Full wwPDB EM Validation Report ⓘ

Apr 12, 2023 – 02:44 PM JST

PDB ID	:	7YFP
EMDB ID	:	EMD-33796
Title	:	The NuA4 histone acetyltransferase complex from S. cerevisiae
Authors	:	Ji, L.T.; Zhao, L.X.; Xu, K.; Gao, H.H.; Zhou, Y.; Kornberg, R.D.; Zhang, H.Q.
Deposited on	:	2022-07-08
Resolution	:	4.00 Å(reported)
Based on initial model	:	5OJS

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:

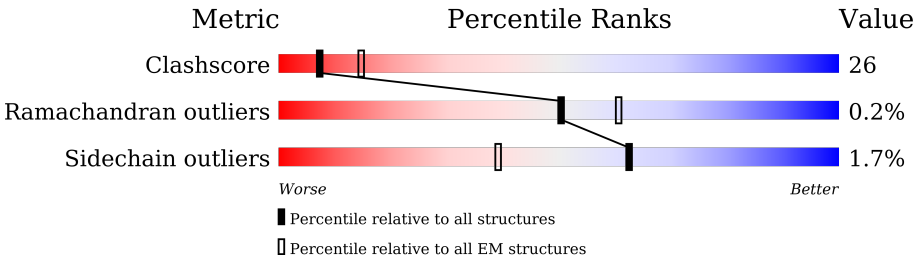
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 4.00 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	372	6% 54% 46%
2	B	481	48% 35% 16%
3	D	982	28% 18% 54%
4	E	476	26% 16% 58%
5	F	832	9% 6% 85%
6	T	3744	21% 48% 43% 7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 40949 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 Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	372	Total	C	N	O	S	0	0
			2904	1841	491	553	19		

- Molecule 2 is a protein called ARP4 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	402	Total	C	N	O	S	0	0
			3172	2024	518	619	11		

- Molecule 3 is a protein called Chromatin modification-related protein EAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	454	Total	C	N	O	S	0	0
			3777	2392	683	691	11		

- Molecule 4 is a protein called SWR1-complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	201	Total	C	N	O	S	0	0
			1668	1069	276	319	4		

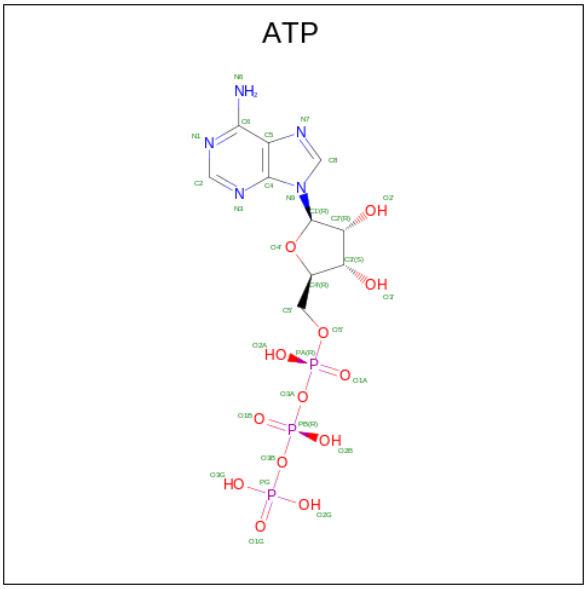
- Molecule 5 is a protein called Enhancer of polycomb-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	124	Total	C	N	O	S	0	0
			1023	653	177	190	3		

- Molecule 6 is a protein called Transcription-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	3475	Total	C	N	O	S	0	0
			28374	18368	4717	5169	120		

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



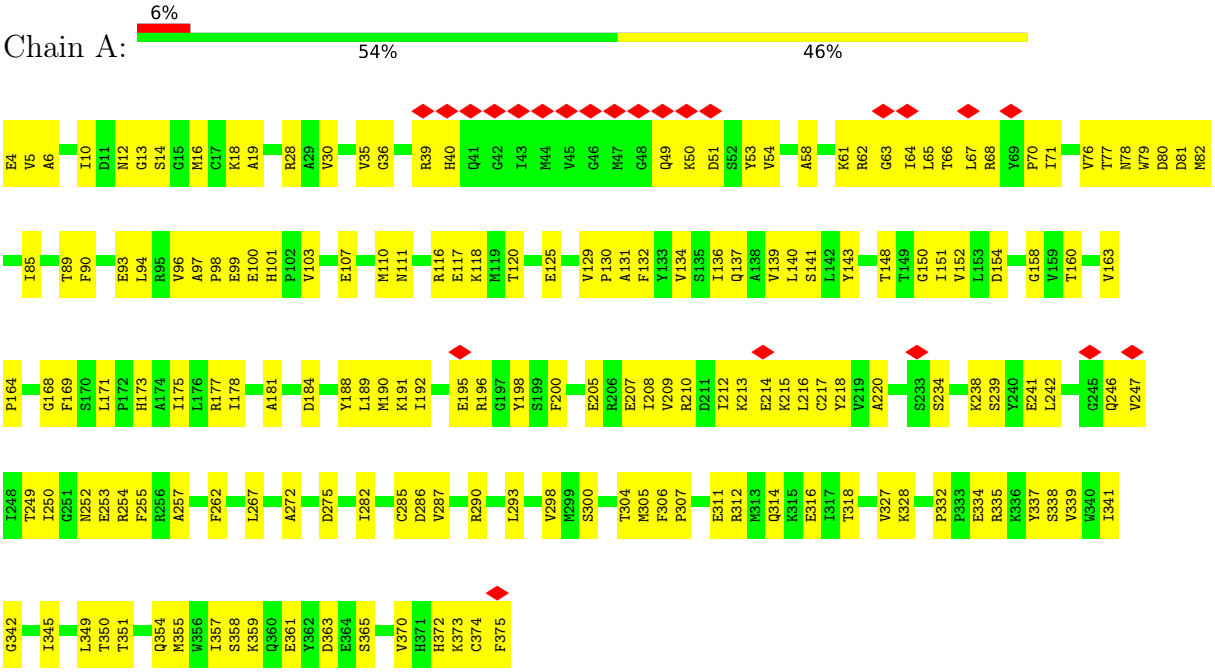
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	B	1	31	10	5	13	3	0

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.

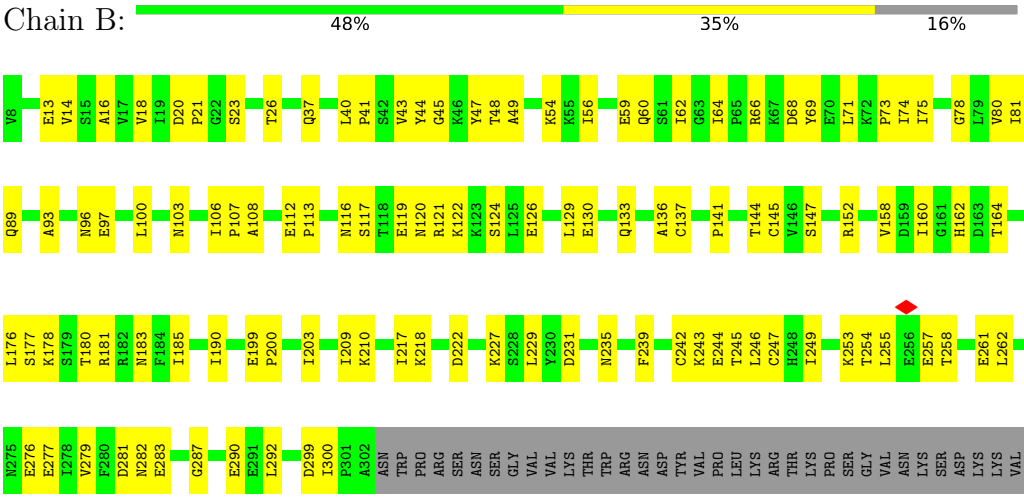
- Molecule 1: Actin

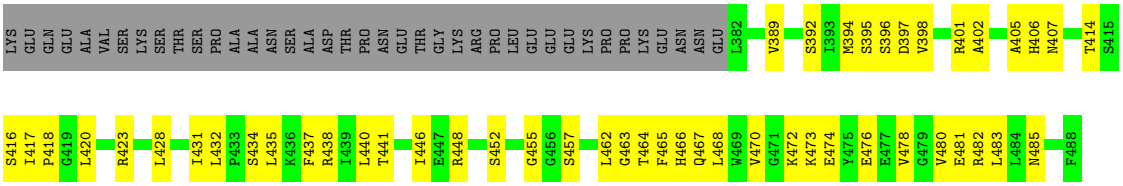
Chain A:



- Molecule 2: ARP4 isoform 1

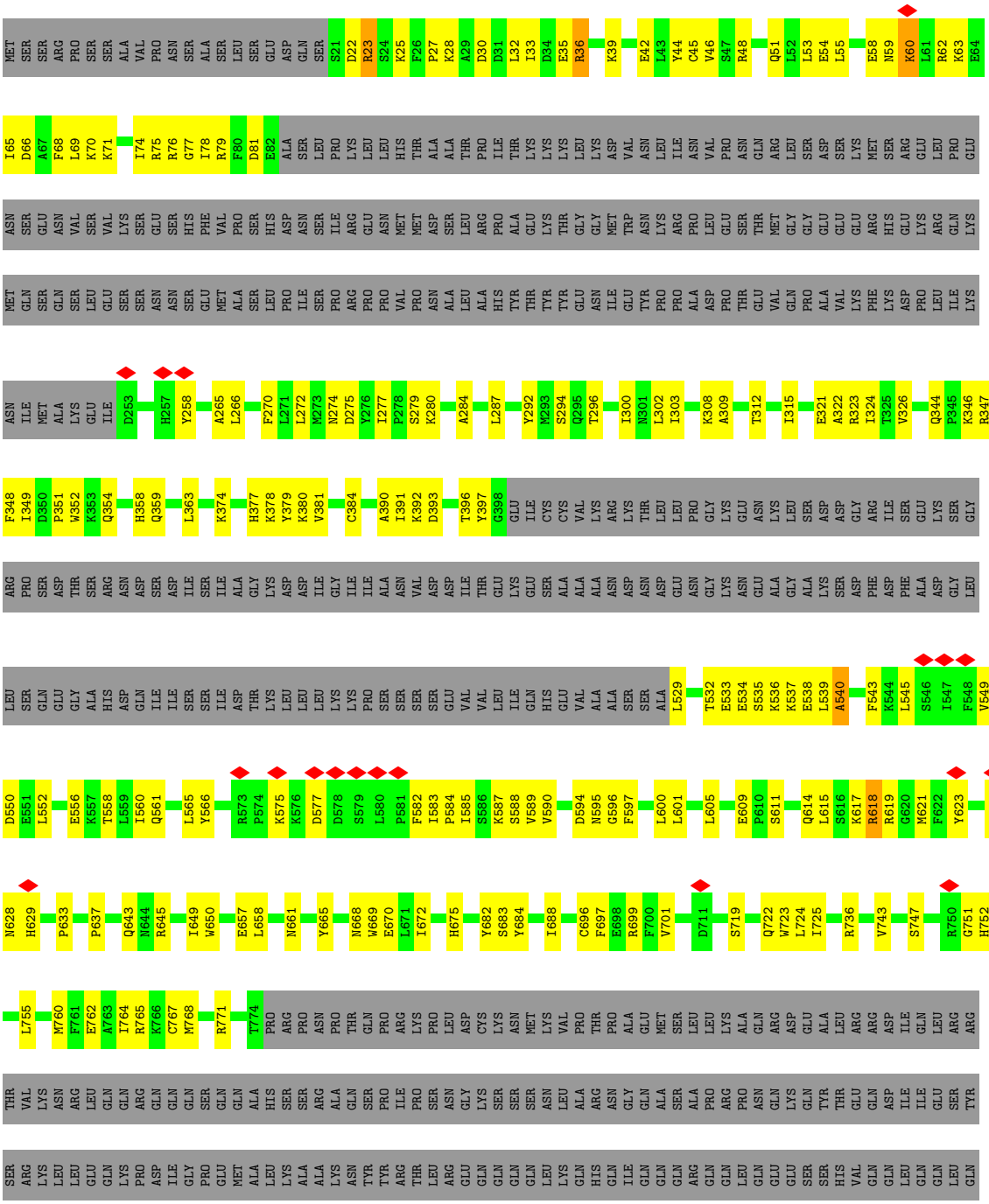
Chain B:

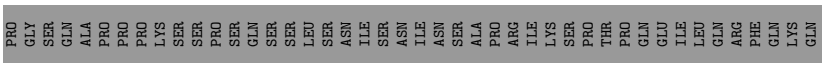




• Molecule 3: Chromatin modification-related protein EAF1

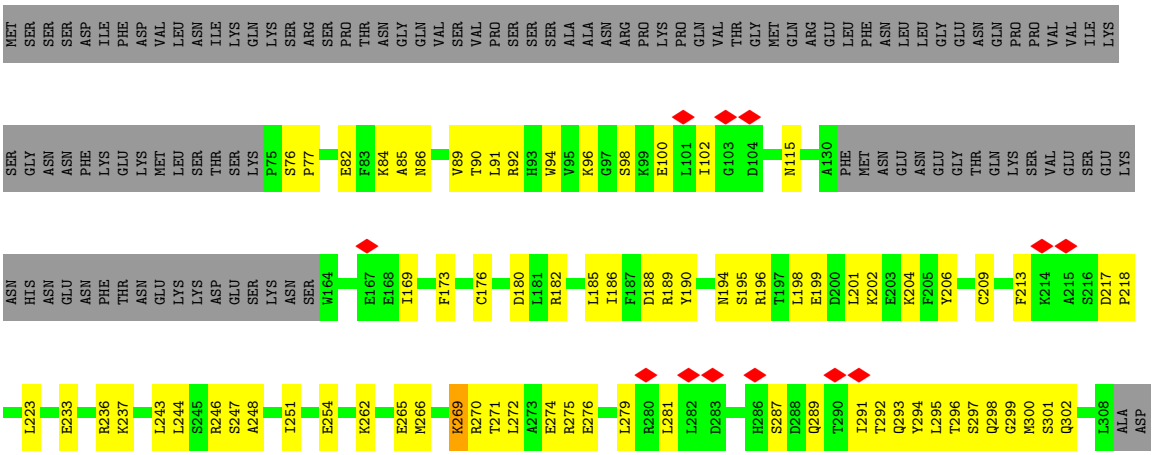
Chain D:

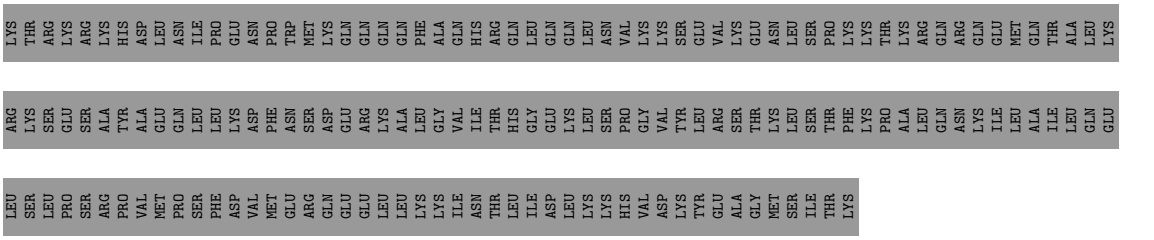




• Molecule 4: SWR1-complex protein 4

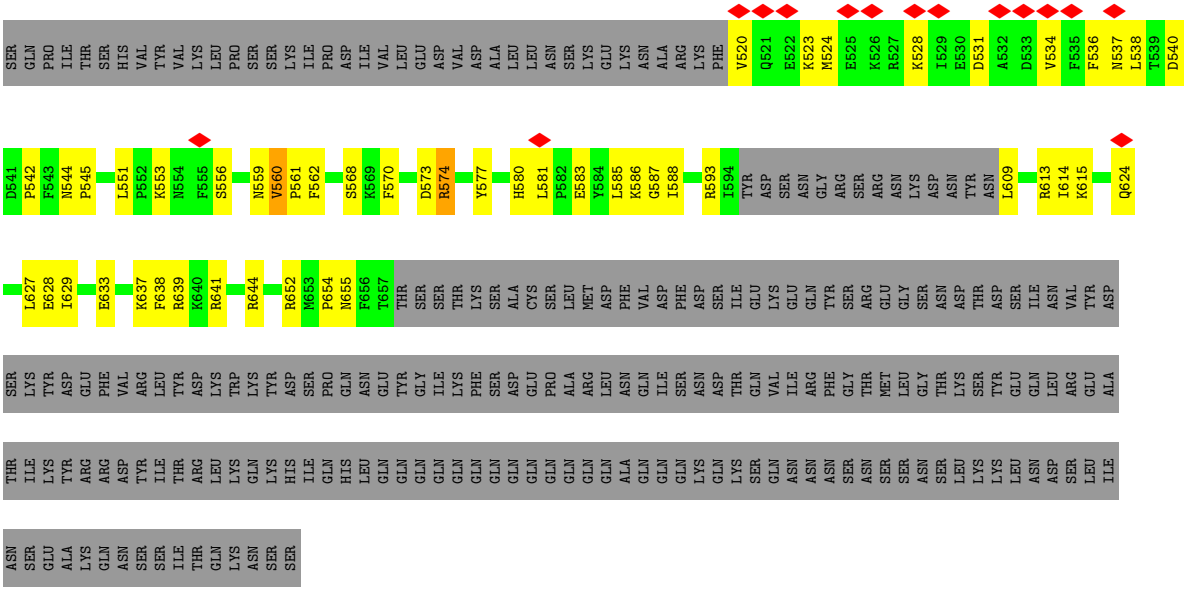
Chain E:





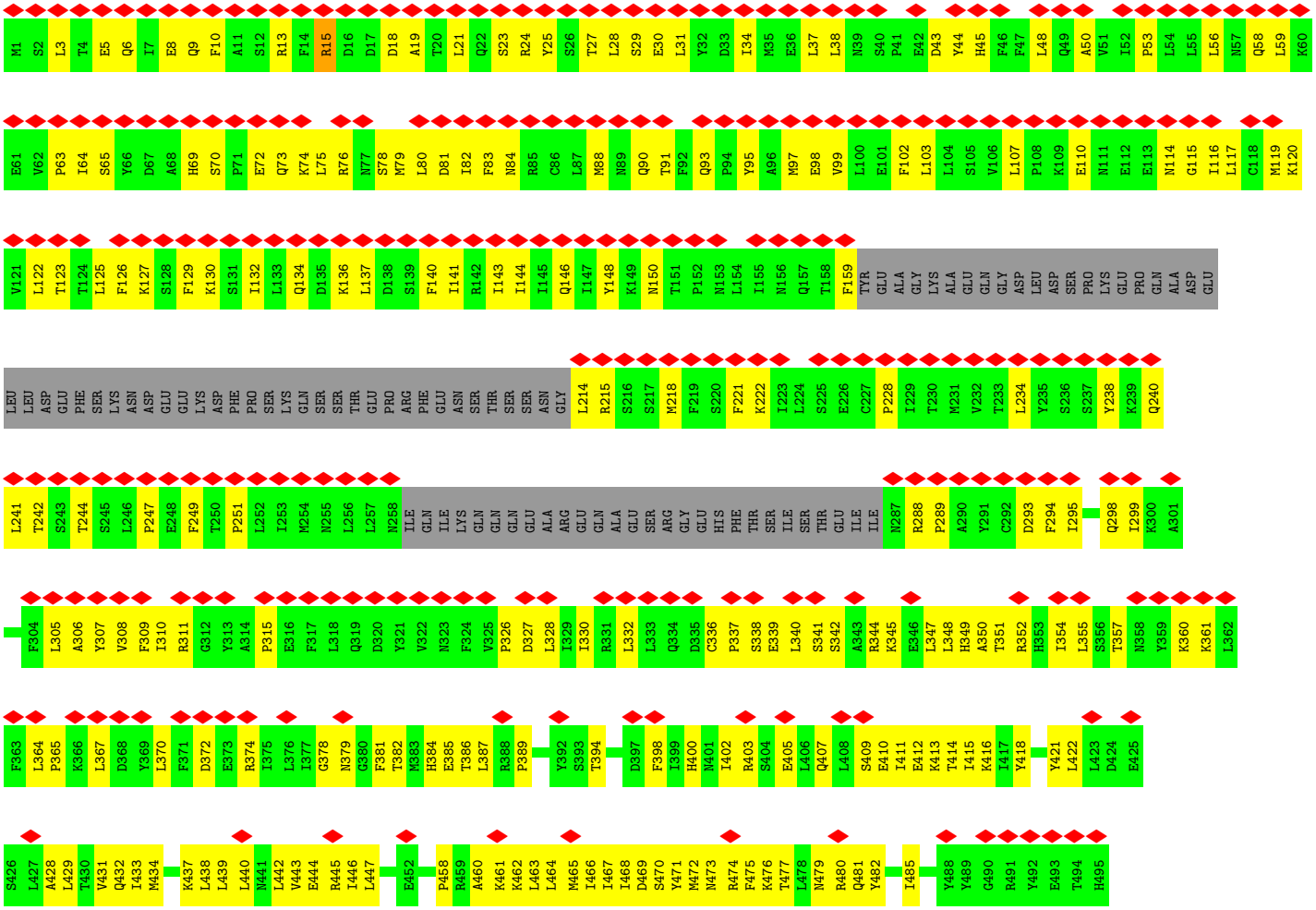
• Molecule 5: Enhancer of polycomb-like protein 1

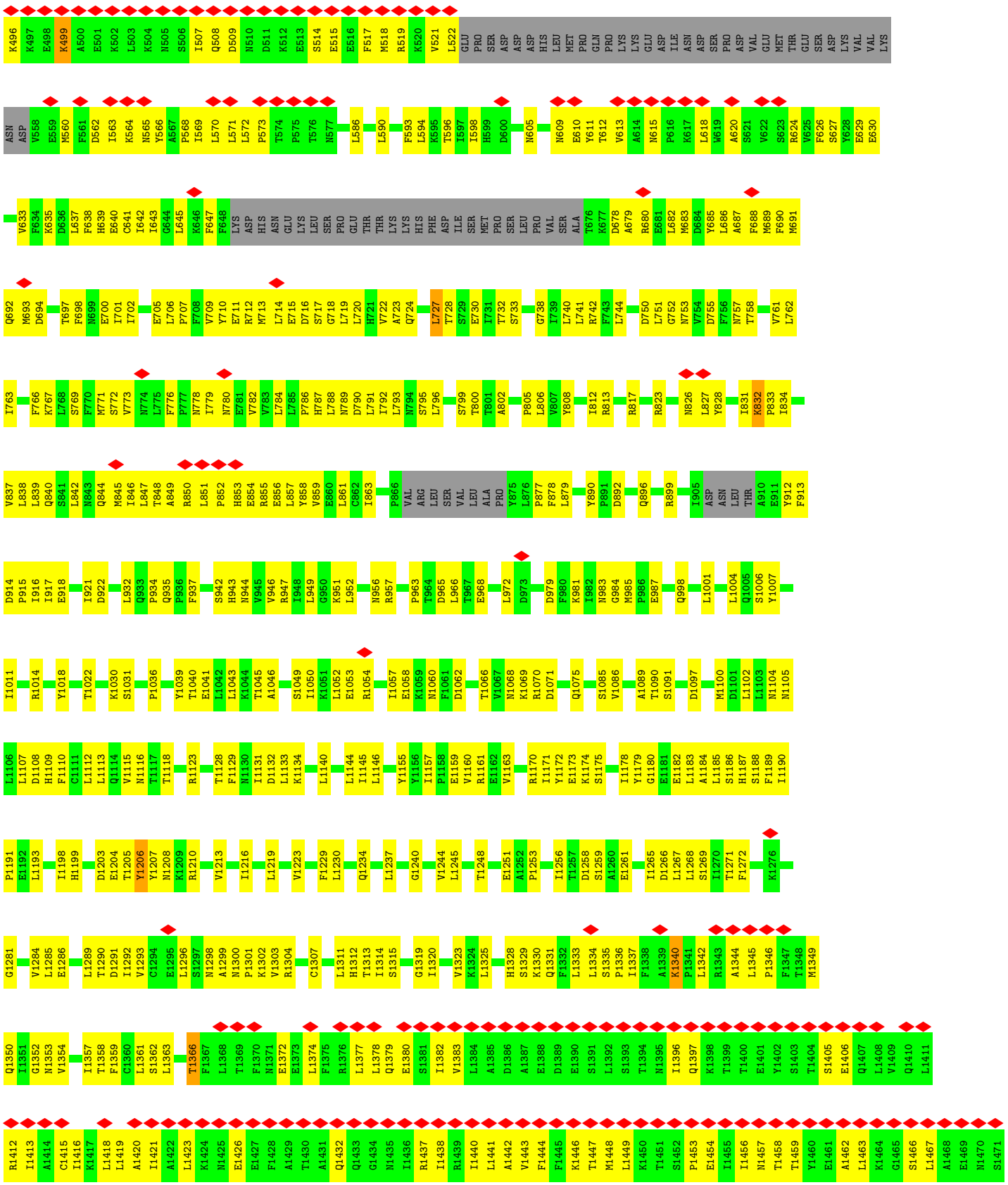
Chain F:



• Molecule 6: Transcription-associated protein 1

Chain T:

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ASN ASP V558 E559 M560 F561 D562 I563 K564 N565 Y566 A567 P568 I569 L570 L571 L572 P573 T574 P575 T576 N577 L586 L590 F593 L594 K595 T596 I597 I598 H599 D600 N605 N609 E610 T612 V613 A614 N615 P616 K617 L618 W619 A620 S621 V622 S623 R624 V625 F626 S627 Y628 E629 E630
V633 F634 K635 D636 L637 F638 H639 E640 C641 I642 I643 G644 L645 K646 F647 F648 LYS ASP HIS ASN GLU LYS LEU SER PRO GLU THR THR LYS LYS HIS PHE ASP ILE SER MET PRO SER LEU PRO VAL SER ALA T676 K677 D678 A679 R680 E681 L682 M683 D684 Y685 L686 A687 F688 M689 F690 M691
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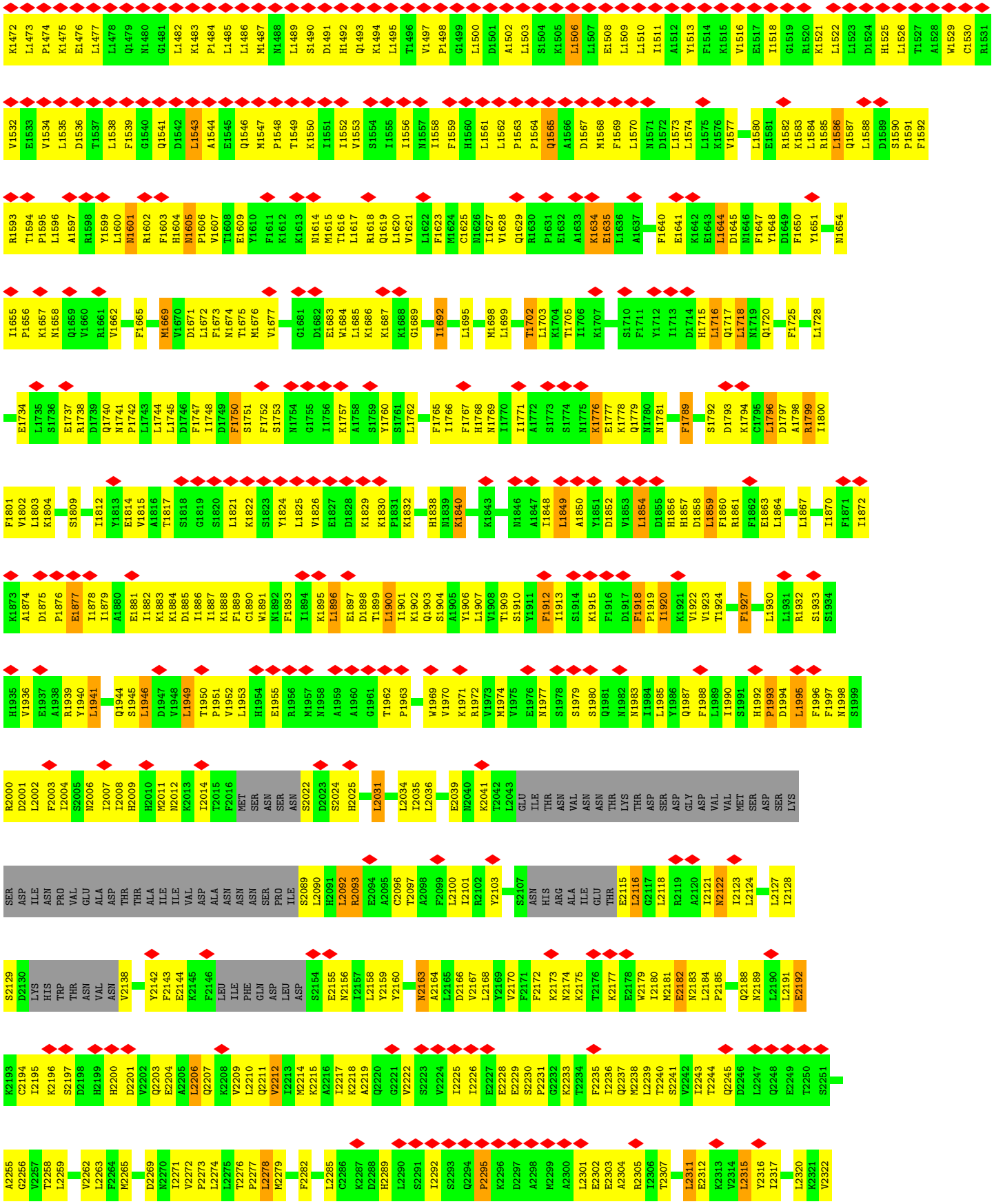
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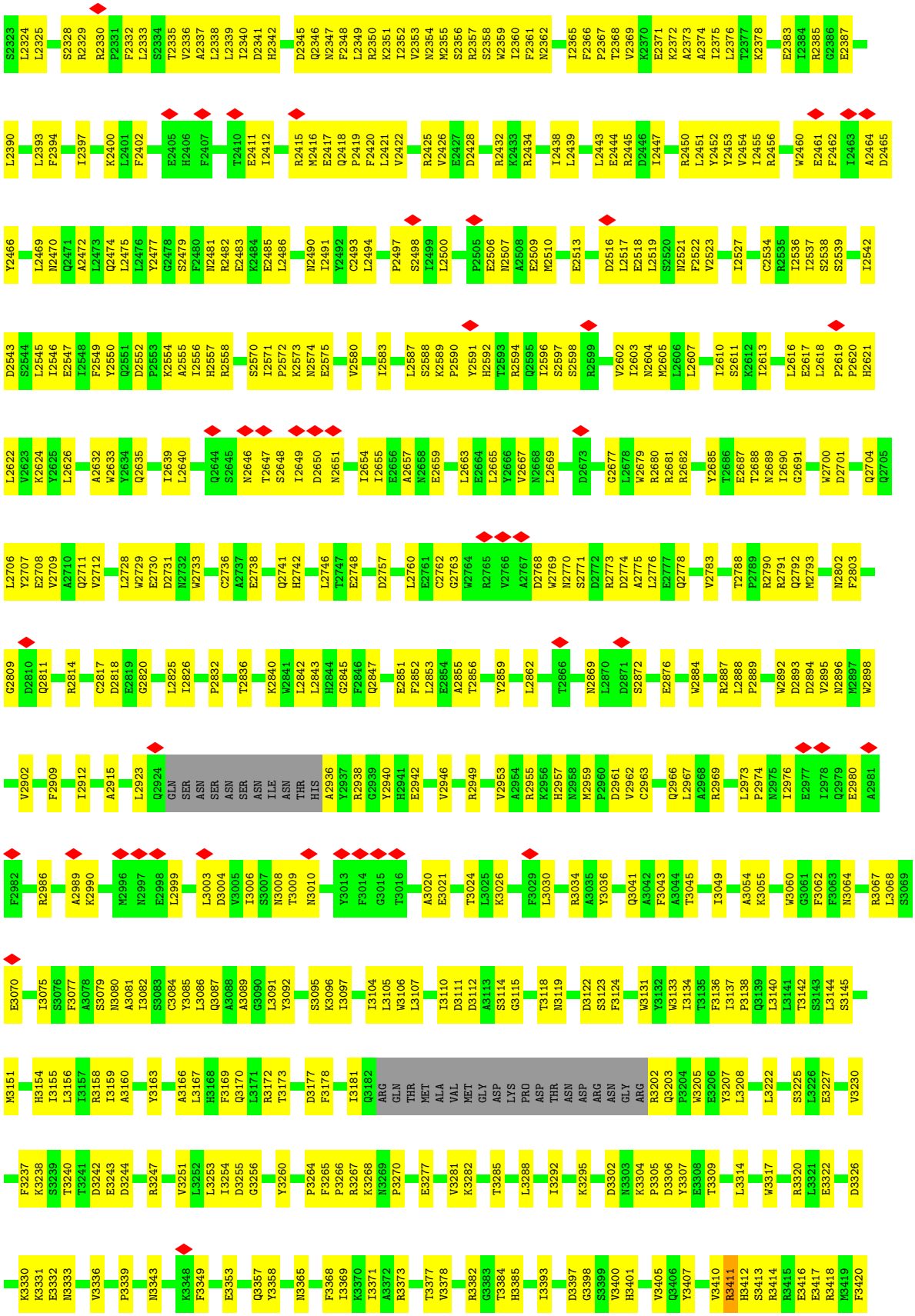
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Y2466 L2469 N2470 Q2471 A2472 L2473 Q2474 L2475 L2476 Y2477 Q2478 S2479 F2480 N2481 R2482 E2483 K2484 E2485 L2486 N2490 I2491 Y2492 C2493 L2494 P2497 S2498 I2499 L2500 P2505 E2506 N2507 A2508 E2509 M2510 E2513 D2516 L2517 E2518 L2519 S2520 N2521 F2522 V2523 I2527 C2534 R2535 I2536 I2537 S2538 S2539 I2542
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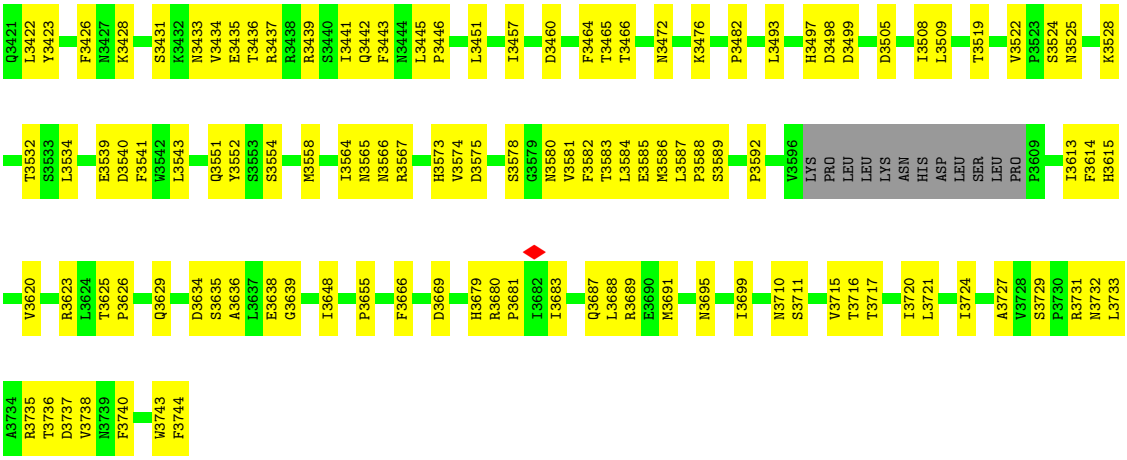
L2622 V2623 K2624 Y2625 L2626 A2632 W2633 Y2634 Q2635 I2639 L2640 Q2644 S2645 N2646 T2647 S2648 I2649 D2650 N2651 I2654 I2655 E2656 A2657 N2658 E2659 L2663 E2664 L2665 Y2666 V2667 N2668 L2669 D2673 G2677 L2678 W2679 R2680 R2681 R2682 Y2685 T2686 E2687 T2688 N2689 I2690 G2691 W2700 D2701 Q2704 Q2705
L2706 Y2707 E2708 V2709 A2710 Q2711 V2712 L2728 W2729 E2730 D2731 N2732 W2733 C2736 A2737 E2738 Q2741 H2742 L2746 T2747 E2748 D2757 L2760 E2761 C2762 G2763 W2764 R2765 V2766 A2767 D2768 W2769 N2770 S2771 D2772 R2773 D2774 A2775 L2776 E2777 Q2778 V2783 T2788 P2789 R2790 R2791 Q2792 M2793 N2802 F2803
G2809 D2810 Q2811 R2814 C2817 D2818 E2819 G2820 L2825 I2826 P2832 T2836 K2840 W2841 L2842 L2843 H2844 G2845 F2846 Q2847 E2851 F2852 L2853 E2854 A2855 T2856 Y2859 L2862 T2866 N2869 L2870 D2871 S2872 E2876 W2884 R2887 L2888 P2889 W2892 D2893 D2894 V2895 N2896 M2897 W2898
V2902 F2909 I2912 A2915 L2923 Q2924 GLN SER ASN SER ASN SER ASN ILE ASN THR HIS A2936 Y2937 R2938 G2939 Y2940 H2941 E2942 V2946 R2949 V2953 A2954 R2955 K2956 H2957 N2958 M2959 P2960 D2961 V2962 C2963 Q2966 L2967 A2968 R2969 L2973 P2974 N2975 I2976 E2977 I2978 Q2979 E2980 A2981
F2982 R2986 A2989 K2990 M2996 N2997 E2998 L2999 L3003 D3004 V3005 I3006 S3007 N3008 T3009 N3010 Y3013 F3014 G3015 T3016 A3020 E3021 T3024 L3025 K3026 F3029 L3030 R3034 A3035 Y3036 Q3041 A3042 F3043 A3044 T3045 I3049 A3054 K3055 W3060 G3061 F3062 F3063 N3064 R3067 L3068 S3069
E3070 I3075 S3076 F3077 A3078 S3079 N3080 A3081 I3082 S3083 C3084 Y3085 L3086 Q3087 A3088 A3089 G3090 L3091 Y3092 S3095 K3096 I3097 I3104 L3105 W3106 L3107 I3110 D3111 D3112 A3113 S3114 G3115 T3118 N3119 D3122 S3123 F3124 W3131 Y3132 W3133 W3134 T3135 F3136 I3137 P3138 Q3139 L3140 L3141 T3142 S3143 L3144 S3145
M3151 H3154 I3155 L3156 Y3157 R3158 I3159 A3160 Y3163 A3166 L3167 H3168 F3169 Q3170 L3171 R3172 T3173 D3177 F3178 I3181 Q3182 ARG GLN THR MET ALA VAL MET GLY ASP LYS PRO ASP THR ASN ASP ARG ASN GLY ARG R3202 Q3203 P3204 W3205 E3206 Y3207 L3208 L3222 S3225 L3226 E3227 V3230
F3237 K3238 S3239 T3240 T3241 D3242 E3243 D3244 R3247 V3251 L3252 L3253 I3254 D3255 G3256 Y3260 P3264 F3265 P3266 R3267 K3268 N3269 P3270 E3277 V3281 K3282 T3285 L3288 I3292 K3295 D3302 N3303 K3304 P3305 D3306 Y3307 E3308 T3309 L3314 W3317 R3320 L3321 E3322 D3326
K3330 K3331 E3332 N3333 V3336 P3339 N3343 K3348 F3349 E3353 Q3357 Y3358 N3365 F3368 I3369 K3370 I3371 A3372 R3373 T3377 V3378 R3382 G3383 T3384 H3385 I3393 D3397 G3398 S3399 V3400 H3401 V3405 Q3406 Y3407 V3410 R3411 H3412 S3413 R3414 R3415 E3416 E3417 R3418 M3419 F3420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T3532 S3533 L3534 E3539 D3540 F3541 W3542 L3543 Q3551 Y3552 S3553 S3554 M3558 I3564 N3565 N3566 R3567 H3573 V3574 D3575 S3578 G3579 N3580 V3581 F3582 T3583 L3584 E3585 M3586 L3587 P3588 S3589 P3592 V3596 LYS PRO LEU LEU LYS ASN HIS ASP LEU SER LEU PRO P3609 I3613 F3614 H3615
V3620 R3623 L3624 T3625 P3626 Q3629 D3634 S3635 A3636 L3637 E3638 G3639 I3648 P3655 F3666 D3669 H3679 R3680 P3681 I3682 I3683 Q3687 L3688 R3689 E3690 M3691 N3695 I3699 N3710 S3711 V3715 T3716 T3717 I3720 L3721 I3724 A3727 V3728 S3729 P3730 R3731 N3732 L3733
A3734 R3735 T3736 D3737 V3738 N3739 F3740 W3743 F3744

