1:A:3898:GLU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2578:ILE:HG21	1:A:2630:TYR:HB2	1.91	0.52
1:A:3911:TRP:HH2	1:A:3926:VAL:CG1	2.23	0.52
1:A:3951:SER:HB2	1:A:4002:LYS:HD2	1.91	0.52
1:A:1803:THR:HG21	1:A:1848:ASP:OD1	2.10	0.52
1:A:4021:LEU:HD23	1:A:4023:ILE:CG1	2.40	0.52
1:A:4065:LEU:HD12	1:A:4065:LEU:O	2.10	0.52
1:A:1939:PHE:HD1	1:A:1939:PHE:H	1.57	0.52
1:A:2115:TYR:OH	1:A:2162:TYR:O	2.23	0.52
1:A:2302:PHE:HA	1:A:2310:LEU:HD11	1.92	0.52
1:A:3995:GLY:HA2	1:A:3998:ILE:HD13	1.91	0.52
1:A:4034:LEU:HD23	1:A:4034:LEU:O	2.10	0.52
1:A:1650:LEU:HD11	1:A:1747:VAL:HG11	1.92	0.51
1:A:3854:TYR:O	1:A:3858:HIS:HB2	2.10	0.51
1:A:1606:GLU:O	1:A:1610:ILE:HG12	2.11	0.51
1:A:2102:TYR:HB2	1:A:2152:VAL:HG22	1.93	0.51
1:A:2494:LEU:HD12	1:A:2494:LEU:O	2.10	0.51
1:A:2645:ILE:CD1	1:A:2686:LEU:HG	2.40	0.51
1:A:1645:PHE:HB2	1:A:1697:LYS:HG3	1.91	0.51
1:A:3934:TRP:CB	1:A:4023:ILE:HD13	2.41	0.51
1:A:1707:HIS:O	1:A:1711:VAL:HG23	2.10	0.51
1:A:1926:SER:HA	1:A:1929:ILE:HD13	1.92	0.51
1:A:3737:THR:OG1	1:A:3740:THR:CB	2.59	0.51
1:A:2177:THR:HG22	1:A:2183:ARG:HG2	1.91	0.51
1:A:3839:ILE:CG2	1:A:3873:MET:HG3	2.41	0.51
1:A:3645:SER:CB	1:A:3890:GLN:HE21	2.19	0.51
1:A:3787:THR:HG22	1:A:3875:MET:HB2	1.93	0.51
1:A:1963:MET:HB3	1:A:1966:TYR:CD2	2.45	0.51
1:A:3877:CYS:SG	1:A:3884:LEU:HD22	2.50	0.51
1:A:1645:PHE:HZ	1:A:1768:ARG:HD2	1.75	0.51
1:A:2084:TRP:HE3	1:A:2088:ILE:HD12	1.76	0.50
1:A:2476:LYS:HZ2	1:A:2528:ARG:HB2	1.76	0.50
1:A:2400:HIS:NE2	1:A:2559:LEU:CD1	2.67	0.50
1:A:2476:LYS:H	1:A:2476:LYS:HD2	1.73	0.50
1:A:3845:GLN:OE1	1:A:3878:HIS:HB2	2.12	0.50
1:A:3855:LEU:HD12	1:A:3859:VAL:HG23	1.93	0.50
1:A:1749:ILE:HD13	1:A:1813:LEU:HD22	1.92	0.50
1:A:1849:GLU:CG	1:A:1899:ASN:HD22	2.22	0.50
1:A:2034:ILE:CD1	1:A:2061:TYR:CZ	2.95	0.50
1:A:2290:LEU:HD23	1:A:2321:SER:HA	1.92	0.50
1:A:2637:PRO:O	1:A:2639:GLN:NE2	2.44	0.50
1:A:3566:LEU:HD11	1:A:3570:LEU:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3645:SER:CB	1:A:3890:GLN:NE2	2.74	0.50
1:A:3737:THR:CB	1:A:3740:THR:CB	2.89	0.50
1:A:1917:ARG:HD2	1:A:3963:PHE:CE2	2.46	0.50
1:A:2034:ILE:CD1	1:A:2061:TYR:CE2	2.95	0.50
1:A:3350:LYS:HA	1:A:3353:LEU:HD12	1.94	0.50
1:A:3848:LEU:HD12	1:A:3884:LEU:HD12	1.93	0.50
1:A:1677:ASP:HA	1:A:1680:ILE:HD12	1.93	0.50
1:A:1706:LEU:HD22	1:A:1935:GLN:HG2	1.93	0.50
1:A:2111:LYS:CD	1:A:2161:GLU:CG	2.84	0.50
1:A:2654:ARG:HH22	1:A:2691:SER:HB2	1.77	0.50
1:A:3323:ASN:HD21	1:A:3361:ASP:H	1.58	0.50
1:A:2109:LEU:HD13	1:A:2129:LEU:HD23	1.94	0.50
1:A:1748:PHE:CE2	1:A:1755:LEU:HD22	2.47	0.50
1:A:2762:SER:O	1:A:2763:ARG:HB2	2.12	0.50
1:A:3725:VAL:HG22	1:A:3731:ASP:HA	1.93	0.50
1:A:2839:ASP:O	1:A:2841:PRO:HD3	2.12	0.49
1:A:2295:ILE:HG12	1:A:2314:ILE:HD12	1.93	0.49
1:A:3911:TRP:HH2	1:A:3926:VAL:HG12	1.77	0.49
1:A:4033:LEU:HD12	1:A:4036:GLN:H	1.77	0.49
1:A:2960:THR:HG22	1:A:2961:ILE:N	2.27	0.49
1:A:3978:ASN:O	1:A:3981:PRO:CD	2.60	0.49
1:A:1570:GLU:HB2	1:A:1585:VAL:HA	1.93	0.49
1:A:1983:LEU:HD21	1:A:2000:ARG:NE	2.27	0.49
1:A:2169:VAL:HG13	1:A:2186:ILE:HG12	1.94	0.49
1:A:2514:GLY:CA	1:A:2523:TRP:CZ2	2.96	0.49
1:A:3979:ASN:C	1:A:3981:PRO:CD	2.80	0.49
1:A:2780:LYS:HD3	1:A:2813:THR:HG22	1.93	0.49
1:A:2385:VAL:HG23	1:A:2574:TYR:HD1	1.77	0.49
1:A:3459:ASP:OD2	1:A:3461:ILE:CG1	2.61	0.49
1:A:2427:ILE:HD12	1:A:2559:LEU:HD22	1.93	0.49
1:A:2860:THR:HG22	1:A:2865:LEU:O	2.13	0.49
1:A:3946:VAL:HA	1:A:3947:PRO:C	2.33	0.49
1:A:1645:PHE:CD2	1:A:1765:ILE:HG22	2.48	0.49
1:A:2448:ASP:CB	1:A:2829:GLU:OE2	2.47	0.49
1:A:3307:LEU:O	1:A:3311:LYS:N	2.27	0.49
1:A:1657:THR:HG21	1:A:1734:PHE:O	2.12	0.49
1:A:1967:HIS:NE2	1:A:2204:PRO:HB3	2.28	0.49
1:A:3373:LEU:O	1:A:3373:LEU:HD23	2.13	0.48
1:A:3692:LYS:HE3	1:A:3898:GLU:O	2.12	0.48
1:A:2645:ILE:HD11	1:A:2686:LEU:HG	1.94	0.48
1:A:1626:CYS:HB2	1:A:1643:TYR:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1911:ASN:OD1	1:A:1912:LEU:HG	2.13	0.48
1:A:2064:GLN:NE2	1:A:2091:MET:CE	2.76	0.48
1:A:2828:LEU:HD13	1:A:2902:MET:SD	2.53	0.48
1:A:2982:VAL:HG12	1:A:2983:GLY:N	2.27	0.48
