



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 10:17 AM BST

PDB ID : 4AKH
Title : Dynein Motor Domain - AMPPNP complex
Authors : Schmidt, H.; Gleave, E.S.; Carter, A.P.
Deposited on : 2012-02-22
Resolution : 3.60 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

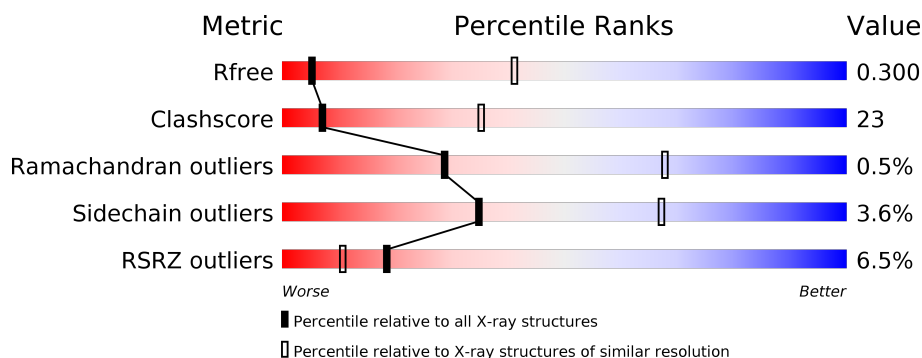
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2695	<div> <div>3%</div> <div>65%</div> <div>31%</div> <div>..</div> </div>
1	B	2695	<div> <div>10%</div> <div>67%</div> <div>30%</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
2	ATP	B	5093	-	-	X	-
4	SO4	A	5095	-	-	X	-
4	SO4	B	5096	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 41642 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.

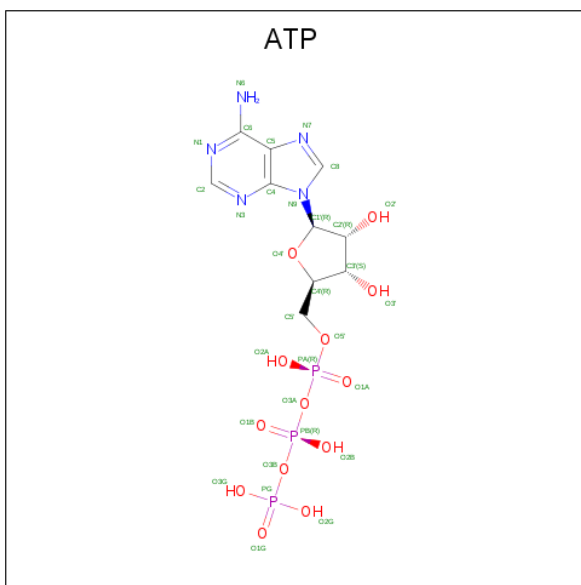
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

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 8 discrepancies between the modelled and reference sequences:

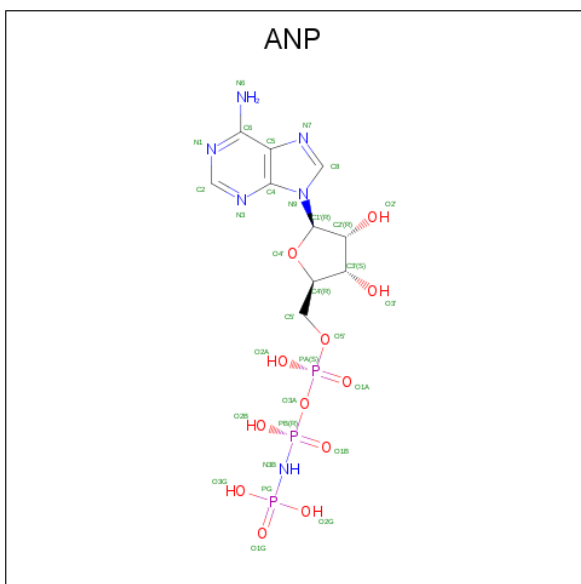
Chain	Residue	Modelled	Actual	Comment	Reference
A	218	SER	-	linker	UNP P36022
A	219	ASP	-	linker	UNP P36022
A	1630	ILE	LEU	conflict	UNP P36022
A	3782	ASP	GLU	conflict	UNP P36022
B	218	SER	-	linker	UNP P36022
B	219	ASP	-	linker	UNP P36022
B	1630	ILE	LEU	conflict	UNP P36022
B	3782	ASP	GLU	conflict	UNP P36022

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



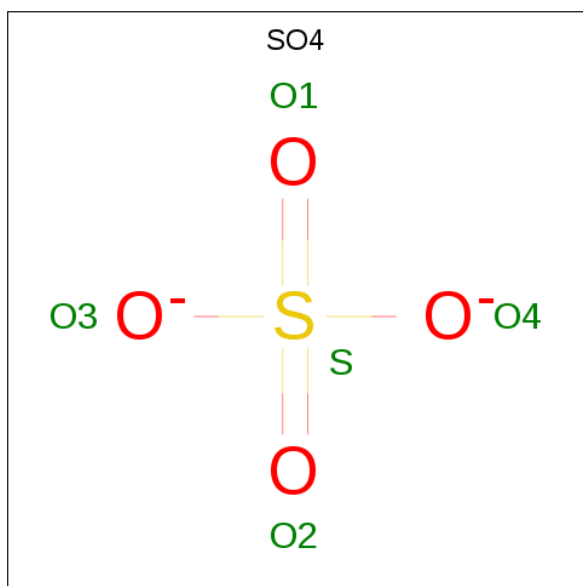
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

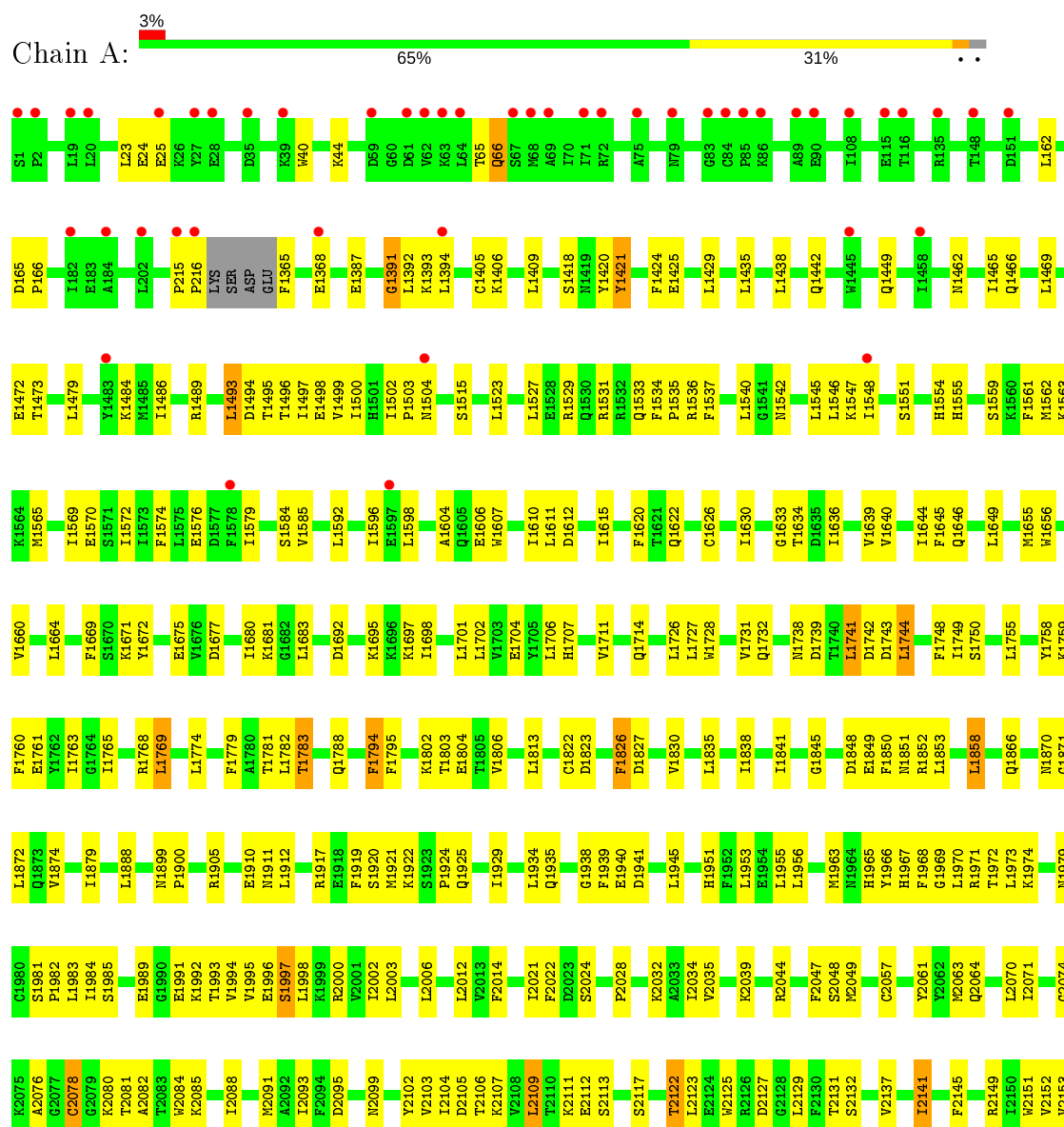
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

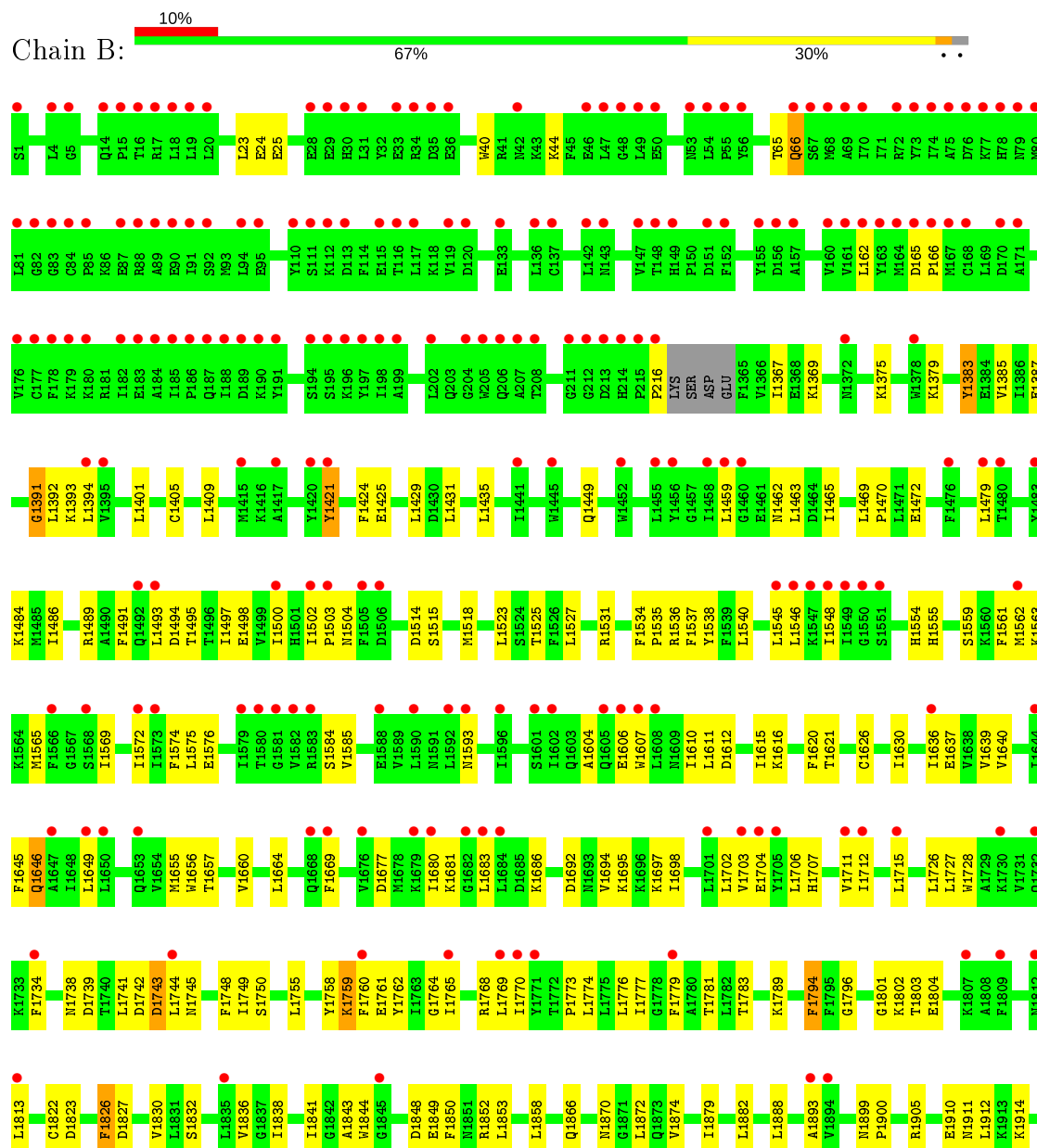
3 Residue-property plots

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







S5400	K3297	PRO	P2841	K2565	S2477	D3889	K2883	S2156	K2085	L1998	R1917
F3406	K3303	GLU	D2842	S2566	D2478	D3890	L2284	E2161	I2088	K1999	E1918
D3409	E3304	VAL	Q2845	Y2571	L2479	V2391	E2285	Y2162	I2088	R2001	F1919
K3425	K3305	LYS	Q2846	E2572	L2482	T2394	V2288	Y2169	M2091	L2003	M1921
K3426	K3306	GLU	R2747	L2573	L2483	L2395	V2289	Y2169	A2092	L2002	K1922
K3427	K3307	LEU	A2748	Y2574	L2484	L2396	L2290	Y2173	I2093	P2004	S1923
K3428	K3308	VAL	Y2849	Y2575	F2485	T2397	L2293	K2174	F2094	S2005	P1924
K3429	K3309	PHE	L2853	A2577	E2488	D3900	H2293	K2174	D2095	L2006	Q1925
K3430	K3310	THR	L2856	L2578	L2489	F2404	I2295	L2175	N2099	G2007	S1926
K3431	K3311	GLU	T2860	E2590	L2490	L2407	F2302	L2177	V2100	D2008	I1929
K3432	K3312	PRO	T2860	E2590	L2491	L2407	F2302	L2178	V2101	L2012	I1929
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K3435	K3315	LEU	L2867	T2623	L2494	S2410	D2306	E2182	I2104	L2013	Q1935
K3436	K3316	LEU	L2867	G2760	D2495	K2411	D2307	R2183	D2105	F2022	I1936
K3437	K3317	LEU	L2867	A2761	K2496	R2412	D2307	R2183	T2106	D2023	M1937
K3438	K3318	LEU	E2870	R2627	D2497	R2412	L2310	T2186	K2107	S2024	G1938
K3439	K3319	LEU	Q2871	Y2630	G2498	I2415	D2311	L2193	V2108	A2025	F1939
K3440	K3320	LEU	Q2872	T2631	S2499	P2420	D2312	L2193	L2109	G2026	E1940
K3441	K3321	LEU	L2873	T2635	V2503	G2421	D2313	E2195	L2110	T2027	D1941
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K3443	K3323	LEU	V2878	P2637	R2567	G2423	I2317	D2197	E2112	K2032	L1945
K3444	K3324	LEU	Q2871	R2638	K2567	Y2424	I2318	D2197	L2114	A2032	I1949
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K3447	K3327	LEU	V2878	T2640	M2510	M2427	L2322	T2202	N2118	K2039	L1956
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K3451	K3331	LEU	H2886	T2655	G2514	L2437	Q2335	L2214	E2124	F2047	Y1966
K3452	K3332	LEU	H2886	T2655	G2514	L2437	Q2335	L2214	H2125	S2048	H1967
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K3462	K3342	LEU	H2886	T2655	G2514	L2437	Q2335	L2214	D2140	L2070	L1983
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K3465	K3345	LEU	H2886	T2655	G2514	L2437	Q2335	L2214	I2141	L2072	G1988
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K3529	K3409	LEU	H2886	T2655	G2514	L2437	Q2335	L2214	L2276	T2083	E1996
K3530	K3410	LEU	H2886	T2655	G2514						

Q4022	I4023	V4024	V4027	R4028	I4029	L4033	E4038	E4039	E4040	L4059	S4060	W4061	W4062	L4063	Q4064	L4065	E4068	S4069	I4070	L4071	I4072	K4079	S4084	T4085	E4086	Q4087	L4088	W4092																					
Y3934	F3935	I3939	T3940	T3943	T3944	L3945	V3946	P3947	H3948	G3949	F3950	S3951	Y3955	D3958	C3959	D3960	F3963	A3964	S3965	L3968	L3972	K3978	I3979	I3980	P3981	W3982	A3983	I3984	Y3985	V3993	Y3994	G3995	I3998	K4002	D4003	L4004	E4005	V4006	K4009	V4014	F4015	V4016	E4017	I4020	L4021				
L3855	H3858	V3859	T3862	A3865	E3866	E3869	K3870	F3871	K3872	M3873	F3874	M3875	T3876	C3877	H3878	D3882	K3883	L3884	P3885	A3886	P3887	L3888	L3889	Q3890	R3894	F3895	Y3896	Y3897	E3898	D3899	T3900	P3901	T3906	W3911	G3912	S3913	Q3914	F3915	F3916	T3917	G3918	K3919	V3923	W3924	S3925	V3926	Y3927	F3930	
N3773	I3774	V3777	V3778	A3779	N3780	N3784	F3785	F3786	T3787	W3788	R3792	T3797	F3798	C3799	L3803	S3807	K3808	E3809	S3810	L3811	K3812	I3813	I3814	P3815	L3816	G3817	S3818	I3819	E3820	N3821	L3822	N3823	S3832	G3836	G3837	W3838	I3839	L3840	L3841	I3844	Q3845	M3846	S3847	L3848	S3849	W3850	V3851	K3852	Y3854
F3641	Y3642	G3643	I3644	S3645	I3646	V3656	F3657	I3658	LYS	LYS	SER	ARG	GLU	THR	ALA	ALA	ARG	T3669	R3670	V3671	I3674	L3677	Y3683	S3687	K3692	K3693	F3694	K3698	A3699	M3700	T3701	M3702	I3714	L3726	S3727	E3728	S3729	T3737	T3740	L3744	F3767	F3768	V3769	W3772					
K3544	D3547	L3548	I3549	K3550	L3551	E3554	Y3555	L3559	K3560	K3564	R3565	L3566	L3567	L3570	N3571	M3577	L3578	E3579	M3580	D3581	E3582	L3583	M3584	L3587	N3588	N3589	L3590	K3591	K3592	E3593	N3596	I3597	E3598	E3605	D3612	N3613	L3614	V3615	Y3618	G3622	K3631	L3632	G3636						

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	175.56Å 118.13Å 201.02Å 90.00° 90.29° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 70.46 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-3.60) 99.2 (70.46-3.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.58Å)	Xtriage
Refinement program	REFMAC 5.7.0019	Depositor
R, R_{free}	0.241 , 0.302 0.236 , 0.300	Depositor DCC
R_{free} test set	4767 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	127.5	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 117.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.074 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	41642	wwPDB-VP
Average B, all atoms (Å ²)	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, ANP, 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	0.53	0/21146	0.77	7/28618 (0.0%)
1	B	0.46	2/21146 (0.0%)	0.68	5/28618 (0.0%)
All	All	0.49	2/42292 (0.0%)	0.73	12/57236 (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	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3306	TRP	CE3-CZ3	-6.25	1.27	1.38
1	B	3306	TRP	CE2-CZ2	-5.22	1.30	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2012	LEU	CA-CB-CG	7.99	133.67	115.30
1	A	1741	LEU	CB-CG-CD1	6.69	122.38	111.00
1	A	3792	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	1782	LEU	CB-CG-CD2	-5.54	101.59	111.00
1	B	2460	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	2865	LEU	CB-CG-CD1	-5.47	101.69	111.00
1	A	2866	LEU	CA-CB-CG	5.27	127.43	115.30
1	B	2494	LEU	CB-CG-CD2	-5.25	102.08	111.00
1	A	2220	CYS	CA-CB-SG	-5.22	104.60	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2279	ARG	NE-CZ-NH1	-5.11	117.74	120.30
1	B	3306	TRP	N-CA-C	-5.02	97.43	111.00
1	B	1463	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2119	LEU	Peptide
1	B	2620	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20748	0	20206	952	0
1	B	20748	0	20206	909	0
2	A	31	0	12	8	0
2	B	31	0	12	17	0
3	A	31	0	13	7	0
3	B	31	0	13	7	0
4	A	10	0	0	3	0
4	B	10	0	0	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	41642	0	40462	1861	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 23.