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	197044	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.170	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0396	Depositor
Map size (Å)	330.0, 330.0, 330.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.66, 0.66, 0.66	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.29	0/2968	0.43	0/4017
2	B	0.32	0/3241	0.46	0/4398
3	D	0.33	0/3859	0.49	0/5212
4	E	0.30	0/1707	0.43	0/2300
5	F	0.34	0/1046	0.57	0/1405
6	T	0.41	0/28991	0.52	1/39278 (0.0%)
All	All	0.39	0/41812	0.50	1/56610 (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
3	D	0	3
5	F	0	1
6	T	0	1
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	T	3592	PRO	N-CA-CB	5.78	110.23	103.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	535	SER	Peptide
3	D	540	ALA	Peptide
3	D	60	LYS	Peptide
5	F	560	VAL	Peptide
6	T	1366	THR	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	2904	0	2874	133	0
2	B	3172	0	3125	132	0
3	D	3777	0	3763	179	0
4	E	1668	0	1630	73	0
5	F	1023	0	999	55	0
6	T	28374	0	28736	1670	0
7	B	31	0	12	4	0
All	All	40949	0	41139	2155	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 26.

All (2155) 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)
6:T:480:ARG:HD3	6:T:1760:TYR:CD1	1.17	1.60
6:T:2320:LEU:CD1	6:T:2355:MET:HB3	1.26	1.58
6:T:480:ARG:CB	6:T:1760:TYR:CZ	1.86	1.55
6:T:480:ARG:HD3	6:T:1760:TYR:CE1	1.40	1.53
6:T:2320:LEU:CD1	6:T:2355:MET:CB	1.85	1.50
6:T:2320:LEU:HD11	6:T:2355:MET:C	1.30	1.46
6:T:2320:LEU:HD13	6:T:2355:MET:CB	1.42	1.44
6:T:1441:LEU:CD1	6:T:1473:LEU:HD13	1.51	1.41
6:T:694:ASP:CG	6:T:1585:ARG:HH11	1.15	1.41
6:T:1441:LEU:HD12	6:T:1473:LEU:CD1	1.49	1.40
6:T:560:MET:HA	6:T:1767:PHE:CZ	1.59	1.37
6:T:2325:LEU:CD2	6:T:2329:ARG:HA	1.53	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:480:ARG:HB3	6:T:1760:TYR:CZ	1.49	1.32
6:T:560:MET:HG2	6:T:1767:PHE:CE1	1.64	1.31
6:T:480:ARG:CD	6:T:1760:TYR:CE1	2.12	1.30
6:T:480:ARG:CD	6:T:1760:TYR:CD1	2.13	1.29
6:T:480:ARG:HB2	6:T:1760:TYR:CZ	1.52	1.28
6:T:2320:LEU:HD21	6:T:2358:SER:OG	1.33	1.27
6:T:2325:LEU:HD21	6:T:2329:ARG:CA	1.69	1.23
6:T:480:ARG:HB2	6:T:1760:TYR:CE1	1.74	1.21
6:T:480:ARG:HB3	6:T:1760:TYR:CE2	1.77	1.20
6:T:694:ASP:OD2	6:T:1585:ARG:NH1	1.73	1.19
6:T:560:MET:HG2	6:T:1767:PHE:CZ	1.76	1.19
6:T:2276:THR:CG2	6:T:2277:PRO:HD3	1.72	1.19
6:T:1594:THR:OG1	6:T:1595:PRO:HD3	1.40	1.18
6:T:694:ASP:CG	6:T:1585:ARG:NH1	2.00	1.13
6:T:1441:LEU:CD1	6:T:1473:LEU:CD1	2.13	1.12
6:T:1441:LEU:HD12	6:T:1473:LEU:HD12	1.28	1.12
6:T:1441:LEU:HD13	6:T:1473:LEU:HD13	1.19	1.11
6:T:629:GLU:CD	6:T:1717:GLN:HB3	1.69	1.11
6:T:381:PHE:HB2	6:T:1858:ASP:OD1	1.50	1.10
6:T:2320:LEU:CD1	6:T:2355:MET:C	2.20	1.10
6:T:480:ARG:CB	6:T:1760:TYR:CE1	2.32	1.09
6:T:480:ARG:CB	6:T:1760:TYR:OH	1.96	1.09
6:T:480:ARG:HB2	6:T:1760:TYR:OH	1.51	1.08
6:T:613:VAL:HG13	6:T:1536:ASP:OD1	1.53	1.07
6:T:1900:LEU:HD23	6:T:1900:LEU:H	1.17	1.06
6:T:1716:LEU:H	6:T:1716:LEU:HD12	1.16	1.05
6:T:1920:ILE:H	6:T:1920:ILE:HD12	1.21	1.05
6:T:1543:LEU:HD22	6:T:1543:LEU:H	1.20	1.05
6:T:1449:LEU:HD22	6:T:1484:PRO:HG2	1.35	1.04
6:T:611:TYR:CZ	6:T:1583:LYS:O	2.10	1.04
6:T:1441:LEU:HB2	6:T:1473:LEU:HD11	1.39	1.04
6:T:560:MET:CA	6:T:1767:PHE:CZ	2.39	1.04
6:T:560:MET:O	6:T:1767:PHE:HE1	1.42	1.03
6:T:480:ARG:NH1	6:T:1760:TYR:HD1	1.55	1.02
6:T:2116:LEU:HD23	6:T:2116:LEU:H	1.22	1.02
6:T:611:TYR:CE1	6:T:1583:LYS:O	2.12	1.02
6:T:694:ASP:OD1	6:T:1585:ARG:NH1	1.91	1.02
6:T:2320:LEU:HD12	6:T:2355:MET:CB	1.84	1.01
6:T:560:MET:CG	6:T:1767:PHE:CE1	2.43	1.01
6:T:2320:LEU:HD11	6:T:2356:SER:N	1.74	1.00
6:T:2276:THR:HG23	6:T:2277:PRO:CD	1.90	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:480:ARG:NH1	6:T:1760:TYR:CD1	2.28	0.99
6:T:480:ARG:NH1	6:T:1760:TYR:HB2	1.77	0.99
6:T:629:GLU:OE1	6:T:1717:GLN:HB3	1.60	0.99
6:T:2320:LEU:CD1	6:T:2355:MET:CA	2.43	0.96
6:T:378:GLY:O	6:T:1856:HIS:NE2	1.99	0.96
6:T:2320:LEU:HD21	6:T:2358:SER:HG	1.27	0.95
6:T:1832:LYS:HE2	6:T:1832:LYS:HA	1.49	0.94
6:T:2320:LEU:CD1	6:T:2355:MET:HB2	1.96	0.94
6:T:694:ASP:OD2	6:T:1585:ARG:CZ	2.16	0.94
6:T:1751:SER:HB2	6:T:1796:LEU:HG	1.48	0.94
6:T:1950:THR:OG1	6:T:1951:PRO:HD3	1.69	0.92
6:T:2325:LEU:HD21	6:T:2329:ARG:HA	0.93	0.92
6:T:339:GLU:CD	6:T:1897:GLU:HG2	1.88	0.92
6:T:629:GLU:HG2	6:T:1720:GLN:OE1	1.69	0.92
6:T:2320:LEU:CD2	6:T:2358:SER:OG	2.17	0.92
6:T:560:MET:HA	6:T:1767:PHE:HZ	0.97	0.92
6:T:1547:MET:HA	6:T:1550:LYS:HE2	1.50	0.92
6:T:480:ARG:C	6:T:1760:TYR:OH	2.08	0.91
6:T:2325:LEU:CD2	6:T:2329:ARG:CA	2.35	0.91
6:T:694:ASP:OD2	6:T:1585:ARG:NE	2.04	0.91
6:T:2276:THR:HG23	6:T:2277:PRO:HD3	0.96	0.91
6:T:2320:LEU:HD12	6:T:2355:MET:HB2	1.47	0.91
6:T:1915:LYS:HA	6:T:1915:LYS:HE2	1.52	0.91
6:T:560:MET:HA	6:T:1767:PHE:CE1	2.05	0.91
6:T:2320:LEU:HD11	6:T:2355:MET:CA	2.01	0.91
6:T:560:MET:CG	6:T:1767:PHE:CZ	2.55	0.90
6:T:2155:GLU:HA	6:T:2158:LEU:HD13	1.54	0.89
6:T:2004:ILE:HG21	6:T:2035:ILE:HD13	1.55	0.89
6:T:1416:ILE:HD13	6:T:1459:THR:OG1	1.72	0.89
6:T:1594:THR:HG1	6:T:1595:PRO:HD3	1.31	0.88
6:T:1628:VAL:HG13	6:T:1675:THR:HG21	1.55	0.88
6:T:2155:GLU:HG3	6:T:2158:LEU:HD22	1.56	0.88
6:T:2207:GLN:HA	6:T:2210:LEU:HD12	1.54	0.88
6:T:560:MET:CA	6:T:1767:PHE:CE1	2.57	0.88
6:T:2115:GLU:OE1	6:T:2115:GLU:N	2.08	0.86
6:T:572:LEU:HA	6:T:1940:TYR:CD2	2.11	0.86
6:T:1553:VAL:HG12	6:T:1592:PHE:HB3	1.56	0.86
6:T:2315:LEU:HD12	6:T:2315:LEU:O	1.76	0.86
6:T:1692:ILE:HA	6:T:1695:LEU:HD12	1.57	0.86
3:D:284:ALA:HB1	4:E:265:GLU:HG2	1.56	0.85
6:T:381:PHE:HD2	6:T:1859:LEU:HD21	1.39	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:2688:THR:HG1	6:T:2729:TRP:HE1	1.20	0.85
6:T:381:PHE:CD2	6:T:1859:LEU:HD21	2.11	0.85
3:D:621:MET:HB3	6:T:2417:GLU:HG3	1.59	0.85
6:T:1799:ARG:N	6:T:1799:ARG:HD2	1.90	0.85
6:T:1493:GLN:HA	6:T:1493:GLN:HE21	1.41	0.85
6:T:572:LEU:CA	6:T:1940:TYR:CD2	2.60	0.84
6:T:1655:ILE:HG12	6:T:1662:VAL:HG12	1.59	0.84
6:T:1995:LEU:HD23	6:T:1995:LEU:H	1.43	0.84
6:T:2325:LEU:HD23	6:T:2329:ARG:HA	1.57	0.83
6:T:560:MET:HG2	6:T:1767:PHE:CD1	2.13	0.83
6:T:2206:LEU:HD12	6:T:2206:LEU:O	1.78	0.83
6:T:560:MET:C	6:T:1767:PHE:HE1	1.81	0.83
6:T:2226:ILE:HD12	6:T:2228:GLU:HB2	1.60	0.83
6:T:1487:MET:HE2	6:T:1487:MET:HA	1.61	0.82
6:T:2239:LEU:HD11	6:T:2259:LEU:HD13	1.60	0.82
6:T:2243:ILE:HG21	6:T:2256:GLY:HA3	1.59	0.82
6:T:1296:LEU:HD13	6:T:1307:CYS:HB2	1.61	0.82
6:T:1449:LEU:HD22	6:T:1484:PRO:CG	2.09	0.82
6:T:1562:LEU:HD12	6:T:1563:PRO:HD2	1.60	0.82
6:T:1801:PHE:HA	6:T:1804:LYS:HD2	1.62	0.82
6:T:2517:LEU:HD12	6:T:2519:LEU:HB2	1.63	0.81
3:D:62:ARG:HD2	3:D:65:ILE:HB	1.61	0.81
6:T:382:THR:HG23	6:T:1900:LEU:HD11	1.63	0.81
6:T:1594:THR:OG1	6:T:1595:PRO:CD	2.28	0.81
6:T:611:TYR:OH	6:T:1583:LYS:O	1.99	0.81
6:T:560:MET:O	6:T:1767:PHE:CE1	2.33	0.80
6:T:1654:ASN:HA	6:T:1657:LYS:HE2	1.63	0.80
6:T:680:ARG:HA	6:T:683:MET:HE2	1.62	0.80
2:B:244:GLU:O	3:D:75:ARG:NH2	2.14	0.80
6:T:838:LEU:HD11	6:T:1251:GLU:HB3	1.64	0.80
6:T:1586:LEU:O	6:T:1586:LEU:HD23	1.83	0.79
6:T:750:ASP:HB2	6:T:753:ASN:HB2	1.64	0.79
6:T:1535:LEU:HD13	6:T:1583:LYS:HE3	1.64	0.79
6:T:1441:LEU:HB2	6:T:1473:LEU:CD1	2.13	0.79
6:T:1979:SER:HA	6:T:1983:ASN:HB2	1.64	0.79
2:B:398:VAL:HA	2:B:401:ARG:HE	1.47	0.79
4:E:246:ARG:NH1	4:E:254:GLU:OE1	2.16	0.79
6:T:799:SER:HB2	6:T:805:PRO:HB3	1.65	0.79
6:T:518:MET:SD	6:T:2317:ILE:HD13	2.23	0.78
3:D:529:LEU:N	3:D:556:GLU:OE2	2.16	0.78
6:T:2168:LEU:HD12	6:T:2212:VAL:HG12	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1493:GLN:HA	6:T:1493:GLN:NE2	1.97	0.78
6:T:1885:ASP:HA	6:T:1888:LYS:HE3	1.65	0.78
6:T:2116:LEU:H	6:T:2116:LEU:CD2	1.97	0.77
6:T:2493:CYS:SG	6:T:2494:LEU:N	2.57	0.77
6:T:573:PRO:HG3	6:T:1940:TYR:CE1	2.20	0.77
6:T:1832:LYS:HE2	6:T:1832:LYS:CA	2.15	0.77
6:T:1562:LEU:CD1	6:T:1563:PRO:HD2	2.13	0.77
6:T:2271:ILE:HG21	6:T:2274:LEU:HD12	1.66	0.77
1:A:188:TYR:HB2	1:A:267:LEU:HD21	1.66	0.77
6:T:773:VAL:HG21	6:T:784:LEU:HD12	1.67	0.77
6:T:730:GLU:HG2	6:T:732:THR:H	1.50	0.76
6:T:340:LEU:O	6:T:344:ARG:NH1	2.18	0.76
6:T:2007:ILE:HG13	6:T:2031:LEU:HD22	1.66	0.76
6:T:351:THR:HA	6:T:354:ILE:HD12	1.67	0.76
6:T:480:ARG:CG	6:T:1760:TYR:CE1	2.69	0.75
6:T:956:ASN:HD21	6:T:2843:LEU:HB3	1.52	0.75
6:T:2241:SER:HA	6:T:2274:LEU:HD21	1.68	0.75
6:T:3412:HIS:NE2	6:T:3585:GLU:OE1	2.20	0.75
6:T:1543:LEU:H	6:T:1543:LEU:CD2	1.96	0.74
6:T:1789:PHE:HB3	6:T:1803:LEU:HD13	1.69	0.74
6:T:570:LEU:HG	6:T:1940:TYR:HE2	1.50	0.74
6:T:2688:THR:OG1	6:T:2729:TRP:NE1	2.17	0.74
6:T:1971:LYS:HE2	6:T:2000:ARG:HG3	1.68	0.74
3:D:62:ARG:NH1	3:D:65:ILE:O	2.21	0.74
6:T:1766:ILE:HD13	6:T:1769:ASN:HD21	1.52	0.74
3:D:585:ILE:HG22	3:D:587:LYS:HZ1	1.52	0.74
6:T:2986:ARG:HH12	6:T:3055:LYS:HE2	1.53	0.74
6:T:3043:PHE:HB3	6:T:3060:TRP:HE3	1.52	0.74
6:T:1449:LEU:CD2	6:T:1484:PRO:HG2	2.15	0.73
6:T:1463:LEU:O	6:T:1463:LEU:HD23	1.89	0.73
5:F:633:GLU:OE2	5:F:655:ASN:ND2	2.21	0.73
6:T:560:MET:C	6:T:1767:PHE:CE1	2.61	0.73
6:T:2090:LEU:HD12	6:T:2093:ARG:HB2	1.70	0.73
6:T:2245:GLN:HA	6:T:2245:GLN:NE2	2.04	0.73
6:T:1543:LEU:HD22	6:T:1543:LEU:N	2.01	0.73
6:T:2116:LEU:HD23	6:T:2116:LEU:N	2.02	0.73
6:T:2329:ARG:HH22	6:T:2367:PRO:HD2	1.53	0.73
3:D:45:CYS:SG	6:T:3497:HIS:NE2	2.62	0.73
6:T:560:MET:CA	6:T:1767:PHE:HZ	1.86	0.73
6:T:1006:SER:O	6:T:1014:ARG:NH1	2.22	0.73
6:T:3054:ALA:H	6:T:3091:LEU:HD22	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:467:GLN:HA	4:E:85:ALA:HB1	1.71	0.72
6:T:917:ILE:HG12	6:T:921:ILE:HG12	1.70	0.72
6:T:65:SER:HA	6:T:76:ARG:HH22	1.54	0.72
6:T:2282:PHE:HB2	6:T:2315:LEU:HD21	1.70	0.72
6:T:2957:HIS:HA	6:T:3434:VAL:HG11	1.72	0.72
1:A:332:PRO:O	1:A:335:ARG:NE	2.23	0.72
6:T:339:GLU:OE2	6:T:1897:GLU:HG2	1.90	0.72
6:T:1482:LEU:HD12	6:T:1485:LEU:HB2	1.70	0.72
6:T:2354:ASN:OD1	6:T:2357:ARG:NH1	2.21	0.72
1:A:107:GLU:OE1	1:A:116:ARG:NH1	2.23	0.71
1:A:285:CYS:SG	1:A:286:ASP:N	2.63	0.71
6:T:381:PHE:CB	6:T:1858:ASP:OD1	2.36	0.71
6:T:2976:ILE:HB	6:T:2980:GLU:HB2	1.71	0.71
6:T:3054:ALA:HB2	6:T:3091:LEU:HB3	1.70	0.71
6:T:2649:ILE:HD12	6:T:2655:ILE:HD13	1.72	0.71
6:T:339:GLU:OE1	6:T:1897:GLU:HG2	1.88	0.71
6:T:1850:ALA:HB1	6:T:1860:PHE:HE2	1.54	0.71
6:T:2138:VAL:HA	6:T:2142:TYR:HB2	1.73	0.71
6:T:560:MET:CB	6:T:1767:PHE:CZ	2.74	0.71
6:T:572:LEU:C	6:T:1940:TYR:CE2	2.64	0.71
6:T:1919:PRO:HG2	6:T:1922:VAL:HB	1.71	0.71
6:T:2811:GLN:HG3	6:T:2814:ARG:HD3	1.73	0.71
6:T:1699:LEU:O	6:T:1699:LEU:HD23	1.90	0.71
6:T:1995:LEU:H	6:T:1995:LEU:CD2	2.02	0.71
6:T:1600:LEU:HD13	6:T:1607:VAL:HG11	1.73	0.70
6:T:1593:ARG:HG2	6:T:1627:ILE:HD11	1.72	0.70
6:T:1829:LYS:O	6:T:1829:LYS:HD3	1.91	0.70
3:D:768:MET:HA	3:D:771:ARG:HG2	1.73	0.70
6:T:2613:ILE:HG21	6:T:2616:LEU:HB2	1.72	0.70
2:B:394:MET:SD	2:B:401:ARG:NH1	2.65	0.70
6:T:1619:GLN:OE1	6:T:1619:GLN:N	2.18	0.70
6:T:1872:ILE:HD11	6:T:1886:ILE:HG21	1.73	0.70
3:D:623:TYR:HB2	3:D:626:ARG:HE	1.54	0.70
6:T:570:LEU:HD11	6:T:1940:TYR:OH	1.92	0.70
6:T:629:GLU:OE2	6:T:1717:GLN:HB3	1.91	0.70
6:T:2700:TRP:HD1	6:T:2736:CYS:HG	1.39	0.70
3:D:35:GLU:OE1	6:T:3731:ARG:NH2	2.25	0.70
6:T:2278:LEU:C	6:T:2278:LEU:HD12	2.12	0.70
6:T:480:ARG:NH1	6:T:1760:TYR:CB	2.55	0.70
6:T:1794:LYS:H	6:T:1794:LYS:HD3	1.56	0.70
6:T:1941:LEU:HD12	6:T:1941:LEU:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:86:ASN:HB2	4:E:89:VAL:HG22	1.74	0.69
6:T:572:LEU:N	6:T:1940:TYR:CD2	2.60	0.69
6:T:3715:VAL:HG23	6:T:3716:THR:H	1.56	0.69
6:T:1635:GLU:H	6:T:1635:GLU:CD	1.93	0.69
6:T:1716:LEU:H	6:T:1716:LEU:CD1	1.94	0.69
6:T:1995:LEU:HD23	6:T:1995:LEU:N	2.07	0.69
6:T:2031:LEU:HD12	6:T:2031:LEU:O	1.93	0.69
3:D:614:GLN:HB2	6:T:2456:ARG:HH12	1.56	0.69
6:T:222:LYS:NZ	6:T:238:TYR:OH	2.24	0.69
6:T:1506:LEU:C	6:T:1506:LEU:HD12	2.13	0.69
6:T:1879:ILE:HB	6:T:1882:ILE:HG12	1.75	0.69
6:T:1915:LYS:HE2	6:T:1915:LYS:CA	2.22	0.69
6:T:2093:ARG:HG2	6:T:2127:LEU:HD11	1.72	0.69
6:T:2325:LEU:HD21	6:T:2329:ARG:N	2.07	0.69
6:T:2320:LEU:O	6:T:2320:LEU:HD23	1.92	0.69
1:A:16:MET:O	1:A:18:LYS:NZ	2.26	0.69
3:D:33:ILE:HD12	3:D:300:ILE:HD11	1.74	0.69
3:D:45:CYS:HG	6:T:3497:HIS:CE1	2.11	0.69
3:D:617:LYS:O	3:D:619:ARG:NH1	2.26	0.69
6:T:966:LEU:HD12	6:T:3540:ASP:HB2	1.72	0.69
6:T:1473:LEU:HD23	6:T:1473:LEU:C	2.14	0.69
6:T:2303:GLU:OE1	6:T:2303:GLU:N	2.19	0.69
6:T:474:ARG:O	6:T:474:ARG:NH2	2.26	0.69
6:T:2320:LEU:HD11	6:T:2355:MET:O	1.90	0.69
2:B:441:THR:OG1	2:B:448:ARG:NH2	2.27	0.68
6:T:1100:MET:O	6:T:1104:ASN:ND2	2.25	0.68
6:T:1900:LEU:H	6:T:1900:LEU:CD2	1.96	0.68
6:T:339:GLU:OE1	6:T:1897:GLU:CG	2.41	0.68
6:T:481:GLN:N	6:T:1760:TYR:OH	2.27	0.68
6:T:1762:LEU:HD23	6:T:1762:LEU:C	2.14	0.68
6:T:2100:LEU:HD23	6:T:2100:LEU:C	2.14	0.68
6:T:1204:GLU:OE1	6:T:3373:ARG:NH1	2.26	0.68
6:T:1300:ASN:HB3	6:T:1303:VAL:HG12	1.76	0.68
6:T:2128:ILE:HG21	6:T:2173:LYS:HB3	1.75	0.68
6:T:1854:LEU:HD23	6:T:1854:LEU:C	2.14	0.68
6:T:3446:PRO:HD3	6:T:3582:PHE:HB2	1.75	0.68
3:D:312:THR:OG1	6:T:3629:GLN:NE2	2.27	0.68
6:T:613:VAL:CG1	6:T:1536:ASP:OD1	2.38	0.68
6:T:1472:LYS:HG3	6:T:1475:LYS:HE2	1.74	0.68
1:A:93:GLU:HG3	1:A:94:LEU:HD12	1.75	0.68
3:D:657:GLU:O	3:D:661:ASN:ND2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:613:VAL:HA	6:T:1536:ASP:OD2	1.94	0.68
6:T:1577:VAL:HG13	6:T:1592:PHE:HE2	1.59	0.68
6:T:2124:LEU:HD23	6:T:2124:LEU:C	2.14	0.68
3:D:670:GLU:OE1	3:D:670:GLU:N	2.26	0.68
6:T:1920:ILE:HD12	6:T:1920:ILE:N	2.04	0.68
6:T:727:LEU:HG	6:T:772:SER:HB3	1.76	0.68
6:T:1907:LEU:HD23	6:T:1907:LEU:C	2.14	0.68
6:T:2955:ARG:HH12	6:T:2990:LYS:HB3	1.59	0.68
1:A:196:ARG:HH12	1:A:250:ILE:HA	1.57	0.67
6:T:2034:LEU:HD23	6:T:2034:LEU:C	2.14	0.67
6:T:2039:GLU:HA	6:T:2039:GLU:OE1	1.94	0.67
1:A:35:VAL:HG21	1:A:81:ASP:HB3	1.76	0.67
4:E:289:GLN:NE2	4:E:291:ILE:O	2.27	0.67
6:T:1361:LEU:HD23	6:T:1421:ILE:HG23	1.76	0.67
6:T:1509:LEU:HD22	6:T:1509:LEU:N	2.09	0.67
2:B:47:TYR:OH	2:B:66:ARG:NH2	2.28	0.67
6:T:2244:THR:HG21	6:T:2274:LEU:HD22	1.77	0.67
6:T:1476:GLU:N	6:T:1476:GLU:OE1	2.28	0.67
6:T:1482:LEU:HG	6:T:1486:LEU:HG	1.77	0.67
6:T:1703:LEU:HD23	6:T:1703:LEU:C	2.15	0.67
2:B:243:LYS:NZ	7:B:501:ATP:O2'	2.28	0.67
6:T:1535:LEU:HD23	6:T:1535:LEU:C	2.14	0.67
1:A:35:VAL:HA	1:A:54:VAL:HG12	1.77	0.67
3:D:48:ARG:HG2	3:D:55:LEU:HD13	1.77	0.67
5:F:537:ASN:O	5:F:538:LEU:HG	1.95	0.67
2:B:112:GLU:OE1	2:B:116:ASN:ND2	2.25	0.67
6:T:1378:LEU:HD12	6:T:1415:CYS:HB2	1.77	0.67
6:T:2387:GLU:OE1	6:T:2390:LEU:N	2.22	0.67
4:E:293:GLN:OE1	4:E:302:GLN:NE2	2.28	0.67
6:T:110:GLU:HG2	6:T:214:LEU:HD13	1.76	0.67
6:T:1941:LEU:HA	6:T:1944:GLN:HE21	1.60	0.66
6:T:2008:ILE:HG12	6:T:2031:LEU:HD21	1.76	0.66
6:T:2320:LEU:HD13	6:T:2355:MET:CA	2.19	0.66
3:D:566:TYR:HH	5:F:638:PHE:HD2	1.43	0.66
6:T:469:ASP:O	6:T:473:ASN:ND2	2.28	0.66
6:T:1586:LEU:HD23	6:T:1586:LEU:C	2.15	0.66
6:T:1777:GLU:OE1	6:T:1777:GLU:HA	1.94	0.66
6:T:1936:VAL:HA	6:T:1939:ARG:HG3	1.77	0.66
6:T:1949:LEU:HD23	6:T:1949:LEU:C	2.15	0.66
6:T:141:ILE:HA	6:T:144:ILE:HD12	1.76	0.66
6:T:968:GLU:OE1	6:T:968:GLU:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1577:VAL:HG21	6:T:1596:LEU:HD11	1.76	0.66
6:T:515:GLU:HA	6:T:518:MET:HE2	1.78	0.66
6:T:1936:VAL:HG23	6:T:1939:ARG:HD3	1.77	0.66
6:T:1485:LEU:HD22	6:T:1503:LEU:HD21	1.77	0.66
6:T:2485:GLU:HG2	6:T:2486:LEU:H	1.61	0.66
5:F:637:LYS:NZ	5:F:654:PRO:O	2.28	0.66
6:T:2014:ILE:HG13	6:T:2024:SER:HB2	1.77	0.66
6:T:2773:ARG:HA	6:T:2776:LEU:HB2	1.78	0.66
6:T:1178:ILE:HD12	6:T:2519:LEU:HD23	1.78	0.65
6:T:1179:TYR:HD2	6:T:1184:ALA:HA	1.61	0.65
6:T:1900:LEU:HD23	6:T:1900:LEU:N	2.01	0.65
6:T:943:HIS:NE2	6:T:2818:ASP:OD1	2.24	0.65
6:T:1570:LEU:HD23	6:T:1570:LEU:C	2.17	0.65
6:T:1315:SER:O	6:T:1319:GLY:HA2	1.94	0.65
6:T:2325:LEU:HD11	6:T:2328:SER:HB3	1.78	0.65
3:D:274:ASN:OD1	3:D:275:ASP:N	2.29	0.65
6:T:2118:LEU:C	6:T:2118:LEU:HD23	2.16	0.65
6:T:1538:LEU:HD22	6:T:1546:GLN:HE22	1.61	0.65
6:T:1546:GLN:HG3	6:T:1548:PRO:HD2	1.79	0.65
6:T:1815:VAL:HG21	6:T:1870:ILE:HD11	1.79	0.65
6:T:2450:ARG:NH1	6:T:2475:LEU:O	2.30	0.65
6:T:339:GLU:CD	6:T:1897:GLU:CG	2.64	0.65
6:T:2604:ASN:HD22	6:T:2632:ALA:HB2	1.62	0.65
6:T:1689:GLY:HA2	6:T:1692:ILE:HG23	1.77	0.65
3:D:45:CYS:O	6:T:3497:HIS:NE2	2.30	0.65
6:T:572:LEU:N	6:T:1940:TYR:HD2	1.95	0.65
6:T:1036:PRO:HD3	6:T:2498:SER:HA	1.79	0.65
6:T:1662:VAL:HG11	6:T:1705:THR:HG21	1.78	0.65
6:T:1718:LEU:C	6:T:1718:LEU:HD12	2.18	0.65
6:T:382:THR:HG22	6:T:1858:ASP:OD2	1.96	0.65
6:T:2184:LEU:O	6:T:2184:LEU:HD23	1.97	0.65
2:B:71:LEU:HD11	2:B:229:LEU:HD23	1.79	0.65
6:T:944:ASN:OD1	6:T:947:ARG:NH2	2.30	0.65
3:D:533:GLU:OE1	3:D:533:GLU:N	2.29	0.64
6:T:813:ARG:HD3	6:T:817:ARG:HD3	1.79	0.64
6:T:1797:ASP:HA	6:T:1800:ILE:HD12	1.79	0.64
6:T:2464:ALA:HA	6:T:2596:ILE:HA	1.78	0.64
2:B:20:ASP:OD2	2:B:452:SER:OG	2.14	0.64
6:T:780:ASN:HB2	6:T:782:VAL:HG12	1.77	0.64
6:T:1848:ILE:HG21	6:T:1852:ASP:H	1.63	0.64
6:T:2803:PHE:HA	6:T:2809:GLY:HA3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:2369:VAL:O	6:T:2415:ARG:NH1	2.29	0.64
6:T:466:ILE:HA	6:T:1716:LEU:HD21	1.80	0.64
6:T:1939:ARG:HB3	6:T:1939:ARG:CZ	2.26	0.64
6:T:2271:ILE:HG12	6:T:2274:LEU:HG	1.80	0.64
6:T:2421:LEU:HD13	6:T:2460:TRP:HB2	1.78	0.64
3:D:615:LEU:HD21	6:T:2452:TYR:HB3	1.79	0.64
5:F:588:ILE:HD11	5:F:593:ARG:HH21	1.63	0.64
6:T:2768:ASP:OD1	6:T:2769:TRP:N	2.31	0.64
1:A:66:THR:OG1	1:A:68:ARG:NH2	2.27	0.64
1:A:154:ASP:HA	1:A:300:SER:O	1.96	0.64
1:A:334:GLU:OE1	1:A:334:GLU:N	2.30	0.64
5:F:581:LEU:HD23	5:F:615:LYS:HE3	1.79	0.64
6:T:1265:ILE:HG23	6:T:1313:THR:HG21	1.79	0.64
6:T:1567:ASP:HB3	6:T:1569:PHE:HD2	1.61	0.64
6:T:2792:GLN:HG2	6:T:2820:GLY:HA2	1.78	0.64
6:T:1487:MET:HA	6:T:1487:MET:CE	2.26	0.64
6:T:1881:GLU:OE1	6:T:1881:GLU:N	2.19	0.64
6:T:2168:LEU:HD23	6:T:2168:LEU:C	2.19	0.64
6:T:1821:LEU:HB3	6:T:1874:ALA:HB1	1.78	0.64
6:T:2869:ASN:O	6:T:2872:SER:OG	2.15	0.64
2:B:93:ALA:O	2:B:97:GLU:HB2	1.97	0.64
6:T:2680:ARG:HE	6:T:2689:ASN:HD22	1.44	0.64
6:T:3004:ASP:O	6:T:3008:ASN:N	2.30	0.64
3:D:561:GLN:OE1	3:D:561:GLN:N	2.31	0.63
4:E:269:LYS:O	4:E:270:ARG:NE	2.31	0.63
6:T:2276:THR:CG2	6:T:2277:PRO:CD	2.63	0.63
6:T:2632:ALA:HB1	6:T:2635:GLN:HB2	1.79	0.63
6:T:934:PRO:HB3	6:T:2825:LEU:HB3	1.81	0.63
3:D:303:ILE:HD13	3:D:315:ILE:HD13	1.79	0.63
6:T:570:LEU:HG	6:T:1940:TYR:CE2	2.34	0.63
6:T:626:PHE:O	6:T:1587:GLN:NE2	2.31	0.63
6:T:1854:LEU:HD23	6:T:1854:LEU:O	1.97	0.63
3:D:347:ARG:NH1	3:D:582:PHE:O	2.32	0.63
6:T:2373:ALA:HA	6:T:2376:LEU:HD12	1.80	0.63
2:B:152:ARG:NH1	2:B:407:ASN:OD1	2.32	0.63
6:T:336:CYS:HB2	6:T:344:ARG:HH21	1.62	0.63
1:A:14:SER:HB2	1:A:158:GLY:H	1.63	0.63
4:E:84:LYS:HG2	4:E:90:THR:HG22	1.79	0.63
6:T:1529:TRP:HB3	6:T:1552:ILE:HD11	1.80	0.63
6:T:1203:ASP:OD1	6:T:1204:GLU:N	2.32	0.63
6:T:1476:GLU:HG2	6:T:1477:LEU:HD22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:2590:PRO:HG2	6:T:2592:HIS:CE1	2.33	0.63
6:T:3060:TRP:O	6:T:3064:ASN:ND2	2.32	0.63
6:T:148:TYR:OH	6:T:218:MET:SD	2.54	0.63
6:T:956:ASN:ND2	6:T:2843:LEU:O	2.31	0.63
6:T:1879:ILE:HG13	6:T:1879:ILE:O	1.99	0.63
6:T:2680:ARG:NH1	6:T:3638:GLU:OE2	2.31	0.63
6:T:480:ARG:CA	6:T:1760:TYR:OH	2.46	0.62
6:T:615:ASN:HB3	6:T:618:LEU:HD13	1.80	0.62
6:T:856:GLU:HA	6:T:859:VAL:HG12	1.80	0.62
6:T:1304:ARG:HH11	6:T:1352:GLY:HA2	1.63	0.62
6:T:3357:GLN:HE22	6:T:3369:ILE:H	1.47	0.62
6:T:3505:ASP:OD2	6:T:3508:ILE:N	2.30	0.62
1:A:97:ALA:O	1:A:101:HIS:NE2	2.32	0.62
6:T:612:THR:OG1	6:T:1583:LYS:NZ	2.32	0.62
6:T:2704:GLN:HG3	6:T:2733:TRP:HE1	1.62	0.62
6:T:2773:ARG:NH1	6:T:2802:ASN:OD1	2.33	0.62
1:A:205:GLU:HA	1:A:208:ILE:HG22	1.81	0.62
2:B:44:TYR:HB3	2:B:74:ILE:HD11	1.82	0.62
3:D:33:ILE:O	3:D:36:ARG:HD3	2.00	0.62
4:E:98:SER:OG	4:E:100:GLU:OE1	2.18	0.62
6:T:568:PRO:HG2	6:T:569:ILE:HD12	1.80	0.62
6:T:767:LYS:O	6:T:771:MET:HG2	1.99	0.62
6:T:3244:ASP:OD1	6:T:3247:ARG:NH2	2.32	0.62
6:T:3410:VAL:HB	6:T:3412:HIS:CE1	2.34	0.62
