



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:49 PM GMT

PDB ID : 4AKI
Title : Dynein Motor Domain - LuAc derivative
Authors : Schmidt, H.; Gleave, E.S.; Carter, A.P.
Deposited on : 2012-02-22
Resolution : 3.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

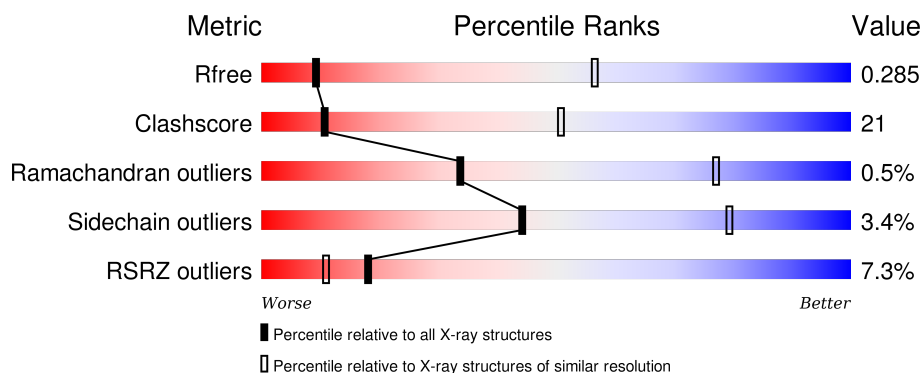
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	2695	<div> <div>6%</div> <div>66%</div> <div>30%</div> <div>..</div> </div>
1	B	2695	<div> <div>8%</div> <div>68%</div> <div>29%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	5094	-	-	X	-
3	SO4	A	5095	-	-	X	X
3	SO4	A	5096	-	-	X	-
3	SO4	B	5095	-	-	X	-
4	MG	A	5097	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 41590 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

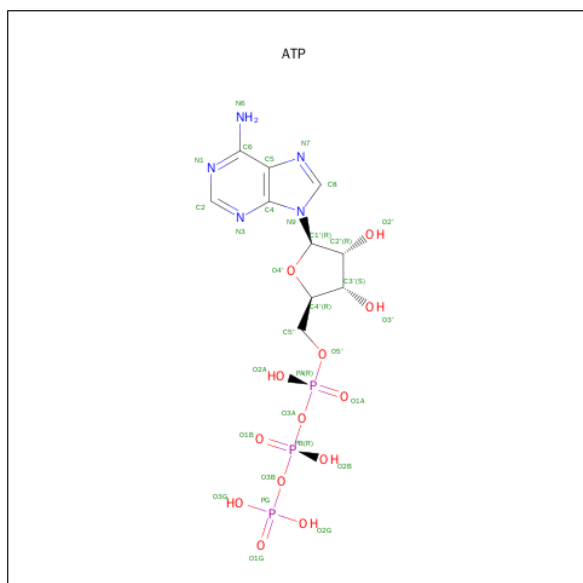
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2650	Total	C	N	O	S	0	0	0
			20748	13268	3472	3915	93			
1	B	2650	Total	C	N	O	S	0	0	0
			20748	13268	3472	3915	93			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1630	ILE	LEU	CONFLICT	UNP P36022
A	3782	ASP	GLU	CONFLICT	UNP P36022
B	1630	ILE	LEU	CONFLICT	UNP P36022
B	3782	ASP	GLU	CONFLICT	UNP P36022

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

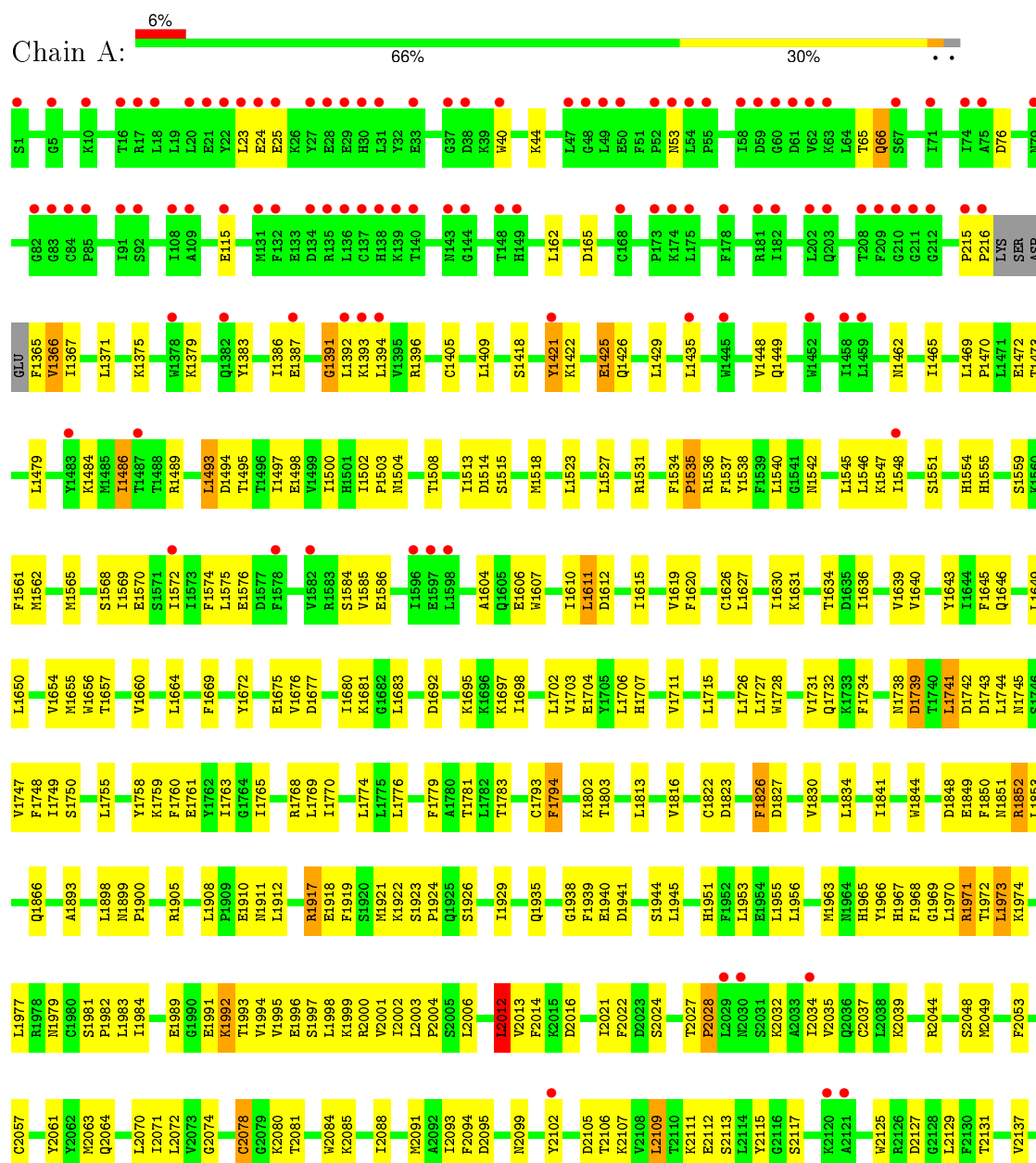
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

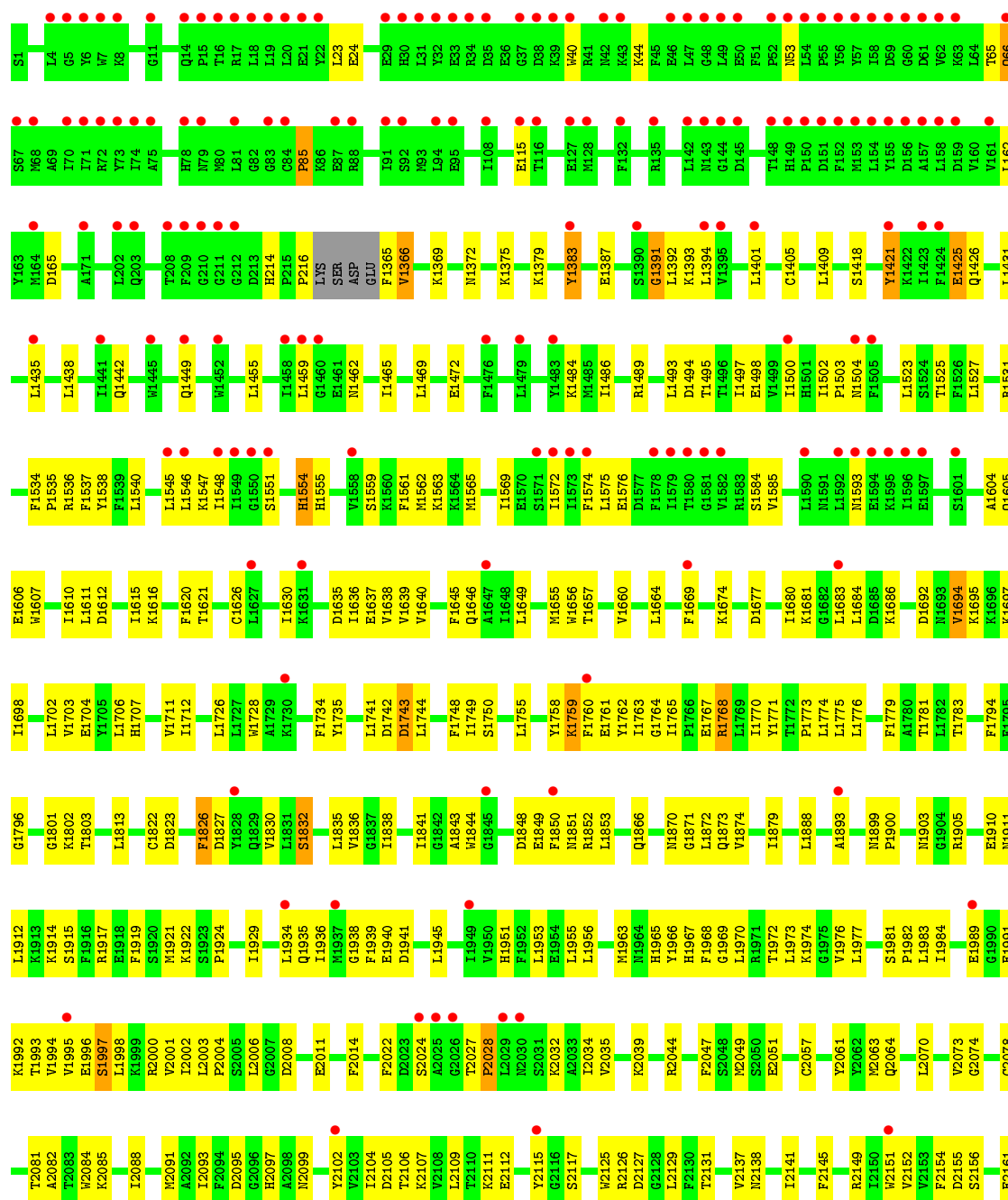
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

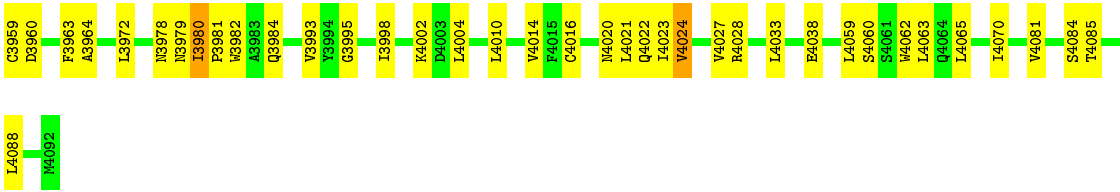
- Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC



T3876	G3877	G3878	L3884	P3885	A3886	P3887	L3888	L3889	Q3890	R3894	F3895	E3898	D3899	T3906	V3911	G3912	F3915	F3916	T3917	K3919	V3923	K3924	S3925	V3926	Y3927	K3934	K3946	S3947	H3948	G3949	F3950	S3951	Y3955	D3960	F3963	A3964	Y3967	N3978												
F3786	T3787		R3792	K3799	L3803	S3807	K3808	K3809	S3810	L3811	L3816	G3817	S3818	L3819	E3820	N3821	L3614	L3822	N3823	N3722	S3825	G3832	S3729	K3833	G3836	G3837	W3838	V3839	Q3845	K3846	S3847	L3848	S3849	K3850	K3851	L3852	L3853	V3854	P3854	H3858	V3859	T3862	A3865	E3869	K3870	A3871	K3872	K3873	N3874	N3875
S3687	L3690	D3691	K3692	K3693	F3694	K3695	K3696	L3697	K3698	K3700	T3701	N3596	L3601	F3607	D3612	N3613	V3615	Y3618	G3622	S3628	M3631	F3641	L3736	T3737	V3738	D3739	T3740	N3741	K3566	F3657	L3658	L3744	L3760	S3766	F3767	T3768	V3769	N3772	N3773	L3774	V3777	V3778	A3779	N3780	K3873	N3874	N3875			
E3582	L3583	N3584	L3587	N3588	N3589	L3590	K3591	K3592	F3593	A3594	N3596	L3601	F3607	D3612	N3613	V3615	Y3618	G3622	S3628	M3631	F3641	L3736	T3737	V3738	D3739	T3740	N3741	K3566	F3657	L3658	L3744	L3760	S3766	F3767	T3768	V3769	N3772	N3773	L3774	V3777	V3778	A3779	N3780	K3873	N3874	N3875				
D3483	V3488	I3505	F3508	L3509	R3510	S3511	K3512	V3513	F3518	V3519	T3520	N3521	I3525	F3530	D3531	L3534	E3537	N3538	M3541	K3542	K3543	K3544	D3547	L3548	L3549	K3550	Y3555	K3556	N3561	L3562	E3563	K3564	L3565	L3566	L3567	E3568	F3569	L3570	N3571	N3572	S3573	M3577	L3578	E3579	N3580	D3581				
E3022	F3023	L3024	N3025	V3028	L3029	L3030	V3031	L3032	L3033	L3034	L3035	L3036	L3037	L3038	L3039	L3040	F3406	L3407	L3408	D3409	R3413	K3414	L3415	T3416	V3417	L3418	L3429	R3439	L3440	F3446	Q3453	D3459	P3460	L3461	L3462	S3463	L3464	L3465	L3466	S3467	F3470	A3473	G3474	N3475	R3476	L3481	G3482			
T2881	T2890	L2891	C2892	K2902	L2903	L2908	R2911	C2912	V2916	K2917	W2920	M2938	T2941	D2942	F2943	I2944	V2945	P2946	G2947	L2948	L2949	L2950	L2951	L2952	L2953	L2954	L2955	L2956	L2957	L2958	L2959	L2960	L2961	D2962	D2963	V2982	G2983	N2984	N2985	R2986	R2987	S2988	P2989	G2990	L3010	F3016	V3017	N3018	L3021	
L2786	R2787	R2788	F2795	L2799	L2808	R2812	T2813	L2816	L2817	L2818	E2819	S2820	L2821	L2822	L2828	E2829	K2832	T2833	L2834	L2835	L2836	L2837	L2838	L2839	L2840	L2841	L2842	L2843	L2844	Q2845	G2846	Y2849	L2852	L2853	L2856	T2860	R2861	L2865	L2866	L2867	D2868	E2872	L2873	V2874	D2875	V2878				
S2643	L2644	L2645	R2646	L2647	R2654	D2658	V2661	V2677	L2686	G2687	S2691	L2694	L2699	L2707	S2663	K2664	K2665	S2666	L2667	S2668	Y2671	L2674	L2675	L2676	L2677	L2678	L2679	K2680	R2686	G2697	S2699	V2502	V2503	L2610	L2611	Q2612	R2627	V2630	L2631	Q2612	R2632	T2635	G2636	P2637	R2638	L2639	T2640			
W2523	F2526	E2527	R2528	L2529	H2530	C2535	N2536	R2543	L2544	R2549	R2552	Y2558	L2559	P2562	K2563	K2564	K2565	S2566	L2567	S2568	L2571	L2574	L2575	L2576	L2577	L2578	L2579	K2580	R2586	G2597	T2609	G2610	L2611	Q2612	R2627	V2630	L2631	Q2612	R2632	T2635	G2636	P2637	R2638	L2639	T2640					
T2425	F2426	M2428	L2437	F2445	S2446	K2447	D2448	T2449	T2450	H2453	L2458	H2461	T2462	T2472	K2476	S2477	D2478	E2488	L2489	L2490	L2491	P2492	K2493	L2494	D2495	K2496	Y2497	G2498	S2499	V2502	V2503	L2407	L2408	N2409	S2410	K2411	R2412	T2415	L2416	Q2417	Q2418	P2419	F2420	G2421	S2422	G2423	E2520			
L2229	L2230	L2241	L2252	P2257	L2262	L2265	F2266	H2274	L2275	L2276	T2280	P2281	N2282	K2283	L2284	E2285	T2286	A2287	L2288	Q2289	L2290	H2293	L2294	T2295	R2299	F2302	L2305	D2306	S2309	L2310	T2314	L2315	L2316	L2317	L2318	S2321	L2322	L2326	Q2332	Q2335	S2336	R2336								
L2141	F2145	K2146	R2149	T2150	W2151	V2152	F2153	D2154	D2155	E2161	Y2162	V2169	N2173	K2174	L2175	L2176	T2177	L2178	E2185	P2179	H2180	G2181	E2182	R2183	L2186	L2193	F2194	E2195	T2196	D2197	L2198	L2199	H2201	T2202	T2203	P2204	A2205	T2206	T2207	L2212	F2215	D2218	V2219	K2220	S2221	L2222	S2223	S2224	K2225	







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	175.77Å 118.19Å 202.68Å 90.00° 90.91° 90.00°	Depositor
Resolution (Å)	49.14 – 3.70 49.09 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.14-3.70) 99.9 (49.09-3.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.7.0019	Depositor
R, R_{free}	0.231 , 0.289 0.226 , 0.285	Depositor DCC
R_{free} test set	4446 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	142.7	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 138.7	EDS
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 88912 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	41590	wwPDB-VP
Average B, all atoms (Å ²)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, 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	0.58	1/21146 (0.0%)	0.80	12/28618 (0.0%)
1	B	0.47	0/21146	0.68	4/28618 (0.0%)
All	All	0.53	1/42292 (0.0%)	0.74	16/57236 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2872	GLU	CG-CD	7.57	1.63	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1741	LEU	CB-CG-CD1	8.44	125.34	111.00
1	A	1973	LEU	CB-CG-CD1	-7.38	98.45	111.00
1	A	2872	GLU	OE1-CD-OE2	-7.25	114.59	123.30
1	A	2866	LEU	CA-CB-CG	6.12	129.38	115.30
1	A	1769	LEU	CA-CB-CG	6.06	129.24	115.30
1	A	2866	LEU	CB-CG-CD1	6.04	121.28	111.00
1	B	3650	LEU	CB-CG-CD1	-5.85	101.06	111.00
1	A	2012	LEU	CA-CB-CG	5.84	128.72	115.30
1	B	2866	LEU	CA-CB-CG	5.76	128.55	115.30
1	A	3577	MET	CG-SD-CE	5.72	109.36	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1611	LEU	CB-CG-CD2	-5.41	101.80	111.00
1	A	1776	LEU	CB-CG-CD1	-5.28	102.03	111.00
1	A	1769	LEU	CB-CG-CD1	5.27	119.96	111.00
1	B	2620	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	2759	ILE	CG1-CB-CG2	-5.23	99.90	111.40
1	A	1917	ARG	NE-CZ-NH2	-5.09	117.76	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1739	ASP	Peptide

5.2 Too-close contacts ⓘ

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	20748	0	20207	891	0
1	B	20748	0	20206	851	0
2	A	31	0	12	4	0
2	B	31	0	12	7	0
3	A	15	0	0	9	0
3	B	15	0	0	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	41590	0	40437	1741	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 21.