1:A:3566:LEU:HD13	1:A:3570:LEU:HD12	1.95	0.48
1:A:3671:VAL:O	1:A:3674:ILE:HG22	2.13	0.48
1:A:2354:SER:OG	1:A:2357:SER:CB	2.61	0.48
1:A:1849:GLU:OE2	1:A:1899:ASN:ND2	2.47	0.48
1:A:2364:ASP:O	1:A:2365:LYS:HG2	2.13	0.48
1:A:3462:ILE:O	1:A:3465:LEU:N	2.44	0.48
1:A:1626:CYS:SG	1:A:1639:VAL:CG1	3.01	0.48
1:A:1683:LEU:HB3	1:A:1702:LEU:HD21	1.96	0.48
1:A:1731:VAL:HG12	1:A:1732:GLN:N	2.29	0.48
1:A:2074:GLY:O	1:A:2197:ASP:HA	2.13	0.48
1:A:4065:LEU:HD12	1:A:4065:LEU:C	2.33	0.48
1:A:1664:LEU:HD23	1:A:1669:PHE:HZ	1.77	0.48
1:A:1826:PHE:CE1	1:A:1853:LEU:CD2	2.96	0.48
1:A:2002:ILE:HB	1:A:2014:PHE:HE2	1.78	0.48
1:A:2112:GLU:CB	1:A:2117:SER:HB2	2.35	0.48
1:A:3737:THR:CB	1:A:3740:THR:HB	2.44	0.48
1:A:4084:SER:O	1:A:4088:LEU:HG	2.14	0.48
1:A:1794:PHE:HD1	1:A:1802:LYS:HB3	1.79	0.48
1:A:3353:LEU:HD23	1:A:3358:VAL:HG11	1.95	0.48
1:A:3721:THR:O	1:A:3725:VAL:HG23	2.14	0.47
1:A:1636:ILE:O	1:A:1640:VAL:HG23	2.15	0.47
1:A:1844:TRP:CD1	1:A:1893:ALA:HB3	2.50	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:3541:MET:HB2	1:A:3607:PHE:HE1	1.78	0.47
1:A:1681:LYS:HE2	1:A:1939:PHE:CE1	2.50	0.47
1:A:2084:TRP:CZ3	1:A:2085:LYS:HG3	2.49	0.47
1:A:2105:ASP:OD2	1:A:2508:GLN:HB2	2.15	0.47
1:A:3967:TYR:HE2	1:A:3985:VAL:HA	1.80	0.47
1:A:2580:LYS:HG2	1:A:2586:ARG:HH22	1.79	0.47
1:A:3612:ASP:O	1:A:3615:VAL:CG2	2.63	0.47
1:A:3415:ILE:HD13	1:A:3453:GLN:HG3	1.97	0.47
1:A:2445:PHE:HA	1:A:2449:THR:HG21	1.97	0.47
1:A:3703:PHE:HE1	1:A:3766:GLU:HG2	1.79	0.47
1:A:3877:CYS:SG	1:A:3884:LEU:HD21	2.55	0.47
1:A:2835:LEU:HD23	1:A:2911:ARG:HB2	1.97	0.46
1:A:2878:VAL:HA	1:A:2881:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3807:SER:O	1:A:3808:LYS:HB2	2.16	0.46
1:A:2654:ARG:NH1	1:A:2658:ASP:OD1	2.49	0.46
1:A:3690:LEU:HD23	1:A:3694:PHE:HB3	1.96	0.46
1:A:3924:TRP:O	1:A:3927:TYR:HB3	2.15	0.46
1:A:2027:THR:HA	1:A:2028:PRO:HD3	1.47	0.46
1:A:3592:LYS:O	1:A:3596:ASN:N	2.48	0.46
1:A:3934:TRP:HB3	1:A:4023:ILE:HD13	1.97	0.46
1:A:2318:ILE:O	1:A:2322:LEU:HB2	2.16	0.46
1:A:3833:LYS:HZ3	1:A:3862:THR:HG21	1.81	0.46
1:A:3889:LEU:HG	1:A:3894:ARG:HD3	1.95	0.46
1:A:1554:HIS:O	1:A:1555:HIS:HB2	2.15	0.46
1:A:1683:LEU:HD22	1:A:1698:ILE:HG23	1.96	0.46
1:A:2125:TRP:CZ2	1:A:2178:LEU:CD1	2.97	0.46
1:A:2627:ARG:NH1	1:A:2630:TYR:CD2	2.84	0.46
1:A:1586:GLU:HG3	1:A:1765:ILE:H	1.81	0.46
1:A:3303:LYS:C	1:A:3306:TRP:CD1	2.74	0.46
1:A:1995:VAL:HG22	1:A:2022:PHE:HE2	1.80	0.46
1:A:2286:THR:HA	1:A:2412:ARG:NE	2.31	0.46
1:A:1660:VAL:HG13	1:A:1728:TRP:CH2	2.51	0.46
1:A:1945:LEU:HD13	1:A:1994:VAL:HG21	1.98	0.46
1:A:1748:PHE:HD2	1:A:1755:LEU:HD22	1.77	0.46
1:A:2274:HIS:CE1	1:A:2326:LEU:O	2.54	0.46
1:A:2571:TYR:HA	1:A:2574:TYR:HB2	1.97	0.46
1:A:3631:MET:HE1	1:A:3698:MET:HG3	1.98	0.45
1:A:1968:PHE:N	1:A:1968:PHE:CD1	2.84	0.45
1:A:3760:LEU:HD21	1:A:4078:ALA:HA	1.99	0.45
1:A:3995:GLY:HA2	1:A:3998:ILE:CD1	2.46	0.45
1:A:1992:LYS:CG	1:A:2024:SER:CB	2.78	0.45
1:A:2199:LEU:O	1:A:2201:HIS:N	2.49	0.45
1:A:2422:SER:H	1:A:2424:LYS:HZ1	1.65	0.45
1:A:2783:GLN:HG2	1:A:2816:ILE:HB	1.99	0.45
1:A:3809:GLU:HB3	1:A:3810:SER:H	1.53	0.45
1:A:2112:GLU:HB3	1:A:2117:SER:OG	2.16	0.45
1:A:1910:GLU:HB2	1:A:3846:MET:HA	1.98	0.45
1:A:2280:THR:HA	1:A:2283:LYS:HD2	1.99	0.45
1:A:2204:PRO:HA	1:A:2207:ILE:HD12	1.97	0.45
1:A:2358:THR:CG2	1:A:2359:ILE:N	2.80	0.45
1:A:3308:ASN:O	1:A:3312:GLN:HB2	2.16	0.45
1:A:3509:LEU:CG	1:A:3513:VAL:HG21	2.45	0.45
1:A:3579:GLU:O	1:A:3582:GLU:N	2.43	0.45
1:A:2984:VAL:C	1:A:2986:PRO:HD3	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3338:ASN:H	1:A:3341:GLU:HB2	1.82	0.45
1:A:1759:LYS:HE3	1:A:1761:GLU:OE2	2.17	0.45
1:A:1953:LEU:HD11	1:A:1973:LEU:HB3	1.98	0.45
1:A:2417:CYS:O	1:A:2558:TYR:HA	2.17	0.45
1:A:3566:LEU:HD23	1:A:3587:LEU:HD11	1.99	0.45
1:A:2197:ASP:HB3	1:A:2549:ARG:HD2	1.99	0.45
1:A:2749:LEU:HD12	1:A:2773:VAL:HG12	1.99	0.45
1:A:3470:PHE:CE1	1:A:3488:VAL:HG21	2.52	0.45
1:A:2021:ILE:HG22	1:A:2022:PHE:HD1	1.82	0.45
1:A:2099:ASN:HA	1:A:2149:ARG:O	2.17	0.44
1:A:2447:LYS:HE3	1:A:2493:LYS:HD3	1.99	0.44
