



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:49 PM GMT

PDB ID : 4AKG
Title : Dynein Motor Domain - ATP complex
Authors : Schmidt, H.; Gleave, E.S.; Carter, A.P.
Deposited on : 2012-02-22
Resolution : 3.30 Å(reported)

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

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

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

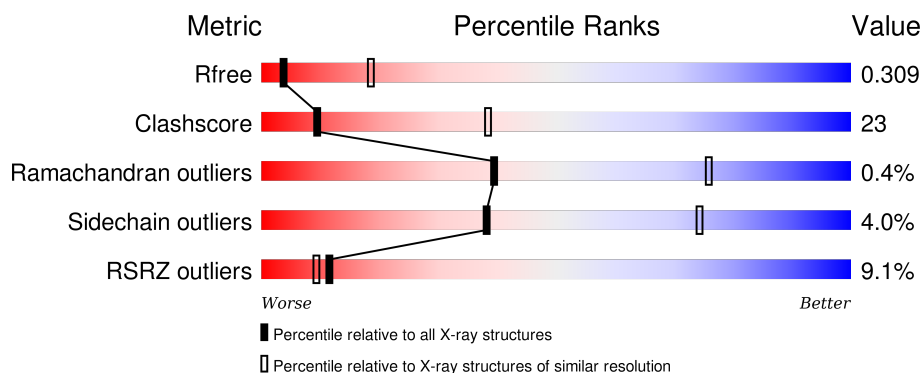
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	2695	<div> <div>5%</div> <div>64%</div> <div>32%</div> <div>..</div> </div>
1	B	2695	<div> <div>12%</div> <div>68%</div> <div>29%</div> <div>..</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ATP	A	5093	-	-	X	-
2	ATP	B	5093	-	-	X	-
4	MG	A	5095	-	-	-	X
4	MG	B	5095	-	-	-	X
5	SO4	A	5096	-	-	-	X
5	SO4	A	5097	-	-	X	-
5	SO4	B	5096	-	-	X	X
5	SO4	B	5097	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 41634 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

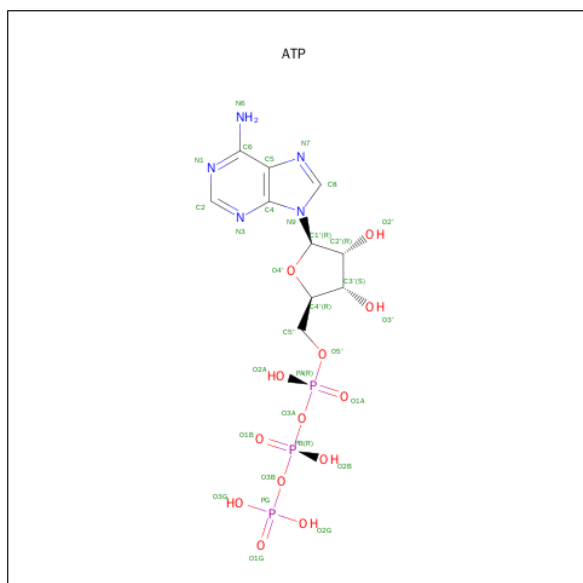
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

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

There are 4 discrepancies between the modelled and reference sequences:

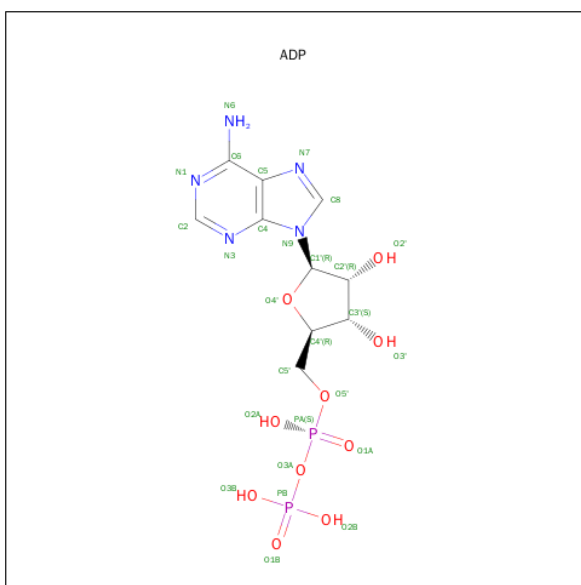
Chain	Residue	Modelled	Actual	Comment	Reference
A	1630	ILE	LEU	CONFLICT	UNP P36022
A	3782	ASP	GLU	CONFLICT	UNP P36022
B	1630	ILE	LEU	CONFLICT	UNP P36022
B	3782	ASP	GLU	CONFLICT	UNP P36022

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 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 ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

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

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



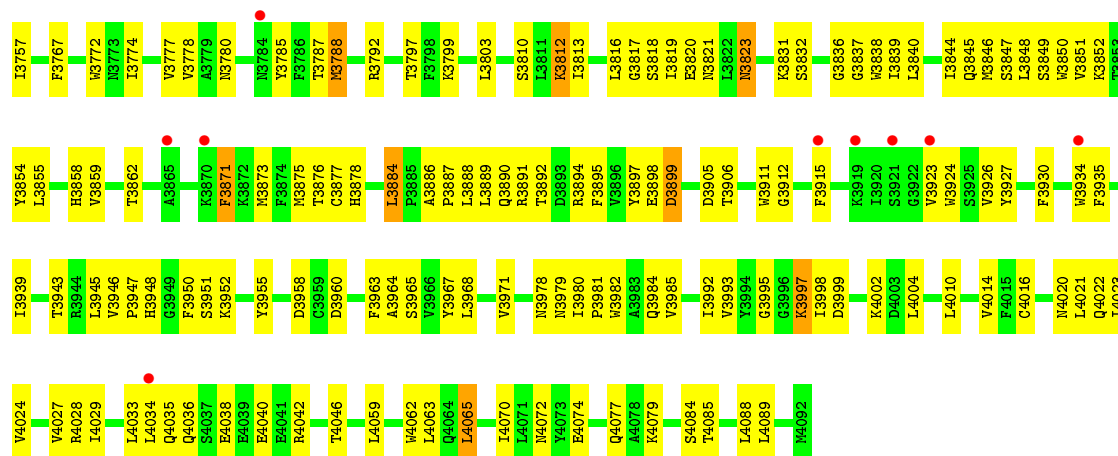
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