All (1861) 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:CB	1:A:1365:PHE:CE1	2.05	1.38
1:B:3303:LYS:HD2	1:B:3306:TRP:CD1	1.67	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1620:PHE:HD1	1:B:1760:PHE:CZ	1.53	1.25
1:A:1368:GLU:HG2	1:A:1424:PHE:CZ	1.69	1.24
1:B:2467:THR:HB	1:B:2473:LEU:CD1	1.66	1.23
1:A:2061:TYR:CE1	1:A:2091:MET:SD	2.35	1.20
1:A:2061:TYR:HE1	1:A:2091:MET:SD	1.65	1.19
1:A:3777:VAL:HG11	1:A:3895:PHE:CE1	1.80	1.16
1:A:1970:LEU:HD13	1:A:1974:LYS:HE3	1.25	1.16
1:B:3534:LEU:CD1	1:B:3618:TYR:HE2	1.58	1.16
1:A:4033:LEU:CD1	1:A:4035:GLN:HB2	1.76	1.16
1:B:2111:LYS:HD3	1:B:2161:GLU:HG3	1.18	1.14
1:B:3023:LYS:CD	1:B:3567:LEU:HD21	1.77	1.14
1:A:2111:LYS:HD3	1:A:2161:GLU:HG3	1.23	1.14
1:B:2141:ILE:HG22	1:B:2145:PHE:HB2	1.27	1.14
1:A:3534:LEU:CD1	1:A:3618:TYR:HE2	1.61	1.13
1:A:215:PRO:CB	1:A:3475:ASN:HD22	1.61	1.13
1:B:2470:GLY:HA3	1:B:2473:LEU:HD21	1.29	1.13
1:A:3303:LYS:HA	1:A:3306:TRP:CD1	1.84	1.12
1:B:1970:LEU:CD2	1:B:1974:LYS:HE2	1.77	1.12
1:B:2404:PHE:CZ	1:B:2428:MET:SD	2.43	1.12
1:B:2107:LYS:HE3	1:B:2495:ASP:OD2	1.49	1.12
1:B:2707:VAL:HB	1:B:2712:LEU:HD11	1.22	1.11
1:A:2707:VAL:HB	1:A:2712:LEU:HD11	1.13	1.11
1:B:1421:TYR:O	1:B:1425:GLU:HB2	1.51	1.10
1:A:1620:PHE:HD1	1:A:1760:PHE:CZ	1.68	1.10
1:B:2112:GLU:HB3	1:B:2117:SER:HB2	1.32	1.10
1:B:2488:GLU:HB3	1:B:2491:LEU:HD12	1.13	1.10
1:A:2488:GLU:HB3	1:A:2491:LEU:HD12	1.09	1.09
1:B:3777:VAL:HG11	1:B:3895:PHE:CE1	1.88	1.09
1:A:2988:SER:HB3	1:A:2989:PRO:CD	1.83	1.09
1:A:1421:TYR:O	1:A:1425:GLU:HB2	1.50	1.08
1:A:2745:ILE:HG23	1:A:2756:MET:HE1	1.33	1.08
1:B:3525:ILE:HD11	1:B:3646:ILE:HG22	1.28	1.08
1:B:1409:LEU:HD21	1:B:1435:LEU:HB3	1.18	1.08
1:B:1992:LYS:HG3	1:B:2024:SER:HB2	1.22	1.08
1:B:3023:LYS:CD	1:B:3567:LEU:CD2	2.31	1.08
1:A:1822:CYS:HB2	1:A:1853:LEU:HD21	1.36	1.08
1:B:3024:LEU:HD11	1:B:3303:LYS:HG3	1.36	1.08
1:A:1992:LYS:CG	1:A:2024:SER:HB2	1.83	1.08
1:B:3777:VAL:HG11	1:B:3895:PHE:HE1	0.96	1.07
1:A:1645:PHE:HB3	1:A:1765:ILE:HG22	1.37	1.07
1:B:1645:PHE:HB3	1:B:1765:ILE:CG2	1.85	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2920:TRP:HB2	1:B:2989:PRO:HG3	1.10	1.07
1:B:2988:SER:HB3	1:B:2989:PRO:CD	1.84	1.07
1:B:2467:THR:HB	1:B:2473:LEU:HD12	1.32	1.06
1:A:1645:PHE:HB3	1:A:1765:ILE:CG2	1.85	1.06
1:B:1645:PHE:HB3	1:B:1765:ILE:HG22	1.34	1.06
1:A:2494:LEU:CD1	1:A:2498:GLY:HA2	1.86	1.05
1:B:2467:THR:CB	1:B:2473:LEU:HD12	1.86	1.05
1:B:1620:PHE:CD1	1:B:1760:PHE:CZ	2.43	1.05
1:B:2061:TYR:HE1	1:B:2091:MET:CE	1.70	1.05
1:A:2494:LEU:HD13	1:A:2498:GLY:CA	1.86	1.05
1:A:2707:VAL:CB	1:A:2712:LEU:HD11	1.86	1.05
1:B:2494:LEU:HD13	1:B:2498:GLY:CA	1.86	1.04
1:A:3777:VAL:HG11	1:A:3895:PHE:HE1	0.90	1.04
1:A:1409:LEU:HD21	1:A:1435:LEU:HB3	1.36	1.03
1:B:2494:LEU:CD1	1:B:2498:GLY:HA2	1.88	1.03
1:A:1823:ASP:HB2	1:A:1852:ARG:O	1.58	1.03
1:A:3303:LYS:O	1:A:3306:TRP:HD1	1.41	1.03
1:B:1620:PHE:CD1	1:B:1760:PHE:HZ	1.73	1.03
1:B:2386:MET:HB2	1:B:2627:ARG:HD3	1.35	1.03
1:A:2476:LYS:H	1:A:2476:LYS:CD	1.66	1.02
1:A:3525:ILE:HD11	1:A:3646:ILE:HG22	1.41	1.02
1:B:2779:LEU:HD23	1:B:2812:ARG:O	1.60	1.02
1:B:3023:LYS:HD3	1:B:3567:LEU:HD21	1.37	1.02
1:B:2061:TYR:CE1	1:B:2091:MET:SD	2.53	1.02
1:A:2920:TRP:HB2	1:A:2989:PRO:HG3	1.03	1.02
1:B:2386:MET:CB	1:B:2627:ARG:HD3	1.90	1.02
1:B:3303:LYS:HD2	1:B:3306:TRP:HD1	0.87	1.02
1:A:3530:PHE:CD1	1:A:3618:TYR:HD2	1.77	1.01
1:B:2391:VAL:HG23	1:B:2426:MET:SD	2.00	1.01
1:A:1983:LEU:HD21	1:A:2000:ARG:HD2	1.36	1.01
1:A:1992:LYS:HG3	1:A:2024:SER:HB2	1.40	1.01
1:A:2988:SER:CB	1:A:2989:PRO:HD2	1.91	1.01
1:A:2107:LYS:HE3	1:A:2495:ASP:OD2	1.58	1.01
1:A:4033:LEU:HD11	1:A:4035:GLN:HB2	1.43	1.00
1:B:2494:LEU:HD13	1:B:2498:GLY:HA2	1.02	1.00
1:B:1421:TYR:CE2	1:B:1425:GLU:CG	2.45	1.00
1:A:2488:GLU:CB	1:A:2491:LEU:HD12	1.89	1.00
1:B:2988:SER:HB3	1:B:2989:PRO:HD2	1.03	1.00
1:B:1822:CYS:HB2	1:B:1853:LEU:HD21	1.41	1.00
1:B:1866:GLN:OE1	1:B:1911:ASN:HB2	1.61	0.99
1:A:1983:LEU:HD22	1:A:1997:SER:OG	1.63	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2081:THR:HB	2:B:5093:ATP:O2A	1.60	0.99
1:A:215:PRO:CB	1:A:3475:ASN:ND2	2.24	0.99
1:B:3023:LYS:HD2	1:B:3567:LEU:CD2	1.92	0.99
1:A:1421:TYR:CE2	1:A:1425:GLU:CG	2.46	0.99
1:A:1421:TYR:CE2	1:A:1425:GLU:HG3	1.97	0.99
1:B:3534:LEU:CD1	1:B:3618:TYR:CE2	2.44	0.99
1:B:2707:VAL:CB	1:B:2712:LEU:HD11	1.92	0.99
1:B:1421:TYR:CE2	1:B:1425:GLU:HG3	1.97	0.99
1:A:3777:VAL:CG1	1:A:3895:PHE:HE1	1.75	0.98
1:A:2988:SER:HB3	1:A:2989:PRO:HD2	1.00	0.98
1:B:3645:SER:HB3	1:B:3890:GLN:HE21	1.26	0.97
1:A:3534:LEU:CD1	1:A:3618:TYR:CE2	2.46	0.97
1:B:1970:LEU:HD21	1:B:1974:LYS:HE2	1.46	0.97
1:A:3534:LEU:HD12	1:A:3618:TYR:HE2	1.26	0.97
1:A:3406:PHE:HB2	1:A:3513:VAL:CG1	1.93	0.97
1:B:1645:PHE:CB	1:B:1765:ILE:HG22	1.94	0.97
1:B:2488:GLU:CB	1:B:2491:LEU:HD12	1.94	0.97
1:A:2494:LEU:HD13	1:A:2498:GLY:HA2	0.98	0.97
1:B:1744:LEU:HA	1:B:1760:PHE:CE2	1.99	0.97
1:B:1823:ASP:HB2	1:B:1852:ARG:O	1.64	0.97
1:B:3737:THR:HB	1:B:3740:THR:OG1	1.65	0.97
1:A:2920:TRP:CB	1:A:2989:PRO:HG3	1.95	0.96
1:A:3024:LEU:HD11	1:A:3303:LYS:HG3	1.43	0.96
1:B:2988:SER:CB	1:B:2989:PRO:HD2	1.95	0.96
1:B:3534:LEU:HD12	1:B:3618:TYR:HE2	1.31	0.96
1:A:3946:VAL:HG12	1:A:3950:PHE:O	1.66	0.96
1:B:1992:LYS:CG	1:B:2024:SER:HB2	1.94	0.96
1:A:2488:GLU:HB3	1:A:2491:LEU:CD1	1.95	0.95
1:B:1983:LEU:HG	1:B:1993:THR:HG23	1.45	0.95
1:A:2787:HIS:HA	1:A:3460:PRO:HD2	1.43	0.95
1:B:2787:HIS:HA	1:B:3460:PRO:HD2	1.47	0.95
1:B:3023:LYS:HE2	1:B:3567:LEU:HG	1.49	0.95
1:B:3530:PHE:CD1	1:B:3618:TYR:HD2	1.85	0.94
1:B:2755:HIS:HB2	1:B:2911:ARG:O	1.66	0.94
1:B:3777:VAL:CG1	1:B:3895:PHE:HE1	1.79	0.94
1:B:1956:LEU:HB3	1:B:1968:PHE:HE2	1.32	0.94
1:A:2332:GLY:HA2	1:A:2335:GLN:HB2	1.50	0.93
1:B:2380:LEU:HD12	1:B:2577:ALA:HB1	1.49	0.93
1:B:1630:ILE:HG22	1:B:1655:MET:SD	2.09	0.93
1:A:2380:LEU:HD12	1:A:2577:ALA:CB	1.98	0.93
1:B:2488:GLU:HB3	1:B:2491:LEU:CD1	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1421:TYR:CZ	1:A:1425:GLU:HG3	2.04	0.93
1:B:3946:VAL:HG12	1:B:3950:PHE:O	1.69	0.93
1:B:3023:LYS:HD2	1:B:3567:LEU:HD21	1.51	0.92
1:B:3534:LEU:HD13	1:B:3618:TYR:HE2	1.31	0.92
1:B:2853:LEU:HD21	1:B:2870:GLU:HG3	1.52	0.92
1:B:1939:PHE:CD2	1:B:1940:GLU:O	2.23	0.92
1:A:3656:VAL:HG13	1:A:3677:LEU:HB3	1.52	0.92
1:A:3303:LYS:HD2	1:A:3306:TRP:CD1	2.04	0.92
1:A:3534:LEU:HD12	1:A:3618:TYR:CE2	2.03	0.92
1:B:1535:PRO:C	1:B:1841:ILE:HD11	1.90	0.92
1:A:2787:HIS:HA	1:A:3460:PRO:CD	1.99	0.91
1:B:2061:TYR:HE1	1:B:2091:MET:SD	1.91	0.91
1:B:2332:GLY:HA2	1:B:2335:GLN:HB2	1.52	0.91
1:A:3303:LYS:HA	1:A:3306:TRP:NE1	1.85	0.91
1:A:3303:LYS:O	1:A:3306:TRP:CD1	2.24	0.91
1:B:1956:LEU:HB3	1:B:1968:PHE:CE2	2.06	0.91
1:A:1645:PHE:CB	1:A:1765:ILE:HG22	2.00	0.91
1:B:1421:TYR:CZ	1:B:1425:GLU:HG3	2.05	0.91
1:A:2707:VAL:HB	1:A:2712:LEU:CD1	2.01	0.91
1:A:3737:THR:HB	1:A:3740:THR:OG1	1.70	0.90
1:A:1983:LEU:HD21	1:A:2000:ARG:CD	2.01	0.90
1:B:2380:LEU:CD1	1:B:2577:ALA:CB	2.49	0.90
1:A:1823:ASP:CB	1:A:1852:ARG:O	2.20	0.90
1:B:2112:GLU:HB3	1:B:2117:SER:CB	2.00	0.90
1:B:2380:LEU:HD12	1:B:2577:ALA:CB	2.01	0.90
1:A:2137:VAL:O	1:A:2141:ILE:HG23	1.72	0.90
1:A:3530:PHE:CD1	1:A:3618:TYR:CD2	2.60	0.90
1:B:2061:TYR:HE1	1:B:2091:MET:HE1	1.37	0.90
1:A:1620:PHE:CD1	1:A:1760:PHE:CZ	2.60	0.90
1:B:3303:LYS:CD	1:B:3306:TRP:HD1	1.82	0.90
1:B:1726:LEU:CD1	1:B:3984:GLN:HB3	2.02	0.89
1:B:1774:LEU:HD21	1:B:1922:LYS:O	1.72	0.89
1:B:2404:PHE:HZ	1:B:2428:MET:SD	1.94	0.89
1:B:2131:THR:HG22	1:B:2176:LEU:HD21	1.55	0.89
1:A:2274:HIS:HE1	1:A:2326:LEU:O	1.54	0.89
1:A:2787:HIS:HA	1:A:3460:PRO:CG	2.02	0.89
1:B:1992:LYS:HE2	1:B:2024:SER:O	1.71	0.89
1:A:2476:LYS:H	1:A:2476:LYS:HD3	1.37	0.89
1:B:2111:LYS:HD3	1:B:2161:GLU:CG	2.00	0.89
1:B:2404:PHE:CE1	1:B:2428:MET:SD	2.66	0.89
1:B:2467:THR:HB	1:B:2473:LEU:HD11	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1939:PHE:CD2	1:A:1940:GLU:O	2.26	0.89
1:A:2757:MET:CE	1:A:2912:CYS:HB2	2.01	0.89
1:B:3303:LYS:CD	1:B:3306:TRP:CD1	2.54	0.89
1:A:2563:SER:HB3	1:A:2566:SER:H	1.37	0.88
1:B:3406:PHE:HB2	1:B:3513:VAL:CG1	2.04	0.88
1:A:1924:PRO:HB2	1:A:1929:ILE:HD11	1.55	0.88
1:A:1940:GLU:HB2	1:A:1989:GLU:O	1.72	0.88
1:B:1535:PRO:HB2	1:B:1841:ILE:HG13	1.53	0.88
1:A:1535:PRO:HB2	1:A:1841:ILE:HG13	1.53	0.88
1:A:2745:ILE:HG23	1:A:2756:MET:CE	2.04	0.88
1:B:1604:ALA:HA	1:B:1607:TRP:CD1	2.09	0.88
1:A:1979:ASN:O	1:A:1983:LEU:HD13	1.73	0.87
1:B:1409:LEU:HD21	1:B:1435:LEU:CB	2.04	0.87
1:B:2224:SER:O	2:B:5093:ATP:H2	1.57	0.87
1:A:1535:PRO:C	1:A:1841:ILE:HD11	1.94	0.87
1:A:1992:LYS:HE2	1:A:2024:SER:O	1.74	0.87
1:A:3024:LEU:CD1	1:A:3303:LYS:HG3	2.03	0.87
1:A:1744:LEU:HA	1:A:1760:PHE:CE2	2.11	0.86
1:B:2563:SER:HB3	1:B:2566:SER:H	1.38	0.86
1:B:3024:LEU:CD1	1:B:3303:LYS:HG3	2.05	0.86
1:A:2111:LYS:HD3	1:A:2161:GLU:CG	2.04	0.86
1:B:2787:HIS:HA	1:B:3460:PRO:CD	2.04	0.86
1:B:3534:LEU:HD12	1:B:3618:TYR:CE2	2.10	0.86
1:A:3534:LEU:HD13	1:A:3618:TYR:HE2	1.39	0.86
1:A:2412:ARG:HH11	1:A:2412:ARG:HB2	1.41	0.86
1:A:3525:ILE:CD1	1:A:3646:ILE:HG22	2.06	0.85
1:B:1744:LEU:HA	1:B:1760:PHE:CD2	2.10	0.85
1:B:1926:SER:CB	1:B:1970:LEU:HD12	2.06	0.85
1:B:2745:ILE:HG23	1:B:2756:MET:HE1	1.57	0.85
1:A:3923:VAL:HG23	1:A:4038:GLU:HA	1.58	0.85
1:B:1996:GLU:O	1:B:2000:ARG:HG3	1.76	0.85
1:B:2787:HIS:HA	1:B:3460:PRO:CG	2.07	0.85
1:A:1368:GLU:HG2	1:A:1424:PHE:HZ	1.36	0.85
1:A:2380:LEU:CD1	1:A:2577:ALA:CB	2.54	0.85
1:A:2380:LEU:HD12	1:A:2577:ALA:HB1	1.56	0.85
1:B:1425:GLU:OE2	1:B:1429:LEU:HG	1.76	0.85
1:A:166:PRO:CB	1:A:3476:ARG:HD3	2.06	0.84
1:B:1726:LEU:HD12	1:B:3984:GLN:HB3	1.57	0.84
1:A:1866:GLN:OE1	1:A:1911:ASN:HB2	1.77	0.84
1:A:2446:SER:H	1:A:2449:THR:CG2	1.90	0.84
1:A:1726:LEU:HD12	1:A:3984:GLN:HB3	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2081:THR:HB	2:B:5093:ATP:PA	2.17	0.84
1:A:216:PRO:CB	1:A:1365:PHE:CZ	2.59	0.84
1:A:1620:PHE:HD1	1:A:1760:PHE:HZ	1.22	0.84
1:A:2061:TYR:CE1	1:A:2091:MET:CE	2.60	0.84
1:B:1425:GLU:OE2	1:B:1429:LEU:CG	2.24	0.84
1:A:2920:TRP:HB2	1:A:2989:PRO:CG	1.99	0.84
1:A:1368:GLU:CG	1:A:1424:PHE:CZ	2.58	0.83
1:A:3303:LYS:CA	1:A:3306:TRP:CD1	2.61	0.83
1:A:2787:HIS:HA	1:A:3460:PRO:HG2	1.57	0.83
1:A:3509:LEU:CD1	1:A:3513:VAL:HG21	2.08	0.83
1:B:1983:LEU:HD23	1:B:1993:THR:O	1.78	0.83
1:B:2141:ILE:HG22	1:B:2145:PHE:CB	2.06	0.83
1:B:2623:THR:HG21	3:B:5094:ANP:O3'	1.78	0.83
1:A:2476:LYS:N	1:A:2476:LYS:HD3	1.90	0.83
1:A:1604:ALA:HA	1:A:1607:TRP:CD1	2.13	0.83
1:B:1421:TYR:O	1:B:1425:GLU:CB	2.26	0.83
1:A:2064:GLN:OE1	1:A:2151:TRP:HH2	1.61	0.83
1:B:2274:HIS:HE1	1:B:2326:LEU:O	1.60	0.83
1:A:1387:GLU:HB3	1:A:1393:LYS:HG2	1.58	0.83
1:A:1409:LEU:HD21	1:A:1435:LEU:CB	2.07	0.83
1:B:1392:LEU:HD13	1:B:1393:LYS:N	1.93	0.83
1:B:1562:MET:HB3	1:B:1569:ILE:HD11	1.61	0.83
1:A:1421:TYR:O	1:A:1425:GLU:CB	2.26	0.83
1:B:2920:TRP:CB	1:B:2989:PRO:HG3	2.04	0.83
1:A:1562:MET:HB3	1:A:1569:ILE:HD11	1.59	0.83
1:A:2386:MET:HB2	1:A:2627:ARG:HD3	1.61	0.83
1:B:2787:HIS:HA	1:B:3460:PRO:HG2	1.59	0.83
1:A:3534:LEU:HD11	1:A:3614:LEU:HD23	1.60	0.83
1:A:1604:ALA:HA	1:A:1607:TRP:NE1	1.94	0.82
1:B:1940:GLU:HB2	1:B:1989:GLU:O	1.77	0.82
1:B:2472:THR:CG2	1:B:2524:VAL:HG22	2.08	0.82
1:B:1409:LEU:CD2	1:B:1435:LEU:HB3	2.06	0.82
1:B:4065:LEU:HD11	1:B:4070:ILE:HD11	1.61	0.82
1:B:1421:TYR:CE2	1:B:1425:GLU:HG2	2.13	0.82
1:B:1574:PHE:HB3	1:B:1576:GLU:H	1.45	0.82
1:A:1392:LEU:HD13	1:A:1393:LYS:N	1.95	0.82
1:A:1569:ILE:HA	1:A:1584:SER:HA	1.59	0.82
1:B:2513:GLN:O	1:B:2526:ILE:HG13	1.78	0.82
1:A:1365:PHE:CZ	1:A:1420:TYR:CD1	2.68	0.82
1:B:1802:LYS:HG2	1:B:1921:MET:HG3	1.61	0.82
1:A:1462:ASN:HB2	1:A:1465:ILE:HG22	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3534:LEU:HD13	1:B:3618:TYR:CE2	2.10	0.82
1:A:1421:TYR:CE2	1:A:1425:GLU:HG2	2.14	0.81
1:A:2755:HIS:HB2	1:A:2911:ARG:O	1.80	0.81
1:B:1924:PRO:HB2	1:B:1929:ILE:HD11	1.61	0.81
1:A:1779:PHE:O	1:A:1783:THR:HG22	1.80	0.81
1:B:3645:SER:HB3	1:B:3890:GLN:NE2	1.96	0.81
1:A:2224:SER:O	2:A:5093:ATP:H2	1.63	0.81
1:B:2106:THR:OG1	1:B:2154:PHE:HB3	1.81	0.81
1:A:1630:ILE:HG22	1:A:1655:MET:SD	2.21	0.81
1:A:1970:LEU:HD13	1:A:1974:LYS:CE	2.08	0.81
1:A:4033:LEU:HD13	1:A:4035:GLN:HB2	1.61	0.81
1:A:1645:PHE:CB	1:A:1765:ILE:CG2	2.57	0.80
1:A:2493:LYS:HG3	1:A:2494:LEU:H	1.45	0.80
1:B:1970:LEU:CD2	1:B:1974:LYS:CE	2.59	0.80
1:B:3799:LYS:O	1:B:3803:LEU:HG	1.80	0.80
1:A:2112:GLU:HB3	1:A:2117:SER:HB2	1.62	0.80
1:B:1823:ASP:CB	1:B:1852:ARG:O	2.29	0.80
1:A:2111:LYS:NZ	1:A:2161:GLU:HG2	1.96	0.80
1:A:2362:ALA:HB3	1:A:2365:LYS:O	1.82	0.80
1:A:3700:MET:HB3	1:A:4085:THR:HG21	1.64	0.80
1:A:2225:LYS:HA	2:A:5093:ATP:C2	2.16	0.80
1:A:1992:LYS:HG2	1:A:2024:SER:HB2	1.62	0.80
1:B:1604:ALA:HA	1:B:1607:TRP:NE1	1.97	0.80
1:B:3509:LEU:CD1	1:B:3513:VAL:HG21	2.12	0.79
1:A:3998:ILE:CG2	1:A:4004:LEU:HG	2.12	0.79
1:A:1822:CYS:SG	1:A:1850:PHE:HA	2.22	0.79
1:B:2141:ILE:CG2	1:B:2145:PHE:HB2	2.09	0.79
1:B:3023:LYS:HD2	1:B:3567:LEU:HD23	1.64	0.79
1:A:2410:SER:C	1:A:2411:LYS:HG3	2.03	0.79
1:A:2386:MET:CB	1:A:2627:ARG:HD3	2.13	0.78
1:A:2513:GLN:O	1:A:2526:ILE:HG13	1.82	0.78
1:B:2111:LYS:NZ	1:B:2161:GLU:HG2	1.99	0.78
1:A:3792:ARG:HB2	1:A:3955:TYR:CD2	2.18	0.78
1:B:1939:PHE:HD2	1:B:1940:GLU:O	1.64	0.78
1:A:2512:LYS:O	1:A:2513:GLN:HB2	1.82	0.78
1:A:4033:LEU:CD1	1:A:4035:GLN:CB	2.61	0.78
1:A:2106:THR:OG1	1:A:2154:PHE:HB3	1.83	0.78
1:A:2631:THR:O	1:A:2635:THR:HG22	1.81	0.78
1:B:3530:PHE:CD1	1:B:3618:TYR:CD2	2.70	0.78
1:B:3656:VAL:HG13	1:B:3677:LEU:HB3	1.64	0.78
1:A:2941:THR:HG22	1:A:2942:ASP:H	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2181:GLY:O	1:A:2182:GLU:HG3	1.84	0.78
1:B:2061:TYR:CE1	1:B:2091:MET:HE1	2.18	0.78
1:A:2552:ARG:HG2	1:A:2552:ARG:HH11	1.48	0.78
1:A:1970:LEU:HD12	1:A:1971:ARG:N	1.98	0.77
1:B:1967:HIS:C	1:B:1968:PHE:HD1	1.88	0.77
1:B:3024:LEU:HD11	1:B:3303:LYS:CG	2.14	0.77
1:A:1922:LYS:NZ	1:A:4004:LEU:HD12	1.99	0.77
1:B:3919:LYS:HZ3	1:B:4038:GLU:CD	1.87	0.77
1:B:2745:ILE:HG12	1:B:2756:MET:HE3	1.66	0.77
1:A:2175:ILE:HG12	1:A:2183:ARG:HB3	1.64	0.77
1:A:2757:MET:HE3	1:A:2912:CYS:HB2	1.64	0.77
1:A:1956:LEU:HB3	1:A:1968:PHE:CE2	2.20	0.77
1:B:3774:ILE:O	1:B:3778:VAL:HG23	1.83	0.77
1:A:1939:PHE:HD2	1:A:1940:GLU:O	1.67	0.77
1:A:2336:ARG:HD3	1:A:2355:ASP:OD2	1.84	0.77
1:A:2446:SER:H	1:A:2449:THR:HG23	1.49	0.77
1:A:2745:ILE:HG12	1:A:2756:MET:HE3	1.66	0.77
1:A:2061:TYR:CD1	1:A:2091:MET:SD	2.78	0.77
1:B:2107:LYS:HE2	1:B:2499:SER:HB3	1.66	0.77
1:B:3871:PHE:CZ	1:B:3873:MET:HB2	2.20	0.77
1:A:3946:VAL:CG1	1:A:3950:PHE:O	2.32	0.76
1:B:2420:PRO:HD3	1:B:2536:ASN:HD21	1.50	0.76
1:A:2103:VAL:CG1	1:A:2155:ASP:OD1	2.33	0.76
1:A:3303:LYS:C	1:A:3306:TRP:HD1	1.87	0.76
1:B:1645:PHE:CB	1:B:1765:ILE:CG2	2.59	0.76
1:B:3946:VAL:CG1	1:B:3950:PHE:O	2.33	0.76
1:A:1495:THR:HG22	1:A:1497:ILE:HG22	1.67	0.76
1:B:2512:LYS:O	1:B:2513:GLN:HB2	1.84	0.76
1:A:216:PRO:CB	1:A:1365:PHE:CD1	2.69	0.76
1:A:1922:LYS:HZ1	1:A:4004:LEU:HD12	1.49	0.76
1:B:3473:ALA:HB3	1:B:3476:ARG:O	1.85	0.76
1:B:3998:ILE:HG21	1:B:4004:LEU:HG	1.66	0.76
1:A:2766:LYS:HE3	1:A:2892:CYS:SG	2.26	0.76
1:B:2380:LEU:HD11	1:B:2577:ALA:CB	2.15	0.76
1:B:3019:VAL:O	1:B:3023:LYS:HG3	1.86	0.76
1:B:3566:LEU:HA	1:B:3583:LEU:CD2	2.16	0.76
1:A:2061:TYR:CD1	1:A:2091:MET:CE	2.69	0.76
1:A:2787:HIS:CA	1:A:3460:PRO:HD2	2.14	0.76
1:A:1849:GLU:HG2	1:A:1899:ASN:ND2	2.01	0.76
1:A:3406:PHE:HB2	1:A:3513:VAL:HG11	1.65	0.75
1:A:3774:ILE:O	1:A:3778:VAL:HG23	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2467:THR:CB	1:B:2473:LEU:CD1	2.50	0.75
1:B:2707:VAL:HB	1:B:2712:LEU:CD1	2.11	0.75
1:B:3923:VAL:HG23	1:B:4038:GLU:HA	1.68	0.75
1:B:2446:SER:H	1:B:2449:THR:HG23	1.52	0.75
1:B:3998:ILE:CG2	1:B:4004:LEU:HG	2.16	0.75
1:A:2107:LYS:HE2	1:A:2499:SER:HB3	1.66	0.75
1:A:2003:LEU:HA	1:A:2006:LEU:HD12	1.66	0.75
1:B:1940:GLU:HG3	1:B:1941:ASP:H	1.52	0.75
1:A:2779:LEU:HD23	1:A:2812:ARG:O	1.87	0.75
1:B:1405:CYS:O	1:B:1409:LEU:HG	1.86	0.75
1:B:2707:VAL:CG1	1:B:2712:LEU:CD1	2.64	0.75
1:B:2176:LEU:O	1:B:2183:ARG:HA	1.87	0.74
1:B:2380:LEU:CD1	1:B:2577:ALA:HB1	2.15	0.74
1:A:2220:CYS:SG	1:A:2224:SER:HB2	2.27	0.74
1:A:3618:TYR:CD1	1:A:3618:TYR:N	2.54	0.74
1:B:2175:ILE:HG12	1:B:2183:ARG:HB3	1.68	0.74
1:B:2476:LYS:HZ1	1:B:2528:ARG:HD2	1.52	0.74
1:B:3023:LYS:HE2	1:B:3567:LEU:CG	2.16	0.74
1:A:3998:ILE:HG21	1:A:4004:LEU:HG	1.69	0.74
1:B:2081:THR:CB	2:B:5093:ATP:O2A	2.28	0.74
1:B:2517:LYS:HE2	1:B:2520:GLU:OE1	1.88	0.74
1:A:1707:HIS:O	1:A:1711:VAL:HG23	1.88	0.74
1:A:1922:LYS:HE2	1:A:3999:ASP:O	1.87	0.74
1:B:1630:ILE:CG2	1:B:1655:MET:SD	2.74	0.74
1:B:2112:GLU:CB	1:B:2117:SER:HB2	2.15	0.74
1:B:2220:CYS:CB	2:B:5093:ATP:C6	2.71	0.74
1:A:2152:VAL:HG12	1:A:2154:PHE:HE1	1.51	0.74
1:A:1965:HIS:HD2	1:A:2212:LEU:HD21	1.53	0.74
1:B:2380:LEU:CD1	1:B:2577:ALA:HB2	2.18	0.73
1:A:3566:LEU:HA	1:A:3583:LEU:CD2	2.18	0.73
1:B:2203:THR:HG22	1:B:2205:ALA:H	1.51	0.73
1:B:3618:TYR:CD1	1:B:3618:TYR:N	2.51	0.73
1:A:1559:SER:HB3	1:A:1572:ILE:HG22	1.70	0.73
1:A:1938:GLY:O	1:A:1989:GLU:HB3	1.88	0.73
1:A:3530:PHE:HD1	1:A:3618:TYR:HD2	1.36	0.73
1:B:1535:PRO:HB2	1:B:1841:ILE:CG1	2.18	0.73
1:B:2032:LYS:O	1:B:2035:VAL:HG12	1.86	0.73
1:B:3792:ARG:HB2	1:B:3955:TYR:CD2	2.23	0.73
1:A:3645:SER:HB3	1:A:3890:GLN:NE2	2.04	0.73
1:A:2425:THR:CG2	3:A:5094:ANP:O3G	2.37	0.73