1:A:3508:PHE:O	1:A:3512:ARG:HG2	2.16	0.44
1:A:1611:LEU:O	1:A:1615:ILE:HG23	2.18	0.44
1:A:1951:HIS:O	1:A:1955:LEU:HB2	2.17	0.44
1:A:2262:LEU:HA	1:A:2265:ILE:HD12	1.99	0.44
1:A:3330:TYR:CD1	1:A:3334:PHE:CD2	3.05	0.44
1:A:1660:VAL:CG1	1:A:1728:TRP:CH2	3.01	0.44
1:A:2386:MET:HB3	1:A:2627:ARG:NE	2.32	0.44
1:A:3319:GLU:HA	1:A:3359:LYS:O	2.17	0.44
1:A:3330:TYR:CE1	1:A:3334:PHE:CD2	3.05	0.44
1:A:3964:ALA:HB2	1:A:3993:VAL:HG11	1.99	0.44
1:A:1803:THR:HG21	1:A:1848:ASP:CG	2.37	0.44
1:A:2155:ASP:OD1	1:A:2195:GLU:HG3	2.17	0.44
1:A:2517:LYS:NZ	1:A:2520:GLU:OE1	2.48	0.44
1:A:2646:ARG:NH1	1:A:2687:GLY:H	2.15	0.44
1:A:2760:GLY:O	1:A:2761:ALA:HB3	2.18	0.44
1:A:1793:CYS:SG	1:A:1918:GLU:HG2	2.57	0.44
1:A:1940:GLU:CG	1:A:1941:ASP:H	2.22	0.44
1:A:2494:LEU:HB2	1:A:2499:SER:N	2.32	0.44
1:A:1559:SER:CB	1:A:1572:ILE:HG22	2.47	0.44
1:A:2037:CYS:SG	1:A:2094:PHE:HB2	2.57	0.44
1:A:3010:LEU:HD22	1:A:3320:LEU:HD12	1.99	0.44
1:A:3821:ASN:O	1:A:3825:ALA:HB2	2.17	0.44
1:A:4034:LEU:HD23	1:A:4034:LEU:C	2.38	0.44
1:A:1973:LEU:O	1:A:1977:LEU:HG	2.18	0.44
1:A:2861:ARG:HD2	1:A:2866:LEU:HD13	2.00	0.44
1:A:3461:ILE:C	1:A:3463:SER:N	2.70	0.44
1:A:3702:MET:HB3	1:A:3767:PHE:HZ	1.83	0.44
1:A:1926:SER:HA	1:A:1929:ILE:CD1	2.48	0.44
1:A:3979:ASN:O	1:A:3981:PRO:CD	2.64	0.44
1:A:1826:PHE:O	1:A:1826:PHE:CG	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2072:LEU:HD11	1:A:2193:LEU:HD23	2.00	0.43
1:A:2354:SER:H	1:A:2357:SER:HB2	1.83	0.43
1:A:2404:PHE:CZ	1:A:2428:MET:HG2	2.53	0.43
1:A:2707:VAL:HG11	1:A:2712:LEU:CD1	2.45	0.43
1:A:2738:MET:HG2	1:A:2769:LEU:HD21	2.00	0.43
1:A:2266:PHE:HD1	1:A:2326:LEU:HD21	1.83	0.43
1:A:2446:SER:N	1:A:2449:THR:HG23	2.19	0.43
1:A:2458:LEU:HG	1:A:2484:LEU:HD21	1.99	0.43
1:A:4033:LEU:CD1	1:A:4035:GLN:N	2.82	0.43
1:A:1672:TYR:O	1:A:1676:VAL:HG23	2.19	0.43
1:A:3869:GLU:O	1:A:3870:LYS:C	2.56	0.43
1:A:4033:LEU:HD13	1:A:4035:GLN:CG	2.49	0.43
1:A:1741:LEU:O	1:A:1742:ASP:HB2	2.19	0.43
1:A:2061:TYR:O	1:A:2064:GLN:HG2	2.17	0.43
1:A:2109:LEU:CD1	1:A:2129:LEU:HD23	2.49	0.43
1:A:2503:VAL:HA	1:A:2506:LEU:HD12	2.01	0.43
1:A:2578:ILE:CG2	1:A:2630:TYR:HB2	2.49	0.43
1:A:2988:SER:CB	1:A:2989:PRO:CD	2.71	0.43
1:A:1646:GLN:OE1	1:A:1763:ILE:HG12	2.18	0.43
1:A:1967:HIS:C	1:A:1968:PHE:CD1	2.85	0.43
1:A:3696:MET:SD	1:A:3760:LEU:HD23	2.59	0.43
1:A:1611:LEU:O	1:A:1615:ILE:HG12	2.19	0.43
1:A:1681:LYS:HE2	1:A:1939:PHE:CZ	2.53	0.43
1:A:1706:LEU:HD21	1:A:1935:GLN:CG	2.48	0.43
1:A:1620:PHE:CA	1:A:1760:PHE:CE1	3.01	0.43
1:A:2178:LEU:HB3	1:A:2179:PRO:HD2	2.01	0.43
1:A:2375:ILE:HG22	1:A:2376:PRO:O	2.18	0.43
1:A:2982:VAL:CG1	1:A:2983:GLY:N	2.82	0.43
1:A:3544:LYS:O	1:A:3548:LEU:HB2	2.19	0.43
1:A:3784:ASN:ND2	1:A:3865:ALA:O	2.52	0.43
1:A:1650:LEU:O	1:A:1654:VAL:HG23	2.19	0.43
1:A:3407:LEU:HD23	1:A:3518:PHE:CE2	2.53	0.43
1:A:1991:GLU:O	1:A:1994:VAL:HB	2.19	0.42
1:A:3767:PHE:HB3	1:A:3769:VAL:HG23	2.00	0.42
1:A:1822:CYS:SG	1:A:1850:PHE:CA	3.04	0.42
1:A:3628:ILE:HG13	1:A:3705:LEU:HD23	2.00	0.42
1:A:3785:TYR:CD1	1:A:3785:TYR:N	2.87	0.42
1:A:4033:LEU:HD12	1:A:4033:LEU:C	2.39	0.42
1:A:4074:GLU:HA	1:A:4077:GLN:HE21	1.84	0.42
1:A:1568:SER:HB2	1:A:1816:VAL:HG21	2.01	0.42
1:A:1781:THR:HG21	1:A:1919:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2111:LYS:HZ3	1:A:2161:GLU:HG2	1.76	0.42
1:A:2178:LEU:HB2	1:A:2182:GLU:H	1.83	0.42
1:A:2707:VAL:HG11	1:A:2712:LEU:HD12	2.00	0.42
1:A:2786:ILE:HD12	1:A:3460:PRO:CG	2.49	0.42
1:A:1715:LEU:HG	1:A:1727:LEU:HD22	2.02	0.42
1:A:1822:CYS:HB2	1:A:1853:LEU:CD2	2.31	0.42
1:A:2306:ASP:HB2	1:A:2309:SER:HB3	2.02	0.42
1:A:2640:THR:O	1:A:2643:SER:HB3	2.20	0.42
1:A:3414:MET:O	1:A:3418:ILE:HG12	2.19	0.42
1:A:1965:HIS:HD2	1:A:2212:LEU:HD23	1.85	0.42
1:A:2510:MET:O	1:A:2513:GLN:NE2	2.53	0.42
1:A:2708:ASN:O	1:A:2712:LEU:HD13	2.20	0.42
1:A:2829:GLU:HA	1:A:2832:ASN:HD22	1.84	0.42
1:A:3464:ARG:O	1:A:3467:SER:O	2.38	0.42
1:A:3810:SER:HB3	1:A:3837:GLY:HA2	2.01	0.42
1:A:2138:ASN:ND2	1:A:2185:PRO:O	2.52	0.42
1:A:3777:VAL:HG12	1:A:3895:PHE:CE1	2.53	0.42
1:A:1939:PHE:CD1	1:A:1939:PHE:N	2.87	0.42