1:A:196:ARG:HD3	1:A:198:TYR:HE2	1.64	0.62
6:T:2329:ARG:HH11	6:T:2368:THR:HG22	1.63	0.62
6:T:3122:ASP:OD1	6:T:3123:SER:N	2.31	0.62
6:T:3589:SER:OG	6:T:3615:HIS:O	2.17	0.62
2:B:119:GLU:HA	2:B:122:LYS:HE2	1.82	0.62
6:T:339:GLU:HA	6:T:1898:ASP:OD1	1.99	0.62
6:T:2762:CYS:SG	6:T:2763:GLY:N	2.72	0.62
1:A:141:SER:HB3	1:A:339:VAL:HG12	1.82	0.62
3:D:550:ASP:OD2	5:F:652:ARG:NH1	2.32	0.62
6:T:1053:GLU:HG2	6:T:1054:ARG:HG2	1.81	0.62
6:T:2303:GLU:H	6:T:2303:GLU:CD	2.02	0.62
6:T:3096:LYS:HD2	6:T:3428:LYS:HG2	1.81	0.62
6:T:3737:ASP:OD1	6:T:3738:VAL:N	2.33	0.62
6:T:1771:ILE:HD12	6:T:1814:GLU:HB2	1.82	0.62
6:T:1884:LYS:HA	6:T:1887:ILE:HD12	1.82	0.62
6:T:2690:ILE:HA	6:T:3715:VAL:HA	1.82	0.62
6:T:114:ASN:O	6:T:215:ARG:NH1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:2302:GLU:OE2	6:T:2302:GLU:N	2.20	0.62
6:T:3060:TRP:HD1	6:T:3084:CYS:HG	1.45	0.62
6:T:2004:ILE:HD13	6:T:2035:ILE:HD13	1.82	0.62
6:T:3578:SER:OG	6:T:3580:ASN:ND2	2.33	0.62
6:T:21:LEU:HD12	6:T:24:ARG:HH12	1.65	0.61
6:T:560:MET:HG2	6:T:1767:PHE:CE2	2.31	0.61
6:T:2537:ILE:HG22	6:T:2539:SER:H	1.65	0.61
6:T:3306:ASP:OD1	6:T:3309:THR:N	2.32	0.61
1:A:304:THR:O	1:A:335:ARG:NH1	2.32	0.61
6:T:1030:LYS:NZ	6:T:2485:GLU:O	2.33	0.61
6:T:1776:LYS:HG2	6:T:1776:LYS:O	1.99	0.61
3:D:70:LYS:HD3	3:D:540:ALA:HB2	1.82	0.61
6:T:1562:LEU:CG	6:T:1563:PRO:HD2	2.29	0.61
6:T:1585:ARG:O	6:T:1585:ARG:HG3	2.00	0.61
6:T:3540:ASP:OD1	6:T:3541:PHE:N	2.33	0.61
6:T:355:LEU:HD13	6:T:364:LEU:HD13	1.83	0.61
6:T:413:LYS:HG3	6:T:416:LYS:HE3	1.81	0.61
6:T:1737:GLU:OE1	6:T:1737:GLU:N	2.19	0.61
5:F:551:LEU:HD13	5:F:627:LEU:HD22	1.81	0.61
6:T:249:PHE:O	6:T:288:ARG:NH1	2.34	0.61
6:T:1903:GLN:HE21	6:T:1941:LEU:HG	1.66	0.61
6:T:2184:LEU:N	6:T:2185:PRO:HD2	2.14	0.61
6:T:2552:ASP:OD2	6:T:2555:ALA:N	2.30	0.61
6:T:1438:ILE:HA	6:T:1473:LEU:CD1	2.31	0.61
6:T:1543:LEU:HG	6:T:1591:PRO:HG3	1.83	0.61
6:T:1881:GLU:H	6:T:1881:GLU:CD	2.04	0.61
6:T:3400:VAL:O	6:T:3401:HIS:ND1	2.34	0.61
4:E:243:LEU:HD23	4:E:246:ARG:HD3	1.83	0.61
6:T:1340:LYS:NZ	6:T:1344:ALA:O	2.33	0.61
6:T:1800:ILE:HG22	6:T:1804:LYS:HE3	1.83	0.61
6:T:2546:ILE:HA	6:T:2549:PHE:HD2	1.64	0.61
2:B:481:GLU:O	2:B:485:ASN:ND2	2.33	0.61
6:T:690:PHE:HA	6:T:693:MET:HE3	1.83	0.61
6:T:2184:LEU:HD23	6:T:2184:LEU:C	2.21	0.61
3:D:649:ILE:HG13	3:D:688:ILE:HD12	1.82	0.60
6:T:1449:LEU:HD13	6:T:1484:PRO:HB2	1.83	0.60
6:T:1574:LEU:HD22	6:T:1623:PHE:HE2	1.65	0.60
6:T:2007:ILE:HD11	6:T:2031:LEU:HD13	1.83	0.60
6:T:3008:ASN:O	6:T:3010:ASN:ND2	2.34	0.60
6:T:10:PHE:HB2	6:T:13:ARG:NE	2.16	0.60
6:T:1337:ILE:HG23	6:T:1353:ASN:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:463:GLY:HA2	2:B:466:HIS:HE1	1.67	0.60
6:T:1757:LYS:HZ1	6:T:1802:VAL:HG13	1.65	0.60
6:T:2324:LEU:O	6:T:2324:LEU:HD12	2.01	0.60
6:T:306:ALA:HA	6:T:309:PHE:CE2	2.35	0.60
6:T:422:LEU:HD13	6:T:432:GLN:HB3	1.83	0.60
6:T:466:ILE:HG12	6:T:1716:LEU:HD11	1.83	0.60
6:T:2175:LYS:HD3	6:T:2175:LYS:N	2.16	0.60
6:T:2315:LEU:HD12	6:T:2315:LEU:C	2.22	0.60
6:T:2465:ASP:OD1	6:T:2466:TYR:N	2.34	0.60
1:A:200:PHE:HD1	1:A:205:GLU:HB2	1.65	0.60
3:D:323:ARG:HH12	5:F:561:PRO:HD3	1.67	0.60
3:D:649:ILE:H	3:D:688:ILE:HG23	1.67	0.60
3:D:719:SER:O	3:D:722:GLN:NE2	2.33	0.60
6:T:693:MET:HG3	6:T:694:ASP:H	1.66	0.60
6:T:957:ARG:NH2	6:T:2893:ASP:OD2	2.33	0.60
6:T:1179:TYR:HB3	6:T:1183:LEU:HG	1.84	0.60
6:T:1300:ASN:HD22	6:T:1303:VAL:H	1.50	0.60
6:T:1913:ILE:HD12	6:T:1923:VAL:HG22	1.83	0.60
6:T:2289:HIS:HA	6:T:2292:ILE:HG12	1.83	0.60
6:T:2474:GLN:OE1	6:T:2546:ILE:HD12	2.02	0.60
1:A:78:ASN:ND2	1:A:81:ASP:OD2	2.35	0.60
6:T:1840:LYS:HD2	6:T:1840:LYS:C	2.22	0.60
6:T:1897:GLU:OE1	6:T:1897:GLU:N	2.33	0.60
4:E:292:THR:HG22	4:E:295:LEU:HD12	1.84	0.60
6:T:1420:ALA:HB2	6:T:1462:ALA:HB1	1.83	0.60
6:T:1814:GLU:HG2	6:T:1821:LEU:HD12	1.84	0.60
6:T:1936:VAL:HG23	6:T:1939:ARG:HH11	1.66	0.60
6:T:1936:VAL:HG22	6:T:1936:VAL:O	2.02	0.60
6:T:2460:TRP:HD1	6:T:2462:PHE:HD1	1.49	0.60
6:T:3067:ARG:NH2	6:T:3077:PHE:O	2.35	0.60
6:T:3151:MET:SD	6:T:3151:MET:N	2.68	0.60
3:D:565:LEU:HB3	5:F:585:LEU:HD13	1.84	0.60
6:T:3260:TYR:HA	6:T:3307:TYR:OH	2.02	0.60
6:T:706:LEU:HG	6:T:707:PRO:HD3	1.83	0.60
6:T:1199:HIS:ND1	6:T:3333:ASN:OD1	2.35	0.60
6:T:1716:LEU:HD12	6:T:1716:LEU:N	2.01	0.60
6:T:1962:THR:OG1	6:T:1963:PRO:HD3	2.01	0.60
6:T:21:LEU:O	6:T:24:ARG:NH1	2.35	0.60
6:T:679:ALA:O	6:T:683:MET:HG3	2.00	0.60
6:T:1112:LEU:O	6:T:1115:VAL:HG12	2.01	0.60
6:T:1244:VAL:O	6:T:1248:THR:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:2516:ASP:OD1	6:T:2517:LEU:N	2.34	0.60
6:T:3333:ASN:HB2	6:T:3336:VAL:HG22	1.82	0.60
1:A:163:VAL:HG22	1:A:175:ILE:HG23	1.84	0.59
3:D:358:HIS:HB2	4:E:115:ASN:HA	1.84	0.59
6:T:344:ARG:HA	6:T:347:LEU:HB3	1.84	0.59
6:T:411:ILE:O	6:T:415:ILE:HG12	2.01	0.59
6:T:573:PRO:HD3	6:T:1940:TYR:CG	2.38	0.59
6:T:2894:ASP:OD1	6:T:2895:VAL:N	2.36	0.59
1:A:220:ALA:O	1:A:312:ARG:NH1	2.35	0.59
2:B:467:GLN:NE2	2:B:468:LEU:HB2	2.18	0.59
6:T:110:GLU:O	6:T:215:ARG:NH1	2.31	0.59
6:T:2218:LYS:HG3	6:T:2218:LYS:O	2.03	0.59
6:T:2587:LEU:O	6:T:2594:ARG:NH2	2.36	0.59
6:T:355:LEU:HD12	6:T:398:PHE:CE1	2.37	0.59
6:T:793:LEU:HD21	6:T:831:ILE:HD11	1.83	0.59
6:T:877:PRO:HA	6:T:916:ILE:HD11	1.83	0.59
6:T:922:ASP:N	6:T:922:ASP:OD1	2.35	0.59
6:T:1634:LYS:HD2	6:T:1634:LYS:C	2.22	0.59
6:T:1825:LEU:HG	6:T:1878:ILE:HG21	1.83	0.59
6:T:1838:HIS:HE1	6:T:1882:ILE:HG23	1.67	0.59
6:T:2301:LEU:HG	6:T:2304:ALA:HB3	1.83	0.59
6:T:3155:ILE:O	6:T:3159:ILE:HG13	2.02	0.59
1:A:100:GLU:OE1	1:A:100:GLU:N	2.35	0.59
6:T:1182:GLU:OE2	6:T:1182:GLU:N	2.26	0.59
6:T:2549:PHE:HD1	6:T:2556:ILE:HG22	1.67	0.59
6:T:3397:ASP:OD1	6:T:3398:GLY:N	2.35	0.59
4:E:169:ILE:O	4:E:173:PHE:HB2	2.03	0.59
6:T:381:PHE:CB	6:T:1859:LEU:HD21	2.33	0.59
6:T:2285:LEU:HD21	6:T:2311:LEU:HD11	1.85	0.59
6:T:2477:TYR:HD2	6:T:2542:ILE:HB	1.67	0.59
1:A:282:ILE:HG23	1:A:293:LEU:HD23	1.85	0.59
6:T:480:ARG:HD2	6:T:1760:TYR:CE1	2.29	0.59
6:T:917:ILE:HG23	6:T:921:ILE:HD11	1.83	0.59
6:T:1441:LEU:CB	6:T:1473:LEU:CD1	2.81	0.59
6:T:2461:GLU:HA	6:T:2592:HIS:CG	2.37	0.59
2:B:78:GLY:O	2:B:113:PRO:HG3	2.02	0.59
6:T:1877:GLU:CD	6:T:1877:GLU:H	2.05	0.59
6:T:2128:ILE:HD12	6:T:2173:LYS:HG3	1.85	0.59
6:T:3472:ASN:HD22	6:T:3482:PRO:HG2	1.68	0.59
1:A:213:LYS:NZ	1:A:214:GLU:OE2	2.35	0.59
6:T:467:ILE:O	6:T:470:SER:OG	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:626:PHE:HB3	6:T:630:GLU:HB2	1.84	0.59
6:T:2347:ASN:OD1	6:T:2348:PHE:N	2.34	0.59
6:T:2647:THR:HG22	6:T:2648:SER:H	1.68	0.59
6:T:1438:ILE:HG23	6:T:1473:LEU:HG	1.84	0.58
6:T:1949:LEU:HG	6:T:1953:LEU:HD23	1.84	0.58
6:T:3277:GLU:O	6:T:3281:VAL:HG23	2.02	0.58
1:A:89:THR:HA	1:A:93:GLU:HB3	1.84	0.58
6:T:2090:LEU:HD12	6:T:2090:LEU:O	2.03	0.58
6:T:2229:GLU:HG3	6:T:2233:LYS:HG3	1.84	0.58
6:T:2611:SER:HA	6:T:2639:ILE:HD11	1.84	0.58
6:T:2894:ASP:OD1	6:T:2896:ASN:N	2.35	0.58
2:B:190:ILE:HD11	2:B:292:LEU:HD22	1.86	0.58
3:D:346:LYS:H	3:D:346:LYS:HD2	1.66	0.58
6:T:18:ASP:O	6:T:23:SER:OG	2.19	0.58
6:T:1350:GLN:O	6:T:1354:VAL:HG23	2.04	0.58
6:T:1793:ASP:HA	6:T:1800:ILE:HD13	1.84	0.58
2:B:416:SER:HA	2:B:448:ARG:HH11	1.68	0.58
6:T:1737:GLU:H	6:T:1737:GLU:CD	2.04	0.58
6:T:716:ASP:OD1	6:T:717:SER:N	2.36	0.58
6:T:776:PHE:HB3	6:T:779:ILE:HG22	1.85	0.58
6:T:2341:ASP:O	6:T:2385:ARG:NH1	2.36	0.58
2:B:178:LYS:N	4:E:188:ASP:OD2	2.34	0.58
6:T:837:VAL:HA	6:T:840:GLN:HE21	1.68	0.58
6:T:2851:GLU:OE1	6:T:2884:TRP:NE1	2.35	0.58
6:T:3465:THR:OG1	6:T:3466:THR:N	2.37	0.58
3:D:377:HIS:O	3:D:381:VAL:HG23	2.04	0.58
6:T:365:PRO:HG3	6:T:398:PHE:HZ	1.67	0.58
6:T:2325:LEU:HG	6:T:2329:ARG:HB3	1.85	0.58
6:T:2335:THR:O	6:T:2339:LEU:HG	2.03	0.58
6:T:2646:ASN:ND2	6:T:2647:THR:OG1	2.36	0.58
3:D:760:MET:O	3:D:764:ILE:HG12	2.04	0.58
6:T:854:GLU:OE1	6:T:854:GLU:N	2.29	0.58
6:T:2158:LEU:H	6:T:2158:LEU:HD12	1.67	0.58
6:T:2704:GLN:O	6:T:2708:GLU:HG2	2.02	0.58
6:T:1323:VAL:HG12	6:T:1366:THR:HG22	1.84	0.58
6:T:2158:LEU:HD12	6:T:2158:LEU:N	2.19	0.58
6:T:2228:GLU:N	6:T:2228:GLU:OE1	2.36	0.58
2:B:14:VAL:HG11	4:E:91:LEU:HD13	1.84	0.58
2:B:262:LEU:O	2:B:282:ASN:ND2	2.37	0.58
2:B:397:ASP:OD1	2:B:398:VAL:N	2.30	0.58
5:F:556:SER:OG	6:T:3519:THR:OG1	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1216:ILE:HD11	6:T:1237:LEU:HD23	1.84	0.58
6:T:1372:GLU:OE2	6:T:1432:GLN:NE2	2.37	0.58
6:T:1568:MET:HE3	6:T:1568:MET:O	2.04	0.58
6:T:1750:PHE:O	6:T:1750:PHE:HD1	1.87	0.58
3:D:78:ILE:HG13	3:D:79:ARG:H	1.68	0.57
6:T:1562:LEU:HG	6:T:1563:PRO:HD2	1.86	0.57
6:T:2460:TRP:HD1	6:T:2462:PHE:CD1	2.21	0.57
6:T:2811:GLN:HE21	6:T:2814:ARG:HD3	1.69	0.57
6:T:3131:TRP:HD1	6:T:3163:TYR:CZ	2.22	0.57
6:T:126:PHE:CZ	6:T:130:LYS:HD3	2.38	0.57
6:T:1281:GLY:HA2	6:T:1285:LEU:HB2	1.86	0.57
6:T:1617:LEU:HB2	6:T:1620:LEU:HB3	1.86	0.57
6:T:2320:LEU:HD23	6:T:2320:LEU:C	2.25	0.57
6:T:851:LEU:HA	6:T:854:GLU:HB3	1.86	0.57
6:T:1173:GLU:OE1	6:T:1174:LYS:NZ	2.37	0.57
6:T:1234:GLN:NE2	6:T:1271:THR:OG1	2.37	0.57
6:T:1821:LEU:HG	6:T:1821:LEU:O	2.02	0.57
1:A:103:VAL:HG12	1:A:129:VAL:HG11	1.86	0.57
4:E:82:GLU:HG3	4:E:92:ARG:HG2	1.85	0.57
6:T:10:PHE:HA	6:T:30:GLU:HG3	1.86	0.57
6:T:19:ALA:O	6:T:23:SER:N	2.37	0.57
6:T:1486:LEU:HD23	6:T:1489:LEU:HD12	1.86	0.57
6:T:2240:THR:HG23	6:T:2259:LEU:HD22	1.85	0.57
6:T:2357:ARG:O	6:T:2360:ILE:HG22	2.05	0.57
6:T:3060:TRP:HD1	6:T:3084:CYS:SG	2.27	0.57
2:B:231:ASP:OD1	2:B:235:ASN:ND2	2.37	0.57
6:T:832:LYS:HG3	6:T:833:PRO:HD3	1.87	0.57
6:T:1490:SER:HA	6:T:1521:LYS:HD2	1.86	0.57
6:T:1930:LEU:HB3	6:T:1946:LEU:HD21	1.85	0.57
6:T:25:TYR:O	6:T:29:SER:OG	2.21	0.57
6:T:480:ARG:HD3	6:T:1760:TYR:CG	2.16	0.57
6:T:698:PHE:O	6:T:702:ILE:HG22	2.04	0.57
6:T:2432:ARG:HD3	6:T:2550:TYR:CZ	2.38	0.57
6:T:80:LEU:HD22	6:T:120:LYS:HB3	1.87	0.57
6:T:612:THR:HB	6:T:1532:VAL:HG11	1.86	0.57
6:T:751:LEU:HB2	6:T:808:TYR:CZ	2.40	0.57
6:T:1510:LEU:HD23	6:T:1513:TYR:HE1	1.70	0.57
6:T:1949:LEU:HD23	6:T:1949:LEU:O	2.03	0.57
2:B:126:GLU:O	2:B:130:GLU:HB3	2.05	0.57
2:B:130:GLU:O	2:B:133:GLN:NE2	2.38	0.57
6:T:2322:VAL:HG23	6:T:2322:VAL:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:2621:HIS:ND1	6:T:2622:LEU:HG	2.20	0.57
6:T:3202:ARG:O	6:T:3205:TRP:NE1	2.36	0.57
6:T:3551:GLN:O	6:T:3554:SER:OG	2.21	0.57
3:D:597:PHE:CD1	5:F:639:ARG:HB2	2.40	0.57
3:D:645:ARG:O	3:D:736:ARG:NH2	2.33	0.57
6:T:1543:LEU:HD12	6:T:1549:THR:HG21	1.86	0.57
6:T:2209:VAL:HA	6:T:2212:VAL:HG13	1.87	0.57
6:T:2481:ASN:OD1	6:T:2482:ARG:N	2.38	0.57
6:T:507:ILE:HG13	6:T:508:GLN:HG2	1.86	0.57
6:T:1036:PRO:HG2	6:T:1039:TYR:HB2	1.87	0.57
6:T:1962:THR:N	6:T:1963:PRO:HD2	2.20	0.57
6:T:3255:ASP:OD1	6:T:3256:GLY:N	2.38	0.57
6:T:146:GLN:OE1	6:T:150:ASN:ND2	2.38	0.56
6:T:892:ASP:OD1	6:T:892:ASP:N	2.38	0.56
6:T:2426:VAL:HG13	6:T:2428:ASP:H	1.70	0.56
3:D:354:GLN:OE1	4:E:182:ARG:NH1	2.38	0.56
6:T:985:MET:HG2	6:T:2570:SER:HB2	1.88	0.56
1:A:363:ASP:OD1	4:E:76:SER:N	2.24	0.56
3:D:675:HIS:NE2	6:T:2622:LEU:HB2	2.20	0.56
4:E:199:GLU:OE1	4:E:199:GLU:N	2.30	0.56
6:T:240:GLN:O	6:T:244:THR:HG23	2.05	0.56
6:T:352:ARG:HD3	6:T:394:THR:HG22	1.88	0.56
6:T:942:SER:O	6:T:946:VAL:HG23	2.05	0.56
6:T:1379:GLN:O	6:T:1383:VAL:HG23	2.05	0.56
6:T:2036:LEU:HD23	6:T:2123:ILE:HD12	1.87	0.56
6:T:2847:GLN:NE2	6:T:2851:GLU:OE2	2.39	0.56
6:T:3688:LEU:HA	6:T:3691:MET:HE2	1.87	0.56
6:T:2680:ARG:HE	6:T:2689:ASN:ND2	2.03	0.56
2:B:222:ASP:N	2:B:222:ASP:OD1	2.38	0.56
5:F:627:LEU:HD13	5:F:629:ILE:HG12	1.87	0.56
6:T:80:LEU:O	6:T:84:ASN:ND2	2.39	0.56
6:T:2332:PHE:O	6:T:2336:VAL:HG23	2.06	0.56
6:T:422:LEU:HD12	6:T:474:ARG:HG2	1.87	0.56
6:T:1040:THR:OG1	6:T:1041:GLU:OE1	2.24	0.56
6:T:1426:GLU:OE1	6:T:1426:GLU:N	2.38	0.56
6:T:2775:ALA:O	6:T:2778:GLN:NE2	2.38	0.56
6:T:99:VAL:HG21	6:T:125:LEU:HD12	1.87	0.56
6:T:755:ASP:OD1	6:T:758:THR:HG22	2.05	0.56
6:T:808:TYR:O	6:T:812:ILE:HG12	2.05	0.56
6:T:1205:THR:O	6:T:1208:ASN:N	2.39	0.56
6:T:2329:ARG:O	6:T:2333:LEU:HG	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:272:LEU:HD11	3:D:566:TYR:HE1	1.71	0.56
3:D:292:TYR:O	3:D:296:THR:HG23	2.05	0.56
3:D:549:VAL:HG23	3:D:550:ASP:H	1.71	0.56
6:T:31:LEU:HD22	6:T:82:ILE:HG12	1.87	0.56
6:T:1271:THR:HG23	6:T:1272:PHE:HD1	1.70	0.56
6:T:2188:GLN:HE21	6:T:2192:GLU:HB3	1.70	0.56
6:T:3155:ILE:HG22	6:T:3159:ILE:HD11	1.87	0.56
6:T:3729:SER:OG	6:T:3732:ASN:OD1	2.23	0.56
6:T:434:MET:O	6:T:438:LEU:HG	2.05	0.56
6:T:1354:VAL:O	6:T:1358:THR:HG23	2.06	0.56
6:T:3384:THR:HG23	6:T:3385:HIS:HD2	1.71	0.56
2:B:287:GLY:HA2	2:B:290:GLU:HB3	1.87	0.56
6:T:834:ILE:H	6:T:834:ILE:HD12	1.71	0.56
6:T:1110:PHE:HB3	6:T:1145:ILE:HD13	1.88	0.56
6:T:1463:LEU:HD23	6:T:1463:LEU:C	2.26	0.56
6:T:1619:GLN:H	6:T:1619:GLN:CD	2.07	0.56
6:T:1641:GLU:HG2	6:T:1676:MET:HE2	1.87	0.56
6:T:2236:ILE:HB	6:T:2259:LEU:HD21	1.87	0.56
1:A:168:GLY:HA3	3:D:384:CYS:HB3	1.87	0.55
2:B:21:PRO:HB2	2:B:75:ILE:HG13	1.88	0.55
6:T:327:ASP:HA	6:T:330:ILE:HG22	1.88	0.55
6:T:3436:THR:HG23	6:T:3441:ILE:HD13	1.86	0.55
6:T:2350:ARG:HA	6:T:2353:VAL:HG22	1.87	0.55
1:A:39:ARG:NH2	1:A:62:ARG:O	2.40	0.55
1:A:117:GLU:OE1	4:E:94:TRP:NE1	2.40	0.55
2:B:210:LYS:N	2:B:217:ILE:O	2.39	0.55
3:D:595:ASN:OD1	3:D:596:GLY:N	2.31	0.55
5:F:577:TYR:O	5:F:580:HIS:N	2.39	0.55
5:F:580:HIS:CG	5:F:581:LEU:N	2.74	0.55
3:D:683:SER:OG	3:D:684:TYR:N	2.40	0.55
6:T:3041:GLN:O	6:T:3045:THR:HG23	2.06	0.55
6:T:826:ASN:OD1	6:T:827:LEU:N	2.38	0.55
6:T:1673:PHE:HZ	6:T:1692:ILE:HG22	1.71	0.55
6:T:1740:GLN:HE22	6:T:1781:ASN:HB2	1.71	0.55
6:T:1895:LYS:H	6:T:1895:LYS:HD2	1.72	0.55
6:T:2482:ARG:HH21	6:T:2539:SER:HA	1.72	0.55
6:T:2892:TRP:CD2	6:T:3437:ARG:HG2	2.42	0.55
3:D:575:LYS:HE2	3:D:577:ASP:HB3	1.88	0.55
6:T:410:GLU:O	6:T:414:THR:HG23	2.07	0.55
6:T:796:LEU:HD13	6:T:838:LEU:HD23	1.88	0.55
6:T:972:LEU:HD23	6:T:998:GLN:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1702:THR:HA	6:T:1705:THR:HG22	1.87	0.55
6:T:2701:ASP:N	6:T:2701:ASP:OD1	2.39	0.55
1:A:358:SER:OG	1:A:361:GLU:N	2.33	0.55
4:E:274:GLU:HB3	4:E:275:ARG:NH2	2.22	0.55
5:F:581:LEU:HG	5:F:615:LYS:HB2	1.88	0.55
6:T:1864:LEU:HD11	6:T:1893:PHE:HZ	1.71	0.55
6:T:2100:LEU:HD21	6:T:2121:ILE:HD13	1.88	0.55
6:T:3154:HIS:O	6:T:3158:ARG:NH1	2.39	0.55
6:T:3416:GLU:HG3	6:T:3420:PHE:CE2	2.42	0.55
6:T:3717:THR:O	6:T:3720:ILE:N	2.40	0.55
2:B:272:SER:OG	2:B:276:GLU:N	2.39	0.55
6:T:572:LEU:CA	6:T:1940:TYR:CE2	2.90	0.55
6:T:1331:GLN:HA	6:T:1334:LEU:HG	1.88	0.55
1:A:51:ASP:OD1	1:A:51:ASP:N	2.39	0.55
1:A:188:TYR:HE2	1:A:257:ALA:HA	1.71	0.55
2:B:177:SER:O	2:B:180:THR:OG1	2.21	0.55
3:D:762:GLU:HA	3:D:765:ARG:HH11	1.71	0.55
6:T:339:GLU:HB3	6:T:1897:GLU:HB3	1.88	0.55
6:T:1030:LYS:HA	6:T:2534:CYS:SG	2.47	0.55
6:T:3564:ILE:HG13	6:T:3565:ASN:H	1.71	0.55
2:B:103:ASN:HA	2:B:106:ILE:HD12	1.89	0.55
3:D:637:PRO:HG2	3:D:723:TRP:NE1	2.21	0.55
6:T:1198:ILE:HD11	6:T:1237:LEU:HG	1.89	0.55
6:T:1532:VAL:HG22	6:T:1583:LYS:HE2	1.89	0.55
6:T:2741:GLN:HG3	6:T:2742:HIS:H	1.72	0.55
6:T:3082:ILE:HD12	6:T:3107:LEU:HB3	1.89	0.55
1:A:58:ALA:HB1	1:A:67:LEU:HD21	1.88	0.54
1:A:152:VAL:HG13	1:A:298:VAL:HG12	1.88	0.54
6:T:337:PRO:O	6:T:344:ARG:NH2	2.40	0.54
6:T:382:THR:HG23	6:T:1900:LEU:CD1	2.36	0.54
6:T:590:LEU:O	6:T:594:LEU:HG	2.07	0.54
6:T:1132:ASP:HA	6:T:3320:ARG:HH22	1.71	0.54
6:T:1146:LEU:HD13	6:T:1193:LEU:HD22	1.88	0.54
6:T:2118:LEU:HD23	6:T:2118:LEU:O	2.08	0.54
6:T:2320:LEU:CD1	6:T:2356:SER:N	2.60	0.54
1:A:110:MET:SD	2:B:37:GLN:NE2	2.81	0.54
2:B:396:SER:OG	2:B:397:ASP:N	2.40	0.54
2:B:480:VAL:HA	2:B:483:LEU:HD12	1.88	0.54
6:T:1159:GLU:O	6:T:1163:VAL:HG23	2.07	0.54
6:T:1485:LEU:HB3	6:T:1503:LEU:HD21	1.89	0.54
6:T:3034:ARG:NH2	6:T:3036:TYR:OH	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLU:OE1	1:A:5:VAL:HG22	2.07	0.54
1:A:136:ILE:HG23	1:A:139:VAL:HG12	1.90	0.54
3:D:66:ASP:HB3	3:D:537:LYS:HE3	1.89	0.54
6:T:709:VAL:O	6:T:713:MET:HG3	2.07	0.54
6:T:1284:VAL:HG13	6:T:1285:LEU:HD22	1.89	0.54
6:T:1487:MET:CE	6:T:1487:MET:CA	2.85	0.54
6:T:1506:LEU:HD12	6:T:1506:LEU:O	2.07	0.54
6:T:3435:GLU:OE2	6:T:3439:ARG:NH1	2.37	0.54
6:T:769:SER:O	6:T:773:VAL:HG23	2.07	0.54
6:T:2089:SER:O	6:T:2089:SER:OG	2.26	0.54
6:T:2748:GLU:OE1	6:T:2748:GLU:N	2.31	0.54
6:T:2847:GLN:O	6:T:2851:GLU:HG2	2.08	0.54
6:T:639:HIS:CE1	6:T:643:ILE:HD11	2.43	0.54
6:T:769:SER:O	6:T:772:SER:OG	2.17	0.54
6:T:934:PRO:HG3	6:T:2826:ILE:HA	1.90	0.54
6:T:1449:LEU:CD2	6:T:1484:PRO:CG	2.82	0.54
6:T:1859:LEU:N	6:T:1859:LEU:HD23	2.22	0.54
6:T:1915:LYS:CA	6:T:1915:LYS:CE	2.86	0.54
6:T:2174:ASN:HB3	6:T:2175:LYS:HE2	1.90	0.54
6:T:3237:PHE:CD2	6:T:3405:VAL:HG21	2.43	0.54
3:D:33:ILE:HG13	3:D:36:ARG:CZ	2.38	0.54
4:E:169:ILE:HA	4:E:196:ARG:HH22	1.73	0.54
6:T:3566:ASN:O	6:T:3567:ARG:NE	2.36	0.54
6:T:10:PHE:HB2	6:T:13:ARG:HE	1.72	0.54
6:T:1004:LEU:HD21	6:T:1089:ALA:HB2	1.89	0.54
6:T:2411:GLU:OE1	6:T:2411:GLU:N	2.41	0.54
6:T:2590:PRO:HD2	6:T:2592:HIS:O	2.07	0.54
6:T:3680:ARG:HD2	6:T:3683:ILE:HG21	1.90	0.54
4:E:298:GLN:NE2	4:E:301:SER:H	2.04	0.54
6:T:480:ARG:CZ	6:T:1760:TYR:CD1	2.91	0.54
6:T:2278:LEU:HD12	6:T:2278:LEU:O	2.07	0.54
6:T:2691:GLY:HA3	6:T:2707:TYR:CE1	2.43	0.54
6:T:15:ARG:HH22	6:T:27:THR:HB	1.71	0.54
6:T:1420:ALA:CB	6:T:1462:ALA:HB1	2.38	0.54
6:T:2189:ASN:HD22	6:T:2189:ASN:N	2.04	0.54
6:T:2191:LEU:HD12	6:T:2194:CYS:HB2	1.90	0.54
6:T:2210:LEU:HD11	6:T:2258:THR:HB	1.88	0.54
3:D:308:LYS:NZ	6:T:2689:ASN:OD1	2.41	0.54
6:T:792:ILE:O	6:T:795:SER:OG	2.19	0.54
6:T:1107:LEU:HD22	6:T:1171:ILE:HD11	1.88	0.54
6:T:1985:LEU:HA	6:T:1988:PHE:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:2206:LEU:HD23	6:T:2255:ALA:HA	1.90	0.54
6:T:3405:VAL:HG12	6:T:3457:ILE:HG22	1.90	0.54
6:T:786:PRO:O	6:T:787:HIS:ND1	2.40	0.53
6:T:846:ILE:HG12	6:T:848:THR:O	2.08	0.53
6:T:1776:LYS:HE2	6:T:1778:LYS:HE3	1.89	0.53
6:T:2332:PHE:O	6:T:2335:THR:OG1	2.23	0.53
6:T:2862:LEU:HD11	6:T:2915:ALA:HB3	1.90	0.53
6:T:480:ARG:NH1	6:T:1760:TYR:CG	2.73	0.53
6:T:629:GLU:CD	6:T:1717:GLN:CB	2.61	0.53
6:T:3551:GLN:NE2	6:T:3580:ASN:OD1	2.41	0.53
1:A:160:THR:HG23	1:A:178:ILE:HB	1.89	0.53
2:B:141:PRO:O	2:B:144:THR:OG1	2.23	0.53
6:T:678:ASP:O	6:T:682:LEU:HG	2.08	0.53
6:T:823:ARG:O	6:T:826:ASN:N	2.24	0.53
6:T:1444:PHE:O	6:T:1448:MET:HG2	2.08	0.53
6:T:1752:PHE:CE1	6:T:1796:LEU:HD21	2.44	0.53
6:T:1801:PHE:CE1	6:T:1859:LEU:HB2	2.43	0.53
6:T:2365:ILE:HG13	6:T:2366:PHE:N	2.23	0.53
6:T:3240:THR:HG23	6:T:3242:ASP:H	1.73	0.53
6:T:3466:THR:HG22	6:T:3573:HIS:CD2	2.43	0.53
6:T:402:ILE:HG13	6:T:403:ARG:H	1.73	0.53
6:T:1300:ASN:ND2	6:T:1303:VAL:H	2.06	0.53
6:T:2452:TYR:OH	6:T:2575:GLU:OE2	2.25	0.53
6:T:2470:ASN:O	6:T:2474:GLN:HG2	2.09	0.53
1:A:207:GLU:HG2	1:A:210:ARG:HH21	1.72	0.53
2:B:183:ASN:HD21	2:B:185:ILE:HB	1.73	0.53
3:D:743:VAL:HG11	3:D:747:SER:H	1.72	0.53
6:T:440:LEU:O	6:T:443:VAL:HG22	2.07	0.53
6:T:1097:ASP:OD1	6:T:1097:ASP:N	2.41	0.53
6:T:1340:LYS:HE2	6:T:1345:LEU:HD13	1.90	0.53
6:T:1825:LEU:HD23	6:T:1875:ASP:HB2	1.90	0.53
6:T:2708:GLU:OE2	6:T:2733:TRP:NE1	2.41	0.53
1:A:200:PHE:HA	1:A:205:GLU:HG3	1.90	0.53
1:A:239:SER:HA	1:A:249:THR:HA	1.91	0.53
2:B:144:THR:O	2:B:147:SER:OG	2.22	0.53
5:F:540:ASP:OD1	5:F:545:PRO:HD3	2.09	0.53
6:T:2862:LEU:HD12	6:T:2912:ILE:HG13	1.90	0.53
4:E:169:ILE:HD13	4:E:204:LYS:HE2	1.90	0.53
6:T:1046:ALA:O	6:T:1049:SER:OG	2.22	0.53
6:T:1899:THR:HA	6:T:1902:LYS:HE2	1.90	0.53
6:T:2486:LEU:HD23	6:T:2536:ILE:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:NH2	1:A:65:LEU:O	2.42	0.53
6:T:8:GLU:OE2	6:T:9:GLN:NE2	2.41	0.53
6:T:37:LEU:HD12	6:T:2009:HIS:CD2	2.44	0.53
6:T:741:LEU:HD23	6:T:787:HIS:CE1	2.43	0.53
6:T:1312:HIS:O	6:T:1315:SER:OG	2.23	0.53
6:T:1438:ILE:HD12	6:T:1473:LEU:HG	1.91	0.53
6:T:2225:ILE:HG22	6:T:2226:ILE:HG23	1.90	0.53
6:T:2245:GLN:HA	6:T:2245:GLN:HE21	1.71	0.53
6:T:2549:PHE:CD1	6:T:2556:ILE:HG22	2.44	0.53
6:T:2898:TRP:CE3	6:T:2953:VAL:HG11	2.43	0.53
6:T:15:ARG:NH2	6:T:18:ASP:OD1	2.43	0.53