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

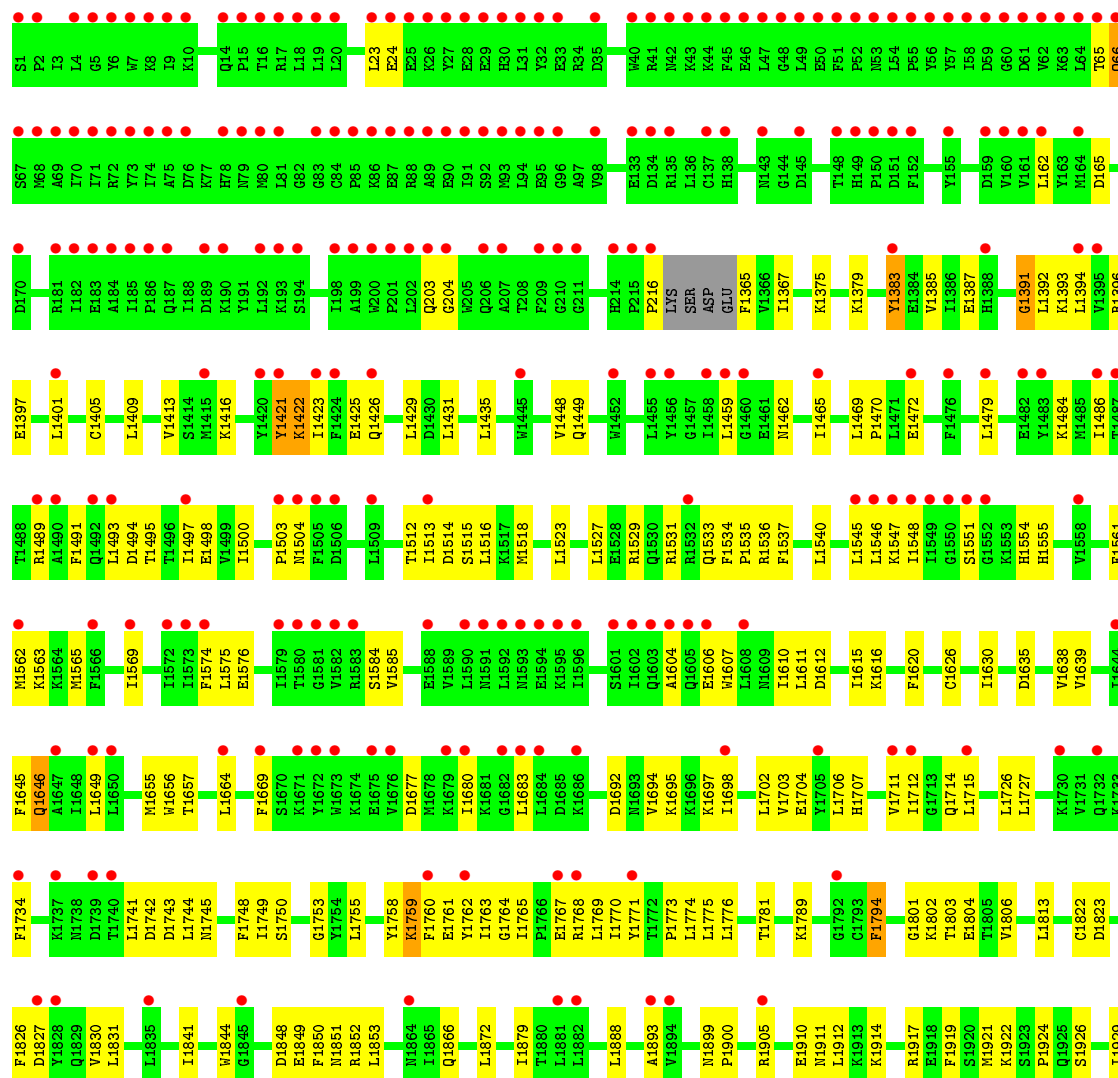
- Chain A: 5% 64% 32%

The visualization displays a hierarchical tree structure of 1000 nodes, each with a unique ID and a color-coded value. The nodes are arranged in a grid-like pattern, with colors ranging from green to red. A legend at the top indicates the color scale: 5% (green), 64% (yellow), and 32% (red). The nodes are organized into a tree structure, with some nodes having multiple children. The nodes are labeled with IDs such as K2055, L2070, G2074, etc. The visualization is a complex network of nodes and edges, representing a hierarchical structure.





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





K4002	F3915	L3841	S3727	L3614
D4003	F3916		E3728	V3615
L4004	T3917	T3844	S3729	
E4005	G3918	Q3845		Y3618
V4006	K3919	K3846	F3734	G3622
	L3920	S3847	K3735	
K4009		L3848	L3736	I3628
	V3923	S3849	T3737	
V4014	K3924	K3850	T3740	M3631
F4015	S3925	V3851		
C4016	V3926		R3745	F3641
G4017	V3927	Y3854		
		L3855	F3767	S3645
N4020	F3930	H3856	F3768	I3646
L4021		K3857	V3769	
Q4022	K3934	H3858		K3654
	F3935	V3859	W3772	R3655
I4023		E3860	K3773	V3656
V4024	I3939		I3774	F3657
		K3865		I3658
V4027	T3943	E3866	V3777	LYS
R4028	K3944		V3778	LYS
I4029	L3945	E3869		SER
	V3946	K3870	A3779	ARG
E4038	P3947	F3871	M3780	ARG
		K3872		GLU
L4049		K3873	Y3785	THR
E4054	F3950	F3874	F3786	ARG
P4055	S3951	K3875	T3787	ALA
	Y3955	T3876		ALA
		C3877	R3792	ARG
L4059	K3958	H3878		T3669
S4060	C3959		K3799	R3670
S4061	D3960	D3882		V3671
W4062		K3883	L3803	
L4063	F3963	L3884		I3674
Q4064	A3964	P3885	S3807	
L4065	S3965	A3886	K3808	L3677
		F3887	E3809	L3678
I4070		L3888	S3810	Y3679
E4074	L3968	L3889	L3811	
	E3969	K3890	K3812	Y3683
Q4077	N3970		I3813	
A4078	V3971	F3895	L3814	S3687
K4079	L3972	V3896	P3615	
		Y3897	L3816	L3690
T4085	N3978	E3898	G3817	D3691
E4086	I3980	D3899	S3818	K3692
Q4087	P3981	I3900	I3819	K3693
L4088	K3982	P3901	E3820	F3694
	A3983		M3821	
	Q3984	D3905	L3822	M3698
	V3985	T3906	N3823	A3699
		K3908		M3700
	V3993		I3834	T3701
	K3994			M3702
	G3995	M3911	G3837	
		G3912	W3838	T3705
		S3913	I3839	
	I3998	Q3914	L3840	L3726

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	175.33Å 117.92Å 202.76Å 90.00° 90.21° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 48.81 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-3.30) 96.1 (48.81-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.33Å)	Xtriage
Refinement program	REFMAC NULL	Depositor
R, R_{free}	0.239 , 0.305 0.239 , 0.309	Depositor DCC
R_{free} test set	5981 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	113.9	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 102.4	EDS
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 119750 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	41634	wwPDB-VP
Average B, all atoms (Å ²)	169.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, SO4, ADP