1:A:1493:LEU:HD23	1:A:1498:GLU:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1527:LEU:CD2	1:A:1545:LEU:HD22	2.18	0.72
1:A:3534:LEU:HD13	1:A:3618:TYR:CE2	2.18	0.72
1:B:2476:LYS:HG2	1:B:2478:ASP:O	1.88	0.72
1:B:1392:LEU:HD13	1:B:1392:LEU:C	2.10	0.72
1:B:3566:LEU:HA	1:B:3583:LEU:HD21	1.71	0.72
1:A:2176:LEU:O	1:A:2183:ARG:HA	1.89	0.72
1:A:3303:LYS:CA	1:A:3306:TRP:HD1	2.03	0.72
1:A:3877:CYS:SG	1:A:3884:LEU:HD22	2.29	0.72
1:B:3406:PHE:HB2	1:B:3513:VAL:HG12	1.70	0.72
1:A:3509:LEU:HD12	1:A:3513:VAL:CG2	2.20	0.72
1:B:2446:SER:H	1:B:2449:THR:CG2	2.01	0.72
1:B:3851:VAL:HG13	1:B:3855:LEU:HD23	1.72	0.72
1:A:3330:TYR:OH	1:A:3346:LEU:HD22	1.90	0.72
1:B:1569:ILE:HA	1:B:1584:SER:HA	1.71	0.72
1:A:3777:VAL:CG1	1:A:3895:PHE:CE1	2.60	0.72
1:A:2107:LYS:CE	1:A:2495:ASP:OD2	2.36	0.71
1:A:2380:LEU:CD1	1:A:2577:ALA:HB2	2.20	0.71
1:B:1706:LEU:HD22	1:B:1935:GLN:HG2	1.72	0.71
1:B:2476:LYS:NZ	1:B:2528:ARG:HD2	2.04	0.71
1:A:2061:TYR:CE1	1:A:2091:MET:HE1	2.24	0.71
1:A:2336:ARG:CD	1:A:2355:ASP:OD2	2.38	0.71
1:B:2448:ASP:HB2	1:B:2829:GLU:OE1	1.91	0.71
1:B:3618:TYR:HD1	1:B:3618:TYR:N	1.87	0.71
1:B:2061:TYR:CE1	1:B:2091:MET:CE	2.63	0.71
1:B:3534:LEU:HD11	1:B:3614:LEU:HD23	1.73	0.71
1:B:3792:ARG:HB2	1:B:3955:TYR:CE2	2.26	0.71
1:A:2293:HIS:CE1	1:A:2409:ASN:HB3	2.25	0.71
1:B:1540:LEU:CD1	1:B:1548:ILE:HD11	2.21	0.71
1:A:2960:THR:HB	1:A:2963:ASP:HB2	1.72	0.71
1:B:1852:ARG:HG3	1:B:1852:ARG:O	1.91	0.71
1:A:1626:CYS:SG	1:A:1639:VAL:HG11	2.31	0.71
1:A:2549:ARG:HE	2:A:5093:ATP:PG	2.13	0.71
1:A:4065:LEU:HD11	1:A:4070:ILE:HD11	1.72	0.71
1:B:1620:PHE:HB2	1:B:1760:PHE:CE1	2.26	0.71
1:B:2111:LYS:CD	1:B:2161:GLU:HG3	2.10	0.71
1:B:2572:GLU:CD	1:B:2590:GLU:HG3	2.11	0.71
1:A:2103:VAL:HG13	1:A:2155:ASP:OD1	1.91	0.71
1:A:3566:LEU:O	1:A:3570:LEU:HG	1.91	0.71
1:B:1738:ASN:O	1:B:1739:ASP:OD1	2.09	0.71
1:B:2787:HIS:CA	1:B:3460:PRO:HD2	2.20	0.71
1:A:2222:ILE:HG23	1:A:2284:LEU:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3024:LEU:HD11	1:A:3303:LYS:CG	2.17	0.70
1:A:3473:ALA:HB3	1:A:3476:ARG:O	1.91	0.70
1:B:2420:PRO:HB2	1:B:2620:ARG:NH2	2.06	0.70
1:A:1620:PHE:CZ	1:A:1743:ASP:HB3	2.25	0.70
1:A:4033:LEU:HD13	1:A:4035:GLN:CB	2.22	0.70
1:B:1938:GLY:O	1:B:1989:GLU:HB3	1.92	0.70
1:B:1953:LEU:CD1	1:B:1973:LEU:HB3	2.21	0.70
1:A:2891:ILE:HD11	1:A:2903:ILE:HD11	1.73	0.70
1:B:3737:THR:HB	1:B:3740:THR:HG1	1.53	0.70
1:A:2563:SER:HB2	1:A:2566:SER:OG	1.92	0.70
1:B:2472:THR:HG21	1:B:2524:VAL:HG22	1.74	0.70
1:A:3459:ASP:OD2	1:A:3461:ILE:HG12	1.92	0.70
1:B:3577:MET:O	1:B:3579:GLU:N	2.24	0.70
1:A:3951:SER:HB2	1:A:4002:LYS:HD2	1.73	0.70
1:B:2064:GLN:OE1	1:B:2151:TRP:HH2	1.74	0.70
1:A:216:PRO:CB	1:A:1365:PHE:HE1	1.99	0.70
1:A:3935:PHE:HB2	1:A:4014:VAL:HG11	1.73	0.70
1:A:2225:LYS:HA	2:A:5093:ATP:N3	2.07	0.70
1:B:3631:MET:CE	1:B:3698:MET:HG3	2.21	0.70
1:B:1620:PHE:HD1	1:B:1760:PHE:HZ	0.81	0.69
1:B:3406:PHE:HB2	1:B:3513:VAL:HG11	1.72	0.69
1:B:1698:ILE:O	1:B:1702:LEU:HG	1.92	0.69
1:B:2745:ILE:HG23	1:B:2756:MET:CE	2.22	0.69
1:B:3645:SER:CB	1:B:3890:GLN:HE21	2.03	0.69
1:A:1574:PHE:HB3	1:A:1576:GLU:H	1.57	0.69
1:B:3330:TYR:OH	1:B:3346:LEU:HD22	1.92	0.69
1:A:3566:LEU:HA	1:A:3583:LEU:HD21	1.74	0.69
1:B:2220:CYS:SG	1:B:2224:SER:CB	2.81	0.69
1:A:1540:LEU:CD1	1:A:1548:ILE:CD1	2.71	0.69
1:A:3848:LEU:HD21	1:A:3852:LYS:HE3	1.73	0.69
1:A:1726:LEU:CD1	1:A:3984:GLN:HB3	2.23	0.69
1:A:1849:GLU:HG2	1:A:1899:ASN:HD22	1.57	0.69
1:A:2632:ALA:HB3	1:A:2647:LEU:HD21	1.75	0.69
1:B:2707:VAL:CG1	1:B:2712:LEU:HD11	2.21	0.69
1:B:3871:PHE:HZ	1:B:3873:MET:HB2	1.57	0.69
1:A:1405:CYS:O	1:A:1409:LEU:HG	1.92	0.69
1:A:2111:LYS:HZ3	1:A:2161:GLU:HG2	1.57	0.69
1:B:1387:GLU:HB3	1:B:1393:LYS:HG2	1.73	0.69
1:A:1392:LEU:HD13	1:A:1392:LEU:C	2.13	0.69
1:A:3799:LYS:O	1:A:3803:LEU:HG	1.93	0.69
1:B:3837:GLY:O	1:B:3871:PHE:HD1	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1802:LYS:NZ	4:A:5095:SO4:O2	2.26	0.69
1:A:1970:LEU:CD1	1:A:1974:LYS:HE3	2.14	0.69
1:A:1562:MET:CB	1:A:1569:ILE:HD11	2.21	0.68
1:B:2061:TYR:CD1	1:B:2091:MET:SD	2.86	0.68
1:A:1368:GLU:HG2	1:A:1424:PHE:CE2	2.25	0.68
1:A:1462:ASN:CB	1:A:1465:ILE:HG22	2.22	0.68
1:A:2109:LEU:HD13	1:A:2129:LEU:HD23	1.75	0.68
1:A:2173:ASN:HB3	1:A:2175:ILE:HG22	1.73	0.68
1:B:1489:ARG:HH12	1:B:1503:PRO:HG2	1.57	0.68
1:B:1540:LEU:CD1	1:B:1548:ILE:CD1	2.71	0.68
1:B:3023:LYS:CD	1:B:3567:LEU:HD23	2.19	0.68
1:A:1394:LEU:HD22	1:A:1449:GLN:HE22	1.57	0.68
1:A:2290:LEU:HD13	1:A:2407:LEU:HD23	1.75	0.68
1:A:2707:VAL:CG1	1:A:2712:LEU:HD11	2.22	0.68
1:B:3819:ILE:O	1:B:3823:ASN:HB2	1.93	0.68
1:A:1995:VAL:HG21	1:A:2024:SER:HB3	1.76	0.68
1:B:2336:ARG:HD3	1:B:2355:ASP:OD2	1.93	0.68
1:B:2181:GLY:O	1:B:2182:GLU:HG3	1.93	0.68
1:A:2476:LYS:NZ	1:A:2528:ARG:HD3	2.09	0.68
1:A:3816:LEU:HD23	1:A:3847:SER:OG	1.93	0.68
1:B:2563:SER:HB2	1:B:2566:SER:OG	1.93	0.68
1:A:2203:THR:HG22	1:A:2205:ALA:H	1.59	0.68
1:B:3459:ASP:OD2	1:B:3461:ILE:HG12	1.93	0.68
1:A:3837:GLY:O	1:A:3871:PHE:HD1	1.76	0.68
1:B:3777:VAL:CG1	1:B:3895:PHE:CE1	2.64	0.68
1:A:2846:GLY:O	1:A:2849:TYR:HB3	1.92	0.68
1:B:3612:ASP:O	1:B:3615:VAL:HG22	1.93	0.68
1:B:3566:LEU:HD13	1:B:3570:LEU:CD1	2.24	0.67
1:B:2620:ARG:HH12	1:B:2910:ASN:CG	1.97	0.67
1:B:3919:LYS:NZ	1:B:4038:GLU:CD	2.47	0.67
1:B:3839:ILE:CG2	1:B:3873:MET:HG3	2.24	0.67
1:A:1645:PHE:CG	1:A:1765:ILE:HG22	2.29	0.67
1:B:1536:ARG:N	1:B:1841:ILE:HD11	2.09	0.67
1:B:1929:ILE:HD13	1:B:1970:LEU:HD11	1.75	0.67
1:B:2293:HIS:CE1	1:B:2409:ASN:HB3	2.29	0.67
1:A:2220:CYS:SG	1:A:2224:SER:CB	2.82	0.67
1:A:3886:ALA:N	1:A:3887:PRO:HD2	2.10	0.67
1:B:1645:PHE:CG	1:B:1765:ILE:HG22	2.28	0.67
1:B:3566:LEU:O	1:B:3570:LEU:HG	1.94	0.67
1:B:3592:LYS:O	1:B:3596:ASN:HB2	1.94	0.67
1:B:1611:LEU:O	1:B:1615:ILE:HG23	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1726:LEU:HD13	1:B:3984:GLN:HB3	1.77	0.67
1:A:2707:VAL:CG1	1:A:2712:LEU:CD1	2.72	0.67
1:A:3979:ASN:C	1:A:3981:PRO:HD2	2.15	0.67
1:B:3886:ALA:N	1:B:3887:PRO:HD2	2.09	0.67
1:A:2380:LEU:HD12	1:A:2577:ALA:HB2	1.75	0.67
1:B:1620:PHE:HA	1:B:1760:PHE:HE1	1.59	0.67
1:B:2394:THR:H	1:B:2397:THR:HB	1.59	0.67
1:A:1744:LEU:HA	1:A:1760:PHE:CD2	2.29	0.67
1:A:2757:MET:HE2	1:A:2912:CYS:HB2	1.75	0.67
1:A:3530:PHE:HD1	1:A:3618:TYR:CD2	2.09	0.67
1:B:3816:LEU:HD23	1:B:3847:SER:OG	1.95	0.67
1:A:2080:LYS:HG2	1:A:2215:PHE:CE1	2.29	0.67
1:A:2131:THR:HG22	1:A:2176:LEU:HD21	1.77	0.67
1:A:2224:SER:O	2:A:5093:ATP:C2	2.48	0.67
1:A:2386:MET:HB3	1:A:2627:ARG:NE	2.10	0.67
1:A:3871:PHE:CZ	1:A:3873:MET:HB2	2.30	0.67
1:B:1612:ASP:HA	1:B:1615:ILE:CD1	2.25	0.67
1:A:1536:ARG:N	1:A:1841:ILE:HD11	2.10	0.66
1:A:1922:LYS:NZ	1:A:4004:LEU:CD1	2.58	0.66
1:B:1649:LEU:CD1	1:B:1704:GLU:HG3	2.25	0.66
1:B:2489:ILE:HG22	1:B:2535:CYS:HB3	1.77	0.66
1:B:1495:THR:HG22	1:B:1497:ILE:HG22	1.77	0.66
1:B:1540:LEU:HD12	1:B:1548:ILE:CD1	2.25	0.66
1:A:1527:LEU:HD23	1:A:1545:LEU:HD22	1.77	0.66
1:A:2112:GLU:HB3	1:A:2117:SER:CB	2.25	0.66
1:B:2936:ILE:HG22	1:B:2962:ARG:HD3	1.78	0.66
1:A:2081:THR:O	1:A:2085:LYS:HB2	1.96	0.66
1:A:1540:LEU:HD11	1:A:1548:ILE:HD11	1.76	0.66
1:A:2425:THR:HG23	3:A:5094:ANP:O3G	1.95	0.66
1:A:1540:LEU:CD1	1:A:1548:ILE:HD11	2.26	0.66
1:A:1466:GLN:CB	1:A:1473:THR:HG21	2.26	0.66
1:A:1531:ARG:HG2	1:A:1537:PHE:HB3	1.77	0.66
1:A:2495:ASP:O	1:A:2498:GLY:N	2.29	0.66
1:A:3303:LYS:HA	1:A:3306:TRP:HE1	1.59	0.66
1:B:3566:LEU:CD1	1:B:3570:LEU:HD11	2.25	0.66
1:B:2109:LEU:CD1	1:B:2129:LEU:HD23	2.26	0.65
1:B:2302:PHE:HA	1:B:2310:LEU:HD11	1.77	0.65
1:B:3023:LYS:CE	1:B:3567:LEU:HG	2.25	0.65
1:A:2095:ASP:CG	1:A:2149:ARG:HH22	2.00	0.65
1:A:3618:TYR:HD1	1:A:3618:TYR:N	1.94	0.65
1:A:1620:PHE:CD1	1:A:1760:PHE:HZ	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2302:PHE:HA	1:A:2310:LEU:HD11	1.76	0.65
1:B:2220:CYS:SG	1:B:2224:SER:HB2	2.36	0.65
1:A:1706:LEU:CD2	1:A:1935:GLN:HG2	2.27	0.65
1:B:1849:GLU:OE2	1:B:1899:ASN:ND2	2.30	0.65
1:B:3850:TRP:NE1	1:B:3854:TYR:HB3	2.12	0.65
1:B:2173:ASN:HB3	1:B:2175:ILE:HG22	1.77	0.65
1:A:1649:LEU:CD1	1:A:1704:GLU:HG3	2.27	0.65
1:A:1706:LEU:HD21	1:A:1935:GLN:HG2	1.79	0.65
1:A:1425:GLU:OE2	1:A:1429:LEU:HD11	1.96	0.65
1:A:2032:LYS:O	1:A:2035:VAL:HG12	1.96	0.65
1:A:2766:LYS:CE	1:A:2892:CYS:SG	2.84	0.65
1:B:2508:GLN:HG3	1:B:2512:LYS:HG3	1.77	0.65
1:B:3460:PRO:O	1:B:3463:SER:HB3	1.97	0.65
1:B:1391:GLY:HA3	1:B:1484:LYS:NZ	2.11	0.65
1:B:2391:VAL:CG2	1:B:2426:MET:SD	2.83	0.65
1:B:2513:GLN:O	1:B:2526:ILE:CG1	2.45	0.65
1:B:1425:GLU:OE2	1:B:1429:LEU:CD2	2.45	0.65
1:B:1748:PHE:CD2	1:B:1755:LEU:HD22	2.32	0.65
1:B:1995:VAL:HG21	1:B:2024:SER:HB3	1.78	0.64
1:B:2941:THR:HG22	1:B:2942:ASP:H	1.62	0.64
1:B:2109:LEU:HD11	1:B:2129:LEU:HD23	1.79	0.64
1:B:2410:SER:C	1:B:2411:LYS:HG3	2.16	0.64
1:B:2637:PRO:O	1:B:2639:GLN:NE2	2.30	0.64
1:A:1535:PRO:HB2	1:A:1841:ILE:CG1	2.27	0.64
1:A:2039:LYS:HG2	1:A:2049:MET:HG3	1.78	0.64
1:A:3979:ASN:O	1:A:3981:PRO:HD2	1.98	0.64
1:A:2728:LEU:HD12	1:A:2771:ARG:NH2	2.12	0.64
1:B:3911:TRP:HH2	1:B:3926:VAL:HG12	1.62	0.64
1:A:1630:ILE:CG2	1:A:1655:MET:SD	2.86	0.64
1:A:3785:TYR:HE2	1:A:3859:VAL:HG22	1.62	0.64
1:B:1726:LEU:CD1	1:B:3984:GLN:CB	2.75	0.64
1:B:2106:THR:HG1	1:B:2154:PHE:HB3	1.62	0.64
1:A:1645:PHE:CD2	1:A:1765:ILE:HG22	2.32	0.64
1:A:3541:MET:HA	1:A:3544:LYS:HG2	1.78	0.64
1:A:1991:GLU:O	1:A:1995:VAL:HG23	1.98	0.64
1:B:1822:CYS:SG	1:B:1849:GLU:O	2.56	0.64
1:B:2003:LEU:HA	1:B:2006:LEU:HD12	1.80	0.64
1:B:1531:ARG:HG2	1:B:1537:PHE:HB3	1.79	0.64
1:B:2293:HIS:NE2	1:B:2409:ASN:HB3	2.13	0.64
1:A:1365:PHE:CZ	1:A:1420:TYR:CE1	2.86	0.63
1:B:1983:LEU:CD2	1:B:1993:THR:O	2.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3737:THR:OG1	1:B:3740:THR:HB	1.98	0.63
1:A:2401:GLU:HG2	1:A:2431:ALA:HB2	1.81	0.63
1:B:3440:LEU:CD2	1:B:3462:ILE:HD12	2.29	0.63
1:B:2623:THR:HB	3:B:5094:ANP:O2'	1.99	0.63
1:A:2257:PHE:HD1	1:A:2262:LEU:HD11	1.61	0.63
1:B:2728:LEU:HD12	1:B:2771:ARG:CZ	2.28	0.63
1:A:2034:ILE:HD12	1:A:2061:TYR:CZ	2.33	0.63
1:B:3509:LEU:HD12	1:B:3513:VAL:CG2	2.28	0.63
1:A:1489:ARG:HH12	1:A:1503:PRO:HG2	1.64	0.63
1:A:2552:ARG:HG2	1:A:2552:ARG:NH1	2.14	0.63
1:A:3679:TYR:HB3	1:A:3767:PHE:HE1	1.64	0.63
1:A:1900:PRO:HB3	1:A:1905:ARG:HA	1.80	0.63
1:B:1744:LEU:HD22	1:B:1760:PHE:CG	2.34	0.63
1:B:2508:GLN:CG	1:B:2512:LYS:HG3	2.28	0.63
1:A:2095:ASP:CG	1:A:2149:ARG:NH2	2.53	0.63
1:B:1421:TYR:O	1:B:1425:GLU:N	2.32	0.63
1:A:1391:GLY:HA3	1:A:1484:LYS:NZ	2.13	0.62
1:A:1965:HIS:HD2	1:A:2212:LEU:CD2	2.11	0.62
1:A:3509:LEU:CD1	1:A:3513:VAL:CG2	2.74	0.62
1:A:3850:TRP:NE1	1:A:3854:TYR:HB3	2.13	0.62
1:B:3925:SER:HB2	1:B:3972:LEU:HD13	1.81	0.62
1:B:2220:CYS:SG	2:B:5093:ATP:C6	2.92	0.62
1:A:3530:PHE:CE1	1:A:3618:TYR:CD2	2.87	0.62
1:B:2109:LEU:HD11	1:B:2129:LEU:CD2	2.29	0.62
1:B:3530:PHE:CE1	1:B:3618:TYR:CD2	2.87	0.62
1:B:3912:GLY:O	1:B:3915:PHE:CZ	2.52	0.62
1:B:1425:GLU:OE2	1:B:1429:LEU:HD21	1.98	0.62
1:A:3737:THR:OG1	1:A:3740:THR:HB	1.99	0.62
1:B:1706:LEU:HD11	1:B:1936:ILE:HG12	1.80	0.62
1:B:2428:MET:SD	1:B:2532:VAL:HG11	2.39	0.62
1:B:3700:MET:HB3	1:B:4085:THR:HG21	1.81	0.62
1:B:1911:ASN:OD1	1:B:1912:LEU:N	2.33	0.62
1:B:3839:ILE:HG23	1:B:3873:MET:HG3	1.81	0.62
1:A:3566:LEU:CD1	1:A:3570:LEU:HD11	2.30	0.62
1:B:2280:THR:HA	1:B:2283:LYS:HD2	1.81	0.62
1:B:2467:THR:OG1	1:B:2473:LEU:HD12	1.99	0.62
1:B:2677:VAL:HG11	1:B:2686:LEU:HD21	1.82	0.62
1:A:1664:LEU:HD23	1:A:1669:PHE:HZ	1.63	0.62
1:A:2151:TRP:HE3	1:A:2193:LEU:HD11	1.63	0.62
1:A:2280:THR:HA	1:A:2283:LYS:HD2	1.80	0.62
1:A:2578:ILE:CG2	1:A:2630:TYR:HB2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2709:LYS:O	1:A:2713:VAL:HG23	1.98	0.62
1:B:3566:LEU:HD13	1:B:3570:LEU:HD11	1.81	0.62
1:B:1726:LEU:HD12	1:B:3984:GLN:CB	2.29	0.62
1:A:1536:ARG:HD3	1:A:1841:ILE:HD13	1.82	0.62
1:A:3787:THR:HG22	1:A:3875:MET:HB2	1.81	0.62
1:B:1748:PHE:HD2	1:B:1755:LEU:HD22	1.65	0.61
1:B:1965:HIS:HD2	1:B:2212:LEU:HD21	1.65	0.61
1:B:2631:THR:O	1:B:2635:THR:HG22	1.99	0.61
1:A:1984:ILE:HG21	1:A:1989:GLU:HG3	1.82	0.61
1:B:3692:LYS:HE3	1:B:3898:GLU:HB3	1.81	0.61
1:A:2578:ILE:HG21	1:A:2630:TYR:HB2	1.82	0.61
1:B:2111:LYS:HZ3	1:B:2161:GLU:HG2	1.63	0.61
1:B:3737:THR:HB	1:B:3740:THR:CB	2.29	0.61
1:A:3813:ILE:HG22	1:A:3840:LEU:HD23	1.83	0.61
1:B:2063:MET:HB3	1:B:2070:LEU:HD11	1.82	0.61
1:A:1612:ASP:HA	1:A:1615:ILE:CD1	2.30	0.61
1:A:2380:LEU:HD11	1:A:2577:ALA:CB	2.30	0.61
1:B:3023:LYS:HD3	1:B:3567:LEU:CD2	2.10	0.61
1:A:1469:LEU:HD13	1:A:1523:LEU:CD2	2.30	0.61
1:A:1802:LYS:HG2	1:A:1921:MET:HG3	1.83	0.61
1:A:3696:MET:SD	1:A:3760:LEU:HD23	2.41	0.61
1:B:2493:LYS:HG3	1:B:2494:LEU:H	1.66	0.61
1:A:2293:HIS:CE1	1:A:2409:ASN:CB	2.84	0.61
1:A:3964:ALA:HB2	1:A:3993:VAL:HG11	1.82	0.61
1:A:4021:LEU:HD23	1:A:4023:ILE:HG12	1.82	0.61
1:B:1493:LEU:O	1:B:1494:ASP:HB2	2.00	0.61
1:B:3023:LYS:CE	1:B:3567:LEU:CD2	2.79	0.61
1:A:2394:THR:H	1:A:2397:THR:HB	1.65	0.61
1:A:1826:PHE:CE1	1:A:1853:LEU:HD22	2.36	0.60
1:A:3839:ILE:CG2	1:A:3873:MET:HG3	2.31	0.60
1:B:1849:GLU:HG2	1:B:1899:ASN:ND2	2.16	0.60
1:B:2386:MET:HB3	1:B:2627:ARG:HD3	1.77	0.60
1:B:2707:VAL:CG1	1:B:2712:LEU:HD12	2.31	0.60
1:A:1849:GLU:OE2	1:A:1899:ASN:ND2	2.34	0.60
1:A:3912:GLY:O	1:A:3915:PHE:CZ	2.55	0.60
1:B:1744:LEU:HD22	1:B:1760:PHE:CD2	2.36	0.60
1:B:3912:GLY:O	1:B:3915:PHE:CE2	2.54	0.60
1:B:1706:LEU:HD22	1:B:1935:GLN:CG	2.30	0.60
1:B:1983:LEU:HD21	1:B:1996:GLU:HB2	1.84	0.60
1:B:3525:ILE:HD11	1:B:3646:ILE:CG2	2.18	0.60
1:A:1493:LEU:HD23	1:A:1498:GLU:CB	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2230:LEU:HD23	1:A:2288:VAL:HG13	1.83	0.60
1:A:3656:VAL:CG1	1:A:3677:LEU:HB3	2.30	0.60
1:B:1991:GLU:O	1:B:1995:VAL:HG23	2.01	0.60
1:B:3330:TYR:CD1	1:B:3334:PHE:CD2	2.90	0.60
1:A:2332:GLY:O	1:A:2336:ARG:HG3	2.01	0.60
1:A:2757:MET:HE1	1:A:2909:PHE:HA	1.83	0.60
1:A:3641:PHE:HA	1:A:3889:LEU:HD21	1.84	0.60
1:A:3566:LEU:HD13	1:A:3570:LEU:CD1	2.32	0.60
1:B:1692:ASP:O	1:B:1695:LYS:HB3	2.01	0.60
1:B:1983:LEU:CG	1:B:1993:THR:HG23	2.25	0.60
1:B:2476:LYS:HD2	1:B:2476:LYS:H	1.67	0.60
1:B:2107:LYS:CE	1:B:2495:ASP:OD2	2.38	0.60
1:A:2125:TRP:CZ2	1:A:2178:LEU:HD13	2.37	0.60
1:B:3728:GLU:HG3	1:B:4079:LYS:HE2	1.82	0.60
1:A:2476:LYS:H	1:A:2476:LYS:HD2	1.64	0.59
1:A:2512:LYS:O	1:A:2513:GLN:CB	2.50	0.59
1:A:3583:LEU:O	1:A:3587:LEU:HG	2.02	0.59
1:A:3819:ILE:O	1:A:3823:ASN:HB2	2.01	0.59
1:A:2446:SER:H	1:A:2449:THR:HG21	1.66	0.59
1:A:3592:LYS:O	1:A:3596:ASN:HB2	2.02	0.59
1:B:2960:THR:HB	1:B:2963:ASP:HB2	1.84	0.59
1:B:3671:VAL:O	1:B:3674:ILE:HG22	2.02	0.59
1:A:1956:LEU:HB3	1:A:1968:PHE:HE2	1.67	0.59
1:A:2757:MET:CE	1:A:2912:CYS:CB	2.77	0.59
1:A:3839:ILE:HG23	1:A:3873:MET:HG3	1.84	0.59
1:B:2131:THR:HG22	1:B:2176:LEU:CD2	2.32	0.59
1:B:2074:GLY:O	1:B:2197:ASP:HA	2.03	0.59
1:B:3612:ASP:O	1:B:3615:VAL:CG2	2.50	0.59
1:B:3631:MET:HE3	1:B:3698:MET:HG3	1.82	0.59
1:A:1493:LEU:O	1:A:1494:ASP:HB2	2.01	0.59
1:A:2197:ASP:HB3	1:A:2549:ARG:HD2	1.84	0.59
1:A:3671:VAL:HA	1:A:3674:ILE:HG22	1.83	0.59
1:A:3785:TYR:CE2	1:A:3859:VAL:HG22	2.37	0.59
1:A:1802:LYS:NZ	4:A:5095:SO4:S	2.75	0.59
1:A:1534:PHE:HD2	1:A:1537:PHE:CE1	2.20	0.59
1:B:1536:ARG:HD2	1:B:1565:MET:O	2.01	0.59
1:B:3877:CYS:SG	1:B:3884:LEU:HD22	2.41	0.59
1:B:2423:GLY:N	3:B:5094:ANP:O1B	2.29	0.59
1:B:2293:HIS:CE1	1:B:2409:ASN:CB	2.86	0.59
1:A:1939:PHE:HD1	1:A:1939:PHE:H	1.51	0.59
1:B:3541:MET:HA	1:B:3544:LYS:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2512:LYS:O	1:B:2513:GLN:CB	2.50	0.59
1:B:3995:GLY:HA2	1:B:3998:ILE:HD13	1.84	0.59
1:A:2080:LYS:HG2	1:A:2215:PHE:CD1	2.38	0.59
1:A:2201:HIS:CE1	1:A:2497:TYR:HA	2.38	0.59
1:A:2757:MET:HE2	1:A:2912:CYS:CB	2.32	0.59
1:B:166:PRO:CB	1:B:1369:LYS:HB3	2.32	0.59
1:B:1926:SER:HB2	1:B:1970:LEU:HD12	1.84	0.59
1:B:2266:PHE:HD1	1:B:2326:LEU:HD21	1.67	0.59
1:B:2856:LEU:HD23	1:B:2873:LEU:HB3	1.84	0.59
1:A:1852:ARG:HG3	1:A:1852:ARG:O	2.03	0.59
1:A:1965:HIS:CD2	1:A:2212:LEU:HD21	2.38	0.59
1:A:2786:ILE:O	1:A:3460:PRO:HB2	2.01	0.59
1:A:3460:PRO:O	1:A:3463:SER:HB3	2.03	0.59
1:B:2274:HIS:CE1	1:B:2326:LEU:O	2.51	0.59
1:B:2503:VAL:HA	1:B:2506:LEU:HD12	1.83	0.59
1:B:3525:ILE:CD1	1:B:3646:ILE:HG22	2.19	0.59
1:A:2425:THR:HG21	3:A:5094:ANP:O3G	2.02	0.58
1:A:3350:LYS:HA	1:A:3353:LEU:HD12	1.84	0.58
1:A:3737:THR:HB	1:A:3740:THR:CB	2.32	0.58
1:B:1620:PHE:HA	1:B:1760:PHE:CE1	2.37	0.58
1:B:3807:SER:O	1:B:3808:LYS:HB2	2.03	0.58
1:A:1392:LEU:HD13	1:A:1393:LYS:C	2.24	0.58
1:A:2102:TYR:HB2	1:A:2152:VAL:HG22	1.84	0.58
1:B:1683:LEU:HB3	1:B:1702:LEU:HD21	1.84	0.58
1:A:1425:GLU:C	1:A:1425:GLU:OE1	2.42	0.58
1:A:1823:ASP:HB2	1:A:1853:LEU:HD23	1.83	0.58
1:A:1967:HIS:C	1:A:1968:PHE:HD1	2.06	0.58
1:B:1649:LEU:HD11	1:B:1704:GLU:HG3	1.82	0.58
1:A:1368:GLU:CG	1:A:1424:PHE:CE2	2.86	0.58
1:B:2517:LYS:CE	1:B:2520:GLU:OE1	2.50	0.58
1:B:3979:ASN:C	1:B:3981:PRO:HD2	2.24	0.58
1:B:3948:HIS:NE2	1:B:4072:ASN:CG	2.57	0.58
1:A:1683:LEU:HD22	1:A:1698:ILE:HG23	1.85	0.58
1:A:2293:HIS:NE2	1:A:2409:ASN:HB3	2.18	0.58
1:A:2842:ASP:O	1:A:2845:GLN:HG2	2.04	0.58
1:B:2655:ILE:HD11	1:B:2747:ARG:HH22	1.68	0.58
1:B:2766:LYS:HE2	1:B:2890:THR:HB	1.85	0.58
1:A:1774:LEU:HD21	1:A:1922:LYS:O	2.03	0.58
1:A:2563:SER:CB	1:A:2566:SER:OG	2.51	0.58
1:A:3409:ASP:HB3	1:A:3518:PHE:HB2	1.85	0.58
1:B:1703:VAL:HG13	1:B:1770:ILE:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2332:GLY:HA2	1:B:2335:GLN:CB	2.30	0.58
1:A:1421:TYR:O	1:A:1425:GLU:N	2.36	0.58