6:T:76:ARG:HB3	6:T:117:LEU:HD11	1.90	0.53
6:T:479:ASN:ND2	6:T:640:GLU:O	2.42	0.53
6:T:2394:PHE:O	6:T:2397:ILE:HG12	2.08	0.53
6:T:3715:VAL:O	6:T:3716:THR:OG1	2.23	0.53
1:A:49:GLN:NE2	1:A:50:LYS:O	2.42	0.52
1:A:100:GLU:HG2	1:A:101:HIS:CE1	2.45	0.52
6:T:1205:THR:HG22	6:T:1207:TYR:HB2	1.92	0.52
3:D:30:ASP:O	3:D:33:ILE:HG22	2.09	0.52
3:D:349:ILE:HG13	3:D:351:PRO:HD3	1.91	0.52
3:D:583:ILE:HB	3:D:584:PRO:HD3	1.91	0.52
6:T:365:PRO:HG3	6:T:398:PHE:CZ	2.45	0.52
6:T:1382:ILE:O	6:T:1412:ARG:NH2	2.34	0.52
6:T:3054:ALA:HB3	6:T:3092:TYR:HB2	1.91	0.52
2:B:48:THR:OG1	2:B:68:ASP:OD1	2.27	0.52
6:T:1359:PHE:O	6:T:1363:LEU:HG	2.10	0.52
6:T:1883:LYS:HB3	6:T:1912:PHE:CZ	2.43	0.52
6:T:3112:ASP:OD1	6:T:3112:ASP:N	2.43	0.52
6:T:59:LEU:HD11	6:T:83:PHE:CE2	2.45	0.52
6:T:75:LEU:O	6:T:79:MET:HG3	2.10	0.52
6:T:640:GLU:HA	6:T:643:ILE:HD12	1.92	0.52
6:T:1281:GLY:O	6:T:1286:GLU:HB2	2.08	0.52
6:T:1454:GLU:H	6:T:1454:GLU:CD	2.12	0.52
6:T:1742:PRO:HA	6:T:1745:LEU:HD12	1.90	0.52
6:T:2783:VAL:HG12	6:T:2791:ARG:HE	1.73	0.52
6:T:3106:TRP:HE3	6:T:3107:LEU:HD22	1.75	0.52
1:A:181:ALA:N	1:A:184:ASP:OD2	2.43	0.52
6:T:473:ASN:O	6:T:477:THR:HG23	2.10	0.52
6:T:572:LEU:CA	6:T:1940:TYR:HD2	2.21	0.52
6:T:1511:ILE:HG23	6:T:1511:ILE:O	2.09	0.52
6:T:1513:TYR:O	6:T:1513:TYR:HD1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1699:LEU:HD23	6:T:1699:LEU:C	2.29	0.52
6:T:1830:LYS:HA	6:T:1832:LYS:HE3	1.91	0.52
3:D:533:GLU:OE2	3:D:552:LEU:N	2.43	0.52
6:T:496:LYS:O	6:T:499:LYS:HG3	2.09	0.52
6:T:507:ILE:HG13	6:T:508:GLN:N	2.24	0.52
6:T:1906:TYR:HA	6:T:1909:THR:HG22	1.91	0.52
6:T:326:PRO:HG2	6:T:367:LEU:HD13	1.92	0.52
6:T:697:THR:O	6:T:701:ILE:HG12	2.10	0.52
6:T:3240:THR:HG23	6:T:3242:ASP:N	2.25	0.52
3:D:265:ALA:O	3:D:266:LEU:HG	2.10	0.52
3:D:682:TYR:HD1	6:T:2667:VAL:HG13	1.74	0.52
6:T:1298:ASN:OD1	6:T:1299:ALA:N	2.39	0.52
6:T:1301:PRO:HA	6:T:1304:ARG:HD2	1.92	0.52
6:T:1441:LEU:HD23	6:T:1444:PHE:HD2	1.74	0.52
6:T:2271:ILE:HG13	6:T:2273:PRO:HD2	1.92	0.52
6:T:2519:LEU:H	6:T:2519:LEU:HD12	1.75	0.52
6:T:2959:MET:O	6:T:2962:VAL:HG12	2.10	0.52
6:T:2966:GLN:HA	6:T:2969:ARG:HH22	1.75	0.52
1:A:218:TYR:HA	1:A:307:PRO:HD2	1.90	0.52
6:T:349:HIS:HD2	6:T:352:ARG:HH12	1.58	0.52
6:T:1178:ILE:HG23	6:T:1179:TYR:CD1	2.45	0.52
6:T:1509:LEU:N	6:T:1509:LEU:CD2	2.73	0.52
6:T:1651:TYR:CE2	6:T:1669:MET:HB3	2.45	0.52
6:T:2359:TRP:O	6:T:2372:LYS:NZ	2.39	0.52
3:D:628:ASN:H	6:T:2591:TYR:HE2	1.57	0.52
6:T:473:ASN:HA	6:T:476:LYS:HE2	1.92	0.52
6:T:1673:PHE:CE2	6:T:1695:LEU:HD11	2.45	0.52
6:T:2195:ILE:HG23	6:T:2239:LEU:HD22	1.91	0.52
6:T:2420:PHE:HE2	6:T:2439:LEU:HD13	1.75	0.52
2:B:181:ARG:NH2	2:B:395:SER:OG	2.43	0.51
3:D:42:GLU:O	3:D:46:VAL:HG12	2.10	0.51
3:D:59:ASN:OD1	3:D:60:LYS:N	2.43	0.51
6:T:72:GLU:HB2	6:T:76:ARG:HH21	1.75	0.51
6:T:979:ASP:N	6:T:979:ASP:OD1	2.43	0.51
6:T:1510:LEU:HD11	6:T:1563:PRO:HD3	1.92	0.51
6:T:1559:PHE:HB3	6:T:1599:TYR:CD1	2.45	0.51
6:T:1673:PHE:CZ	6:T:1692:ILE:HG22	2.45	0.51
6:T:2687:GLU:OE1	6:T:2687:GLU:N	2.23	0.51
1:A:13:GLY:HA2	1:A:137:GLN:HE22	1.75	0.51
6:T:222:LYS:HZ1	6:T:234:LEU:HD22	1.75	0.51
6:T:381:PHE:CE1	6:T:1856:HIS:CE1	2.98	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:752:GLY:HA3	6:T:802:ALA:HB1	1.92	0.51
6:T:856:GLU:HB3	6:T:890:TYR:CE1	2.45	0.51
6:T:984:GLY:HA3	6:T:2447:ILE:HG22	1.91	0.51
1:A:286:ASP:OD1	1:A:287:VAL:N	2.40	0.51
2:B:253:LYS:HE3	2:B:257:GLU:HG3	1.93	0.51
6:T:2180:ILE:O	6:T:2180:ILE:HG13	2.10	0.51
6:T:3087:GLN:HG2	6:T:3124:PHE:HE1	1.75	0.51
2:B:23:SER:N	7:B:501:ATP:O3G	2.43	0.51
3:D:751:GLY:HA2	3:D:755:LEU:HD22	1.92	0.51
5:F:560:VAL:O	5:F:562:PHE:N	2.44	0.51
6:T:1939:ARG:NH1	6:T:1939:ARG:CB	2.73	0.51
6:T:2621:HIS:CE1	6:T:2657:ALA:HB1	2.45	0.51
6:T:2650:ASP:OD1	6:T:2650:ASP:N	2.44	0.51
6:T:3172:ARG:NH2	6:T:3227:GLU:OE1	2.43	0.51
2:B:21:PRO:HA	2:B:26:THR:HG23	1.92	0.51
3:D:643:GLN:CD	3:D:643:GLN:H	2.14	0.51
6:T:1353:ASN:O	6:T:1357:ILE:HG13	2.11	0.51
6:T:1601:ASN:HD22	6:T:1601:ASN:N	2.07	0.51
6:T:2143:PHE:CZ	6:T:2170:VAL:HG11	2.45	0.51
6:T:2164:ALA:HA	6:T:2167:VAL:HG22	1.92	0.51
6:T:2669:LEU:HD22	6:T:2836:THR:HG21	1.91	0.51
6:T:3156:LEU:HA	6:T:3159:ILE:HD12	1.93	0.51
6:T:3493:LEU:HG	6:T:3509:LEU:HD21	1.92	0.51
1:A:70:PRO:O	1:A:77:THR:N	2.43	0.51
1:A:372:HIS:HE1	5:F:644:ARG:CZ	2.24	0.51
6:T:443:VAL:HA	6:T:446:ILE:HD12	1.92	0.51
6:T:1045:THR:HG21	6:T:2510:MET:HA	1.93	0.51
6:T:1625:CYS:HA	6:T:1628:VAL:HG12	1.93	0.51
6:T:3736:THR:HG21	6:T:3740:PHE:HD2	1.75	0.51
1:A:275:ASP:N	1:A:275:ASP:OD1	2.40	0.51
1:A:311:GLU:OE1	1:A:311:GLU:N	2.43	0.51
3:D:272:LEU:HD11	3:D:566:TYR:CE1	2.46	0.51
6:T:381:PHE:O	6:T:385:GLU:N	2.41	0.51
6:T:2182:GLU:H	6:T:2182:GLU:CD	2.13	0.51
6:T:2206:LEU:HD12	6:T:2206:LEU:C	2.31	0.51
6:T:3203:GLN:HG3	6:T:3207:TYR:HE2	1.75	0.51
1:A:151:ILE:HA	1:A:164:PRO:HA	1.91	0.51
3:D:633:PRO:HB3	3:D:697:PHE:CZ	2.46	0.51
4:E:98:SER:O	4:E:102:ILE:HG12	2.10	0.51
6:T:80:LEU:HD13	6:T:120:LYS:HG2	1.93	0.51
6:T:519:ARG:HA	6:T:522:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1131:ILE:HG23	6:T:3320:ARG:HG2	1.93	0.51
6:T:1132:ASP:HA	6:T:3320:ARG:NH2	2.26	0.51
6:T:1159:GLU:OE1	6:T:1159:GLU:N	2.39	0.51
6:T:2469:LEU:HD12	6:T:2605:MET:HE3	1.93	0.51
4:E:294:TYR:HB3	6:T:2712:VAL:HG11	1.93	0.51
6:T:1715:HIS:HD1	6:T:1717:GLN:HG2	1.76	0.51
6:T:1848:ILE:HB	6:T:1852:ASP:HB2	1.93	0.51
6:T:2271:ILE:HG23	6:T:2274:LEU:HB2	1.93	0.51
1:A:82:MET:HA	1:A:85:ILE:HD12	1.93	0.51
2:B:116:ASN:OD1	2:B:117:SER:N	2.44	0.51
3:D:277:ILE:HG23	5:F:577:TYR:OH	2.11	0.51
3:D:347:ARG:HD2	3:D:585:ILE:HD11	1.92	0.51
6:T:381:PHE:N	6:T:1858:ASP:OD1	2.43	0.51
6:T:477:THR:O	6:T:481:GLN:HG2	2.10	0.51
6:T:1062:ASP:OD1	6:T:1062:ASP:N	2.38	0.51
6:T:1157:ILE:O	6:T:1160:VAL:HG22	2.10	0.51
6:T:1423:LEU:HD12	6:T:1466:SER:OG	2.11	0.51
6:T:3304:LYS:N	6:T:3305:PRO:HD2	2.26	0.51
1:A:242:LEU:HD13	1:A:246:GLN:HB3	1.93	0.50
2:B:41:PRO:HD3	2:B:59:GLU:HB2	1.94	0.50
3:D:762:GLU:HA	3:D:765:ARG:HD3	1.93	0.50
6:T:379:ASN:OD1	6:T:1856:HIS:HA	2.12	0.50
6:T:570:LEU:HD23	6:T:570:LEU:H	1.77	0.50
6:T:3412:HIS:CD2	6:T:3587:LEU:HD21	2.46	0.50
5:F:520:VAL:O	5:F:524:MET:HG3	2.11	0.50
6:T:858:TYR:HA	6:T:861:LEU:HD12	1.92	0.50
6:T:1405:SER:OG	6:T:1406:GLU:OE1	2.27	0.50
6:T:1516:VAL:HG11	6:T:1562:LEU:HD21	1.93	0.50
6:T:2197:SER:HA	6:T:2200:HIS:CE1	2.47	0.50
4:E:218:PRO:HA	4:E:223:LEU:HD12	1.93	0.50
6:T:24:ARG:NH2	6:T:70:SER:O	2.45	0.50
6:T:711:GLU:O	6:T:714:LEU:HB2	2.11	0.50
6:T:757:ASN:O	6:T:761:VAL:HG23	2.11	0.50
6:T:942:SER:OG	6:T:943:HIS:ND1	2.44	0.50
6:T:1655:ILE:N	6:T:1656:PRO:HD2	2.26	0.50
1:A:164:PRO:HG2	1:A:171:LEU:HD12	1.94	0.50
2:B:247:CYS:HB2	2:B:417:ILE:HD12	1.93	0.50
3:D:378:LYS:NZ	3:D:536:LYS:O	2.30	0.50
6:T:918:GLU:HA	6:T:921:ILE:HG13	1.94	0.50
6:T:1641:GLU:HB3	6:T:1684:TRP:CZ2	2.45	0.50
6:T:3613:ILE:HG22	6:T:3614:PHE:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:609:GLU:O	3:D:611:SER:N	2.44	0.50
3:D:619:ARG:HD2	3:D:619:ARG:N	2.27	0.50
6:T:598:ILE:HD11	6:T:689:MET:HB3	1.93	0.50
6:T:912:TYR:O	6:T:915:PRO:HD2	2.12	0.50
6:T:1449:LEU:HD22	6:T:1484:PRO:CB	2.40	0.50
6:T:1482:LEU:HG	6:T:1482:LEU:O	2.12	0.50
6:T:2156:ASN:HA	6:T:2159:TYR:CD2	2.46	0.50
6:T:2342:HIS:O	6:T:2385:ARG:NH2	2.29	0.50
6:T:3266:PRO:HA	6:T:3498:ASP:HB3	1.93	0.50
6:T:3413:SER:OG	6:T:3417:GLU:OE2	2.30	0.50
1:A:169:PHE:HZ	3:D:381:VAL:HG22	1.77	0.50
1:A:196:ARG:NH1	1:A:253:GLU:OE2	2.43	0.50
2:B:209:ILE:HA	2:B:218:LYS:HA	1.94	0.50
3:D:684:TYR:CD2	6:T:2757:ASP:HB2	2.46	0.50
4:E:298:GLN:HE22	4:E:301:SER:H	1.59	0.50
6:T:307:TYR:OH	6:T:347:LEU:HB2	2.11	0.50
6:T:434:MET:HA	6:T:437:LYS:HD2	1.94	0.50
6:T:1437:ARG:HA	6:T:1440:ILE:HG22	1.93	0.50
6:T:1570:LEU:HD23	6:T:1570:LEU:O	2.12	0.50
6:T:1977:ASN:HD21	6:T:1983:ASN:HA	1.76	0.50
6:T:2337:ALA:HA	6:T:2340:ILE:HD12	1.93	0.50
6:T:2338:LEU:HG	6:T:2342:HIS:NE2	2.26	0.50
2:B:43:VAL:HG12	2:B:73:PRO:HA	1.93	0.50
2:B:478:VAL:HG22	2:B:482:ARG:HG2	1.94	0.50
3:D:71:LYS:HA	3:D:74:ILE:HG22	1.93	0.50
6:T:477:THR:HA	6:T:480:ARG:HD2	1.94	0.50
6:T:1115:VAL:HA	6:T:1118:THR:HG22	1.94	0.50
6:T:1210:ARG:HB2	6:T:1256:ILE:HD12	1.93	0.50
6:T:2616:LEU:O	6:T:2617:GLU:HG2	2.11	0.50
6:T:2619:PRO:N	6:T:2620:PRO:HD2	2.26	0.50
6:T:3306:ASP:OD1	6:T:3309:THR:HG22	2.11	0.50
1:A:98:PRO:HA	1:A:101:HIS:HD2	1.76	0.50
5:F:574:ARG:HG2	5:F:574:ARG:O	2.12	0.50
6:T:103:LEU:HD22	6:T:122:LEU:HG	1.93	0.50
1:A:80:ASP:OD1	1:A:81:ASP:N	2.44	0.50
3:D:543:PHE:O	3:D:545:LEU:HG	2.12	0.50
6:T:99:VAL:O	6:T:103:LEU:HG	2.11	0.50
6:T:381:PHE:HE1	6:T:1856:HIS:CE1	2.30	0.50
6:T:1912:PHE:CD1	6:T:1912:PHE:C	2.85	0.50
6:T:2189:ASN:N	6:T:2189:ASN:ND2	2.60	0.50
6:T:2320:LEU:HD13	6:T:2355:MET:HB3	0.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:2588:SER:OG	6:T:2589:LYS:N	2.45	0.50
5:F:524:MET:O	5:F:528:LYS:HG2	2.12	0.49
6:T:562:ASP:OD1	6:T:565:ASN:ND2	2.31	0.49
6:T:847:LEU:H	6:T:1207:TYR:HE2	1.59	0.49
6:T:1001:LEU:HD21	6:T:1085:SER:HB2	1.94	0.49
6:T:1102:LEU:HA	6:T:1105:ASN:HD22	1.76	0.49
6:T:1335:SER:OG	6:T:1336:PRO:HD3	2.12	0.49
6:T:1832:LYS:HE2	6:T:1832:LYS:N	2.27	0.49
6:T:1858:ASP:OD1	6:T:1858:ASP:N	2.45	0.49
6:T:2006:ASN:HA	6:T:2009:HIS:CD2	2.47	0.49
6:T:2282:PHE:HE1	6:T:2335:THR:HB	1.77	0.49
6:T:2311:LEU:C	6:T:2311:LEU:HD12	2.33	0.49
6:T:2588:SER:O	6:T:2594:ARG:NH2	2.35	0.49
6:T:2633:TRP:CD1	6:T:2832:PRO:HD3	2.46	0.49
2:B:16:ALA:HB2	2:B:107:PRO:HG2	1.94	0.49
4:E:272:LEU:O	4:E:276:GLU:HG2	2.12	0.49
6:T:1750:PHE:C	6:T:1750:PHE:CD1	2.85	0.49
6:T:2138:VAL:HG22	6:T:2142:TYR:CD1	2.48	0.49
6:T:3020:ALA:O	6:T:3024:THR:HG23	2.11	0.49
6:T:624:ARG:O	6:T:1585:ARG:HD2	2.12	0.49
6:T:1378:LEU:HB3	6:T:1415:CYS:SG	2.52	0.49
6:T:1491:ASP:HA	6:T:1525:HIS:CE1	2.48	0.49
6:T:1605:ASN:H	6:T:1606:PRO:CD	2.25	0.49
6:T:1765:PHE:HA	6:T:1768:HIS:CE1	2.46	0.49
3:D:752:HIS:H	3:D:755:LEU:HB3	1.77	0.49
4:E:274:GLU:HB3	4:E:275:ARG:HH22	1.77	0.49
6:T:339:GLU:CD	6:T:1897:GLU:CB	2.80	0.49
6:T:612:THR:O	6:T:1532:VAL:CG1	2.60	0.49
6:T:789:ASN:HB3	6:T:828:TYR:CE1	2.47	0.49
6:T:1857:HIS:HB3	6:T:1859:LEU:HG	1.94	0.49
6:T:1875:ASP:HB3	6:T:1878:ILE:HG22	1.95	0.49
6:T:2124:LEU:HD23	6:T:2124:LEU:O	2.12	0.49
6:T:2999:LEU:HD23	6:T:3003:LEU:HD23	1.94	0.49
6:T:3441:ILE:HG21	6:T:3648:ILE:HD11	1.94	0.49
5:F:581:LEU:HD21	5:F:613:ARG:HA	1.94	0.49
6:T:137:LEU:HD21	6:T:228:PRO:HG2	1.95	0.49
6:T:796:LEU:O	6:T:800:THR:HG23	2.12	0.49
6:T:1483:LYS:HB3	6:T:1484:PRO:HD3	1.94	0.49
6:T:2361:PHE:HZ	6:T:2400:LYS:HG2	1.78	0.49
6:T:2973:LEU:HD12	6:T:2974:PRO:HD2	1.95	0.49
6:T:34:ILE:HB	6:T:38:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1419:LEU:O	6:T:1423:LEU:HG	2.12	0.49
6:T:1564:PRO:HA	6:T:1603:PHE:CE1	2.47	0.49
6:T:1748:ILE:HD11	6:T:1789:PHE:HZ	1.78	0.49
6:T:2160:TYR:HA	6:T:2163:ASN:ND2	2.28	0.49
6:T:2708:GLU:O	6:T:2712:VAL:HG23	2.13	0.49
6:T:3460:ASP:HA	6:T:3464:PHE:HZ	1.76	0.49
3:D:39:LYS:HA	6:T:3508:ILE:HG21	1.95	0.49
6:T:72:GLU:O	6:T:76:ARG:HG3	2.12	0.49
6:T:789:ASN:OD1	6:T:790:ASP:N	2.42	0.49
6:T:849:ALA:C	6:T:851:LEU:H	2.14	0.49
6:T:965:ASP:N	6:T:965:ASP:OD1	2.46	0.49
6:T:1546:GLN:HG2	6:T:1549:THR:HG23	1.93	0.49
6:T:1821:LEU:HD11	6:T:1824:TYR:HB2	1.94	0.49
6:T:2143:PHE:HZ	6:T:2170:VAL:HG11	1.76	0.49
6:T:2329:ARG:HG3	6:T:2330:ARG:N	2.28	0.49
6:T:2461:GLU:HA	6:T:2592:HIS:CD2	2.47	0.49
6:T:2626:LEU:HD23	6:T:2626:LEU:O	2.12	0.49
6:T:3422:LEU:HB2	6:T:3666:PHE:HD2	1.78	0.49
6:T:3423:TYR:CD2	6:T:3558:MET:HG2	2.48	0.49
1:A:125:GLU:OE2	4:E:77:PRO:HA	2.13	0.49
2:B:261:GLU:OE1	2:B:261:GLU:N	2.45	0.49
2:B:277:GLU:OE1	2:B:279:VAL:HG23	2.13	0.49
3:D:22:ASP:OD1	3:D:23:ARG:N	2.45	0.49
3:D:379:TYR:CZ	3:D:532:THR:HG21	2.48	0.49
3:D:722:GLN:HA	3:D:725:ILE:HG22	1.95	0.49
6:T:129:PHE:HA	6:T:132:ILE:HG12	1.95	0.49
6:T:686:LEU:HA	6:T:689:MET:SD	2.53	0.49
6:T:715:GLU:OE1	6:T:715:GLU:N	2.45	0.49
6:T:1179:TYR:HB2	6:T:1184:ALA:HB2	1.95	0.49
6:T:1776:LYS:HE2	6:T:1778:LYS:CE	2.43	0.49
6:T:1778:LYS:HA	6:T:1781:ASN:ND2	2.28	0.49
6:T:2790:ARG:NH1	6:T:2793:MET:SD	2.86	0.49
1:A:19:ALA:O	1:A:28:ARG:N	2.43	0.49
2:B:242:CYS:HB3	2:B:246:LEU:HD12	1.95	0.49
6:T:129:PHE:HZ	6:T:136:LYS:H	1.59	0.49
6:T:311:ARG:HH21	6:T:315:PRO:HD3	1.78	0.49
6:T:458:PRO:O	6:T:462:LYS:HG3	2.13	0.49
6:T:461:LYS:O	6:T:465:MET:HG2	2.12	0.49
6:T:1039:TYR:CZ	6:T:1043:LEU:HD21	2.48	0.49
6:T:1832:LYS:CA	6:T:1832:LYS:CE	2.85	0.49
6:T:1864:LEU:HD11	6:T:1893:PHE:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1903:GLN:HB3	6:T:1941:LEU:HD21	1.94	0.49
6:T:1992:HIS:HB2	6:T:1993:PRO:HD3	1.95	0.49
6:T:2573:LYS:O	6:T:2574:ASN:HB3	2.13	0.49
6:T:2855:ALA:HB1	6:T:2859:TYR:HE2	1.78	0.49
6:T:3080:ASN:OD1	6:T:3081:ALA:N	2.41	0.49
1:A:152:VAL:HG22	1:A:298:VAL:HB	1.94	0.49
3:D:32:LEU:HD23	3:D:300:ILE:HB	1.94	0.49
6:T:95:TYR:HA	6:T:98:GLU:HG3	1.94	0.49
6:T:560:MET:CB	6:T:1767:PHE:CE1	2.96	0.49
6:T:730:GLU:HB3	6:T:733:SER:OG	2.13	0.49
6:T:1809:SER:HA	6:T:1812:ILE:HG12	1.95	0.49
6:T:1918:PHE:CE2	6:T:1920:ILE:HG13	2.48	0.49
6:T:1927:PHE:HA	6:T:1930:LEU:CD1	2.43	0.49
6:T:2031:LEU:HD12	6:T:2031:LEU:C	2.32	0.49
6:T:2659:GLU:HB3	6:T:2682:ARG:HD2	1.93	0.49
1:A:18:LYS:HG2	1:A:30:VAL:HG12	1.94	0.48
3:D:292:TYR:HE2	5:F:524:MET:HG2	1.78	0.48
6:T:789:ASN:HB3	6:T:828:TYR:HE1	1.77	0.48
6:T:1109:HIS:O	6:T:1113:LEU:HG	2.13	0.48
6:T:1747:PHE:HA	6:T:1750:PHE:CE2	2.48	0.48
6:T:1798:ALA:HA	6:T:1801:PHE:HD2	1.77	0.48
6:T:2172:PHE:HB2	6:T:2215:LYS:HD3	1.94	0.48
6:T:2272:VAL:N	6:T:2273:PRO:CD	2.75	0.48
6:T:2419:PRO:O	6:T:2422:VAL:HG12	2.12	0.48
6:T:2817:CYS:SG	6:T:2853:LEU:HD21	2.53	0.48
1:A:99:GLU:H	1:A:99:GLU:CD	2.14	0.48
6:T:24:ARG:NE	6:T:74:LYS:HB2	2.28	0.48
6:T:326:PRO:HB2	6:T:367:LEU:HD22	1.93	0.48
6:T:1522:LEU:C	6:T:1522:LEU:HD23	2.34	0.48
6:T:3169:PHE:O	6:T:3173:THR:HG23	2.12	0.48
6:T:3225:SER:HB3	6:T:3349:PHE:HE1	1.78	0.48
6:T:3270:PRO:HG2	6:T:3307:TYR:CD2	2.48	0.48
3:D:585:ILE:HD12	3:D:585:ILE:H	1.76	0.48
3:D:628:ASN:OD1	3:D:629:HIS:N	2.40	0.48
6:T:594:LEU:HD13	6:T:637:LEU:HD11	1.95	0.48
6:T:742:ARG:CZ	6:T:1544:ALA:CB	2.90	0.48
6:T:2711:GLN:NE2	6:T:2730:GLU:HA	2.28	0.48
6:T:3238:LYS:HG2	6:T:3407:TYR:CZ	2.49	0.48
3:D:312:THR:H	6:T:3629:GLN:NE2	2.12	0.48
4:E:173:PHE:HA	4:E:176:CYS:HB2	1.94	0.48
4:E:281:LEU:HD13	6:T:2685:TYR:C	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:370:LEU:O	6:T:374:ARG:NH1	2.47	0.48
6:T:573:PRO:HD3	6:T:1940:TYR:CD2	2.48	0.48
6:T:851:LEU:N	6:T:852:PRO:HD3	2.28	0.48
6:T:1128:THR:OG1	6:T:1129:PHE:N	2.46	0.48
6:T:1590:SER:HB3	6:T:1593:ARG:CD	2.43	0.48
6:T:3679:HIS:O	6:T:3681:PRO:HD3	2.14	0.48
3:D:51:GLN:HE21	3:D:54:GLU:CD	2.16	0.48
3:D:308:LYS:HZ1	4:E:281:LEU:HD21	1.78	0.48
6:T:63:PRO:O	6:T:64:ILE:HD13	2.14	0.48
6:T:629:GLU:OE2	6:T:1717:GLN:CB	2.59	0.48
6:T:1039:TYR:CE1	6:T:2497:PRO:HB2	2.49	0.48
6:T:1123:ARG:HH11	6:T:1133:LEU:HD22	1.78	0.48
6:T:1800:ILE:HA	6:T:1803:LEU:CD1	2.43	0.48
6:T:1895:LYS:HD2	6:T:1895:LYS:N	2.28	0.48
6:T:2285:LEU:CD2	6:T:2311:LEU:HD11	2.44	0.48
5:F:627:LEU:HD12	5:F:628:GLU:N	2.28	0.48
6:T:247:PRO:HG2	6:T:251:PRO:HD3	1.95	0.48
6:T:462:LYS:O	6:T:466:ILE:HG13	2.13	0.48
6:T:842:LEU:HA	6:T:845:MET:HB3	1.95	0.48
6:T:2788:THR:HG22	6:T:2791:ARG:HH11	1.78	0.48
6:T:2852:PHE:O	6:T:2856:THR:HG23	2.13	0.48
6:T:3114:SER:OG	6:T:3115:GLY:N	2.46	0.48
6:T:3365:ASN:HB2	6:T:3368:PHE:CE2	2.49	0.48
1:A:169:PHE:CZ	3:D:381:VAL:HG22	2.49	0.48
2:B:175:THR:O	4:E:189:ARG:NH1	2.46	0.48
2:B:267:LYS:HD3	2:B:281:ASP:HA	1.96	0.48
3:D:594:ASP:OD1	3:D:594:ASP:N	2.45	0.48
6:T:572:LEU:N	6:T:1940:TYR:CE2	2.82	0.48
6:T:1031:SER:HB2	6:T:2493:CYS:SG	2.53	0.48
6:T:1359:PHE:HA	6:T:1362:SER:OG	2.13	0.48
6:T:2460:TRP:CG	6:T:2461:GLU:N	2.81	0.48
6:T:3302:ASP:C	6:T:3304:LYS:H	2.17	0.48
3:D:558:THR:HB	3:D:561:GLN:HB2	1.95	0.48
3:D:661:ASN:O	3:D:665:TYR:HB2	2.13	0.48
6:T:378:GLY:O	6:T:1856:HIS:CD2	2.67	0.48
6:T:466:ILE:CA	6:T:1716:LEU:HD21	2.42	0.48
6:T:509:ASP:OD1	6:T:509:ASP:N	2.42	0.48
6:T:629:GLU:OE2	6:T:1717:GLN:N	2.46	0.48
6:T:2700:TRP:HD1	6:T:2736:CYS:SG	2.36	0.48
6:T:3177:ASP:O	6:T:3181:ILE:HG13	2.13	0.48
6:T:3371:ILE:HG22	6:T:3393:ILE:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:THR:HG21	1:A:370:VAL:HB	1.96	0.48
2:B:299:ASP:H	2:B:300:ILE:HD12	1.78	0.48
3:D:684:TYR:OH	6:T:2738:GLU:OE1	2.21	0.48
6:T:249:PHE:CG	6:T:289:PRO:HG3	2.49	0.48
6:T:480:ARG:CZ	6:T:1760:TYR:HB2	2.41	0.48
6:T:613:VAL:HA	6:T:1536:ASP:CG	2.34	0.48
6:T:1300:ASN:ND2	6:T:1302:LYS:HB2	2.29	0.48
6:T:1591:PRO:HG2	6:T:1592:PHE:HD1	1.78	0.48
6:T:1974:MET:HA	6:T:1977:ASN:HB2	1.95	0.48
6:T:2244:THR:HB	6:T:2277:PRO:HB3	1.96	0.48
6:T:3151:MET:HA	6:T:3154:HIS:HD2	1.78	0.48
1:A:363:ASP:O	4:E:96:LYS:NZ	2.28	0.48
6:T:44:TYR:HB3	6:T:48:LEU:HD22	1.96	0.48
6:T:472:MET:HA	6:T:475:PHE:CE2	2.49	0.48
6:T:740:LEU:O	6:T:744:LEU:HD23	2.14	0.48
6:T:951:LYS:HA	6:T:2887:ARG:HE	1.79	0.48
6:T:1330:LYS:HG3	6:T:1331:GLN:N	2.29	0.48
6:T:1738:ARG:NE	6:T:1738:ARG:HA	2.29	0.48
6:T:1990:ILE:HG13	6:T:1997:PHE:CZ	2.49	0.48
6:T:1996:PHE:C	6:T:1996:PHE:CD2	2.87	0.48
6:T:2898:TRP:HZ3	6:T:2949:ARG:HG3	1.79	0.48
6:T:2989:ALA:HA	6:T:3006:ILE:HD12	1.96	0.48
1:A:14:SER:HB2	1:A:158:GLY:N	2.28	0.47
1:A:349:LEU:HD12	1:A:350:THR:H	1.78	0.47
3:D:697:PHE:O	3:D:701:VAL:HG23	2.14	0.47
5:F:573:ASP:OD1	5:F:574:ARG:HD3	2.14	0.47
6:T:120:LYS:O	6:T:123:THR:OG1	2.28	0.47
6:T:1190:ILE:HG23	6:T:1191:PRO:HD3	1.95	0.47
6:T:1516:VAL:CG2	6:T:1562:LEU:HD11	2.44	0.47
6:T:1879:ILE:HD12	6:T:1882:ILE:HG21	1.96	0.47
6:T:1924:THR:HA	6:T:1927:PHE:CD2	2.49	0.47
3:D:628:ASN:N	6:T:2591:TYR:HE2	2.12	0.47
5:F:520:VAL:N	5:F:523:LYS:HB3	2.29	0.47
6:T:1086:VAL:O	6:T:1090:THR:HG23	2.14	0.47
6:T:1516:VAL:HG21	6:T:1562:LEU:HD11	1.95	0.47
1:A:39:ARG:O	1:A:40:HIS:ND1	2.47	0.47
1:A:139:VAL:HG13	1:A:140:LEU:HD22	1.94	0.47
3:D:765:ARG:NE	4:E:300:MET:SD	2.74	0.47
4:E:296:THR:OG1	4:E:297:SER:N	2.48	0.47
6:T:45:HIS:HB2	6:T:88:MET:HE1	1.96	0.47
6:T:1108:ASP:HB2	6:T:2522:PHE:HZ	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1651:TYR:HE2	6:T:1669:MET:HB3	1.78	0.47
6:T:1741:ASN:HB3	6:T:1742:PRO:HD3	1.96	0.47
6:T:1872:ILE:HD12	6:T:1912:PHE:CD2	2.49	0.47
6:T:1919:PRO:HD2	6:T:1923:VAL:HG23	1.96	0.47
6:T:3464:PHE:HB3	6:T:3575:ASP:HA	1.95	0.47
6:T:3731:ARG:H	6:T:3731:ARG:HD2	1.80	0.47
4:E:298:GLN:OE1	4:E:299:GLY:N	2.47	0.47
6:T:428:ALA:HB3	6:T:431:VAL:HG12	1.96	0.47
6:T:1040:THR:OG1	6:T:1041:GLU:N	2.47	0.47
6:T:1290:THR:HG22	6:T:1329:SER:OG	2.15	0.47
6:T:1547:MET:N	6:T:1548:PRO:CD	2.78	0.47
6:T:1644:LEU:HA	6:T:1647:PHE:CD2	2.50	0.47
6:T:1747:PHE:HA	6:T:1750:PHE:CZ	2.50	0.47
6:T:2096:CYS:SG	6:T:2097:THR:N	2.88	0.47
6:T:2122:ASN:N	6:T:2122:ASN:ND2	2.60	0.47
6:T:2177:LYS:NZ	6:T:2179:TRP:HB3	2.30	0.47
6:T:2961:ASP:OD1	6:T:2961:ASP:N	2.47	0.47
6:T:3371:ILE:HG13	6:T:3371:ILE:O	2.15	0.47
1:A:36:GLY:HA3	1:A:53:TYR:HB2	1.96	0.47
5:F:580:HIS:CG	5:F:581:LEU:H	2.32	0.47
6:T:242:THR:HB	6:T:328:LEU:HD21	1.97	0.47
6:T:678:ASP:OD1	6:T:679:ALA:N	2.48	0.47
6:T:1240:GLY:O	6:T:1244:VAL:HG23	2.14	0.47
6:T:1556:ILE:HD12	6:T:1573:LEU:HD21	1.95	0.47
6:T:1744:LEU:HA	6:T:1747:PHE:CD2	2.50	0.47
6:T:1744:LEU:HD13	6:T:1747:PHE:CE2	2.50	0.47
6:T:1985:LEU:HA	6:T:1988:PHE:CZ	2.49	0.47
6:T:2003:PHE:HA	6:T:2006:ASN:ND2	2.29	0.47
6:T:2158:LEU:H	6:T:2158:LEU:CD1	2.28	0.47
6:T:2557:HIS:ND1	6:T:2605:MET:HG2	2.29	0.47
6:T:3464:PHE:HB2	6:T:3574:VAL:O	2.14	0.47
1:A:30:VAL:HG11	1:A:337:TYR:CE1	2.50	0.47
1:A:39:ARG:NE	1:A:63:GLY:O	2.48	0.47
1:A:252:ASN:HA	1:A:255:PHE:CE2	2.49	0.47
3:D:623:TYR:HD1	3:D:626:ARG:HH21	1.63	0.47
6:T:638:PHE:O	6:T:642:ILE:HG12	2.14	0.47
6:T:1068:ASN:ND2	6:T:1071:ASP:OD2	2.46	0.47
6:T:1219:LEU:O	6:T:1223:VAL:HG12	2.14	0.47
6:T:1289:LEU:O	6:T:1293:VAL:HG12	2.15	0.47
6:T:1658:ASN:HD21	6:T:1665:PHE:HZ	1.61	0.47
6:T:2679:TRP:CZ3	6:T:2728:LEU:HD22	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:2959:MET:O	6:T:2959:MET:HG2	2.15	0.47