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	0.62	7/21146 (0.0%)	0.85	21/28618 (0.1%)
1	B	0.51	2/21146 (0.0%)	0.72	4/28618 (0.0%)
All	All	0.57	9/42292 (0.0%)	0.79	25/57236 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2064	GLN	CA-C	-8.38	1.31	1.52
1	B	2841	PRO	N-CD	-7.95	1.36	1.47
1	A	2495	ASP	C-N	-7.35	1.17	1.34
1	B	1759	LYS	C-O	6.47	1.35	1.23
1	A	2488	GLU	CD-OE1	5.63	1.31	1.25
1	A	3459	ASP	CB-CG	-5.33	1.40	1.51
1	A	2412	ARG	CA-C	-5.27	1.39	1.52
1	A	2412	ARG	CZ-NH2	-5.20	1.26	1.33
1	A	1783	THR	CB-CG2	-5.10	1.35	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2412	ARG	NE-CZ-NH2	9.64	125.12	120.30
1	B	2471	LEU	CA-CB-CG	8.90	135.76	115.30
1	A	3459	ASP	CB-CG-OD2	-8.07	111.03	118.30
1	A	2012	LEU	CA-CB-CG	7.53	132.62	115.30
1	A	2212	LEU	CB-CG-CD1	-7.18	98.80	111.00
1	A	1769	LEU	CA-CB-CG	6.83	131.00	115.30
1	A	2064	GLN	O-C-N	6.68	133.39	122.70
1	A	2487	ASP	CB-CG-OD1	6.48	124.14	118.30
1	A	2412	ARG	NH1-CZ-NH2	-6.29	112.48	119.40
1	A	1741	LEU	CB-CG-CD1	6.08	121.34	111.00
1	A	1973	LEU	CB-CG-CD1	-6.01	100.78	111.00
1	A	2220	CYS	CA-CB-SG	-5.99	103.22	114.00
1	A	2336	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	A	1463	LEU	CA-CB-CG	5.85	128.75	115.30
1	A	1659	LEU	CB-CG-CD2	-5.73	101.27	111.00
1	A	2078	CYS	CA-CB-SG	-5.69	103.76	114.00
1	B	2999	LEU	CA-CB-CG	5.66	128.31	115.30
1	A	2176	LEU	CA-CB-CG	5.43	127.79	115.30
1	A	4065	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	A	1973	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	2866	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	2012	LEU	CB-CG-CD2	-5.18	102.19	111.00
1	A	1531	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	B	1938	GLY	N-CA-C	-5.07	100.42	113.10
1	B	2460	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ASP	Peptide
1	A	2007	GLY	Peptide
1	A	2521	ASN	Peptide
1	B	2727	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20748	0	20205	957	0
1	B	20748	0	20206	896	0
2	A	31	0	12	10	0
2	B	31	0	12	24	0
3	A	27	0	12	2	0
3	B	27	0	12	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	10	0	0	2	0
5	B	10	0	0	4	0
All	All	41634	0	40459	1855	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 (1855) 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:2380:LEU:CD2	1:A:2390:ILE:HD11	1.55	1.33
1:B:1826:PHE:CE2	1:B:1831:LEU:HB2	1.66	1.29
1:B:1620:PHE:HD1	1:B:1760:PHE:CZ	1.55	1.24
1:B:216:PRO:O	1:B:1365:PHE:HD1	1.21	1.22
1:B:216:PRO:O	1:B:1365:PHE:CD1	1.94	1.20
1:B:3458:PHE:CE1	1:B:3459:ASP:O	1.96	1.19
1:B:1421:TYR:O	1:B:1425:GLU:HB2	1.42	1.18
1:B:2707:VAL:HB	1:B:2712:LEU:HD11	1.24	1.18
1:B:1416:LYS:HA	1:B:1421:TYR:CZ	1.77	1.18
1:B:1826:PHE:CZ	1:B:1831:LEU:HB2	1.78	1.16
1:A:4033:LEU:CD1	1:A:4035:GLN:HB2	1.76	1.16
1:B:2354:SER:OG	1:B:2357:SER:HB2	1.43	1.16
1:A:3777:VAL:HG11	1:A:3895:PHE:CE1	1.82	1.15
1:B:2988:SER:HB3	1:B:2989:PRO:CD	1.77	1.14
1:A:3777:VAL:HG11	1:A:3895:PHE:HE1	0.97	1.13
1:B:1726:LEU:HD12	1:B:3984:GLN:HB3	1.30	1.13
1:B:2488:GLU:HB3	1:B:2491:LEU:HD12	1.17	1.13
1:A:2289:GLN:OE1	1:A:2412:ARG:HG2	1.49	1.13
1:A:1926:SER:HB2	1:A:1970:LEU:HD13	1.28	1.12
1:A:2111:LYS:HD3	1:A:2161:GLU:HG3	1.23	1.12
1:B:3534:LEU:CD1	1:B:3618:TYR:HE2	1.62	1.12
1:A:2707:VAL:HB	1:A:2712:LEU:HD11	1.19	1.12
1:A:3303:LYS:HA	1:A:3306:TRP:CD1	1.83	1.12
1:A:2757:MET:HG2	1:A:2889:PHE:HB2	1.29	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2488:GLU:HB3	1:A:2491:LEU:HD12	1.16	1.12
1:B:2822:ILE:O	1:B:2822:ILE:HG13	1.51	1.11
1:B:2380:LEU:HD13	1:B:2390:ILE:HD11	1.33	1.10
1:B:2111:LYS:HD3	1:B:2161:GLU:HG3	1.23	1.10
1:B:1645:PHE:HB3	1:B:1765:ILE:HG22	1.33	1.09
1:B:2380:LEU:HD22	1:B:2384:GLU:OE1	1.49	1.09
1:B:1409:LEU:HD21	1:B:1435:LEU:HB3	1.17	1.09
1:B:3777:VAL:HG11	1:B:3895:PHE:HE1	0.99	1.08
1:B:1645:PHE:HB3	1:B:1765:ILE:CG2	1.84	1.08
1:B:1992:LYS:HG3	1:B:2024:SER:HB2	1.24	1.08
1:A:2988:SER:HB3	1:A:2989:PRO:CD	1.84	1.08
1:B:2920:TRP:HB2	1:B:2989:PRO:HG3	1.33	1.07
1:B:3303:LYS:O	1:B:3306:TRP:HD1	1.37	1.07
1:A:3534:LEU:CD1	1:A:3618:TYR:HE2	1.67	1.06
1:B:3303:LYS:HA	1:B:3306:TRP:CD1	1.90	1.06
1:A:1992:LYS:HG3	1:A:2024:SER:HB2	1.32	1.06
1:A:2494:LEU:HD13	1:A:2498:GLY:HA2	1.11	1.06
1:A:1562:MET:HB3	1:A:1569:ILE:HD11	1.32	1.05
1:B:2112:GLU:HB3	1:B:2117:SER:HB2	1.32	1.05
1:B:3777:VAL:HG11	1:B:3895:PHE:CE1	1.92	1.05