1:B:1929:ILE:HD13	1:B:1970:LEU:CD1	2.34	0.58
1:B:2127:ASP:O	1:B:2131:THR:OG1	2.22	0.58
1:B:3530:PHE:HD1	1:B:3618:TYR:HD2	1.49	0.58
1:A:2755:HIS:O	1:A:2913:ILE:HG13	2.03	0.58
1:A:3792:ARG:HB2	1:A:3955:TYR:CE2	2.39	0.58
1:B:1534:PHE:CE2	1:B:1536:ARG:HB2	2.39	0.58
1:B:2846:GLY:O	1:B:2849:TYR:HB3	2.02	0.58
1:A:1559:SER:CB	1:A:1572:ILE:HG22	2.34	0.58
1:A:2420:PRO:HD3	1:A:2536:ASN:HD21	1.69	0.58
1:B:1707:HIS:O	1:B:1711:VAL:HG23	2.04	0.58
1:B:1940:GLU:HG3	1:B:1941:ASP:N	2.19	0.58
1:B:2786:ILE:O	1:B:3460:PRO:HB2	2.04	0.58
1:A:1409:LEU:CD2	1:A:1435:LEU:HB3	2.24	0.57
1:A:1620:PHE:HA	1:A:1760:PHE:CE1	2.39	0.57
1:A:1953:LEU:CD1	1:A:1973:LEU:HB3	2.33	0.57
1:A:3449:VAL:HG22	1:A:3493:LYS:HB2	1.85	0.57
1:B:2224:SER:C	2:B:5093:ATP:H2	2.07	0.57
1:A:2064:GLN:OE1	1:A:2151:TRP:CH2	2.51	0.57
1:A:3912:GLY:O	1:A:3915:PHE:CE2	2.57	0.57
1:B:1984:ILE:HG21	1:B:1989:GLU:HG3	1.86	0.57
1:B:2095:ASP:CG	1:B:2149:ARG:NH2	2.57	0.57
1:B:4020:ASN:HB3	1:B:4028:ARG:HH11	1.68	0.57
1:A:2266:PHE:HD1	1:A:2326:LEU:HD21	1.69	0.57
1:A:2382:ALA:O	1:A:2385:VAL:HG12	2.04	0.57
1:A:3810:SER:O	1:A:3838:TRP:HB2	2.03	0.57
1:A:1493:LEU:CD2	1:A:1498:GLU:HB3	2.33	0.57
1:A:1612:ASP:HA	1:A:1615:ILE:HD11	1.86	0.57
1:A:1611:LEU:O	1:A:1615:ILE:HG23	2.05	0.57
1:A:1738:ASN:O	1:A:1739:ASP:OD1	2.23	0.57
1:A:1945:LEU:HD13	1:A:1994:VAL:HG21	1.86	0.57
1:B:1940:GLU:CB	1:B:1989:GLU:O	2.52	0.57
1:B:2755:HIS:NE2	1:B:2835:LEU:HG	2.20	0.57
1:B:3350:LYS:HA	1:B:3353:LEU:HD12	1.87	0.57
1:A:1698:ILE:O	1:A:1702:LEU:HG	2.05	0.57
1:A:2225:LYS:HG2	1:A:2229:LEU:HD12	1.87	0.57
1:A:3566:LEU:HD13	1:A:3570:LEU:HD11	1.87	0.57
1:A:4021:LEU:HD23	1:A:4023:ILE:CG1	2.34	0.57
1:B:1953:LEU:HD11	1:B:1973:LEU:HB3	1.86	0.57
1:A:1469:LEU:HB3	1:A:1472:GLU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2274:HIS:CE1	1:A:2326:LEU:O	2.47	0.57
1:B:2788:ARG:HB2	1:B:3459:ASP:HB3	1.87	0.57
1:B:1620:PHE:CB	1:B:1760:PHE:CE1	2.87	0.57
1:B:2084:TRP:HE3	1:B:2088:ILE:HD12	1.70	0.57
1:B:2563:SER:CB	1:B:2566:SER:OG	2.52	0.57
1:B:2620:ARG:O	1:B:2623:THR:HG22	2.04	0.57
1:A:2127:ASP:O	1:A:2131:THR:OG1	2.23	0.57
1:A:2437:LEU:H	1:A:2437:LEU:HD12	1.70	0.57
1:A:2637:PRO:O	1:A:2639:GLN:NE2	2.38	0.57
1:A:4020:ASN:ND2	1:A:4028:ARG:HD3	2.20	0.57
1:B:2034:ILE:HD12	1:B:2061:TYR:CZ	2.39	0.57
1:B:3353:LEU:HD23	1:B:3358:VAL:HG11	1.85	0.57
1:A:2047:PHE:CE2	1:A:2082:ALA:HB1	2.40	0.57
1:A:2137:VAL:O	1:A:2141:ILE:CG2	2.51	0.57
1:B:1392:LEU:HD13	1:B:1393:LYS:C	2.25	0.57
1:B:1527:LEU:CD2	1:B:1545:LEU:HD22	2.35	0.57
1:B:1744:LEU:HA	1:B:1760:PHE:HE2	1.66	0.57
1:B:2536:ASN:HB2	1:B:2543:ARG:HE	1.70	0.57
1:A:1535:PRO:O	1:A:1841:ILE:HD11	2.05	0.56
1:A:1794:PHE:HD1	1:A:1802:LYS:HB3	1.69	0.56
1:A:2290:LEU:HD23	1:A:2321:SER:HA	1.86	0.56
1:B:1823:ASP:HB2	1:B:1853:LEU:HD23	1.86	0.56
1:B:2755:HIS:CB	1:B:2911:ARG:O	2.47	0.56
1:B:3017:VAL:HG21	1:B:3313:PHE:CE2	2.40	0.56
1:B:3330:TYR:CE1	1:B:3334:PHE:CD2	2.93	0.56
1:B:3810:SER:O	1:B:3838:TRP:HB2	2.04	0.56
1:A:2517:LYS:HG2	1:A:2520:GLU:HB2	1.87	0.56
1:A:3618:TYR:O	1:A:3622:GLY:N	2.37	0.56
1:B:3583:LEU:O	1:B:3587:LEU:HG	2.05	0.56
1:B:1394:LEU:HD22	1:B:1449:GLN:NE2	2.20	0.56
1:B:1813:LEU:HD12	1:B:1844:TRP:HH2	1.71	0.56
1:A:1394:LEU:HD22	1:A:1449:GLN:NE2	2.20	0.56
1:A:1645:PHE:HZ	1:A:1768:ARG:HD2	1.69	0.56
1:B:1612:ASP:HA	1:B:1615:ILE:HD11	1.86	0.56
1:B:3519:VAL:HG13	1:B:3521:ASN:ND2	2.20	0.56
1:A:1704:GLU:OE2	1:A:1768:ARG:NH1	2.39	0.56
1:A:1963:MET:HB3	1:A:1966:TYR:CD2	2.41	0.56
1:A:2581:LEU:HD13	1:A:2633:ILE:HG22	1.87	0.56
1:B:1469:LEU:HB3	1:B:1472:GLU:HB2	1.87	0.56
1:B:1781:THR:HG21	1:B:1919:PHE:CE1	2.40	0.56
1:B:1803:THR:HG21	1:B:1848:ASP:OD1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2842:ASP:O	1:B:2845:GLN:HG2	2.05	0.56
1:B:1998:LEU:HD11	1:B:2022:PHE:HZ	1.71	0.56
1:B:3919:LYS:NZ	1:B:4038:GLU:CG	2.69	0.56
1:B:2225:LYS:HA	2:B:5093:ATP:N3	2.21	0.56
1:A:1462:ASN:HB2	1:A:1465:ILE:CG2	2.32	0.56
1:A:1967:HIS:O	1:A:1968:PHE:HD1	1.88	0.56
1:A:2386:MET:CB	1:A:2627:ARG:CD	2.84	0.56
1:A:2356:TYR:CE1	1:A:2395:ILE:HG22	2.41	0.56
1:A:2445:PHE:HA	1:A:2449:THR:HG21	1.88	0.56
1:A:3566:LEU:HD23	1:A:3587:LEU:HD11	1.87	0.56
1:B:3440:LEU:HD23	1:B:3462:ILE:HD12	1.87	0.56
1:A:2513:GLN:O	1:A:2526:ILE:CG1	2.50	0.56
1:A:3519:VAL:HG13	1:A:3521:ASN:ND2	2.20	0.56
1:A:2741:HIS:HA	1:A:2744:ARG:HD2	1.87	0.56
1:A:1418:SER:HB2	1:A:3446:PHE:HB3	1.87	0.56
1:B:1981:SER:HB3	1:B:1982:PRO:HD3	1.87	0.56
1:A:3612:ASP:O	1:A:3615:VAL:HG22	2.06	0.56
1:B:3919:LYS:NZ	1:B:4038:GLU:HG3	2.21	0.56
1:A:2106:THR:HG1	1:A:2154:PHE:HB3	1.70	0.56
1:A:3481:ILE:O	1:A:3483:ASP:N	2.35	0.56
1:B:3845:GLN:OE1	1:B:3878:HIS:HB2	2.06	0.56
1:A:1394:LEU:CD2	1:A:1449:GLN:HE22	2.19	0.55
1:A:2380:LEU:CD1	1:A:2577:ALA:HB1	2.30	0.55
1:A:3833:LYS:HZ3	1:A:3862:THR:HG21	1.70	0.55
1:A:3871:PHE:HZ	1:A:3873:MET:HB2	1.71	0.55
1:B:216:PRO:CB	1:B:1424:PHE:CG	2.89	0.55
1:B:3537:GLU:OE1	1:B:3618:TYR:OH	2.24	0.55
1:B:3930:PHE:HE2	1:B:4029:ILE:HD13	1.71	0.55
1:A:2048:SER:H	2:A:5093:ATP:HN62	1.54	0.55
1:A:2339:ILE:HG12	1:A:2353:LEU:HD23	1.87	0.55
1:A:2762:SER:O	1:A:2763:ARG:HB2	2.06	0.55
1:B:1527:LEU:HD22	1:B:1545:LEU:HD22	1.88	0.55
1:B:2225:LYS:HA	2:B:5093:ATP:C2	2.40	0.55
1:B:2362:ALA:HB3	1:B:2365:LYS:O	2.07	0.55
1:B:2728:LEU:HD12	1:B:2771:ARG:NH2	2.21	0.55
1:B:3566:LEU:CA	1:B:3583:LEU:HD21	2.36	0.55
1:A:1604:ALA:HA	1:A:1607:TRP:HE1	1.71	0.55
1:B:2386:MET:CB	1:B:2627:ARG:CD	2.77	0.55
1:A:2320:ARG:NH1	1:A:2406:ASP:OD2	2.30	0.55
1:A:3303:LYS:C	1:A:3306:TRP:CD1	2.72	0.55
1:B:2472:THR:CB	1:B:2524:VAL:HG22	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2201:HIS:CE1	1:B:2497:TYR:HA	2.41	0.55
1:A:1365:PHE:CE2	1:A:1420:TYR:CE2	2.94	0.55
1:A:1922:LYS:HZ2	1:A:4004:LEU:CD1	2.18	0.55
1:A:2795:PHE:CE2	1:A:2799:LEU:HD11	2.42	0.55
1:A:3810:SER:HB3	1:A:3837:GLY:HA2	1.87	0.55
1:A:3998:ILE:HG22	1:A:4004:LEU:HG	1.89	0.55
1:A:1851:ASN:HD21	1:A:1899:ASN:HB2	1.71	0.55
1:A:1911:ASN:OD1	1:A:1912:LEU:N	2.39	0.55
1:B:1939:PHE:O	1:B:1940:GLU:HB3	2.06	0.55
1:B:1970:LEU:HD23	1:B:1974:LYS:CE	2.35	0.55
1:B:2220:CYS:SG	2:B:5093:ATP:N1	2.79	0.55
1:B:2252:LEU:HD21	1:B:2310:LEU:HD23	1.87	0.55
1:A:1781:THR:HG21	1:A:1919:PHE:CD1	2.42	0.55
1:A:3631:MET:CE	1:A:3698:MET:HG3	2.37	0.55
1:B:1534:PHE:HD2	1:B:1537:PHE:CE1	2.25	0.55
1:B:1620:PHE:CA	1:B:1760:PHE:CE1	2.90	0.55
1:B:2420:PRO:HB2	1:B:2620:ARG:HH21	1.69	0.55
1:B:2495:ASP:O	1:B:2498:GLY:N	2.39	0.55
1:B:2787:HIS:CA	1:B:3460:PRO:HG2	2.35	0.55
1:A:1365:PHE:CD1	1:A:1365:PHE:N	2.74	0.55
1:A:2339:ILE:HG23	1:A:2353:LEU:HB3	1.89	0.55
1:A:2354:SER:OG	1:A:2357:SER:HB2	2.07	0.55
1:A:2825:THR:O	1:A:2829:GLU:HG2	2.06	0.55
1:A:3911:TRP:HH2	1:A:3926:VAL:CG1	2.20	0.55
1:B:2151:TRP:HE3	1:B:2193:LEU:HD11	1.72	0.55
1:B:2201:HIS:NE2	1:B:2497:TYR:O	2.40	0.55
1:B:2336:ARG:HA	1:B:2339:ILE:HD12	1.88	0.55
1:B:3323:ASN:HD21	1:B:3361:ASP:H	1.55	0.55
1:A:1940:GLU:CB	1:A:1989:GLU:O	2.51	0.55
1:A:2490:ASN:HB3	1:A:2546:MET:CE	2.37	0.55
1:A:3509:LEU:HD11	1:A:3513:VAL:HG21	1.89	0.55
1:B:1970:LEU:HD23	1:B:1974:LYS:HE2	1.78	0.55
1:B:2780:LYS:HD3	1:B:2813:THR:HG22	1.88	0.55
1:B:2891:ILE:HG21	1:B:2902:MET:HG3	1.89	0.55
1:B:3656:VAL:CG1	1:B:3677:LEU:HB3	2.35	0.55
1:B:4065:LEU:HD11	1:B:4070:ILE:CD1	2.34	0.55
1:A:1970:LEU:C	1:A:1970:LEU:HD12	2.27	0.55
1:A:2257:PHE:CD1	1:A:2262:LEU:HD11	2.41	0.55
1:A:2728:LEU:HD12	1:A:2771:ARG:CZ	2.37	0.55
1:A:3945:LEU:O	1:A:3948:HIS:O	2.24	0.55
1:A:3978:ASN:O	1:A:3981:PRO:CD	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1462:ASN:HB2	1:B:1465:ILE:HG22	1.89	0.55
1:B:1562:MET:CB	1:B:1569:ILE:HD11	2.36	0.55
1:A:1660:VAL:HG13	1:A:1728:TRP:CH2	2.42	0.54
1:A:3460:PRO:O	1:A:3463:SER:CB	2.55	0.54
1:A:3817:GLY:H	1:A:3821:ASN:HB2	1.72	0.54
1:A:3851:VAL:HG13	1:A:3855:LEU:HD23	1.88	0.54
1:B:1802:LYS:NZ	4:B:5096:SO4:O4	2.40	0.54
1:A:1540:LEU:HD12	1:A:1548:ILE:CD1	2.37	0.54
1:A:3303:LYS:HD2	1:A:3306:TRP:HD1	1.66	0.54
1:A:3537:GLU:OE1	1:A:3618:TYR:OH	2.24	0.54
1:B:1750:SER:HB2	1:B:1755:LEU:CD2	2.37	0.54
1:B:3023:LYS:HE2	1:B:3567:LEU:CD2	2.37	0.54
1:B:3509:LEU:HD12	1:B:3513:VAL:HG21	1.86	0.54
1:A:1741:LEU:O	1:A:1742:ASP:HB2	2.07	0.54
1:A:3541:MET:HB2	1:A:3607:PHE:HE1	1.72	0.54
1:B:3303:LYS:O	1:B:3306:TRP:CD1	2.60	0.54
1:A:1826:PHE:HE1	1:A:1853:LEU:HD22	1.72	0.54
1:A:1969:GLY:O	1:A:1972:THR:HB	2.07	0.54
1:A:1649:LEU:HD11	1:A:1704:GLU:HG3	1.88	0.54
1:A:4084:SER:O	1:A:4088:LEU:HG	2.07	0.54
1:B:2081:THR:O	1:B:2085:LYS:HB2	2.06	0.54
1:B:2424:LYS:HE2	1:B:2534:ALA:HB1	1.88	0.54
1:B:3645:SER:CB	1:B:3890:GLN:NE2	2.65	0.54
1:A:1996:GLU:O	1:A:2000:ARG:HG3	2.07	0.54
1:A:2386:MET:HB3	1:A:2627:ARG:CD	2.38	0.54
1:A:3797:THR:HG23	1:A:3840:LEU:HD21	1.90	0.54
1:A:1497:ILE:O	1:A:1500:ILE:HG12	2.07	0.54
1:A:2064:GLN:HE22	1:A:2091:MET:HG3	1.73	0.54
1:A:2448:ASP:HB2	1:A:2829:GLU:OE2	2.08	0.54
1:A:3671:VAL:O	1:A:3674:ILE:HG22	2.07	0.54
1:B:1965:HIS:HD2	1:B:2212:LEU:CD2	2.21	0.54
1:A:2566:SER:O	1:A:2570:ILE:HD12	2.08	0.54
1:B:3330:TYR:CE1	1:B:3334:PHE:CE2	2.95	0.54
1:B:3945:LEU:O	1:B:3948:HIS:O	2.25	0.54
1:A:1826:PHE:O	1:A:1826:PHE:CG	2.61	0.54
1:B:1493:LEU:HD23	1:B:1498:GLU:CB	2.38	0.54
1:B:1620:PHE:CZ	1:B:1743:ASP:HB3	2.42	0.54
1:B:1900:PRO:HB3	1:B:1905:ARG:HA	1.90	0.54
1:B:1926:SER:HB3	1:B:1970:LEU:HD12	1.86	0.54
1:B:2708:ASN:O	1:B:2712:LEU:HD13	2.08	0.54
1:B:3964:ALA:HB2	1:B:3993:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2412:ARG:HH11	1:A:2412:ARG:CB	2.16	0.54
1:A:3010:LEU:HD22	1:A:3320:LEU:HD12	1.90	0.54
1:B:2412:ARG:HH11	1:B:2412:ARG:HB2	1.73	0.54
1:B:2420:PRO:CB	1:B:2620:ARG:NH2	2.71	0.54
1:B:2385:VAL:O	1:B:2574:TYR:HE1	1.91	0.54
1:B:3785:TYR:CE2	1:B:3859:VAL:HG22	2.42	0.54
1:A:1692:ASP:O	1:A:1695:LYS:HB3	2.07	0.53
1:A:4020:ASN:HB3	1:A:4028:ARG:HH11	1.73	0.53
1:B:1769:LEU:HD11	1:B:1804:GLU:HB3	1.90	0.53
1:B:1965:HIS:CD2	1:B:2212:LEU:HD21	2.42	0.53
1:B:2425:THR:HG23	1:B:2485:PHE:HE2	1.71	0.53
1:B:2514:GLY:HA3	1:B:2525:THR:HA	1.90	0.53
1:B:3429:LEU:HD21	1:B:3439:ARG:HB3	1.89	0.53
1:B:3702:MET:HB3	1:B:3767:PHE:HZ	1.71	0.53
1:B:3946:VAL:HA	1:B:3947:PRO:C	2.28	0.53
1:A:2112:GLU:CB	1:A:2117:SER:HB2	2.37	0.53
1:B:3509:LEU:HD11	1:B:3513:VAL:HG21	1.90	0.53
1:B:4060:SER:HB3	1:B:4070:ILE:HG13	1.90	0.53
1:B:3612:ASP:C	1:B:3615:VAL:HG22	2.29	0.53
1:B:3855:LEU:HD12	1:B:3859:VAL:HG23	1.90	0.53
1:A:2336:ARG:HA	1:A:2339:ILE:HD12	1.91	0.53
1:A:2391:VAL:HG23	1:A:2426:MET:SD	2.47	0.53
1:A:3406:PHE:HB2	1:A:3513:VAL:HG12	1.83	0.53
1:A:2154:PHE:HD1	1:A:2154:PHE:N	2.05	0.53
1:A:2252:LEU:HD21	1:A:2310:LEU:HD23	1.89	0.53
1:A:4024:VAL:HG11	1:A:4062:TRP:CD2	2.44	0.53
1:B:2808:LEU:HD21	1:B:2856:LEU:HD12	1.91	0.53
1:A:1911:ASN:OD1	1:A:1912:LEU:HG	2.09	0.53
1:A:2410:SER:O	1:A:2411:LYS:CG	2.57	0.53
1:A:2640:THR:HG23	1:A:2643:SER:H	1.74	0.53
1:A:3323:ASN:HD21	1:A:3361:ASP:H	1.55	0.53
1:B:1645:PHE:CD2	1:B:1765:ILE:HG22	2.44	0.53
1:B:3530:PHE:HD1	1:B:3618:TYR:CD2	2.24	0.53
1:B:3683:TYR:O	1:B:3687:SER:HB2	2.09	0.53
1:B:3911:TRP:HH2	1:B:3926:VAL:CG1	2.21	0.53
1:A:1365:PHE:CE2	1:A:1420:TYR:CZ	2.97	0.53
1:A:2151:TRP:CE3	1:A:2193:LEU:HD11	2.44	0.53
1:A:2154:PHE:CD1	1:A:2154:PHE:N	2.74	0.53
1:A:2410:SER:O	1:A:2411:LYS:HG3	2.08	0.53
1:B:1425:GLU:OE2	1:B:1429:LEU:CD1	2.57	0.53
1:B:2467:THR:O	1:B:2471:LEU:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1991:GLU:O	1:A:1994:VAL:HB	2.08	0.53
1:A:1995:VAL:HG22	1:A:2022:PHE:CE2	2.44	0.53
1:A:2424:LYS:HE2	3:A:5094:ANP:O1G	2.08	0.53
1:A:3965:SER:HA	1:A:3968:LEU:HD12	1.91	0.53
1:B:1759:LYS:HE3	1:B:1761:GLU:OE2	2.09	0.53
1:B:1879:ILE:HG12	1:B:1888:LEU:HB2	1.89	0.53
1:B:1914:LYS:HD3	1:B:3959:CYS:SG	2.48	0.53
1:B:3978:ASN:O	1:B:3981:PRO:CD	2.57	0.53
1:A:1849:GLU:CG	1:A:1899:ASN:HD22	2.20	0.53
1:A:2111:LYS:HZ2	1:A:2161:GLU:HG2	1.70	0.53
1:A:2220:CYS:SG	1:A:2221:SER:N	2.82	0.53
1:A:2332:GLY:HA2	1:A:2335:GLN:CB	2.30	0.53
1:A:2492:PRO:CB	1:A:2502:VAL:HG11	2.39	0.53
1:A:2536:ASN:HB2	1:A:2543:ARG:HE	1.73	0.53
1:A:3555:TYR:HE1	1:A:3593:GLU:HG2	1.72	0.53
1:A:1827:ASP:HB3	1:A:1830:VAL:HG12	1.90	0.53
1:A:1929:ILE:H	1:A:1929:ILE:HD12	1.74	0.53
1:A:3807:SER:O	1:A:3808:LYS:HB2	2.09	0.53
1:B:2224:SER:O	2:B:5093:ATP:C2	2.53	0.53
1:B:4021:LEU:HD23	1:B:4023:ILE:HG12	1.91	0.53
1:A:3924:TRP:O	1:A:3927:TYR:HB3	2.09	0.52
1:B:2472:THR:HG21	1:B:2524:VAL:CG2	2.39	0.52
1:B:3923:VAL:CG2	1:B:4038:GLU:HA	2.37	0.52
1:B:2354:SER:OG	1:B:2357:SER:HB2	2.10	0.52
1:B:3459:ASP:OD2	1:B:3461:ILE:CG1	2.57	0.52
1:B:3924:TRP:O	1:B:3927:TYR:HB3	2.09	0.52
1:A:1981:SER:HB3	1:A:1982:PRO:HD3	1.91	0.52
1:A:2673:LEU:O	1:A:2677:VAL:HG23	2.10	0.52
1:B:1527:LEU:HD21	1:B:1546:LEU:HD21	1.91	0.52
1:B:1963:MET:HB3	1:B:1966:TYR:CD2	2.44	0.52
1:B:3785:TYR:HE2	1:B:3859:VAL:HG22	1.74	0.52
1:A:1983:LEU:HD21	1:A:2000:ARG:NE	2.24	0.52
1:A:3772:TRP:HZ3	1:A:3780:ASN:HD22	1.57	0.52
1:A:1531:ARG:HG2	1:A:1537:PHE:CB	2.39	0.52
1:A:1849:GLU:CG	1:A:1899:ASN:ND2	2.70	0.52
1:A:1995:VAL:HG22	1:A:2022:PHE:CD2	2.44	0.52
1:A:2780:LYS:HD3	1:A:2813:THR:HG22	1.92	0.52
1:B:1612:ASP:HA	1:B:1615:ILE:HG12	1.92	0.52
1:A:3010:LEU:HD21	1:A:3317:SER:HB3	1.90	0.52
1:A:3845:GLN:OE1	1:A:3878:HIS:HB2	2.09	0.52
1:B:2458:LEU:HD11	1:B:2484:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3632:LEU:HD13	1:B:3644:ILE:HD13	1.92	0.52
1:B:3951:SER:HB2	1:B:4002:LYS:HD2	1.91	0.52
1:A:1391:GLY:HA3	1:A:1484:LYS:HZ1	1.75	0.52
1:A:1535:PRO:O	1:A:1841:ILE:CD1	2.58	0.52
1:A:2386:MET:HB3	1:A:2627:ARG:HD3	1.89	0.52
1:B:1502:ILE:HG23	1:B:1503:PRO:HD2	1.91	0.52
1:B:1531:ARG:HG2	1:B:1537:PHE:CB	2.39	0.52
1:B:1606:GLU:O	1:B:1610:ILE:HG12	2.10	0.52
1:B:1781:THR:HG21	1:B:1919:PHE:CD1	2.45	0.52
1:B:2476:LYS:CD	1:B:2476:LYS:H	2.23	0.52
1:B:3737:THR:CB	1:B:3740:THR:CB	2.87	0.52
1:B:1844:TRP:CD1	1:B:1893:ALA:HB3	2.44	0.52
1:B:2448:ASP:HB2	1:B:2829:GLU:CD	2.31	0.52
1:B:3460:PRO:O	1:B:3463:SER:CB	2.58	0.52
1:A:1559:SER:HB3	1:A:1572:ILE:CG2	2.40	0.52
1:A:1748:PHE:CE2	1:A:1755:LEU:HD22	2.44	0.52
1:A:1870:ASN:O	1:A:1874:VAL:HG23	2.09	0.52
1:A:2494:LEU:O	1:A:2494:LEU:HD12	2.10	0.52
1:A:2834:LEU:HD21	1:A:2885:LEU:HD21	1.92	0.52
1:A:3631:MET:HE3	1:A:3698:MET:HG3	1.91	0.52
1:B:2111:LYS:CD	1:B:2161:GLU:CG	2.82	0.52
1:A:1531:ARG:HD3	1:A:1537:PHE:O	2.10	0.52
1:A:2181:GLY:O	1:A:2182:GLU:CG	2.56	0.52
1:A:65:THR:O	1:A:66:GLN:CB	2.57	0.52
1:B:3618:TYR:O	1:B:3622:GLY:N	2.38	0.52
1:A:2580:LYS:HG2	1:A:2586:ARG:HH22	1.74	0.51
1:A:3330:TYR:CE1	1:A:3334:PHE:CD2	2.98	0.51
1:A:3330:TYR:CD1	1:A:3334:PHE:CD2	2.99	0.51
1:A:3566:LEU:CD2	1:A:3587:LEU:HD11	2.41	0.51
1:B:1826:PHE:CE1	1:B:1853:LEU:HD22	2.45	0.51
1:B:1910:GLU:HB2	1:B:3846:MET:CB	2.39	0.51
1:B:2220:CYS:HB2	2:B:5093:ATP:C6	2.45	0.51
1:B:2867:LEU:HB3	1:B:2872:GLU:HB3	1.92	0.51
1:B:3810:SER:HB3	1:B:3837:GLY:HA2	1.92	0.51
1:A:2201:HIS:NE2	1:A:2497:TYR:O	2.43	0.51
1:A:2849:TYR:O	1:A:2853:LEU:HB2	2.11	0.51
1:B:1563:LYS:HE2	1:B:1585:VAL:HG12	1.91	0.51
1:A:1992:LYS:HG2	1:A:2024:SER:CB	2.38	0.51
1:B:2428:MET:HE2	1:B:2485:PHE:HD1	1.74	0.51
1:B:2428:MET:HE2	1:B:2485:PHE:CD1	2.45	0.51
1:B:3854:TYR:O	1:B:3858:HIS:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3939:ILE:HG23	1:B:3950:PHE:HE2	1.75	0.51
1:B:65:THR:O	1:B:66:GLN:CB	2.58	0.51
1:A:2002:ILE:HG22	1:A:2006:LEU:HD11	1.92	0.51
1:A:2177:THR:HG22	1:A:2183:ARG:HG2	1.93	0.51
1:A:3566:LEU:CA	1:A:3583:LEU:HD21	2.38	0.51
1:B:1968:PHE:N	1:B:1968:PHE:HD1	2.08	0.51
1:B:2154:PHE:CD1	1:B:2154:PHE:N	2.78	0.51
1:B:2470:GLY:CA	1:B:2473:LEU:HD21	2.20	0.51
1:B:2425:THR:HG23	1:B:2485:PHE:CE2	2.45	0.51
1:A:2385:VAL:O	1:A:2574:TYR:HE1	1.93	0.51
1:A:2655:ILE:HD11	1:A:2747:ARG:HH22	1.76	0.51
1:B:1826:PHE:HE1	1:B:1853:LEU:HD22	1.76	0.51
1:B:1917:ARG:HD2	1:B:3963:PHE:CE2	2.46	0.51
1:B:2084:TRP:CZ3	1:B:2085:LYS:HG3	2.45	0.51
1:B:2494:LEU:HB2	1:B:2499:SER:N	2.25	0.51
1:B:2741:HIS:HA	1:B:2744:ARG:HD2	1.91	0.51
1:B:3509:LEU:CD1	1:B:3513:VAL:CG2	2.83	0.51
1:B:1469:LEU:HD13	1:B:1523:LEU:CD2	2.40	0.51
1:B:2707:VAL:HG12	1:B:2712:LEU:CD1	2.41	0.51
1:B:2788:ARG:HG3	1:B:3459:ASP:HA	1.91	0.51
1:B:3737:THR:CB	1:B:3740:THR:HB	2.41	0.51
1:A:3737:THR:CB	1:A:3740:THR:CB	2.88	0.51
1:B:1540:LEU:HD11	1:B:1561:PHE:HB3	1.93	0.51
1:B:2368:PHE:N	1:B:2368:PHE:CD1	2.77	0.51
1:B:3308:ASN:O	1:B:3312:GLN:HB2	2.11	0.51
1:B:3353:LEU:HD23	1:B:3358:VAL:CG1	2.41	0.51
1:B:3817:GLY:H	1:B:3821:ASN:HB2	1.76	0.51
1:A:3725:VAL:HG22	1:A:3731:ASP:HA	1.93	0.51
1:B:1646:GLN:NE2	1:B:1758:TYR:OH	2.43	0.51
1:B:2382:ALA:O	1:B:2385:VAL:HG12	2.11	0.51
1:B:2620:ARG:NH1	1:B:2910:ASN:ND2	2.58	0.51
1:A:2084:TRP:HE3	1:A:2088:ILE:HD12	1.76	0.51
1:A:2141:ILE:HG22	1:A:2145:PHE:HB2	1.91	0.51
1:B:1744:LEU:CD2	1:B:1760:PHE:CD2	2.94	0.51
1:B:2125:TRP:CZ2	1:B:2178:LEU:HD13	2.46	0.51
1:B:3023:LYS:CE	1:B:3567:LEU:HD23	2.41	0.51
1:B:3330:TYR:CE2	1:B:3346:LEU:HD13	2.44	0.51
1:B:2002:ILE:HB	1:B:2014:PHE:CE2	2.46	0.51
1:B:2472:THR:HB	1:B:2524:VAL:HG22	1.92	0.51
1:B:4024:VAL:HG11	1:B:4062:TRP:CD2	2.46	0.51
1:B:1462:ASN:CB	1:B:1465:ILE:HG22	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2201:HIS:CE1	1:A:2497:TYR:CA	2.94	0.50
1:A:2984:VAL:C	1:A:2986:PRO:HD3	2.30	0.50
1:A:3017:VAL:HG21	1:A:3313:PHE:CE2	2.46	0.50
1:A:3569:GLU:O	1:A:3573:SER:OG	2.22	0.50
1:A:2336:ARG:HG2	1:A:2355:ASP:OD1	2.11	0.50
1:B:1929:ILE:HD12	1:B:1929:ILE:H	1.75	0.50