2:B:152:ARG:NH2	2:B:440:LEU:HD11	2.30	0.47
3:D:346:LYS:HE2	5:F:536:PHE:HD2	1.79	0.47
4:E:271:THR:O	4:E:275:ARG:HG2	2.13	0.47
6:T:28:LEU:HG	6:T:78:SER:HB3	1.97	0.47
6:T:159:PHE:HE1	6:T:298:GLN:HE22	1.62	0.47
6:T:638:PHE:HB2	6:T:690:PHE:CZ	2.49	0.47
6:T:687:ALA:O	6:T:691:MET:HG2	2.15	0.47
6:T:1998:ASN:ND2	6:T:2041:LYS:HG2	2.29	0.47
6:T:2168:LEU:HD11	6:T:2211:GLN:CG	2.45	0.47
6:T:2177:LYS:HZ3	6:T:2179:TRP:HB3	1.79	0.47
6:T:2238:MET:SD	6:T:2239:LEU:N	2.88	0.47
6:T:2325:LEU:HD11	6:T:2328:SER:C	2.35	0.47
6:T:2374:ALA:O	6:T:2378:LYS:HG2	2.14	0.47
6:T:3110:ILE:HG22	6:T:3112:ASP:H	1.78	0.47
6:T:3418:ARG:NH1	6:T:3669:ASP:HB3	2.30	0.47
6:T:3564:ILE:HA	6:T:3588:PRO:HA	1.95	0.47
6:T:3731:ARG:O	6:T:3735:ARG:HG3	2.14	0.47
3:D:590:VAL:HA	5:F:570:PHE:CE2	2.50	0.47
4:E:169:ILE:O	4:E:173:PHE:CB	2.63	0.47
4:E:194:ASN:OD1	4:E:195:SER:N	2.48	0.47
6:T:1794:LYS:HD3	6:T:1794:LYS:N	2.27	0.47
6:T:2008:ILE:CG1	6:T:2031:LEU:HD21	2.44	0.47
6:T:2129:SER:HB3	6:T:2173:LYS:NZ	2.30	0.47
6:T:2304:ALA:HA	6:T:2307:THR:HG22	1.96	0.47
1:A:242:LEU:HB2	1:A:246:GLN:HB3	1.96	0.47
3:D:533:GLU:HG2	3:D:533:GLU:O	2.15	0.47
6:T:328:LEU:O	6:T:332:LEU:HG	2.15	0.47
6:T:2235:PHE:HA	6:T:2238:MET:HG3	1.97	0.47
1:A:190:MET:HG3	1:A:200:PHE:HB2	1.96	0.47
2:B:183:ASN:ND2	2:B:185:ILE:HB	2.31	0.47
6:T:338:SER:O	6:T:338:SER:OG	2.31	0.47
6:T:418:TYR:HA	6:T:421:TYR:CD2	2.50	0.47
6:T:744:LEU:HD12	6:T:766:PHE:CE2	2.50	0.47
6:T:1751:SER:HA	6:T:1799:ARG:NE	2.30	0.47
6:T:1864:LEU:HD13	6:T:1889:PHE:CZ	2.50	0.47
6:T:2594:ARG:HH12	6:T:2603:ILE:HD12	1.80	0.47
6:T:3420:PHE:HE1	6:T:3446:PRO:HD2	1.80	0.47
1:A:349:LEU:HD21	3:D:390:ALA:HB1	1.97	0.46
3:D:51:GLN:NE2	3:D:54:GLU:OE2	2.42	0.46
3:D:323:ARG:NH1	5:F:561:PRO:HD3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:76:ARG:O	6:T:80:LEU:HG	2.16	0.46
6:T:857:LEU:O	6:T:861:LEU:HG	2.15	0.46
6:T:1053:GLU:OE1	6:T:1053:GLU:N	2.48	0.46
6:T:1641:GLU:CG	6:T:1676:MET:HE2	2.44	0.46
6:T:1876:PRO:HA	6:T:1883:LYS:HE2	1.96	0.46
6:T:2236:ILE:HD12	6:T:2263:LEU:HD22	1.97	0.46
6:T:2316:TYR:CE2	6:T:2348:PHE:CD2	3.03	0.46
6:T:2348:PHE:O	6:T:2352:ILE:HG23	2.15	0.46
6:T:2545:LEU:HG	6:T:2549:PHE:CE2	2.49	0.46
6:T:2610:ILE:HG21	6:T:2618:LEU:HD23	1.96	0.46
6:T:3136:PHE:O	6:T:3140:LEU:HG	2.15	0.46
6:T:3322:GLU:OE2	6:T:3382:ARG:NH2	2.48	0.46
6:T:382:THR:HG21	6:T:1901:ILE:HD11	1.98	0.46
6:T:1796:LEU:HD12	6:T:1799:ARG:HD3	1.98	0.46
6:T:1941:LEU:HD12	6:T:1941:LEU:C	2.35	0.46
6:T:2214:MET:C	6:T:2214:MET:SD	2.94	0.46
6:T:2422:VAL:HA	6:T:2425:ARG:HG2	1.98	0.46
6:T:3332:GLU:HB2	6:T:3378:VAL:HG13	1.97	0.46
1:A:94:LEU:HB3	1:A:96:VAL:HG12	1.98	0.46
3:D:53:LEU:HA	3:D:53:LEU:HD23	1.62	0.46
3:D:588:SER:OG	3:D:589:VAL:N	2.48	0.46
4:E:186:ILE:O	4:E:190:TYR:HB3	2.15	0.46
4:E:206:TYR:HA	4:E:209:CYS:SG	2.56	0.46
6:T:381:PHE:HD2	6:T:1859:LEU:CD2	2.21	0.46
6:T:1860:PHE:HD2	6:T:1861:ARG:HD2	1.80	0.46
6:T:1867:LEU:C	6:T:1867:LEU:HD12	2.36	0.46
6:T:2101:ILE:HD12	6:T:2166:ASP:HB3	1.96	0.46
6:T:3081:ALA:HB1	6:T:3085:TYR:HE1	1.81	0.46
1:A:216:LEU:HB3	1:A:254:ARG:HE	1.78	0.46
1:A:342:GLY:HA2	1:A:345:ILE:HD12	1.96	0.46
2:B:108:ALA:O	2:B:137:CYS:HA	2.15	0.46
6:T:471:TYR:HE2	6:T:593:PHE:HD2	1.63	0.46
6:T:481:GLN:O	6:T:485:ILE:HG13	2.16	0.46
6:T:1442:ALA:O	6:T:1446:LYS:HG3	2.15	0.46
6:T:1799:ARG:N	6:T:1799:ARG:CD	2.73	0.46
6:T:2007:ILE:CD1	6:T:2031:LEU:HD13	2.45	0.46
6:T:2182:GLU:HG2	6:T:2183:ASN:ND2	2.30	0.46
6:T:3423:TYR:HB2	6:T:3445:LEU:HD13	1.97	0.46
6:T:3499:ASP:N	6:T:3499:ASP:OD1	2.48	0.46
1:A:338:SER:HA	1:A:341:ILE:HD12	1.96	0.46
2:B:13:GLU:OE2	5:F:644:ARG:NH1	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:587:LYS:HD2	4:E:244:LEU:HD21	1.97	0.46
3:D:650:TRP:CE3	3:D:699:ARG:HG2	2.50	0.46
6:T:384:HIS:CD2	6:T:387:LEU:HD12	2.51	0.46
6:T:438:LEU:O	6:T:442:LEU:HG	2.16	0.46
6:T:517:PHE:O	6:T:521:VAL:HG22	2.15	0.46
6:T:719:LEU:HA	6:T:722:VAL:HG23	1.98	0.46
6:T:723:ALA:O	6:T:727:LEU:HD22	2.16	0.46
6:T:742:ARG:NH2	6:T:1544:ALA:HB3	2.30	0.46
6:T:963:PRO:HD2	6:T:3543:LEU:HD21	1.97	0.46
6:T:1518:ILE:HA	6:T:1521:LYS:CE	2.46	0.46
6:T:2282:PHE:HD2	6:T:2315:LEU:HG	1.81	0.46
1:A:312:ARG:O	1:A:316:GLU:HG2	2.16	0.46
2:B:45:GLY:HA3	2:B:69:TYR:OH	2.16	0.46
3:D:767:CYS:SG	6:T:2704:GLN:NE2	2.89	0.46
6:T:37:LEU:HD23	6:T:37:LEU:H	1.80	0.46
6:T:345:LYS:O	6:T:349:HIS:ND1	2.30	0.46
6:T:1268:LEU:O	6:T:1272:PHE:HB2	2.15	0.46
6:T:3021:GLU:OE1	6:T:3021:GLU:N	2.48	0.46
6:T:3733:LEU:O	6:T:3736:THR:HG22	2.15	0.46
1:A:61:LYS:HG2	1:A:64:ILE:HD11	1.98	0.46
1:A:213:LYS:HD3	1:A:306:PHE:CZ	2.51	0.46
6:T:685:TYR:O	6:T:689:MET:HG3	2.15	0.46
6:T:1188:SER:OG	6:T:1189:PHE:N	2.48	0.46
6:T:1510:LEU:HA	6:T:1513:TYR:CE1	2.50	0.46
6:T:1535:LEU:HD23	6:T:1535:LEU:O	2.16	0.46
6:T:1597:ALA:HB2	6:T:1627:ILE:HG23	1.97	0.46
6:T:2229:GLU:HA	6:T:2229:GLU:OE2	2.15	0.46
6:T:3339:PRO:O	6:T:3343:ASN:ND2	2.48	0.46
6:T:3416:GLU:OE1	6:T:3586:MET:N	2.49	0.46
2:B:83:TRP:CH2	2:B:124:SER:HB3	2.51	0.46
6:T:69:HIS:HA	6:T:73:GLN:HG3	1.97	0.46
6:T:293:ASP:OD1	6:T:294:PHE:N	2.49	0.46
6:T:611:TYR:OH	6:T:1584:LEU:C	2.54	0.46
6:T:683:MET:HB3	6:T:722:VAL:HG22	1.97	0.46
6:T:700:GLU:OE1	6:T:1587:GLN:N	2.42	0.46
6:T:1110:PHE:CZ	6:T:1144:LEU:HD11	2.50	0.46
6:T:1320:ILE:HG13	6:T:1325:LEU:HD21	1.97	0.46
6:T:1640:PHE:HB3	6:T:1672:LEU:HD21	1.96	0.46
6:T:2485:GLU:HG2	6:T:2486:LEU:N	2.28	0.46
6:T:3416:GLU:HG3	6:T:3420:PHE:HE2	1.80	0.46
6:T:3721:LEU:HA	6:T:3724:ILE:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:THR:HG22	1:A:132:PHE:HE2	1.81	0.46
3:D:534:GLU:OE2	5:F:641:ARG:NH2	2.30	0.46
5:F:586:LYS:HE2	5:F:586:LYS:HB2	1.78	0.46
6:T:148:TYR:CG	6:T:241:LEU:HD11	2.51	0.46
6:T:480:ARG:HH11	6:T:1760:TYR:HD1	0.71	0.46
6:T:1185:LEU:HD21	6:T:1229:PHE:HB3	1.98	0.46
6:T:1453:PRO:HA	6:T:1456:ILE:HG12	1.98	0.46
6:T:1629:GLN:HA	6:T:1675:THR:HG23	1.98	0.46
6:T:1910:SER:HA	6:T:1913:ILE:CD1	2.45	0.46
6:T:2704:GLN:HG3	6:T:2733:TRP:NE1	2.29	0.46
6:T:3170:GLN:O	6:T:3173:THR:OG1	2.27	0.46
2:B:462:LEU:HD11	2:B:465:PHE:HB2	1.98	0.46
3:D:683:SER:HB2	6:T:2731:ASP:HB3	1.99	0.46
6:T:382:THR:N	6:T:1858:ASP:OD2	2.44	0.46
6:T:848:THR:OG1	6:T:849:ALA:N	2.49	0.46
6:T:1311:LEU:HD13	6:T:1314:ILE:HD11	1.98	0.46
6:T:1358:THR:HA	6:T:1418:LEU:HD13	1.98	0.46
6:T:1526:LEU:CD2	6:T:1552:ILE:HG23	2.46	0.46
6:T:1645:ASP:HA	6:T:1648:TYR:HD2	1.79	0.46
6:T:2538:SER:O	6:T:2542:ILE:HG12	2.16	0.46
6:T:2665:LEU:HD12	6:T:2665:LEU:HA	1.80	0.46
6:T:3331:LYS:HE2	6:T:3377:THR:HB	1.97	0.46
2:B:462:LEU:HD12	2:B:464:THR:H	1.80	0.45
3:D:258:TYR:HB2	5:F:627:LEU:HD21	1.98	0.45
6:T:93:GLN:O	6:T:97:MET:HG2	2.16	0.45
6:T:444:GLU:O	6:T:447:LEU:HG	2.16	0.45
6:T:1438:ILE:HA	6:T:1473:LEU:HD11	1.98	0.45
6:T:1939:ARG:CZ	6:T:1939:ARG:CB	2.94	0.45
6:T:2011:MET:HA	6:T:2014:ILE:HG12	1.97	0.45
6:T:2174:ASN:HB3	6:T:2175:LYS:NZ	2.31	0.45
6:T:2393:LEU:O	6:T:2397:ILE:HG23	2.16	0.45
6:T:2651:ASN:O	6:T:2654:ILE:HG22	2.15	0.45
6:T:3411:ARG:NH1	6:T:3412:HIS:HB3	2.32	0.45
1:A:173:HIS:CD2	2:B:446:ILE:HG21	2.51	0.45
6:T:73:GLN:HE22	6:T:116:ILE:HD11	1.80	0.45
6:T:952:LEU:O	6:T:956:ASN:N	2.49	0.45
6:T:1223:VAL:HG13	6:T:1230:LEU:HD21	1.98	0.45
6:T:1441:LEU:CB	6:T:1473:LEU:HD11	2.26	0.45
6:T:2180:ILE:CD1	6:T:2183:ASN:HB2	2.46	0.45
6:T:2454:VAL:HG21	6:T:2472:ALA:HA	1.98	0.45
4:E:289:GLN:HE22	4:E:292:THR:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1267:LEU:O	6:T:1271:THR:HG22	2.17	0.45
6:T:1412:ARG:O	6:T:1416:ILE:HG13	2.16	0.45
6:T:1564:PRO:HA	6:T:1603:PHE:HE1	1.81	0.45
6:T:1848:ILE:CB	6:T:1852:ASP:HB2	2.46	0.45
6:T:2179:TRP:HA	6:T:2181:MET:CE	2.46	0.45
6:T:2279:MET:HA	6:T:2279:MET:HE3	1.97	0.45
6:T:3687:GLN:O	6:T:3691:MET:HG3	2.15	0.45
2:B:60:GLN:NE2	2:B:60:GLN:O	2.50	0.45
3:D:59:ASN:ND2	3:D:63:LYS:HG3	2.32	0.45
6:T:123:THR:O	6:T:127:LYS:HG3	2.16	0.45
6:T:515:GLU:OE2	6:T:519:ARG:NH2	2.50	0.45
6:T:570:LEU:HD21	6:T:1940:TYR:OH	2.17	0.45
6:T:853:HIS:HB3	6:T:856:GLU:CG	2.45	0.45
6:T:1060:ASN:HD22	6:T:1134:LYS:NZ	2.15	0.45
6:T:1172:TYR:HD2	6:T:1190:ILE:HD12	1.81	0.45
6:T:1299:ALA:HA	6:T:1304:ARG:NH1	2.31	0.45
6:T:1449:LEU:CD2	6:T:1484:PRO:CB	2.94	0.45
6:T:1546:GLN:CG	6:T:1548:PRO:HD2	2.46	0.45
6:T:1677:VAL:HG21	6:T:1728:LEU:HD11	1.98	0.45
6:T:2285:LEU:HD13	6:T:2312:GLU:HG3	1.99	0.45
6:T:2366:PHE:O	6:T:2368:THR:N	2.50	0.45
2:B:160:ILE:HG22	2:B:414:THR:OG1	2.16	0.45
2:B:431:ILE:HG23	2:B:432:LEU:H	1.81	0.45
2:B:473:LYS:H	2:B:473:LYS:HD2	1.81	0.45
3:D:302:LEU:HD21	4:E:279:LEU:HB3	1.98	0.45
6:T:593:PHE:O	6:T:596:THR:OG1	2.31	0.45
6:T:1330:LYS:HG3	6:T:1331:GLN:H	1.82	0.45
6:T:1618:ARG:HA	6:T:1621:VAL:HG22	1.99	0.45
6:T:2461:GLU:HG3	6:T:2592:HIS:CB	2.47	0.45
6:T:2542:ILE:O	6:T:2546:ILE:HG12	2.16	0.45
6:T:2663:LEU:HD13	6:T:2679:TRP:NE1	2.31	0.45
6:T:3620:VAL:HG23	6:T:3727:ALA:HA	1.98	0.45
6:T:3635:SER:OG	6:T:3636:ALA:N	2.49	0.45
1:A:96:VAL:HG22	1:A:101:HIS:HE2	1.81	0.45
1:A:215:LYS:HB3	1:A:216:LEU:HD12	1.99	0.45
3:D:321:GLU:O	3:D:324:ILE:HG22	2.16	0.45
6:T:766:PHE:O	6:T:769:SER:OG	2.27	0.45
6:T:849:ALA:HB3	6:T:854:GLU:CB	2.47	0.45
6:T:1864:LEU:HD13	6:T:1889:PHE:HZ	1.82	0.45
6:T:1939:ARG:HE	6:T:1985:LEU:HD22	1.81	0.45
6:T:2369:VAL:HG12	6:T:2372:LYS:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:2597:SER:OG	6:T:2598:SER:N	2.49	0.45
6:T:3160:ALA:HA	6:T:3167:LEU:HD21	1.97	0.45
1:A:357:ILE:HD11	1:A:373:LYS:HB2	1.98	0.45
2:B:472:LYS:O	2:B:476:GLU:HG2	2.16	0.45
6:T:76:ARG:HA	6:T:79:MET:SD	2.57	0.45
6:T:460:ALA:O	6:T:464:LEU:HG	2.17	0.45
6:T:466:ILE:CG1	6:T:1716:LEU:HD11	2.46	0.45
6:T:850:ARG:NH2	6:T:1007:TYR:HB2	2.31	0.45
6:T:1715:HIS:ND1	6:T:1717:GLN:HG2	2.31	0.45
6:T:2325:LEU:CD2	6:T:2329:ARG:CB	2.95	0.45
6:T:2353:VAL:HA	6:T:2356:SER:OG	2.16	0.45
6:T:2506:GLU:OE1	6:T:2507:ASN:ND2	2.50	0.45
6:T:2681:ARG:HH11	6:T:3634:ASP:HB2	1.81	0.45
6:T:3087:GLN:HG2	6:T:3124:PHE:CE1	2.50	0.45
6:T:3288:LEU:O	6:T:3292:ILE:HG22	2.16	0.45
2:B:23:SER:OG	7:B:501:ATP:O3B	2.30	0.45
2:B:172:ASP:OD2	4:E:182:ARG:NH1	2.50	0.45
4:E:213:PHE:O	4:E:217:ASP:N	2.50	0.45
6:T:949:LEU:HD23	6:T:949:LEU:HA	1.78	0.45
6:T:1491:ASP:HA	6:T:1525:HIS:NE2	2.32	0.45
6:T:1650:PHE:CD2	6:T:1650:PHE:C	2.90	0.45
6:T:1800:ILE:HA	6:T:1803:LEU:HD12	1.98	0.45
6:T:2184:LEU:C	6:T:2184:LEU:CD2	2.86	0.45
6:T:2418:GLN:HB3	6:T:2419:PRO:HD3	1.99	0.45
6:T:2554:LYS:HE3	6:T:2558:ARG:HH21	1.82	0.45
1:A:66:THR:HG1	1:A:68:ARG:HH22	1.61	0.45
1:A:287:VAL:HA	1:A:290:ARG:NE	2.32	0.45
1:A:354:GLN:HG3	1:A:355:MET:SD	2.56	0.45
3:D:23:ARG:HH21	3:D:27:PRO:HG3	1.82	0.45
6:T:90:GLN:HG2	6:T:91:THR:HG23	1.97	0.45
6:T:409:SER:O	6:T:412:GLU:HG3	2.16	0.45
6:T:629:GLU:O	6:T:633:VAL:HG13	2.16	0.45
6:T:641:CYS:O	6:T:645:LEU:HG	2.17	0.45
6:T:1266:ASP:O	6:T:1269:SER:OG	2.30	0.45
6:T:1564:PRO:HD3	6:T:1602:ARG:CZ	2.47	0.45
6:T:1952:VAL:HA	6:T:1955:GLU:HG2	1.99	0.45
6:T:2677:GLY:HA3	6:T:3639:GLY:HA3	1.98	0.45
6:T:3295:LYS:HG3	6:T:3317:TRP:HZ2	1.82	0.45
1:A:177:ARG:NH2	2:B:96:ASN:O	2.40	0.45
2:B:402:ALA:HA	2:B:435:LEU:HD22	1.99	0.45
3:D:669:TRP:CZ2	3:D:697:PHE:HD1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:422:LEU:O	6:T:432:GLN:NE2	2.51	0.45
6:T:705:GLU:O	6:T:709:VAL:HG23	2.17	0.45
6:T:738:GLY:O	6:T:742:ARG:HG3	2.16	0.45
6:T:854:GLU:HG2	6:T:855:ARG:N	2.32	0.45
6:T:1133:LEU:HD23	6:T:1133:LEU:HA	1.80	0.45
6:T:1258:ASP:OD1	6:T:1259:SER:N	2.51	0.45
6:T:1605:ASN:N	6:T:1606:PRO:CD	2.80	0.45
6:T:1918:PHE:CD1	6:T:1923:VAL:HG21	2.51	0.45
6:T:1939:ARG:HB3	6:T:1939:ARG:NH1	2.31	0.45
6:T:2279:MET:HA	6:T:2279:MET:CE	2.47	0.45
6:T:2412:ILE:O	6:T:2415:ARG:HG2	2.17	0.45
6:T:2518:GLU:OE1	6:T:2521:ASN:ND2	2.48	0.45
2:B:249:ILE:HD12	2:B:420:LEU:HA	1.98	0.44
2:B:434:SER:HA	4:E:251:ILE:HD12	1.99	0.44
4:E:82:GLU:OE1	4:E:82:GLU:N	2.50	0.44
6:T:249:PHE:HB3	6:T:288:ARG:NE	2.32	0.44
6:T:778:ASN:OD1	6:T:778:ASN:N	2.50	0.44
6:T:1180:GLY:HA3	6:T:1183:LEU:HD21	1.98	0.44
6:T:1508:GLU:HB2	6:T:1561:LEU:HD12	1.99	0.44
6:T:1580:LEU:HD11	6:T:1592:PHE:CZ	2.52	0.44
6:T:2122:ASN:N	6:T:2122:ASN:HD22	2.14	0.44
6:T:2179:TRP:O	6:T:2179:TRP:CE3	2.70	0.44
6:T:2345:ASP:H	6:T:2348:PHE:HE1	1.65	0.44
6:T:3222:LEU:HD12	6:T:3222:LEU:HA	1.81	0.44
1:A:312:ARG:NE	1:A:316:GLU:OE2	2.50	0.44
2:B:49:ALA:H	2:B:68:ASP:CG	2.20	0.44
3:D:585:ILE:HG22	3:D:587:LYS:NZ	2.28	0.44
4:E:194:ASN:ND2	4:E:196:ARG:HD3	2.32	0.44
6:T:339:GLU:CB	6:T:1897:GLU:HB3	2.47	0.44
6:T:386:THR:O	6:T:389:PRO:HD2	2.18	0.44
6:T:1018:TYR:O	6:T:1022:THR:HG23	2.17	0.44
6:T:1186:SER:OG	6:T:1187:HIS:N	2.51	0.44
6:T:1440:ILE:HA	6:T:1443:VAL:HG12	1.98	0.44
6:T:1804:LYS:HD3	6:T:1863:GLU:HG2	1.99	0.44
6:T:2412:ILE:HG23	6:T:2415:ARG:H	1.83	0.44
6:T:2542:ILE:HG13	6:T:2543:ASP:N	2.32	0.44
6:T:2596:ILE:HG13	6:T:2602:VAL:HG11	1.98	0.44
6:T:2909:PHE:O	6:T:2912:ILE:HG22	2.18	0.44
1:A:217:CYS:HA	1:A:254:ARG:HB3	1.99	0.44
3:D:58:GLU:HG3	3:D:59:ASN:N	2.32	0.44
3:D:605:LEU:HD21	5:F:614:ILE:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:665:TYR:HE2	3:D:675:HIS:CE1	2.35	0.44
6:T:932:LEU:HG	6:T:2825:LEU:HD11	1.98	0.44
6:T:1532:VAL:HG22	6:T:1583:LYS:NZ	2.32	0.44
6:T:1532:VAL:HG22	6:T:1583:LYS:CE	2.47	0.44
6:T:1748:ILE:HD11	6:T:1789:PHE:CZ	2.53	0.44
6:T:1856:HIS:CG	6:T:1856:HIS:O	2.70	0.44
6:T:1924:THR:HA	6:T:1927:PHE:CE2	2.52	0.44
6:T:2092:LEU:H	6:T:2092:LEU:HG	1.61	0.44
6:T:2230:SER:N	6:T:2231:PRO:CD	2.81	0.44
6:T:2620:PRO:O	6:T:2622:LEU:N	2.50	0.44
6:T:2663:LEU:HD23	6:T:2663:LEU:HA	1.71	0.44
6:T:3251:VAL:HA	6:T:3254:ILE:HG22	1.99	0.44
6:T:3353:GLU:OE2	6:T:3358:TYR:HE2	2.00	0.44
6:T:3565:ASN:OD1	6:T:3566:ASN:N	2.45	0.44
6:T:3710:ASN:OD1	6:T:3711:SER:N	2.48	0.44
6:T:357:THR:O	6:T:361:LYS:HG3	2.18	0.44
6:T:474:ARG:NH2	6:T:477:THR:OG1	2.51	0.44
6:T:518:MET:SD	6:T:2317:ILE:HG21	2.57	0.44
6:T:563:ILE:HG23	6:T:564:LYS:H	1.83	0.44
6:T:611:TYR:CE1	6:T:1585:ARG:HB3	2.52	0.44
6:T:1041:GLU:O	6:T:1045:THR:HG23	2.17	0.44
6:T:1286:GLU:OE2	6:T:1328:HIS:NE2	2.51	0.44
6:T:3253:LEU:HD12	6:T:3314:LEU:HB3	1.98	0.44
1:A:305:MET:HA	1:A:335:ARG:NH1	2.32	0.44
2:B:18:VAL:HG21	2:B:457:SER:HA	1.99	0.44
2:B:245:THR:HA	3:D:75:ARG:NH2	2.33	0.44
2:B:406:HIS:O	2:B:438:ARG:HG2	2.17	0.44
3:D:352:TRP:N	3:D:352:TRP:CD1	2.85	0.44
6:T:730:GLU:HG2	6:T:732:THR:N	2.24	0.44
6:T:806:LEU:HD12	6:T:806:LEU:H	1.82	0.44
6:T:1066:THR:N	6:T:3476:LYS:HZ2	2.15	0.44
6:T:1493:GLN:HE21	6:T:1493:GLN:CA	2.12	0.44
6:T:1539:PHE:CD2	6:T:1539:PHE:O	2.70	0.44
6:T:1685:LEU:HD12	6:T:1689:GLY:H	1.83	0.44
6:T:1699:LEU:C	6:T:1699:LEU:CD2	2.86	0.44
6:T:2175:LYS:HD3	6:T:2175:LYS:H	1.82	0.44
6:T:2320:LEU:CD2	6:T:2320:LEU:C	2.86	0.44
6:T:3075:ILE:HG23	6:T:3077:PHE:H	1.83	0.44
6:T:3134:ILE:HG12	6:T:3166:ALA:HB1	2.00	0.44
2:B:40:LEU:HD23	2:B:40:LEU:HA	1.83	0.44
2:B:74:ILE:O	2:B:81:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:762:GLU:N	3:D:762:GLU:OE1	2.50	0.44
6:T:571:LEU:C	6:T:1940:TYR:HD2	2.19	0.44
6:T:724:GLN:O	6:T:728:THR:HG23	2.18	0.44
6:T:1041:GLU:HB3	6:T:2513:GLU:HB2	1.99	0.44
6:T:1570:LEU:C	6:T:1570:LEU:CD2	2.86	0.44
6:T:1798:ALA:HA	6:T:1801:PHE:CD2	2.52	0.44
6:T:1815:VAL:HG21	6:T:1870:ILE:CD1	2.47	0.44
6:T:1849:LEU:HD13	6:T:1896:LEU:HD23	2.00	0.44
6:T:1876:PRO:HA	6:T:1883:LYS:NZ	2.33	0.44
6:T:1903:GLN:HB3	6:T:1941:LEU:CD2	2.48	0.44
6:T:3583:THR:HG22	6:T:3584:LEU:H	1.83	0.44
1:A:191:LYS:O	1:A:195:GLU:HG2	2.17	0.44
3:D:537:LYS:HE3	3:D:537:LYS:HB2	1.67	0.44
3:D:558:THR:O	3:D:560:ILE:HD12	2.18	0.44
3:D:615:LEU:H	6:T:2456:ARG:NH1	2.15	0.44
4:E:247:SER:OG	4:E:248:ALA:N	2.51	0.44
4:E:269:LYS:HB3	5:F:624:GLN:HE22	1.83	0.44
6:T:562:ASP:HB3	6:T:566:TYR:HD2	1.81	0.44
6:T:1838:HIS:CE1	6:T:1882:ILE:HD12	2.52	0.44
6:T:2036:LEU:CD2	6:T:2123:ILE:HG23	2.48	0.44
6:T:2282:PHE:HA	6:T:2285:LEU:HD12	1.99	0.44
6:T:2285:LEU:HD13	6:T:2312:GLU:CG	2.48	0.44
6:T:2432:ARG:NH1	6:T:2547:GLU:OE2	2.51	0.44
6:T:2434:ARG:O	6:T:2438:ILE:HG12	2.18	0.44
6:T:2509:GLU:N	6:T:2509:GLU:OE1	2.50	0.44
6:T:2876:GLU:OE1	6:T:2876:GLU:N	2.33	0.44
6:T:3026:LYS:O	6:T:3030:LEU:HG	2.17	0.44
1:A:6:ALA:O	1:A:101:HIS:HB3	2.17	0.44
1:A:110:MET:HB3	2:B:37:GLN:HE21	1.83	0.44
1:A:272:ALA:H	2:B:60:GLN:HE21	1.66	0.44
2:B:80:VAL:HB	2:B:120:ASN:HD21	1.83	0.44
3:D:36:ARG:HE	3:D:322:ALA:HB1	1.83	0.44
3:D:60:LYS:HD2	3:D:60:LYS:HA	1.68	0.44
3:D:81:ASP:N	3:D:81:ASP:OD1	2.51	0.44
3:D:312:THR:OG1	6:T:3626:PRO:HG3	2.18	0.44
3:D:359:GLN:O	3:D:363:LEU:HG	2.18	0.44
4:E:294:TYR:HB2	4:E:302:GLN:HG2	1.99	0.44
6:T:125:LEU:HD11	6:T:140:PHE:CZ	2.53	0.44
6:T:344:ARG:O	6:T:348:LEU:HG	2.18	0.44
6:T:1762:LEU:C	6:T:1762:LEU:CD2	2.85	0.44
6:T:2090:LEU:HA	6:T:2093:ARG:CD	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:2330:ARG:NH2	6:T:2371:GLU:OE2	2.50	0.44
6:T:2372:LYS:O	6:T:2375:ILE:HG12	2.18	0.44
6:T:2402:PHE:CZ	6:T:2416:MET:HB3	2.53	0.44
6:T:3230:VAL:HG23	6:T:3451:LEU:HD22	2.00	0.44
6:T:3426:PHE:HD1	6:T:3426:PHE:HA	1.71	0.44
1:A:10:ILE:HD11	1:A:90:PHE:CE1	2.52	0.44
6:T:712:ARG:HD3	6:T:712:ARG:HA	1.72	0.44
6:T:1345:LEU:O	6:T:1350:GLN:HG3	2.18	0.44
6:T:1879:ILE:HB	6:T:1882:ILE:CG1	2.47	0.44
6:T:1904:SER:N	6:T:1941:LEU:HD21	2.33	0.44
6:T:1918:PHE:CD2	6:T:1918:PHE:O	2.71	0.44
6:T:2490:ASN:OD1	6:T:2490:ASN:N	2.48	0.44
6:T:2889:PRO:HB2	6:T:2898:TRP:NE1	2.33	0.44
6:T:2923:LEU:HD11	6:T:2938:ARG:HG2	2.00	0.44
6:T:3433:ASN:OD1	6:T:3434:VAL:N	2.51	0.44
1:A:213:LYS:HA	1:A:217:CYS:SG	2.57	0.43
2:B:158:VAL:HG22	2:B:167:VAL:HG22	2.00	0.43
2:B:434:SER:HA	4:E:251:ILE:CD1	2.48	0.43
3:D:277:ILE:HD12	5:F:577:TYR:CZ	2.52	0.43
3:D:597:PHE:HE1	5:F:639:ARG:NE	2.16	0.43
3:D:615:LEU:HD12	3:D:619:ARG:HH12	1.83	0.43
5:F:540:ASP:OD1	5:F:544:ASN:HB3	2.18	0.43
5:F:559:ASN:N	5:F:559:ASN:OD1	2.47	0.43
6:T:349:HIS:CD2	6:T:352:ARG:HH12	2.35	0.43
6:T:629:GLU:OE2	6:T:1717:GLN:CA	2.66	0.43
6:T:1473:LEU:C	6:T:1473:LEU:CD2	2.85	0.43
6:T:2100:LEU:C	6:T:2100:LEU:CD2	2.86	0.43
6:T:2607:LEU:HD21	6:T:2624:LYS:HE3	1.99	0.43
6:T:2783:VAL:HG12	6:T:2791:ARG:NE	2.33	0.43
6:T:2840:LYS:HE3	6:T:2840:LYS:HB2	1.80	0.43
6:T:3086:LEU:HD23	6:T:3104:ILE:HD13	1.99	0.43
1:A:241:GLU:HA	1:A:247:VAL:HA	2.00	0.43
2:B:416:SER:HA	2:B:448:ARG:NH1	2.32	0.43
4:E:169:ILE:HG21	4:E:204:LYS:HE2	2.00	0.43
6:T:116:ILE:O	6:T:120:LYS:HD3	2.18	0.43
6:T:981:LYS:N	6:T:2483:GLU:OE1	2.50	0.43
6:T:1890:CYS:SG	6:T:1891:TRP:N	2.90	0.43
6:T:1936:VAL:CG2	6:T:1939:ARG:HD3	2.44	0.43
6:T:2174:ASN:HB3	6:T:2175:LYS:CE	2.47	0.43
6:T:2191:LEU:HA	6:T:2194:CYS:SG	2.58	0.43
6:T:3464:PHE:HB3	6:T:3575:ASP:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:O	1:A:192:ILE:HG12	2.18	0.43
2:B:253:LYS:HE2	2:B:258:THR:HG22	2.00	0.43
3:D:76:ARG:HD2	3:D:77:GLY:N	2.33	0.43
3:D:294:SER:HB2	3:D:321:GLU:OE2	2.19	0.43
4:E:198:LEU:HA	4:E:201:LEU:HB3	2.01	0.43
5:F:609:LEU:N	5:F:613:ARG:HH21	2.16	0.43
6:T:942:SER:OG	6:T:943:HIS:N	2.52	0.43
6:T:1210:ARG:HA	6:T:1213:VAL:HG12	1.99	0.43
6:T:1300:ASN:HD21	6:T:1302:LYS:HB2	1.82	0.43
6:T:1473:LEU:N	6:T:1474:PRO:HD2	2.33	0.43
6:T:1738:ARG:HA	6:T:1738:ARG:HE	1.81	0.43
6:T:1913:ILE:HD12	6:T:1923:VAL:CG2	2.48	0.43
6:T:2022:SER:HB3	6:T:2025:HIS:HE1	1.82	0.43
6:T:3089:ALA:HB1	6:T:3097:ILE:HD12	2.00	0.43
6:T:3225:SER:HB3	6:T:3349:PHE:CE1	2.53	0.43
1:A:98:PRO:HA	1:A:101:HIS:CD2	2.53	0.43
2:B:69:TYR:HE2	2:B:229:LEU:HD21	1.84	0.43
6:T:24:ARG:HE	6:T:74:LYS:HB2	1.82	0.43
6:T:688:PHE:O	6:T:692:GLN:NE2	2.51	0.43
6:T:1333:LEU:O	6:T:1336:PRO:HD2	2.18	0.43
6:T:1463:LEU:C	6:T:1463:LEU:CD2	2.86	0.43
6:T:1492:HIS:ND1	6:T:1494:LYS:HB2	2.34	0.43
6:T:3282:LYS:O	6:T:3285:THR:HG22	2.19	0.43
6:T:952:LEU:O	6:T:952:LEU:HD12	2.19	0.43
6:T:1043:LEU:HD11	6:T:1115:VAL:HG11	2.00	0.43
6:T:1175:SER:HA	6:T:1178:ILE:HG22	2.00	0.43
6:T:1378:LEU:O	6:T:1382:ILE:HG12	2.18	0.43
6:T:1413:ILE:HD11	6:T:1458:THR:HG21	1.99	0.43
6:T:1588:LEU:HG	6:T:1588:LEU:O	2.19	0.43
6:T:1757:LYS:HD3	6:T:1802:VAL:HG22	2.00	0.43