1:A:2225:LYS:HD2	1:A:2281:PHE:CZ	2.55	0.42
1:A:2411:LYS:HG2	1:A:2530:HIS:CE1	2.41	0.42
1:A:2609:THR:HA	1:A:2612:GLN:O	2.20	0.42
1:A:3505:ILE:O	1:A:3510:ARG:NH1	2.53	0.42
1:A:3728:GLU:CG	1:A:4079:LYS:HE2	2.49	0.42
1:A:3785:TYR:CE2	1:A:3859:VAL:HG13	2.54	0.42
1:A:1998:LEU:CD1	1:A:2022:PHE:HZ	2.32	0.42
1:A:2088:ILE:HG12	1:A:2151:TRP:CZ2	2.55	0.42
1:A:2141:ILE:CG2	1:A:2145:PHE:HB2	2.49	0.42
1:A:2385:VAL:HG23	1:A:2574:TYR:CD1	2.53	0.42
1:A:2755:HIS:HB3	1:A:2912:CYS:SG	2.60	0.42
1:A:2905:SER:HA	1:A:2906:PRO:HD2	1.85	0.42
1:A:3848:LEU:O	1:A:3849:SER:C	2.59	0.42
1:A:1575:LEU:O	1:A:1576:GLU:HB3	2.20	0.42
1:A:1727:LEU:O	1:A:1731:VAL:HG23	2.20	0.42
1:A:1830:VAL:O	1:A:1834:LEU:HG	2.19	0.42
1:A:2001:VAL:O	1:A:2004:PRO:HD2	2.20	0.42
1:A:2044:ARG:HH21	1:A:2093:ILE:HD11	1.85	0.42
1:A:2489:ILE:HD11	1:A:2506:LEU:HD13	2.02	0.42
1:A:2575:TYR:HD1	1:A:2578:ILE:HD11	1.83	0.42
1:A:2760:GLY:HA3	1:A:2766:LYS:HD3	2.01	0.42
1:A:4045:LEU:O	1:A:4048:ILE:HG22	2.20	0.42
1:A:2053:PHE:HB2	1:A:2219:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3534:LEU:HD12	1:A:3618:TYR:CZ	2.52	0.41
1:A:2095:ASP:OD1	1:A:2149:ARG:NH2	2.53	0.41
1:A:2492:PRO:CB	1:A:2502:VAL:HG11	2.49	0.41
1:A:2758:LEU:HD22	1:A:2917:MET:SD	2.60	0.41
1:A:3461:ILE:C	1:A:3463:SER:H	2.22	0.41
1:A:3978:ASN:O	1:A:3981:PRO:HD3	2.20	0.41
1:A:1898:LEU:HD11	1:A:1908:LEU:CD2	2.50	0.41
1:A:3612:ASP:C	1:A:3615:VAL:HG22	2.41	0.41
1:A:2012:LEU:HD12	1:A:2013:VAL:N	2.35	0.41
1:A:2568:SER:HA	1:A:2597:VAL:HG21	2.02	0.41
1:A:2786:ILE:HD12	1:A:3460:PRO:HG2	2.02	0.41
1:A:3365:ARG:HD2	1:A:3368:ASP:OD2	2.19	0.41
1:A:1965:HIS:HD2	1:A:2212:LEU:HD21	1.85	0.41
1:A:2034:ILE:HD12	1:A:2061:TYR:CE2	2.55	0.41
1:A:3808:LYS:HA	1:A:3808:LYS:HD3	1.89	0.41
1:A:2109:LEU:HB3	1:A:2113:SER:HB2	2.03	0.41
1:A:2420:PRO:HD3	1:A:2536:ASN:HD21	1.85	0.41
1:A:2512:LYS:O	1:A:2513:GLN:CB	2.66	0.41
1:A:3544:LYS:HE3	1:A:3607:PHE:CD1	2.55	0.41
1:A:3799:LYS:HG3	1:A:3803:LEU:HD11	2.03	0.41
1:A:2276:LEU:HD21	1:A:2415:ILE:HG21	2.03	0.41
1:A:2563:SER:C	1:A:2565:LYS:H	2.23	0.41
1:A:2574:TYR:HB3	1:A:2626:VAL:HG11	2.03	0.41
1:A:2762:SER:O	1:A:2763:ARG:CB	2.68	0.41
1:A:2860:THR:HG21	1:A:2867:LEU:HD12	2.02	0.41
1:A:3833:LYS:NZ	1:A:3862:THR:HG21	2.36	0.41
1:A:4020:ASN:ND2	1:A:4028:ARG:HD3	2.35	0.41
1:A:1702:LEU:HA	1:A:1702:LEU:HD23	1.86	0.41
1:A:2225:LYS:HG2	1:A:2229:LEU:HD12	2.02	0.41
1:A:1966:TYR:CZ	1:A:2006:LEU:HD23	2.55	0.41
1:A:2418:GLY:O	1:A:2424:LYS:HE3	2.21	0.41
1:A:2766:LYS:CE	1:A:2890:THR:HB	2.39	0.41
1:A:2852:LEU:HG	1:A:2856:LEU:HD13	2.03	0.41
1:A:2891:ILE:HD11	1:A:2903:ILE:HD11	2.03	0.41
1:A:2985:ASN:N	1:A:2986:PRO:CD	2.84	0.41
1:A:3846:MET:HG3	1:A:3847:SER:N	2.35	0.41
1:A:3939:ILE:HG13	1:A:4010:LEU:HD23	1.98	0.41
1:A:3413:HIS:O	1:A:3417:VAL:HG23	2.21	0.41
1:A:3671:VAL:HA	1:A:3674:ILE:HG22	2.03	0.41
1:A:3772:TRP:HZ3	1:A:3780:ASN:HD22	1.68	0.41
1:A:4033:LEU:CD1	1:A:4035:GLN:H	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4054:GLU:HA	1:A:4055:PRO:HD3	1.97	0.41
1:A:2977:TYR:HD1	1:A:2981:LYS:HG3	1.86	0.40
1:A:3590:LEU:HD12	1:A:3593:GLU:HB2	2.02	0.40
1:A:2175:ILE:HG13	1:A:2184:LEU:C	2.42	0.40
1:A:2229:LEU:HD11	1:A:2285:GLU:HG3	2.02	0.40
1:A:2488:GLU:HB3	1:A:2491:LEU:CG	2.51	0.40
1:A:3330:TYR:CZ	1:A:3346:LEU:HD13	2.55	0.40
1:A:1794:PHE:CD1	1:A:1802:LYS:HB3	2.56	0.40
1:A:2332:GLY:HA2	1:A:2335:GLN:CG	2.52	0.40
1:A:2336:ARG:HG2	1:A:2355:ASP:CG	2.41	0.40
1:A:2761:ALA:O	1:A:2892:CYS:CB	2.69	0.40
1:A:2819:GLU:HB3	1:A:2891:ILE:HG22	2.03	0.40
1:A:3570:LEU:HD23	1:A:3580:ASN:CG	2.41	0.40
1:A:3813:ILE:HG22	1:A:3840:LEU:HD23	2.04	0.40
1:A:3951:SER:HB3	1:A:4003:ASP:OD2	2.22	0.40
1:A:2039:LYS:HG2	1:A:2049:MET:HG3	2.03	0.40
1:A:2581:LEU:HD13	1:A:2633:ILE:HG22	2.03	0.40
1:A:3024:LEU:HD13	1:A:3303:LYS:HG3	1.92	0.40
1:A:3330:TYR:O	1:A:3334:PHE:HB2	2.22	0.40
1:A:3832:SER:O	1:A:3836:GLY:N	2.45	0.40
1:A:1835:LEU:O	1:A:1838:ILE:HG22	2.22	0.40
1:A:3708:PHE:CZ	1:A:3720:LEU:HD21	2.57	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%)	41 77