All (1741) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:PRO:C	1:A:3475:ASN:HB3	1.39	1.40
1:B:1620:PHE:HD1	1:B:1760:PHE:CZ	1.53	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1620:PHE:HD1	1:A:1760:PHE:CZ	1.58	1.21
1:B:3534:LEU:CD1	1:B:3618:TYR:HE2	1.53	1.21
1:B:1409:LEU:HD21	1:B:1435:LEU:HB3	1.24	1.18
1:A:3777:VAL:HG11	1:A:3895:PHE:HE1	1.06	1.18
1:A:4033:LEU:CD1	1:A:4035:GLN:HB2	1.76	1.16
1:A:3534:LEU:CD1	1:A:3618:TYR:HE2	1.59	1.15
1:B:1992:LYS:HG3	1:B:2024:SER:HB2	1.23	1.15
1:A:3525:ILE:HD11	1:A:3646:ILE:HG22	1.25	1.14
1:B:3525:ILE:HD11	1:B:3646:ILE:HG22	1.23	1.14
1:B:2111:LYS:HD3	1:B:2161:GLU:HG3	1.25	1.14
1:A:2111:LYS:HD3	1:A:2161:GLU:HG3	1.18	1.13
1:B:2473:LEU:HD23	1:B:2475:PRO:HD3	1.31	1.12
1:A:2707:VAL:HB	1:A:2712:LEU:HD11	1.19	1.11
1:B:2707:VAL:HB	1:B:2712:LEU:HD11	1.17	1.10
1:A:1992:LYS:HG3	1:A:2024:SER:HB2	1.17	1.09
1:A:3024:LEU:HD11	1:A:3303:LYS:HG3	1.31	1.09
1:A:2380:LEU:HD13	1:A:2390:ILE:HD11	1.34	1.08
1:B:3777:VAL:HG11	1:B:3895:PHE:HE1	0.97	1.08
1:A:2141:ILE:HD12	1:A:2146:LYS:HE2	1.20	1.07
1:A:3303:LYS:HA	1:A:3306:TRP:CD1	1.89	1.07
1:A:2494:LEU:HD13	1:A:2498:GLY:CA	1.85	1.07
1:B:1620:PHE:CD1	1:B:1760:PHE:CZ	2.42	1.06
1:A:2107:LYS:HE3	1:A:2495:ASP:OD2	1.51	1.06
1:B:2488:GLU:HB3	1:B:2491:LEU:HD12	1.12	1.06
1:B:1620:PHE:CD1	1:B:1760:PHE:HZ	1.73	1.06
1:B:3777:VAL:HG11	1:B:3895:PHE:CE1	1.90	1.06
1:A:1386:ILE:HG21	1:A:1396:ARG:HD2	1.32	1.06
1:A:3530:PHE:CD1	1:A:3618:TYR:HD2	1.71	1.06
1:B:1645:PHE:HB3	1:B:1765:ILE:HG22	1.37	1.06
1:A:1645:PHE:HB3	1:A:1765:ILE:CG2	1.86	1.05
1:B:2494:LEU:HD13	1:B:2498:GLY:CA	1.86	1.05
1:A:2380:LEU:HD22	1:A:2384:GLU:OE1	1.54	1.05
1:B:3534:LEU:CD1	1:B:3618:TYR:CE2	2.40	1.04
1:A:2494:LEU:CD1	1:A:2498:GLY:HA2	1.86	1.04
1:A:1645:PHE:HB3	1:A:1765:ILE:HG22	1.34	1.04
1:B:3534:LEU:HD12	1:B:3618:TYR:HE2	1.20	1.04
1:B:1645:PHE:HB3	1:B:1765:ILE:CG2	1.87	1.04
1:A:1983:LEU:HD22	1:A:1997:SER:OG	1.58	1.04
1:A:216:PRO:C	1:A:3475:ASN:CB	2.24	1.03
1:B:2473:LEU:CD2	1:B:2475:PRO:HD3	1.87	1.03
1:A:1992:LYS:CG	1:A:2024:SER:HB2	1.87	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2988:SER:HB3	1:A:2989:PRO:HD2	1.04	1.03
1:A:2488:GLU:HB3	1:A:2491:LEU:HD12	1.36	1.03
1:B:3303:LYS:HA	1:B:3306:TRP:CD1	1.93	1.03
1:B:1992:LYS:CG	1:B:2024:SER:HB2	1.89	1.03
1:B:2494:LEU:CD1	1:B:2498:GLY:HA2	1.89	1.02
1:A:1823:ASP:HB2	1:A:1852:ARG:O	1.56	1.02
1:A:2920:TRP:HB2	1:A:2989:PRO:HG3	1.06	1.02
1:B:1983:LEU:HD12	1:B:1997:SER:OG	1.59	1.02
1:A:2707:VAL:CB	1:A:2712:LEU:HD11	1.89	1.01
1:B:3024:LEU:HD11	1:B:3303:LYS:HG3	1.39	1.01
1:B:3530:PHE:CD1	1:B:3618:TYR:HD2	1.77	1.01
1:B:2707:VAL:CB	1:B:2712:LEU:HD11	1.88	1.01
1:A:2386:MET:HB2	1:A:2627:ARG:HD3	1.42	1.01
1:B:2488:GLU:CB	1:B:2491:LEU:HD12	1.91	1.00
1:B:2107:LYS:HE3	1:B:2495:ASP:OD2	1.60	1.00
1:A:1535:PRO:HB2	1:A:1841:ILE:HG13	1.44	1.00
1:A:2448:ASP:HB2	1:A:2829:GLU:OE2	1.59	1.00
1:A:3303:LYS:O	1:A:3306:TRP:HD1	1.43	1.00
1:B:1823:ASP:HB2	1:B:1852:ARG:O	1.61	1.00
1:A:2988:SER:HB3	1:A:2989:PRO:CD	1.90	1.00
1:A:3777:VAL:HG11	1:A:3895:PHE:CE1	1.97	0.99
1:A:1620:PHE:CD1	1:A:1760:PHE:CZ	2.50	0.99
1:B:3534:LEU:HD12	1:B:3618:TYR:CE2	1.97	0.99
1:B:2488:GLU:HB3	1:B:2491:LEU:CD1	1.92	0.99
1:A:3777:VAL:CG1	1:A:3895:PHE:HE1	1.74	0.99
1:B:2787:HIS:HA	1:B:3460:PRO:HD2	1.42	0.99
1:A:3534:LEU:CD1	1:A:3618:TYR:CE2	2.45	0.99
1:B:2064:GLN:HE22	1:B:2091:MET:CE	1.76	0.98
1:A:2380:LEU:CD1	1:A:2390:ILE:HD11	1.93	0.98
1:A:1409:LEU:HD21	1:A:1435:LEU:HB3	1.44	0.98
1:B:2745:ILE:HG23	1:B:2756:MET:HE2	1.43	0.97
1:B:2988:SER:HB3	1:B:2989:PRO:HD2	1.45	0.97
1:A:1970:LEU:HD13	1:A:1974:LYS:HE3	1.46	0.96
1:A:2064:GLN:OE1	1:A:2091:MET:HE1	1.64	0.96
1:A:3406:PHE:HB2	1:A:3513:VAL:CG1	1.94	0.96
1:B:1822:CYS:HB2	1:B:1853:LEU:HD21	1.43	0.96
1:A:2476:LYS:H	1:A:2476:LYS:CD	1.74	0.96
1:A:1822:CYS:HB2	1:A:1853:LEU:HD21	1.43	0.96
1:A:3024:LEU:CD1	1:A:3303:LYS:HG3	1.96	0.96
1:A:3534:LEU:HD12	1:A:3618:TYR:HE2	1.24	0.96
1:B:1744:LEU:HA	1:B:1760:PHE:CE2	1.99	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2112:GLU:HB3	1:B:2117:SER:HB2	1.48	0.95
1:B:1992:LYS:HE2	1:B:2024:SER:O	1.64	0.95
1:A:1386:ILE:HG21	1:A:1396:ARG:CD	1.95	0.95
1:B:1956:LEU:HB3	1:B:1968:PHE:HE2	1.31	0.95
1:A:4033:LEU:HD11	1:A:4035:GLN:HB2	1.47	0.95
1:A:2988:SER:CB	1:A:2989:PRO:HD2	1.97	0.95
1:B:1939:PHE:CD2	1:B:1940:GLU:O	2.19	0.95
1:A:3534:LEU:HD12	1:A:3618:TYR:CE2	2.01	0.95
1:B:3777:VAL:CG1	1:B:3895:PHE:HE1	1.78	0.95
1:A:1620:PHE:HD1	1:A:1760:PHE:HZ	1.07	0.94
1:A:2386:MET:CB	1:A:2627:ARG:HD3	1.95	0.94
1:B:1630:ILE:HG22	1:B:1655:MET:SD	2.06	0.94
1:A:2476:LYS:H	1:A:2476:LYS:HD3	1.26	0.94
1:A:2745:ILE:HG23	1:A:2756:MET:HE1	1.47	0.94
1:A:1645:PHE:CB	1:A:1765:ILE:HG22	1.96	0.94
1:A:1409:LEU:HD21	1:A:1435:LEU:CB	1.98	0.94
1:B:1645:PHE:CB	1:B:1765:ILE:HG22	1.97	0.94
1:B:2473:LEU:HD11	1:B:2527:GLU:CG	1.96	0.94
1:B:1535:PRO:HB2	1:B:1841:ILE:HG13	1.50	0.94
1:B:1866:GLN:OE1	1:B:1911:ASN:HB2	1.68	0.93
1:B:2472:THR:CG2	1:B:2524:VAL:HG22	1.99	0.93
1:A:3460:PRO:O	1:A:3463:SER:HB2	1.67	0.93
1:B:2494:LEU:HD13	1:B:2498:GLY:HA2	0.95	0.93
1:B:1774:LEU:HD21	1:B:1922:LYS:O	1.68	0.93
1:A:3530:PHE:CD1	1:A:3618:TYR:CD2	2.56	0.93
1:A:1802:LYS:HG2	1:A:1921:MET:HG3	1.47	0.93
1:A:2137:VAL:O	1:A:2141:ILE:HG23	1.69	0.93
1:A:3509:LEU:CD1	1:A:3513:VAL:HG21	1.98	0.93
1:B:2081:THR:HB	2:B:5093:ATP:PA	2.09	0.92
1:A:4065:LEU:HD11	1:A:4070:ILE:HD11	1.48	0.92
1:A:2111:LYS:HD3	1:A:2161:GLU:CG	2.00	0.92
1:B:1983:LEU:HD21	1:B:2000:ARG:NE	1.84	0.91
1:B:2787:HIS:HA	1:B:3460:PRO:CD	2.00	0.91
1:A:2400:HIS:CD2	1:A:2559:LEU:HD13	2.06	0.91
1:A:1992:LYS:HE2	1:A:2024:SER:O	1.71	0.91
1:B:3534:LEU:HD13	1:B:3618:TYR:HE2	1.35	0.91
1:B:2332:GLY:HA2	1:B:2335:GLN:HB2	1.50	0.91
1:B:2064:GLN:NE2	1:B:2091:MET:CE	2.33	0.91
1:B:3534:LEU:HD11	1:B:3614:LEU:HD23	1.50	0.90
1:A:2787:HIS:HA	1:A:3460:PRO:HD2	1.49	0.90
1:A:3737:THR:HB	1:A:3740:THR:OG1	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2400:HIS:NE2	1:A:2559:LEU:HD13	1.86	0.90
1:B:3737:THR:HB	1:B:3740:THR:OG1	1.69	0.90
1:B:1535:PRO:C	1:B:1841:ILE:HD11	1.90	0.90
1:A:2563:SER:HB3	1:A:2566:SER:H	1.35	0.90
1:B:2473:LEU:HD23	1:B:2475:PRO:CD	2.02	0.90
1:A:2494:LEU:HD13	1:A:2498:GLY:HA2	0.94	0.90
1:B:1726:LEU:CD1	1:B:3984:GLN:HB3	2.02	0.89
1:B:2473:LEU:HD11	1:B:2527:GLU:HG2	1.52	0.89
1:B:1802:LYS:HG2	1:B:1921:MET:HG3	1.54	0.89
1:A:1939:PHE:CD2	1:A:1940:GLU:O	2.26	0.89
1:B:2755:HIS:HB2	1:B:2911:ARG:O	1.72	0.89
1:A:4033:LEU:HD13	1:A:4035:GLN:HB2	1.54	0.88
1:A:1535:PRO:C	1:A:1841:ILE:HD11	1.92	0.88
1:A:1823:ASP:CB	1:A:1852:ARG:O	2.20	0.88
1:A:3946:VAL:HG12	1:A:3950:PHE:O	1.72	0.88
1:B:1604:ALA:HA	1:B:1607:TRP:CD1	2.09	0.88
1:A:2787:HIS:HA	1:A:3460:PRO:CG	2.02	0.88
1:A:1562:MET:HB3	1:A:1569:ILE:HD11	1.55	0.88
1:A:2920:TRP:HB2	1:A:2989:PRO:CG	1.99	0.87
1:A:2787:HIS:HA	1:A:3460:PRO:CD	2.03	0.87
1:A:3534:LEU:HD13	1:A:3618:TYR:HE2	1.38	0.87
1:B:1940:GLU:HB2	1:B:1989:GLU:O	1.73	0.87
1:A:2446:SER:H	1:A:2449:THR:CG2	1.86	0.87
1:A:1649:LEU:HD11	1:A:1704:GLU:HG3	1.56	0.87
1:A:1866:GLN:OE1	1:A:1911:ASN:HB2	1.74	0.87
1:A:2920:TRP:CB	1:A:2989:PRO:HG3	2.01	0.87
1:A:2064:GLN:NE2	1:A:2091:MET:SD	2.47	0.87
1:B:2476:LYS:CD	1:B:2476:LYS:H	1.87	0.87
1:B:2627:ARG:NH1	1:B:2631:THR:CG2	2.38	0.87
1:B:1956:LEU:HB3	1:B:1968:PHE:CE2	2.09	0.86
1:A:1924:PRO:HB2	1:A:1929:ILE:HD11	1.55	0.86
1:B:2988:SER:HB3	1:B:2989:PRO:CD	2.04	0.86
1:A:2787:HIS:HA	1:A:3460:PRO:HG2	1.56	0.86
1:B:1392:LEU:HD13	1:B:1393:LYS:N	1.90	0.86
1:B:2473:LEU:HD21	1:B:2527:GLU:HB2	1.55	0.86
1:B:2274:HIS:HE1	1:B:2326:LEU:O	1.59	0.86
1:A:2766:LYS:HE2	1:A:2890:THR:HB	1.58	0.86
1:B:3530:PHE:CD1	1:B:3618:TYR:CD2	2.64	0.85
1:B:2787:HIS:HA	1:B:3460:PRO:CG	2.06	0.85
1:B:3645:SER:HB3	1:B:3890:GLN:HE21	1.41	0.85
1:A:1726:LEU:HD12	1:A:3984:GLN:HB3	1.55	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2141:ILE:CD1	1:A:2146:LYS:HE2	2.06	0.85
1:A:1387:GLU:HB3	1:A:1393:LYS:HG2	1.58	0.85
1:A:1392:LEU:HD13	1:A:1393:LYS:N	1.91	0.85
1:B:3946:VAL:HG12	1:B:3950:PHE:O	1.76	0.85
1:B:2627:ARG:NH1	1:B:2630:TYR:CD2	2.45	0.85
1:A:3656:VAL:HG13	1:A:3677:LEU:HB3	1.59	0.85
1:A:3024:LEU:HD11	1:A:3303:LYS:CG	2.07	0.85
1:B:2131:THR:HG22	1:B:2176:LEU:HD21	1.57	0.85
1:A:3303:LYS:O	1:A:3306:TRP:CD1	2.28	0.84
1:A:1940:GLU:HB2	1:A:1989:GLU:O	1.77	0.84
1:A:2131:THR:HG22	1:A:2176:LEU:HD21	1.59	0.84
1:A:2446:SER:H	1:A:2449:THR:HG23	1.39	0.84
1:B:3406:PHE:HB2	1:B:3513:VAL:CG1	2.06	0.84
1:B:2563:SER:HB3	1:B:2566:SER:H	1.41	0.84
1:A:2112:GLU:HB3	1:A:2117:SER:HB2	1.57	0.84
1:B:1365:PHE:O	1:B:1366:VAL:HG22	1.78	0.84
1:B:2627:ARG:HH11	1:B:2630:TYR:HD2	1.25	0.84
1:A:2336:ARG:HD3	1:A:2355:ASP:OD2	1.77	0.84
1:B:2446:SER:H	1:B:2449:THR:HG23	1.43	0.83
1:B:1823:ASP:CB	1:B:1852:ARG:O	2.25	0.83
1:B:2745:ILE:HG23	1:B:2756:MET:CE	2.08	0.83
1:A:2274:HIS:HE1	1:A:2326:LEU:O	1.61	0.83
1:B:2111:LYS:HD3	1:B:2161:GLU:CG	2.07	0.83
1:A:2488:GLU:CB	1:A:2491:LEU:HD12	2.09	0.83
1:A:2106:THR:OG1	1:A:2154:PHE:HB3	1.78	0.83
1:A:1649:LEU:CD1	1:A:1704:GLU:HG3	2.07	0.83
1:B:2787:HIS:HA	1:B:3460:PRO:HG2	1.61	0.83
1:B:3024:LEU:CD1	1:B:3303:LYS:HG3	2.09	0.83
1:A:2755:HIS:HB2	1:A:2911:ARG:O	1.79	0.82
1:B:1574:PHE:HB3	1:B:1576:GLU:H	1.43	0.82
1:B:3998:ILE:HG21	1:B:4004:LEU:HG	1.59	0.82
1:A:2111:LYS:NZ	1:A:2161:GLU:HG2	1.94	0.82
1:B:1425:GLU:OE1	1:B:1426:GLN:HA	1.79	0.82
1:B:3919:LYS:HZ3	1:B:4038:GLU:CD	1.83	0.82
1:A:2488:GLU:HB3	1:A:2491:LEU:CD1	2.08	0.82
1:B:2081:THR:HB	2:B:5093:ATP:O2A	1.78	0.82
1:B:3509:LEU:CD1	1:B:3513:VAL:HG21	2.10	0.82
1:A:1425:GLU:OE1	1:A:1426:GLN:HA	1.78	0.82
1:B:2627:ARG:NH1	1:B:2631:THR:HG23	1.94	0.82
1:A:1604:ALA:HA	1:A:1607:TRP:NE1	1.95	0.81
1:A:3645:SER:HB3	1:A:3890:GLN:HE21	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:PRO:O	1:A:216:PRO:CB	2.28	0.81
1:A:2476:LYS:HZ1	1:A:2528:ARG:HD2	1.43	0.81
1:B:3566:LEU:HA	1:B:3583:LEU:HD21	1.61	0.81
1:A:2362:ALA:HB3	1:A:2365:LYS:O	1.81	0.81
1:B:2106:THR:OG1	1:B:2154:PHE:HB3	1.80	0.81
1:A:1849:GLU:HG2	1:A:1899:ASN:ND2	1.95	0.81
1:A:2064:GLN:OE1	1:A:2091:MET:CE	2.29	0.81
1:A:3923:VAL:HG23	1:A:4038:GLU:HA	1.62	0.81
1:B:2627:ARG:NH1	1:B:2630:TYR:CE2	2.48	0.81
1:A:1630:ILE:HG22	1:A:1655:MET:SD	2.21	0.81
1:B:3566:LEU:HA	1:B:3583:LEU:CD2	2.10	0.81
1:B:3792:ARG:HB2	1:B:3955:TYR:CD1	2.15	0.81
1:A:1493:LEU:HD23	1:A:1498:GLU:HB3	1.63	0.81
1:B:2111:LYS:NZ	1:B:2161:GLU:HG2	1.96	0.81
1:B:1604:ALA:HA	1:B:1607:TRP:NE1	1.95	0.80
1:B:2446:SER:H	1:B:2449:THR:CG2	1.93	0.80
1:B:1939:PHE:HD2	1:B:1940:GLU:O	1.62	0.80
1:B:3998:ILE:CG2	1:B:4004:LEU:HG	2.12	0.80
1:B:2707:VAL:CG1	1:B:2712:LEU:CD1	2.59	0.80
1:B:2473:LEU:CD2	1:B:2475:PRO:CD	2.57	0.79
1:A:3303:LYS:HA	1:A:3306:TRP:NE1	1.95	0.79
1:A:3303:LYS:C	1:A:3306:TRP:HD1	1.84	0.79
1:B:2112:GLU:HB3	1:B:2117:SER:CB	2.12	0.79
1:A:3303:LYS:CA	1:A:3306:TRP:CD1	2.65	0.79
1:A:2476:LYS:NZ	1:A:2528:ARG:HD2	1.97	0.79
1:A:1421:TYR:O	1:A:1425:GLU:CB	2.30	0.79
1:A:2181:GLY:O	1:A:2182:GLU:HG3	1.83	0.79
1:A:2332:GLY:HA2	1:A:2335:GLN:HB2	1.62	0.79
1:A:1394:LEU:HD22	1:A:1449:GLN:HE22	1.48	0.79
1:B:1744:LEU:HA	1:B:1760:PHE:CD2	2.18	0.79
1:A:3530:PHE:HD1	1:A:3618:TYR:HD2	1.31	0.78
1:A:2707:VAL:CG1	1:A:2712:LEU:CD1	2.61	0.78
1:A:3799:LYS:O	1:A:3803:LEU:HG	1.82	0.78
1:B:2707:VAL:HB	1:B:2712:LEU:CD1	2.08	0.78
1:A:1956:LEU:HB3	1:A:1968:PHE:CE2	2.18	0.78
1:B:1562:MET:HB3	1:B:1569:ILE:HD11	1.64	0.78
1:B:3303:LYS:O	1:B:3306:TRP:HD1	1.66	0.78
1:B:1996:GLU:O	1:B:2000:ARG:HG3	1.81	0.78
1:B:2380:LEU:HD12	1:B:2577:ALA:HB1	1.65	0.78
1:B:1924:PRO:HB2	1:B:1929:ILE:HD11	1.64	0.78
1:B:1409:LEU:CD2	1:B:1435:LEU:HB3	2.09	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1970:LEU:HD12	1:A:1971:ARG:N	1.98	0.78
1:B:2493:LYS:HG3	1:B:2494:LEU:H	1.48	0.78
1:B:2137:VAL:O	1:B:2141:ILE:HG23	1.84	0.78
1:A:1386:ILE:CG2	1:A:1396:ARG:CD	2.62	0.78
1:A:1620:PHE:CD1	1:A:1760:PHE:HZ	1.96	0.78
1:B:3923:VAL:HG23	1:B:4038:GLU:HA	1.66	0.78
1:B:2472:THR:HG21	1:B:2524:VAL:HG22	1.65	0.77
1:A:1604:ALA:HA	1:A:1607:TRP:CD1	2.18	0.77
1:A:1421:TYR:O	1:A:1425:GLU:HB2	1.84	0.77
1:B:3473:ALA:HB3	1:B:3476:ARG:O	1.85	0.77
1:B:1953:LEU:CD1	1:B:1973:LEU:HB3	2.14	0.77
1:A:3509:LEU:HD12	1:A:3513:VAL:CG2	2.13	0.77
1:B:1387:GLU:HB3	1:B:1393:LYS:HG2	1.66	0.77
1:B:1405:CYS:O	1:B:1409:LEU:HG	1.85	0.77
1:A:2476:LYS:HG2	1:A:2478:ASP:O	1.85	0.77
1:B:1849:GLU:HG2	1:B:1899:ASN:ND2	2.00	0.76
1:A:2064:GLN:OE1	1:A:2151:TRP:HH2	1.67	0.76
1:B:1421:TYR:O	1:B:1425:GLU:CB	2.32	0.76
1:B:2293:HIS:CE1	1:B:2409:ASN:HB3	2.20	0.76
1:B:1409:LEU:HD21	1:B:1435:LEU:CB	2.11	0.76
1:B:1645:PHE:CB	1:B:1765:ILE:CG2	2.61	0.76
1:B:1421:TYR:O	1:B:1425:GLU:HB2	1.85	0.76
1:B:2473:LEU:HD23	1:B:2474:LEU:N	2.01	0.76
1:B:2476:LYS:HG2	1:B:2478:ASP:O	1.86	0.76
1:B:2476:LYS:NZ	1:B:2528:ARG:HD2	2.00	0.76
1:B:3871:PHE:CZ	1:B:3873:MET:HB2	2.21	0.76
1:A:3460:PRO:O	1:A:3463:SER:CB	2.32	0.76
1:B:2572:GLU:CD	1:B:2590:GLU:HG3	2.05	0.76
1:B:2787:HIS:CA	1:B:3460:PRO:HD2	2.15	0.76
1:B:2920:TRP:HB2	1:B:2989:PRO:HG3	1.67	0.76
1:A:2411:LYS:HG2	1:A:2530:HIS:HE1	1.51	0.76
1:A:2563:SER:HB2	1:A:2566:SER:OG	1.86	0.75
1:A:3946:VAL:CG1	1:A:3950:PHE:O	2.34	0.75
1:A:1540:LEU:CD1	1:A:1548:ILE:CD1	2.64	0.75
1:A:3939:ILE:HG13	1:A:4010:LEU:CD2	2.16	0.75
1:B:3534:LEU:HD13	1:B:3618:TYR:CE2	2.15	0.75
1:B:2064:GLN:HE22	1:B:2091:MET:HE3	1.49	0.75
1:B:1366:VAL:HG13	1:B:1369:LYS:HE3	1.68	0.75
1:B:2003:LEU:HA	1:B:2006:LEU:HD12	1.69	0.75
1:B:2064:GLN:NE2	1:B:2091:MET:HE3	2.00	0.75