1:B:2312:ASP:HB3	1:B:2351:GLN:HG3	1.93	0.50
1:B:2336:ARG:CD	1:B:2355:ASP:OD2	2.59	0.50
1:A:1749:ILE:O	1:A:1755:LEU:HA	2.12	0.50
1:A:2488:GLU:CD	1:A:2491:LEU:HD11	2.32	0.50
1:A:1714:GLN:HB3	1:A:1727:LEU:HD11	1.92	0.50
1:A:1660:VAL:CG1	1:A:1728:TRP:CH2	2.95	0.50
1:A:1822:CYS:SG	1:A:1849:GLU:O	2.69	0.50
1:A:2109:LEU:CD1	1:A:2129:LEU:HD23	2.41	0.50
1:A:3547:ASP:HA	1:A:3550:LYS:HB3	1.93	0.50
1:A:3737:THR:OG1	1:A:3740:THR:CB	2.59	0.50
1:A:3757:ILE:HD11	1:A:4074:GLU:HG2	1.91	0.50
1:A:1534:PHE:CE2	1:A:1536:ARG:HB2	2.47	0.50
1:A:2048:SER:H	2:A:5093:ATP:N6	2.08	0.50
1:A:2410:SER:O	1:A:2411:LYS:CB	2.57	0.50
1:A:2514:GLY:HA3	1:A:2525:THR:HA	1.93	0.50
1:A:3939:ILE:HG13	1:A:4010:LEU:CD2	2.41	0.50
1:B:1939:PHE:HD1	1:B:1939:PHE:H	1.58	0.50
1:B:1968:PHE:CD1	1:B:1968:PHE:N	2.79	0.50
1:B:2220:CYS:SG	1:B:2224:SER:HB3	2.51	0.50
1:B:2941:THR:HG22	1:B:2942:ASP:N	2.25	0.50
1:B:2960:THR:HG22	1:B:2961:ILE:N	2.27	0.50
1:A:1622:GLN:HE22	1:A:1644:ILE:H	1.59	0.50
1:A:162:LEU:HA	1:A:165:ASP:O	2.11	0.50
1:A:1822:CYS:SG	1:A:1850:PHE:CA	2.97	0.50
1:A:2839:ASP:O	1:A:2841:PRO:HD3	2.12	0.50
1:B:1998:LEU:CD1	1:B:2022:PHE:HZ	2.25	0.50
1:A:1611:LEU:O	1:A:1615:ILE:HG12	2.12	0.50
1:A:2201:HIS:CE1	1:A:2497:TYR:HB3	2.47	0.50
1:A:2787:HIS:CA	1:A:3460:PRO:HG2	2.35	0.50
1:B:2833:THR:HG21	1:B:2841:PRO:HD2	1.94	0.50
1:B:3767:PHE:HB3	1:B:3769:VAL:HG23	1.94	0.50
1:A:1646:GLN:NE2	1:A:1758:TYR:OH	2.45	0.50
1:A:2489:ILE:HG22	1:A:2535:CYS:HB3	1.93	0.50
1:B:2262:LEU:HA	1:B:2265:ILE:HD12	1.93	0.50
1:B:4006:VAL:HA	1:B:4009:LYS:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1387:GLU:HA	1:A:1393:LYS:HA	1.94	0.49
1:B:1394:LEU:CD2	1:B:1449:GLN:HE22	2.25	0.49
1:B:1611:LEU:O	1:B:1615:ILE:HG12	2.11	0.49
1:B:2620:ARG:HH12	1:B:2910:ASN:ND2	2.10	0.49
1:B:3566:LEU:HD11	1:B:3570:LEU:HD11	1.93	0.49
1:A:1748:PHE:CD2	1:A:1755:LEU:HD22	2.47	0.49
1:A:1749:ILE:HD13	1:A:1813:LEU:HD22	1.93	0.49
1:A:2003:LEU:HD23	1:A:2006:LEU:HD12	1.93	0.49
1:A:2492:PRO:HB2	1:A:2502:VAL:HG11	1.93	0.49
1:A:3817:GLY:H	1:A:3821:ASN:CB	2.25	0.49
1:A:3848:LEU:CD2	1:A:3852:LYS:HE3	2.41	0.49
1:B:1425:GLU:OE2	1:B:1429:LEU:HD11	2.13	0.49
1:B:1822:CYS:HB2	1:B:1853:LEU:CD2	2.29	0.49
1:B:1536:ARG:HE	1:B:1841:ILE:HD13	1.77	0.49
1:B:1926:SER:CA	1:B:1970:LEU:HD12	2.42	0.49
1:A:1731:VAL:HG12	1:A:1732:GLN:N	2.27	0.49
1:A:2249:LEU:HD21	1:A:2302:PHE:HD2	1.77	0.49
1:A:2708:ASN:O	1:A:2712:LEU:HD13	2.12	0.49
1:A:3737:THR:CB	1:A:3740:THR:HB	2.43	0.49
1:B:3979:ASN:O	1:B:3981:PRO:HD2	2.11	0.49
1:A:2141:ILE:HG22	1:A:2145:PHE:CB	2.42	0.49
1:A:2318:ILE:O	1:A:2322:LEU:HB2	2.12	0.49
1:A:2563:SER:C	1:A:2565:LYS:H	2.15	0.49
1:A:3683:TYR:O	1:A:3687:SER:HB2	2.12	0.49
1:B:1983:LEU:HD11	1:B:2000:ARG:HH21	1.76	0.49
1:B:3461:ILE:C	1:B:3463:SER:H	2.15	0.49
1:A:1803:THR:HG21	1:A:1848:ASP:CG	2.33	0.49
1:B:1535:PRO:O	1:B:1841:ILE:HD11	2.13	0.49
1:B:2421:GLY:C	3:B:5094:ANP:O1B	2.51	0.49
1:B:2640:THR:HG23	1:B:2643:SER:H	1.77	0.49
1:B:2908:LEU:O	1:B:2912:CYS:HB2	2.12	0.49
1:B:4059:LEU:HA	1:B:4063:LEU:HD13	1.93	0.49
1:A:2853:LEU:HD21	1:A:2870:GLU:HG3	1.94	0.49
1:A:2941:THR:HG22	1:A:2942:ASP:N	2.24	0.49
1:A:1917:ARG:HD2	1:A:3963:PHE:CE2	2.48	0.49
1:B:2380:LEU:HD11	1:B:2577:ALA:HB2	1.88	0.49
1:B:2620:ARG:NH1	1:B:2910:ASN:CG	2.65	0.49
1:A:2099:ASN:HA	1:A:2149:ARG:O	2.12	0.49
1:A:2784:PRO:HG2	1:A:2817:ILE:HD13	1.94	0.49
1:A:2808:LEU:HD21	1:A:2856:LEU:HD12	1.95	0.49
1:A:2936:ILE:HG22	1:A:2962:ARG:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2835:LEU:HD23	1:B:2911:ARG:HB2	1.95	0.49
1:B:4084:SER:O	1:B:4088:LEU:HG	2.13	0.49
1:A:1502:ILE:HG23	1:A:1503:PRO:HD2	1.94	0.49
1:A:4074:GLU:HA	1:A:4077:GLN:HE21	1.78	0.49
1:B:3303:LYS:HA	1:B:3306:TRP:CD1	2.47	0.49
1:A:2080:LYS:O	1:A:2084:TRP:CD1	2.65	0.49
1:A:2819:GLU:HB3	1:A:2891:ILE:HG22	1.95	0.49
1:A:3461:ILE:C	1:A:3463:SER:H	2.15	0.49
1:B:2136:ARG:O	1:B:2140:ASP:O	2.30	0.49
1:B:2154:PHE:N	1:B:2154:PHE:HD1	2.10	0.49
1:A:2833:THR:HG21	1:A:2841:PRO:HD2	1.94	0.49
1:A:2988:SER:CB	1:A:2989:PRO:CD	2.66	0.49
1:A:3429:LEU:HD21	1:A:3439:ARG:HB3	1.95	0.49
1:A:3693:LYS:HE3	1:A:4080:GLU:HB3	1.94	0.49
1:B:1375:LYS:HE3	1:B:1431:LEU:HD13	1.94	0.49
1:B:162:LEU:HA	1:B:165:ASP:O	2.12	0.49
1:B:3409:ASP:HB3	1:B:3518:PHE:HB2	1.95	0.49
1:A:2152:VAL:HG12	1:A:2154:PHE:CE1	2.39	0.48
1:A:2407:LEU:HB2	1:A:2414:ILE:HD11	1.94	0.48
1:A:2878:VAL:HA	1:A:2881:ILE:HD12	1.95	0.48
1:A:3440:LEU:CD2	1:A:3462:ILE:HD12	2.42	0.48
1:B:1801:GLY:N	4:B:5096:SO4:O4	2.46	0.48
1:B:2339:ILE:HG23	1:B:2353:LEU:HB3	1.94	0.48
1:A:1630:ILE:HA	1:A:1634:THR:HG22	1.95	0.48
1:B:2177:THR:HG22	1:B:2183:ARG:HG2	1.94	0.48
1:A:1953:LEU:HD11	1:A:1973:LEU:HB3	1.94	0.48
1:A:2034:ILE:CD1	1:A:2061:TYR:CE2	2.95	0.48
1:A:2226:ILE:HG23	1:A:2288:VAL:HG21	1.95	0.48
1:A:2305:LEU:HD11	1:A:2368:PHE:CG	2.48	0.48
1:A:2856:LEU:HD23	1:A:2873:LEU:HB3	1.95	0.48
1:B:1911:ASN:OD1	1:B:1912:LEU:HG	2.13	0.48
1:B:2441:VAL:HB	1:B:2484:LEU:HD23	1.95	0.48
1:B:3848:LEU:HD21	1:B:3852:LYS:HE3	1.95	0.48
1:B:1802:LYS:NZ	4:B:5096:SO4:S	2.86	0.48
1:B:2046:GLY:O	1:B:2228:HIS:HB2	2.13	0.48
1:B:2838:ALA:HB3	1:B:2878:VAL:HG13	1.94	0.48
1:A:2109:LEU:CD1	1:A:2129:LEU:CD2	2.92	0.48
1:A:2822:ILE:O	1:A:2822:ILE:HG13	2.14	0.48
1:B:1497:ILE:O	1:B:1500:ILE:HG12	2.14	0.48
1:B:1926:SER:HA	1:B:1970:LEU:HD12	1.94	0.48
1:B:2122:THR:O	1:B:2123:LEU:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2489:ILE:HD11	1:B:2506:LEU:HD13	1.94	0.48
1:B:4024:VAL:HG23	1:B:4027:VAL:H	1.78	0.48
1:A:1645:PHE:CB	1:A:1765:ILE:HG21	2.41	0.48
1:A:2074:GLY:O	1:A:2197:ASP:HA	2.13	0.48
1:A:2175:ILE:HG13	1:A:2184:LEU:C	2.34	0.48
1:A:4033:LEU:HD12	1:A:4036:GLN:H	1.79	0.48
1:B:2100:VAL:HG12	1:B:2102:TYR:CE2	2.48	0.48
1:B:2833:THR:CG2	1:B:2841:PRO:HD2	2.43	0.48
1:B:3023:LYS:NZ	1:B:3571:ASN:HD21	2.11	0.48
1:B:2623:THR:CB	3:B:5094:ANP:O2'	2.61	0.48
1:A:1826:PHE:O	1:A:1826:PHE:CD1	2.67	0.48
1:A:1939:PHE:O	1:A:1940:GLU:HB3	2.13	0.48
1:A:2071:ILE:HB	1:A:2212:LEU:HD12	1.96	0.48
1:A:2314:ILE:HG22	1:A:2318:ILE:HD12	1.96	0.48
1:A:2387:ARG:O	1:A:2390:ILE:HG22	2.13	0.48
1:B:1493:LEU:HD23	1:B:1498:GLU:HB2	1.94	0.48
1:B:1995:VAL:HG22	1:B:2022:PHE:CE2	2.47	0.48
1:B:2102:TYR:HB2	1:B:2152:VAL:HG22	1.95	0.48
1:B:2252:LEU:HD22	1:B:2314:ILE:HG13	1.96	0.48
1:B:2473:LEU:CD2	1:B:2525:THR:HB	2.43	0.48
1:B:3406:PHE:CZ	1:B:3505:ILE:HG21	2.49	0.48
1:A:1409:LEU:CD2	1:A:1435:LEU:CB	2.86	0.48
1:A:2425:THR:OG1	3:A:5094:ANP:O2A	2.31	0.48
1:B:2111:LYS:HZ2	1:B:2161:GLU:HG2	1.73	0.48
1:B:2290:LEU:HD23	1:B:2321:SER:HA	1.96	0.48
1:B:2780:LYS:HB3	1:B:2813:THR:HG22	1.94	0.48
1:B:2755:HIS:CE1	1:B:2835:LEU:HG	2.49	0.48
1:B:3348:ILE:HA	1:B:3351:ARG:HG2	1.95	0.48
1:B:1604:ALA:HA	1:B:1607:TRP:HE1	1.75	0.48
1:B:2445:PHE:HA	1:B:2449:THR:HG21	1.96	0.48
1:A:2488:GLU:CG	1:A:2491:LEU:HD12	2.41	0.48
1:B:1392:LEU:C	1:B:1392:LEU:CD1	2.81	0.48
1:B:2106:THR:HG1	1:B:2154:PHE:HD2	1.61	0.48
1:B:23:LEU:O	1:B:25:GLU:N	2.47	0.48
1:B:4022:GLN:HG2	1:B:4022:GLN:O	2.14	0.48
1:A:2294:LEU:HB3	1:A:2317:LEU:HD22	1.94	0.47
1:A:4059:LEU:HA	1:A:4063:LEU:HD13	1.96	0.47
1:B:1803:THR:HG21	1:B:1848:ASP:CG	2.34	0.47
1:B:2305:LEU:HB3	1:B:2310:LEU:HD12	1.95	0.47
1:B:3566:LEU:HD13	1:B:3570:LEU:HD12	1.96	0.47
1:A:1466:GLN:HB3	1:A:1473:THR:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1534:PHE:CD2	1:A:1537:PHE:CE1	3.02	0.47
1:A:1649:LEU:HD13	1:A:1704:GLU:HG3	1.96	0.47
1:A:2354:SER:OG	1:A:2357:SER:CB	2.62	0.47
1:A:2582:VAL:O	1:A:2582:VAL:HG23	2.14	0.47
1:B:1822:CYS:SG	1:B:1850:PHE:HA	2.54	0.47
1:B:3671:VAL:HA	1:B:3674:ILE:HG22	1.95	0.47
1:A:2707:VAL:CG1	1:A:2712:LEU:HD12	2.45	0.47
1:B:2099:ASN:HA	1:B:2149:ARG:O	2.14	0.47
1:B:3787:THR:HG22	1:B:3875:MET:HB2	1.96	0.47
1:B:3978:ASN:O	1:B:3981:PRO:HD2	2.14	0.47
1:A:1421:TYR:CD2	1:A:1425:GLU:CG	2.97	0.47
1:A:1645:PHE:HB2	1:A:1697:LYS:HG3	1.95	0.47
1:A:2375:ILE:HG22	1:A:2376:PRO:O	2.14	0.47
1:A:3443:ALA:HB1	1:A:3450:VAL:HG21	1.96	0.47
1:A:3728:GLU:HG3	1:A:4079:LYS:HE2	1.95	0.47
1:A:3812:LYS:HB2	1:A:3839:ILE:HD12	1.97	0.47
1:A:3911:TRP:HH2	1:A:3926:VAL:HG13	1.79	0.47
1:B:1469:LEU:HD13	1:B:1523:LEU:HD21	1.96	0.47
1:B:2002:ILE:HG22	1:B:2006:LEU:HD11	1.96	0.47
1:B:2420:PRO:HD3	1:B:2536:ASN:ND2	2.25	0.47
1:B:2563:SER:CB	1:B:2566:SER:H	2.16	0.47
1:B:3772:TRP:HZ3	1:B:3780:ASN:HD22	1.62	0.47
1:B:40:TRP:O	1:B:44:LYS:N	2.48	0.47
1:A:1495:THR:CG2	1:A:1497:ILE:HG22	2.41	0.47
1:A:1527:LEU:HD21	1:A:1546:LEU:HD23	1.96	0.47
1:A:2677:VAL:HG11	1:A:2686:LEU:HD21	1.95	0.47
1:A:3728:GLU:CG	1:A:4079:LYS:HE2	2.44	0.47
1:B:1967:HIS:O	1:B:1968:PHE:HD1	1.97	0.47
1:B:2760:GLY:O	1:B:2761:ALA:HB3	2.14	0.47
1:A:1951:HIS:O	1:A:1955:LEU:HB2	2.14	0.47
1:A:2169:VAL:HG13	1:A:2186:ILE:HG12	1.96	0.47
1:A:2463:ASN:O	1:A:2475:PRO:HD2	2.15	0.47
1:A:3854:TYR:O	1:A:3858:HIS:HB2	2.15	0.47
1:B:2282:ASN:HB3	1:B:2552:ARG:HG3	1.97	0.47
1:B:3737:THR:OG1	1:B:3740:THR:CB	2.62	0.47
1:A:3365:ARG:HD2	1:A:3368:ASP:OD2	2.15	0.47
1:B:1387:GLU:HA	1:B:1393:LYS:HA	1.97	0.47
1:B:1657:THR:HG21	1:B:1734:PHE:O	2.15	0.47
1:B:2795:PHE:CE2	1:B:2799:LEU:HD11	2.49	0.47
1:A:1365:PHE:HE2	1:A:1420:TYR:CZ	2.33	0.47
1:A:2122:THR:O	1:A:2123:LEU:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2860:THR:HG22	1:A:2865:LEU:O	2.15	0.47
1:B:2437:LEU:H	1:B:2437:LEU:HD12	1.79	0.47
1:A:1822:CYS:SG	1:A:1849:GLU:C	2.93	0.47
1:A:2839:ASP:HB3	1:A:2878:VAL:HG22	1.97	0.47
1:B:2061:TYR:O	1:B:2064:GLN:HG2	2.14	0.47
1:B:2967:ASN:HB3	1:B:3356:PHE:CE2	2.49	0.47
1:B:2785:LYS:HD3	1:B:3482:GLY:O	2.15	0.47
1:A:1656:TRP:O	1:A:1660:VAL:HG12	2.15	0.47
1:A:2358:THR:HG22	1:A:2359:ILE:N	2.29	0.47
1:B:2472:THR:CG2	1:B:2524:VAL:CG2	2.86	0.47
1:A:1750:SER:HA	1:A:1755:LEU:HD23	1.96	0.47
1:A:2761:ALA:O	1:A:2892:CYS:HB3	2.15	0.47
1:A:3307:LEU:HA	1:A:3310:THR:HB	1.97	0.47
1:A:3466:ILE:HD13	1:A:3509:LEU:HD13	1.97	0.47
1:A:2422:SER:N	3:A:5094:ANP:O1B	2.47	0.47
1:B:2276:LEU:CD2	1:B:2415:ILE:HG21	2.45	0.47
1:B:2472:THR:HG22	1:B:2524:VAL:HG13	1.96	0.47
1:B:4020:ASN:ND2	1:B:4028:ARG:HD3	2.30	0.47
1:A:2034:ILE:CD1	1:A:2061:TYR:CZ	2.98	0.46
1:A:2757:MET:HE3	1:A:2912:CYS:CB	2.38	0.46
1:A:3632:LEU:HD13	1:A:3644:ILE:HD13	1.96	0.46
1:A:3844:ILE:HG12	1:A:3851:VAL:HG21	1.96	0.46
1:B:1656:TRP:HE1	1:B:1712:ILE:HD11	1.81	0.46
1:B:1822:CYS:SG	1:B:1849:GLU:C	2.94	0.46
1:B:2155:ASP:O	1:B:2549:ARG:NH1	2.46	0.46
1:B:2318:ILE:O	1:B:2322:LEU:HB2	2.14	0.46
1:B:2441:VAL:HG21	1:B:2482:LEU:HD21	1.96	0.46
1:B:2758:LEU:HD23	1:B:2915:ASN:HB3	1.96	0.46
1:B:3307:LEU:HA	1:B:3310:THR:HB	1.97	0.46
1:A:1592:LEU:CD1	1:A:1596:ILE:HD12	2.45	0.46
1:A:2178:LEU:HD12	1:A:2182:GLU:HB2	1.97	0.46
1:A:2516:TRP:CZ3	1:A:2523:TRP:HB2	2.51	0.46
1:A:2758:LEU:HD23	1:A:2915:ASN:HB3	1.96	0.46
1:B:2354:SER:OG	1:B:2357:SER:CB	2.63	0.46
1:B:2860:THR:HG22	1:B:2865:LEU:O	2.15	0.46
1:B:2938:MET:SD	1:B:3321:ILE:HG21	2.55	0.46
1:B:3547:ASP:HA	1:B:3550:LYS:HB3	1.97	0.46
1:A:1871:GLY:HA3	1:A:1879:ILE:HG21	1.98	0.46
1:A:2761:ALA:O	1:A:2892:CYS:CB	2.63	0.46
1:B:1636:ILE:O	1:B:1640:VAL:HG23	2.16	0.46
1:B:2464:TYR:CE1	1:B:2524:VAL:HG11	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3372:THR:HG23	1:B:3375:GLU:HB2	1.97	0.46
1:A:1479:LEU:HD11	1:A:1515:SER:HB3	1.97	0.46
1:A:1527:LEU:HD21	1:A:1546:LEU:CD2	2.45	0.46
1:A:1606:GLU:O	1:A:1610:ILE:HG12	2.16	0.46
1:A:1727:LEU:O	1:A:1731:VAL:HG23	2.15	0.46
1:A:2225:LYS:HD2	1:A:2281:PHE:CZ	2.51	0.46
1:A:3869:GLU:O	1:A:3870:LYS:C	2.54	0.46
1:A:3979:ASN:C	1:A:3981:PRO:CD	2.84	0.46
1:B:1367:ILE:HD12	1:B:1367:ILE:H	1.80	0.46
1:B:1593:ASN:HD21	1:B:1621:THR:CB	2.29	0.46
1:B:2220:CYS:HG	1:B:2224:SER:HB3	1.80	0.46
1:B:2761:ALA:O	1:B:2892:CYS:SG	2.73	0.46
1:B:3641:PHE:HA	1:B:3889:LEU:HD21	1.96	0.46
1:A:1540:LEU:HD11	1:A:1561:PHE:HB3	1.97	0.46
1:A:1744:LEU:HA	1:A:1760:PHE:HE2	1.75	0.46
1:A:3461:ILE:C	1:A:3463:SER:N	2.67	0.46
1:A:3911:TRP:CH2	1:A:3926:VAL:HG13	2.50	0.46
1:B:1612:ASP:HA	1:B:1615:ILE:CG1	2.46	0.46
1:B:1983:LEU:HD13	1:B:2000:ARG:HE	1.80	0.46
1:B:2137:VAL:O	1:B:2141:ILE:HG23	2.16	0.46
1:A:2061:TYR:CD1	1:A:2091:MET:HE3	2.47	0.46
1:A:2476:LYS:HZ1	1:A:2528:ARG:HD3	1.81	0.46
1:A:3470:PHE:CE1	1:A:3488:VAL:HG21	2.51	0.46
1:B:1421:TYR:O	1:B:1425:GLU:CA	2.63	0.46
1:B:2112:GLU:HB3	1:B:2117:SER:OG	2.14	0.46
1:B:2493:LYS:HG3	1:B:2494:LEU:N	2.30	0.46
1:B:2107:LYS:CE	1:B:2499:SER:HB3	2.43	0.46
1:B:2464:TYR:HE1	1:B:2524:VAL:HG11	1.80	0.46
1:B:2737:SER:HB2	1:B:2924:THR:HG21	1.97	0.46
1:A:2084:TRP:CH2	1:A:2153:VAL:HG21	2.50	0.46
1:B:1392:LEU:HD13	1:B:1393:LYS:CA	2.45	0.46
1:B:1514:ASP:O	1:B:1518:MET:HG2	2.15	0.46
1:B:1681:LYS:HE2	1:B:1939:PHE:CZ	2.51	0.46
1:B:2169:VAL:HG13	1:B:2186:ILE:HG12	1.98	0.46
1:B:3869:GLU:O	1:B:3870:LYS:C	2.52	0.46
1:A:1626:CYS:SG	1:A:1639:VAL:CG1	3.01	0.46
1:A:1910:GLU:HB2	1:A:3846:MET:HA	1.97	0.46
1:A:2063:MET:HB3	1:A:2070:LEU:HD11	1.98	0.46
1:A:2305:LEU:CD1	1:A:2368:PHE:CD1	2.98	0.46
1:A:3319:GLU:HA	1:A:3359:LYS:O	2.15	0.46
1:A:3473:ALA:HB3	1:A:3476:ARG:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3889:LEU:HG	1:A:3894:ARG:HD3	1.97	0.46
1:A:4033:LEU:HD13	1:A:4035:GLN:CG	2.46	0.46
1:A:1802:LYS:NZ	4:A:5095:SO4:O1	2.40	0.46
1:B:1620:PHE:HB2	1:B:1760:PHE:CZ	2.50	0.46
1:B:2563:SER:C	1:B:2565:LYS:H	2.18	0.46
1:B:4017:GLY:HA3	1:B:4021:LEU:HD12	1.97	0.46
1:B:1969:GLY:O	1:B:1972:THR:HB	2.15	0.46
1:B:3889:LEU:HG	1:B:3894:ARG:HD3	1.97	0.46
1:A:3509:LEU:HD12	1:A:3513:VAL:HG23	1.94	0.46
1:B:1706:LEU:CD1	1:B:1936:ILE:HG12	2.45	0.46
1:B:1956:LEU:CB	1:B:1968:PHE:CE2	2.90	0.46
1:B:3815:PRO:O	1:B:3821:ASN:HB3	2.16	0.46
1:B:3935:PHE:HB2	1:B:4014:VAL:HG11	1.97	0.46
1:A:1529:ARG:O	1:A:1533:GLN:HG2	2.16	0.45
1:A:1802:LYS:O	1:A:1806:VAL:HG23	2.16	0.45
1:A:2755:HIS:HB3	1:A:2912:CYS:SG	2.56	0.45
1:A:215:PRO:C	1:A:3475:ASN:ND2	2.69	0.45
1:B:1827:ASP:HB3	1:B:1830:VAL:HG12	1.98	0.45
1:B:2488:GLU:CG	1:B:2491:LEU:HD12	2.45	0.45
1:B:2761:ALA:O	1:B:2892:CYS:CB	2.64	0.45
1:A:2241:LEU:HD13	1:A:2299:ARG:HH11	1.80	0.45
1:A:2788:ARG:HG3	1:A:3459:ASP:HA	1.96	0.45
1:A:3308:ASN:O	1:A:3312:GLN:HB2	2.15	0.45
1:A:3322:GLY:HA2	1:A:3325:ILE:HD12	1.98	0.45
1:A:3692:LYS:HE3	1:A:3898:GLU:HB3	1.98	0.45
1:B:1392:LEU:HD22	1:B:1393:LYS:H	1.82	0.45
1:B:1813:LEU:HD12	1:B:1844:TRP:CH2	2.50	0.45
1:B:2109:LEU:HD13	1:B:2129:LEU:HD23	1.97	0.45
1:B:2380:LEU:HD12	1:B:2577:ALA:HB2	1.85	0.45
1:B:2571:TYR:HA	1:B:2574:TYR:HB2	1.98	0.45
1:B:2420:PRO:CB	1:B:2620:ARG:HH21	2.29	0.45
1:B:3338:ASN:HD22	1:B:3341:GLU:HG2	1.81	0.45
1:A:1365:PHE:CZ	1:A:1420:TYR:CG	3.05	0.45
1:A:1706:LEU:HD22	1:A:1935:GLN:HG2	1.98	0.45
1:A:2490:ASN:HB3	1:A:2546:MET:HE1	1.98	0.45
1:A:2563:SER:CB	1:A:2566:SER:H	2.19	0.45
1:B:1626:CYS:SG	1:B:1639:VAL:HG11	2.56	0.45
1:B:3538:ASN:HB3	1:B:3541:MET:HG2	1.98	0.45
1:A:1365:PHE:HZ	1:A:1420:TYR:CE1	2.31	0.45
1:A:1563:LYS:HA	1:A:1569:ILE:O	2.17	0.45
1:A:1563:LYS:HE2	1:A:1585:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2081:THR:HG22	1:A:2085:LYS:HD2	1.98	0.45
1:A:3592:LYS:O	1:A:3596:ASN:N	2.49	0.45
1:A:3721:THR:O	1:A:3725:VAL:HG23	2.16	0.45
1:A:3832:SER:O	1:A:3836:GLY:N	2.43	0.45
1:B:1554:HIS:O	1:B:1555:HIS:HB2	2.17	0.45
1:B:1704:GLU:OE2	1:B:1768:ARG:NH1	2.49	0.45
1:B:2471:LEU:O	1:B:2473:LEU:HG	2.16	0.45
1:B:3965:SER:HA	1:B:3968:LEU:HD12	1.98	0.45
1:A:1570:GLU:HB2	1:A:1585:VAL:HA	1.99	0.45
1:A:2204:PRO:HA	1:A:2207:ILE:HD12	1.97	0.45
1:A:2419:PRO:O	1:A:2424:LYS:NZ	2.50	0.45
1:A:23:LEU:O	1:A:25:GLU:N	2.50	0.45
1:A:3342:ARG:NH2	1:A:3393:ASN:OD1	2.47	0.45
1:A:3926:VAL:HG11	1:A:4042:ARG:HG2	1.97	0.45
1:B:1749:ILE:HD13	1:B:1813:LEU:HD22	1.99	0.45
1:B:2201:HIS:CE1	1:B:2497:TYR:HB3	2.52	0.45
1:B:2494:LEU:HD12	1:B:2494:LEU:O	2.17	0.45
1:B:2839:ASP:O	1:B:2841:PRO:HD3	2.17	0.45
1:A:1677:ASP:HA	1:A:1680:ILE:HD12	1.98	0.45
1:A:2412:ARG:HD3	1:A:2555:ALA:HB2	1.99	0.45
1:A:2938:MET:SD	1:A:3321:ILE:HG21	2.57	0.45
1:A:1919:PHE:CD1	1:A:3996:GLY:HA2	2.51	0.45
1:A:4033:LEU:HD12	1:A:4035:GLN:N	2.32	0.45
1:A:4065:LEU:HD12	1:A:4065:LEU:C	2.37	0.45
1:B:1495:THR:HB	1:B:1498:GLU:CG	2.47	0.45
1:B:1940:GLU:CG	1:B:1941:ASP:H	2.18	0.45
1:B:3461:ILE:C	1:B:3463:SER:N	2.68	0.45
1:A:2493:LYS:HG3	1:A:2494:LEU:N	2.22	0.45
1:B:1383:TYR:CE2	1:B:1401:LEU:HD13	2.52	0.45
1:B:1531:ARG:CD	1:B:1538:TYR:HA	2.47	0.45
1:B:3946:VAL:HB	1:B:3947:PRO:HA	1.98	0.45
1:A:1750:SER:HB2	1:A:1755:LEU:CD2	2.47	0.45
1:A:1803:THR:HG21	1:A:1848:ASP:OD1	2.17	0.45
1:A:1934:LEU:HD22	1:A:1945:LEU:HD12	1.98	0.45
1:A:1984:ILE:CG2	1:A:1989:GLU:HG3	2.46	0.45
1:A:2385:VAL:HG23	1:A:2574:TYR:HD1	1.82	0.45
1:A:2755:HIS:O	1:A:2913:ILE:N	2.48	0.45
1:A:3353:LEU:HD23	1:A:3358:VAL:HG11	1.98	0.45
1:A:3509:LEU:CG	1:A:3513:VAL:HG21	2.46	0.45
1:A:3628:ILE:HG22	1:A:3649:PHE:HE2	1.82	0.45
1:A:3903:ILE:O	1:A:3907:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3994:TYR:O	1:A:3998:ILE:HD12	2.16	0.45
1:A:4022:GLN:O	1:A:4023:ILE:C	2.56	0.45
1:B:2155:ASP:OD1	1:B:2195:GLU:OE2	2.34	0.45
1:B:2354:SER:H	1:B:2357:SER:HB2	1.81	0.45
1:B:2386:MET:HB3	1:B:2627:ARG:CD	2.45	0.45
1:B:2474:LEU:HB3	1:B:2526:ILE:HG22	1.99	0.45
1:B:2225:LYS:HG3	2:B:5093:ATP:H1'	1.99	0.45
1:A:1392:LEU:HD13	1:A:1393:LYS:CA	2.46	0.45
1:A:1469:LEU:HD13	1:A:1523:LEU:HD21	1.99	0.45
1:A:1998:LEU:HD11	1:A:2022:PHE:HZ	1.82	0.45
1:A:2002:ILE:HB	1:A:2014:PHE:CE2	2.52	0.45
1:A:2084:TRP:CZ3	1:A:2085:LYS:HG3	2.52	0.45