1:B:1983:LEU:HG	1:B:1993:THR:HG23	1.08	1.05
1:A:3946:VAL:HG12	1:A:3950:PHE:O	1.57	1.04
1:B:1416:LYS:HG2	1:B:1421:TYR:OH	1.57	1.04
1:B:1620:PHE:CD1	1:B:1760:PHE:CZ	2.45	1.04
1:B:2988:SER:HB3	1:B:2989:PRO:HD2	1.05	1.04
1:A:2380:LEU:HD21	1:A:2390:ILE:CD1	1.86	1.03
1:A:1421:TYR:O	1:A:1425:GLU:HB2	1.58	1.03
1:B:2494:LEU:HD13	1:B:2498:GLY:HA2	1.04	1.03
1:A:3303:LYS:HD2	1:A:3306:TRP:CD1	1.92	1.03
1:A:2745:ILE:HG23	1:A:2756:MET:HE1	1.37	1.03
1:A:2476:LYS:HD2	1:A:2476:LYS:N	1.69	1.03
1:A:1645:PHE:HB3	1:A:1765:ILE:CG2	1.89	1.02
1:B:2494:LEU:HD13	1:B:2498:GLY:CA	1.88	1.02
1:A:2060:PHE:CZ	1:A:2064:GLN:NE2	2.27	1.02
1:B:1866:GLN:OE1	1:B:1911:ASN:HB2	1.59	1.02
1:B:3525:ILE:HD11	1:B:3646:ILE:HG22	1.40	1.01
1:A:2707:VAL:CB	1:A:2712:LEU:HD11	1.90	1.01
1:A:2920:TRP:HB2	1:A:2989:PRO:HG3	1.04	1.01
1:A:2988:SER:CB	1:A:2989:PRO:HD2	1.90	1.01
1:B:2728:LEU:HD12	1:B:2771:ARG:NH2	1.76	1.01
1:A:1421:TYR:CE2	1:A:1425:GLU:CG	2.43	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2494:LEU:CD1	1:B:2498:GLY:HA2	1.91	1.01
1:B:1983:LEU:CG	1:B:1993:THR:HG23	1.90	1.00
1:A:1645:PHE:HB3	1:A:1765:ILE:HG22	1.42	1.00
1:B:1620:PHE:CD1	1:B:1760:PHE:HZ	1.76	1.00
1:A:3024:LEU:HD11	1:A:3303:LYS:HG3	1.39	1.00
1:A:1620:PHE:HD2	1:A:1760:PHE:CZ	1.80	1.00
1:A:1992:LYS:CG	1:A:2024:SER:HB2	1.92	0.99
1:A:1630:ILE:HG22	1:A:1655:MET:SD	2.01	0.99
1:B:1422:LYS:O	1:B:1425:GLU:HB3	1.63	0.99
1:B:1822:CYS:HB2	1:B:1853:LEU:HD21	1.39	0.99
1:B:1645:PHE:CB	1:B:1765:ILE:HG22	1.92	0.99
1:A:3460:PRO:O	1:A:3463:SER:HB2	1.60	0.99
1:A:3525:ILE:HD11	1:A:3646:ILE:HG22	1.45	0.99
1:B:3024:LEU:HD11	1:B:3303:LYS:HG3	1.45	0.98
1:A:2378:VAL:HG22	1:A:2380:LEU:HD13	1.43	0.98
1:A:2494:LEU:CD1	1:A:2498:GLY:HA2	1.92	0.98
1:B:2471:LEU:O	1:B:2473:LEU:HD13	1.63	0.98
1:A:2920:TRP:CB	1:A:2989:PRO:HG3	1.93	0.98
1:A:1970:LEU:HD12	1:A:1973:LEU:HG	1.46	0.97
1:B:2386:MET:HB2	1:B:2627:ARG:HD3	1.45	0.97
1:A:3777:VAL:CG1	1:A:3895:PHE:HE1	1.76	0.97
1:B:1744:LEU:HA	1:B:1760:PHE:CE2	1.99	0.97
1:A:3530:PHE:CD1	1:A:3618:TYR:HD2	1.82	0.97
1:A:2988:SER:HB3	1:A:2989:PRO:HD2	0.97	0.97
1:B:1726:LEU:CD1	1:B:3984:GLN:HB3	1.94	0.97
1:B:2988:SER:CB	1:B:2989:PRO:HD2	1.95	0.96
1:B:2470:GLY:CA	1:B:2473:LEU:HD11	1.96	0.96
1:A:3303:LYS:O	1:A:3306:TRP:HD1	1.47	0.96
1:B:1823:ASP:HB2	1:B:1852:ARG:O	1.66	0.96
1:B:2470:GLY:HA3	1:B:2473:LEU:HD11	1.47	0.96
1:B:1616:LYS:NZ	1:B:1759:LYS:HE3	1.78	0.96
1:A:3534:LEU:HD12	1:A:3618:TYR:HE2	1.30	0.96
1:A:1421:TYR:CE2	1:A:1425:GLU:HG3	1.98	0.96
1:B:3460:PRO:O	1:B:3463:SER:HB2	1.65	0.96
1:B:2787:HIS:HA	1:B:3460:PRO:HD2	1.45	0.95
1:A:2064:GLN:NE2	1:A:2151:TRP:CZ3	2.35	0.95
1:A:2378:VAL:CG2	1:A:2380:LEU:HD13	1.96	0.95
1:B:3946:VAL:HG12	1:B:3950:PHE:O	1.66	0.95
1:B:3534:LEU:CD1	1:B:3618:TYR:CE2	2.51	0.94
1:B:3534:LEU:HD12	1:B:3618:TYR:HE2	1.32	0.94
1:A:2787:HIS:HA	1:A:3460:PRO:HD2	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3406:PHE:HB2	1:A:3513:VAL:CG1	1.97	0.94
1:B:2064:GLN:NE2	1:B:2070:LEU:HG	1.82	0.94
1:B:2080:LYS:HD2	1:B:2195:GLU:HB2	1.48	0.94
1:B:2707:VAL:CB	1:B:2712:LEU:HD11	1.97	0.93
1:A:2378:VAL:CG2	1:A:2380:LEU:CD1	2.46	0.93
1:B:3737:THR:HB	1:B:3740:THR:OG1	1.69	0.93
1:B:1826:PHE:HE2	1:B:1831:LEU:HB2	1.27	0.93
1:A:2488:GLU:CB	1:A:2491:LEU:HD12	1.96	0.93
1:A:4033:LEU:HD11	1:A:4035:GLN:HB2	1.48	0.93
1:B:1630:ILE:HG22	1:B:1655:MET:SD	2.09	0.93
1:A:3656:VAL:HG13	1:A:3677:LEU:HB3	1.50	0.93
1:B:2488:GLU:CB	1:B:2491:LEU:HD12	1.98	0.93
1:A:1421:TYR:CZ	1:A:1425:GLU:HG3	2.04	0.92
1:A:2060:PHE:CE2	1:A:2064:GLN:NE2	2.37	0.92
1:B:3777:VAL:CG1	1:B:3895:PHE:HE1	1.82	0.92
1:B:2755:HIS:HB2	1:B:2911:ARG:O	1.68	0.92
1:B:3303:LYS:O	1:B:3306:TRP:CD1	2.22	0.92
1:A:1535:PRO:HB2	1:A:1841:ILE:HG13	1.52	0.92
1:A:1924:PRO:HB2	1:A:1929:ILE:HD11	1.51	0.91
1:A:2920:TRP:HB2	1:A:2989:PRO:CG	1.98	0.91
1:B:3303:LYS:HD2	1:B:3306:TRP:CD1	2.06	0.91
1:A:2493:LYS:HG3	1:A:2494:LEU:H	1.36	0.91
1:A:2494:LEU:HD13	1:A:2498:GLY:CA	2.00	0.91
1:B:2472:THR:C	1:B:2473:LEU:HD12	1.89	0.91
1:B:1992:LYS:CG	1:B:2024:SER:HB2	2.01	0.91
1:A:1726:LEU:HD12	1:A:3984:GLN:HB3	1.51	0.91
1:B:2380:LEU:CD1	1:B:2390:ILE:HD11	2.00	0.91
1:B:2386:MET:CB	1:B:2627:ARG:HD3	2.01	0.91
1:B:3530:PHE:CD1	1:B:3618:TYR:HD2	1.88	0.91
1:A:3534:LEU:CD1	1:A:3618:TYR:CE2	2.53	0.91
1:A:3737:THR:HB	1:A:3740:THR:OG1	1.70	0.91