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2990	GLY
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 (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	2039/2078 (98%)	1967 (96%)	72 (4%)	36 59

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1794	PHE
1	A	1826	PHE
1	A	1852	ARG
1	A	1923	SER
1	A	1944	SER
1	A	1971	ARG
1	A	1992	LYS
1	A	1999	LYS
1	A	2012	LEU
1	A	2057	CYS
1	A	2078	CYS
1	A	2109	LEU
1	A	2202	THR
1	A	2218	ASP
1	A	2295	ILE
1	A	2346	PHE
1	A	2357	SER
1	A	2386	MET
1	A	2424	LYS
1	A	2428	MET

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Mol	Chain	Res	Type
1	A	2461	HIS
1	A	2472	THR
1	A	2476	LYS
1	A	2526	ILE
1	A	2544	ILE
1	A	2563	SER
1	A	2566	SER
1	A	2611	LEU
1	A	2638	ARG
1	A	2694	LEU
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	2875	ASP
1	A	2911	ARG
1	A	2920	TRP
1	A	3301	PHE
1	A	3329	ILE
1	A	3332	THR
1	A	3355	LYS
1	A	3372	THR
1	A	3400	SER
1	A	3418	ILE
1	A	3531	ASP
1	A	3538	ASN
1	A	3548	LEU
1	A	3565	ARG
1	A	3601	LEU
1	A	3618	TYR
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	3871	PHE
1	A	3884	LEU