1:A:1939:PHE:HD2	1:A:1940:GLU:O	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1489:ARG:HH12	1:B:1503:PRO:HG2	1.52	0.75
1:A:4033:LEU:CD1	1:A:4035:GLN:CB	2.60	0.75
1:B:1967:HIS:C	1:B:1968:PHE:HD1	1.90	0.75
1:A:3816:LEU:HD23	1:A:3847:SER:OG	1.86	0.75
1:B:3774:ILE:O	1:B:3778:VAL:HG23	1.86	0.75
1:A:3777:VAL:CG1	1:A:3895:PHE:CE1	2.63	0.75
1:A:2707:VAL:HB	1:A:2712:LEU:CD1	2.09	0.75
1:B:2707:VAL:CG1	1:B:2712:LEU:HD11	2.16	0.75
1:B:1983:LEU:HD11	1:B:2000:ARG:HD2	1.66	0.75
1:B:3525:ILE:CD1	1:B:3646:ILE:HG22	2.11	0.75
1:A:2032:LYS:O	1:A:2035:VAL:HG12	1.85	0.75
1:B:1392:LEU:HD13	1:B:1392:LEU:C	2.06	0.75
1:A:2107:LYS:HE2	1:A:2499:SER:HB3	1.67	0.74
1:A:3406:PHE:HB2	1:A:3513:VAL:HG11	1.68	0.74
1:B:2380:LEU:HD11	1:B:2577:ALA:CB	2.17	0.74
1:B:3799:LYS:O	1:B:3803:LEU:HG	1.87	0.74
1:A:1940:GLU:HG3	1:A:1941:ASP:H	1.52	0.74
1:B:2032:LYS:O	1:B:2035:VAL:HG12	1.85	0.74
1:B:3303:LYS:CA	1:B:3306:TRP:CD1	2.70	0.74
1:A:1983:LEU:HD21	1:A:2000:ARG:HD2	1.69	0.74
1:A:3525:ILE:CD1	1:A:3646:ILE:HG22	2.13	0.74
1:A:3406:PHE:HB2	1:A:3513:VAL:HG12	1.69	0.74
1:B:2476:LYS:HD2	1:B:2476:LYS:H	1.51	0.74
1:B:3645:SER:HB3	1:B:3890:GLN:NE2	2.00	0.74
1:A:3534:LEU:HD11	1:A:3614:LEU:HD23	1.67	0.74
1:A:1744:LEU:HA	1:A:1760:PHE:CE2	2.23	0.74
1:A:1392:LEU:HD13	1:A:1392:LEU:C	2.07	0.74
1:B:2175:ILE:HG12	1:B:2183:ARG:HB3	1.70	0.74
1:B:2380:LEU:CD1	1:B:2577:ALA:CB	2.65	0.74
1:A:3871:PHE:CZ	1:A:3873:MET:HB2	2.22	0.74
1:B:2512:LYS:HB3	1:B:2523:TRP:HH2	1.52	0.74
1:A:1956:LEU:HB3	1:A:1968:PHE:HE2	1.53	0.74
1:B:2512:LYS:O	1:B:2513:GLN:HB2	1.88	0.74
1:A:2745:ILE:HG23	1:A:2756:MET:CE	2.17	0.73
1:A:1569:ILE:HA	1:A:1584:SER:HA	1.70	0.73
1:B:1726:LEU:HD12	1:B:3984:GLN:HB3	1.66	0.73
1:B:3946:VAL:CG1	1:B:3950:PHE:O	2.36	0.73
1:B:3303:LYS:C	1:B:3306:TRP:HD1	1.91	0.73
1:A:3566:LEU:HA	1:A:3583:LEU:CD2	2.18	0.73
1:A:2112:GLU:HB3	1:A:2117:SER:CB	2.19	0.73
1:A:2707:VAL:CG1	1:A:2712:LEU:HD11	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2785:LYS:HD3	1:B:3482:GLY:O	1.89	0.73
1:B:3618:TYR:CD1	1:B:3618:TYR:N	2.54	0.73
1:A:3303:LYS:CA	1:A:3306:TRP:HD1	2.02	0.73
1:A:1802:LYS:NZ	3:A:5096:SO4:S	2.61	0.73
1:B:2203:THR:HG22	1:B:2205:ALA:H	1.54	0.73
1:A:1405:CYS:O	1:A:1409:LEU:HG	1.88	0.73
1:A:2176:LEU:O	1:A:2183:ARG:HA	1.88	0.73
1:B:3792:ARG:HB2	1:B:3955:TYR:CE1	2.23	0.73
1:B:2380:LEU:CD1	1:B:2577:ALA:HB1	2.18	0.73
1:B:1630:ILE:CG2	1:B:1655:MET:SD	2.76	0.72
1:B:1569:ILE:HA	1:B:1584:SER:HA	1.70	0.72
1:B:3656:VAL:HG13	1:B:3677:LEU:HB3	1.70	0.72
1:A:2201:HIS:CE1	1:A:2497:TYR:HA	2.24	0.72
1:B:3690:LEU:HD23	1:B:3694:PHE:HB3	1.70	0.72
1:A:1822:CYS:SG	1:A:1850:PHE:HA	2.29	0.72
1:B:1849:GLU:HG2	1:B:1899:ASN:HD22	1.54	0.72
1:B:2627:ARG:NH1	1:B:2631:THR:HG22	2.04	0.72
1:B:2176:LEU:O	1:B:2183:ARG:HA	1.89	0.72
1:B:3024:LEU:HD11	1:B:3303:LYS:CG	2.18	0.72
1:A:1849:GLU:HG2	1:A:1899:ASN:HD22	1.53	0.72
1:B:1726:LEU:HD13	1:B:3984:GLN:HB3	1.69	0.72
1:B:1706:LEU:HD22	1:B:1935:GLN:HG2	1.70	0.72
1:A:3509:LEU:CD1	1:A:3513:VAL:CG2	2.68	0.71
1:B:2476:LYS:HZ1	1:B:2528:ARG:HD2	1.54	0.71
1:B:1620:PHE:HA	1:B:1760:PHE:HE1	1.55	0.71
1:A:1645:PHE:CB	1:A:1765:ILE:CG2	2.61	0.71
1:B:216:PRO:CB	1:B:1365:PHE:HD2	2.03	0.71
1:B:2563:SER:HB2	1:B:2566:SER:OG	1.91	0.71
1:B:3737:THR:OG1	1:B:3740:THR:HB	1.90	0.71
1:A:3530:PHE:HD1	1:A:3618:TYR:CD2	2.04	0.71
1:B:3330:TYR:OH	1:B:3346:LEU:HD22	1.89	0.71
1:B:1983:LEU:HD21	1:B:2000:ARG:CZ	2.19	0.71
1:B:1983:LEU:HB3	1:B:1993:THR:HG23	1.72	0.71
1:B:2448:ASP:HB2	1:B:2829:GLU:OE1	1.91	0.71
1:B:2107:LYS:HE2	1:B:2499:SER:HB3	1.72	0.71
1:B:3631:MET:CE	1:B:3698:MET:HG3	2.21	0.71
1:B:3566:LEU:O	1:B:3570:LEU:HG	1.91	0.71
1:A:1540:LEU:HD11	1:A:1548:ILE:HD11	1.73	0.71
1:A:2960:THR:HB	1:A:2963:ASP:HB2	1.73	0.70
1:B:1698:ILE:O	1:B:1702:LEU:HG	1.91	0.70
1:B:1970:LEU:HD13	1:B:1974:LYS:HE2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3774:ILE:O	1:A:3778:VAL:HG23	1.91	0.70
1:A:3792:ARG:HB2	1:A:3955:TYR:CD1	2.26	0.70
1:A:3871:PHE:HZ	1:A:3873:MET:HB2	1.56	0.70
1:A:2003:LEU:HA	1:A:2006:LEU:HD12	1.74	0.70
1:B:2514:GLY:O	1:B:2523:TRP:CH2	2.44	0.70
1:A:1774:LEU:HD21	1:A:1922:LYS:O	1.91	0.70
1:B:3303:LYS:O	1:B:3306:TRP:CD1	2.44	0.70
1:B:1535:PRO:HB2	1:B:1841:ILE:CG1	2.19	0.70
1:B:3406:PHE:HB2	1:B:3513:VAL:HG11	1.73	0.70
1:A:3618:TYR:CD1	1:A:3618:TYR:N	2.54	0.70
1:B:2745:ILE:HG12	1:B:2756:MET:HE1	1.73	0.70
1:A:1493:LEU:HD23	1:A:1498:GLU:CB	2.22	0.70
1:B:2410:SER:C	1:B:2411:LYS:HG3	2.12	0.70
1:B:1536:ARG:N	1:B:1841:ILE:HD11	2.07	0.70
1:A:3305:ARG:O	1:A:3307:LEU:N	2.24	0.70
1:B:1611:LEU:O	1:B:1615:ILE:HG23	1.91	0.70
1:A:2294:LEU:HB3	1:A:2317:LEU:HD22	1.74	0.70
1:A:1495:THR:HG22	1:A:1497:ILE:HG22	1.73	0.70
1:A:1612:ASP:HA	1:A:1615:ILE:CD1	2.21	0.69
1:A:2203:THR:HG22	1:A:2205:ALA:H	1.56	0.69
1:A:3645:SER:HB3	1:A:3890:GLN:NE2	2.06	0.69
1:B:1612:ASP:HA	1:B:1615:ILE:CD1	2.22	0.69
1:A:3330:TYR:OH	1:A:3346:LEU:HD22	1.92	0.69
1:B:1649:LEU:HD11	1:B:1704:GLU:HG3	1.73	0.69
1:B:1495:THR:HG22	1:B:1497:ILE:HG22	1.73	0.69
1:B:3919:LYS:NZ	1:B:4038:GLU:CD	2.46	0.69
1:A:3785:TYR:HE2	1:A:3859:VAL:HG22	1.57	0.69
1:B:3871:PHE:HZ	1:B:3873:MET:HB2	1.57	0.69
1:A:2107:LYS:CE	1:A:2495:ASP:OD2	2.37	0.69
1:B:1822:CYS:SG	1:B:1849:GLU:O	2.51	0.69
1:A:1970:LEU:HD13	1:A:1974:LYS:CE	2.20	0.69
1:A:2175:ILE:HG12	1:A:2183:ARG:HB3	1.74	0.69
1:A:3979:ASN:O	1:A:3981:PRO:HD2	1.92	0.69
1:B:1540:LEU:CD1	1:B:1548:ILE:CD1	2.71	0.69
1:A:2285:GLU:HB2	1:A:2412:ARG:NH2	2.08	0.69
1:A:1646:GLN:NE2	1:A:1758:TYR:OH	2.26	0.69
1:B:2081:THR:HB	2:B:5093:ATP:O1A	1.92	0.69
1:B:1365:PHE:O	1:B:1366:VAL:CG2	2.41	0.69
1:A:2514:GLY:O	1:A:2523:TRP:CH2	2.45	0.69
1:A:3534:LEU:HD13	1:A:3618:TYR:CE2	2.19	0.68
1:A:2125:TRP:CZ2	1:A:2178:LEU:HD13	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3777:VAL:CG1	1:B:3895:PHE:CE1	2.65	0.68
1:B:1649:LEU:CD1	1:B:1704:GLU:HG3	2.23	0.68
1:B:1983:LEU:CD1	1:B:1997:SER:OG	2.39	0.68
1:B:2081:THR:CB	2:B:5093:ATP:O2A	2.41	0.68
1:B:3566:LEU:HD13	1:B:3570:LEU:CD1	2.23	0.68
1:A:3850:TRP:NE1	1:A:3854:TYR:HB3	2.08	0.68
1:A:1995:VAL:HG21	1:A:2024:SER:HB3	1.74	0.68
1:A:2419:PRO:O	1:A:2424:LYS:HE3	1.93	0.68
1:B:3303:LYS:CA	1:B:3306:TRP:HD1	2.04	0.68
1:A:1967:HIS:C	1:A:1968:PHE:HD1	1.97	0.68
1:B:3851:VAL:HG13	1:B:3855:LEU:HD23	1.76	0.68
1:A:1802:LYS:NZ	3:A:5096:SO4:O2	2.26	0.68
1:A:4033:LEU:HD13	1:A:4035:GLN:CB	2.21	0.68
1:A:1983:LEU:HB3	1:A:1993:THR:HG23	1.75	0.68
1:A:3837:GLY:O	1:A:3871:PHE:HD1	1.77	0.68
1:B:3592:LYS:O	1:B:3596:ASN:HB2	1.94	0.68
1:B:1620:PHE:HB2	1:B:1760:PHE:CE1	2.29	0.68
1:A:3848:LEU:HD21	1:A:3852:LYS:HE3	1.75	0.68
1:A:1698:ILE:O	1:A:1702:LEU:HG	1.94	0.68
1:B:3886:ALA:N	1:B:3887:PRO:HD2	2.09	0.68
1:A:2787:HIS:CA	1:A:3460:PRO:HD2	2.20	0.68
1:B:1620:PHE:HD1	1:B:1760:PHE:HZ	0.81	0.68
1:B:2224:SER:O	2:B:5093:ATP:H2	1.76	0.68
1:B:1425:GLU:OE1	1:B:1426:GLN:CA	2.42	0.68
1:A:3566:LEU:HA	1:A:3583:LEU:HD21	1.76	0.67
1:A:3935:PHE:HB2	1:A:4014:VAL:HG11	1.76	0.67
1:A:2293:HIS:NE2	1:A:2409:ASN:HB3	2.09	0.67
1:A:1744:LEU:HA	1:A:1760:PHE:CD2	2.29	0.67
1:B:1540:LEU:CD1	1:B:1548:ILE:HD11	2.25	0.67
1:A:1462:ASN:HB2	1:A:1465:ILE:HG22	1.75	0.67
1:A:2293:HIS:CE1	1:A:2409:ASN:HB3	2.29	0.67
1:B:2766:LYS:HE2	1:B:2890:THR:HB	1.75	0.67
1:B:3530:PHE:HD1	1:B:3618:TYR:HD2	1.42	0.67
1:A:1822:CYS:SG	1:A:1849:GLU:O	2.53	0.67
1:B:3458:PHE:CE1	1:B:3459:ASP:O	2.47	0.67
1:A:2080:LYS:HG2	1:A:2215:PHE:CE1	2.30	0.67
1:A:1630:ILE:HA	1:A:1634:THR:HG22	1.75	0.67
1:B:3816:LEU:HD23	1:B:3847:SER:OG	1.94	0.67
1:B:1527:LEU:HD23	1:B:1545:LEU:HD22	1.75	0.67
1:A:2305:LEU:HD11	1:A:2368:PHE:CG	2.29	0.67
1:A:2493:LYS:HG3	1:A:2494:LEU:H	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:PRO:O	1:A:3475:ASN:HB3	1.95	0.67
1:A:2252:LEU:HD21	1:A:2310:LEU:HD23	1.76	0.67
1:A:2386:MET:HB3	1:A:2627:ARG:HD3	1.75	0.67
1:A:1489:ARG:HH12	1:A:1503:PRO:HG2	1.59	0.67
1:B:2394:THR:H	1:B:2397:THR:HB	1.58	0.67
1:B:3303:LYS:HA	1:B:3306:TRP:NE1	2.10	0.67
1:B:3837:GLY:O	1:B:3871:PHE:HD1	1.77	0.67
1:B:1527:LEU:CD2	1:B:1545:LEU:HD22	2.24	0.67
1:A:3525:ILE:HD11	1:A:3646:ILE:CG2	2.16	0.67
1:B:1531:ARG:HG2	1:B:1537:PHE:HB3	1.76	0.67
1:B:3566:LEU:CD1	1:B:3570:LEU:HD11	2.24	0.67
1:B:2941:THR:HG22	1:B:2942:ASP:H	1.60	0.66
1:A:1536:ARG:N	1:A:1841:ILE:HD11	2.09	0.66
1:B:1425:GLU:OE1	1:B:1426:GLN:N	2.28	0.66
1:A:1540:LEU:CD1	1:A:1548:ILE:HD11	2.25	0.66
1:A:3979:ASN:C	1:A:3981:PRO:HD2	2.16	0.66
1:A:1703:VAL:HG13	1:A:1770:ILE:HD13	1.78	0.66
1:B:2181:GLY:O	1:B:2182:GLU:HG3	1.96	0.66
1:B:1645:PHE:CG	1:B:1765:ILE:HG22	2.31	0.66
1:B:3850:TRP:NE1	1:B:3854:TYR:HB3	2.10	0.66
1:B:2779:LEU:HD23	1:B:2812:ARG:O	1.96	0.66
1:B:3819:ILE:O	1:B:3823:ASN:HB2	1.94	0.66
1:A:3998:ILE:HG21	1:A:4004:LEU:HG	1.77	0.66
1:B:1620:PHE:HA	1:B:1760:PHE:CE1	2.31	0.66
1:A:1425:GLU:OE1	1:A:1426:GLN:CA	2.43	0.66
1:A:1493:LEU:CD2	1:A:1498:GLU:HB3	2.25	0.66
1:A:1612:ASP:HA	1:A:1615:ILE:HD11	1.78	0.66
1:A:2631:THR:O	1:A:2635:THR:HG22	1.96	0.66
1:B:216:PRO:CB	1:B:1365:PHE:CD2	2.79	0.65
1:A:2382:ALA:O	1:A:2385:VAL:HG12	1.96	0.65
1:A:1626:CYS:SG	1:A:1639:VAL:HG11	2.35	0.65
1:B:3935:PHE:HB2	1:B:4014:VAL:HG11	1.77	0.65
1:B:2707:VAL:CG1	1:B:2712:LEU:HD12	2.27	0.65
1:A:2514:GLY:HA3	1:A:2523:TRP:CZ2	2.32	0.65
1:A:3998:ILE:CG2	1:A:4004:LEU:HG	2.27	0.65
1:A:1527:LEU:CD2	1:A:1545:LEU:HD22	2.26	0.65
1:B:3406:PHE:HB2	1:B:3513:VAL:HG12	1.76	0.65
1:A:3566:LEU:O	1:A:3570:LEU:HG	1.97	0.65
1:B:3979:ASN:O	1:B:3981:PRO:HD2	1.97	0.65
1:A:2220:CYS:SG	1:A:2224:SER:HB2	2.36	0.65
1:B:3839:ILE:HG23	1:B:3873:MET:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2728:LEU:HD12	1:A:2771:ARG:CZ	2.27	0.65
1:A:2290:LEU:HD13	1:A:2407:LEU:HD23	1.79	0.65
1:A:3459:ASP:OD2	1:A:3461:ILE:HG12	1.97	0.65
1:B:2489:ILE:HG22	1:B:2535:CYS:HB3	1.78	0.65
1:B:2336:ARG:HD3	1:B:2355:ASP:OD2	1.97	0.65
1:A:1645:PHE:CG	1:A:1765:ILE:HG22	2.32	0.65
1:A:3566:LEU:HD13	1:A:3570:LEU:CD1	2.27	0.65
1:A:2512:LYS:O	1:A:2513:GLN:HB2	1.97	0.65
1:A:2448:ASP:HB2	1:A:2829:GLU:CD	2.17	0.65
1:A:3010:LEU:HD21	1:A:3317:SER:HB3	1.79	0.65
1:B:2707:VAL:CB	1:B:2712:LEU:CD1	2.72	0.64
1:A:1706:LEU:CD2	1:A:1935:GLN:HG2	2.27	0.64
1:A:2842:ASP:O	1:A:2845:GLN:HG2	1.97	0.64
1:A:3473:ALA:HB3	1:A:3476:ARG:O	1.96	0.64
1:B:2920:TRP:HB2	1:B:2989:PRO:CG	2.26	0.64
1:A:3509:LEU:HD11	1:A:3513:VAL:HG21	1.76	0.64
1:B:2112:GLU:CB	1:B:2117:SER:HB2	2.25	0.64
1:A:3819:ILE:O	1:A:3823:ASN:HB2	1.96	0.64
1:A:2707:VAL:CG1	1:A:2712:LEU:HD12	2.26	0.64
1:B:1534:PHE:CE2	1:B:1536:ARG:HB2	2.33	0.64
1:B:3509:LEU:HD12	1:B:3513:VAL:CG2	2.28	0.64
1:A:2779:LEU:HD23	1:A:2812:ARG:O	1.97	0.64
1:B:3530:PHE:CE1	1:B:3618:TYR:CD2	2.85	0.64
1:A:2315:THR:HG21	1:A:2350:SER:HB3	1.80	0.64
1:B:2536:ASN:HB2	1:B:2543:ARG:HE	1.63	0.64
1:A:3566:LEU:CD1	1:A:3570:LEU:HD11	2.26	0.64
1:A:2095:ASP:CG	1:A:2149:ARG:NH2	2.50	0.64
1:A:2222:ILE:HG23	1:A:2284:LEU:HD11	1.80	0.64
1:A:3618:TYR:HD1	1:A:3618:TYR:N	1.94	0.64
1:A:2495:ASP:O	1:A:2498:GLY:N	2.30	0.64
1:B:2252:LEU:HD21	1:B:2310:LEU:HD23	1.79	0.64
1:A:2141:ILE:HD12	1:A:2146:LYS:CE	2.12	0.64
1:A:3785:TYR:CE2	1:A:3859:VAL:HG22	2.33	0.64
1:B:1748:PHE:CD2	1:B:1755:LEU:HD22	2.32	0.64
1:A:2111:LYS:HZ3	1:A:2161:GLU:HG2	1.60	0.63
1:A:3792:ARG:HB2	1:A:3955:TYR:CE1	2.33	0.63
1:A:2285:GLU:HB2	1:A:2412:ARG:HH22	1.62	0.63
1:B:2111:LYS:CD	1:B:2161:GLU:HG3	2.17	0.63
1:B:1706:LEU:HD11	1:B:1936:ILE:HG12	1.79	0.63
1:A:1953:LEU:CD1	1:A:1973:LEU:HB3	2.27	0.63
1:A:3641:PHE:HA	1:A:3889:LEU:HD21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1992:LYS:HG3	1:A:2024:SER:CB	2.11	0.63
1:A:1995:VAL:HG22	1:A:2022:PHE:CE2	2.33	0.63
1:A:3737:THR:OG1	1:A:3740:THR:HB	1.98	0.63
1:A:1738:ASN:O	1:A:1739:ASP:OD1	2.16	0.63
1:B:3530:PHE:HD1	1:B:3618:TYR:CD2	2.17	0.63
1:A:2632:ALA:HB3	1:A:2647:LEU:HD21	1.80	0.63
1:B:2846:GLY:O	1:B:2849:TYR:HB3	1.98	0.63
1:A:1562:MET:CB	1:A:1569:ILE:HD11	2.29	0.63
1:A:2536:ASN:HB2	1:A:2543:ARG:HE	1.64	0.63
1:A:3409:ASP:HB3	1:A:3518:PHE:HB2	1.81	0.63
1:B:3618:TYR:HD1	1:B:3618:TYR:N	1.94	0.63
1:A:1991:GLU:O	1:A:1995:VAL:HG23	1.99	0.62
1:A:2151:TRP:HE3	1:A:2193:LEU:HD11	1.64	0.62
1:A:3700:MET:HB3	1:A:4085:THR:HG21	1.81	0.62
1:A:1938:GLY:O	1:A:1989:GLU:HB3	1.98	0.62
1:A:1421:TYR:O	1:A:1425:GLU:N	2.33	0.62
1:B:3566:LEU:HD13	1:B:3570:LEU:HD11	1.80	0.62
1:B:3912:GLY:O	1:B:3915:PHE:CZ	2.53	0.62
1:B:2276:LEU:HD21	1:B:2415:ILE:HG21	1.81	0.62
1:A:1826:PHE:HE1	1:A:1853:LEU:HD22	1.62	0.62
1:B:2034:ILE:HD12	1:B:2061:TYR:CZ	2.34	0.62
1:B:3951:SER:HB2	1:B:4002:LYS:HD2	1.82	0.62
1:A:1827:ASP:HB3	1:A:1830:VAL:HG12	1.81	0.62
1:A:1826:PHE:CE1	1:A:1853:LEU:HD22	2.35	0.62
1:A:1535:PRO:HB2	1:A:1841:ILE:CG1	2.25	0.62
1:B:1984:ILE:HG21	1:B:1989:GLU:HG3	1.80	0.62
1:B:1706:LEU:HD22	1:B:1935:GLN:CG	2.29	0.62
1:A:3912:GLY:O	1:A:3915:PHE:CE2	2.53	0.62
1:A:3303:LYS:HD2	1:A:3306:TRP:CD1	2.33	0.62
1:A:3307:LEU:HA	1:A:3310:THR:HB	1.81	0.62
1:B:2420:PRO:HD3	1:B:2536:ASN:HD21	1.65	0.62
1:A:2394:THR:H	1:A:2397:THR:HB	1.64	0.62
1:A:2386:MET:CB	1:A:2627:ARG:CD	2.77	0.62
1:A:1970:LEU:CD1	1:A:1974:LYS:HE3	2.24	0.62
1:B:1391:GLY:HA3	1:B:1484:LYS:NZ	2.14	0.62
1:A:1421:TYR:CD2	1:A:1425:GLU:HB2	2.33	0.62
1:B:3839:ILE:CG2	1:B:3873:MET:HG3	2.29	0.62
1:A:1748:PHE:CD2	1:A:1755:LEU:HD22	2.34	0.62
1:B:2111:LYS:HZ2	1:B:2161:GLU:HG2	1.62	0.62
1:B:2473:LEU:HD11	1:B:2527:GLU:HG3	1.81	0.62
1:A:1996:GLU:O	1:A:2000:ARG:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1938:GLY:O	1:B:1989:GLU:HB3	1.99	0.62
1:B:2472:THR:HG21	1:B:2524:VAL:CG2	2.30	0.62