1:A:3303:LYS:O	1:A:3306:TRP:CD1	2.23	0.90
1:A:1983:LEU:HG	1:A:1993:THR:HG23	1.49	0.90
1:A:2757:MET:HG2	1:A:2889:PHE:CB	2.01	0.90
1:B:3406:PHE:HB2	1:B:3513:VAL:CG1	2.01	0.90
1:B:2112:GLU:HB3	1:B:2117:SER:CB	2.01	0.90
1:A:1940:GLU:HB2	1:A:1989:GLU:O	1.70	0.90
1:B:1956:LEU:HB3	1:B:1968:PHE:HE2	1.37	0.90
1:B:1774:LEU:HD21	1:B:1922:LYS:O	1.72	0.90
1:A:2380:LEU:HD21	1:A:2390:ILE:HD11	0.92	0.89
1:B:1983:LEU:CD2	1:B:1993:THR:O	2.20	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1983:LEU:HD23	1:B:1993:THR:O	1.72	0.89
1:A:1939:PHE:CD2	1:A:1940:GLU:O	2.25	0.89
1:B:2488:GLU:HB3	1:B:2491:LEU:CD1	2.02	0.89
1:A:1822:CYS:SG	1:A:1850:PHE:HA	2.13	0.89
1:A:3458:PHE:CE1	1:A:3459:ASP:O	2.26	0.88
1:A:2106:THR:OG1	1:A:2154:PHE:HB3	1.74	0.88
1:B:1535:PRO:HB2	1:B:1841:ILE:HG13	1.54	0.88
1:B:2225:LYS:HA	2:B:5093:ATP:C2	2.09	0.88
1:B:2563:SER:HB3	1:B:2566:SER:H	1.39	0.88
1:B:2080:LYS:HE2	1:B:2195:GLU:OE1	1.73	0.88
1:A:1425:GLU:OE2	1:A:1429:LEU:CG	2.21	0.88
1:A:2378:VAL:HG22	1:A:2380:LEU:CD1	2.03	0.88
1:A:1823:ASP:HB2	1:A:1853:LEU:HD23	1.56	0.88
1:A:2512:LYS:O	1:A:2513:GLN:HB2	1.74	0.88
1:A:2137:VAL:O	1:A:2141:ILE:HG23	1.74	0.88
1:B:1744:LEU:HA	1:B:1760:PHE:CD2	2.09	0.87
1:A:4033:LEU:HD13	1:A:4035:GLN:HB2	1.54	0.87
1:A:3303:LYS:HA	1:A:3306:TRP:NE1	1.89	0.87
1:A:2380:LEU:CD2	1:A:2390:ILE:CD1	2.47	0.87
1:B:1409:LEU:HD21	1:B:1435:LEU:CB	2.04	0.87
1:B:1939:PHE:CD2	1:B:1940:GLU:O	2.28	0.87
1:A:1425:GLU:OE2	1:A:1429:LEU:HG	1.74	0.87
1:A:1822:CYS:HB2	1:A:1853:LEU:HD21	1.55	0.87
1:A:1421:TYR:CE2	1:A:1425:GLU:HG2	2.08	0.87
1:A:1983:LEU:CG	1:A:1993:THR:HG23	2.04	0.87
1:B:1535:PRO:C	1:B:1841:ILE:HD11	1.94	0.87
1:A:1866:GLN:OE1	1:A:1911:ASN:HB2	1.75	0.87
1:A:3534:LEU:HD12	1:A:3618:TYR:CE2	2.09	0.87
1:B:2332:GLY:HA2	1:B:2335:GLN:HB2	1.57	0.86
1:A:3303:LYS:CA	1:A:3306:TRP:CD1	2.58	0.86
1:B:1992:LYS:HE2	1:B:2024:SER:O	1.75	0.86
1:A:3530:PHE:CD1	1:A:3618:TYR:CD2	2.64	0.86
1:A:3509:LEU:CD1	1:A:3513:VAL:HG21	2.05	0.86
1:B:3998:ILE:HG21	1:B:4004:LEU:HG	1.57	0.86
1:B:1956:LEU:HB3	1:B:1968:PHE:CE2	2.11	0.86
1:B:1604:ALA:HA	1:B:1607:TRP:CD1	2.11	0.86
1:A:2787:HIS:HA	1:A:3460:PRO:CD	2.06	0.86
1:B:2853:LEU:HD21	1:B:2870:GLU:HG3	1.58	0.86
1:A:1409:LEU:HD21	1:A:1435:LEU:HB3	1.58	0.85
1:B:3534:LEU:HD13	1:B:3618:TYR:HE2	1.37	0.85
1:A:1707:HIS:O	1:A:1711:VAL:HG23	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2472:THR:O	1:B:2473:LEU:HD12	1.76	0.85
1:A:2787:HIS:HA	1:A:3460:PRO:HG2	1.59	0.85
1:B:2141:ILE:HG22	1:B:2145:PHE:HB2	1.58	0.85
1:A:1970:LEU:HD12	1:A:1973:LEU:CG	2.07	0.84
1:A:2332:GLY:HA2	1:A:2335:GLN:HB2	1.59	0.84
1:A:2631:THR:O	1:A:2635:THR:HG22	1.76	0.84
1:A:2755:HIS:HB2	1:A:2911:ARG:O	1.77	0.84
1:A:1645:PHE:CB	1:A:1765:ILE:HG22	2.07	0.84
1:B:3303:LYS:HA	1:B:3306:TRP:NE1	1.91	0.84
1:B:2787:HIS:HA	1:B:3460:PRO:CD	2.07	0.84
1:A:1621:THR:HA	1:A:1624:ARG:NH1	1.92	0.84
1:B:1924:PRO:HB2	1:B:1929:ILE:HD11	1.59	0.84
1:B:3024:LEU:CD1	1:B:3303:LYS:HG3	2.07	0.83
1:B:1940:GLU:HB2	1:B:1989:GLU:O	1.78	0.83
1:A:2787:HIS:HA	1:A:3460:PRO:CG	2.07	0.83
1:A:3566:LEU:HD23	1:A:3587:LEU:HD11	1.61	0.83
1:A:2563:SER:HB3	1:A:2566:SER:H	1.42	0.83
1:A:2941:THR:HG22	1:A:2942:ASP:H	1.42	0.83
1:A:3946:VAL:CG1	1:A:3950:PHE:O	2.28	0.82
1:A:2274:HIS:HE1	1:A:2326:LEU:O	1.61	0.82
1:B:3534:LEU:HD12	1:B:3618:TYR:CE2	2.13	0.82
1:A:2107:LYS:HE2	1:A:2499:SER:HB3	1.61	0.82
1:B:2512:LYS:O	1:B:2513:GLN:HB2	1.77	0.82
1:A:2488:GLU:HB3	1:A:2491:LEU:CD1	2.07	0.82
1:B:2274:HIS:HE1	1:B:2326:LEU:O	1.62	0.82
1:A:2745:ILE:HG23	1:A:2756:MET:CE	2.09	0.82
1:A:2757:MET:HG2	1:A:2889:PHE:CD2	2.14	0.82
1:A:3534:LEU:HD13	1:A:3618:TYR:HE2	1.44	0.82
1:A:1992:LYS:HE2	1:A:2024:SER:O	1.78	0.82
1:B:3656:VAL:HG13	1:B:3677:LEU:HB3	1.60	0.81
1:A:1387:GLU:HB3	1:A:1393:LYS:HG2	1.61	0.81
1:A:1783:THR:HG22	1:A:1809:PHE:HZ	1.44	0.81
1:B:1409:LEU:CD2	1:B:1435:LEU:HB3	2.06	0.81
1:A:1562:MET:CB	1:A:1569:ILE:HD11	2.09	0.81
1:A:1569:ILE:HA	1:A:1584:SER:HA	1.59	0.81
1:A:2112:GLU:HB3	1:A:2117:SER:HB2	1.60	0.81
1:B:3566:LEU:HA	1:B:3583:LEU:HD21	1.62	0.81
1:A:3024:LEU:CD1	1:A:3303:LYS:HG3	2.11	0.81
1:A:2386:MET:HB2	1:A:2627:ARG:HD3	1.62	0.81
1:B:2111:LYS:HD3	1:B:2161:GLU:CG	2.08	0.80
1:A:2476:LYS:CD	1:A:2476:LYS:N	2.40	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1802:LYS:HG2	1:B:1921:MET:HG3	1.61	0.80