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Mol	Chain	Res	Type
1	A	3899	ASP
1	A	3906	THR
1	A	3917	THR
1	A	3943	THR
1	A	3950	PHE
1	A	3960	ASP
1	A	3982	TRP
1	A	4004	LEU
1	A	4016	CYS
1	A	4040	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1622	GLN
1	A	1646	GLN
1	A	1736	GLN
1	A	1745	ASN
1	A	1851	ASN
1	A	1873	GLN
1	A	1899	ASN
1	A	1951	HIS
1	A	1965	HIS
1	A	1979	ASN
1	A	2068	GLN
1	A	2099	ASN
1	A	2274	HIS
1	A	2282	ASN
1	A	2293	HIS
1	A	2383	HIS
1	A	2409	ASN
1	A	2459	HIS
1	A	2530	HIS
1	A	2536	ASN
1	A	2634	ASN
1	A	2683	ASN
1	A	2688	ASN
1	A	3323	ASN
1	A	3338	ASN
1	A	3420	ASN
1	A	3497	HIS
1	A	3521	ASN

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Mol	Chain	Res	Type
1	A	3542	GLN
1	A	3588	ASN
1	A	3624	HIS
1	A	3780	ASN
1	A	3890	GLN
1	A	4020	ASN
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 monosaccharides 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.

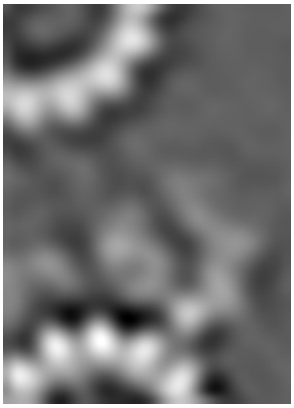
5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

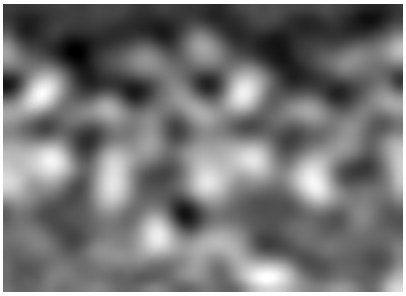
6 Tomogram visualisation (i)

This section contains visualisations of the EMDB entry EMD-5757. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections (i)