1:A:2563:SER:CB	1:A:2566:SER:OG	2.47	0.62
1:B:2563:SER:CB	1:B:2566:SER:OG	2.48	0.62
1:B:3925:SER:HB2	1:B:3972:LEU:HD13	1.82	0.62
1:A:3583:LEU:O	1:A:3587:LEU:HG	2.00	0.62
1:B:1540:LEU:HD12	1:B:1548:ILE:CD1	2.29	0.62
1:A:1692:ASP:O	1:A:1695:LYS:HB3	2.00	0.62
1:B:3330:TYR:CE2	1:B:3346:LEU:HD13	2.34	0.61
1:B:3979:ASN:C	1:B:3981:PRO:HD2	2.20	0.61
1:B:2728:LEU:HD12	1:B:2728:LEU:O	1.99	0.61
1:B:3541:MET:HA	1:B:3544:LYS:HG2	1.82	0.61
1:B:2064:GLN:NE2	1:B:2091:MET:SD	2.73	0.61
1:B:1801:GLY:N	3:B:5096:SO4:O2	2.29	0.61
1:A:1574:PHE:HB3	1:A:1576:GLU:H	1.65	0.61
1:B:1744:LEU:HD22	1:B:1760:PHE:CD2	2.36	0.61
1:A:1531:ARG:HG2	1:A:1537:PHE:HB3	1.82	0.61
1:B:2508:GLN:HG3	1:B:2512:LYS:HD2	1.81	0.61
1:B:3736:LEU:HD11	1:B:3745:ARG:HG3	1.82	0.61
1:B:1616:LYS:HE3	1:B:1761:GLU:HG3	1.82	0.61
1:B:1493:LEU:HD23	1:B:1498:GLU:CB	2.29	0.61
1:A:1983:LEU:HD21	1:A:2000:ARG:CD	2.31	0.61
1:B:1744:LEU:HA	1:B:1760:PHE:HE2	1.61	0.61
1:B:1365:PHE:C	1:B:1366:VAL:CG2	2.68	0.61
1:A:1967:HIS:O	1:A:1968:PHE:HD1	1.82	0.61
1:B:1703:VAL:HG13	1:B:1770:ILE:HD13	1.83	0.61
1:B:2960:THR:HB	1:B:2963:ASP:HB2	1.82	0.61
1:B:2472:THR:CG2	1:B:2524:VAL:CG2	2.77	0.61
1:A:3530:PHE:CE1	1:A:3618:TYR:CD2	2.88	0.61
1:B:2495:ASP:O	1:B:2498:GLY:N	2.34	0.61
1:B:2786:ILE:O	1:B:3460:PRO:HB2	1.99	0.61
1:A:4065:LEU:HD11	1:A:4070:ILE:CD1	2.29	0.61
1:A:2421:GLY:N	3:A:5094:SO4:O1	2.31	0.61
1:A:2339:ILE:HG23	1:A:2353:LEU:HB3	1.83	0.61
1:A:3429:LEU:HD21	1:A:3439:ARG:HB3	1.83	0.61
1:A:2785:LYS:HD3	1:A:3482:GLY:O	2.01	0.61
1:A:3541:MET:HA	1:A:3544:LYS:HG2	1.83	0.61
1:B:2473:LEU:HD22	1:B:2475:PRO:HD3	1.82	0.61
1:A:2427:ILE:HD12	1:A:2559:LEU:CD2	2.31	0.61
1:A:3330:TYR:CE2	1:A:3346:LEU:HD13	2.36	0.61
1:A:1469:LEU:HD13	1:A:1523:LEU:HD21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2386:MET:HB2	1:B:2627:ARG:HD3	1.83	0.61
1:B:1612:ASP:HA	1:B:1615:ILE:HD11	1.83	0.61
1:B:1852:ARG:HG3	1:B:1852:ARG:O	2.01	0.60
1:A:1540:LEU:HD12	1:A:1548:ILE:CD1	2.31	0.60
1:A:2293:HIS:CE1	1:A:2409:ASN:CB	2.84	0.60
1:B:1692:ASP:O	1:B:1695:LYS:HB3	2.01	0.60
1:B:3612:ASP:O	1:B:3615:VAL:HG22	2.00	0.60
1:B:3429:LEU:HD21	1:B:3439:ARG:HB3	1.82	0.60
1:A:1527:LEU:HD23	1:A:1545:LEU:HD22	1.83	0.60
1:A:1656:TRP:O	1:A:1660:VAL:HG12	2.01	0.60
1:B:2424:LYS:HA	1:B:2559:LEU:HD12	1.81	0.60
1:B:2445:PHE:HA	1:B:2449:THR:HG21	1.83	0.60
1:B:3700:MET:HB3	1:B:4085:THR:HG21	1.82	0.60
1:B:3330:TYR:CE1	1:B:3334:PHE:CD2	2.89	0.60
1:A:1462:ASN:CB	1:A:1465:ILE:HG22	2.31	0.60
1:B:3911:TRP:HH2	1:B:3926:VAL:HG12	1.65	0.60
1:B:2838:ALA:HB3	1:B:2878:VAL:HG13	1.83	0.60
1:B:1469:LEU:HD13	1:B:1523:LEU:CD2	2.31	0.60
1:B:3350:LYS:HA	1:B:3353:LEU:HD12	1.84	0.60
1:A:2380:LEU:HD11	1:A:2390:ILE:HD11	1.83	0.60
1:B:2332:GLY:HA2	1:B:2335:GLN:CB	2.27	0.60
1:B:3737:THR:HB	1:B:3740:THR:CB	2.31	0.60
1:A:1969:GLY:O	1:A:1972:THR:HB	2.01	0.60
1:A:1851:ASN:HD21	1:A:1899:ASN:HB2	1.66	0.60
1:A:1409:LEU:HD21	1:A:1435:LEU:HB2	1.79	0.60
1:A:3817:GLY:H	1:A:3821:ASN:HB2	1.66	0.60
1:A:2282:ASN:HB3	1:A:2552:ARG:HG3	1.81	0.60
1:B:3702:MET:HB3	1:B:3767:PHE:HZ	1.67	0.60
1:B:1620:PHE:CZ	1:B:1743:ASP:HB3	2.35	0.60
1:B:3459:ASP:OD2	1:B:3461:ILE:HG12	2.01	0.60
1:B:2637:PRO:O	1:B:2639:GLN:NE2	2.35	0.60
1:B:2125:TRP:CZ2	1:B:2178:LEU:HD13	2.36	0.60
1:B:1991:GLU:O	1:B:1995:VAL:HG23	2.02	0.60
1:A:1536:ARG:HD2	1:A:1565:MET:O	2.02	0.60
1:A:2081:THR:O	1:A:2085:LYS:HB2	2.02	0.60
1:A:3509:LEU:HD12	1:A:3513:VAL:HG21	1.75	0.60
1:A:1391:GLY:HA3	1:A:1484:LYS:NZ	2.17	0.60
1:B:3855:LEU:HD12	1:B:3859:VAL:HG23	1.83	0.60
1:B:4065:LEU:HD11	1:B:4070:ILE:HD11	1.84	0.60
1:B:3509:LEU:CD1	1:B:3513:VAL:CG2	2.79	0.59
1:A:3886:ALA:N	1:A:3887:PRO:HD2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3919:LYS:NZ	1:B:4038:GLU:CG	2.65	0.59
1:A:3948:HIS:NE2	1:A:4072:ASN:CG	2.55	0.59
1:A:162:LEU:HA	1:A:165:ASP:O	2.02	0.59
1:A:1425:GLU:OE1	1:A:1426:GLN:N	2.36	0.59
1:A:2354:SER:OG	1:A:2357:SER:HB2	2.02	0.59
1:B:3692:LYS:HE3	1:B:3898:GLU:HB3	1.84	0.59
1:A:1534:PHE:HD2	1:A:1537:PHE:CE1	2.21	0.59
1:A:2755:HIS:NE2	1:A:2835:LEU:HG	2.17	0.59
1:B:3845:GLN:OE1	1:B:3878:HIS:HB2	2.01	0.59
1:A:2941:THR:HG22	1:A:2942:ASP:H	1.67	0.59
1:A:3537:GLU:OE1	1:A:3618:TYR:OH	2.21	0.59
1:A:1421:TYR:CE2	1:A:1425:GLU:HG3	2.37	0.59
1:A:3851:VAL:HG13	1:A:3855:LEU:HD23	1.85	0.59
1:A:2728:LEU:HD12	1:A:2771:ARG:NH2	2.17	0.59
1:A:3945:LEU:O	1:A:3948:HIS:O	2.21	0.59
1:B:2723:PHE:O	1:B:2727:GLU:HB2	2.02	0.59
1:B:2842:ASP:O	1:B:2845:GLN:HG2	2.02	0.59
1:A:2677:VAL:HG11	1:A:2686:LEU:HD21	1.83	0.59
1:A:1620:PHE:HA	1:A:1760:PHE:CE1	2.37	0.59
1:B:1536:ARG:HD2	1:B:1565:MET:O	2.02	0.59
1:A:1900:PRO:HB3	1:A:1905:ARG:HA	1.83	0.59
1:A:2787:HIS:CA	1:A:3460:PRO:HG2	2.32	0.59
1:A:1630:ILE:CG2	1:A:1655:MET:SD	2.89	0.59
1:A:1394:LEU:CD2	1:A:1449:GLN:HE22	2.14	0.59
1:A:2784:PRO:HG2	1:A:2817:ILE:HD13	1.84	0.59
1:A:2034:ILE:HD12	1:A:2061:TYR:CZ	2.38	0.59
1:B:1911:ASN:OD1	1:B:1912:LEU:N	2.36	0.59
1:A:3810:SER:O	1:A:3838:TRP:HB2	2.03	0.59
1:A:2489:ILE:HG22	1:A:2535:CYS:HB3	1.84	0.59
1:B:1998:LEU:HD11	1:B:2022:PHE:HZ	1.67	0.59
1:B:2707:VAL:HG12	1:B:2712:LEU:CD1	2.33	0.59
1:A:1536:ARG:HD3	1:A:1841:ILE:HD13	1.85	0.59
1:B:2290:LEU:HD23	1:B:2321:SER:HA	1.83	0.59
1:A:4033:LEU:HD12	1:A:4035:GLN:N	2.18	0.58
1:A:3737:THR:HB	1:A:3740:THR:CB	2.33	0.58
1:B:2293:HIS:CE1	1:B:2409:ASN:CB	2.86	0.58
1:B:2761:ALA:O	1:B:2892:CYS:HB3	2.02	0.58
1:B:2780:LYS:HD3	1:B:2813:THR:HG22	1.85	0.58
1:A:2549:ARG:HE	2:A:5093:ATP:PG	2.25	0.58
1:B:1910:GLU:HB2	1:B:3846:MET:CB	2.33	0.58
1:B:3566:LEU:CA	1:B:3583:LEU:HD21	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2332:GLY:HA2	1:A:2335:GLN:CB	2.31	0.58
1:B:1900:PRO:HB3	1:B:1905:ARG:HA	1.85	0.58
1:B:3618:TYR:O	1:B:3622:GLY:N	2.33	0.58
1:B:3919:LYS:HZ3	1:B:4038:GLU:CG	2.16	0.58
1:B:3583:LEU:O	1:B:3587:LEU:HG	2.04	0.58
1:A:1984:ILE:HG21	1:A:1989:GLU:HG3	1.84	0.58
1:B:3978:ASN:O	1:B:3981:PRO:CD	2.51	0.58
1:A:2640:THR:HG23	1:A:2643:SER:H	1.67	0.58
1:B:1744:LEU:HD22	1:B:1760:PHE:CG	2.39	0.58
1:B:3525:ILE:HD11	1:B:3646:ILE:CG2	2.16	0.58
1:A:2745:ILE:HG12	1:A:2756:MET:HE3	1.85	0.58
1:A:2446:SER:H	1:A:2449:THR:HG21	1.67	0.58
1:B:1849:GLU:OE2	1:B:1899:ASN:ND2	2.36	0.58
1:B:3330:TYR:CD1	1:B:3334:PHE:CD2	2.92	0.58
1:B:3631:MET:HE1	1:B:3698:MET:HG3	1.84	0.58
1:A:2155:ASP:OD1	1:A:2549:ARG:NH2	2.35	0.58
1:A:3592:LYS:O	1:A:3596:ASN:HB2	2.03	0.58
1:B:1394:LEU:HD22	1:B:1449:GLN:NE2	2.18	0.58
1:B:1620:PHE:CA	1:B:1760:PHE:CE1	2.86	0.58
1:B:3537:GLU:OE1	1:B:3618:TYR:OH	2.20	0.58
1:B:2472:THR:CB	1:B:2524:VAL:HG22	2.34	0.58
1:B:3912:GLY:O	1:B:3915:PHE:CE2	2.57	0.58
1:A:1779:PHE:O	1:A:1783:THR:HG22	2.03	0.58
1:B:4084:SER:O	1:B:4088:LEU:HG	2.03	0.58
1:B:1967:HIS:O	1:B:1968:PHE:HD1	1.86	0.58
1:B:3440:LEU:CD2	1:B:3462:ILE:HD12	2.33	0.58
1:B:1726:LEU:CD1	1:B:3984:GLN:CB	2.79	0.58
1:B:3330:TYR:OH	1:B:3346:LEU:HD13	2.04	0.58
1:B:3612:ASP:O	1:B:3615:VAL:CG2	2.52	0.58
1:B:162:LEU:HA	1:B:165:ASP:O	2.04	0.58
1:B:3683:TYR:O	1:B:3687:SER:HB2	2.04	0.58
1:A:1704:GLU:OE2	1:A:1768:ARG:NH1	2.37	0.57
1:B:2627:ARG:NH1	1:B:2630:TYR:HE2	1.98	0.57
1:B:2127:ASP:O	1:B:2131:THR:OG1	2.22	0.57
1:B:1750:SER:HB2	1:B:1755:LEU:CD2	2.34	0.57
1:A:2846:GLY:O	1:A:2849:TYR:HB3	2.04	0.57
1:B:2111:LYS:HZ3	1:B:2161:GLU:HG2	1.68	0.57
1:B:1826:PHE:CE1	1:B:1853:LEU:HD22	2.39	0.57
1:A:3839:ILE:HG23	1:A:3873:MET:HG3	1.86	0.57
1:A:2201:HIS:NE2	1:A:2497:TYR:O	2.37	0.57
1:A:3912:GLY:O	1:A:3915:PHE:CZ	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1981:SER:HB3	1:B:1982:PRO:HD3	1.87	0.57
1:A:1781:THR:HG21	1:A:1919:PHE:CD1	2.39	0.57
1:B:2891:ILE:HD11	1:B:2903:ILE:HD11	1.84	0.57
1:A:3303:LYS:C	1:A:3306:TRP:CD1	2.74	0.57
1:B:1940:GLU:HG3	1:B:1941:ASP:H	1.69	0.57
1:B:2627:ARG:HH11	1:B:2631:THR:HG23	1.64	0.57
1:B:2131:THR:HG22	1:B:2176:LEU:CD2	2.30	0.57
1:A:2257:PHE:HD1	1:A:2262:LEU:HD11	1.69	0.57
1:A:2808:LEU:HD21	1:A:2856:LEU:HD12	1.86	0.57
1:A:2437:LEU:H	1:A:2437:LEU:HD12	1.69	0.57
1:A:2137:VAL:O	1:A:2141:ILE:CG2	2.50	0.57
1:A:2476:LYS:CD	1:A:2476:LYS:N	2.52	0.57
1:A:1493:LEU:O	1:A:1494:ASP:HB2	2.04	0.57
1:B:1683:LEU:HB3	1:B:1702:LEU:HD21	1.85	0.57
1:B:2302:PHE:HA	1:B:2310:LEU:HD11	1.85	0.57
1:A:3555:TYR:HE1	1:A:3593:GLU:HG2	1.68	0.57
1:A:3519:VAL:HG13	1:A:3521:ASN:ND2	2.19	0.57
1:A:2111:LYS:CD	1:A:2161:GLU:HG3	2.13	0.57
1:B:1849:GLU:CG	1:B:1899:ASN:HD22	2.18	0.57
1:A:1394:LEU:HD22	1:A:1449:GLN:NE2	2.19	0.57
1:A:1965:HIS:HD2	1:A:2212:LEU:CD2	2.18	0.57
1:A:3618:TYR:O	1:A:3622:GLY:N	2.34	0.57
1:A:3303:LYS:HA	1:A:3306:TRP:HE1	1.67	0.57
1:A:2380:LEU:HD13	1:A:2390:ILE:CD1	2.23	0.57
1:A:2563:SER:CB	1:A:2566:SER:H	2.15	0.57
1:A:4024:VAL:HG11	1:A:4062:TRP:CD2	2.38	0.57
1:A:1559:SER:HB3	1:A:1572:ILE:HG22	1.86	0.57
1:B:1620:PHE:CB	1:B:1760:PHE:CE1	2.88	0.57
1:B:3995:GLY:HA2	1:B:3998:ILE:HD13	1.86	0.57
1:B:2473:LEU:HG	1:B:2525:THR:O	2.05	0.57
1:B:2472:THR:HG22	1:B:2524:VAL:HG13	1.86	0.57
1:A:2419:PRO:O	1:A:2424:LYS:CE	2.52	0.57
1:B:3785:TYR:HE2	1:B:3859:VAL:HG22	1.69	0.57
1:A:2048:SER:H	2:A:5093:ATP:HN62	1.52	0.57
1:B:3784:ASN:ND2	1:B:3865:ALA:O	2.37	0.57
1:B:2382:ALA:O	1:B:2385:VAL:HG12	2.04	0.57
1:A:4021:LEU:HD23	1:A:4023:ILE:HG13	1.85	0.57
1:A:1940:GLU:HG3	1:A:1941:ASP:N	2.18	0.57
1:A:1706:LEU:HD21	1:A:1935:GLN:HG2	1.86	0.57
1:A:1469:LEU:HB3	1:A:1472:GLU:HB2	1.87	0.57
1:B:2293:HIS:NE2	1:B:2409:ASN:HB3	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3566:LEU:HD13	1:A:3570:LEU:HD11	1.86	0.57
1:A:3538:ASN:HB3	1:A:3541:MET:HG2	1.87	0.57
1:A:2071:ILE:HB	1:A:2212:LEU:HD12	1.85	0.57
1:A:1911:ASN:OD1	1:A:1912:LEU:N	2.38	0.56
1:A:2127:ASP:O	1:A:2131:THR:OG1	2.23	0.56
1:B:2106:THR:HG1	1:B:2154:PHE:HB3	1.68	0.56
1:A:4017:GLY:HA3	1:A:4021:LEU:HD12	1.87	0.56
1:B:2755:HIS:NE2	1:B:2835:LEU:HG	2.20	0.56
1:A:3939:ILE:HG13	1:A:4010:LEU:HD22	1.86	0.56
1:B:2063:MET:HB3	1:B:2070:LEU:HD11	1.86	0.56
1:A:3833:LYS:HZ3	1:A:3862:THR:HG21	1.70	0.56
1:A:2241:LEU:HD13	1:A:2299:ARG:HH11	1.68	0.56
1:B:3409:ASP:HB3	1:B:3518:PHE:HB2	1.87	0.56
1:A:1620:PHE:CZ	1:A:1743:ASP:HB3	2.40	0.56
1:A:1995:VAL:HG22	1:A:2022:PHE:CD2	2.40	0.56
1:B:1531:ARG:HG2	1:B:1537:PHE:CB	2.36	0.56
1:A:3631:MET:CE	1:A:3698:MET:HG3	2.36	0.56
1:A:2938:MET:SD	1:A:3321:ILE:HG21	2.45	0.56
1:A:4022:GLN:HG2	1:A:4022:GLN:O	2.05	0.56
1:A:1939:PHE:O	1:A:1940:GLU:HB3	2.05	0.56
1:B:2512:LYS:O	1:B:2513:GLN:CB	2.52	0.56
1:B:1748:PHE:HD2	1:B:1755:LEU:HD22	1.69	0.56
1:A:1726:LEU:CD1	1:A:3984:GLN:HB3	2.30	0.56
1:B:1493:LEU:HD23	1:B:1498:GLU:HB3	1.86	0.56
1:B:3017:VAL:HG21	1:B:3313:PHE:CE2	2.41	0.56
1:B:1462:ASN:HB2	1:B:1465:ILE:HG22	1.88	0.56
1:A:2627:ARG:NH1	1:A:2630:TYR:CE2	2.74	0.56
1:B:2380:LEU:HD12	1:B:2577:ALA:CB	2.31	0.56
1:B:1493:LEU:O	1:B:1494:ASP:HB2	2.06	0.56
1:B:1995:VAL:HG22	1:B:2022:PHE:CE2	2.41	0.56
1:A:3509:LEU:HD12	1:A:3513:VAL:HG23	1.88	0.56
1:B:1392:LEU:HD13	1:B:1393:LYS:C	2.26	0.56
1:A:1619:VAL:HG12	1:A:1760:PHE:HD1	1.70	0.56
1:B:3785:TYR:CE2	1:B:3859:VAL:HG22	2.41	0.56
1:A:2305:LEU:HD11	1:A:2368:PHE:CD1	2.41	0.56
1:A:2868:ASP:HB2	1:A:2872:GLU:OE1	2.06	0.56
1:B:1998:LEU:CD1	1:B:2022:PHE:HZ	2.18	0.56
1:B:3919:LYS:NZ	1:B:4038:GLU:HG3	2.21	0.55
1:A:1497:ILE:O	1:A:1500:ILE:HG12	2.05	0.55
1:A:2514:GLY:C	1:A:2523:TRP:CH2	2.80	0.55
1:B:3737:THR:CB	1:B:3740:THR:HB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2489:ILE:HD11	1:B:2506:LEU:HD13	1.88	0.55
1:A:2111:LYS:HZ2	1:A:2161:GLU:HG2	1.67	0.55
1:A:1983:LEU:HB3	1:A:1993:THR:CG2	2.36	0.55
1:A:2220:CYS:SG	1:A:2224:SER:CB	2.94	0.55
1:B:3911:TRP:HH2	1:B:3926:VAL:CG1	2.19	0.55
1:B:1646:GLN:NE2	1:B:1758:TYR:OH	2.40	0.55
1:A:2386:MET:HB3	1:A:2627:ARG:CD	2.36	0.55
1:A:3683:TYR:O	1:A:3687:SER:HB2	2.07	0.55
1:B:3645:SER:CB	1:B:3890:GLN:NE2	2.69	0.55
1:A:2002:ILE:HB	1:A:2014:PHE:CE2	2.42	0.55
1:B:2336:ARG:HA	1:B:2339:ILE:HD12	1.88	0.55
1:B:2362:ALA:HB3	1:B:2365:LYS:O	2.07	0.55
1:A:1425:GLU:OE1	1:A:1429:LEU:HD12	2.06	0.55
1:A:1527:LEU:HD21	1:A:1546:LEU:CD2	2.36	0.55
1:B:3845:GLN:NE2	1:B:3882:ASP:O	2.39	0.55
1:B:2155:ASP:OD1	1:B:2549:ARG:NH2	2.40	0.55
1:B:3787:THR:HG22	1:B:3875:MET:HB2	1.88	0.55
1:B:2109:LEU:CD1	1:B:2129:LEU:HD23	2.36	0.55
1:B:1563:LYS:HE2	1:B:1585:VAL:HG12	1.87	0.55
1:A:4037:SER:HB3	1:A:4040:GLU:HB3	1.87	0.55
1:A:2410:SER:O	1:A:2411:LYS:HB2	2.06	0.55
1:A:1365:PHE:C	1:A:1366:VAL:HG23	2.27	0.55
1:A:2763:ARG:N	3:A:5095:SO4:O1	2.38	0.55
1:A:2151:TRP:CE3	1:A:2193:LEU:HD11	2.41	0.55
1:A:2788:ARG:HG3	1:A:3459:ASP:HA	1.89	0.55
1:B:115:GLU:CB	1:B:1372:ASN:OD1	2.55	0.55
1:A:1531:ARG:HD3	1:A:1537:PHE:O	2.07	0.55
1:A:1535:PRO:O	1:A:1841:ILE:CD1	2.55	0.55
1:B:2447:LYS:HE3	1:B:2493:LYS:HD3	1.89	0.55
1:A:2064:GLN:CD	1:A:2091:MET:CE	2.75	0.55
1:B:1421:TYR:O	1:B:1425:GLU:N	2.40	0.55
1:A:1502:ILE:HG23	1:A:1503:PRO:HD2	1.89	0.55
1:A:2078:CYS:N	2:A:5093:ATP:O2B	2.31	0.55
1:A:4023:ILE:HD12	1:A:4029:ILE:HD11	1.87	0.55
1:B:4024:VAL:HG11	1:B:4062:TRP:CD2	2.42	0.55
1:A:3440:LEU:HD23	1:A:3462:ILE:HD12	1.88	0.55
1:A:2786:ILE:O	1:A:3460:PRO:HB2	2.07	0.54
1:A:1627:LEU:HD11	1:A:1631:LYS:HE3	1.89	0.54
1:A:2002:ILE:HG22	1:A:2006:LEU:HD11	1.88	0.54
1:A:2400:HIS:NE2	1:A:2559:LEU:CD1	2.67	0.54
1:B:2476:LYS:N	1:B:2476:LYS:CD	2.63	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2131:THR:HG22	1:A:2176:LEU:CD2	2.34	0.54
1:A:2336:ARG:CD	1:A:2355:ASP:OD2	2.51	0.54
1:A:2707:VAL:HG12	1:A:2712:LEU:CD1	2.37	0.54
1:A:1823:ASP:HB2	1:A:1853:LEU:HD23	1.88	0.54
1:B:1956:LEU:CB	1:B:1968:PHE:CE2	2.88	0.54
1:B:1911:ASN:OD1	1:B:1912:LEU:HG	2.08	0.54