1:A:2111:LYS:HD3	1:A:2161:GLU:CG	2.10	0.80
1:A:2707:VAL:HB	1:A:2712:LEU:CD1	2.07	0.80
1:B:2048:SER:H	2:B:5093:ATP:HN62	1.29	0.80
1:A:4021:LEU:HD23	1:A:4023:ILE:HG12	1.61	0.80
1:B:1392:LEU:HD13	1:B:1393:LYS:N	1.97	0.80
1:B:1983:LEU:HG	1:B:1993:THR:CG2	2.03	0.80
1:A:2175:ILE:HG12	1:A:2183:ARG:HB3	1.62	0.80
1:A:3525:ILE:CD1	1:A:3646:ILE:HG22	2.10	0.80
1:B:1823:ASP:CB	1:B:1852:ARG:O	2.30	0.79
1:B:2471:LEU:O	1:B:2473:LEU:CD1	2.31	0.79
1:B:2728:LEU:HD12	1:B:2771:ARG:HH22	1.44	0.79
1:A:1604:ALA:HA	1:A:1607:TRP:NE1	1.97	0.79
1:A:3534:LEU:HD11	1:A:3614:LEU:HD23	1.63	0.79
1:B:2354:SER:OG	1:B:2357:SER:CB	2.28	0.79
1:B:1996:GLU:O	1:B:2000:ARG:HG3	1.81	0.79
1:B:3303:LYS:C	1:B:3306:TRP:HD1	1.86	0.79
1:A:1620:PHE:CE1	1:A:1624:ARG:HD3	2.18	0.79
1:B:1970:LEU:CD2	1:B:1974:LYS:HE2	2.13	0.79
1:B:2745:ILE:HG12	1:B:2756:MET:HE3	1.65	0.79
1:B:216:PRO:C	1:B:1365:PHE:CD1	2.56	0.79
1:B:2106:THR:OG1	1:B:2154:PHE:HB3	1.82	0.79
1:A:1604:ALA:HA	1:A:1607:TRP:CD1	2.18	0.78
1:A:2003:LEU:HA	1:A:2006:LEU:HD12	1.62	0.78
1:A:2048:SER:H	2:A:5093:ATP:HN62	1.31	0.78
1:A:3406:PHE:HB2	1:A:3513:VAL:HG11	1.65	0.78
1:A:1462:ASN:HB2	1:A:1465:ILE:HG22	1.64	0.78
1:A:2220:CYS:SG	1:A:2224:SER:HB2	2.23	0.78
1:A:1630:ILE:CG2	1:A:1655:MET:SD	2.71	0.78
1:B:1616:LYS:HZ1	1:B:1759:LYS:HE3	1.47	0.78
1:B:1416:LYS:CG	1:B:1421:TYR:OH	2.31	0.78
1:B:2224:SER:O	2:B:5093:ATP:H2	1.66	0.78
1:A:1783:THR:HG22	1:A:1809:PHE:CZ	2.19	0.78
1:B:3645:SER:HB3	1:B:3890:GLN:NE2	1.99	0.78
1:A:4033:LEU:CD1	1:A:4035:GLN:CB	2.62	0.78
1:A:2446:SER:H	1:A:2449:THR:HG23	1.49	0.78
1:A:2380:LEU:HG	1:A:2384:GLU:OE1	1.84	0.77
1:B:1826:PHE:CZ	1:B:1831:LEU:CB	2.66	0.77
1:B:3946:VAL:CG1	1:B:3950:PHE:O	2.32	0.77
1:A:1392:LEU:HD13	1:A:1393:LYS:N	1.99	0.77
1:A:2176:LEU:O	1:A:2183:ARG:HA	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3777:VAL:CG1	1:A:3895:PHE:CE1	2.57	0.77
1:A:2289:GLN:OE1	1:A:2412:ARG:CG	2.32	0.77
1:A:2152:VAL:HG12	1:A:2154:PHE:HE1	1.49	0.77
1:B:3303:LYS:CA	1:B:3306:TRP:CD1	2.66	0.77
1:A:3618:TYR:CD1	1:A:3618:TYR:N	2.51	0.77
1:B:1421:TYR:O	1:B:1425:GLU:CB	2.28	0.77
1:A:2446:SER:H	1:A:2449:THR:CG2	1.97	0.77
1:B:4065:LEU:HD11	1:B:4070:ILE:HD11	1.65	0.77
1:B:1826:PHE:CE2	1:B:1831:LEU:CB	2.60	0.77
1:B:3998:ILE:CG2	1:B:4004:LEU:HG	2.13	0.77
1:B:1604:ALA:HA	1:B:1607:TRP:NE1	1.99	0.77
1:A:1626:CYS:SG	1:A:1639:VAL:HG11	2.24	0.77
1:A:3700:MET:HB3	1:A:4085:THR:HG21	1.67	0.77
1:A:3458:PHE:HE1	1:A:3462:ILE:HB	1.50	0.77
1:B:1616:LYS:NZ	1:B:1759:LYS:CE	2.48	0.77
1:B:3406:PHE:HB2	1:B:3513:VAL:HG11	1.67	0.77
1:B:1645:PHE:CB	1:B:1765:ILE:CG2	2.58	0.76
1:B:1616:LYS:HZ2	1:B:1759:LYS:HE3	1.47	0.76
1:A:1535:PRO:C	1:A:1841:ILE:HD11	2.05	0.76
1:A:1463:LEU:HA	1:A:1466:GLN:HG2	1.66	0.76
1:B:2111:LYS:NZ	1:B:2161:GLU:HG2	2.01	0.76
1:B:1759:LYS:CE	1:B:1761:GLU:OE2	2.33	0.76
1:A:1531:ARG:HG2	1:A:1537:PHE:HB3	1.67	0.76
1:B:2779:LEU:HD23	1:B:2812:ARG:O	1.84	0.76
1:B:2787:HIS:HA	1:B:3460:PRO:CG	2.15	0.76
1:A:2111:LYS:NZ	1:A:2161:GLU:HG2	2.01	0.76
1:A:1649:LEU:CD1	1:A:1704:GLU:HG3	2.16	0.76
1:A:1645:PHE:CB	1:A:1765:ILE:CG2	2.62	0.76
1:A:3566:LEU:HA	1:A:3583:LEU:CD2	2.16	0.76
1:B:1940:GLU:HG3	1:B:1941:ASP:H	1.50	0.76
1:A:2197:ASP:HB3	1:A:2549:ARG:HD2	1.67	0.76
1:A:3774:ILE:O	1:A:3778:VAL:HG23	1.86	0.75
1:A:2107:LYS:HE3	1:A:2495:ASP:OD2	1.85	0.75
1:B:3566:LEU:HA	1:B:3583:LEU:CD2	2.16	0.75
1:B:3792:ARG:HB2	1:B:3955:TYR:CD2	2.21	0.75
1:A:2757:MET:CG	1:A:2889:PHE:HB2	2.14	0.75
1:A:3509:LEU:HD12	1:A:3513:VAL:CG2	2.16	0.75
1:B:216:PRO:C	1:B:1365:PHE:HA	2.06	0.75
1:B:1421:TYR:O	1:B:1421:TYR:CG	2.37	0.75
1:A:1620:PHE:HE1	1:A:1624:ARG:HD3	1.50	0.75
1:A:2779:LEU:HD23	1:A:2812:ARG:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3792:ARG:HB2	1:B:3955:TYR:CE2	2.22	0.75
1:B:1562:MET:HB3	1:B:1569:ILE:HD11	1.69	0.75
1:B:3530:PHE:CD1	1:B:3618:TYR:CD2	2.74	0.75
1:B:3799:LYS:O	1:B:3803:LEU:HG	1.86	0.75
1:B:2137:VAL:O	1:B:2141:ILE:HG23	1.86	0.74
1:B:1574:PHE:HB3	1:B:1576:GLU:H	1.51	0.74
1:A:1965:HIS:HD2	1:A:2212:LEU:HD21	1.52	0.74
1:B:1405:CYS:O	1:B:1409:LEU:HG	1.86	0.74
1:B:2707:VAL:CG1	1:B:2712:LEU:CD1	2.65	0.74
1:B:2080:LYS:NZ	2:B:5093:ATP:O3G	2.21	0.74
1:B:2203:THR:HG22	1:B:2205:ALA:H	1.51	0.74
1:B:2920:TRP:CB	1:B:2989:PRO:HG3	2.14	0.74