6:T:1872:ILE:HD12	6:T:1912:PHE:HD2	1.84	0.43
6:T:2118:LEU:C	6:T:2118:LEU:CD2	2.86	0.43
6:T:2245:GLN:NE2	6:T:2245:GLN:CA	2.73	0.43
6:T:2621:HIS:CE1	6:T:2622:LEU:HG	2.54	0.43
6:T:2746:LEU:H	6:T:2746:LEU:HD23	1.83	0.43
6:T:2774:ASP:OD1	6:T:2775:ALA:N	2.49	0.43
6:T:2986:ARG:HH12	6:T:2990:LYS:HZ1	1.65	0.43
6:T:3626:PRO:HA	6:T:3629:GLN:HG2	2.00	0.43
3:D:393:ASP:HA	3:D:396:THR:HG22	2.00	0.43
3:D:537:LYS:HG3	3:D:538:GLU:H	1.83	0.43
6:T:381:PHE:CG	6:T:1859:LEU:HD21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1091:SER:O	6:T:1091:SER:OG	2.33	0.43
6:T:1107:LEU:HD23	6:T:1107:LEU:HA	1.83	0.43
6:T:1582:ARG:HD3	6:T:1582:ARG:C	2.39	0.43
6:T:1962:THR:N	6:T:1963:PRO:CD	2.81	0.43
6:T:2182:GLU:OE1	6:T:2182:GLU:N	2.37	0.43
6:T:2244:THR:CG2	6:T:2274:LEU:HD22	2.48	0.43
6:T:2451:LEU:HD12	6:T:2451:LEU:HA	1.79	0.43
6:T:2842:LEU:O	6:T:2845:GLY:N	2.52	0.43
1:A:314:GLN:HE22	1:A:328:LYS:HA	1.84	0.43
2:B:199:GLU:N	2:B:200:PRO:HD2	2.34	0.43
2:B:441:THR:HG22	3:D:68:PHE:HA	2.01	0.43
2:B:474:GLU:O	2:B:478:VAL:HG12	2.19	0.43
3:D:379:TYR:OH	3:D:532:THR:HG21	2.19	0.43
6:T:1448:MET:CE	6:T:1456:ILE:HB	2.48	0.43
6:T:1483:LYS:N	6:T:1484:PRO:CD	2.82	0.43
6:T:1546:GLN:OE1	6:T:1546:GLN:HA	2.19	0.43
6:T:1703:LEU:C	6:T:1703:LEU:CD2	2.85	0.43
6:T:2204:GLU:H	6:T:2204:GLU:HG3	1.63	0.43
6:T:2282:PHE:HE1	6:T:2335:THR:CB	2.31	0.43
6:T:2325:LEU:HD21	6:T:2328:SER:C	2.39	0.43
6:T:3111:ASP:OD1	6:T:3111:ASP:N	2.48	0.43
2:B:162:HIS:HB2	7:B:501:ATP:O3'	2.19	0.43
5:F:581:LEU:HD11	5:F:613:ARG:HA	2.01	0.43
6:T:23:SER:HA	6:T:27:THR:HG23	2.01	0.43
6:T:80:LEU:HA	6:T:83:PHE:HB2	2.00	0.43
6:T:341:SER:OG	6:T:344:ARG:HB2	2.18	0.43
6:T:627:SER:H	6:T:630:GLU:CD	2.22	0.43
6:T:913:PHE:HZ	6:T:917:ILE:HD12	1.83	0.43
6:T:1075:GLN:NE2	6:T:2491:ILE:O	2.46	0.43
6:T:1300:ASN:O	6:T:1303:VAL:HG12	2.18	0.43
6:T:1377:LEU:O	6:T:1380:GLU:HG3	2.19	0.43
6:T:1497:VAL:N	6:T:1498:PRO:CD	2.81	0.43
6:T:1703:LEU:HD23	6:T:1703:LEU:O	2.18	0.43
6:T:1932:ARG:HE	6:T:1933:SER:H	1.67	0.43
6:T:2124:LEU:C	6:T:2124:LEU:CD2	2.86	0.43
6:T:2387:GLU:HB3	6:T:2390:LEU:HB3	2.01	0.43
6:T:2482:ARG:HD2	6:T:2539:SER:HB2	2.01	0.43
6:T:2580:VAL:HA	6:T:2583:ILE:HG22	2.00	0.43
6:T:3095:SER:O	6:T:3096:LYS:HE2	2.18	0.43
6:T:3178:PHE:HA	6:T:3181:ILE:HD12	2.00	0.43
6:T:3267:ARG:NH1	6:T:3498:ASP:OD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:ALA:O	2:B:89:GLN:HB3	2.19	0.43
3:D:44:TYR:HD1	3:D:44:TYR:HA	1.71	0.43
3:D:600:LEU:HD13	3:D:600:LEU:HA	1.82	0.43
6:T:6:GLN:NE2	6:T:43:ASP:OD2	2.52	0.43
6:T:635:LYS:HB2	6:T:701:ILE:HD12	2.01	0.43
6:T:1541:GLN:OE1	6:T:1541:GLN:HA	2.18	0.43
6:T:2383:GLU:OE1	6:T:2383:GLU:N	2.52	0.43
6:T:2888:LEU:HD12	6:T:2888:LEU:HA	1.92	0.43
6:T:3414:ARG:NH2	6:T:3417:GLU:OE1	2.51	0.43
3:D:537:LYS:HG3	3:D:538:GLU:N	2.34	0.43
5:F:637:LYS:NZ	5:F:655:ASN:HB3	2.34	0.43
6:T:429:LEU:O	6:T:433:ILE:HG13	2.19	0.43
6:T:776:PHE:HB3	6:T:779:ILE:CG2	2.48	0.43
6:T:844:GLN:N	6:T:844:GLN:OE1	2.52	0.43
6:T:896:GLN:HA	6:T:899:ARG:HD2	2.01	0.43
6:T:1104:ASN:HB3	6:T:1170:ARG:NE	2.34	0.43
6:T:1346:PRO:O	6:T:1349:MET:N	2.52	0.43
6:T:1969:TRP:HA	6:T:1972:ARG:HB2	2.01	0.43
6:T:2770:ASN:OD1	6:T:2771:SER:N	2.52	0.43
1:A:150:GLY:HA2	1:A:293:LEU:HD12	2.01	0.42
2:B:418:PRO:HG3	3:D:75:ARG:HH12	1.83	0.42
3:D:287:LEU:HB2	4:E:265:GLU:OE1	2.18	0.42
6:T:222:LYS:NZ	6:T:234:LEU:HD22	2.34	0.42
6:T:330:ILE:HD13	6:T:372:ASP:HB3	2.01	0.42
6:T:518:MET:CE	6:T:2317:ILE:HD13	2.48	0.42
6:T:570:LEU:O	6:T:571:LEU:HG	2.19	0.42
6:T:788:LEU:O	6:T:791:LEU:HB3	2.19	0.42
6:T:1518:ILE:HA	6:T:1521:LYS:HE2	2.01	0.42
6:T:1936:VAL:HG23	6:T:1939:ARG:NH1	2.34	0.42
6:T:3551:GLN:HB3	6:T:3581:VAL:HG12	2.01	0.42
2:B:129:LEU:HD23	2:B:129:LEU:HA	1.73	0.42
3:D:536:LYS:HD2	3:D:536:LYS:HA	1.76	0.42
3:D:601:LEU:HD23	3:D:601:LEU:HA	1.78	0.42
3:D:723:TRP:HE3	3:D:724:LEU:HD22	1.84	0.42
6:T:3:LEU:HG	6:T:5:GLU:H	1.84	0.42
6:T:349:HIS:O	6:T:352:ARG:HG2	2.19	0.42
6:T:400:HIS:HB2	6:T:438:LEU:HD22	2.01	0.42
6:T:439:LEU:O	6:T:443:VAL:HG13	2.18	0.42
6:T:1011:ILE:HA	6:T:1014:ARG:HD3	2.01	0.42
6:T:1776:LYS:NZ	6:T:1778:LYS:HG3	2.33	0.42
6:T:1815:VAL:HG21	6:T:1870:ILE:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1907:LEU:C	6:T:1907:LEU:CD2	2.85	0.42
6:T:1949:LEU:C	6:T:1949:LEU:CD2	2.85	0.42
6:T:1970:VAL:HG12	6:T:2003:PHE:CE2	2.54	0.42
6:T:2034:LEU:C	6:T:2034:LEU:CD2	2.86	0.42
6:T:3105:LEU:HD21	6:T:3133:TRP:HZ3	1.83	0.42
1:A:253:GLU:H	1:A:253:GLU:CD	2.21	0.42
2:B:203:ILE:HA	2:B:274:TRP:CH2	2.55	0.42
2:B:472:LYS:HE2	2:B:476:GLU:HG3	2.01	0.42
3:D:308:LYS:NZ	4:E:281:LEU:HD21	2.34	0.42
3:D:374:LYS:O	3:D:378:LYS:HG3	2.19	0.42
4:E:198:LEU:O	4:E:202:LYS:HG2	2.19	0.42
6:T:1157:ILE:O	6:T:1161:ARG:HG3	2.19	0.42
6:T:1206:TYR:CE2	6:T:1253:PRO:HD2	2.54	0.42
6:T:1474:PRO:HG3	6:T:1511:ILE:HD13	2.00	0.42
6:T:1559:PHE:HB3	6:T:1599:TYR:CE1	2.53	0.42
6:T:1564:PRO:HD3	6:T:1602:ARG:NH2	2.35	0.42
6:T:1600:LEU:N	6:T:1600:LEU:HD23	2.34	0.42
6:T:1673:PHE:HA	6:T:1676:MET:HG2	2.01	0.42
6:T:1930:LEU:CB	6:T:1946:LEU:HD21	2.48	0.42
6:T:2115:GLU:HB2	6:T:2116:LEU:HD23	2.00	0.42
6:T:2219:ALA:HB3	6:T:2222:VAL:CG1	2.50	0.42
6:T:2640:LEU:HD23	6:T:2640:LEU:HA	1.78	0.42
6:T:3240:THR:CG2	6:T:3243:GLU:H	2.31	0.42
1:A:361:GLU:O	1:A:365:SER:OG	2.26	0.42
3:D:25:LYS:O	3:D:28:LYS:N	2.50	0.42
5:F:627:LEU:O	5:F:628:GLU:HG3	2.18	0.42
6:T:3:LEU:HD23	6:T:3:LEU:H	1.84	0.42
6:T:72:GLU:OE1	6:T:76:ARG:NH2	2.53	0.42
6:T:471:TYR:CE2	6:T:590:LEU:HD22	2.54	0.42
6:T:719:LEU:HA	6:T:722:VAL:CG2	2.49	0.42
6:T:934:PRO:HD3	6:T:2825:LEU:HG	2.01	0.42
6:T:1039:TYR:HE1	6:T:2497:PRO:HB2	1.84	0.42
6:T:1671:ASP:HA	6:T:1674:ASN:HD22	1.84	0.42
6:T:1750:PHE:O	6:T:1750:PHE:CD1	2.70	0.42
6:T:1822:LYS:HB2	6:T:1822:LYS:HE3	1.82	0.42
6:T:2191:LEU:HD12	6:T:2194:CYS:SG	2.60	0.42
6:T:2359:TRP:HA	6:T:2362:ASN:CG	2.40	0.42
6:T:2707:TYR:O	6:T:2711:GLN:HG3	2.17	0.42
6:T:2825:LEU:HD12	6:T:2825:LEU:HA	1.85	0.42
6:T:3142:THR:O	6:T:3145:SER:OG	2.18	0.42
6:T:3528:LYS:O	6:T:3532:THR:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:3583:THR:HG22	6:T:3584:LEU:N	2.33	0.42
2:B:47:TYR:HD2	2:B:54:LYS:HG3	1.84	0.42
2:B:254:THR:HG22	2:B:423:ARG:NH2	2.34	0.42
3:D:619:ARG:HD3	6:T:2443:LEU:HD23	2.00	0.42
4:E:82:GLU:OE2	4:E:92:ARG:NH1	2.52	0.42
6:T:310:ILE:HD13	6:T:350:ALA:HB1	2.00	0.42
6:T:332:LEU:O	6:T:336:CYS:HB3	2.19	0.42
6:T:357:THR:OG1	6:T:360:LYS:HB2	2.19	0.42
6:T:466:ILE:HA	6:T:1716:LEU:CD2	2.49	0.42
6:T:913:PHE:CZ	6:T:917:ILE:HD12	2.54	0.42
6:T:1066:THR:H	6:T:3476:LYS:HZ2	1.67	0.42
6:T:1849:LEU:HD21	6:T:1893:PHE:HA	2.01	0.42
6:T:1860:PHE:HA	6:T:1863:GLU:HG3	2.01	0.42
6:T:1902:LYS:HB3	6:T:1906:TYR:CE2	2.55	0.42
6:T:1919:PRO:CG	6:T:1922:VAL:HB	2.47	0.42
6:T:1987:GLN:HE21	6:T:2007:ILE:HG22	1.83	0.42
6:T:2022:SER:HB3	6:T:2025:HIS:CE1	2.55	0.42
6:T:2182:GLU:CD	6:T:2182:GLU:N	2.73	0.42
6:T:2365:ILE:HG13	6:T:2366:PHE:H	1.84	0.42
6:T:2620:PRO:O	6:T:2621:HIS:CG	2.72	0.42
6:T:2892:TRP:HA	6:T:3434:VAL:HG23	2.02	0.42
6:T:2936:ALA:HB3	6:T:2938:ARG:NH2	2.34	0.42
6:T:3079:SER:HA	6:T:3082:ILE:HG22	2.01	0.42
6:T:3422:LEU:HD12	6:T:3666:PHE:HB2	2.01	0.42
1:A:130:PRO:O	1:A:359:LYS:N	2.52	0.42
2:B:164:THR:O	2:B:164:THR:OG1	2.36	0.42
3:D:270:PHE:O	5:F:587:GLY:N	2.32	0.42
6:T:56:LEU:HB2	6:T:102:PHE:HZ	1.84	0.42
6:T:58:GLN:HG2	6:T:79:MET:HG2	2.01	0.42
6:T:81:ASP:HA	6:T:84:ASN:HD21	1.83	0.42
6:T:1140:LEU:HB2	6:T:2493:CYS:O	2.20	0.42
6:T:1654:ASN:HB3	6:T:1665:PHE:CZ	2.55	0.42
6:T:2214:MET:HA	6:T:2217:ILE:HG22	2.01	0.42
6:T:2444:GLU:HG3	6:T:2445:ARG:H	1.85	0.42
6:T:3137:ILE:HG23	6:T:3138:PRO:HD3	2.02	0.42
6:T:3137:ILE:HA	6:T:3140:LEU:HD12	2.01	0.42
2:B:227:LYS:HD3	2:B:227:LYS:HA	1.78	0.42
6:T:407:GLN:O	6:T:411:ILE:HG12	2.20	0.42
6:T:605:ASN:HD22	6:T:620:ALA:C	2.22	0.42
6:T:956:ASN:HD21	6:T:2843:LEU:CB	2.25	0.42
6:T:987:GLU:OE1	6:T:987:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1456:ILE:HD12	6:T:1502:ALA:HB2	2.01	0.42
6:T:2369:VAL:HA	6:T:2372:LYS:HD3	2.02	0.42
6:T:2959:MET:HG2	6:T:2962:VAL:HG12	2.02	0.42
6:T:3081:ALA:HB1	6:T:3085:TYR:CE1	2.54	0.42
6:T:3326:ASP:OD2	6:T:3382:ARG:NH1	2.47	0.42
1:A:107:GLU:OE2	1:A:111:ASN:ND2	2.52	0.42
3:D:59:ASN:HA	5:F:568:SER:O	2.19	0.42
3:D:74:ILE:HD12	3:D:74:ILE:HA	1.95	0.42
3:D:309:ALA:HB3	6:T:2681:ARG:NH2	2.34	0.42
3:D:623:TYR:HB2	3:D:626:ARG:NE	2.27	0.42
4:E:262:LYS:O	4:E:266:MET:HG3	2.20	0.42
4:E:287:SER:O	4:E:287:SER:OG	2.37	0.42
6:T:618:LEU:H	6:T:618:LEU:HD12	1.85	0.42
6:T:935:GLN:C	6:T:937:PHE:N	2.73	0.42
6:T:1416:ILE:HG21	6:T:1459:THR:OG1	2.20	0.42
6:T:1449:LEU:CD1	6:T:1484:PRO:HB2	2.48	0.42
6:T:1683:GLU:HG3	6:T:1686:LYS:H	1.84	0.42
6:T:2243:ILE:HD13	6:T:2243:ILE:HA	1.85	0.42
6:T:2262:VAL:HA	6:T:2265:MET:SD	2.59	0.42
6:T:2474:GLN:OE1	6:T:2546:ILE:HG23	2.19	0.42
6:T:3464:PHE:CB	6:T:3575:ASP:HA	2.49	0.42
6:T:3623:ARG:NH2	6:T:3744:PHE:O	2.42	0.42
2:B:243:LYS:HA	2:B:247:CYS:SG	2.60	0.42
2:B:389:VAL:O	2:B:392:SER:OG	2.29	0.42
6:T:218:MET:HA	6:T:221:PHE:CD2	2.55	0.42
6:T:683:MET:O	6:T:686:LEU:HG	2.20	0.42
6:T:758:THR:O	6:T:762:LEU:HD23	2.20	0.42
6:T:879:LEU:HD13	6:T:879:LEU:HA	1.90	0.42
6:T:1342:LEU:HA	6:T:1342:LEU:HD12	1.78	0.42
6:T:1617:LEU:HD12	6:T:1620:LEU:HD23	2.02	0.42
6:T:1814:GLU:HA	6:T:1817:THR:HG22	2.02	0.42
6:T:2316:TYR:CE2	6:T:2348:PHE:HD2	2.38	0.42
6:T:2760:LEU:HD11	6:T:2790:ARG:HH21	1.84	0.42
6:T:3524:SER:OG	6:T:3525:ASN:N	2.53	0.42
1:A:375:PHE:CD1	3:D:380:LYS:HB2	2.54	0.42
2:B:431:ILE:HG23	2:B:432:LEU:N	2.35	0.42
5:F:583:GLU:OE1	5:F:583:GLU:N	2.52	0.42
6:T:72:GLU:CB	6:T:76:ARG:HE	2.33	0.42
6:T:295:ILE:O	6:T:299:ILE:HG12	2.20	0.42
6:T:1821:LEU:CD1	6:T:1824:TYR:HB2	2.50	0.42
6:T:2195:ILE:CG2	6:T:2239:LEU:HD22	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:2443:LEU:HD11	6:T:2453:TYR:CD2	2.55	0.42
6:T:2523:VAL:O	6:T:2527:ILE:HG12	2.20	0.42
6:T:2546:ILE:HA	6:T:2546:ILE:HD13	1.86	0.42
1:A:12:ASN:HD21	1:A:71:ILE:HG21	1.85	0.41
1:A:238:LYS:HE3	1:A:238:LYS:HB3	1.93	0.41
2:B:16:ALA:CB	2:B:107:PRO:HG2	2.50	0.41
3:D:537:LYS:HG3	3:D:538:GLU:OE1	2.20	0.41
3:D:618:ARG:C	3:D:619:ARG:HD2	2.39	0.41
6:T:382:THR:H	6:T:1858:ASP:CG	2.23	0.41
6:T:474:ARG:HA	6:T:474:ARG:HD2	1.89	0.41
6:T:700:GLU:OE1	6:T:1587:GLN:O	2.37	0.41
6:T:713:MET:HE1	6:T:720:LEU:HD23	2.02	0.41
6:T:1155:TYR:CD2	6:T:1160:VAL:HG21	2.55	0.41
6:T:1396:ILE:HG13	6:T:1397:GLN:H	1.84	0.41
6:T:1448:MET:HA	6:T:1456:ILE:HG22	2.02	0.41
6:T:1454:GLU:HA	6:T:1457:ASN:HD21	1.85	0.41
6:T:1543:LEU:CB	6:T:1591:PRO:HG3	2.50	0.41
6:T:1568:MET:O	6:T:1568:MET:SD	2.78	0.41
6:T:1792:SER:HA	6:T:1794:LYS:NZ	2.34	0.41
2:B:49:ALA:N	2:B:68:ASP:OD2	2.53	0.41
2:B:281:ASP:OD2	2:B:283:GLU:HB3	2.20	0.41
2:B:405:ALA:O	2:B:437:PHE:HA	2.20	0.41
3:D:70:LYS:NZ	3:D:539:LEU:H	2.18	0.41
3:D:258:TYR:CZ	5:F:553:LYS:HB2	2.54	0.41
3:D:650:TRP:CZ3	3:D:699:ARG:HG2	2.55	0.41
4:E:180:ASP:HB3	4:E:182:ARG:NE	2.35	0.41
6:T:470:SER:HA	6:T:473:ASN:HD21	1.85	0.41
6:T:482:TYR:HD1	6:T:647:PHE:CE1	2.38	0.41
6:T:1574:LEU:HD22	6:T:1623:PHE:CE2	2.49	0.41
6:T:3009:THR:HG23	6:T:3010:ASN:H	1.86	0.41
6:T:3036:TYR:OH	6:T:3070:GLU:OE1	2.26	0.41
3:D:348:PHE:H	4:E:236:ARG:NH1	2.19	0.41
6:T:611:TYR:OH	6:T:1584:LEU:O	2.37	0.41
6:T:2571:ILE:HD12	6:T:2571:ILE:HA	1.95	0.41
6:T:3295:LYS:HG3	6:T:3317:TRP:CZ2	2.56	0.41
1:A:318:THR:HA	1:A:327:VAL:HG21	2.02	0.41
1:A:351:THR:O	1:A:354:GLN:HG2	2.21	0.41
6:T:50:ALA:O	6:T:53:PRO:HD2	2.20	0.41
6:T:914:ASP:HB2	6:T:915:PRO:HD3	2.02	0.41
6:T:1046:ALA:O	6:T:1050:ILE:HG12	2.20	0.41
6:T:1601:ASN:HA	6:T:1604:HIS:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1684:TRP:CE3	6:T:1684:TRP:O	2.72	0.41
6:T:1932:ARG:HE	6:T:1932:ARG:HA	1.85	0.41
6:T:2325:LEU:CD1	6:T:2328:SER:HB3	2.46	0.41
6:T:2999:LEU:HD23	6:T:2999:LEU:O	2.21	0.41
6:T:3020:ALA:HB2	6:T:3049:ILE:HG21	2.02	0.41
6:T:3322:GLU:HG3	6:T:3382:ARG:HD3	2.01	0.41
2:B:56:ILE:H	2:B:56:ILE:HD12	1.85	0.41
3:D:279:SER:OG	3:D:280:LYS:N	2.54	0.41
4:E:292:THR:HB	4:E:295:LEU:HB2	2.02	0.41
5:F:560:VAL:HB	5:F:561:PRO:CD	2.51	0.41
6:T:464:LEU:HA	6:T:467:ILE:HG22	2.02	0.41
6:T:854:GLU:HG2	6:T:855:ARG:H	1.85	0.41
6:T:1529:TRP:HA	6:T:1529:TRP:CE3	2.56	0.41
6:T:1565:GLN:HE21	6:T:1565:GLN:HB2	1.55	0.41
6:T:1591:PRO:HG2	6:T:1592:PHE:CD1	2.55	0.41
6:T:1651:TYR:CD1	6:T:1665:PHE:HB3	2.55	0.41
6:T:2852:PHE:O	6:T:2855:ALA:HB3	2.20	0.41
1:A:209:VAL:HA	1:A:212:ILE:HD12	2.03	0.41
1:A:272:ALA:H	2:B:60:GLN:NE2	2.19	0.41
2:B:64:ILE:O	2:B:66:ARG:NH1	2.51	0.41
4:E:185:LEU:HD23	4:E:185:LEU:H	1.84	0.41
4:E:246:ARG:HE	4:E:246:ARG:HB2	1.54	0.41
5:F:585:LEU:C	5:F:586:LYS:HD3	2.41	0.41
6:T:132:ILE:HD12	6:T:134:GLN:HG2	2.01	0.41
6:T:840:GLN:OE1	6:T:878:PHE:HB3	2.20	0.41
6:T:859:VAL:O	6:T:863:ILE:HG12	2.21	0.41
6:T:913:PHE:CE1	6:T:917:ILE:HB	2.56	0.41
6:T:934:PRO:HG3	6:T:2825:LEU:O	2.21	0.41
6:T:1057:ILE:HG22	6:T:1058:GLU:N	2.36	0.41
6:T:1848:ILE:HG21	6:T:1852:ASP:N	2.31	0.41
6:T:1877:GLU:CD	6:T:1877:GLU:N	2.73	0.41
6:T:2204:GLU:HA	6:T:2207:GLN:NE2	2.35	0.41
6:T:2320:LEU:HD21	6:T:2355:MET:O	2.21	0.41
6:T:3140:LEU:O	6:T:3144:LEU:HG	2.20	0.41
2:B:100:LEU:HD21	2:B:106:ILE:HD13	2.03	0.41
2:B:145:CYS:O	2:B:455:GLY:HA3	2.21	0.41
2:B:290:GLU:OE1	2:B:423:ARG:NH1	2.39	0.41
2:B:432:LEU:HD23	2:B:432:LEU:HA	1.95	0.41
3:D:617:LYS:HD2	3:D:617:LYS:HA	1.76	0.41
5:F:531:ASP:HA	5:F:534:VAL:HG12	2.02	0.41
6:T:129:PHE:CD1	6:T:132:ILE:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:464:LEU:O	6:T:468:ILE:HG12	2.19	0.41
6:T:1328:HIS:O	6:T:1328:HIS:ND1	2.54	0.41
6:T:1342:LEU:HB2	6:T:1377:LEU:HD11	2.02	0.41
6:T:1617:LEU:HD12	6:T:1620:LEU:CD2	2.49	0.41
6:T:1703:LEU:CD1	6:T:1753:SER:HB2	2.51	0.41
6:T:1798:ALA:HB3	6:T:1799:ARG:HH11	1.85	0.41
6:T:1876:PRO:HA	6:T:1883:LYS:CE	2.50	0.41
6:T:2349:LEU:O	6:T:2353:VAL:HG13	2.20	0.41
1:A:143:TYR:CE1	3:D:391:ILE:HG13	2.56	0.41
3:D:396:THR:HG23	3:D:397:TYR:CD1	2.56	0.41
4:E:198:LEU:HD23	4:E:198:LEU:H	1.85	0.41
6:T:586:LEU:O	6:T:590:LEU:HG	2.21	0.41
6:T:611:TYR:CZ	6:T:1585:ARG:HB3	2.55	0.41
6:T:1049:SER:HA	6:T:1052:LEU:HG	2.03	0.41
6:T:1750:PHE:HD1	6:T:1750:PHE:C	2.24	0.41
6:T:1832:LYS:N	6:T:1832:LYS:CE	2.84	0.41
6:T:2768:ASP:HB2	6:T:2770:ASN:OD1	2.20	0.41
6:T:3623:ARG:NH1	6:T:3625:THR:HB	2.35	0.41
1:A:70:PRO:HB3	1:A:78:ASN:HB3	2.02	0.41
1:A:118:LYS:HE3	1:A:118:LYS:HB2	1.90	0.41
2:B:48:THR:OG1	2:B:49:ALA:N	2.54	0.41
2:B:64:ILE:HB	2:B:66:ARG:NH1	2.36	0.41
2:B:75:ILE:HD13	2:B:75:ILE:HA	1.87	0.41
2:B:116:ASN:OD1	2:B:120:ASN:HB3	2.21	0.41
2:B:121:ARG:O	2:B:124:SER:OG	2.29	0.41
3:D:68:PHE:CE2	3:D:69:LEU:HG	2.56	0.41
3:D:344:GLN:O	5:F:538:LEU:HD13	2.20	0.41
3:D:539:LEU:HD23	3:D:539:LEU:HA	1.78	0.41
3:D:658:LEU:HD13	3:D:696:CYS:SG	2.61	0.41
4:E:173:PHE:HA	4:E:176:CYS:CB	2.51	0.41
4:E:233:GLU:O	4:E:237:LYS:HG2	2.21	0.41
6:T:5:GLU:O	6:T:8:GLU:HG3	2.20	0.41
6:T:5:GLU:O	6:T:9:GLN:HG2	2.20	0.41
6:T:342:SER:HA	6:T:345:LYS:HG3	2.03	0.41
6:T:706:LEU:HA	6:T:709:VAL:HB	2.03	0.41
6:T:744:LEU:HD12	6:T:766:PHE:CZ	2.56	0.41
6:T:1001:LEU:HD23	6:T:1001:LEU:HA	1.82	0.41
6:T:1069:LYS:HZ1	6:T:3330:LYS:HD3	1.86	0.41
6:T:1070:ARG:NH1	6:T:3534:LEU:HD13	2.35	0.41
6:T:1116:ASN:OD1	6:T:2500:LEU:HB3	2.21	0.41
6:T:1291:ASP:OD1	6:T:1292:ILE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1495:LEU:HB3	6:T:1500:LEU:HD11	2.03	0.41
6:T:1513:TYR:O	6:T:1513:TYR:CD1	2.70	0.41
6:T:1535:LEU:C	6:T:1535:LEU:CD2	2.86	0.41
6:T:1635:GLU:OE1	6:T:1635:GLU:N	2.53	0.41
6:T:1662:VAL:HG21	6:T:1705:THR:HG23	2.02	0.41
6:T:3106:TRP:CH2	6:T:3689:ARG:HD2	2.55	0.41
6:T:3420:PHE:HA	6:T:3445:LEU:HD11	2.03	0.41
6:T:3431:SER:HB2	6:T:3442:GLN:OE1	2.21	0.41
6:T:3472:ASN:ND2	6:T:3482:PRO:HG2	2.33	0.41
6:T:3695:ASN:O	6:T:3699:ILE:HG12	2.20	0.41
2:B:178:LYS:H	4:E:188:ASP:CG	2.22	0.41
6:T:1357:ILE:HD13	6:T:1374:LEU:HD13	2.02	0.41
6:T:1467:LEU:O	6:T:1467:LEU:HG	2.21	0.41
6:T:1473:LEU:N	6:T:1474:PRO:CD	2.83	0.41
6:T:1907:LEU:HD12	6:T:1945:SER:HB3	2.03	0.41
6:T:3045:THR:O	6:T:3049:ILE:HG12	2.21	0.41
6:T:3062:PHE:HD1	6:T:3085:TYR:HH	1.68	0.41
6:T:3118:THR:OG1	6:T:3119:ASN:N	2.54	0.41
6:T:3265:PHE:O	6:T:3267:ARG:HG3	2.21	0.41
1:A:134:VAL:HG12	1:A:374:CYS:SG	2.61	0.40
2:B:235:ASN:HA	2:B:239:PHE:CD2	2.56	0.40
3:D:323:ARG:O	3:D:326:VAL:HG12	2.20	0.40
5:F:574:ARG:HD3	5:F:574:ARG:H	1.87	0.40
6:T:305:LEU:O	6:T:308:VAL:HG12	2.21	0.40
6:T:463:LEU:HA	6:T:466:ILE:HD12	2.03	0.40
6:T:473:ASN:HA	6:T:476:LYS:HB3	2.03	0.40
6:T:514:SER:O	6:T:518:MET:HG3	2.22	0.40
6:T:609:ASN:OD1	6:T:610:GLU:N	2.54	0.40
6:T:839:LEU:HD23	6:T:839:LEU:HA	1.86	0.40
6:T:983:ASN:ND2	6:T:2479:SER:OG	2.51	0.40
6:T:1129:PHE:CD2	6:T:1131:ILE:HG12	2.56	0.40
6:T:1698:MET:O	6:T:1698:MET:SD	2.79	0.40
6:T:2461:GLU:HG3	6:T:2592:HIS:HB3	2.03	0.40
6:T:2620:PRO:C	6:T:2622:LEU:H	2.24	0.40
6:T:2940:TYR:O	6:T:2942:GLU:N	2.54	0.40
1:A:131:ALA:HA	1:A:357:ILE:O	2.20	0.40
2:B:136:ALA:HB1	2:B:470:VAL:O	2.21	0.40
2:B:176:LEU:O	2:B:180:THR:HG23	2.21	0.40
2:B:255:LEU:HB2	2:B:290:GLU:HG2	2.03	0.40
6:T:93:GLN:HG3	6:T:136:LYS:HZ3	1.86	0.40
6:T:710:TYR:HA	6:T:713:MET:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:763:ILE:HD13	6:T:763:ILE:HA	1.93	0.40
6:T:1703:LEU:HD11	6:T:1753:SER:HB2	2.03	0.40
6:T:2271:ILE:HG12	6:T:2274:LEU:CG	2.47	0.40
6:T:2571:ILE:HG13	6:T:2572:PRO:HD2	2.03	0.40
1:A:234:SER:O	1:A:234:SER:OG	2.33	0.40
1:A:262:PHE:CE2	1:A:312:ARG:HG2	2.56	0.40
6:T:218:MET:HA	6:T:221:PHE:CE2	2.57	0.40
6:T:405:GLU:H	6:T:445:ARG:NH2	2.19	0.40
6:T:1245:LEU:HD11	6:T:1261:GLU:HB3	2.03	0.40
6:T:1486:LEU:HD23	6:T:1486:LEU:HA	1.95	0.40
6:T:1744:LEU:HA	6:T:1744:LEU:HD13	1.84	0.40
6:T:2346:GLN:O	6:T:2350:ARG:HG2	2.21	0.40
6:T:2455:ILE:HD13	6:T:2455:ILE:HA	1.89	0.40
6:T:2963:CYS:O	6:T:2967:LEU:HD23	2.21	0.40
6:T:3266:PRO:HB2	6:T:3268:LYS:NZ	2.37	0.40
6:T:3434:VAL:HG22	6:T:3435:GLU:H	1.87	0.40
1:A:99:GLU:O	1:A:130:PRO:HD3	2.22	0.40
1:A:148:THR:HG21	3:D:392:LYS:HD2	2.03	0.40
2:B:59:GLU:O	2:B:62:ILE:HG22	2.21	0.40
2:B:152:ARG:CZ	2:B:440:LEU:HD11	2.51	0.40
2:B:428:LEU:HD12	2:B:437:PHE:CZ	2.57	0.40
3:D:668:ASN:O	3:D:672:ILE:HG13	2.21	0.40
6:T:718:GLY:O	6:T:722:VAL:HG23	2.22	0.40
6:T:1213:VAL:HA	6:T:1216:ILE:HG22	2.04	0.40
6:T:1615:MET:HB2	6:T:1650:PHE:CZ	2.57	0.40
6:T:1907:LEU:HD23	6:T:1907:LEU:O	2.20	0.40
6:T:1950:THR:N	6:T:1951:PRO:CD	2.84	0.40
6:T:1962:THR:OG1	6:T:1963:PRO:CD	2.69	0.40
6:T:1994:ASP:HA	6:T:1997:PHE:HD2	1.85	0.40
6:T:2138:VAL:O	6:T:2138:VAL:HG12	2.21	0.40
6:T:2348:PHE:HA	6:T:2351:LYS:HB2	2.03	0.40
6:T:2706:LEU:O	6:T:2709:VAL:HG12	2.21	0.40
6:T:2902:VAL:HG13	6:T:2946:VAL:HG12	2.03	0.40
6:T:3208:LEU:HA	6:T:3208:LEU:HD12	1.83	0.40
6:T:3522:VAL:HG21	6:T:3743:TRP:CD1	2.57	0.40
1:A:76:VAL:HG21	1:A:79:TRP:CE3	2.56	0.40
1:A:160:THR:CG2	1:A:178:ILE:HB	2.52	0.40
6:T:58:GLN:O	6:T:79:MET:HE1	2.22	0.40
6:T:107:LEU:HD22	6:T:143:ILE:HD12	2.04	0.40
6:T:115:GLY:O	6:T:119:MET:HG2	2.21	0.40
6:T:1251:GLU:H	6:T:1251:GLU:CD	2.17	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1447:THR:O	6:T:1456:ILE:HG22	2.22	0.40
6:T:1883:LYS:HB3	6:T:1912:PHE:HZ	1.83	0.40
6:T:1895:LYS:H	6:T:1895:LYS:CD	2.34	0.40
6:T:1910:SER:HA	6:T:1913:ILE:HD11	2.02	0.40
6:T:2004:ILE:H	6:T:2004:ILE:HG13	1.67	0.40
6:T:2236:ILE:HD12	6:T:2263:LEU:CD2	2.52	0.40
6:T:2292:ILE:C	6:T:2295:PRO:HD2	2.42	0.40
6:T:2477:TYR:CD2	6:T:2542:ILE:HB	2.52	0.40
6:T:2681:ARG:HD2	6:T:2681:ARG:HA	1.83	0.40
6:T:3067:ARG:HH12	6:T:3075:ILE:HG21	1.85	0.40
6:T:3552:TYR:OH	6:T:3623:ARG:O	2.35	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	370/372 (100%)	346 (94%)	24 (6%)	0	100	100
2	B	398/481 (83%)	365 (92%)	33 (8%)	0	100	100
3	D	448/982 (46%)	357 (80%)	91 (20%)	0	100	100
4	E	197/476 (41%)	174 (88%)	23 (12%)	0	100	100
5	F	120/832 (14%)	93 (78%)	26 (22%)	1 (1%)	19	58
6	T	3445/3744 (92%)	3069 (89%)	366 (11%)	10 (0%)	41	75
All	All	4978/6887 (72%)	4404 (88%)	563 (11%)	11 (0%)	50	79