1:B:3737:THR:CB	1:B:3740:THR:CB	2.85	0.54
1:A:1940:GLU:CB	1:A:1989:GLU:O	2.51	0.54
1:B:3946:VAL:HA	1:B:3947:PRO:C	2.27	0.54
1:A:1535:PRO:O	1:A:1841:ILE:HD11	2.08	0.54
1:A:2112:GLU:CB	1:A:2117:SER:HB2	2.35	0.54
1:A:1604:ALA:HA	1:A:1607:TRP:HE1	1.72	0.54
1:A:3566:LEU:CA	1:A:3583:LEU:HD21	2.37	0.54
1:A:2201:HIS:CE1	1:A:2497:TYR:CA	2.91	0.54
1:B:1462:ASN:CB	1:B:1465:ILE:HG22	2.37	0.54
1:B:3924:TRP:O	1:B:3927:TYR:HB3	2.08	0.54
1:A:1392:LEU:HD13	1:A:1393:LYS:C	2.27	0.54
1:B:1421:TYR:CD2	1:B:1425:GLU:HB2	2.42	0.54
1:B:1394:LEU:CD2	1:B:1449:GLN:HE22	2.20	0.54
1:A:2063:MET:HB3	1:A:2070:LEU:HD11	1.90	0.54
1:A:1852:ARG:O	1:A:1852:ARG:HG3	2.06	0.54
1:B:1983:LEU:HD21	1:B:2000:ARG:HE	1.66	0.54
1:B:3737:THR:OG1	1:B:3740:THR:CB	2.55	0.54
1:B:2761:ALA:O	1:B:2892:CYS:CB	2.55	0.54
1:B:2936:ILE:HG22	1:B:2962:ARG:HD3	1.89	0.54
1:A:2786:ILE:HG12	1:A:2821:ASN:HA	1.90	0.54
1:B:3645:SER:CB	1:B:3890:GLN:HE21	2.18	0.54
1:A:2181:GLY:C	1:A:2182:GLU:HG3	2.27	0.54
1:A:3877:CYS:SG	1:A:3884:LEU:CD2	2.96	0.54
1:A:2115:TYR:OH	1:A:2162:TYR:O	2.23	0.54
1:A:1386:ILE:CG2	1:A:1396:ARG:HD3	2.37	0.54
1:B:2274:HIS:CE1	1:B:2326:LEU:O	2.50	0.54
1:A:3645:SER:CB	1:A:3890:GLN:HE21	2.19	0.54
1:B:3330:TYR:CE1	1:B:3334:PHE:CE2	2.96	0.54
1:B:2960:THR:HG22	1:B:2961:ILE:N	2.23	0.54
1:A:2448:ASP:CB	1:A:2829:GLU:OE2	2.47	0.54
1:B:2151:TRP:HE3	1:B:2193:LEU:HD11	1.73	0.54
1:B:3810:SER:O	1:B:3838:TRP:HB2	2.07	0.54
1:B:3656:VAL:CG1	1:B:3677:LEU:HB3	2.38	0.54
1:B:1527:LEU:HD21	1:B:1546:LEU:HD21	1.88	0.54
1:B:2728:LEU:HG	1:B:2771:ARG:HH22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3323:ASN:HD21	1:B:3361:ASP:H	1.56	0.54
1:A:2707:VAL:HG12	1:A:2712:LEU:HD12	1.89	0.53
1:A:1645:PHE:CZ	1:A:1649:LEU:HD22	2.43	0.53
1:B:1823:ASP:HB2	1:B:1853:LEU:HD23	1.90	0.53
1:A:2064:GLN:OE1	1:A:2151:TRP:CH2	2.55	0.53
1:B:2220:CYS:SG	1:B:2224:SER:CB	2.96	0.53
1:A:4059:LEU:HA	1:A:4063:LEU:HD13	1.89	0.53
1:B:2835:LEU:HD23	1:B:2911:ARG:HB2	1.91	0.53
1:A:3307:LEU:O	1:A:3311:LYS:N	2.27	0.53
1:B:3854:TYR:O	1:B:3858:HIS:HB2	2.08	0.53
1:B:1759:LYS:HE3	1:B:1761:GLU:OE2	2.08	0.53
1:A:3440:LEU:CD2	1:A:3462:ILE:HD12	2.38	0.53
1:B:2074:GLY:O	1:B:2197:ASP:HA	2.09	0.53
1:B:3509:LEU:HD11	1:B:3513:VAL:HG21	1.90	0.53
1:A:2106:THR:HG1	1:A:2154:PHE:HB3	1.72	0.53
1:B:1953:LEU:HD11	1:B:1973:LEU:HB3	1.91	0.53
1:A:3703:PHE:CE1	1:A:3766:GLU:HG2	2.43	0.53
1:A:2141:ILE:HG22	1:A:2145:PHE:HB2	1.90	0.53
1:A:2305:LEU:CD1	1:A:2368:PHE:CD1	2.91	0.53
1:B:2741:HIS:HA	1:B:2744:ARG:HD2	1.89	0.53
1:B:1744:LEU:CD2	1:B:1760:PHE:CD2	2.92	0.53
1:B:2002:ILE:HB	1:B:2014:PHE:CE2	2.43	0.53
1:B:2181:GLY:O	1:B:2182:GLU:CG	2.57	0.53
1:B:3767:PHE:HB3	1:B:3769:VAL:HG23	1.90	0.53
1:A:3612:ASP:O	1:A:3615:VAL:HG22	2.08	0.53
1:A:1534:PHE:CE2	1:A:1536:ARG:HB2	2.43	0.53
1:A:2336:ARG:HG2	1:A:2355:ASP:OD1	2.08	0.53
1:A:2419:PRO:O	1:A:2424:LYS:NZ	2.42	0.53
1:A:3017:VAL:HG21	1:A:3313:PHE:CE2	2.44	0.53
1:B:2201:HIS:CE1	1:B:2497:TYR:HA	2.44	0.53
1:A:1409:LEU:CD2	1:A:1435:LEU:HB2	2.39	0.53
1:A:1970:LEU:C	1:A:1970:LEU:HD12	2.28	0.53
1:B:3330:TYR:CZ	1:B:3346:LEU:HD13	2.44	0.53
1:A:3817:GLY:H	1:A:3821:ASN:CB	2.21	0.53
1:B:1914:LYS:HD3	1:B:3959:CYS:SG	2.48	0.53
1:A:2488:GLU:CD	1:A:2491:LEU:HD11	2.29	0.53
1:A:2177:THR:HG22	1:A:2183:ARG:HG2	1.91	0.53
1:A:2048:SER:H	2:A:5093:ATP:N6	2.06	0.53
1:A:2795:PHE:CE2	1:A:2799:LEU:HD11	2.44	0.53
1:B:1995:VAL:HG22	1:B:2022:PHE:CD2	2.44	0.52
1:A:1979:ASN:O	1:A:1983:LEU:HD13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2788:ARG:HB2	1:A:3459:ASP:HB3	1.90	0.52
1:A:2339:ILE:HG12	1:A:2353:LEU:HD23	1.90	0.52
1:A:2450:THR:H	1:A:2453:HIS:CE1	2.27	0.52
1:B:3308:ASN:O	1:B:3312:GLN:HB2	2.09	0.52
1:B:2476:LYS:H	1:B:2476:LYS:HD3	1.72	0.52
1:B:2201:HIS:NE2	1:B:2497:TYR:O	2.42	0.52
1:B:3772:TRP:HZ3	1:B:3780:ASN:HD22	1.56	0.52
1:A:1822:CYS:SG	1:A:1849:GLU:C	2.88	0.52
1:A:2787:HIS:HB3	1:A:3461:ILE:HG23	1.91	0.52
1:B:2493:LYS:HG3	1:B:2494:LEU:N	2.19	0.52
1:B:1822:CYS:HB2	1:B:1853:LEU:CD2	2.29	0.52
1:B:1939:PHE:HD1	1:B:1939:PHE:H	1.56	0.52
1:A:2173:ASN:HB3	1:A:2175:ILE:HG22	1.90	0.52
1:A:3877:CYS:SG	1:A:3884:LEU:HD22	2.50	0.52
1:A:2290:LEU:HD23	1:A:2321:SER:HA	1.92	0.52
1:A:4021:LEU:HD23	1:A:4023:ILE:CG1	2.39	0.52
1:A:1981:SER:HB3	1:A:1982:PRO:HD3	1.91	0.52
1:A:3692:LYS:HE3	1:A:3898:GLU:HB3	1.91	0.52
1:B:2860:THR:HG22	1:B:2865:LEU:O	2.09	0.52
1:A:2230:LEU:HD23	1:A:2288:VAL:HG13	1.90	0.52
1:B:3461:ILE:C	1:B:3463:SER:H	2.12	0.52
1:B:2173:ASN:HB3	1:B:2175:ILE:HG22	1.91	0.52
1:A:2285:GLU:CB	1:A:2412:ARG:NH2	2.73	0.52
1:B:2571:TYR:HA	1:B:2574:TYR:HB2	1.91	0.52
1:A:1486:ILE:HG12	1:A:1508:THR:HG21	1.91	0.52
1:B:3519:VAL:HG13	1:B:3521:ASN:ND2	2.24	0.52
1:A:2462:THR:HG22	1:A:2476:LYS:HA	1.90	0.52
1:A:2095:ASP:CG	1:A:2149:ARG:HH22	2.11	0.52
1:B:2220:CYS:SG	1:B:2224:SER:HB2	2.50	0.52
1:A:1926:SER:HA	1:A:1929:ILE:HD13	1.92	0.52
1:B:1392:LEU:C	1:B:1392:LEU:CD1	2.77	0.52
1:B:1365:PHE:C	1:B:1366:VAL:HG23	2.30	0.52
1:B:2109:LEU:HD13	1:B:2129:LEU:HD23	1.92	0.52
1:A:2012:LEU:HD13	1:A:2016:ASP:OD2	2.10	0.52
1:B:3641:PHE:HA	1:B:3889:LEU:HD21	1.91	0.52
1:A:3951:SER:HB2	1:A:4002:LYS:HD2	1.91	0.52
1:A:3547:ASP:HA	1:A:3550:LYS:HB3	1.90	0.52
1:A:4034:LEU:O	1:A:4034:LEU:HD23	2.10	0.52
1:A:3911:TRP:HH2	1:A:3926:VAL:CG1	2.23	0.52
1:A:1620:PHE:HA	1:A:1760:PHE:HE1	1.74	0.52
1:A:1536:ARG:HB3	1:A:1565:MET:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3656:VAL:CG1	1:A:3677:LEU:HB3	2.36	0.52
1:A:3995:GLY:HA2	1:A:3998:ILE:HD13	1.91	0.52
1:B:1394:LEU:HD22	1:B:1449:GLN:HE22	1.74	0.52
1:A:2833:THR:HG21	1:A:2841:PRO:HD2	1.91	0.52
1:A:2494:LEU:O	1:A:2494:LEU:HD12	2.10	0.52
1:B:1604:ALA:HA	1:B:1607:TRP:HE1	1.72	0.52
1:B:2631:THR:O	1:B:2635:THR:HG22	2.10	0.52
1:A:3854:TYR:O	1:A:3858:HIS:HB2	2.10	0.52
1:A:2578:ILE:HG21	1:A:2630:TYR:HB2	1.91	0.52
1:B:3460:PRO:O	1:B:3463:SER:CB	2.58	0.52
1:B:2064:GLN:NE2	1:B:2091:MET:HE1	2.24	0.52
1:B:1681:LYS:HE2	1:B:1939:PHE:CZ	2.44	0.52
1:A:1650:LEU:HD11	1:A:1747:VAL:HG11	1.92	0.52
1:B:2620:ARG:NH2	3:B:5095:SO4:O3	2.43	0.52
1:B:1983:LEU:HD11	1:B:2000:ARG:CD	2.39	0.51
1:B:2786:ILE:HG12	1:B:2821:ASN:HA	1.92	0.51
1:A:1963:MET:HB3	1:A:1966:TYR:CD2	2.45	0.51
1:A:2645:ILE:CD1	1:A:2686:LEU:HG	2.40	0.51
1:A:1514:ASP:O	1:A:1518:MET:HG3	2.10	0.51
1:A:1707:HIS:O	1:A:1711:VAL:HG23	2.10	0.51
1:A:1677:ASP:HA	1:A:1680:ILE:HD12	1.93	0.51
1:A:1645:PHE:HZ	1:A:1768:ARG:HD2	1.75	0.51
1:B:3978:ASN:O	1:B:3981:PRO:HD3	2.10	0.51
1:B:1781:THR:HG21	1:B:1919:PHE:CE1	2.45	0.51
1:B:1940:GLU:CB	1:B:1989:GLU:O	2.51	0.51
1:B:1469:LEU:HB3	1:B:1472:GLU:HB2	1.91	0.51
1:B:1707:HIS:O	1:B:1711:VAL:HG23	2.10	0.51
1:B:2061:TYR:O	1:B:2064:GLN:HG2	2.10	0.51
1:A:3737:THR:CB	1:A:3740:THR:CB	2.89	0.51
1:A:3737:THR:OG1	1:A:3740:THR:CB	2.59	0.51
1:B:2266:PHE:HD1	1:B:2326:LEU:HD21	1.76	0.51
1:B:1493:LEU:CD2	1:B:1498:GLU:HB3	2.41	0.51
1:A:2780:LYS:HD3	1:A:2813:THR:HG22	1.93	0.51
1:B:2312:ASP:HB3	1:B:2351:GLN:HG3	1.91	0.51
1:A:1939:PHE:HD1	1:A:1939:PHE:H	1.57	0.51
1:A:2302:PHE:HA	1:A:2310:LEU:HD11	1.92	0.51
1:A:65:THR:O	1:A:66:GLN:CB	2.59	0.51
1:B:2795:PHE:CE2	1:B:2799:LEU:HD11	2.46	0.51
1:B:2787:HIS:CA	1:B:3460:PRO:HG2	2.37	0.51
1:B:2034:ILE:CD1	1:B:2061:TYR:CE2	2.94	0.51
1:A:3946:VAL:HB	1:A:3947:PRO:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3645:SER:CB	1:A:3890:GLN:NE2	2.74	0.51
1:A:3839:ILE:CG2	1:A:3873:MET:HG3	2.41	0.51
1:A:3934:TRP:CB	1:A:4023:ILE:HD13	2.41	0.51
1:A:3787:THR:HG22	1:A:3875:MET:HB2	1.93	0.51
1:A:1749:ILE:HD13	1:A:1813:LEU:HD22	1.92	0.51
1:A:2427:ILE:HD12	1:A:2559:LEU:HD22	1.92	0.51
1:B:3509:LEU:O	1:B:3513:VAL:HG23	2.11	0.51
1:B:1606:GLU:O	1:B:1610:ILE:HG12	2.11	0.51
1:A:1917:ARG:HD2	1:A:3963:PHE:CE2	2.46	0.51
1:B:2708:ASN:O	1:B:2712:LEU:HD13	2.10	0.51
1:B:2464:TYR:HE1	1:B:2524:VAL:HG11	1.75	0.51
1:A:4065:LEU:O	1:A:4065:LEU:HD12	2.10	0.51
1:B:4022:GLN:HG2	1:B:4022:GLN:O	2.11	0.51
1:A:2084:TRP:HE3	1:A:2088:ILE:HD12	1.76	0.51
1:B:2448:ASP:HB2	1:B:2829:GLU:CD	2.31	0.51
1:B:4024:VAL:HG23	1:B:4027:VAL:H	1.75	0.51
1:A:2637:PRO:O	1:A:2639:GLN:NE2	2.44	0.51
1:A:1645:PHE:HB2	1:A:1697:LYS:HG3	1.91	0.51
1:B:2494:LEU:HD12	1:B:2494:LEU:O	2.11	0.51
1:B:2107:LYS:CE	1:B:2499:SER:HB3	2.40	0.51
1:B:2512:LYS:HB3	1:B:2523:TRP:CH2	2.40	0.51
1:A:2102:TYR:HB2	1:A:2152:VAL:HG22	1.93	0.51
1:A:1803:THR:HG21	1:A:1848:ASP:OD1	2.10	0.51
1:A:3566:LEU:HD11	1:A:3570:LEU:HD11	1.92	0.50
1:A:1706:LEU:HD22	1:A:1935:GLN:HG2	1.93	0.50
1:B:1635:ASP:HB2	1:B:1638:VAL:HG23	1.93	0.50
1:A:3845:GLN:OE1	1:A:3878:HIS:HB2	2.11	0.50
1:A:1606:GLU:O	1:A:1610:ILE:HG12	2.11	0.50
1:B:2640:THR:HG23	1:B:2643:SER:H	1.76	0.50
1:B:3307:LEU:HA	1:B:3310:THR:HB	1.92	0.50
1:B:1612:ASP:HA	1:B:1615:ILE:HG12	1.94	0.50
1:A:2422:SER:H	1:A:2424:LYS:HZ1	1.59	0.50
1:B:2201:HIS:CE1	1:B:2497:TYR:HB3	2.47	0.50
1:B:3547:ASP:HA	1:B:3550:LYS:HB3	1.92	0.50
1:B:1803:THR:HG21	1:B:1848:ASP:OD1	2.11	0.50
1:B:2627:ARG:HH12	1:B:2631:THR:HG22	1.73	0.50
1:B:1575:LEU:O	1:B:1576:GLU:HB3	2.11	0.50
1:B:1502:ILE:HG23	1:B:1503:PRO:HD2	1.93	0.50
1:A:3725:VAL:HG22	1:A:3731:ASP:HA	1.93	0.50
1:B:2488:GLU:CD	1:B:2491:LEU:HD11	2.32	0.50
1:B:1822:CYS:SG	1:B:1849:GLU:C	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2034:ILE:HD12	1:B:2061:TYR:CE2	2.46	0.50
1:A:2034:ILE:CD1	1:A:2061:TYR:CZ	2.95	0.50
1:B:2785:LYS:HE2	1:B:3480:GLU:OE1	2.11	0.50
1:B:2784:PRO:HG2	1:B:2817:ILE:HD13	1.93	0.50
1:A:2982:VAL:HG12	1:A:2983:GLY:N	2.27	0.50
1:B:1826:PHE:HE1	1:B:1853:LEU:HD22	1.76	0.50
1:B:2336:ARG:CD	1:B:2355:ASP:OD2	2.59	0.50
1:A:3911:TRP:HH2	1:A:3926:VAL:HG12	1.77	0.50
1:B:2354:SER:H	1:B:2357:SER:HB2	1.76	0.50
1:B:3671:VAL:O	1:B:3674:ILE:HG22	2.11	0.50
1:B:2749:LEU:HD12	1:B:2773:VAL:HG12	1.94	0.50
1:A:2111:LYS:CD	1:A:2161:GLU:CG	2.84	0.50
1:B:2707:VAL:HG12	1:B:2712:LEU:HD12	1.91	0.50
1:A:1849:GLU:CG	1:A:1899:ASN:ND2	2.70	0.50
1:A:1531:ARG:CD	1:A:1538:TYR:HA	2.42	0.50
1:B:2788:ARG:HG3	1:B:3459:ASP:HA	1.93	0.50
1:A:2034:ILE:CD1	1:A:2061:TYR:CE2	2.95	0.50
1:A:2645:ILE:HD11	1:A:2686:LEU:HG	1.94	0.50
1:B:3440:LEU:HD23	1:B:3462:ILE:HD12	1.93	0.50
1:A:2476:LYS:N	1:A:2476:LYS:HD3	2.09	0.50
1:A:3323:ASN:HD21	1:A:3361:ASP:H	1.58	0.50
1:A:1535:PRO:C	1:A:1841:ILE:CD1	2.75	0.50
1:B:2290:LEU:HD13	1:B:2407:LEU:HD23	1.93	0.50
1:A:2762:SER:O	1:A:2763:ARG:HB2	2.12	0.50
1:B:2262:LEU:HA	1:B:2265:ILE:HD12	1.94	0.50
1:A:1570:GLU:HB2	1:A:1585:VAL:HA	1.93	0.50
1:B:1387:GLU:HA	1:B:1393:LYS:HA	1.94	0.49
1:A:3692:LYS:HE3	1:A:3898:GLU:O	2.12	0.49
1:B:4020:ASN:HB3	1:B:4028:ARG:HH11	1.77	0.49
1:A:1983:LEU:HD21	1:A:2000:ARG:NE	2.27	0.49
1:A:2002:ILE:HB	1:A:2014:PHE:HE2	1.78	0.49
1:A:2385:VAL:HG23	1:A:2574:TYR:HD1	1.77	0.49
1:A:2654:ARG:HH22	1:A:2691:SER:HB2	1.77	0.49
1:A:1392:LEU:CD1	1:A:1392:LEU:C	2.78	0.49
1:B:3566:LEU:HD13	1:B:3570:LEU:HD12	1.94	0.49
1:A:3979:ASN:C	1:A:3981:PRO:CD	2.80	0.49
1:B:1995:VAL:HG21	1:B:2024:SER:HB3	1.93	0.49
1:A:1657:THR:HG21	1:A:1734:PHE:O	2.12	0.49
1:A:2295:ILE:HG12	1:A:2314:ILE:HD12	1.93	0.49
1:A:3353:LEU:HD23	1:A:3358:VAL:HG11	1.95	0.49
1:A:4033:LEU:HD12	1:A:4036:GLN:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1645:PHE:CD2	1:B:1765:ILE:HG22	2.47	0.49
1:A:1849:GLU:CG	1:A:1899:ASN:HD22	2.22	0.49
1:A:2064:GLN:NE2	1:A:2091:MET:CE	2.76	0.49
1:B:2105:ASP:OD2	1:B:2508:GLN:HB2	2.12	0.49
1:A:3566:LEU:HD13	1:A:3570:LEU:HD12	1.95	0.49
1:A:2960:THR:HG22	1:A:2961:ILE:N	2.27	0.49
1:A:3350:LYS:HA	1:A:3353:LEU:HD12	1.94	0.49
1:B:3319:GLU:HA	1:B:3359:LYS:O	2.13	0.49
1:A:1531:ARG:HG2	1:A:1537:PHE:CB	2.42	0.49
1:B:2552:ARG:NH2	2:B:5093:ATP:O2G	2.45	0.49
1:A:1421:TYR:CZ	1:A:1425:GLU:HG3	2.46	0.49
1:A:1540:LEU:HD11	1:A:1561:PHE:HB3	1.95	0.49
1:A:3848:LEU:HD12	1:A:3884:LEU:HD12	1.93	0.49
1:B:2170:LEU:HB3	1:B:2209:ARG:HD3	1.95	0.49
1:A:3855:LEU:HD12	1:A:3859:VAL:HG23	1.93	0.49
1:A:2514:GLY:CA	1:A:2523:TRP:CZ2	2.96	0.49
1:A:1626:CYS:SG	1:A:1639:VAL:CG1	3.01	0.49
1:A:1748:PHE:CE2	1:A:1755:LEU:HD22	2.47	0.49
1:B:2517:LYS:NZ	1:B:2520:GLU:OE1	2.45	0.49
1:B:3459:ASP:OD2	1:B:3461:ILE:CG1	2.60	0.49
1:A:2364:ASP:O	1:A:2365:LYS:HG2	2.13	0.49
1:A:2074:GLY:O	1:A:2197:ASP:HA	2.13	0.49
1:A:1448:VAL:HG22	1:A:1513:ILE:HB	1.94	0.49
1:B:1844:TRP:CD1	1:B:1893:ALA:HB3	2.48	0.49
1:B:1838:ILE:HG13	1:B:1843:ALA:HB3	1.95	0.49
1:B:2472:THR:HB	1:B:2524:VAL:HG22	1.94	0.49
1:A:3737:THR:HB	1:A:3740:THR:HG1	1.77	0.49
1:B:2385:VAL:O	1:B:2574:TYR:HE1	1.96	0.49
1:B:3817:GLY:H	1:B:3821:ASN:HB2	1.78	0.49
1:A:3481:ILE:O	1:A:3483:ASP:N	2.36	0.49
1:B:2095:ASP:CG	1:B:2149:ARG:NH2	2.66	0.49
1:A:3946:VAL:HA	1:A:3947:PRO:C	2.33	0.49
1:A:1626:CYS:HB2	1:A:1643:TYR:CD2	2.48	0.49
1:A:3889:LEU:HG	1:A:3894:ARG:HD3	1.95	0.49
1:B:3555:TYR:HE1	1:B:3593:GLU:HG2	1.77	0.49
1:B:1657:THR:HG21	1:B:1734:PHE:O	2.13	0.49
1:B:3460:PRO:O	1:B:3463:SER:HB3	2.13	0.48
1:A:3978:ASN:O	1:A:3981:PRO:CD	2.60	0.48
1:B:2760:GLY:O	1:B:2761:ALA:HB3	2.13	0.48
1:A:76:ASP:CB	1:B:85:PRO:CB	2.90	0.48
1:A:3671:VAL:O	1:A:3674:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2828:LEU:HD13	1:A:2902:MET:SD	2.53	0.48
1:B:2044:ARG:HH21	1:B:2093:ILE:HD11	1.76	0.48
1:B:2737:SER:HB2	1:B:2924:THR:HG21	1.95	0.48
1:A:1469:LEU:CD1	1:A:1523:LEU:HD21	2.43	0.48
1:A:1664:LEU:HD23	1:A:1669:PHE:HZ	1.77	0.48
1:A:1645:PHE:CD2	1:A:1765:ILE:HG22	2.48	0.48
1:B:2446:SER:H	1:B:2449:THR:HG21	1.74	0.48
1:A:2354:SER:OG	1:A:2357:SER:CB	2.61	0.48
1:A:2839:ASP:O	1:A:2841:PRO:HD3	2.12	0.48
1:B:23:LEU:O	1:B:24:GLU:CB	2.62	0.48
1:B:65:THR:O	1:B:66:GLN:CB	2.60	0.48