1:B:1849:GLU:HG2	1:B:1899:ASN:HD22	1.82	0.45
1:B:3897:TYR:CZ	1:B:3899:ASP:HB3	2.52	0.45
1:A:1365:PHE:CE2	1:A:1420:TYR:CD2	3.04	0.45
1:A:1970:LEU:HD12	1:A:1971:ARG:CA	2.47	0.45
1:A:3330:TYR:CE1	1:A:3334:PHE:CE2	3.04	0.45
1:B:1677:ASP:HA	1:B:1680:ILE:HD12	1.99	0.45
1:B:2047:PHE:CE2	1:B:2082:ALA:HB1	2.52	0.45
1:B:2104:ILE:O	1:B:2154:PHE:HA	2.16	0.45
1:B:2203:THR:HG23	1:B:2204:PRO:HD2	1.99	0.45
1:B:2294:LEU:HB3	1:B:2317:LEU:HD22	1.98	0.45
1:B:2447:LYS:HE3	1:B:2493:LYS:HD3	1.98	0.45
1:B:2508:GLN:HG2	1:B:2512:LYS:HG3	1.97	0.45
1:B:2755:HIS:HD2	1:B:2911:ARG:HB3	1.82	0.45
1:B:3862:THR:HB	1:B:3865:ALA:HB2	1.99	0.45
1:A:1940:GLU:HG3	1:A:1941:ASP:H	1.82	0.44
1:A:2654:ARG:NH1	1:A:2658:ASP:OD1	2.50	0.44
1:A:3330:TYR:CE2	1:A:3346:LEU:HD13	2.51	0.44
1:B:1421:TYR:CD2	1:B:1425:GLU:CG	2.98	0.44
1:B:2654:ARG:HH22	1:B:2691:SER:HB2	1.81	0.44
1:A:1527:LEU:HD22	1:A:1545:LEU:HD22	1.97	0.44
1:A:2424:LYS:HA	1:A:2559:LEU:HD12	1.99	0.44
1:A:2745:ILE:HG12	1:A:2756:MET:CE	2.42	0.44
1:A:3372:THR:HG23	1:A:3375:GLU:HB2	2.00	0.44
1:B:1392:LEU:HD23	1:B:1484:LYS:HA	1.99	0.44
1:B:1612:ASP:CA	1:B:1615:ILE:HG12	2.47	0.44
1:B:2109:LEU:HB3	1:B:2113:SER:HB2	2.00	0.44
1:B:3481:ILE:O	1:B:3483:ASP:N	2.46	0.44
1:B:3817:GLY:H	1:B:3821:ASN:CB	2.29	0.44
1:B:3845:GLN:NE2	1:B:3882:ASP:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1967:HIS:C	1:A:1968:PHE:CD1	2.87	0.44
1:A:2356:TYR:CE1	1:A:2399:LYS:HD2	2.52	0.44
1:A:3505:ILE:O	1:A:3510:ARG:NH1	2.51	0.44
1:B:1995:VAL:HG22	1:B:2022:PHE:CD2	2.52	0.44
1:A:3968:LEU:HA	1:A:3971:VAL:HG12	2.00	0.44
1:B:3010:LEU:HD22	1:B:3320:LEU:HD12	1.99	0.44
1:A:1392:LEU:CD1	1:A:1392:LEU:C	2.83	0.44
1:A:1536:ARG:HD3	1:A:1841:ILE:CD1	2.47	0.44
1:A:1849:GLU:CD	1:A:1899:ASN:HD22	2.20	0.44
1:A:1982:PRO:O	1:A:1985:SER:HB2	2.18	0.44
1:A:2960:THR:HG22	1:A:2961:ILE:N	2.32	0.44
1:A:3671:VAL:HA	1:A:3674:ILE:CG2	2.46	0.44
1:B:2707:VAL:HG12	1:B:2712:LEU:HD12	1.99	0.44
1:B:3636:GLY:CA	1:B:3642:TYR:O	2.66	0.44
1:B:1531:ARG:HD3	1:B:1537:PHE:O	2.17	0.44
1:B:1715:LEU:HG	1:B:1727:LEU:HD22	2.00	0.44
1:B:1779:PHE:O	1:B:1783:THR:HG22	2.18	0.44
1:B:3330:TYR:OH	1:B:3346:LEU:HD13	2.17	0.44
1:B:3998:ILE:HG22	1:B:4004:LEU:HG	1.97	0.44
1:A:2982:VAL:HG12	1:A:2983:GLY:N	2.32	0.44
1:B:2421:GLY:CA	3:B:5094:ANP:O1B	2.66	0.44
1:B:2783:GLN:HG2	1:B:2816:ILE:HB	2.00	0.44
1:B:3330:TYR:CZ	1:B:3346:LEU:HD13	2.53	0.44
1:A:1706:LEU:HD21	1:A:1935:GLN:CG	2.47	0.44
1:A:2044:ARG:HH21	1:A:2093:ILE:HD11	1.82	0.44
1:A:2105:ASP:OD2	1:A:2508:GLN:HB2	2.17	0.44
1:A:2838:ALA:HB3	1:A:2878:VAL:HG13	2.00	0.44
1:A:3798:PHE:HA	1:A:3801:ILE:HG12	2.00	0.44
1:A:2423:GLY:N	3:A:5094:ANP:O1B	2.39	0.44
1:B:1385:VAL:HG21	1:B:1491:PHE:CD1	2.53	0.44
1:A:1540:LEU:HD23	1:A:1540:LEU:HA	1.71	0.44
1:A:1646:GLN:OE1	1:A:1763:ILE:HG12	2.18	0.44
1:A:1983:LEU:HB3	1:A:1993:THR:HG23	2.00	0.44
1:A:2127:ASP:HB3	1:A:2132:SER:HB3	2.00	0.44
1:A:3473:ALA:CB	1:A:3476:ARG:HG3	2.48	0.44
1:A:3930:PHE:HE2	1:A:4029:ILE:CD1	2.31	0.44
1:B:1375:LYS:O	1:B:1379:LYS:HG2	2.18	0.44
1:B:2389:ASP:HB3	1:B:2433:ARG:HH11	1.83	0.44
1:B:2572:GLU:CG	1:B:2590:GLU:HG3	2.47	0.44
1:B:2755:HIS:HB3	1:B:2912:CYS:SG	2.58	0.44
1:A:1636:ILE:O	1:A:1640:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2088:ILE:HG12	1:A:2151:TRP:CZ2	2.53	0.43
1:A:2383:HIS:CE1	1:A:2384:GLU:HG3	2.53	0.43
1:A:2941:THR:CG2	1:A:2942:ASP:H	2.25	0.43
1:A:4045:LEU:O	1:A:4048:ILE:HG22	2.18	0.43
1:B:1495:THR:CG2	1:B:1497:ILE:HG22	2.48	0.43
1:B:1645:PHE:HB2	1:B:1697:LYS:HG3	2.00	0.43
1:B:3911:TRP:CH2	1:B:3926:VAL:CG1	3.01	0.43
1:B:4020:ASN:HB3	1:B:4028:ARG:NH1	2.33	0.43
1:A:1744:LEU:HD22	1:A:1760:PHE:CD2	2.53	0.43
1:A:2201:HIS:CE1	1:A:2497:TYR:O	2.71	0.43
1:A:2565:LYS:O	1:A:2569:GLN:HG3	2.19	0.43
1:A:3833:LYS:NZ	1:A:3862:THR:HG21	2.33	0.43
1:A:3845:GLN:NE2	1:A:3882:ASP:O	2.51	0.43
1:B:2984:VAL:C	1:B:2986:PRO:HD3	2.39	0.43
1:A:1759:LYS:HE3	1:A:1761:GLU:OE2	2.18	0.43
1:A:2034:ILE:HD12	1:A:2061:TYR:CE2	2.52	0.43
1:A:2099:ASN:HB3	1:A:2151:TRP:HE1	1.83	0.43
1:A:2203:THR:HG23	1:A:2204:PRO:HD2	1.99	0.43
1:A:2760:GLY:O	1:A:2761:ALA:HB3	2.18	0.43
1:A:3471:ASN:HB2	1:A:3478:THR:HG23	2.00	0.43
1:A:3978:ASN:O	1:A:3981:PRO:HD3	2.17	0.43
1:B:1394:LEU:HD22	1:B:1449:GLN:HE22	1.83	0.43
1:B:1540:LEU:HA	1:B:1540:LEU:HD23	1.72	0.43
1:B:3592:LYS:O	1:B:3596:ASN:N	2.51	0.43
1:B:3832:SER:O	1:B:3836:GLY:N	2.46	0.43
1:B:3848:LEU:O	1:B:3849:SER:C	2.57	0.43
1:A:1536:ARG:CD	1:A:1841:ILE:HD13	2.48	0.43
1:A:2104:ILE:O	1:A:2154:PHE:HA	2.18	0.43
1:A:4033:LEU:CD1	1:A:4035:GLN:H	2.31	0.43
1:B:1535:PRO:O	1:B:1841:ILE:CD1	2.65	0.43
1:B:2152:VAL:HG12	1:B:2154:PHE:HE1	1.83	0.43
1:B:2201:HIS:CE1	1:B:2497:TYR:CA	3.01	0.43
1:B:3555:TYR:HE1	1:B:3593:GLU:HG2	1.83	0.43
1:B:3886:ALA:N	1:B:3887:PRO:CD	2.78	0.43
1:A:1421:TYR:O	1:A:1425:GLU:CA	2.65	0.43
1:A:1934:LEU:HD13	1:A:1945:LEU:HB2	2.01	0.43
1:A:3544:LYS:O	1:A:3548:LEU:HB2	2.19	0.43
1:A:3800:LEU:HA	1:A:3803:LEU:HD12	1.99	0.43
1:A:3967:TYR:HE2	1:A:3985:VAL:HA	1.83	0.43
1:A:4034:LEU:O	1:A:4036:GLN:HG3	2.19	0.43
1:B:1794:PHE:HB3	1:B:1919:PHE:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3544:LYS:O	1:B:3548:LEU:HB2	2.18	0.43
1:B:4065:LEU:HD12	1:B:4065:LEU:C	2.39	0.43
1:A:2141:ILE:CG2	1:A:2145:PHE:HB2	2.49	0.43
1:A:2787:HIS:HB3	1:A:3461:ILE:HG23	2.00	0.43
1:B:1826:PHE:O	1:B:1826:PHE:CG	2.71	0.43
1:B:2517:LYS:HD2	1:B:2524:VAL:CG2	2.49	0.43
1:B:3462:ILE:O	1:B:3465:LEU:N	2.51	0.43
1:A:1835:LEU:O	1:A:1838:ILE:HG22	2.18	0.43
1:A:1872:LEU:HG	1:A:1888:LEU:HD21	2.00	0.43
1:A:3459:ASP:OD2	1:A:3461:ILE:CG1	2.65	0.43
1:A:3566:LEU:HD11	1:A:3570:LEU:HD11	1.99	0.43
1:A:3690:LEU:HD23	1:A:3694:PHE:HB3	2.01	0.43
1:A:3785:TYR:CE2	1:A:3859:VAL:HG13	2.54	0.43
1:A:4021:LEU:CD2	1:A:4023:ILE:HG12	2.49	0.43
1:B:1741:LEU:O	1:B:1742:ASP:HB2	2.18	0.43
1:B:2425:THR:CG2	1:B:2485:PHE:HE2	2.32	0.43
1:B:2761:ALA:O	1:B:2892:CYS:HB3	2.19	0.43
1:A:2252:LEU:HD22	1:A:2314:ILE:HG13	2.01	0.43
1:A:2788:ARG:HB2	1:A:3459:ASP:HB3	2.01	0.43
1:A:3788:MET:HG3	1:A:3788:MET:O	2.19	0.43
1:B:1391:GLY:HA3	1:B:1484:LYS:HZ3	1.81	0.43
1:B:2220:CYS:SG	1:B:2221:SER:N	2.92	0.43
1:B:2510:MET:O	1:B:2513:GLN:NE2	2.52	0.43
1:B:3930:PHE:CE2	1:B:4029:ILE:HD13	2.51	0.43
1:A:1794:PHE:CD1	1:A:1802:LYS:HB3	2.51	0.43
1:A:1953:LEU:HA	1:A:1956:LEU:HD12	2.01	0.43
1:A:2141:ILE:HG22	1:A:2145:PHE:CG	2.54	0.43
1:B:1789:LYS:HD3	1:B:1872:LEU:O	2.19	0.43
1:B:2129:LEU:O	1:B:2133:ILE:HG12	2.19	0.43
1:B:2152:VAL:HG12	1:B:2154:PHE:CE1	2.54	0.43
1:B:2446:SER:H	1:B:2449:THR:HG21	1.80	0.43
1:B:3505:ILE:O	1:B:3510:ARG:NH1	2.52	0.43
1:A:1438:LEU:O	1:A:1442:GLN:HB2	2.19	0.43
1:A:2061:TYR:O	1:A:2064:GLN:HG2	2.19	0.43
1:B:1409:LEU:CD2	1:B:1435:LEU:CB	2.80	0.43
1:B:1536:ARG:HD3	1:B:1536:ARG:HA	1.67	0.43
1:B:2034:ILE:CD1	1:B:2061:TYR:CE2	3.02	0.43
1:B:2368:PHE:O	1:B:2369:SER:OG	2.25	0.43
1:A:1469:LEU:CD1	1:A:1523:LEU:CD2	2.97	0.42
1:A:1645:PHE:CZ	1:A:1768:ARG:HD2	2.52	0.42
1:A:2170:LEU:HB3	1:A:2209:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2220:CYS:SG	1:A:2224:SER:HB3	2.59	0.42
1:A:4023:ILE:HG13	1:A:4029:ILE:HD12	2.01	0.42
1:B:1616:LYS:HE3	1:B:1761:GLU:HG3	2.01	0.42
1:A:1702:LEU:HD23	1:A:1702:LEU:HA	1.85	0.42
1:A:1744:LEU:HD22	1:A:1760:PHE:CG	2.54	0.42
1:A:3326:ILE:HG22	1:A:3330:TYR:CE2	2.54	0.42
1:A:3629:PHE:O	1:A:3633:GLU:HB2	2.20	0.42
1:A:3930:PHE:HE2	1:A:4029:ILE:HD13	1.83	0.42
1:B:2001:VAL:O	1:B:2004:PRO:HD2	2.19	0.42
1:B:2027:THR:HA	1:B:2028:PRO:HD3	1.55	0.42
1:B:2151:TRP:CE3	1:B:2193:LEU:HD11	2.54	0.42
1:B:2220:CYS:HB2	2:B:5093:ATP:N6	2.33	0.42
1:B:2707:VAL:HG11	1:B:2712:LEU:HD12	2.00	0.42
1:B:3979:ASN:C	1:B:3981:PRO:CD	2.86	0.42
1:B:2220:CYS:SG	2:B:5093:ATP:N6	2.93	0.42
1:A:2742:ILE:HG23	1:A:2773:VAL:HG22	2.00	0.42
1:A:3409:ASP:HA	1:A:3410:PRO:HD3	1.93	0.42
1:A:3897:TYR:CZ	1:A:3899:ASP:HB3	2.54	0.42
1:B:1630:ILE:HG21	1:B:1655:MET:SD	2.57	0.42
1:B:1870:ASN:O	1:B:1874:VAL:HG23	2.19	0.42
1:B:3930:PHE:HE2	1:B:4029:ILE:CD1	2.31	0.42
1:A:1392:LEU:HD23	1:A:1484:LYS:HA	2.01	0.42
1:A:1554:HIS:O	1:A:1555:HIS:HB2	2.19	0.42
1:A:1822:CYS:HB2	1:A:1853:LEU:CD2	2.27	0.42
1:A:4022:GLN:HG2	1:A:4022:GLN:O	2.19	0.42
1:B:2224:SER:C	2:B:5093:ATP:C2	2.92	0.42
1:B:2747:ARG:O	1:B:2751:GLN:HG2	2.19	0.42
1:B:3431:PHE:CZ	1:B:3458:PHE:HD1	2.38	0.42
1:B:3459:ASP:HB2	1:B:3460:PRO:HD2	2.01	0.42
1:A:1365:PHE:N	1:A:1365:PHE:HD1	2.17	0.42
1:A:2109:LEU:HD11	1:A:2129:LEU:CD2	2.50	0.42
1:A:2378:VAL:HG11	1:A:2392:ILE:HD12	2.00	0.42
1:A:2707:VAL:HG12	1:A:2708:ASN:N	2.35	0.42
1:A:4006:VAL:HG13	1:A:4009:LYS:HE2	2.01	0.42
1:A:4037:SER:HB3	1:A:4040:GLU:HB3	2.01	0.42
1:B:4033:LEU:HD23	1:B:4033:LEU:HA	1.84	0.42
1:A:1536:ARG:HD2	1:A:1565:MET:O	2.19	0.42
1:A:3784:ASN:ND2	1:A:3865:ALA:O	2.52	0.42
1:B:1656:TRP:O	1:B:1660:VAL:HG12	2.18	0.42
1:B:3813:ILE:HG22	1:B:3840:LEU:HD23	2.01	0.42
1:A:1672:TYR:O	1:A:1675:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2653:TRP:HB3	1:A:2654:ARG:NH1	2.34	0.42
1:A:2737:SER:HB2	1:A:2924:THR:HG21	2.01	0.42
1:A:3570:LEU:HD23	1:A:3580:ASN:CG	2.40	0.42
1:A:3645:SER:CB	1:A:3890:GLN:NE2	2.80	0.42
1:B:1459:LEU:HD23	1:B:1465:ILE:HG13	2.02	0.42
1:B:1762:TYR:CZ	1:B:1764:GLY:HA2	2.55	0.42
1:B:1849:GLU:CD	1:B:1899:ASN:HD22	2.23	0.42
1:B:23:LEU:C	1:B:25:GLU:N	2.73	0.42
1:B:2467:THR:HG22	1:B:2468:SER:N	2.34	0.42
1:B:3848:LEU:O	1:B:3851:VAL:N	2.53	0.42
1:A:1706:LEU:HD23	1:A:1706:LEU:HA	1.90	0.42
1:A:3612:ASP:C	1:A:3615:VAL:HG22	2.40	0.42
1:A:3628:ILE:HD11	1:A:3679:TYR:CZ	2.55	0.42
1:A:4022:GLN:HA	1:A:4028:ARG:HA	2.01	0.42
1:B:1531:ARG:HD2	1:B:1538:TYR:HA	2.01	0.42
1:B:1660:VAL:CG1	1:B:1728:TRP:CH2	3.02	0.42
1:B:2114:LEU:HA	1:B:2129:LEU:HB3	2.02	0.42
1:A:1769:LEU:HD11	1:A:1804:GLU:HB3	2.01	0.42
1:A:2354:SER:H	1:A:2357:SER:HB2	1.85	0.42
1:A:2799:LEU:HD13	1:A:2840:ILE:CD1	2.49	0.42
1:A:3304:GLU:C	1:A:3306:TRP:H	2.23	0.42
1:A:3462:ILE:O	1:A:3465:LEU:N	2.48	0.42
1:A:3509:LEU:HG	1:A:3513:VAL:HG21	2.02	0.42
1:A:3845:GLN:O	1:A:3848:LEU:HB2	2.20	0.42
1:A:4033:LEU:CD1	1:A:4035:GLN:N	2.83	0.42
1:B:1750:SER:CB	1:B:1755:LEU:HD23	2.50	0.42
1:B:1838:ILE:HG13	1:B:1843:ALA:HB3	2.02	0.42
1:B:2106:THR:H	1:B:2156:SER:HB2	1.83	0.42
1:A:1645:PHE:CZ	1:A:1649:LEU:HD22	2.55	0.42
1:A:3600:LYS:HA	1:A:3603:GLU:HG2	2.01	0.42
1:A:3671:VAL:CA	1:A:3674:ILE:HG22	2.49	0.42
1:B:1593:ASN:ND2	1:B:1621:THR:OG1	2.47	0.42
1:B:2336:ARG:HG2	1:B:2355:ASP:OD1	2.19	0.42
1:A:3725:VAL:HA	1:A:3730:SER:O	2.19	0.41
1:A:3886:ALA:N	1:A:3887:PRO:CD	2.80	0.41
1:A:40:TRP:O	1:A:44:LYS:N	2.53	0.41
1:B:1575:LEU:O	1:B:1576:GLU:HB3	2.19	0.41
1:B:1992:LYS:CG	1:B:2024:SER:CB	2.83	0.41
1:B:1983:LEU:CD1	1:B:2000:ARG:HH21	2.33	0.41
1:B:2707:VAL:CB	1:B:2712:LEU:CD1	2.76	0.41
1:B:2754:GLY:HA3	1:B:2886:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2965:VAL:HA	1:B:2968:ILE:HD12	2.01	0.41
1:B:3002:LEU:HD21	1:B:3370:LEU:HD11	2.02	0.41
1:B:3303:LYS:O	1:B:3306:TRP:HD1	2.03	0.41
1:B:3319:GLU:HA	1:B:3359:LYS:O	2.19	0.41
1:A:1823:ASP:HB3	1:A:1852:ARG:O	2.15	0.41
1:A:2034:ILE:HG13	1:A:2061:TYR:CE2	2.55	0.41
1:A:2226:ILE:HG23	1:A:2288:VAL:CG2	2.49	0.41
1:A:2828:LEU:HD13	1:A:2902:MET:SD	2.60	0.41
1:A:2755:HIS:NE2	1:A:2835:LEU:HG	2.35	0.41
1:A:3373:LEU:HD13	1:A:3557:LEU:HD13	2.02	0.41
1:A:3979:ASN:OD1	1:A:3979:ASN:N	2.51	0.41
1:B:1479:LEU:HD11	1:B:1515:SER:HB3	2.02	0.41
1:B:3901:PRO:HG2	1:B:3906:THR:HG23	2.01	0.41
1:A:1542:ASN:O	1:A:1546:LEU:HG	2.20	0.41
1:A:1671:LYS:HD3	1:A:1671:LYS:HA	1.96	0.41
1:A:1681:LYS:HE2	1:A:1939:PHE:CZ	2.55	0.41
1:A:2109:LEU:HB3	1:A:2113:SER:HB2	2.02	0.41
1:A:3406:PHE:CZ	1:A:3505:ILE:HG21	2.56	0.41
1:A:3538:ASN:HB3	1:A:3541:MET:HG2	2.02	0.41
1:A:3946:VAL:HB	1:A:3947:PRO:HA	2.02	0.41
1:B:1939:PHE:CD1	1:B:1939:PHE:N	2.88	0.41
1:B:1934:LEU:HD22	1:B:1945:LEU:HD12	2.01	0.41
1:B:3919:LYS:HZ3	1:B:4038:GLU:CG	2.31	0.41
1:A:1697:LYS:O	1:A:1701:LEU:HG	2.20	0.41
1:A:2279:ARG:HH11	1:A:2279:ARG:HD2	1.66	0.41
1:A:2078:CYS:N	2:A:5093:ATP:O2B	2.49	0.41
1:B:1535:PRO:C	1:B:1841:ILE:CD1	2.77	0.41
1:B:1536:ARG:NE	1:B:1841:ILE:HD13	2.35	0.41
1:B:2661:VAL:HG12	1:B:2916:TRP:CD2	2.55	0.41
1:B:2938:MET:SD	1:B:3321:ILE:CG2	3.09	0.41
1:A:1940:GLU:HG3	1:A:1941:ASP:N	2.35	0.41
1:A:2099:ASN:HB3	1:A:2151:TRP:NE1	2.34	0.41
1:A:2282:ASN:HB3	1:A:2552:ARG:HG3	2.02	0.41
1:A:2494:LEU:HD12	1:A:2495:ASP:O	2.20	0.41
1:B:2080:LYS:O	1:B:2081:THR:C	2.59	0.41
1:B:2748:ALA:O	1:B:2751:GLN:HG3	2.19	0.41
1:B:4022:GLN:O	1:B:4023:ILE:C	2.58	0.41
1:A:1392:LEU:N	1:A:1484:LYS:HE2	2.36	0.41
1:A:2761:ALA:O	1:A:2892:CYS:SG	2.78	0.41
1:A:3024:LEU:HD13	1:A:3303:LYS:HG3	1.92	0.41
1:A:3367:ILE:O	1:A:3371:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3930:PHE:CE2	1:A:4029:ILE:HD13	2.55	0.41
1:B:1774:LEU:HA	1:B:1777:ILE:HD12	2.02	0.41
1:B:1832:SER:HB3	1:B:1882:LEU:HD22	2.03	0.41
1:B:2181:GLY:C	1:B:2182:GLU:HG3	2.40	0.41
1:B:3584:MET:HA	1:B:3587:LEU:HD12	2.03	0.41
1:A:1496:THR:O	1:A:1499:VAL:HG23	2.21	0.41
1:A:1866:GLN:O	1:A:1870:ASN:HB2	2.21	0.41
1:A:2021:ILE:HG22	1:A:2022:PHE:HD1	1.85	0.41
1:A:2762:SER:O	1:A:2763:ARG:CB	2.69	0.41
1:B:1392:LEU:N	1:B:1484:LYS:HE2	2.35	0.41
1:B:1949:ILE:HD11	1:B:1994:VAL:HG11	2.03	0.41
1:B:2034:ILE:CD1	1:B:2061:TYR:CZ	3.03	0.41
1:B:2290:LEU:HD13	1:B:2407:LEU:HD23	2.02	0.41
1:B:2464:TYR:CZ	1:B:2474:LEU:HD12	2.55	0.41
1:B:3924:TRP:CD1	1:B:3924:TRP:C	2.94	0.41
1:A:1406:LYS:HB3	1:A:1406:LYS:HE2	1.95	0.41
1:A:1547:LYS:O	1:A:1551:SER:HB3	2.20	0.41
1:A:1795:PHE:CE1	1:A:1920:SER:HB3	2.55	0.41
1:A:2316:LEU:HD13	1:A:2351:GLN:HB3	2.01	0.41
1:A:2076:ALA:HB2	1:A:2549:ARG:HG2	2.02	0.41
1:A:2571:TYR:HA	1:A:2574:TYR:HB2	2.03	0.41
1:A:215:PRO:C	1:A:3475:ASN:HD21	2.24	0.41
1:B:1826:PHE:CE1	1:B:1853:LEU:CD2	3.04	0.41
1:B:2044:ARG:HH21	1:B:2093:ILE:HD11	1.85	0.41
1:B:2230:LEU:HD23	1:B:2288:VAL:HG13	2.03	0.41
1:B:2428:MET:HG2	1:B:2485:PHE:CE1	2.55	0.41
1:B:3846:MET:HG3	1:B:3847:SER:N	2.35	0.41
1:B:2079:GLY:HA2	2:B:5093:ATP:H5'2	2.02	0.41
1:A:2938:MET:HG2	1:A:3321:ILE:HG12	2.03	0.41
1:A:3430:SER:HB2	1:A:3453:GLN:HB3	2.02	0.41
1:B:1559:SER:HB3	1:B:1572:ILE:HG22	2.02	0.41
1:B:1702:LEU:O	1:B:1706:LEU:HG	2.21	0.41
1:B:2000:ARG:O	1:B:2004:PRO:HG2	2.21	0.41
1:B:2295:ILE:HG12	1:B:2314:ILE:HD12	2.02	0.41
1:B:2422:SER:N	3:B:5094:ANP:O1B	2.54	0.41
1:B:2491:LEU:HD23	1:B:2491:LEU:HA	1.78	0.41
1:B:2572:GLU:HG3	1:B:2590:GLU:HG3	2.02	0.41
1:B:2787:HIS:HB3	1:B:3461:ILE:HG23	2.02	0.41
1:B:3462:ILE:O	1:B:3465:LEU:HB3	2.21	0.41
1:A:3772:TRP:HZ3	1:A:3780:ASN:ND2	2.19	0.41
1:B:2578:ILE:CG2	1:B:2630:TYR:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2707:VAL:HG11	1:B:2712:LEU:CD1	2.46	0.41
1:B:3551:LEU:HA	1:B:3554:GLU:HB3	2.02	0.41
1:A:1535:PRO:C	1:A:1841:ILE:CD1	2.79	0.41
1:A:1620:PHE:CE1	1:A:1743:ASP:HB3	2.55	0.41
1:A:1968:PHE:N	1:A:1968:PHE:CD1	2.88	0.41
1:A:2320:ARG:O	1:A:2323:LEU:HB3	2.20	0.41
1:A:3642:TYR:CD1	1:A:3642:TYR:N	2.87	0.41
1:B:1637:GLU:HG2	1:B:1686:LYS:HG3	2.03	0.41
1:B:2488:GLU:CD	1:B:2491:LEU:HD11	2.41	0.41
1:A:1704:GLU:O	1:A:1707:HIS:HB3	2.21	0.40
1:A:1838:ILE:HD11	1:A:1845:GLY:N	2.37	0.40
1:A:1853:LEU:HB2	1:A:1858:LEU:HD12	2.03	0.40
1:A:2199:LEU:O	1:A:2200:ASP:C	2.59	0.40
1:A:2415:ILE:O	1:A:2556:ILE:HA	2.21	0.40
1:A:3848:LEU:O	1:A:3849:SER:C	2.57	0.40
1:A:3862:THR:HB	1:A:3865:ALA:HB2	2.03	0.40
1:A:4065:LEU:O	1:A:4065:LEU:HD12	2.21	0.40
1:B:2039:LYS:HG2	1:B:2049:MET:HG3	2.02	0.40
1:B:2115:TYR:OH	1:B:2162:TYR:O	2.28	0.40
1:B:2178:LEU:HB2	1:B:2182:GLU:H	1.86	0.40
1:B:2476:LYS:N	1:B:2476:LYS:CD	2.84	0.40
1:A:1592:LEU:HD13	1:A:1596:ILE:CD1	2.50	0.40
1:A:1579:ILE:HG13	1:A:1598:LEU:HD11	2.03	0.40
1:A:1620:PHE:HA	1:A:1760:PHE:HE1	1.86	0.40
1:A:2510:MET:O	1:A:2513:GLN:NE2	2.53	0.40
1:A:2627:ARG:NH1	1:A:2630:TYR:CE2	2.89	0.40
1:A:3978:ASN:O	1:A:3981:PRO:HD2	2.19	0.40
1:B:1664:LEU:HD23	1:B:1669:PHE:HZ	1.86	0.40
1:B:1743:ASP:C	1:B:1745:ASN:N	2.74	0.40
1:B:1987:PHE:HB3	1:B:1988:GLY:H	1.73	0.40
1:B:2752:VAL:HG13	1:B:2883:LYS:CB	2.50	0.40
1:B:3784:ASN:ND2	1:B:3865:ALA:O	2.54	0.40
1:A:1939:PHE:CD1	1:A:1939:PHE:N	2.81	0.40
1:A:2125:TRP:CE2	1:A:2178:LEU:HD13	2.56	0.40
1:A:3534:LEU:HD12	1:A:3618:TYR:CZ	2.54	0.40
1:A:4033:LEU:HD13	1:A:4035:GLN:H	1.87	0.40
1:B:1734:PHE:CD2	1:B:1749:ILE:HG12	2.56	0.40
1:B:2012:LEU:HD12	1:B:2013:VAL:N	2.36	0.40
1:B:23:LEU:C	1:B:25:GLU:H	2.25	0.40
1:B:2820:SER:O	1:B:2823:LEU:HD12	2.21	0.40
1:A:2071:ILE:HB	1:A:2212:LEU:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3443:ALA:HB1	1:A:3450:VAL:CG2	2.50	0.40
1:A:3564:LYS:O	1:A:3568:GLU:HG2	2.21	0.40
1:B:1750:SER:HB2	1:B:1755:LEU:HD23	2.03	0.40
1:B:1826:PHE:CD1	1:B:1826:PHE:O	2.75	0.40
1:B:2759:ILE:HG21	1:B:2916:TRP:CZ2	2.56	0.40
1:A:2378:VAL:HG11	1:A:2392:ILE:CD1	2.51	0.40
1:A:3566:LEU:HD13	1:A:3570:LEU:HD12	2.02	0.40
1:A:3939:ILE:CG1	1:A:4010:LEU:CD2	2.99	0.40
1:B:1773:PRO:HA	1:B:1776:LEU:HD12	2.03	0.40
1:B:1832:SER:O	1:B:1836:VAL:HG23	2.21	0.40
1:B:1796:GLY:O	1:B:1900:PRO:HD3	2.22	0.40
1:B:2463:ASN:O	1:B:2475:PRO:HD2	2.21	0.40
1:B:2653:TRP:HB3	1:B:2654:ARG:NH1	2.35	0.40
1:B:3566:LEU:HA	1:B:3583:LEU:HD23	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	2518 (95%)	110 (4%)	12 (0%)	29	68
1	B	2640/2695 (98%)	2515 (95%)	111 (4%)	14 (0%)	29	68
All	All	5280/5390 (98%)	5033 (95%)	221 (4%)	26 (0%)	29	68