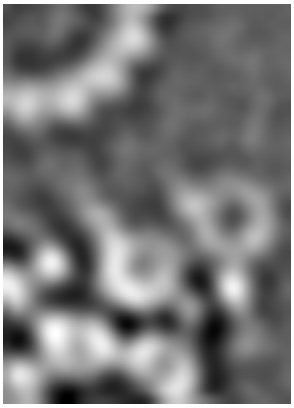

X

Y

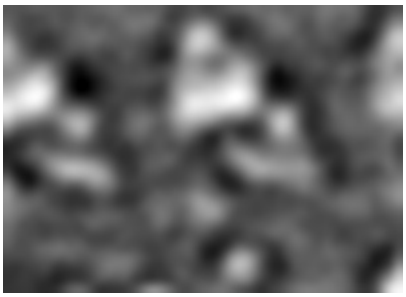

Z

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)

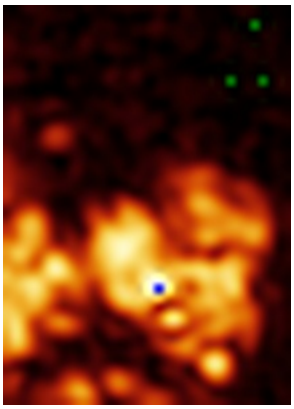
X Index: 29

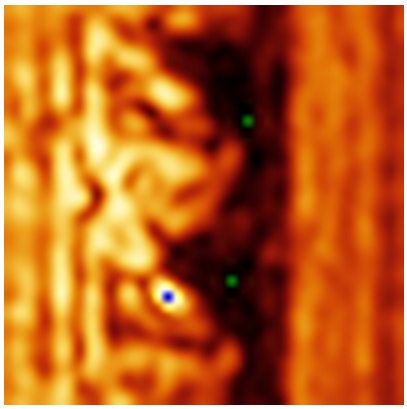
Y Index: 16

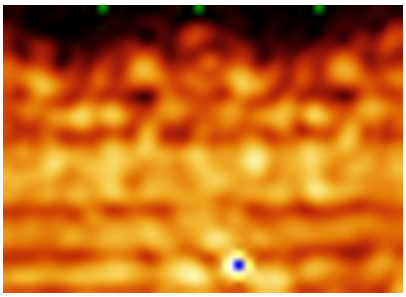
Z Index: 7

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.

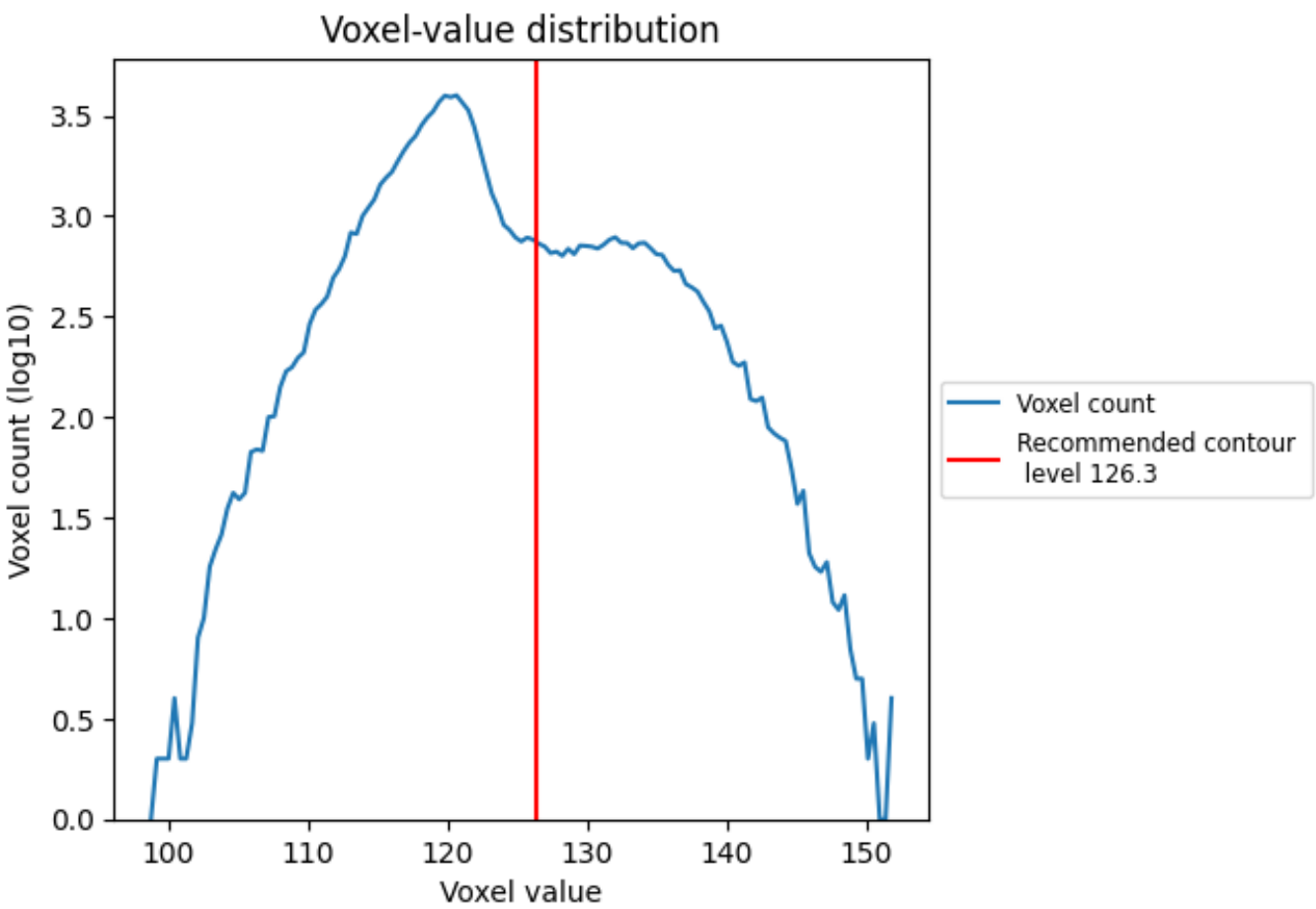
6.5 Mask visualisation (i)

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.