1:A:3737:THR:CB	1:A:3740:THR:HB	2.44	0.48
1:A:1911:ASN:OD1	1:A:1912:LEU:HG	2.13	0.48
1:B:3946:VAL:HB	1:B:3947:PRO:HA	1.95	0.48
1:B:2177:THR:HG22	1:B:2183:ARG:HG2	1.94	0.48
1:B:3810:SER:HB3	1:B:3837:GLY:HA2	1.96	0.48
1:A:2425:THR:HG23	3:A:5094:SO4:O2	2.14	0.48
1:B:2109:LEU:HD11	1:B:2129:LEU:CD2	2.44	0.48
1:B:2894:PRO:HG3	1:B:2916:TRP:CH2	2.49	0.48
1:B:2654:ARG:HH22	1:B:2691:SER:HB2	1.79	0.48
1:A:1794:PHE:HD1	1:A:1802:LYS:HB3	1.79	0.48
1:A:1683:LEU:HB3	1:A:1702:LEU:HD21	1.96	0.48
1:A:3721:THR:O	1:A:3725:VAL:HG23	2.14	0.48
1:B:2008:ASP:HA	1:B:2011:GLU:HB2	1.96	0.48
1:B:1531:ARG:HD3	1:B:1537:PHE:O	2.13	0.48
1:B:1559:SER:HB3	1:B:1572:ILE:HG22	1.96	0.48
1:A:3024:LEU:HD13	1:A:3303:LYS:HG3	1.92	0.48
1:B:2464:TYR:CE1	1:B:2524:VAL:HG11	2.48	0.48
1:B:2563:SER:CB	1:B:2566:SER:H	2.20	0.48
1:B:3979:ASN:C	1:B:3981:PRO:CD	2.81	0.48
1:B:3612:ASP:C	1:B:3615:VAL:HG22	2.34	0.48
1:A:2763:ARG:HA	3:A:5095:SO4:O1	2.14	0.48
1:B:3934:TRP:CB	1:B:4023:ILE:HD13	2.43	0.48
1:A:2109:LEU:HD13	1:A:2129:LEU:HD23	1.94	0.48
1:A:3690:LEU:HD23	1:A:3694:PHE:HB3	1.96	0.48
1:B:2655:ILE:HD11	1:B:2747:ARG:HH22	1.78	0.48
1:A:1826:PHE:CE1	1:A:1853:LEU:CD2	2.96	0.48
1:A:1967:HIS:NE2	1:A:2204:PRO:HB3	2.28	0.48
1:B:2380:LEU:HD12	1:B:2380:LEU:O	2.13	0.48
1:A:3541:MET:HB2	1:A:3607:PHE:HE1	1.78	0.48
1:A:2169:VAL:HG13	1:A:2186:ILE:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4059:LEU:HA	1:B:4063:LEU:HD13	1.95	0.48
1:A:2084:TRP:CZ3	1:A:2085:LYS:HG3	2.49	0.48
1:A:4065:LEU:HD12	1:A:4065:LEU:C	2.33	0.48
1:A:1421:TYR:CE2	1:A:1425:GLU:CG	2.96	0.48
1:B:3592:LYS:O	1:B:3596:ASN:N	2.46	0.48
1:B:3818:SER:O	1:B:3820:GLU:N	2.46	0.48
1:B:2027:THR:HA	1:B:2028:PRO:HD3	1.49	0.48
1:B:3461:ILE:C	1:B:3463:SER:N	2.66	0.48
1:B:3566:LEU:HD11	1:B:3570:LEU:HD11	1.94	0.48
1:A:1540:LEU:CD1	1:A:1548:ILE:HD12	2.41	0.48
1:B:1706:LEU:CD1	1:B:1936:ILE:HG12	2.43	0.48
1:B:1637:GLU:HG2	1:B:1686:LYS:HG3	1.96	0.48
1:A:2860:THR:HG22	1:A:2865:LEU:O	2.13	0.48
1:A:2741:HIS:O	1:A:2745:ILE:HG13	2.15	0.47
1:B:1540:LEU:HD11	1:B:1561:PHE:HB3	1.95	0.47
1:B:2316:LEU:HD13	1:B:2351:GLN:HB3	1.95	0.47
1:A:3373:LEU:O	1:A:3373:LEU:HD23	2.13	0.47
1:B:2514:GLY:HA3	1:B:2523:TRP:CZ2	2.49	0.47
1:B:1849:GLU:CG	1:B:1899:ASN:ND2	2.74	0.47
1:B:1534:PHE:HD2	1:B:1537:PHE:CE1	2.33	0.47
1:A:3459:ASP:OD2	1:A:3461:ILE:CG1	2.61	0.47
1:B:2220:CYS:SG	1:B:2221:SER:N	2.88	0.47
1:A:1683:LEU:HD22	1:A:1698:ILE:HG23	1.96	0.47
1:A:3703:PHE:HE1	1:A:3766:GLU:HG2	1.79	0.47
1:B:1781:THR:HG21	1:B:1919:PHE:CD1	2.49	0.47
1:B:1969:GLY:O	1:B:1972:THR:HB	2.14	0.47
1:B:2280:THR:HA	1:B:2283:LYS:HD2	1.95	0.47
1:A:2027:THR:HA	1:A:2028:PRO:HD3	1.48	0.47
1:A:1849:GLU:OE2	1:A:1899:ASN:ND2	2.47	0.47
1:B:1939:PHE:O	1:B:1940:GLU:HB3	2.14	0.47
1:A:1554:HIS:O	1:A:1555:HIS:HB2	2.15	0.47
1:B:2473:LEU:HD23	1:B:2475:PRO:N	2.29	0.47
1:B:1645:PHE:HB2	1:B:1697:LYS:HG3	1.97	0.47
1:B:1646:GLN:OE1	1:B:1763:ILE:HG12	2.14	0.47
1:B:4021:LEU:HD23	1:B:4023:ILE:CG1	2.45	0.47
1:B:2724:CYS:SG	1:B:2729:GLU:OE2	2.72	0.47
1:B:1620:PHE:HB2	1:B:1760:PHE:CZ	2.49	0.47
1:A:1542:ASN:O	1:A:1546:LEU:HG	2.14	0.47
1:A:1731:VAL:HG12	1:A:1732:GLN:N	2.28	0.47
1:B:1934:LEU:HD22	1:B:1945:LEU:HD12	1.97	0.47
1:B:1726:LEU:HD13	1:B:3984:GLN:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2380:LEU:C	1:B:2380:LEU:HD12	2.35	0.47
1:B:2761:ALA:O	1:B:2892:CYS:SG	2.72	0.47
1:B:2828:LEU:HD13	1:B:2902:MET:SD	2.54	0.47
1:B:40:TRP:O	1:B:44:LYS:N	2.47	0.47
1:B:3010:LEU:HD22	1:B:3320:LEU:HD12	1.96	0.47
1:A:4084:SER:O	1:A:4088:LEU:HG	2.14	0.47
1:B:2064:GLN:OE1	1:B:2151:TRP:HH2	1.98	0.47
1:A:2424:LYS:H	1:A:2424:LYS:HG3	1.52	0.47
1:B:2452:GLU:HA	1:B:2455:LEU:HD12	1.97	0.47
1:A:1636:ILE:O	1:A:1640:VAL:HG23	2.15	0.47
1:A:1386:ILE:HD12	1:A:1396:ARG:HH11	1.80	0.47
1:A:1681:LYS:HE2	1:A:1939:PHE:CE1	2.50	0.47
1:A:2517:LYS:NZ	1:A:2520:GLU:OE1	2.48	0.47
1:B:1392:LEU:HD13	1:B:1393:LYS:CA	2.45	0.47
1:A:3877:CYS:SG	1:A:3884:LEU:HD21	2.55	0.47
1:B:4021:LEU:HD23	1:B:4023:ILE:HG12	1.96	0.47
1:B:3818:SER:O	1:B:3821:ASN:N	2.43	0.47
1:A:1375:LYS:O	1:A:1379:LYS:HG2	2.15	0.47
1:B:2494:LEU:HB2	1:B:2499:SER:N	2.30	0.46
1:B:3306:TRP:HH2	1:B:3594:ALA:HB1	1.80	0.46
1:B:3509:LEU:CG	1:B:3513:VAL:HG21	2.45	0.46
1:A:3934:TRP:HB3	1:A:4023:ILE:HD13	1.97	0.46
1:A:2580:LYS:HG2	1:A:2586:ARG:HH22	1.79	0.46
1:B:1973:LEU:O	1:B:1977:LEU:HG	2.15	0.46
1:B:1459:LEU:HD23	1:B:1465:ILE:HG13	1.96	0.46
1:A:2358:THR:HG22	1:A:2359:ILE:N	2.29	0.46
1:B:2467:THR:O	1:B:2471:LEU:N	2.48	0.46
1:A:3967:TYR:HE2	1:A:3985:VAL:HA	1.80	0.46
1:B:1917:ARG:HD2	1:B:3963:PHE:CE2	2.50	0.46
1:A:2105:ASP:OD2	1:A:2508:GLN:HB2	2.15	0.46
1:B:1425:GLU:OE1	1:B:1425:GLU:C	2.53	0.46
1:A:1422:LYS:O	1:A:1425:GLU:HB3	2.15	0.46
1:B:3566:LEU:HA	1:B:3583:LEU:HD23	1.95	0.46
1:B:1929:ILE:HD12	1:B:1929:ILE:H	1.81	0.46
1:A:3995:GLY:HA2	1:A:3998:ILE:CD1	2.46	0.46
1:B:2252:LEU:HD22	1:B:2314:ILE:HG13	1.97	0.46
1:A:2763:ARG:CA	3:A:5095:SO4:O1	2.64	0.46
1:A:2878:VAL:HA	1:A:2881:ILE:HD12	1.97	0.46
1:A:2571:TYR:HA	1:A:2574:TYR:HB2	1.97	0.46
1:B:2849:TYR:O	1:B:2853:LEU:HB2	2.15	0.46
1:A:3592:LYS:O	1:A:3596:ASN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1694:VAL:HG23	1:B:1697:LYS:HE2	1.97	0.46
1:A:1409:LEU:CD2	1:A:1435:LEU:CB	2.82	0.46
1:A:2476:LYS:HZ2	1:A:2528:ARG:HB2	1.80	0.46
1:A:2445:PHE:HA	1:A:2449:THR:HG21	1.96	0.46
1:B:2201:HIS:CE1	1:B:2497:TYR:CA	2.98	0.46
1:A:3415:ILE:HD13	1:A:3453:GLN:HG3	1.97	0.46
1:B:2580:LYS:HG2	1:B:2586:ARG:HH22	1.79	0.46
1:A:3509:LEU:CG	1:A:3513:VAL:HG21	2.45	0.46
1:B:1984:ILE:CG2	1:B:1989:GLU:HG3	2.44	0.46
1:B:3509:LEU:HG	1:B:3513:VAL:HG21	1.96	0.46
1:A:2112:GLU:HB3	1:A:2117:SER:OG	2.16	0.46
1:A:2125:TRP:CZ2	1:A:2178:LEU:CD1	2.97	0.46
1:B:1611:LEU:O	1:B:1615:ILE:HG12	2.15	0.46
1:A:3924:TRP:O	1:A:3927:TYR:HB3	2.15	0.46
1:A:1995:VAL:HG22	1:A:2022:PHE:HE2	1.80	0.46
1:B:2988:SER:CB	1:B:2989:PRO:CD	2.85	0.46
1:A:2835:LEU:HD23	1:A:2911:ARG:HB2	1.97	0.46
1:A:1425:GLU:C	1:A:1425:GLU:OE1	2.54	0.46
1:B:2503:VAL:HA	1:B:2506:LEU:HD12	1.97	0.46
1:B:3541:MET:HB2	1:B:3607:PHE:HE1	1.81	0.46
1:A:2654:ARG:NH1	1:A:2658:ASP:OD1	2.49	0.46
1:B:1734:PHE:CD2	1:B:1749:ILE:HG12	2.50	0.46
1:A:40:TRP:O	1:A:44:LYS:N	2.49	0.46
1:A:1418:SER:HB2	1:A:3446:PHE:HB3	1.96	0.46
1:B:1827:ASP:HB3	1:B:1830:VAL:HG12	1.97	0.46
1:B:1421:TYR:CE2	1:B:1425:GLU:HG3	2.50	0.46
1:B:2099:ASN:HA	1:B:2149:ARG:O	2.16	0.46
1:A:2318:ILE:O	1:A:2322:LEU:HB2	2.16	0.46
1:B:1547:LYS:O	1:B:1551:SER:HB3	2.16	0.46
1:A:2627:ARG:NH1	1:A:2630:TYR:CD2	2.84	0.46
1:A:1527:LEU:HD21	1:A:1546:LEU:HD23	1.97	0.46
1:A:3612:ASP:O	1:A:3615:VAL:CG2	2.63	0.46
1:B:1612:ASP:HA	1:B:1615:ILE:CG1	2.46	0.46
1:A:1748:PHE:HD2	1:A:1755:LEU:HD22	1.77	0.46
1:A:3508:PHE:O	1:A:3512:ARG:HG2	2.16	0.46
1:B:3813:ILE:HG22	1:B:3840:LEU:HD23	1.98	0.46
1:A:1945:LEU:HD13	1:A:1994:VAL:HG21	1.98	0.45
1:A:1586:GLU:HG3	1:A:1765:ILE:H	1.81	0.45
1:B:1535:PRO:C	1:B:1841:ILE:CD1	2.75	0.45
1:A:1392:LEU:HD23	1:A:1484:LYS:HA	1.97	0.45
1:A:2204:PRO:HA	1:A:2207:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2785:LYS:NZ	1:B:3480:GLU:CD	2.69	0.45
1:A:1462:ASN:HB2	1:A:1465:ILE:CG2	2.44	0.45
1:A:1660:VAL:HG13	1:A:1728:TRP:CH2	2.51	0.45
1:A:3807:SER:O	1:A:3808:LYS:HB2	2.16	0.45
1:B:1992:LYS:HG2	1:B:2024:SER:HB2	1.88	0.45
1:A:2199:LEU:O	1:A:2201:HIS:N	2.49	0.45
1:B:2425:THR:HG23	3:B:5095:SO4:O2	2.17	0.45
1:B:1965:HIS:HD2	1:B:2212:LEU:HD21	1.81	0.45
1:A:1534:PHE:CD2	1:A:1537:PHE:CE1	3.02	0.45
1:B:1968:PHE:CD1	1:B:1968:PHE:N	2.84	0.45
1:B:1535:PRO:O	1:B:1841:ILE:HD11	2.14	0.45
1:A:2286:THR:HA	1:A:2412:ARG:NE	2.31	0.45
1:A:1844:TRP:CD1	1:A:1893:ALA:HB3	2.50	0.45
1:A:1951:HIS:O	1:A:1955:LEU:HB2	2.17	0.45
1:A:3330:TYR:CE1	1:A:3334:PHE:CD2	3.05	0.45
1:B:2354:SER:OG	1:B:2357:SER:HB2	2.16	0.45
1:A:2458:LEU:HG	1:A:2484:LEU:HD21	1.99	0.45
1:B:3462:ILE:O	1:B:3465:LEU:HB3	2.17	0.45
1:A:1387:GLU:HA	1:A:1393:LYS:HA	1.98	0.45
1:A:1391:GLY:HA3	1:A:1484:LYS:HZ1	1.82	0.45
1:B:1540:LEU:HD11	1:B:1548:ILE:HD11	1.99	0.45
1:B:2472:THR:HG22	1:B:2524:VAL:CG1	2.47	0.45
1:A:2766:LYS:CE	1:A:2890:THR:HB	2.39	0.45
1:A:2783:GLN:HG2	1:A:2816:ILE:HB	1.99	0.45
1:B:3343:ALA:O	1:B:3347:VAL:HG23	2.17	0.45
1:A:1822:CYS:HB2	1:A:1853:LEU:CD2	2.31	0.45
1:B:1826:PHE:O	1:B:1826:PHE:CG	2.70	0.45
1:B:1822:CYS:SG	1:B:1850:PHE:HA	2.56	0.45
1:B:1968:PHE:N	1:B:1968:PHE:HD1	2.15	0.45
1:B:1535:PRO:O	1:B:1841:ILE:CD1	2.65	0.45
1:B:3584:MET:HA	1:B:3587:LEU:HD12	1.98	0.45
1:A:1910:GLU:HB2	1:A:3846:MET:HA	1.98	0.45
1:B:1684:LEU:HD21	1:B:1936:ILE:O	2.16	0.45
1:B:1750:SER:CB	1:B:1755:LEU:HD23	2.46	0.45
1:B:1910:GLU:HB2	1:B:3846:MET:HB3	1.98	0.45
1:A:3470:PHE:CE1	1:A:3488:VAL:HG21	2.52	0.45
1:A:3308:ASN:O	1:A:3312:GLN:HB2	2.16	0.45
1:A:2494:LEU:HB2	1:A:2499:SER:N	2.32	0.45
1:A:2446:SER:N	1:A:2449:THR:HG23	2.19	0.45
1:A:3462:ILE:O	1:A:3465:LEU:N	2.45	0.45
1:A:2358:THR:CG2	1:A:2359:ILE:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2280:THR:HA	1:A:2283:LYS:HD2	1.99	0.45
1:A:1759:LYS:HE3	1:A:1761:GLU:OE2	2.17	0.45
1:B:1677:ASP:HA	1:B:1680:ILE:HD12	1.99	0.45
1:A:3832:SER:O	1:A:3836:GLY:N	2.45	0.45
1:A:3461:ILE:C	1:A:3463:SER:N	2.70	0.45
1:B:2552:ARG:HG2	1:B:2552:ARG:HH11	1.81	0.45
1:A:3010:LEU:HD22	1:A:3320:LEU:HD12	1.99	0.45
1:B:2354:SER:OG	1:B:2357:SER:CB	2.65	0.45
1:A:2984:VAL:C	1:A:2986:PRO:HD3	2.37	0.45
1:B:1656:TRP:HE1	1:B:1712:ILE:HD11	1.81	0.45
1:A:2707:VAL:HG11	1:A:2712:LEU:CD1	2.45	0.45
1:A:2386:MET:HB3	1:A:2627:ARG:NE	2.32	0.45
1:B:2081:THR:O	1:B:2085:LYS:HB2	2.17	0.45
1:A:1527:LEU:HD21	1:A:1546:LEU:HD21	1.98	0.45
1:A:1793:CYS:SG	1:A:1918:GLU:HG2	2.57	0.45
1:B:2039:LYS:HG2	1:B:2049:MET:HG3	1.98	0.45
1:B:3342:ARG:NH2	1:B:3393:ASN:OD1	2.47	0.45
1:B:2707:VAL:HG11	1:B:2712:LEU:HD12	1.98	0.44
1:B:1849:GLU:CD	1:B:1899:ASN:HD22	2.21	0.44
1:B:1826:PHE:CE1	1:B:1853:LEU:CD2	3.00	0.44
1:A:1392:LEU:HD13	1:A:1393:LYS:CA	2.46	0.44
1:A:3330:TYR:CD1	1:A:3334:PHE:CD2	3.05	0.44
1:A:2099:ASN:HA	1:A:2149:ARG:O	2.17	0.44
1:A:2155:ASP:OD1	1:A:2195:GLU:HG3	2.17	0.44
1:B:4020:ASN:ND2	1:B:4028:ARG:HD3	2.32	0.44
1:B:3481:ILE:O	1:B:3483:ASP:N	2.47	0.44
1:B:2492:PRO:HB2	1:B:2502:VAL:HG11	1.99	0.44
1:B:3725:VAL:HG22	1:B:3731:ASP:HA	1.97	0.44
1:B:3462:ILE:O	1:B:3465:LEU:N	2.48	0.44
1:B:1681:LYS:HE2	1:B:1939:PHE:HZ	1.83	0.44
1:B:1536:ARG:HD3	1:B:1536:ARG:HA	1.72	0.44
1:A:1968:PHE:CD1	1:A:1968:PHE:N	2.84	0.44
1:B:1562:MET:CB	1:B:1569:ILE:HD11	2.40	0.44
1:B:3449:VAL:HG13	1:B:3493:LYS:HB2	1.99	0.44
1:B:2473:LEU:CD2	1:B:2474:LEU:N	2.76	0.44
1:B:1796:GLY:O	1:B:1900:PRO:HD3	2.17	0.44
1:A:23:LEU:O	1:A:25:GLU:N	2.50	0.44
1:B:1626:CYS:SG	1:B:1639:VAL:HG11	2.57	0.44
1:A:2021:ILE:HG22	1:A:2022:PHE:HD1	1.82	0.44
1:B:1612:ASP:CA	1:B:1615:ILE:HG12	2.48	0.44
1:B:2960:THR:CG2	1:B:2961:ILE:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3579:GLU:O	1:A:3582:GLU:N	2.43	0.44
1:A:2646:ARG:NH1	1:A:2687:GLY:H	2.14	0.44
1:A:2749:LEU:HD12	1:A:2773:VAL:HG12	1.99	0.44
1:B:3869:GLU:O	1:B:3870:LYS:C	2.56	0.44
1:B:1832:SER:O	1:B:1836:VAL:HG23	2.18	0.44
1:B:2002:ILE:HG22	1:B:2006:LEU:HD11	2.00	0.44
1:A:3407:LEU:HD23	1:A:3518:PHE:CE2	2.53	0.44
1:B:2728:LEU:C	1:B:2728:LEU:HD12	2.38	0.44
1:B:1469:LEU:HD13	1:B:1523:LEU:HD21	1.97	0.44
1:B:2084:TRP:HE3	1:B:2088:ILE:HD12	1.82	0.44
1:A:1547:LYS:O	1:A:1551:SER:HB3	2.18	0.44
1:A:2861:ARG:HD2	1:A:2866:LEU:HD13	2.00	0.44
1:B:2437:LEU:H	1:B:2437:LEU:HD12	1.82	0.44
1:A:1826:PHE:O	1:A:1826:PHE:CG	2.70	0.44
1:B:2112:GLU:HB3	1:B:2117:SER:OG	2.18	0.44
1:B:4060:SER:HB3	1:B:4070:ILE:HG13	1.98	0.44
1:A:1559:SER:CB	1:A:1572:ILE:HG22	2.47	0.44
1:B:1593:ASN:HD21	1:B:1621:THR:CB	2.30	0.44
1:B:3964:ALA:HB2	1:B:3993:VAL:HG11	2.00	0.44
1:A:1421:TYR:O	1:A:1425:GLU:CA	2.65	0.44
1:A:1611:LEU:O	1:A:1615:ILE:HG23	2.18	0.44
1:B:1748:PHE:CE2	1:B:1755:LEU:HD22	2.52	0.44
1:A:4034:LEU:C	1:A:4034:LEU:HD23	2.38	0.44
1:B:1870:ASN:O	1:B:1874:VAL:HG23	2.17	0.44
1:A:3760:LEU:HD21	1:A:4078:ALA:HA	1.99	0.44
1:A:3767:PHE:HB3	1:A:3769:VAL:HG23	2.00	0.44
1:B:1664:LEU:HD23	1:B:1669:PHE:HZ	1.82	0.44
1:A:2707:VAL:HG11	1:A:2712:LEU:HD12	2.00	0.44
1:B:2788:ARG:HB2	1:B:3459:ASP:HB3	2.00	0.44
1:B:2034:ILE:CD1	1:B:2061:TYR:CZ	3.00	0.44
1:B:1967:HIS:C	1:B:1968:PHE:CD1	2.82	0.44
1:B:2755:HIS:CB	1:B:2911:ARG:O	2.56	0.44
1:A:3566:LEU:HD23	1:A:3587:LEU:HD11	1.99	0.44
1:A:1646:GLN:OE1	1:A:1763:ILE:HG12	2.18	0.44
1:B:2758:LEU:HD13	1:B:2766:LYS:HB2	1.99	0.44
1:A:3821:ASN:O	1:A:3825:ALA:HB2	2.17	0.44
1:A:2354:SER:H	1:A:2357:SER:HB2	1.83	0.44
1:A:3631:MET:HE1	1:A:3698:MET:HG3	2.00	0.44
1:A:1803:THR:HG21	1:A:1848:ASP:CG	2.37	0.44
1:B:3671:VAL:HA	1:B:3674:ILE:HG22	1.99	0.44
1:A:2037:CYS:SG	1:A:2094:PHE:HB2	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2783:GLN:HG2	1:B:2816:ILE:HB	1.99	0.44
1:B:2241:LEU:HD13	1:B:2299:ARG:HH11	1.82	0.44
1:B:3786:PHE:CD1	1:B:3895:PHE:HE2	2.36	0.44
1:A:2141:ILE:CD1	1:A:2146:LYS:CE	2.86	0.44
1:B:3458:PHE:HE1	1:B:3462:ILE:HB	1.82	0.44
1:A:1681:LYS:HE2	1:A:1939:PHE:CZ	2.53	0.44
1:B:2410:SER:O	1:B:2411:LYS:HG3	2.17	0.44
1:B:2339:ILE:HG23	1:B:2353:LEU:HB3	2.00	0.44
1:A:1660:VAL:CG1	1:A:1728:TRP:CH2	3.01	0.44
1:A:3702:MET:HB3	1:A:3767:PHE:HZ	1.83	0.44
1:B:1375:LYS:HE3	1:B:1431:LEU:HD13	1.99	0.44
1:B:1645:PHE:CZ	1:B:1649:LEU:HD22	2.52	0.43
1:A:1531:ARG:HD3	1:A:1538:TYR:HA	2.00	0.43
1:B:1531:ARG:HD2	1:B:1538:TYR:HA	2.00	0.43
1:A:1926:SER:HA	1:A:1929:ILE:CD1	2.48	0.43
1:A:2266:PHE:HD1	1:A:2326:LEU:HD21	1.83	0.43