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1391	GLY
1	B	1391	GLY
1	B	3578	LEU
1	A	24	GLU

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Mol	Chain	Res	Type
1	A	1633	GLY
1	A	2513	GLN
1	A	3482	GLY
1	B	24	GLU
1	B	2513	GLN
1	B	2990	GLY
1	B	3482	GLY
1	A	2990	GLY
1	A	66	GLN
1	A	1744	LEU
1	A	2519	PRO
1	B	66	GLN
1	B	3914	GLN
1	B	2519	PRO
1	B	2562	PRO
1	B	3809	GLU
1	A	3980	ILE
1	B	3305	ARG
1	A	2028	PRO
1	B	3980	ILE
1	A	2562	PRO
1	B	1470	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%)	2138 (96%)	80 (4%)	35	67
1	B	2218/2453 (90%)	2137 (96%)	81 (4%)	34	66
All	All	4436/4906 (90%)	4275 (96%)	161 (4%)	35	67

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1421	TYR

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Mol	Chain	Res	Type
1	A	1486	ILE
1	A	1493	LEU
1	A	1504	ASN
1	A	1769	LEU
1	A	1783	THR
1	A	1788	GLN
1	A	1794	PHE
1	A	1826	PHE
1	A	1858	LEU
1	A	1925	GLN
1	A	1997	SER
1	A	2057	CYS
1	A	2078	CYS
1	A	2109	LEU
1	A	2122	THR
1	A	2141	ILE
1	A	2154	PHE
1	A	2155	ASP
1	A	2202	THR
1	A	2229	LEU
1	A	2295	ILE
1	A	2352	GLU
1	A	2357	SER
1	A	2387	ARG
1	A	2395	ILE
1	A	2397	THR
1	A	2411	LYS
1	A	2412	ARG
1	A	2428	MET
1	A	2476	LYS
1	A	2482	LEU
1	A	2544	ILE
1	A	2548	GLU
1	A	2566	SER
1	A	2576	LYS
1	A	2623	THR
1	A	2626	VAL
1	A	2627	ARG
1	A	2681	LEU
1	A	2689	ILE
1	A	2694	LEU
1	A	2822	ILE

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Mol	Chain	Res	Type
1	A	2833	THR
1	A	2843	LEU
1	A	2856	LEU
1	A	2866	LEU
1	A	2967	ASN
1	A	2999	LEU
1	A	3002	LEU
1	A	3301	PHE
1	A	3329	ILE
1	A	3332	THR
1	A	3340	ARG
1	A	3372	THR
1	A	3400	SER
1	A	3560	LYS
1	A	3578	LEU
1	A	3601	LEU
1	A	3618	TYR
1	A	3634	LYS
1	A	3673	GLU
1	A	3677	LEU
1	A	3729	SER
1	A	3737	THR
1	A	3788	MET
1	A	3805	LYS
1	A	3823	ASN
1	A	3871	PHE
1	A	3876	THR
1	A	3899	ASP
1	A	3906	THR
1	A	3940	THR
1	A	3943	THR
1	A	3958	ASP
1	A	3960	ASP
1	A	3980	ILE
1	A	3982	TRP
1	A	3997	LYS
1	A	4016	CYS
1	B	1383	TYR
1	B	1421	TYR
1	B	1486	ILE
1	B	1504	ASN
1	B	1525	THR

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Mol	Chain	Res	Type
1	B	1646	GLN
1	B	1694	VAL
1	B	1743	ASP
1	B	1759	LYS
1	B	1794	PHE
1	B	1826	PHE
1	B	1858	LEU
1	B	1936	ILE
1	B	2008	ASP
1	B	2068	GLN
1	B	2075	LYS
1	B	2109	LEU
1	B	2141	ILE
1	B	2154	PHE
1	B	2155	ASP
1	B	2202	THR
1	B	2229	LEU
1	B	2285	GLU
1	B	2295	ILE
1	B	2307	ASP
1	B	2310	LEU
1	B	2351	GLN
1	B	2357	SER
1	B	2368	PHE
1	B	2381	GLU
1	B	2390	ILE
1	B	2395	ILE
1	B	2412	ARG
1	B	2425	THR
1	B	2476	LYS
1	B	2479	ILE
1	B	2496	LYS
1	B	2512	LYS
1	B	2566	SER
1	B	2574	TYR
1	B	2681	LEU
1	B	2689	ILE
1	B	2769	LEU
1	B	2822	ILE
1	B	2829	GLU
1	B	2853	LEU
1	B	2920	TRP

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Mol	Chain	Res	Type
1	B	2967	ASN
1	B	2969	LEU
1	B	3305	ARG
1	B	3329	ILE
1	B	3360	TYR
1	B	3372	THR
1	B	3380	LEU
1	B	3391	LEU
1	B	3400	SER
1	B	3502	SER
1	B	3559	LEU
1	B	3581	ASP
1	B	3598	GLU
1	B	3605	GLU
1	B	3618	TYR
1	B	3729	SER
1	B	3737	THR
1	B	3744	LEU
1	B	3811	LEU
1	B	3844	ILE
1	B	3871	PHE
1	B	3899	ASP
1	B	3906	THR
1	B	3917	THR
1	B	3940	THR
1	B	3943	THR
1	B	3958	ASP
1	B	3960	ASP
1	B	3982	TRP
1	B	4016	CYS
1	B	4024	VAL
1	B	4040	GLU
1	B	4068	GLU
1	B	4087	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1533	GLN
1	A	1605	GLN
1	A	1622	GLN
1	A	1646	GLN

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Mol	Chain	Res	Type
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	2064	GLN
1	A	2068	GLN
1	A	2099	ASN
1	A	2274	HIS
1	A	2282	ASN
1	A	2293	HIS
1	A	2351	GLN
1	A	2383	HIS
1	A	2409	ASN
1	A	2444	ASN
1	A	2459	HIS
1	A	2536	ASN
1	A	2601	ASN
1	A	2634	ASN
1	A	2688	ASN
1	A	2896	ASN
1	A	3323	ASN
1	A	3420	ASN
1	A	3475	ASN
1	A	3521	ASN
1	A	3624	HIS
1	A	3780	ASN
1	A	3890	GLN
1	A	3962	GLN
1	A	3970	ASN
1	A	4020	ASN
1	A	4077	GLN
1	B	1501	HIS
1	B	1622	GLN
1	B	1646	GLN
1	B	1707	HIS
1	B	1736	GLN
1	B	1864	ASN
1	B	1873	GLN
1	B	1899	ASN

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Mol	Chain	Res	Type
1	B	1951	HIS
1	B	2068	GLN
1	B	2274	HIS
1	B	2282	ASN
1	B	2293	HIS
1	B	2409	ASN
1	B	2444	ASN
1	B	2536	ASN
1	B	2598	HIS
1	B	2634	ASN
1	B	2751	GLN
1	B	2753	GLN
1	B	2755	HIS
1	B	2896	ASN
1	B	2910	ASN
1	B	3323	ASN
1	B	3338	ASN
1	B	3471	ASN
1	B	3521	ASN
1	B	3542	GLN
1	B	3571	ASN
1	B	3624	HIS
1	B	3685	GLN
1	B	3780	ASN
1	B	3783	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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	5	26,33,33	1.01	1 (3%)	31,52,52	1.65	5 (16%)
2	ATP	B	5093	5	26,33,33	1.02	2 (7%)	31,52,52	1.65	5 (16%)
4	SO4	B	5095	-	4,4,4	0.33	0	6,6,6	0.46	0
4	SO4	A	5095	-	4,4,4	0.52	0	6,6,6	0.69	0
3	ANP	A	5094	-	29,33,33	2.43	5 (17%)	31,52,52	1.56	7 (22%)
3	ANP	B	5094	-	29,33,33	2.48	5 (17%)	31,52,52	1.52	4 (12%)
4	SO4	A	5096	-	4,4,4	0.45	0	6,6,6	0.24	0
4	SO4	B	5096	-	4,4,4	0.35	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
3	ANP	A	5094	-	-	8/14/38/38	0/3/3/3
3	ANP	B	5094	-	-	6/14/38/38	0/3/3/3
2	ATP	B	5093	5	-	7/18/38/38	0/3/3/3
2	ATP	A	5093	5	-	5/18/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5094	ANP	PG-O1G	9.66	1.61	1.46
3	A	5094	ANP	PG-O1G	9.47	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5094	ANP	PG-N3B	4.66	1.75	1.63
3	A	5094	ANP	PG-N3B	4.66	1.75	1.63
3	B	5094	ANP	PB-N3B	4.60	1.75	1.63
3	A	5094	ANP	PB-N3B	4.34	1.74	1.63
3	B	5094	ANP	PG-O3G	-3.08	1.48	1.56
3	A	5094	ANP	PG-O3G	-3.04	1.48	1.56
2	A	5093	ATP	C5-C4	2.73	1.48	1.40
2	B	5093	ATP	C5-C4	2.62	1.47	1.40
3	B	5094	ANP	C5-C4	2.52	1.47	1.40
3	A	5094	ANP	C5-C4	2.43	1.47	1.40
2	B	5093	ATP	O4'-C1'	2.24	1.44	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5093	ATP	C3'-C2'-C1'	3.97	106.96	100.98
2	B	5093	ATP	C3'-C2'-C1'	3.77	106.65	100.98
2	B	5093	ATP	PB-O3B-PG	-3.71	120.08	132.83
2	B	5093	ATP	PA-O3A-PB	-3.69	120.16	132.83
2	A	5093	ATP	PB-O3B-PG	-3.60	120.49	132.83
3	B	5094	ANP	C3'-C2'-C1'	3.55	106.32	100.98
2	A	5093	ATP	PA-O3A-PB	-3.45	120.98	132.83
3	B	5094	ANP	PA-O3A-PB	-3.43	120.54	132.62
3	A	5094	ANP	N3-C2-N1	-3.36	123.42	128.68
3	A	5094	ANP	PA-O3A-PB	-3.30	120.99	132.62
3	B	5094	ANP	N3-C2-N1	-3.15	123.75	128.68
2	A	5093	ATP	N3-C2-N1	-3.14	123.77	128.68
2	B	5093	ATP	N3-C2-N1	-3.06	123.89	128.68
3	A	5094	ANP	C4-C5-N7	-2.82	106.46	109.40
3	B	5094	ANP	C4-C5-N7	-2.71	106.57	109.40
3	A	5094	ANP	C2'-C3'-C4'	2.70	107.90	102.64
2	B	5093	ATP	C4-C5-N7	-2.68	106.60	109.40
2	A	5093	ATP	C4-C5-N7	-2.63	106.66	109.40
3	A	5094	ANP	C3'-C2'-C1'	2.39	104.57	100.98
3	A	5094	ANP	O2A-PA-O1A	2.09	122.58	112.24
3	A	5094	ANP	O3G-PG-O1G	-2.08	108.23	113.45

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5093	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	A	5094	ANP	PB-N3B-PG-O1G
3	A	5094	ANP	C5'-O5'-PA-O2A
3	B	5094	ANP	PB-N3B-PG-O1G
3	B	5094	ANP	C5'-O5'-PA-O1A
3	B	5094	ANP	C5'-O5'-PA-O2A
3	B	5094	ANP	O4'-C4'-C5'-O5'
2	A	5093	ATP	O4'-C4'-C5'-O5'
2	A	5093	ATP	C3'-C4'-C5'-O5'
2	B	5093	ATP	O4'-C4'-C5'-O5'
2	B	5093	ATP	C3'-C4'-C5'-O5'
3	B	5094	ANP	C3'-C4'-C5'-O5'
3	A	5094	ANP	PB-O3A-PA-O1A
3	A	5094	ANP	O4'-C4'-C5'-O5'
2	B	5093	ATP	C5'-O5'-PA-O3A
3	A	5094	ANP	C5'-O5'-PA-O3A
2	B	5093	ATP	PA-O3A-PB-O1B
3	A	5094	ANP	C5'-O5'-PA-O1A
3	A	5094	ANP	PB-O3A-PA-O2A
2	A	5093	ATP	PA-O3A-PB-O1B
2	A	5093	ATP	C5'-O5'-PA-O3A
3	B	5094	ANP	C5'-O5'-PA-O3A
3	A	5094	ANP	C3'-C4'-C5'-O5'
2	B	5093	ATP	PA-O3A-PB-O2B
2	A	5093	ATP	C5'-O5'-PA-O1A
2	B	5093	ATP	C5'-O5'-PA-O2A

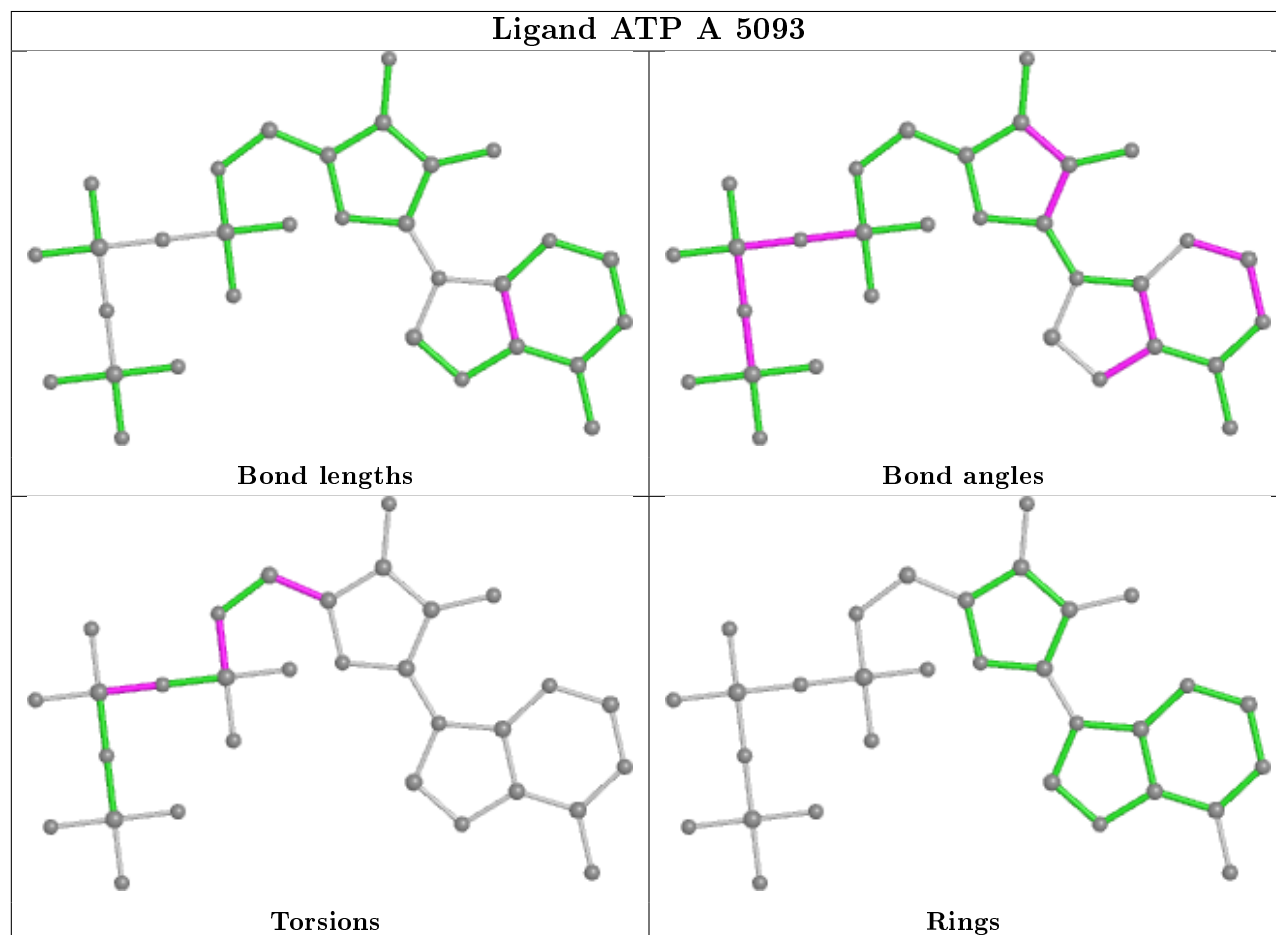
There are no ring outliers.