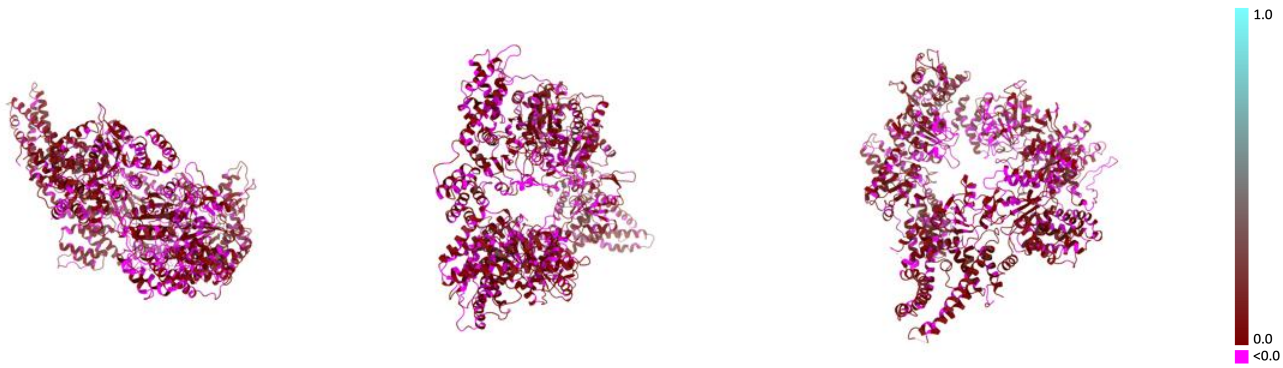
8 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-5757 and PDB model 3J67. 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)



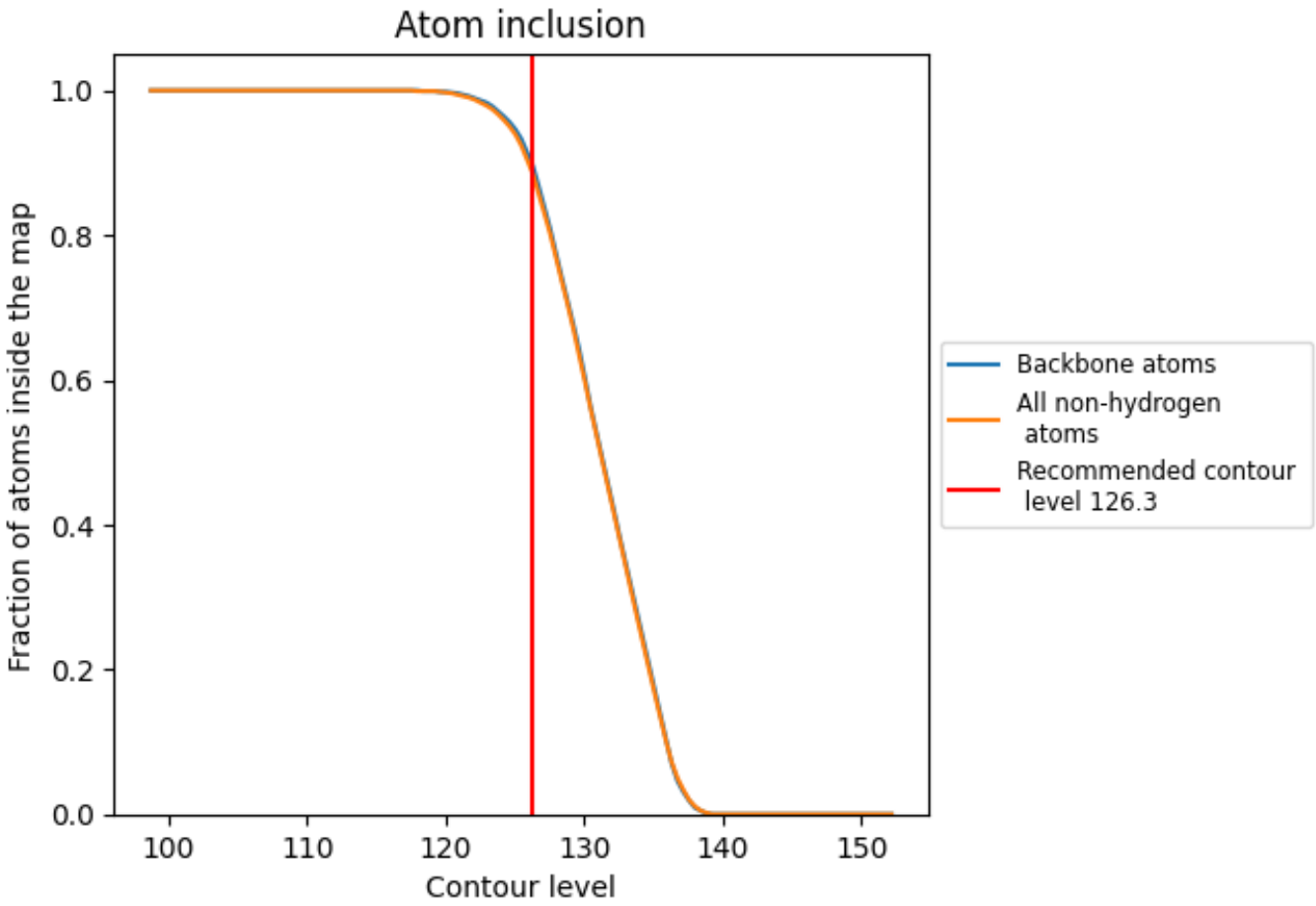
X Y Z

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.

8.3 Atom inclusion mapped to coordinate model (i)

This section was not generated.

8.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (126.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8850	0.0340
A	0.8850	0.0340