1:A:4033:LEU:HD13	1:A:4035:GLN:CB	2.18	0.74
1:B:2425:THR:HB	3:B:5094:ADP:O1A	1.85	0.74
1:A:3645:SER:HB3	1:A:3890:GLN:NE2	2.03	0.74
1:B:1929:ILE:HD13	1:B:1970:LEU:CD1	2.18	0.74
1:B:3871:PHE:CZ	1:B:3873:MET:HB2	2.22	0.74
1:B:1939:PHE:HD2	1:B:1940:GLU:O	1.69	0.74
1:A:1409:LEU:HD21	1:A:1435:LEU:CB	2.18	0.74
1:A:2411:LYS:HG2	1:A:2530:HIS:HE1	1.53	0.74
1:B:2420:PRO:HD3	1:B:2536:ASN:HD21	1.51	0.74
1:B:3534:LEU:HD13	1:B:3618:TYR:CE2	2.18	0.73
1:A:2707:VAL:CG1	1:A:2712:LEU:CD1	2.66	0.73
1:A:1939:PHE:HD2	1:A:1940:GLU:O	1.68	0.73
1:B:3728:GLU:HG3	1:B:4079:LYS:HE2	1.69	0.73
1:B:4020:ASN:HB3	1:B:4028:ARG:HH11	1.51	0.73
1:B:3774:ILE:O	1:B:3778:VAL:HG23	1.88	0.73
1:B:3458:PHE:CD1	1:B:3459:ASP:O	2.41	0.73
1:A:3923:VAL:HG23	1:A:4038:GLU:HA	1.70	0.73
1:A:2386:MET:HB3	1:A:2627:ARG:NE	2.04	0.73
1:B:2175:ILE:HG12	1:B:2183:ARG:HB3	1.71	0.73
1:A:3303:LYS:C	1:A:3306:TRP:HD1	1.90	0.73
1:A:3566:LEU:HA	1:A:3583:LEU:HD21	1.71	0.73
1:A:2048:SER:N	2:A:5093:ATP:HN62	1.86	0.73
1:A:2064:GLN:NE2	1:A:2151:TRP:HZ3	1.86	0.73
1:B:1616:LYS:HZ1	1:B:1759:LYS:CE	2.02	0.73
1:B:2155:ASP:OD1	1:B:2549:ARG:NH2	2.22	0.73
1:B:2080:LYS:HG2	2:B:5093:ATP:O1B	1.89	0.73
1:B:2745:ILE:HG23	1:B:2756:MET:CE	2.18	0.73
1:B:2787:HIS:HA	1:B:3460:PRO:HG2	1.71	0.72
1:A:1983:LEU:CD2	1:A:1993:THR:HG23	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1726:LEU:HD12	1:B:3984:GLN:CB	2.14	0.72
1:A:2757:MET:HG2	1:A:2889:PHE:CG	2.24	0.72
1:A:1620:PHE:CD2	1:A:1760:PHE:CZ	2.72	0.72
1:B:1879:ILE:HG12	1:B:1888:LEU:HB2	1.68	0.72
1:B:2631:THR:O	1:B:2635:THR:HG22	1.88	0.72
1:B:2220:CYS:SG	1:B:2224:SER:CB	2.77	0.72
1:B:1929:ILE:HD13	1:B:1970:LEU:HD11	1.72	0.72
1:A:2386:MET:CB	1:A:2627:ARG:HD3	2.20	0.72
1:A:3303:LYS:CA	1:A:3306:TRP:HD1	2.00	0.72
1:A:1421:TYR:O	1:A:1425:GLU:CB	2.34	0.72
1:A:1394:LEU:HD22	1:A:1449:GLN:HE22	1.53	0.72
1:A:1938:GLY:O	1:A:1989:GLU:HB3	1.88	0.72
1:A:4065:LEU:HD11	1:A:4070:ILE:HD11	1.70	0.72
1:B:2572:GLU:CD	1:B:2590:GLU:HG3	2.09	0.72
1:B:1953:LEU:CD1	1:B:1973:LEU:HB3	2.19	0.72
1:B:1926:SER:CB	1:B:1970:LEU:HD12	2.19	0.72
1:A:3799:LYS:O	1:A:3803:LEU:HG	1.90	0.72
1:A:2080:LYS:HG2	1:A:2215:PHE:CE1	2.25	0.72
1:A:2745:ILE:HG12	1:A:2756:MET:HE3	1.72	0.71
1:B:1630:ILE:CG2	1:B:1655:MET:SD	2.77	0.71
1:B:1620:PHE:HD1	1:B:1760:PHE:HZ	0.84	0.71
1:A:1466:GLN:CB	1:A:1473:THR:HG21	2.20	0.71
1:B:3458:PHE:CZ	1:B:3459:ASP:O	2.43	0.71
1:A:3998:ILE:CG2	1:A:4004:LEU:HG	2.21	0.71
1:B:3618:TYR:CD1	1:B:3618:TYR:N	2.53	0.71
1:A:2106:THR:HG1	1:A:2154:PHE:HB3	1.53	0.71
1:B:2513:GLN:O	1:B:2526:ILE:HG13	1.91	0.71
1:B:2220:CYS:SG	1:B:2224:SER:HB2	2.31	0.71
1:A:2302:PHE:HA	1:A:2310:LEU:HD11	1.71	0.71
1:B:2446:SER:H	1:B:2449:THR:HG23	1.56	0.71
1:A:1849:GLU:OE2	1:A:1899:ASN:ND2	2.23	0.71
1:A:3024:LEU:HD11	1:A:3303:LYS:CG	2.19	0.71
1:A:2549:ARG:HE	2:A:5093:ATP:PG	2.14	0.71
1:A:3839:ILE:HG23	1:A:3873:MET:HG3	1.73	0.71
1:A:2846:GLY:O	1:A:2849:TYR:HB3	1.90	0.71
1:A:1738:ASN:O	1:A:1739:ASP:OD1	2.09	0.71
1:A:1781:THR:HG21	1:A:1919:PHE:CD1	2.26	0.71
1:B:1425:GLU:OE2	1:B:1429:LEU:HD11	1.90	0.71
1:A:3618:TYR:HD1	1:A:3618:TYR:N	1.89	0.71
1:A:2787:HIS:CA	1:A:3460:PRO:HD2	2.21	0.71
1:A:3566:LEU:O	1:A:3570:LEU:HG	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2476:LYS:NZ	1:B:2528:ARG:HD2	2.05	0.71
1:A:1493:LEU:HD23	1:A:1498:GLU:HB3	1.72	0.71
1:B:1970:LEU:HD21	1:B:1974:LYS:HE2	1.72	0.71
1:A:3330:TYR:OH	1:A:3346:LEU:HD22	1.91	0.71
1:B:1540:LEU:CD1	1:B:1548:ILE:HD11	2.21	0.71
1:A:3406:PHE:HB2	1:A:3513:VAL:HG12	1.72	0.70
1:B:2476:LYS:HD2	1:B:2476:LYS:H	1.56	0.70
1:B:1965:HIS:HD2	1:B:2212:LEU:HD21	1.55	0.70
1:A:3303:LYS:HD2	1:A:3306:TRP:HD1	1.53	0.70
1:A:1462:ASN:CB	1:A:1465:ILE:HG22	2.20	0.70
1:B:2446:SER:H	1:B:2449:THR:CG2	2.03	0.70
1:A:3353:LEU:HD23	1:A:3358:VAL:HG11	1.73	0.70
1:A:1726:LEU:CD1	1:A:3984:GLN:HB3	2.22	0.70
1:B:1535:PRO:HB2	1:B:1841:ILE:CG1	2.21	0.70
1:A:1620:PHE:CZ	1:A:1743:ASP:HB3	2.27	0.70
1:A:1826:PHE:CE1	1:A:1853:LEU:HD22	2.26	0.70
1:B:2476:LYS:HG2	1:B:2478:ASP:O	1.91	0.70
1:A:2728:LEU:HD12	1:A:2771:ARG:NH2	2.07	0.70
1:B:1698:ILE:O	1:B:1702:LEU:HG	1.91	0.70
1:B:2787:HIS:CA	1:B:3460:PRO:HD2	2.21	0.70
1:B:3303:LYS:CA	1:B:3306:TRP:HD1	2.05	0.70
1:A:1744:LEU:HA	1:A:1760:PHE:CE1	2.25	0.70
1:A:2707:VAL:CG1	1:A:2712:LEU:HD11	2.21	0.70
1:A:2563:SER:HB2	1:A:2566:SER:OG	1.92	0.70