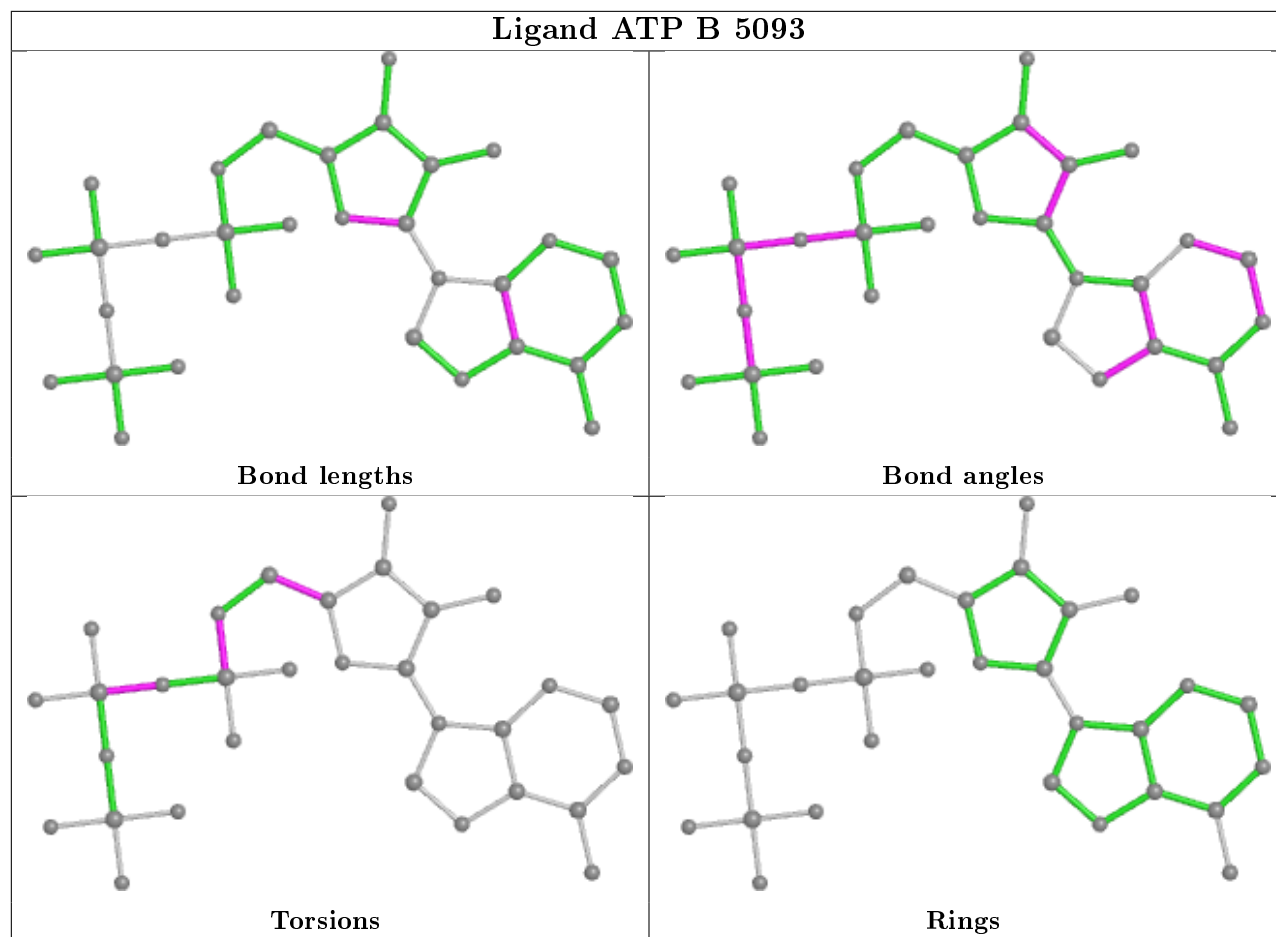
6 monomers are involved in 45 short contacts:

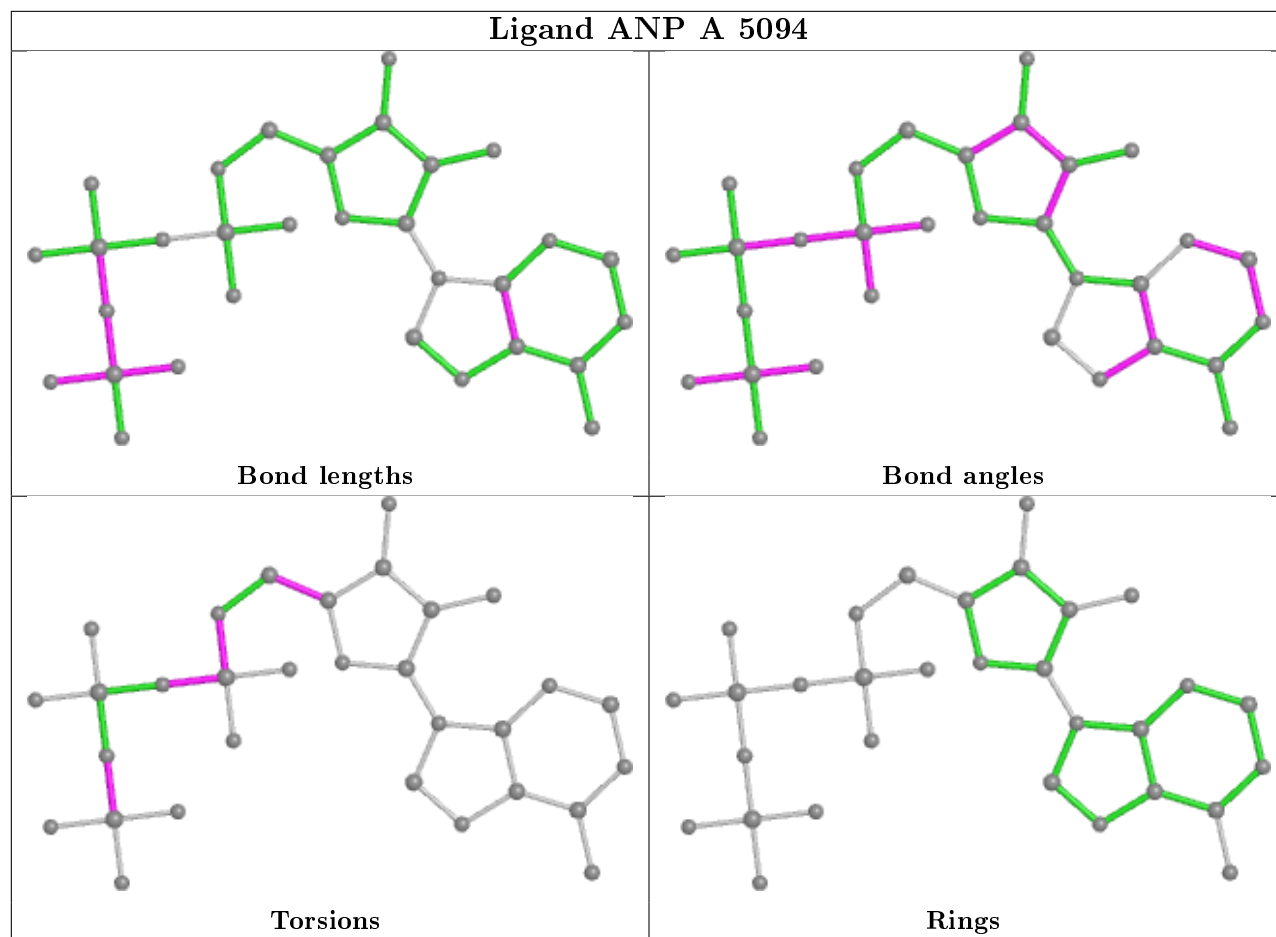
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5093	ATP	8	0
2	B	5093	ATP	17	0
4	A	5095	SO4	3	0
3	A	5094	ANP	7	0
3	B	5094	ANP	7	0
4	B	5096	SO4	3	0

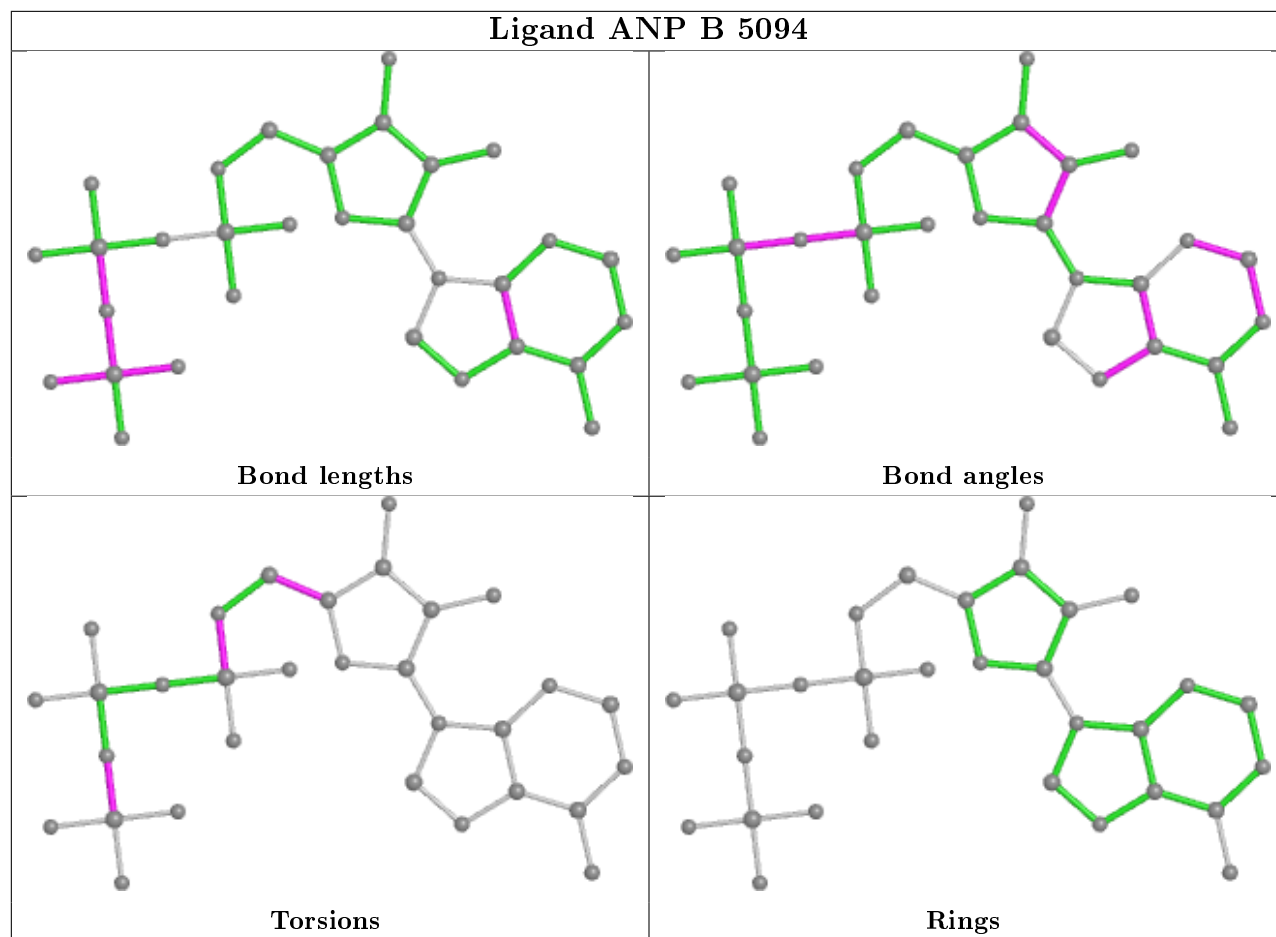
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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%)	0.11	69 (2%) 56 40	69, 151, 281, 423	0
1	B	2650/2695 (98%)	0.64	277 (10%) 6 3	92, 193, 357, 500	0
All	All	5300/5390 (98%)	0.37	346 (6%) 18 11	69, 172, 321, 500	0

All (346) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	165	ASP	24.7
1	B	164	MET	22.6
1	B	213	ASP	20.8
1	B	29	GLU	19.9
1	B	163	TYR	19.7
1	B	161	VAL	19.2
1	B	84	CYS	18.3
1	B	49	LEU	16.9
1	B	214	HIS	16.0
1	B	142	LEU	15.4
1	B	206	GLN	14.4
1	B	166	PRO	14.2
1	B	48	GLY	14.0
1	B	80	MET	14.0
1	B	143	ASN	13.1
1	A	2	PRO	12.6
1	B	168	CYS	12.6
1	B	19	LEU	12.5
1	B	162	LEU	12.3
1	B	69	ALA	12.2
1	B	18	LEU	12.1
1	B	83	GLY	11.9
1	B	151	ASP	11.8
1	B	53	ASN	11.1

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Mol	Chain	Res	Type	RSRZ
1	B	215	PRO	10.9
1	B	70	ILE	10.9
1	B	76	ASP	10.6
1	B	78	HIS	10.6
1	B	212	GLY	10.1
1	B	4	LEU	9.8
1	B	1683	LEU	9.5
1	B	30	HIS	9.3
1	A	2364	ASP	8.9
1	B	1572	ILE	8.7
1	B	184	ALA	8.6
1	B	167	MET	8.2
1	B	120	ASP	8.2
1	B	90	GLU	8.1
1	B	197	TYR	8.1
1	A	63	LYS	8.1
1	B	185	ILE	8.0
1	B	73	TYR	7.9
1	B	188	ILE	7.8
1	B	1549	ILE	7.8
1	B	208	THR	7.7
1	B	115	GLU	7.7
1	B	148	THR	7.7
1	A	1	SER	7.5
1	B	1644	ILE	7.4
1	B	216	PRO	7.4
1	B	205	TRP	7.3
1	B	1937	MET	7.3
1	A	1483	TYR	7.2
1	A	115	GLU	7.2
1	B	74	ILE	7.1
1	B	14	GLN	7.1
1	B	186	PRO	7.1
1	B	68	MET	7.0
1	B	92	SER	6.9
1	B	79	ASN	6.8
1	B	1459	LEU	6.7
1	B	160	VAL	6.6
1	A	71	ILE	6.5
1	B	189	ASP	6.5
1	B	133	GLU	6.5
1	B	1680	ILE	6.5

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Mol	Chain	Res	Type	RSRZ
1	B	81	LEU	6.4
1	A	28	GLU	6.3
1	B	1590	LEU	6.3
1	B	1582	VAL	6.3
1	B	1679	LYS	6.3
1	B	171	ALA	6.3
1	B	1732	GLN	6.2
1	B	157	ALA	6.1
1	B	50	GLU	6.1
1	B	116	THR	6.0
1	B	67	SER	5.9
1	B	46	GLU	5.9
1	B	33	GLU	5.8
1	B	1550	GLY	5.8
1	B	1684	LEU	5.8
1	B	1581	GLY	5.7
1	B	1669	PHE	5.7
1	B	190	LYS	5.7
1	B	147	VAL	5.7
1	B	177	CYS	5.6
1	B	82	GLY	5.6
1	B	91	ILE	5.6
1	B	111	SER	5.4
1	B	34	ARG	5.4
1	A	86	LYS	5.4
1	B	207	ALA	5.4
1	A	85	PRO	5.4
1	A	27	TYR	5.3
1	B	75	ALA	5.3
1	B	1458	ILE	5.3
1	B	3580	ASN	5.3
1	B	180	LYS	5.3
1	B	77	LYS	5.2
1	B	194	SER	5.2
1	B	3555	TYR	5.1
1	B	1601	SER	5.1
1	B	1596	ILE	5.0
1	B	1730	LYS	4.9
1	B	119	VAL	4.9
1	B	1705	TYR	4.9
1	B	195	SER	4.9
1	B	196	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	3563	GLU	4.9
1	B	1545	LEU	4.8
1	B	16	THR	4.8
1	B	1649	LEU	4.8
1	B	35	ASP	4.7
1	B	66	GLN	4.7
1	A	216	PRO	4.7
1	B	1606	GLU	4.7
1	B	1483	TYR	4.7
1	B	1566	PHE	4.7
1	B	3866	GLU	4.7
1	B	1452	TRP	4.6
1	A	215	PRO	4.6
1	B	1456	TYR	4.6
1	B	47	LEU	4.5
1	B	54	LEU	4.5
1	B	204	GLY	4.4
1	B	1771	TYR	4.4
1	B	85	PRO	4.4
1	B	1415	MET	4.4
1	B	17	ARG	4.3
1	B	1647	ALA	4.3
1	B	170	ASP	4.3
1	B	179	LYS	4.3
1	A	25	GLU	4.3
1	A	3580	ASN	4.1
1	B	1770	ILE	4.1
1	A	35	ASP	4.1
1	B	1476	PHE	4.1
1	B	117	LEU	4.1
1	B	1548	ILE	4.1
1	B	1893	ALA	4.0
1	B	3482	GLY	4.0
1	A	62	VAL	3.9
1	B	1894	VAL	3.9
1	B	28	GLU	3.8
1	B	3304	GLU	3.8
1	B	3393	ASN	3.8
1	B	1394	LEU	3.8
1	A	151	ASP	3.7
1	B	211	GLY	3.7
1	B	1701	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	3588	ASN	3.7
1	B	15	PRO	3.7
1	A	116	THR	3.6
1	B	2938	MET	3.6
1	A	148	THR	3.6
1	B	1460	GLY	3.6
1	B	1546	LEU	3.6
1	A	84	CYS	3.6
1	B	3846	MET	3.5
1	B	183	GLU	3.5
1	A	83	GLY	3.4
1	B	56	TYR	3.4
1	A	1394	LEU	3.4
1	A	3979	ASN	3.4
1	B	112	LYS	3.4
1	B	1933	ILE	3.4
1	B	1734	PHE	3.4
1	B	187	GLN	3.4
1	A	69	ALA	3.3
1	A	20	LEU	3.3
1	B	1441	ILE	3.3
1	A	1597	GLU	3.3
1	A	61	ASP	3.2
1	B	178	PHE	3.2
1	B	152	PHE	3.2
1	B	4023	ILE	3.2
1	B	1	SER	3.2
1	A	3330	TYR	3.2
1	A	2918	GLY	3.2
1	B	89	ALA	3.1
1	A	72	ARG	3.1
1	B	1835	LEU	3.1
1	B	1636	ILE	3.1
1	B	1812	ASN	3.1
1	B	1653	GLN	3.1
1	A	90	GLU	3.1
1	A	64	LEU	3.1
1	B	191	TYR	3.1
1	B	198	ILE	3.1
1	B	2000	ARG	3.0
1	B	1445	TRP	3.0
1	B	1935	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	202	LEU	3.0
1	B	1760	PHE	3.0
1	B	1676	VAL	3.0
1	B	1845	GLY	3.0
1	B	1608	LEU	3.0
1	B	5	GLY	3.0
1	B	2213	LEU	3.0
1	B	1602	ILE	3.0
1	B	1372	ASN	3.0
1	B	1579	ILE	2.9
1	B	1650	LEU	2.9
1	B	3726	LEU	2.9
1	B	42	ASN	2.9
1	B	1395	VAL	2.9
1	B	3391	LEU	2.9
1	B	1744	LEU	2.9
1	B	155	TYR	2.8
1	B	1715	LEU	2.8
1	B	2669	PHE	2.8
1	B	1605	GLN	2.8
1	B	3326	ILE	2.8
1	B	113	ASP	2.8
1	B	1813	LEU	2.8
1	B	1765	ILE	2.8
1	A	3334	PHE	2.8
1	B	1703	VAL	2.8
1	B	1936	ILE	2.8
1	A	79	ASN	2.7
1	B	87	GLU	2.7
1	B	110	TYR	2.7
1	B	1562	MET	2.7
1	A	3418	ILE	2.7
1	B	1682	GLY	2.7
1	B	1704	GLU	2.7
1	A	1548	ILE	2.7
1	B	3325	ILE	2.7
1	A	2194	PHE	2.7
1	B	36	GLU	2.7
1	B	2770	THR	2.7
1	B	1378	TRP	2.7
1	B	3919	LYS	2.7
1	B	1506	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	1420	TYR	2.7
1	A	3564	LYS	2.7
1	A	202	LEU	2.7
1	B	3841	LEU	2.7
1	A	1368	GLU	2.7
1	B	72	ARG	2.6
1	B	1493	LEU	2.6
1	B	1607	TRP	2.6
1	B	3589	ASN	2.6
1	A	59	ASP	2.6
1	B	1592	LEU	2.6
1	B	1593	ASN	2.6
1	B	3788	MET	2.6
1	B	1568	SER	2.6
1	A	1458	ILE	2.6
1	B	55	PRO	2.6
1	A	67	SER	2.6
1	A	3495	PHE	2.6
1	A	75	ALA	2.5
1	B	199	ALA	2.5
1	B	156	ASP	2.5
1	B	3847	SER	2.5
1	B	20	LEU	2.5
1	B	1711	VAL	2.5
1	B	2353	LEU	2.5
1	B	3839	ILE	2.5
1	B	1505	PHE	2.5
1	B	2428	MET	2.5
1	A	3567	LEU	2.5
1	B	4029	ILE	2.5
1	B	94	LEU	2.5
1	A	89	ALA	2.5
1	A	68	MET	2.5
1	B	1479	LEU	2.4
1	A	3784	ASN	2.4
1	B	3714	GLN	2.4
1	B	3024	LEU	2.4
1	A	135	ARG	2.4
1	B	1809	PHE	2.4
1	B	31	LEU	2.4
1	B	1492	GLN	2.4
1	B	136	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	3590	LEU	2.4
1	B	2026	GLY	2.3
1	B	2918	GLY	2.3
1	A	182	ILE	2.3
1	B	182	ILE	2.3
1	B	2072	LEU	2.3
1	A	108	ILE	2.3
1	B	1421	TYR	2.3
1	A	2928	VAL	2.3
1	B	3425	LYS	2.3
1	B	3785	TYR	2.3
1	B	1547	LYS	2.3
1	B	2058	MET	2.3
1	B	1500	ILE	2.3
1	B	3597	ILE	2.3
1	B	1551	SER	2.3
1	B	3618	TYR	2.3
1	B	1417	ALA	2.3
1	B	3560	LYS	2.3
1	B	1503	PRO	2.3
1	B	3694	PHE	2.3
1	B	1712	ILE	2.3
1	A	1445	TRP	2.2
1	B	1573	ILE	2.2
1	A	184	ALA	2.2
1	A	3321	ILE	2.2
1	B	1580	THR	2.2
1	B	2214	TRP	2.2
1	B	1583	ARG	2.2
1	B	137	CYS	2.2
1	B	176	VAL	2.2
1	B	3571	ASN	2.2
1	B	1807	LYS	2.2
1	B	3466	ILE	2.2
1	B	3591	LYS	2.2
1	B	149	HIS	2.2
1	A	1504	ASN	2.2
1	B	3427	VAL	2.2
1	B	3915	PHE	2.2
1	A	3494	LEU	2.2
1	B	88	ARG	2.2
1	B	1769	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	3927	TYR	2.1
1	B	95	GLU	2.1
1	B	1588	GLU	2.1
1	B	2212	LEU	2.1
1	A	1578	PHE	2.1
1	A	19	LEU	2.1
1	B	1502	ILE	2.1
1	B	2660	LEU	2.1
1	B	3884	LEU	2.1
1	B	3564	LYS	2.1
1	B	3934	TRP	2.1
1	B	2889	PHE	2.1
1	B	3985	VAL	2.1
1	A	39	LYS	2.1
1	A	3329	ILE	2.1
1	B	3327	SER	2.0
1	B	1480	THR	2.0
1	A	2470	GLY	2.0
1	B	3330	TYR	2.0
1	B	3844	ILE	2.0
1	A	3545	ARG	2.0
1	B	1668	GLN	2.0
1	B	1455	LEU	2.0
1	B	1779	PHE	2.0
1	A	3325	ILE	2.0
1	B	3797	THR	2.0
1	A	3546	GLU	2.0
1	A	3796	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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. The B-factors column lists the minimum,

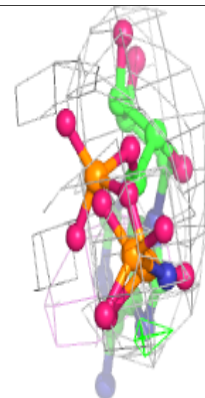
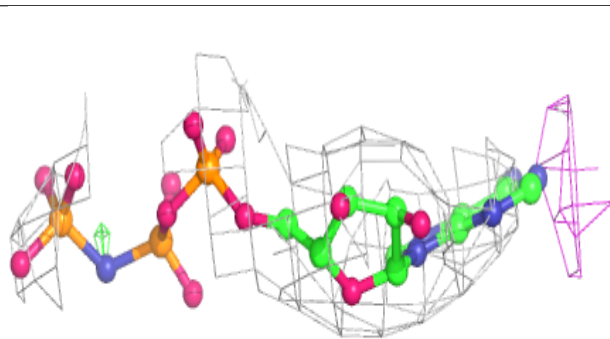
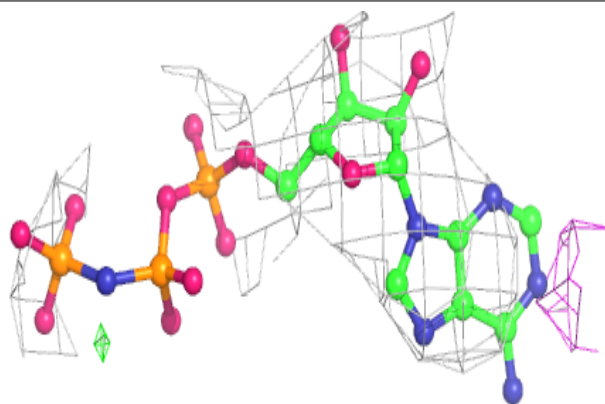
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	B	5095	5/5	0.84	0.18	152,154,166,167	0
3	ANP	B	5094	31/31	0.89	0.29	112,145,237,257	0
2	ATP	B	5093	31/31	0.92	0.24	99,141,184,200	0
3	ANP	A	5094	31/31	0.94	0.27	111,140,238,248	0
2	ATP	A	5093	31/31	0.95	0.29	88,123,185,204	0
4	SO4	B	5096	5/5	0.95	0.14	155,168,174,176	0
4	SO4	A	5096	5/5	0.96	0.20	115,130,143,145	0
4	SO4	A	5095	5/5	0.96	0.25	84,98,104,105	0
5	MG	B	5097	1/1	0.97	0.18	66,66,66,66	0
5	MG	A	5097	1/1	0.99	0.22	62,62,62,62	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

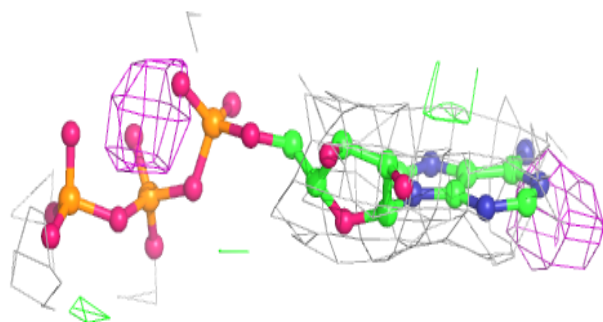
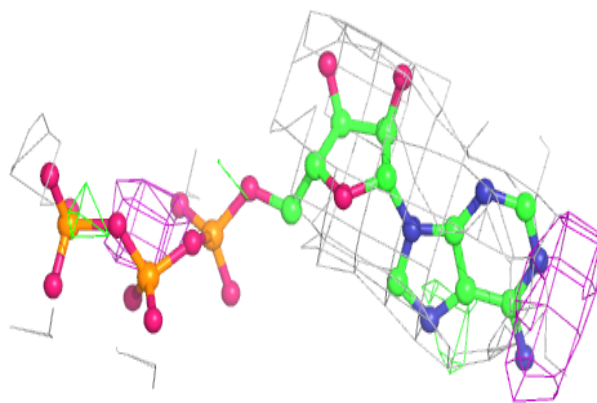
Electron density around ANP B 5094:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

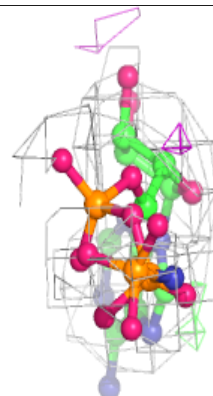
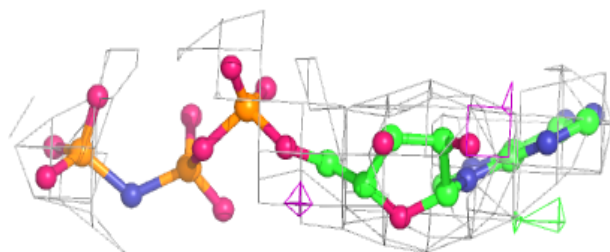
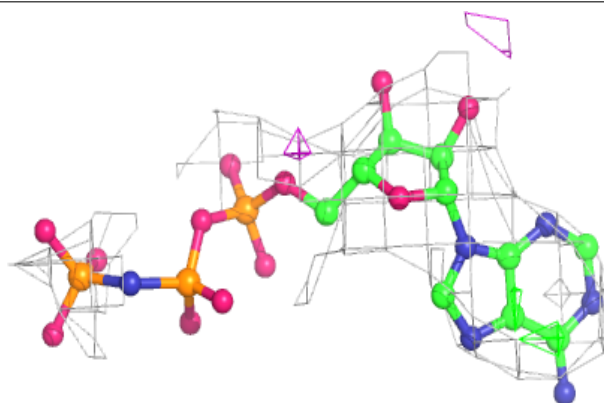


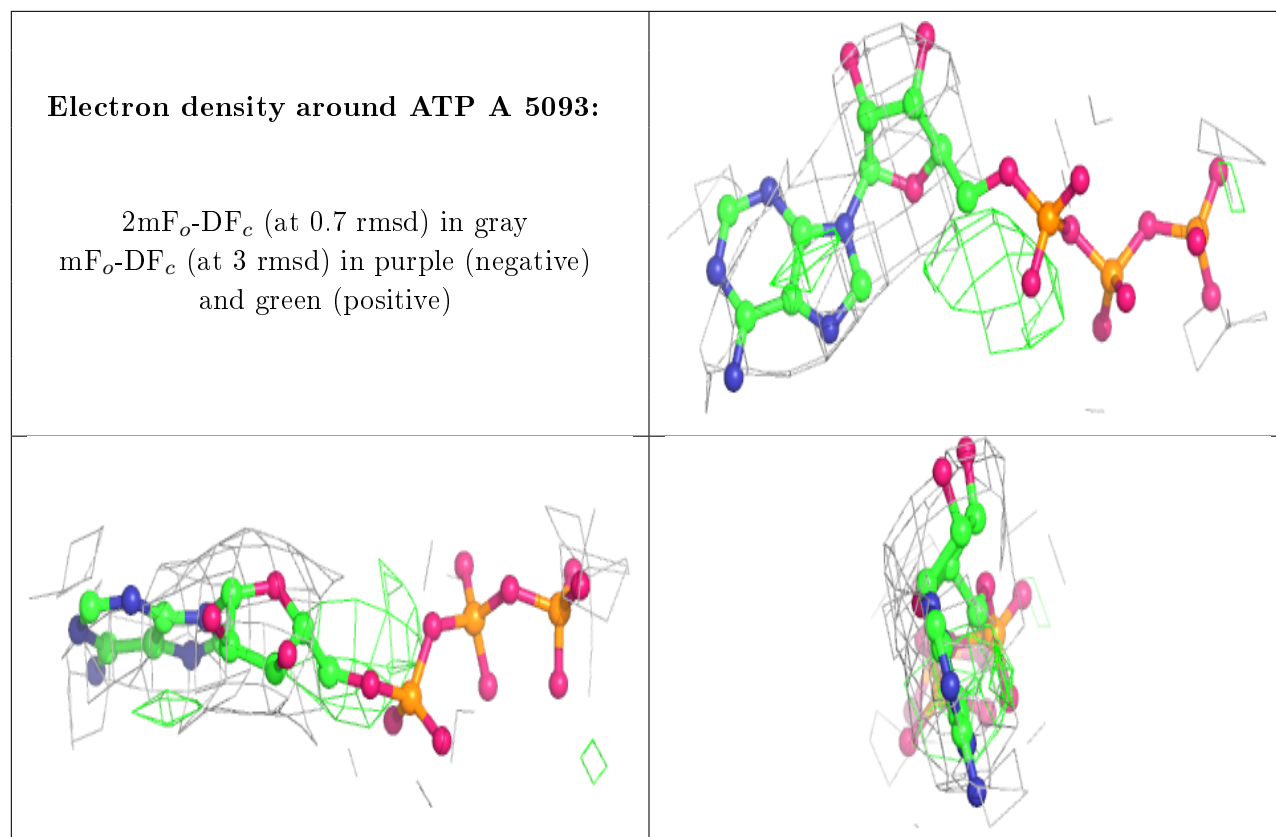
Electron density around ATP B 5093:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ANP A 5094:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.