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	T	1796	LEU

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Mol	Chain	Res	Type
6	T	1980	SER
5	F	542	PRO
6	T	1993	PRO
6	T	1206	TYR
6	T	3443	PHE
6	T	3539	GLU
6	T	2295	PRO
6	T	3655	PRO
6	T	1605	ASN
6	T	3264	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	317/317 (100%)	317 (100%)	0	100	100
2	B	354/428 (83%)	354 (100%)	0	100	100
3	D	414/892 (46%)	411 (99%)	3 (1%)	84	90
4	E	184/441 (42%)	183 (100%)	1 (0%)	88	93
5	F	114/769 (15%)	113 (99%)	1 (1%)	78	88
6	T	3188/3452 (92%)	3114 (98%)	74 (2%)	50	70
All	All	4571/6299 (73%)	4492 (98%)	79 (2%)	62	78

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	23	ARG
3	D	36	ARG
3	D	618	ARG
4	E	269	LYS
5	F	574	ARG
6	T	15	ARG
6	T	499	LYS
6	T	727	LEU

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Mol	Chain	Res	Type
6	T	832	LYS
6	T	1340	LYS
6	T	1506	LEU
6	T	1530	CYS
6	T	1534	VAL
6	T	1543	LEU
6	T	1558	ILE
6	T	1565	GLN
6	T	1586	LEU
6	T	1601	ASN
6	T	1609	GLU
6	T	1614	ASN
6	T	1616	THR
6	T	1634	LYS
6	T	1635	GLU
6	T	1644	LEU
6	T	1669	MET
6	T	1687	LYS
6	T	1692	ILE
6	T	1702	THR
6	T	1716	LEU
6	T	1718	LEU
6	T	1725	PHE
6	T	1734	GLU
6	T	1750	PHE
6	T	1776	LYS
6	T	1779	GLN
6	T	1789	PHE
6	T	1799	ARG
6	T	1826	VAL
6	T	1840	LYS
6	T	1849	LEU
6	T	1854	LEU
6	T	1859	LEU
6	T	1877	GLU
6	T	1896	LEU
6	T	1900	LEU
6	T	1912	PHE
6	T	1918	PHE
6	T	1920	ILE
6	T	1927	PHE
6	T	1941	LEU

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Mol	Chain	Res	Type
6	T	1946	LEU
6	T	1949	LEU
6	T	1995	LEU
6	T	2001	ASP
6	T	2002	LEU
6	T	2012	ASN
6	T	2031	LEU
6	T	2092	LEU
6	T	2093	ARG
6	T	2103	TYR
6	T	2116	LEU
6	T	2122	ASN
6	T	2144	GLU
6	T	2163	ASN
6	T	2182	GLU
6	T	2192	GLU
6	T	2196	LYS
6	T	2201	ASP
6	T	2203	GLN
6	T	2206	LEU
6	T	2212	VAL
6	T	2237	GLN
6	T	2269	ASP
6	T	2278	LEU
6	T	2305	ARG
6	T	2311	LEU
6	T	2315	LEU
6	T	3068	LEU
6	T	3411	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	49	GLN
1	A	87	HIS
1	A	372	HIS
2	B	60	GLN
2	B	91	GLN
2	B	95	GLN
2	B	103	ASN
2	B	120	ASN

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Mol	Chain	Res	Type
2	B	248	HIS
2	B	275	ASN
2	B	406	HIS
3	D	72	ASN
3	D	262	ASN
3	D	360	ASN
3	D	644	ASN
4	E	289	GLN
4	E	302	GLN
5	F	580	HIS
5	F	624	GLN
6	T	6	GLN
6	T	39	ASN
6	T	84	ASN
6	T	146	GLN
6	T	150	ASN
6	T	605	ASN
6	T	615	ASN
6	T	639	HIS
6	T	983	ASN
6	T	1060	ASN
6	T	1104	ASN
6	T	1105	ASN
6	T	1287	ASN
6	T	1300	ASN
6	T	1312	HIS
6	T	1379	GLN
6	T	1407	GLN
6	T	1432	GLN
6	T	1470	ASN
6	T	1493	GLN
6	T	1565	GLN
6	T	1571	ASN
6	T	1601	ASN
6	T	1605	ASN
6	T	1659	GLN
6	T	1674	ASN
6	T	1709	ASN
6	T	1740	GLN
6	T	1768	HIS
6	T	1769	ASN
6	T	1805	ASN

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Mol	Chain	Res	Type
6	T	1838	HIS
6	T	1903	GLN
6	T	1944	GLN
6	T	1977	ASN
6	T	1981	GLN
6	T	1987	GLN
6	T	1992	HIS
6	T	1998	ASN
6	T	2009	HIS
6	T	2122	ASN
6	T	2174	ASN
6	T	2183	ASN
6	T	2188	GLN
6	T	2189	ASN
6	T	2200	HIS
6	T	2207	GLN
6	T	2245	GLN
6	T	2266	ASN
6	T	2418	GLN
6	T	2507	ASN
6	T	2592	HIS
6	T	2646	ASN
6	T	2651	ASN
6	T	2704	GLN
6	T	2742	HIS
6	T	2811	GLN
6	T	2848	GLN
6	T	2863	HIS
6	T	2957	HIS
6	T	3010	ASN
6	T	3059	GLN
6	T	3119	ASN
6	T	3139	GLN
6	T	3154	HIS
6	T	3357	GLN
6	T	3385	HIS
6	T	3421	GLN
6	T	3444	ASN
6	T	3468	HIS
6	T	3472	ASN
6	T	3537	GLN
6	T	3629	GLN

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Mol	Chain	Res	Type
6	T	3644	ASN
6	T	3657	ASN
6	T	3695	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	ATP	B	501	2	26,33,33	0.90	1 (3%)	31,52,52	1.68	5 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ATP	B	501	2	-	2/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	501	ATP	C5-C4	2.23	1.46	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	501	ATP	PA-O3A-PB	-4.60	117.03	132.83
7	B	501	ATP	PB-O3B-PG	-3.81	119.74	132.83
7	B	501	ATP	C3'-C2'-C1'	3.31	105.97	100.98
7	B	501	ATP	N3-C2-N1	-3.01	123.97	128.68
7	B	501	ATP	C4-C5-N7	-2.47	106.83	109.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	501	ATP	O4'-C4'-C5'-O5'
7	B	501	ATP	C5'-O5'-PA-O1A

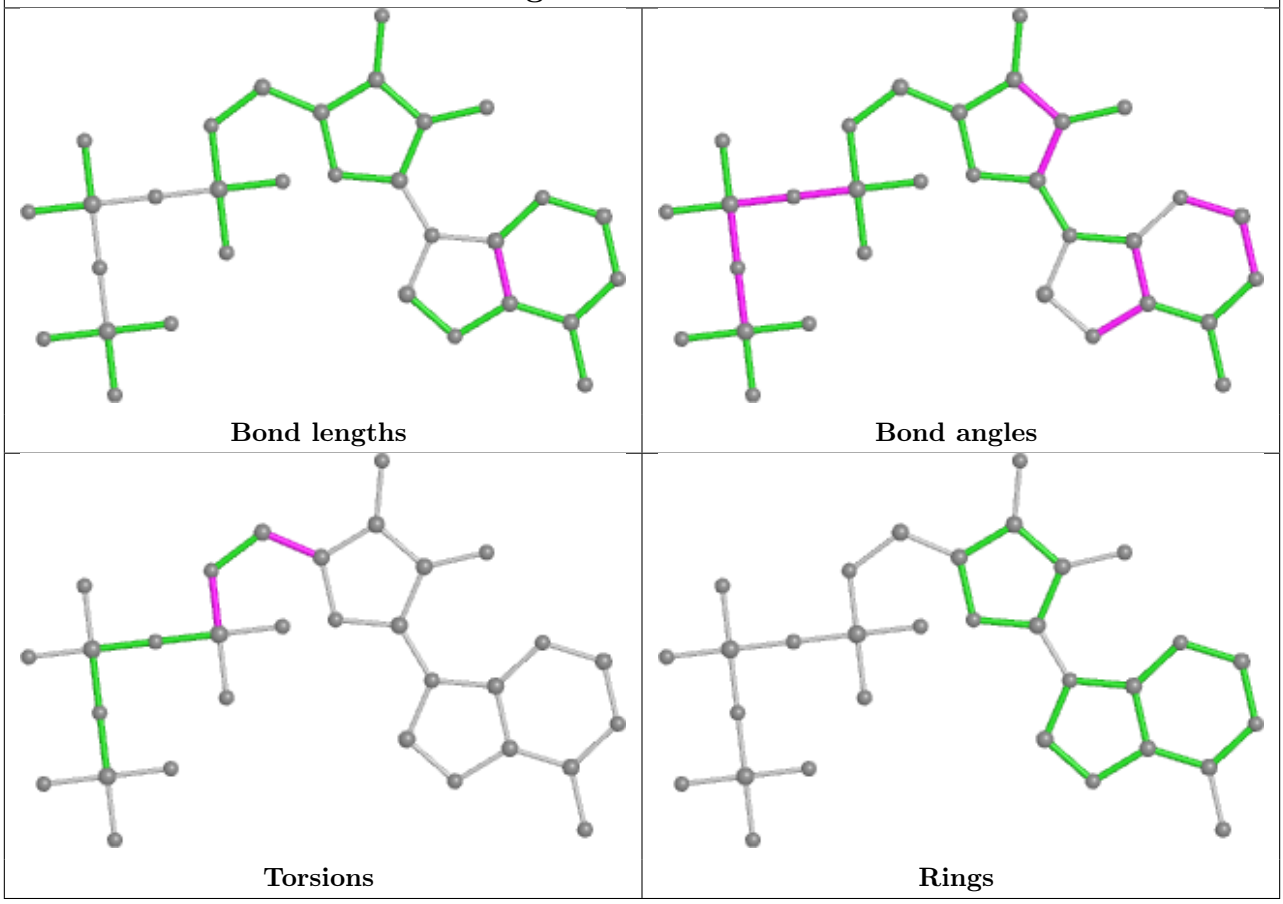
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	501	ATP	4	0

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

Ligand ATP B 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

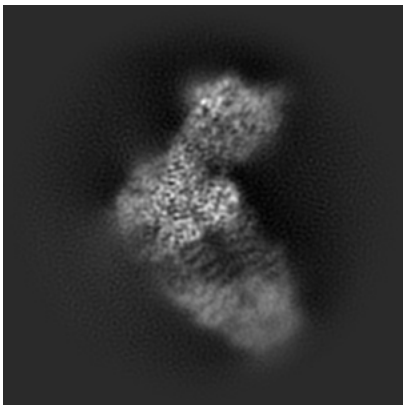
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33796. These allow visual inspection of the internal detail of the map and identification of artifacts.