1:A:2512:LYS:O	1:A:2513:GLN:CB	2.66	0.43
1:A:2375:ILE:HG22	1:A:2376:PRO:O	2.18	0.43
1:B:3897:TYR:CZ	1:B:3899:ASP:HB3	2.53	0.43
1:A:3319:GLU:HA	1:A:3359:LYS:O	2.17	0.43
1:B:1992:LYS:CG	1:B:2024:SER:CB	2.79	0.43
1:B:2476:LYS:HZ2	1:B:2528:ARG:HD2	1.77	0.43
1:A:2262:LEU:HA	1:A:2265:ILE:HD12	1.98	0.43
1:B:1418:SER:HB2	1:B:3446:PHE:HB3	1.99	0.43
1:A:2417:CYS:O	1:A:2558:TYR:HA	2.17	0.43
1:A:2404:PHE:CZ	1:A:2428:MET:HG2	2.53	0.43
1:A:4033:LEU:HD13	1:A:4035:GLN:CG	2.49	0.43
1:B:1976:VAL:HG11	1:B:1998:LEU:HD23	2.00	0.43
1:B:2563:SER:C	1:B:2565:LYS:H	2.21	0.43
1:B:3839:ILE:HG22	1:B:3871:PHE:HE1	1.83	0.43
1:B:2410:SER:O	1:B:2411:LYS:CB	2.66	0.43
1:A:1973:LEU:O	1:A:1977:LEU:HG	2.18	0.43
1:A:2197:ASP:HB3	1:A:2549:ARG:HD2	1.99	0.43
1:A:3964:ALA:HB2	1:A:3993:VAL:HG11	1.99	0.43
1:A:2578:ILE:CG2	1:A:2630:TYR:HB2	2.48	0.43
1:A:1531:ARG:HD2	1:A:1538:TYR:HA	2.01	0.43
1:A:2061:TYR:O	1:A:2064:GLN:HG2	2.17	0.43
1:A:1611:LEU:O	1:A:1615:ILE:HG12	2.19	0.43
1:A:3785:TYR:N	1:A:3785:TYR:CD1	2.87	0.43
1:B:3544:LYS:O	1:B:3548:LEU:HB2	2.18	0.43
1:B:1835:LEU:O	1:B:1838:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1749:ILE:HD13	1:B:1813:LEU:HD22	2.00	0.43
1:A:3628:ILE:HG13	1:A:3705:LEU:HD23	2.00	0.43
1:B:2984:VAL:C	1:B:2986:PRO:HD3	2.38	0.43
1:A:1540:LEU:HD12	1:A:1548:ILE:HD12	2.00	0.43
1:B:1750:SER:HB2	1:B:1755:LEU:HD23	2.01	0.43
1:B:3939:ILE:HG12	1:B:4010:LEU:CD2	2.49	0.43
1:B:2833:THR:CG2	1:B:2841:PRO:HD2	2.48	0.43
1:B:2419:PRO:O	1:B:2424:LYS:NZ	2.51	0.43
1:B:2201:HIS:CE1	1:B:2497:TYR:O	2.72	0.43
1:A:2982:VAL:CG1	1:A:2983:GLY:N	2.82	0.43
1:A:4033:LEU:C	1:A:4033:LEU:HD12	2.39	0.43
1:B:2151:TRP:CE3	1:B:2193:LEU:HD11	2.54	0.43
1:A:2274:HIS:CE1	1:A:2326:LEU:O	2.54	0.43
1:B:1803:THR:HG21	1:B:1848:ASP:CG	2.39	0.43
1:B:2653:TRP:HB3	1:B:2654:ARG:NH1	2.34	0.43
1:A:2109:LEU:CD1	1:A:2129:LEU:HD23	2.49	0.43
1:B:1383:TYR:CZ	1:B:1401:LEU:HD13	2.54	0.43
1:A:3338:ASN:H	1:A:3341:GLU:HB2	1.82	0.43
1:A:2447:LYS:HE3	1:A:2493:LYS:HD3	2.00	0.43
1:A:2575:TYR:HD1	1:A:2578:ILE:HD11	1.83	0.43
1:B:1391:GLY:HA3	1:B:1484:LYS:HZ1	1.81	0.43
1:A:2178:LEU:HB3	1:A:2179:PRO:HD2	2.01	0.43
1:A:3810:SER:HB3	1:A:3837:GLY:HA2	2.01	0.43
1:B:2853:LEU:HD21	1:B:2870:GLU:HG3	2.00	0.43
1:A:2503:VAL:HA	1:A:2506:LEU:HD12	2.01	0.43
1:B:2760:GLY:HA2	1:B:2917:MET:HB2	2.00	0.43
1:A:1650:LEU:O	1:A:1654:VAL:HG23	2.19	0.43
1:B:2226:ILE:HG12	1:B:2284:LEU:HD22	2.01	0.43
1:A:1367:ILE:HG22	1:A:1371:LEU:HD12	2.00	0.43
1:A:2072:LEU:HD11	1:A:2193:LEU:HD23	2.01	0.43
1:B:2081:THR:OG1	2:B:5093:ATP:O1B	2.37	0.43
1:A:2760:GLY:O	1:A:2761:ALA:HB3	2.18	0.43
1:B:2380:LEU:CD1	1:B:2577:ALA:HB2	2.46	0.43
1:A:3696:MET:SD	1:A:3760:LEU:HD23	2.59	0.43
1:A:3869:GLU:O	1:A:3870:LYS:C	2.56	0.43
1:B:3636:GLY:CA	1:B:3642:TYR:O	2.67	0.43
1:B:2463:ASN:O	1:B:2475:PRO:HD2	2.19	0.43
1:B:2707:VAL:HG11	1:B:2712:LEU:CD1	2.45	0.43
1:B:1704:GLU:OE2	1:B:1768:ARG:NH1	2.52	0.43
1:A:2829:GLU:HA	1:A:2832:ASN:HD22	1.84	0.43
1:B:3886:ALA:N	1:B:3887:PRO:CD	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1735:TYR:HB2	1:B:1748:PHE:CZ	2.53	0.43
1:A:1830:VAL:O	1:A:1834:LEU:HG	2.19	0.43
1:B:2936:ILE:CG2	1:B:2962:ARG:HD3	2.48	0.43
1:B:4022:GLN:O	1:B:4023:ILE:C	2.57	0.43
1:B:3721:THR:O	1:B:3725:VAL:HG23	2.19	0.43
1:B:2001:VAL:O	1:B:2004:PRO:HD2	2.19	0.43
1:A:1741:LEU:O	1:A:1742:ASP:HB2	2.19	0.43
1:B:1636:ILE:O	1:B:1640:VAL:HG23	2.19	0.43
1:A:1392:LEU:N	1:A:1484:LYS:HE2	2.34	0.42
1:A:2411:LYS:HG2	1:A:2530:HIS:CE1	2.41	0.42
1:A:2385:VAL:HG23	1:A:2574:TYR:CD1	2.53	0.42
1:B:3889:LEU:HG	1:B:3894:ARG:HD3	2.01	0.42
1:A:2492:PRO:CB	1:A:2502:VAL:HG11	2.49	0.42
1:A:4033:LEU:CD1	1:A:4035:GLN:N	2.82	0.42
1:B:2410:SER:O	1:B:2411:LYS:CG	2.67	0.42
1:A:1715:LEU:HG	1:A:1727:LEU:HD22	2.02	0.42
1:B:3719:VAL:HB	1:B:3744:LEU:HD11	2.01	0.42
1:B:1554:HIS:O	1:B:1555:HIS:HB2	2.18	0.42
1:B:1762:TYR:CZ	1:B:1764:GLY:HA2	2.54	0.42
1:A:4033:LEU:HD12	1:A:4035:GLN:H	1.84	0.42
1:A:1991:GLU:O	1:A:1994:VAL:HB	2.19	0.42
1:A:1998:LEU:CD1	1:A:2022:PHE:HZ	2.32	0.42
1:B:1941:ASP:O	1:B:1945:LEU:HG	2.18	0.42
1:A:2760:GLY:HA3	1:A:2766:LYS:HD3	2.01	0.42
1:B:3566:LEU:CD2	1:B:3587:LEU:HD11	2.49	0.42
1:B:1970:LEU:CD1	1:B:1974:LYS:HE2	2.45	0.42
1:A:3785:TYR:CE2	1:A:3859:VAL:HG13	2.54	0.42
1:A:1953:LEU:HD11	1:A:1973:LEU:HB3	1.98	0.42
1:A:1781:THR:HG21	1:A:1919:PHE:CE1	2.55	0.42
1:B:3815:PRO:O	1:B:3821:ASN:HB3	2.19	0.42
1:A:4045:LEU:O	1:A:4048:ILE:HG22	2.19	0.42
1:A:1672:TYR:O	1:A:1676:VAL:HG23	2.19	0.42
1:A:2707:VAL:CB	1:A:2712:LEU:CD1	2.72	0.42
1:B:1983:LEU:HB3	1:B:1993:THR:CG2	2.47	0.42
1:B:2104:ILE:O	1:B:2154:PHE:HA	2.19	0.42
1:A:3735:LYS:H	1:A:3735:LYS:HG2	1.69	0.42
1:A:1939:PHE:CD1	1:A:1939:PHE:N	2.87	0.42
1:A:2225:LYS:HD2	1:A:2281:PHE:CZ	2.55	0.42
1:A:2738:MET:HG2	1:A:2769:LEU:HD21	2.00	0.42
1:A:3461:ILE:C	1:A:3463:SER:H	2.22	0.42
1:B:2106:THR:H	1:B:2156:SER:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1575:LEU:O	1:A:1576:GLU:HB3	2.20	0.42
1:B:3701:THR:OG1	1:B:4085:THR:HG22	2.19	0.42
1:A:2640:THR:O	1:A:2643:SER:HB3	2.20	0.42
1:B:3407:LEU:HD23	1:B:3518:PHE:CE2	2.55	0.42
1:A:3365:ARG:HD2	1:A:3368:ASP:OD2	2.19	0.42
1:B:2073:VAL:HG21	1:B:2199:LEU:HD11	2.01	0.42
1:A:2306:ASP:HB2	1:A:2309:SER:HB3	2.02	0.42
1:B:3413:HIS:O	1:B:3417:VAL:HG23	2.20	0.42
1:A:1620:PHE:CA	1:A:1760:PHE:CE1	3.01	0.42
1:B:1645:PHE:HZ	1:B:1768:ARG:HD2	1.84	0.42
1:B:1851:ASN:HD21	1:B:1899:ASN:HB2	1.84	0.42
1:B:2745:ILE:HG12	1:B:2756:MET:CE	2.45	0.42
1:B:2141:ILE:HG22	1:B:2145:PHE:HB2	2.02	0.42
1:A:2423:GLY:CA	3:A:5094:SO4:O3	2.68	0.42
1:B:2941:THR:HG22	1:B:2942:ASP:N	2.30	0.42
1:A:1965:HIS:HD2	1:A:2212:LEU:HD23	1.85	0.42
1:B:2354:SER:OG	1:B:2357:SER:CA	2.68	0.42
1:A:2860:THR:HG21	1:A:2867:LEU:HD12	2.02	0.42
1:B:2115:TYR:OH	1:B:2162:TYR:O	2.27	0.42
1:B:1741:LEU:O	1:B:1742:ASP:HB2	2.19	0.42
1:A:2493:LYS:HG3	1:A:2494:LEU:N	2.33	0.42
1:A:1822:CYS:SG	1:A:1850:PHE:CA	3.04	0.42
1:B:2095:ASP:HB3	1:B:2097:HIS:ND1	2.35	0.42
1:B:2730:VAL:HA	1:B:2731:PRO:HD3	1.81	0.42
1:A:4074:GLU:HA	1:A:4077:GLN:HE21	1.84	0.42
1:A:3414:MET:O	1:A:3418:ILE:HG12	2.19	0.42
1:B:1409:LEU:CD2	1:B:1435:LEU:CB	2.83	0.42
1:A:2708:ASN:O	1:A:2712:LEU:HD13	2.20	0.42
1:A:2563:SER:C	1:A:2565:LYS:H	2.23	0.42
1:A:2178:LEU:HB2	1:A:2182:GLU:H	1.83	0.42
1:A:1540:LEU:HD23	1:A:1540:LEU:HA	1.65	0.42
1:B:1612:ASP:C	1:B:1615:ILE:HG12	2.39	0.42
1:A:2095:ASP:OD1	1:A:2149:ARG:NH2	2.53	0.42
1:A:1365:PHE:O	1:A:1366:VAL:CB	2.68	0.42
1:B:2492:PRO:CB	1:B:2502:VAL:HG11	2.49	0.42
1:B:1871:GLY:HA3	1:B:1879:ILE:HG21	2.02	0.42
1:A:2609:THR:HA	1:A:2612:GLN:O	2.20	0.42
1:A:3784:ASN:ND2	1:A:3865:ALA:O	2.52	0.42
1:A:1568:SER:HB2	1:A:1816:VAL:HG21	2.01	0.42
1:A:2755:HIS:HB3	1:A:2912:CYS:SG	2.60	0.42
1:A:1967:HIS:C	1:A:1968:PHE:CD1	2.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3978:ASN:O	1:A:3981:PRO:HD3	2.20	0.42
1:A:2229:LEU:HD11	1:A:2285:GLU:HG3	2.02	0.42
1:A:2510:MET:O	1:A:2513:GLN:NE2	2.53	0.42
1:A:3590:LEU:HD12	1:A:3593:GLU:HB2	2.02	0.42
1:B:3817:GLY:H	1:B:3821:ASN:CB	2.33	0.42
1:A:1727:LEU:O	1:A:1731:VAL:HG23	2.20	0.42
1:B:1951:HIS:O	1:B:1955:LEU:HB2	2.20	0.42
1:B:2169:VAL:HG13	1:B:2186:ILE:HG12	2.02	0.42
1:A:3728:GLU:CG	1:A:4079:LYS:HE2	2.49	0.42
1:B:1998:LEU:CD1	1:B:2022:PHE:CZ	3.02	0.41
1:A:3505:ILE:O	1:A:3510:ARG:NH1	2.53	0.41
1:B:2578:ILE:CG2	1:B:2630:TYR:HB2	2.50	0.41
1:B:1392:LEU:HD23	1:B:1484:LYS:HA	2.02	0.41
1:B:1375:LYS:O	1:B:1379:LYS:HG2	2.20	0.41
1:B:2908:LEU:O	1:B:2912:CYS:HB2	2.20	0.41
1:B:2700:LEU:HD13	1:B:2707:VAL:HG11	2.01	0.41
1:A:2141:ILE:CG2	1:A:2145:PHE:HB2	2.49	0.41
1:A:2034:ILE:HD12	1:A:2061:TYR:CE2	2.55	0.41
1:B:1531:ARG:CD	1:B:1538:TYR:HA	2.50	0.41
1:A:2786:ILE:HD12	1:A:3460:PRO:CG	2.49	0.41
1:B:1497:ILE:O	1:B:1500:ILE:HG12	2.19	0.41
1:B:3017:VAL:HG21	1:B:3313:PHE:HE2	1.83	0.41
1:B:1540:LEU:HA	1:B:1540:LEU:HD23	1.74	0.41
1:B:3551:LEU:HA	1:B:3554:GLU:HB3	2.01	0.41
1:A:2001:VAL:O	1:A:2004:PRO:HD2	2.20	0.41
1:A:2758:LEU:HD22	1:A:2917:MET:SD	2.60	0.41
1:A:2044:ARG:HH21	1:A:2093:ILE:HD11	1.85	0.41
1:B:1392:LEU:N	1:B:1484:LYS:HE2	2.34	0.41
1:A:2424:LYS:NZ	3:A:5094:SO4:O1	2.54	0.41
1:A:3544:LYS:HE3	1:A:3607:PHE:CD1	2.55	0.41
1:A:23:LEU:O	1:A:24:GLU:C	2.58	0.41
1:B:2047:PHE:CE2	1:B:2082:ALA:HB1	2.55	0.41
1:B:2138:ASN:ND2	1:B:2185:PRO:O	2.53	0.41
1:B:1873:GLN:HE22	1:B:1915:SER:HA	1.84	0.41
1:B:2763:ARG:HD3	1:B:3512:ARG:NH1	2.35	0.41
1:A:1536:ARG:HA	1:A:1536:ARG:HD3	1.79	0.41
1:A:2786:ILE:HD12	1:A:3460:PRO:HG2	2.02	0.41
1:B:3570:LEU:HD23	1:B:3580:ASN:CG	2.40	0.41
1:A:3544:LYS:O	1:A:3548:LEU:HB2	2.19	0.41
1:B:115:GLU:CB	1:B:1372:ASN:CG	2.88	0.41
1:A:2012:LEU:HD12	1:A:2013:VAL:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2609:THR:HA	1:B:2612:GLN:O	2.20	0.41
1:A:3413:HIS:O	1:A:3417:VAL:HG23	2.21	0.41
1:A:2141:ILE:HG22	1:A:2145:PHE:CB	2.51	0.41
1:B:2508:GLN:O	1:B:2512:LYS:HB2	2.20	0.41
1:B:2276:LEU:CD2	1:B:2415:ILE:HG21	2.47	0.41
1:A:2489:ILE:HD11	1:A:2506:LEU:HD13	2.02	0.41
1:B:2517:LYS:HD2	1:B:2520:GLU:OE1	2.20	0.41
1:A:2109:LEU:HB3	1:A:2113:SER:HB2	2.03	0.41
1:B:2839:ASP:O	1:B:2841:PRO:HD3	2.20	0.41
1:B:2852:LEU:HG	1:B:2856:LEU:HD13	2.03	0.41
1:A:2039:LYS:HG2	1:A:2049:MET:HG3	2.03	0.41
1:B:2102:TYR:HB2	1:B:2152:VAL:HG22	2.02	0.41
1:A:3534:LEU:HD12	1:A:3618:TYR:CZ	2.52	0.41
1:A:2761:ALA:O	1:A:2892:CYS:CB	2.69	0.41
1:A:2336:ARG:HG2	1:A:2355:ASP:CG	2.41	0.41
1:A:1966:TYR:CZ	1:A:2006:LEU:HD23	2.55	0.41
1:A:3330:TYR:CZ	1:A:3346:LEU:HD13	2.55	0.41
1:A:2225:LYS:HG2	1:A:2229:LEU:HD12	2.02	0.41
1:A:3833:LYS:NZ	1:A:3862:THR:HG21	2.36	0.41
1:B:2044:ARG:NH2	1:B:2093:ILE:HD11	2.35	0.41
1:A:2568:SER:HA	1:A:2597:VAL:HG21	2.02	0.41
1:A:4020:ASN:ND2	1:A:4028:ARG:HD3	2.35	0.41
1:B:2982:VAL:HG12	1:B:2983:GLY:N	2.36	0.41
1:A:2476:LYS:H	1:A:2476:LYS:HD2	1.73	0.41
1:B:3919:LYS:HZ1	1:B:4038:GLU:HG3	1.83	0.41
1:A:1706:LEU:HD21	1:A:1935:GLN:CG	2.48	0.41
1:A:2762:SER:O	1:A:2763:ARG:CB	2.68	0.41
1:A:23:LEU:C	1:A:25:GLU:N	2.74	0.41
1:B:1963:MET:HB3	1:B:1966:TYR:CD2	2.55	0.41
1:A:1479:LEU:HD11	1:A:1515:SER:HB3	2.03	0.41
1:A:4054:GLU:HA	1:A:4055:PRO:HD3	1.98	0.41
1:A:2891:ILE:HD11	1:A:2903:ILE:HD11	2.03	0.41
1:A:2276:LEU:HD21	1:A:2415:ILE:HG21	2.03	0.41
1:A:4033:LEU:CD1	1:A:4035:GLN:H	2.34	0.41
1:B:1939:PHE:CD1	1:B:1939:PHE:N	2.86	0.41
1:B:1531:ARG:HD2	1:B:1538:TYR:CD1	2.55	0.41
1:A:3737:THR:CB	1:A:3740:THR:OG1	2.56	0.41
1:A:1929:ILE:HD12	1:A:1929:ILE:H	1.86	0.41
1:B:3839:ILE:HG22	1:B:3871:PHE:CE1	2.56	0.41
1:A:3570:LEU:HD23	1:A:3580:ASN:CG	2.41	0.41
1:B:4065:LEU:HD12	1:B:4065:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2852:LEU:HG	1:A:2856:LEU:HD13	2.03	0.41
1:B:3636:GLY:HA2	1:B:3642:TYR:O	2.20	0.41
1:A:1742:ASP:HB3	1:A:1745:ASN:HD22	1.85	0.41
1:B:1771:TYR:HA	1:B:1775:LEU:HD13	2.03	0.41
1:A:1898:LEU:HD11	1:A:1908:LEU:CD2	2.50	0.41
1:A:3772:TRP:HZ3	1:A:3780:ASN:HD22	1.68	0.41
1:B:1438:LEU:O	1:B:1442:GLN:HB2	2.20	0.41
1:B:2229:LEU:HD11	1:B:2285:GLU:HG3	2.02	0.41
1:B:3848:LEU:HD21	1:B:3852:LYS:HE3	2.02	0.41
1:B:2752:VAL:O	1:B:2883:LYS:HA	2.21	0.41
1:B:4033:LEU:HD23	1:B:4033:LEU:HA	1.80	0.41
1:B:3688:THR:HG21	1:B:3777:VAL:CG2	2.50	0.41
1:B:2494:LEU:HD12	1:B:2494:LEU:C	2.41	0.41
1:A:2088:ILE:HG12	1:A:2151:TRP:CZ2	2.55	0.41
1:B:2552:ARG:HG2	1:B:2552:ARG:NH1	2.36	0.41
1:B:1674:LYS:HA	1:B:1677:ASP:HB3	2.03	0.41
1:B:1779:PHE:O	1:B:1783:THR:HG22	2.21	0.41
1:B:1872:LEU:HG	1:B:1888:LEU:HD21	2.04	0.41
1:A:3464:ARG:O	1:A:3467:SER:O	2.38	0.41
1:B:2111:LYS:CD	1:B:2161:GLU:CG	2.87	0.40
1:A:1992:LYS:CG	1:A:2024:SER:CB	2.78	0.40
1:A:2488:GLU:HB3	1:A:2491:LEU:CG	2.51	0.40
1:B:3431:PHE:CZ	1:B:3458:PHE:HD1	2.40	0.40
1:B:1534:PHE:CZ	1:B:1536:ARG:HB2	2.57	0.40
1:B:3785:TYR:CD1	1:B:3785:TYR:N	2.89	0.40
1:B:3978:ASN:O	1:B:3981:PRO:HD2	2.21	0.40
1:B:1493:LEU:HD23	1:B:1498:GLU:HB2	2.00	0.40
1:B:3353:LEU:HD23	1:B:3358:VAL:HG11	2.02	0.40
1:B:1383:TYR:CE2	1:B:1401:LEU:HD13	2.57	0.40
1:B:1773:PRO:HA	1:B:1776:LEU:HD12	2.03	0.40
1:B:2514:GLY:CA	1:B:2523:TRP:CZ2	3.05	0.40
1:B:1527:LEU:HD23	1:B:1545:LEU:CD2	2.50	0.40
1:B:1469:LEU:HD13	1:B:1523:LEU:HD23	2.02	0.40
1:B:2109:LEU:HD11	1:B:2129:LEU:HD23	2.03	0.40
1:A:3846:MET:HG3	1:A:3847:SER:N	2.35	0.40
1:B:2032:LYS:HA	1:B:2032:LYS:HD3	1.89	0.40
1:B:4081:VAL:O	1:B:4085:THR:HG23	2.22	0.40
1:A:3951:SER:HB3	1:A:4003:ASP:OD2	2.22	0.40
1:B:3821:ASN:O	1:B:3825:ALA:HB2	2.22	0.40
1:A:2819:GLU:HB3	1:A:2891:ILE:HG22	2.03	0.40
1:B:3703:PHE:CE1	1:B:3766:GLU:HG2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1660:VAL:HG13	1:B:1728:TRP:CH2	2.57	0.40
1:A:1620:PHE:HB2	1:A:1760:PHE:CE1	2.57	0.40
1:B:1991:GLU:O	1:B:1994:VAL:HB	2.21	0.40
1:A:1750:SER:HB2	1:A:1755:LEU:CD2	2.52	0.40
1:A:3612:ASP:C	1:A:3615:VAL:HG22	2.41	0.40
1:B:3772:TRP:HZ3	1:B:3780:ASN:ND2	2.20	0.40
1:A:3924:TRP:CD1	1:A:3924:TRP:C	2.95	0.40
1:A:2661:VAL:HG12	1:A:2916:TRP:CE2	2.57	0.40
1:B:2378:VAL:HG11	1:B:2392:ILE:HD12	2.02	0.40
1:B:2107:LYS:CD	1:B:2499:SER:HB3	2.52	0.40
1:A:3406:PHE:CZ	1:A:3505:ILE:HG21	2.57	0.40
1:B:1612:ASP:O	1:B:1615:ILE:HG12	2.21	0.40
1:A:2418:GLY:O	1:A:2424:LYS:HE3	2.21	0.40
1:B:2336:ARG:HG2	1:B:2355:ASP:OD1	2.21	0.40
1:A:1365:PHE:O	1:A:1366:VAL:HB	2.21	0.40
1:A:1672:TYR:O	1:A:1675:GLU:HB3	2.22	0.40
1:A:2053:PHE:HB2	1:A:2219:VAL:HB	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	2640/2695 (98%)	2519 (95%)	107 (4%)	14 (0%)	34	77
1	B	2640/2695 (98%)	2522 (96%)	104 (4%)	14 (0%)	34	77
All	All	5280/5390 (98%)	5041 (96%)	211 (4%)	28 (0%)	34	77