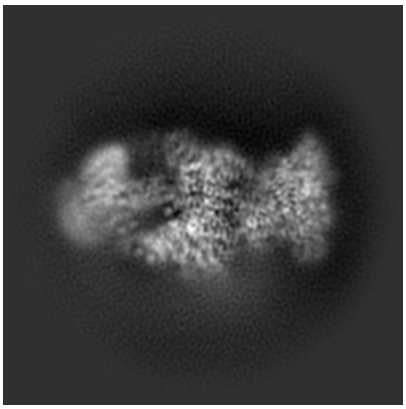
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

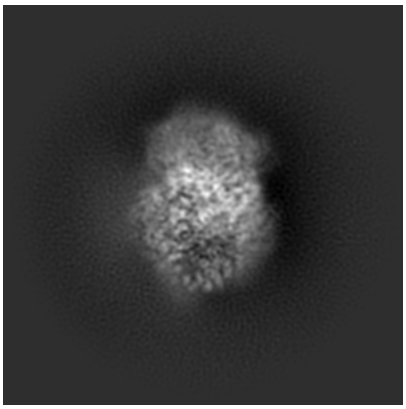
6.1.1 Primary map



X

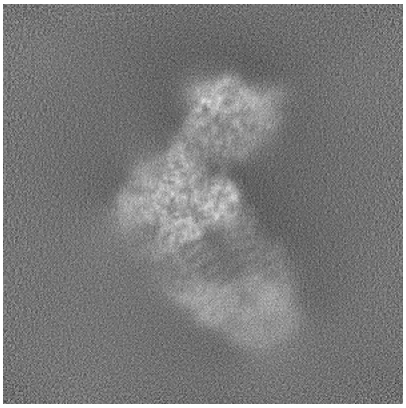


Y

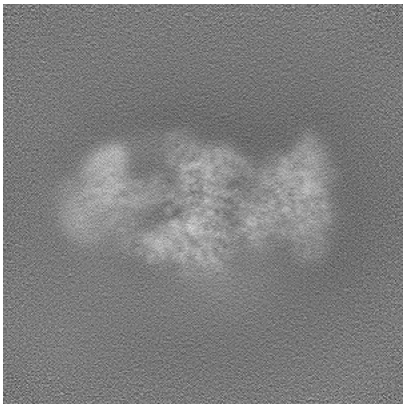


Z

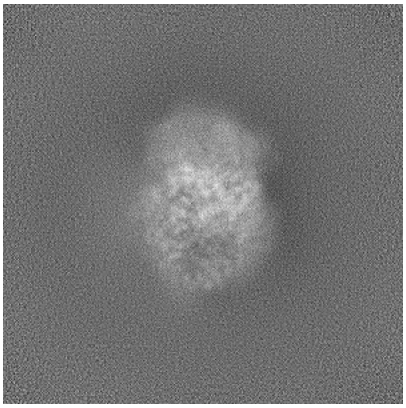
6.1.2 Raw map



X



Y

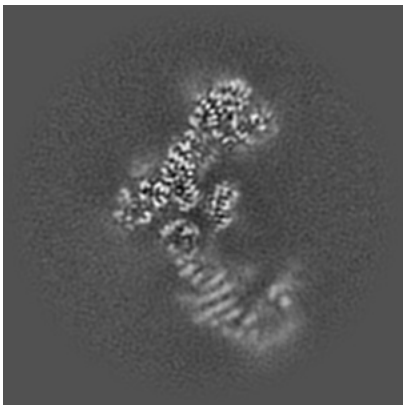


Z

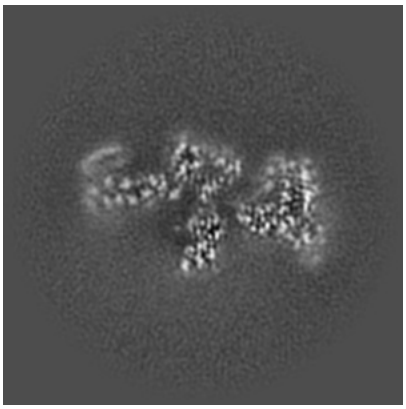
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

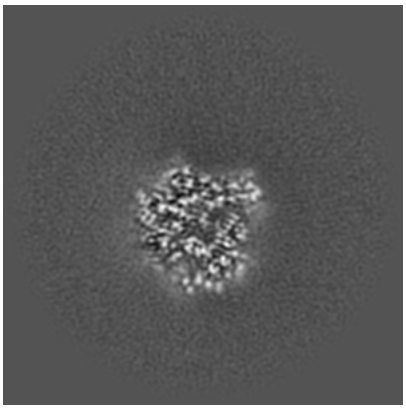
6.2.1 Primary map



X Index: 250

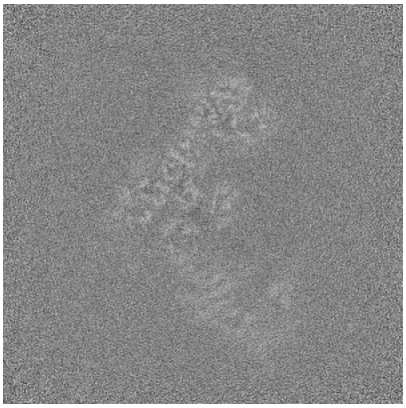


Y Index: 250

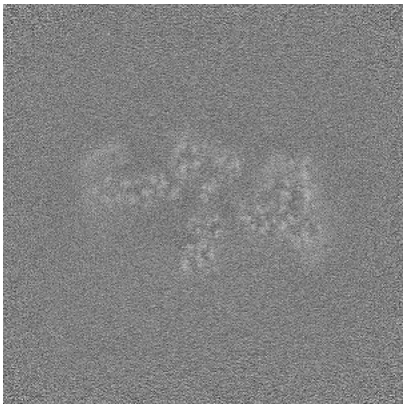


Z Index: 250

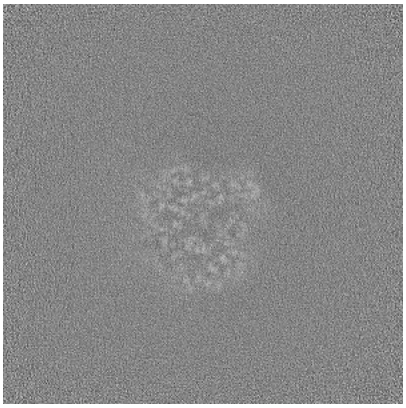
6.2.2 Raw map



X Index: 250



Y Index: 250

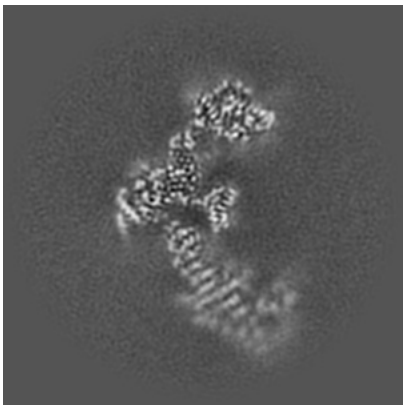


Z Index: 250

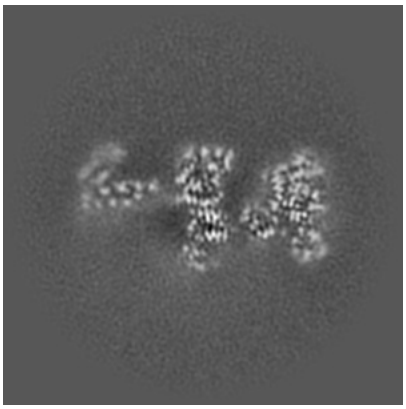
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

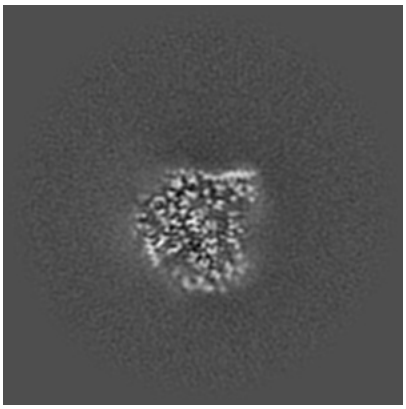
6.3.1 Primary map



X Index: 256

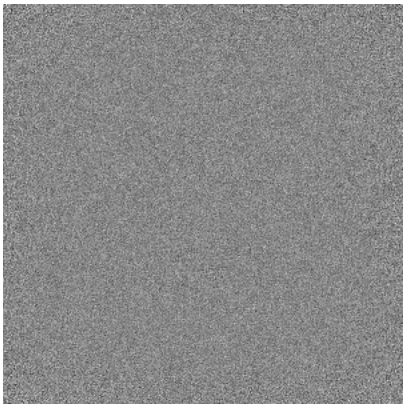


Y Index: 264

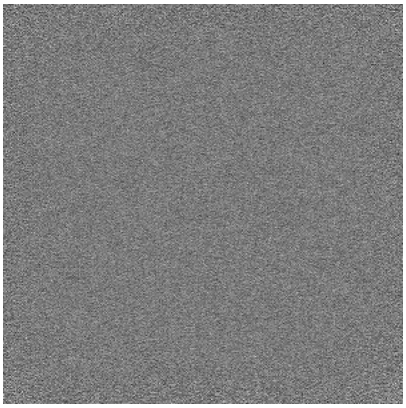


Z Index: 257

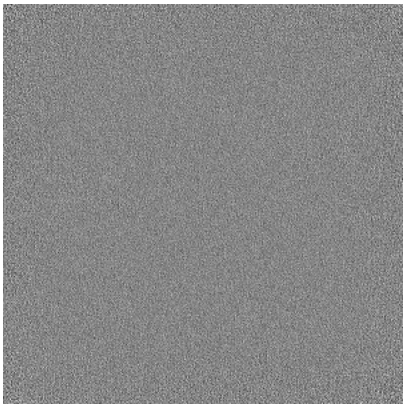
6.3.2 Raw map



X Index: 0



Y Index: 0

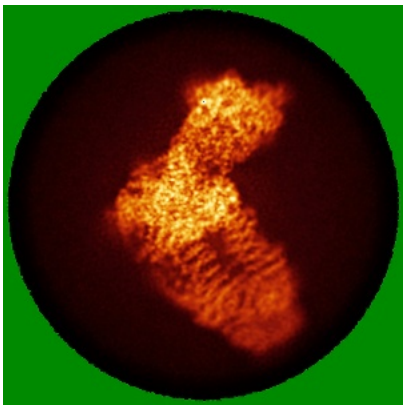


Z Index: 0

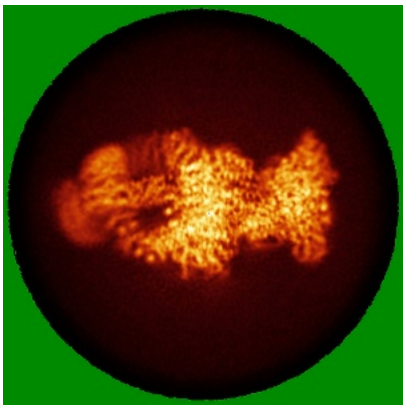
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

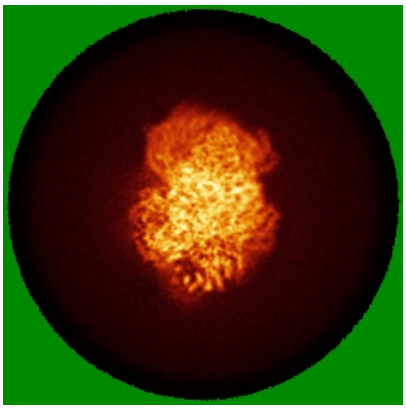
6.4.1 Primary map



X

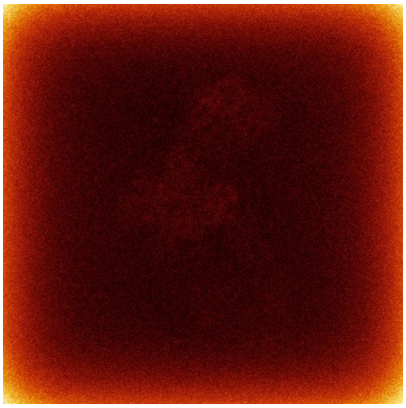


Y

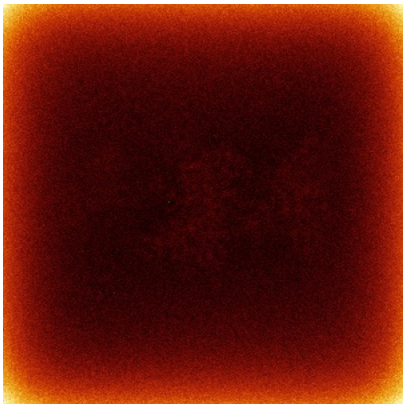


Z

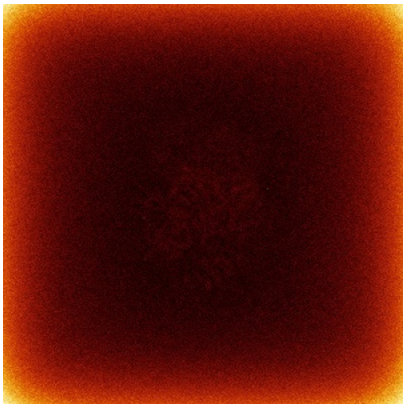
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

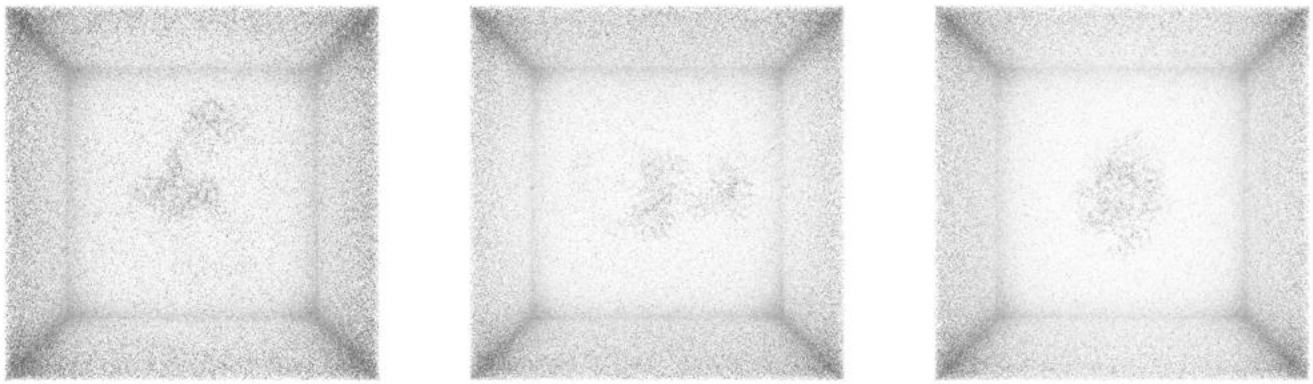
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0396. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

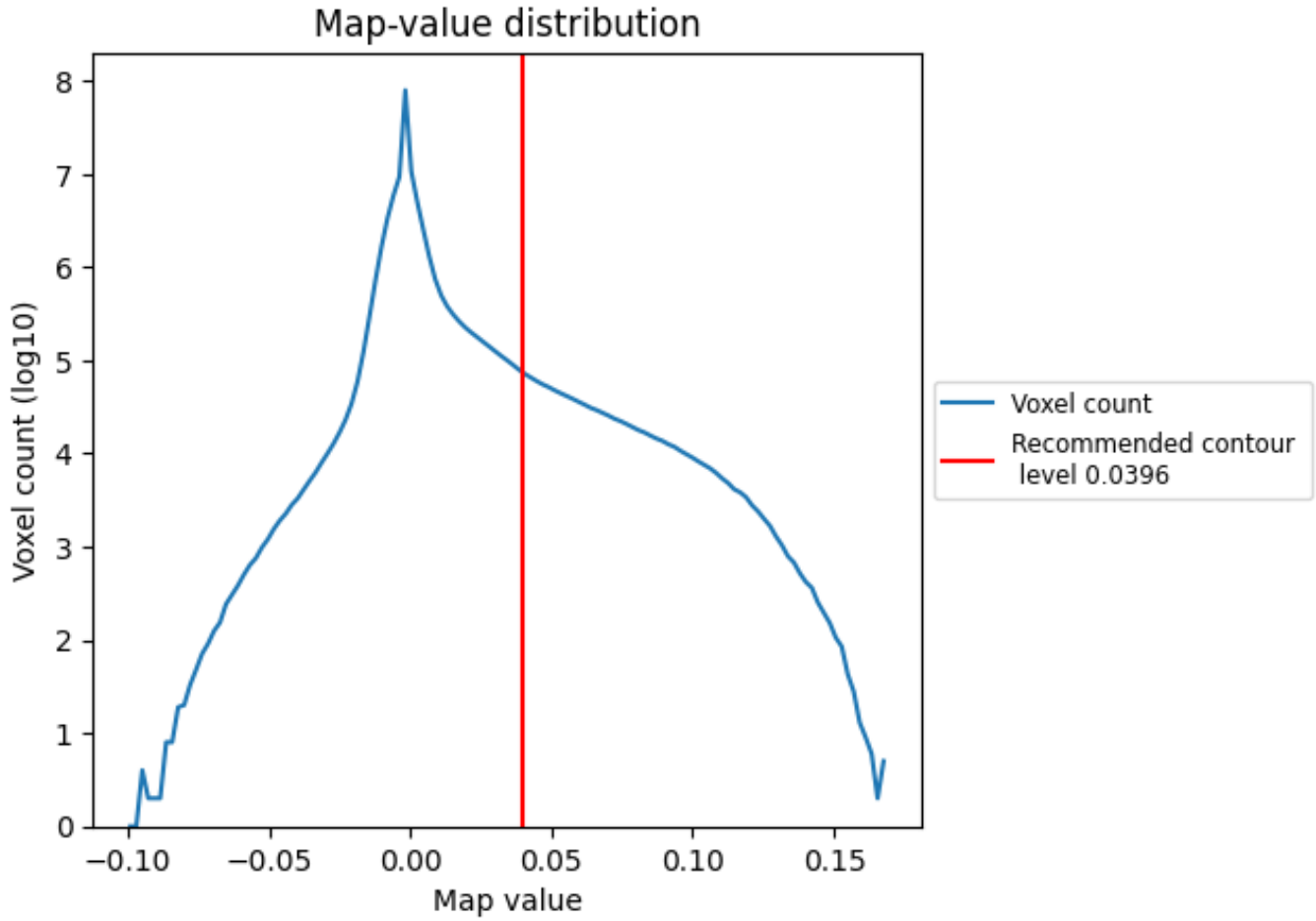
6.6 Mask visualisation (i)

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

7 Map analysis

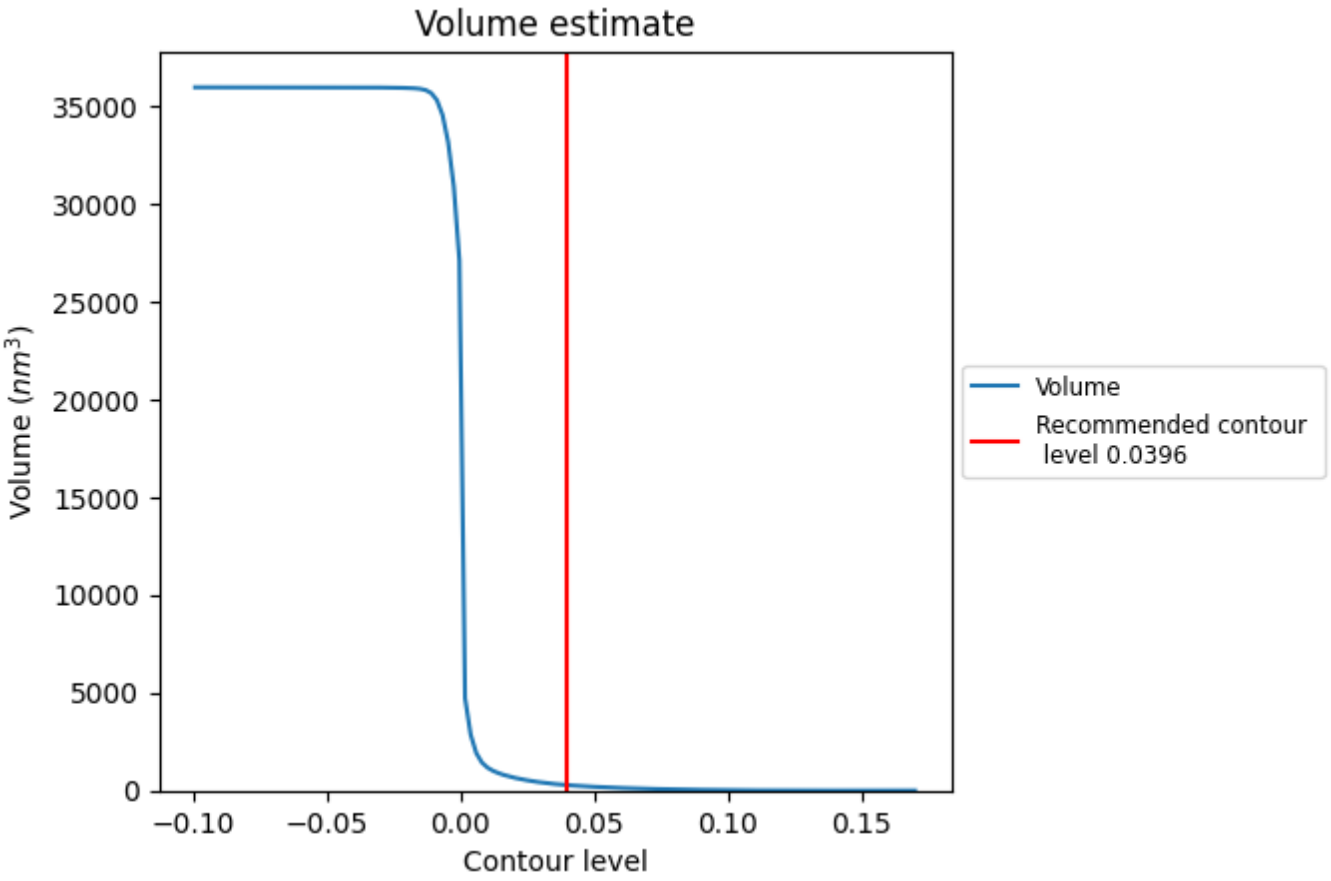
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

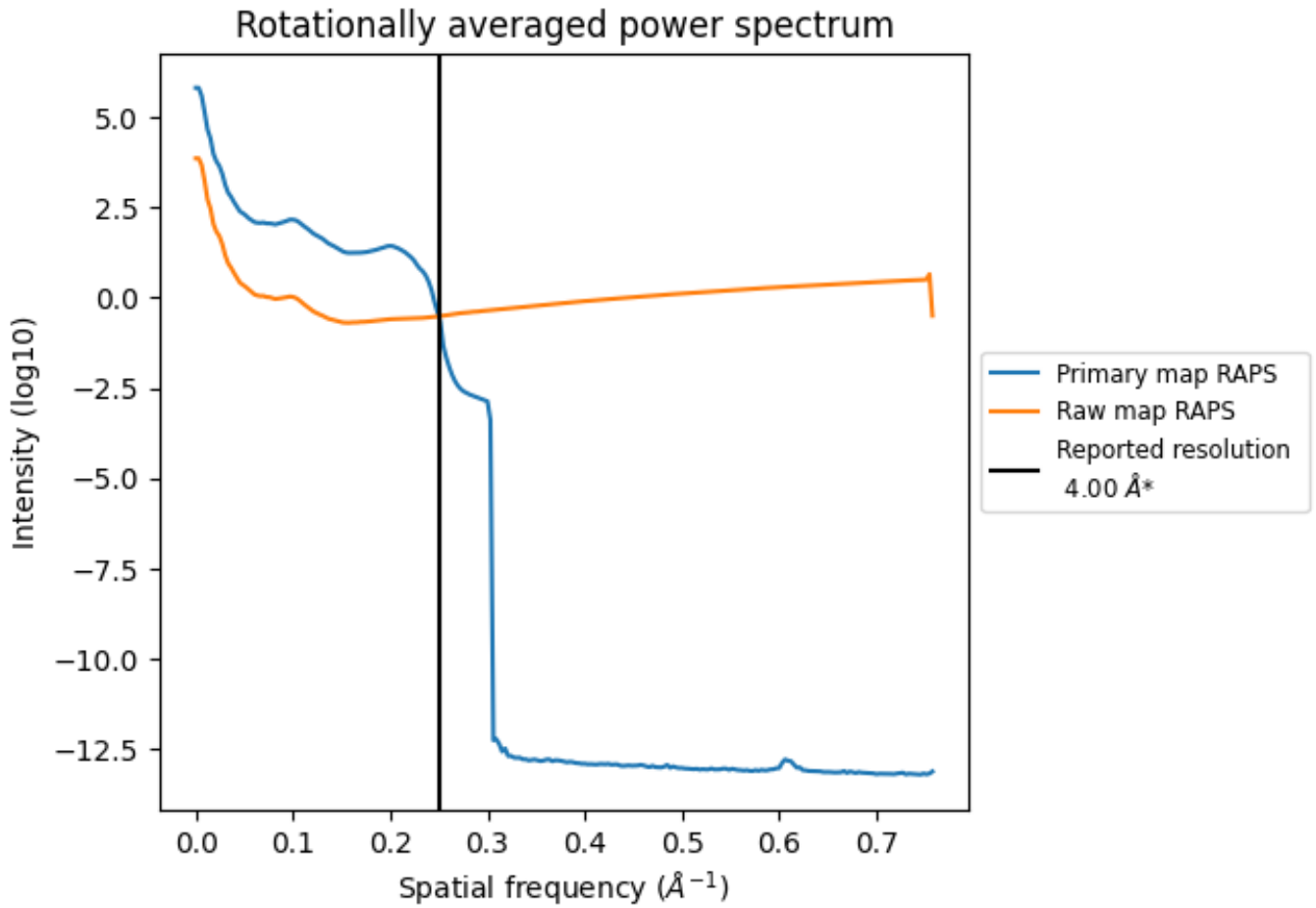
7.2 Volume estimate



The volume at the recommended contour level is 282 nm^3; this corresponds to an approximate mass of 255 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

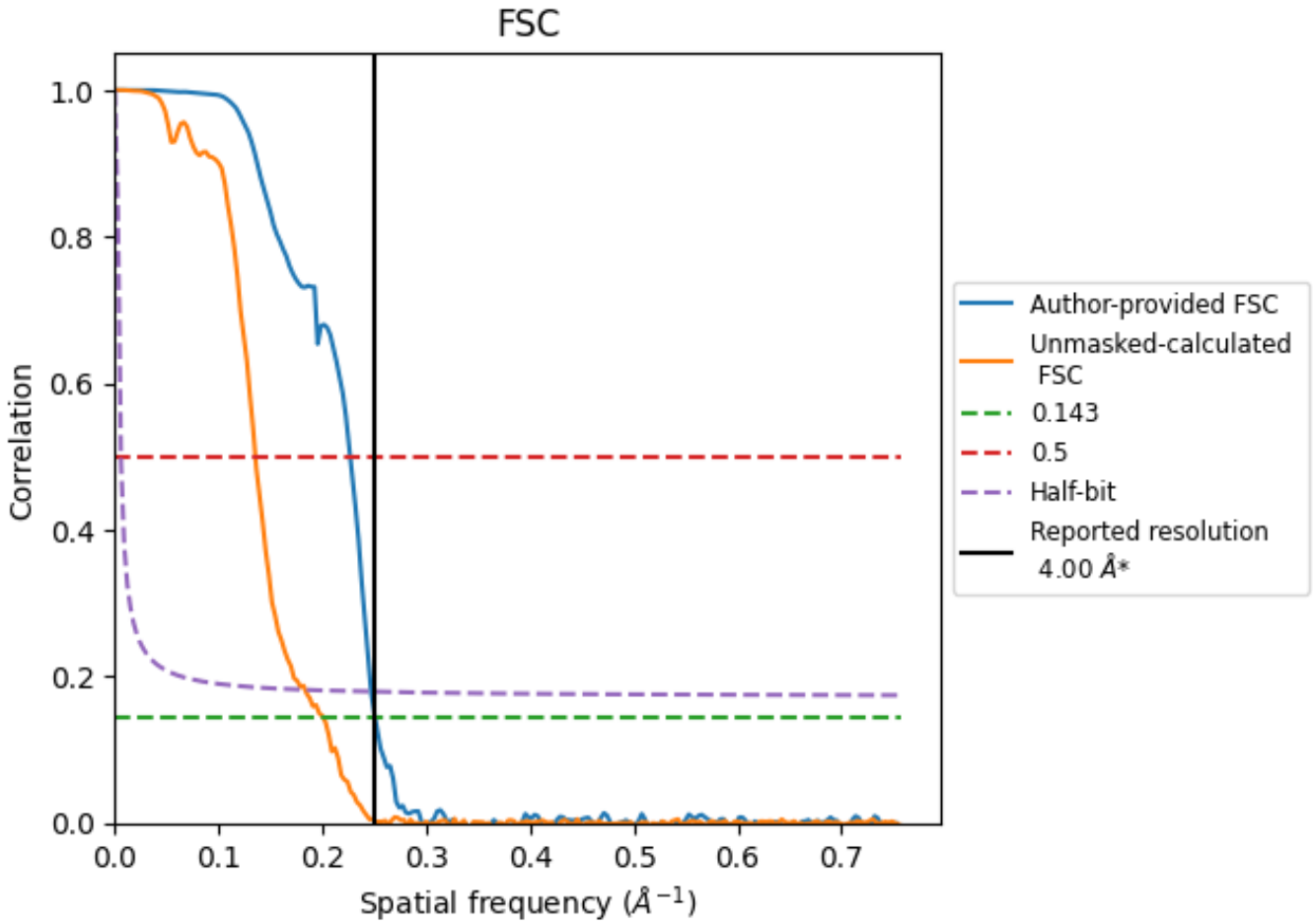


*Reported resolution corresponds to spatial frequency of 0.250 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8.2 Resolution estimates (i)

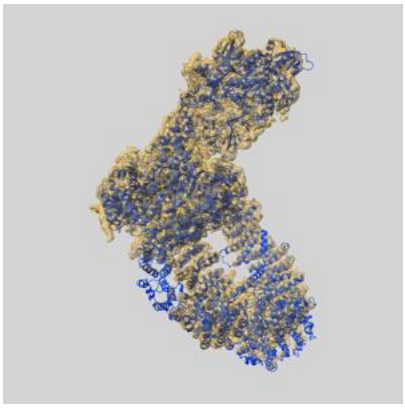
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.99	4.41	4.05
Unmasked-calculated*	4.98	7.39	5.45

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.98 differs from the reported value 4.0 by more than 10 %

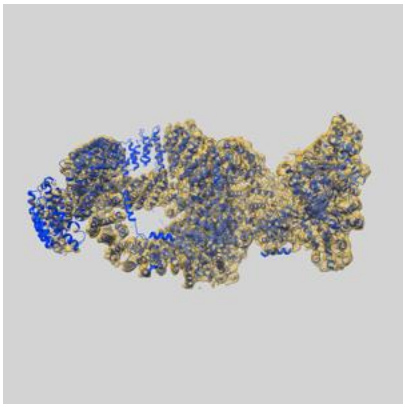
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33796 and PDB model 7YFP. Per-residue inclusion information can be found in section 3 on page 5.

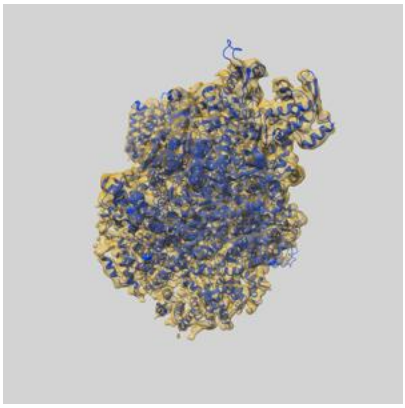
9.1 Map-model overlay



X



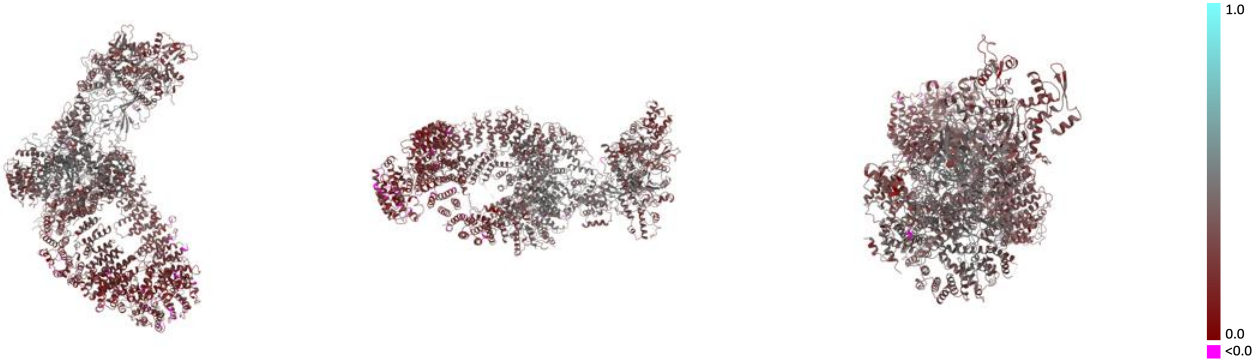
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0396 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

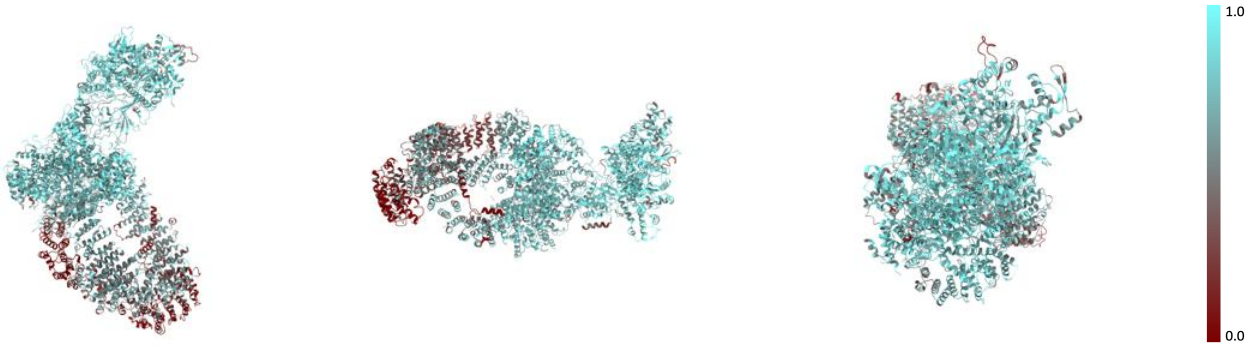
9.2 Q-score mapped to coordinate model (i)



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.

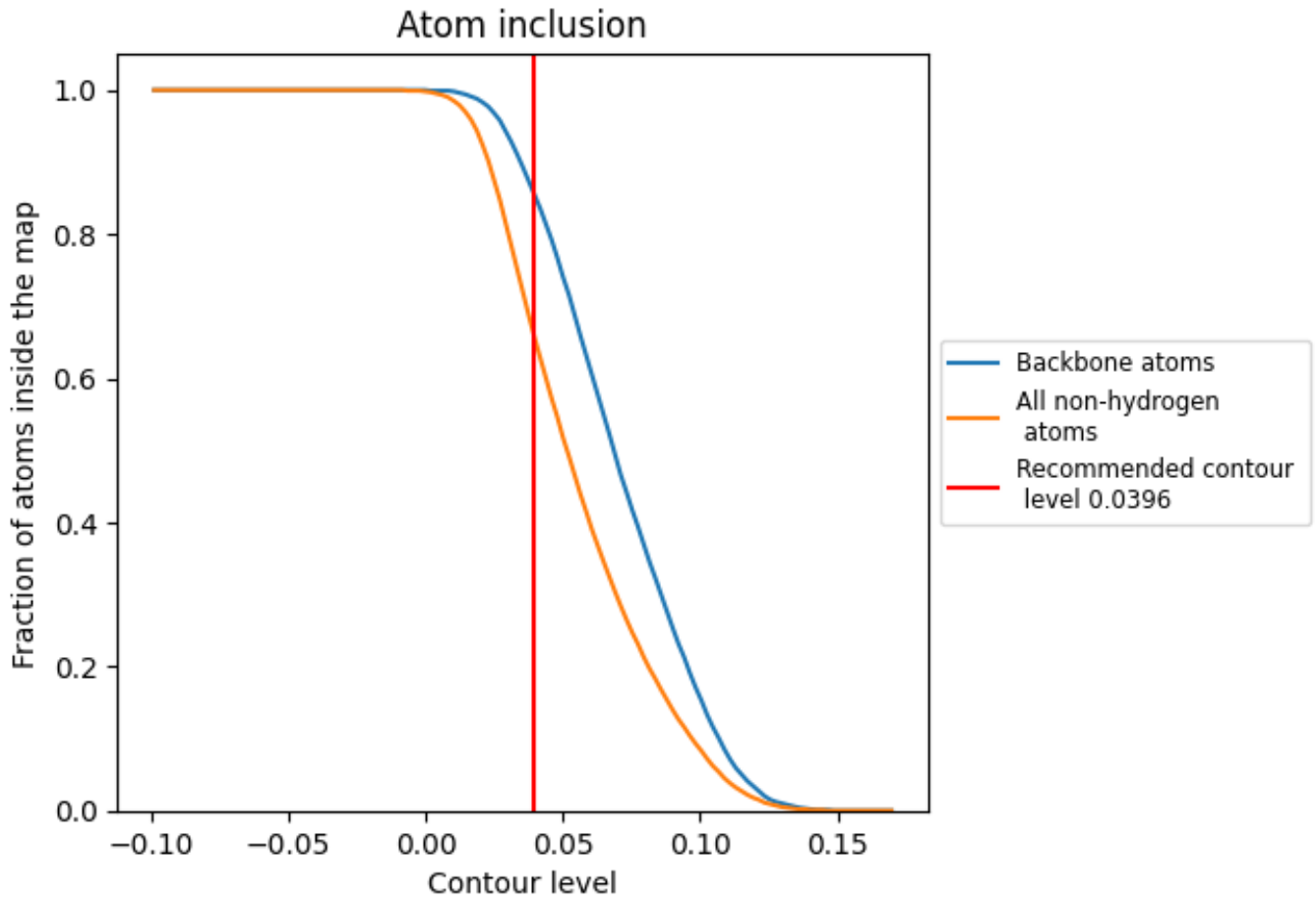
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0396).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0396) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6570	0.3340
A	0.7470	0.3330
B	0.8340	0.3930
D	0.7720	0.3870
E	0.7870	0.3540
F	0.7500	0.4060
T	0.6020	0.3170