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1391	GLY

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Mol	Chain	Res	Type
1	B	214	HIS
1	B	1366	VAL
1	B	1391	GLY
1	A	1366	VAL
1	A	2990	GLY
1	A	3306	TRP
1	A	3482	GLY
1	B	3482	GLY
1	A	53	ASN
1	B	53	ASN
1	B	2562	PRO
1	B	2731	PRO
1	A	115	GLU
1	A	2519	PRO
1	B	66	GLN
1	B	2519	PRO
1	A	66	GLN
1	B	3914	GLN
1	B	3980	ILE
1	A	3980	ILE
1	B	85	PRO
1	A	2562	PRO
1	B	3819	ILE
1	A	1470	PRO
1	A	1535	PRO
1	A	2028	PRO
1	B	2028	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	2218/2453 (90%)	2140 (96%)	78 (4%)	43	78
1	B	2218/2453 (90%)	2144 (97%)	74 (3%)	45	79
All	All	4436/4906 (90%)	4284 (97%)	152 (3%)	44	79

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1383	TYR
1	A	1421	TYR
1	A	1425	GLU
1	A	1473	THR
1	A	1486	ILE
1	A	1493	LEU
1	A	1504	ASN
1	A	1794	PHE
1	A	1826	PHE
1	A	1852	ARG
1	A	1923	SER
1	A	1944	SER
1	A	1971	ARG
1	A	1992	LYS
1	A	1999	LYS
1	A	2012	LEU
1	A	2057	CYS
1	A	2078	CYS
1	A	2109	LEU
1	A	2202	THR
1	A	2218	ASP
1	A	2295	ILE
1	A	2346	PHE
1	A	2357	SER
1	A	2386	MET
1	A	2424	LYS
1	A	2428	MET
1	A	2461	HIS
1	A	2472	THR
1	A	2476	LYS
1	A	2526	ILE
1	A	2544	ILE
1	A	2563	SER
1	A	2566	SER
1	A	2611	LEU
1	A	2638	ARG
1	A	2694	LEU
1	A	2822	ILE
1	A	2833	THR
1	A	2843	LEU
1	A	2853	LEU
1	A	2856	LEU

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Mol	Chain	Res	Type
1	A	2865	LEU
1	A	2873	LEU
1	A	2875	ASP
1	A	2911	ARG
1	A	2920	TRP
1	A	3301	PHE
1	A	3329	ILE
1	A	3332	THR
1	A	3355	LYS
1	A	3372	THR
1	A	3400	SER
1	A	3418	ILE
1	A	3531	ASP
1	A	3538	ASN
1	A	3548	LEU
1	A	3565	ARG
1	A	3601	LEU
1	A	3618	TYR
1	A	3677	LEU
1	A	3717	GLU
1	A	3729	SER
1	A	3735	LYS
1	A	3737	THR
1	A	3744	LEU
1	A	3811	LEU
1	A	3871	PHE
1	A	3884	LEU
1	A	3906	THR
1	A	3917	THR
1	A	3943	THR
1	A	3950	PHE
1	A	3960	ASP
1	A	3982	TRP
1	A	4004	LEU
1	A	4016	CYS
1	A	4040	GLU
1	B	1383	TYR
1	B	1421	TYR
1	B	1425	GLU
1	B	1455	LEU
1	B	1486	ILE
1	B	1504	ASN

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Mol	Chain	Res	Type
1	B	1525	THR
1	B	1554	HIS
1	B	1605	GLN
1	B	1694	VAL
1	B	1743	ASP
1	B	1759	LYS
1	B	1767	GLU
1	B	1768	ARG
1	B	1794	PHE
1	B	1826	PHE
1	B	1832	SER
1	B	1903	ASN
1	B	1997	SER
1	B	2051	GLU
1	B	2057	CYS
1	B	2078	CYS
1	B	2126	ARG
1	B	2229	LEU
1	B	2285	GLU
1	B	2295	ILE
1	B	2307	ASP
1	B	2346	PHE
1	B	2351	GLN
1	B	2369	SER
1	B	2390	ILE
1	B	2395	ILE
1	B	2397	THR
1	B	2424	LYS
1	B	2428	MET
1	B	2476	LYS
1	B	2566	SER
1	B	2576	LYS
1	B	2613	SER
1	B	2681	LEU
1	B	2694	LEU
1	B	2822	ILE
1	B	2843	LEU
1	B	2856	LEU
1	B	2865	LEU
1	B	2866	LEU
1	B	2873	LEU
1	B	2875	ASP

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Mol	Chain	Res	Type
1	B	2920	TRP
1	B	3301	PHE
1	B	3329	ILE
1	B	3372	THR
1	B	3391	LEU
1	B	3400	SER
1	B	3502	SER
1	B	3560	LYS
1	B	3598	GLU
1	B	3605	GLU
1	B	3673	GLU
1	B	3677	LEU
1	B	3729	SER
1	B	3737	THR
1	B	3744	LEU
1	B	3871	PHE
1	B	3899	ASP
1	B	3905	ASP
1	B	3906	THR
1	B	3917	THR
1	B	3943	THR
1	B	3960	ASP
1	B	3980	ILE
1	B	3982	TRP
1	B	4016	CYS
1	B	4024	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1449	GLN
1	A	1622	GLN
1	A	1646	GLN
1	A	1736	GLN
1	A	1745	ASN
1	A	1851	ASN
1	A	1873	GLN
1	A	1899	ASN
1	A	1951	HIS
1	A	1965	HIS
1	A	1979	ASN
1	A	2068	GLN

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Mol	Chain	Res	Type
1	A	2099	ASN
1	A	2228	HIS
1	A	2274	HIS
1	A	2282	ASN
1	A	2293	HIS
1	A	2383	HIS
1	A	2409	ASN
1	A	2459	HIS
1	A	2530	HIS
1	A	2536	ASN
1	A	2634	ASN
1	A	2683	ASN
1	A	2688	ASN
1	A	3323	ASN
1	A	3338	ASN
1	A	3497	HIS
1	A	3521	ASN
1	A	3542	GLN
1	A	3588	ASN
1	A	3624	HIS
1	A	3780	ASN
1	A	3890	GLN
1	A	4020	ASN
1	A	4077	GLN
1	B	1533	GLN
1	B	1605	GLN
1	B	1622	GLN
1	B	1646	GLN
1	B	1851	ASN
1	B	1864	ASN
1	B	1873	GLN
1	B	1899	ASN
1	B	2064	GLN
1	B	2068	GLN
1	B	2099	ASN
1	B	2228	HIS
1	B	2274	HIS
1	B	2282	ASN
1	B	2293	HIS
1	B	2383	HIS
1	B	2409	ASN
1	B	2536	ASN

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Mol	Chain	Res	Type
1	B	2598	HIS
1	B	2634	ASN
1	B	2683	ASN
1	B	2753	GLN
1	B	3323	ASN
1	B	3336	HIS
1	B	3521	ASN
1	B	3542	GLN
1	B	3624	HIS
1	B	3685	GLN
1	B	3780	ASN
1	B	3890	GLN
1	B	3962	GLN
1	B	3970	ASN
1	B	4020	ASN
1	B	4077	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	A	5093	4	24,33,33	1.10	2 (8%)	31,52,52	2.57	7 (22%)
3	SO4	A	5094	-	4,4,4	0.60	0	6,6,6	0.54	0
3	SO4	A	5095	-	4,4,4	0.78	0	6,6,6	0.80	0
3	SO4	A	5096	-	4,4,4	0.41	0	6,6,6	0.45	0
2	ATP	B	5093	4	24,33,33	1.01	2 (8%)	31,52,52	2.01	5 (16%)
3	SO4	B	5094	-	4,4,4	0.56	0	6,6,6	0.56	0
3	SO4	B	5095	-	4,4,4	0.42	0	6,6,6	0.29	0
3	SO4	B	5096	-	4,4,4	0.23	0	6,6,6	0.20	0

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
2	ATP	A	5093	4	-	0/18/38/38	0/3/3/3
3	SO4	A	5094	-	-	0/0/0/0	0/0/0/0
3	SO4	A	5095	-	-	0/0/0/0	0/0/0/0
3	SO4	A	5096	-	-	0/0/0/0	0/0/0/0
2	ATP	B	5093	4	-	0/18/38/38	0/3/3/3
3	SO4	B	5094	-	-	0/0/0/0	0/0/0/0
3	SO4	B	5095	-	-	0/0/0/0	0/0/0/0
3	SO4	B	5096	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5093	ATP	PG-O2G	-2.08	1.47	1.54
2	B	5093	ATP	O4'-C1'	2.31	1.44	1.41
2	A	5093	ATP	C5-C4	2.31	1.45	1.40
2	B	5093	ATP	C5-C4	2.94	1.47	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5093	ATP	N3-C2-N1	-8.68	122.25	128.89
2	B	5093	ATP	N3-C2-N1	-7.44	123.20	128.89
2	A	5093	ATP	PA-O3A-PB	-5.37	117.66	132.73
2	A	5093	ATP	PB-O3B-PG	-4.21	118.56	132.67
2	B	5093	ATP	PB-O3B-PG	-3.78	119.98	132.67
2	B	5093	ATP	PA-O3A-PB	-3.67	122.42	132.73
2	A	5093	ATP	C2'-C1'-N9	-3.65	108.72	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5093	ATP	C2'-C1'-N9	-2.92	109.84	114.29
2	A	5093	ATP	C4-C5-N7	-2.84	106.87	109.48
2	B	5093	ATP	C4-C5-N7	-2.41	107.26	109.48
2	A	5093	ATP	O4'-C1'-N9	3.23	114.87	108.10
2	A	5093	ATP	O3A-PA-O5'	4.45	114.73	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5093	ATP	4	0
3	A	5094	SO4	4	0
3	A	5095	SO4	3	0
3	A	5096	SO4	2	0
2	B	5093	ATP	7	0
3	B	5095	SO4	2	0
3	B	5096	SO4	1	0

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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2650/2695 (98%)	0.16	160 (6%) 25 15	80, 163, 325, 500	0
1	B	2650/2695 (98%)	0.40	229 (8%) 13 9	117, 210, 355, 500	0
All	All	5300/5390 (98%)	0.28	389 (7%) 18 11	80, 189, 342, 500	0

All (389) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	148	THR	18.5
1	B	35	ASP	17.4
1	B	155	TYR	17.3
1	B	143	ASN	16.6
1	B	67	SER	16.2
1	B	31	LEU	16.2
1	A	210	GLY	15.6
1	B	71	ILE	15.1
1	A	211	GLY	14.7
1	B	151	ASP	12.4
1	B	30	HIS	12.2
1	B	59	ASP	11.7
1	B	18	LEU	11.7
1	A	84	CYS	11.6
1	B	152	PHE	11.4
1	B	29	GLU	10.9
1	B	17	ARG	9.9
1	A	209	PHE	9.9
1	B	19	LEU	9.5
1	A	202	LEU	9.4
1	B	73	TYR	9.1
1	A	54	LEU	8.7
1	B	1579	ILE	8.4
1	B	154	LEU	8.4

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Mol	Chain	Res	Type	RSRZ
1	B	1581	GLY	7.9
1	B	1596	ILE	7.8
1	B	159	ASP	7.7
1	B	1572	ILE	7.7
1	A	216	PRO	7.6
1	B	34	ARG	7.5
1	B	158	LEU	7.5
1	B	72	ARG	7.5
1	B	74	ILE	7.4
1	A	215	PRO	7.4
1	A	85	PRO	7.3
1	B	1580	THR	7.1
1	B	1549	ILE	6.7
1	B	149	HIS	6.7
1	B	70	ILE	6.7
1	B	58	ILE	6.5
1	B	47	LEU	6.4
1	B	3580	ASN	6.3
1	B	94	LEU	6.3
1	B	1574	PHE	6.2
1	B	1483	TYR	6.1
1	B	20	LEU	6.1
1	B	2024	SER	5.9
1	B	14	GLN	5.8
1	A	1597	GLU	5.8
1	A	138	HIS	5.6
1	B	3582	GLU	5.6
1	B	1452	TRP	5.6
1	B	56	TYR	5.6
1	B	95	GLU	5.5
1	B	2025	ALA	5.5
1	B	1459	LEU	5.4
1	A	135	ARG	5.4
1	A	3580	ASN	5.4
1	A	143	ASN	5.4
1	B	2298	TYR	5.3
1	B	61	ASP	5.3
1	B	2844	PHE	5.3
1	A	59	ASP	5.3
1	B	75	ALA	5.3
1	A	3537	GLU	5.3
1	A	58	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	3581	ASP	5.2
1	B	87	GLU	5.1
1	B	49	LEU	5.1
1	A	3594	ALA	5.1
1	A	131	MET	5.1
1	B	1597	GLU	5.1
1	A	1487	THR	5.0
1	B	5	GLY	5.0
1	B	211	GLY	5.0
1	A	212	GLY	5.0
1	B	3839	ILE	4.9
1	B	1558	VAL	4.9
1	A	134	ASP	4.9
1	A	3584	MET	4.8
1	B	1546	LEU	4.8
1	B	81	LEU	4.8
1	B	1601	SER	4.7
1	B	22	TYR	4.7
1	B	21	GLU	4.7
1	B	1582	VAL	4.6
1	A	83	GLY	4.6
1	B	144	GLY	4.6
1	B	2808	LEU	4.6
1	B	1424	PHE	4.6
1	B	53	ASN	4.5
1	B	108	ILE	4.5
1	A	208	THR	4.5
1	A	3567	LEU	4.5
1	A	3587	LEU	4.5
1	A	29	GLU	4.4
1	A	3563	GLU	4.4
1	A	3740	THR	4.4
1	B	40	TRP	4.4
1	A	1483	TYR	4.4
1	A	132	PHE	4.3
1	A	16	THR	4.3
1	B	60	GLY	4.3
1	B	1573	ILE	4.3
1	A	168	CYS	4.2
1	B	1548	ILE	4.2
1	A	47	LEU	4.2
1	B	202	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	24	GLU	4.2
1	A	3025	ASN	4.2
1	A	74	ILE	4.1
1	B	116	THR	4.1
1	B	210	GLY	4.1
1	A	203	GLN	4.1
1	A	2364	ASP	4.1
1	B	33	GLU	4.1
1	B	6	TYR	4.0
1	B	1545	LEU	4.0
1	B	16	THR	4.0
1	A	27	TYR	4.0
1	A	139	LYS	4.0
1	B	145	ASP	3.9
1	A	108	ILE	3.9
1	B	54	LEU	3.9
1	B	1845	GLY	3.9
1	A	1598	LEU	3.9
1	B	84	CYS	3.8
1	A	109	ALA	3.8
1	A	63	LYS	3.8
1	A	52	PRO	3.8
1	A	2029	LEU	3.8
1	B	38	ASP	3.8
1	B	3534	LEU	3.8
1	B	1395	VAL	3.7
1	B	1594	GLU	3.7
1	B	3540	GLU	3.7
1	A	3744	LEU	3.7
1	A	61	ASP	3.6
1	B	42	ASN	3.6
1	B	3618	TYR	3.6
1	B	43	LYS	3.6
1	B	2863	LEU	3.6
1	B	2026	GLY	3.6
1	A	67	SER	3.6
1	A	2868	ASP	3.6
1	B	2115	TYR	3.6
1	B	142	LEU	3.6
1	B	46	GLU	3.6
1	B	3571	ASN	3.6
1	A	3589	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	3581	ASP	3.5
1	B	37	GLY	3.5
1	A	173	PRO	3.5
1	A	3741	ASN	3.5
1	B	91	ILE	3.4
1	B	1551	SER	3.4
1	B	1937	MET	3.4
1	A	148	THR	3.4
1	B	1550	GLY	3.4
1	B	3579	GLU	3.4
1	B	1592	LEU	3.4
1	B	157	ALA	3.4
1	A	2030	ASN	3.4
1	A	1572	ILE	3.4
1	A	3784	ASN	3.4
1	B	2179	PRO	3.4
1	A	3731	ASP	3.4
1	B	2355	ASP	3.3
1	B	8	LYS	3.3
1	B	1590	LEU	3.3
1	B	55	PRO	3.3
1	B	1647	ALA	3.3
1	A	3571	ASN	3.3
1	A	1378	TRP	3.3
1	B	83	GLY	3.3
1	B	156	ASP	3.3
1	A	3875	MET	3.3
1	B	1401	LEU	3.2
1	A	140	THR	3.2
1	A	1393	LYS	3.2
1	B	52	PRO	3.2
1	B	132	PHE	3.2
1	A	37	GLY	3.2
1	A	3734	PRO	3.2
1	B	50	GLU	3.2
1	A	22	TYR	3.2
1	B	1683	LEU	3.2
1	B	3436	PHE	3.2
1	B	88	ARG	3.1
1	B	1500	ILE	3.1
1	A	3566	LEU	3.1
1	A	23	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	3475	ASN	3.1
1	B	3583	LEU	3.1
1	B	161	VAL	3.1
1	B	2302	PHE	3.1
1	B	212	GLY	3.1
1	B	1850	PHE	3.1
1	B	2241	LEU	3.1
1	A	1458	ILE	3.0
1	A	82	GLY	3.0
1	A	115	GLU	3.0
1	A	62	VAL	3.0
1	A	79	ASN	3.0
1	B	3538	ASN	3.0
1	B	92	SER	3.0
1	B	164	MET	3.0
1	B	209	PHE	3.0
1	A	5	GLY	3.0
1	A	3919	LYS	3.0
1	B	2859	LYS	3.0
1	B	1669	PHE	3.0
1	B	3840	LEU	3.0
1	B	66	GLN	3.0
1	A	3722	MET	2.9
1	B	135	ARG	2.9
1	A	53	ASN	2.9
1	A	18	LEU	2.9
1	A	1459	LEU	2.9
1	A	60	GLY	2.9
1	B	1476	PHE	2.9
1	B	1989	GLU	2.9
1	A	49	LEU	2.9
1	A	1382	GLN	2.9
1	A	25	GLU	2.9
1	A	17	ARG	2.9
1	B	3578	LEU	2.9
1	A	31	LEU	2.9
1	B	203	GLN	2.9
1	B	3816	LEU	2.8
1	B	57	TYR	2.8
1	A	3899	ASP	2.8
1	B	3841	LEU	2.8
1	B	32	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	3865	ALA	2.8
1	A	40	TRP	2.8
1	B	2839	ASP	2.8
1	A	1445	TRP	2.8
1	A	3300	THR	2.8
1	B	3533	THR	2.8
1	A	3739	ASP	2.8
1	B	2795	PHE	2.8
1	B	1394	LEU	2.7
1	A	3570	LEU	2.7
1	B	63	LYS	2.7
1	B	2151	TRP	2.7
1	B	2029	LEU	2.7
1	A	55	PRO	2.7
1	A	1394	LEU	2.7
1	B	11	GLY	2.7
1	B	2030	ASN	2.7
1	A	30	HIS	2.7
1	B	150	PRO	2.7
1	B	3564	LYS	2.7
1	B	1445	TRP	2.7
1	A	33	GLU	2.7
1	A	91	ILE	2.7
1	B	3584	MET	2.7
1	A	3321	ILE	2.7
1	A	3917	THR	2.7
1	B	1458	ILE	2.6
1	B	1631	LYS	2.6
1	B	3954	TYR	2.6
1	A	174	LYS	2.6
1	A	2942	ASP	2.6
1	A	3555	TYR	2.6
1	A	20	LEU	2.6
1	A	2034	ILE	2.6
1	B	3617	GLU	2.6
1	B	3873	MET	2.6
1	A	2363	ASN	2.6
1	B	2246	LEU	2.6
1	A	3556	LYS	2.6
1	A	149	HIS	2.6
1	A	2120	LYS	2.6
1	A	3024	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1595	LYS	2.6
1	B	15	PRO	2.6
1	A	3297	LYS	2.5
1	B	2102	TYR	2.5
1	A	3561	ASN	2.5
1	B	1893	ALA	2.5
1	B	2840	ILE	2.5
1	B	2941	THR	2.5
1	A	71	ILE	2.5
1	A	137	CYS	2.5
1	B	1593	ASN	2.5
1	A	175	LEU	2.5
1	B	1505	PHE	2.5
1	B	1760	PHE	2.5
1	A	3572	ASN	2.5
1	B	115	GLU	2.5
1	A	3016	PHE	2.5
1	B	3541	MET	2.5
1	B	1479	LEU	2.4
1	A	4035	GLN	2.4
1	B	1730	LYS	2.4
1	A	92	SER	2.4
1	B	68	MET	2.4
1	A	3018	ASN	2.4
1	B	127	GLU	2.4
1	B	3874	PHE	2.4
1	B	1627	LEU	2.4
1	B	62	VAL	2.4
1	B	3359	LYS	2.4
1	A	178	PHE	2.4
1	A	28	GLU	2.4
1	A	3874	PHE	2.4
1	B	2295	ILE	2.4
1	A	3979	ASN	2.4
1	B	1934	LEU	2.4
1	B	1383	TYR	2.4
1	A	10	LYS	2.3
1	A	1392	LEU	2.3
1	B	79	ASN	2.3
1	A	3299	LEU	2.3
1	B	4	LEU	2.3
1	A	136	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	3542	GLN	2.3
1	B	1390	SER	2.3
1	A	38	ASP	2.3
1	A	3542	GLN	2.3
1	B	48	GLY	2.3
1	B	2439	ASP	2.3
1	A	3022	GLU	2.3
1	A	3588	ASN	2.2
1	B	2245	GLU	2.2
1	B	1949	ILE	2.2
1	A	21	GLU	2.2
1	B	208	THR	2.2
1	A	144	GLY	2.2
1	B	171	ALA	2.2
1	B	1828	TYR	2.2
1	B	1435	LEU	2.2
1	B	2257	PHE	2.2
1	B	2817	ILE	2.2
1	A	3569	GLU	2.2
1	A	2179	PRO	2.2
1	B	3923	VAL	2.2
1	A	1596	ILE	2.2
1	A	3021	LEU	2.2
1	A	48	GLY	2.2
1	A	3298	SER	2.2
1	B	1995	VAL	2.2
1	B	2856	LEU	2.2
1	A	3737	THR	2.2
1	A	2102	TYR	2.2
1	B	3566	LEU	2.2
1	A	2121	ALA	2.2
1	A	3573	SER	2.2
1	B	2256	SER	2.2
1	A	182	ILE	2.1
1	B	2299	ARG	2.1
1	B	7	TRP	2.1
1	B	1449	GLN	2.1
1	B	3565	ARG	2.1
1	A	1387	GLU	2.1
1	A	1421	TYR	2.1
1	B	39	LYS	2.1
1	A	2362	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	75	ALA	2.1
1	A	50	GLU	2.1
1	B	3814	ILE	2.1
1	B	2845	GLN	2.1
1	B	2918	GLY	2.1
1	B	1571	SER	2.1
1	A	3593	GLU	2.1
1	B	1441	ILE	2.1
1	B	1421	TYR	2.1
1	B	3574	GLN	2.1
1	B	78	HIS	2.1
1	B	3537	GLU	2.1
1	A	1	SER	2.1
1	B	153	MET	2.1
1	B	128	MET	2.0
1	B	2843	LEU	2.0
1	B	2318	ILE	2.0
1	A	1578	PHE	2.0
1	B	1423	ILE	2.0
1	A	1452	TRP	2.0
1	B	1504	ASN	2.0
1	A	1582	VAL	2.0
1	B	1578	PHE	2.0
1	B	2889	PHE	2.0
1	B	2810	GLU	2.0
1	A	1548	ILE	2.0
1	A	181	ARG	2.0
1	A	1435	LEU	2.0
1	B	1460	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MG	A	5097	1/1	0.99	0.40	3.20	59,59,59,59	0
3	SO4	A	5095	5/5	0.95	0.40	2.26	108,128,132,133	0
2	ATP	A	5093	31/31	0.95	0.32	1.55	72,125,180,196	0
3	SO4	B	5095	5/5	0.90	0.24	1.14	155,178,186,207	0
3	SO4	A	5094	5/5	0.95	0.29	0.93	109,114,153,161	0
2	ATP	B	5093	31/31	0.93	0.28	0.68	115,184,238,261	0
4	MG	B	5097	1/1	0.98	0.24	0.43	127,127,127,127	0
3	SO4	B	5094	5/5	0.86	0.30	0.27	151,165,190,192	0
3	SO4	A	5096	5/5	0.83	0.22	0.14	128,136,144,154	0
3	SO4	B	5096	5/5	0.96	0.14	-0.53	158,193,224,235	0

6.5 Other polymers ⓘ

There are no such residues in this entry.