1:B:2131:THR:HG22	1:B:2176:LEU:HD21	1.72	0.70
1:B:2476:LYS:CD	1:B:2476:LYS:H	2.04	0.70
1:B:1392:LEU:HD13	1:B:1392:LEU:C	2.13	0.70
1:A:2048:SER:H	2:A:5093:ATP:N6	1.88	0.70
1:B:3631:MET:CE	1:B:3698:MET:HG3	2.21	0.70
1:A:3534:LEU:HD13	1:A:3618:TYR:CE2	2.22	0.69
1:A:2112:GLU:HB3	1:A:2117:SER:CB	2.21	0.69
1:A:2891:ILE:HD11	1:A:2903:ILE:HD11	1.74	0.69
1:A:7:TRP:O	1:A:9:ILE:N	2.25	0.69
1:B:1822:CYS:SG	1:B:1849:GLU:O	2.50	0.69
1:A:3509:LEU:HD12	1:A:3513:VAL:HG21	1.74	0.69
1:B:1489:ARG:HH12	1:B:1503:PRO:HG2	1.57	0.69
1:A:3787:THR:HG22	1:A:3875:MET:HB2	1.73	0.69
1:B:3024:LEU:HD11	1:B:3303:LYS:CG	2.20	0.69
1:A:2064:GLN:NE2	1:A:2151:TRP:CH2	2.61	0.69
1:A:1983:LEU:CD2	1:A:1993:THR:O	2.40	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:3871:PHE:CZ	1:A:3873:MET:HB2	2.28	0.69
1:A:2181:GLY:O	1:A:2182:GLU:HG3	1.92	0.69
1:B:2032:LYS:O	1:B:2035:VAL:HG12	1.92	0.69
1:A:1823:ASP:CB	1:A:1852:ARG:O	2.41	0.69
1:A:1495:THR:HG22	1:A:1497:ILE:HG22	1.74	0.69
1:A:3473:ALA:HB3	1:A:3476:ARG:O	1.93	0.69
1:B:3566:LEU:O	1:B:3570:LEU:HG	1.93	0.68
1:B:3850:TRP:NE1	1:B:3854:TYR:HB3	2.09	0.68
1:B:1569:ILE:HA	1:B:1584:SER:HA	1.73	0.68
1:A:2709:LYS:O	1:A:2713:VAL:HG23	1.93	0.68
1:A:3010:LEU:HD21	1:A:3317:SER:HB3	1.76	0.68
1:B:3618:TYR:HD1	1:B:3618:TYR:N	1.91	0.68
1:B:2176:LEU:O	1:B:2183:ARG:HA	1.93	0.68
1:A:1418:SER:HB2	1:A:3446:PHE:HB3	1.73	0.68
1:B:1759:LYS:HE2	1:B:1761:GLU:OE2	1.92	0.68
1:B:1540:LEU:CD1	1:B:1548:ILE:CD1	2.71	0.68
1:A:1956:LEU:HB3	1:A:1968:PHE:CE2	2.28	0.68
1:A:1995:VAL:HG22	1:A:2022:PHE:CE2	2.29	0.68
1:B:3566:LEU:CD1	1:B:3570:LEU:HD11	2.24	0.68
1:B:1387:GLU:HB3	1:B:1393:LYS:HG2	1.74	0.68
1:A:1922:LYS:NZ	1:A:4004:LEU:HD12	2.08	0.68
1:B:2489:ILE:HG22	1:B:2535:CYS:HB3	1.76	0.68
1:B:1826:PHE:HE2	1:B:1831:LEU:CB	2.04	0.68
1:A:3886:ALA:N	1:A:3887:PRO:HD2	2.09	0.68
1:B:2941:THR:HG22	1:B:2942:ASP:H	1.57	0.68
1:B:2111:LYS:CD	1:B:2161:GLU:HG3	2.12	0.68
1:B:3871:PHE:HZ	1:B:3873:MET:HB2	1.59	0.68
1:A:1849:GLU:HG2	1:A:1899:ASN:HD22	1.59	0.68
1:A:2276:LEU:HD23	1:A:2556:ILE:HD13	1.76	0.68
1:B:2707:VAL:CG1	1:B:2712:LEU:HD11	2.24	0.67
1:A:2173:ASN:HB3	1:A:2175:ILE:HG22	1.75	0.67
1:B:3645:SER:HB3	1:B:3890:GLN:HE21	1.57	0.67
1:B:3683:TYR:O	1:B:3687:SER:HB2	1.95	0.67
1:A:1965:HIS:HD2	1:A:2212:LEU:CD2	2.08	0.67
1:B:2177:THR:HG22	1:B:2183:ARG:HG2	1.76	0.67
1:B:3816:LEU:HD23	1:B:3847:SER:OG	1.95	0.67
1:B:1612:ASP:HA	1:B:1615:ILE:CD1	2.24	0.67
1:A:2762:SER:O	1:A:2763:ARG:HB2	1.95	0.67
1:A:2391:VAL:HG22	1:A:2430:ASN:OD1	1.95	0.67
1:A:1620:PHE:HD1	1:A:1624:ARG:NH1	1.93	0.67
1:B:2467:THR:HB	1:B:2473:LEU:HD22	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2081:THR:HB	2:B:5093:ATP:O1A	1.93	0.67
1:A:2463:ASN:HB2	1:A:2477:SER:HA	1.77	0.67
1:A:2760:GLY:HA3	1:A:2766:LYS:HD3	1.77	0.67
1:B:1620:PHE:HB2	1:B:1760:PHE:CE1	2.30	0.67
1:B:2472:THR:CG2	1:B:2524:VAL:HG22	2.25	0.67
1:B:2224:SER:O	2:B:5093:ATP:C2	2.47	0.67
1:B:3923:VAL:HG23	1:B:4038:GLU:HA	1.77	0.67
1:B:3473:ALA:HB3	1:B:3476:ARG:O	1.94	0.67
1:B:4017:GLY:HA3	1:B:4021:LEU:HD12	1.76	0.67
1:B:3919:LYS:NZ	1:B:4038:GLU:CD	2.48	0.67
1:B:1645:PHE:CG	1:B:1765:ILE:HG22	2.29	0.66
1:A:1991:GLU:O	1:A:1995:VAL:HG23	1.95	0.66
1:B:3350:LYS:HA	1:B:3353:LEU:HD12	1.77	0.66
1:B:1967:HIS:C	1:B:1968:PHE:HD1	1.97	0.66
1:B:1611:LEU:O	1:B:1615:ILE:HG23	1.95	0.66
1:B:1849:GLU:OE2	1:B:1899:ASN:ND2	2.28	0.66
1:B:2552:ARG:NH2	2:B:5093:ATP:O2G	2.28	0.66
1:B:1536:ARG:N	1:B:1841:ILE:HD11	2.09	0.66
1:B:3919:LYS:HZ2	1:B:4038:GLU:CD	1.98	0.66
1:B:2517:LYS:HE3	1:B:2519:PRO:HD2	1.76	0.66
1:A:3530:PHE:HD1	1:A:3618:TYR:HD2	1.43	0.66
1:A:3460:PRO:O	1:A:3463:SER:CB	2.40	0.66
1:B:1970:LEU:CD2	1:B:1974:LYS:CE	2.73	0.66
1:A:2220:CYS:SG	1:A:2224:SER:CB	2.83	0.66
1:B:2448:ASP:HB2	1:B:2829:GLU:OE1	1.95	0.66
1:A:1995:VAL:HG21	1:A:2024:SER:HB3	1.78	0.66
1:B:2107:LYS:HE2	1:B:2499:SER:HB3	1.78	0.66
1:B:2745:ILE:HG23	1:B:2756:MET:HE1	1.77	0.66
1:B:2106:THR:HG1	1:B:2154:PHE:HB3	1.59	0.66
1:A:3816:LEU:HD23	1:A:3847:SER:OG	1.96	0.66
1:B:3566:LEU:HD13	1:B:3570:LEU:HD11	1.77	0.66
1:A:2677:VAL:HG11	1:A:2686:LEU:HD21	1.77	0.66
1:A:3459:ASP:OD2	1:A:3461:ILE:HG12	1.95	0.66
1:B:3566:LEU:HD13	1:B:3570:LEU:CD1	2.25	0.66
1:A:3979:ASN:C	1:A:3981:PRO:HD2	2.16	0.66
1:A:1983:LEU:HD23	1:A:1993:THR:O	1.96	0.66
1:A:1823:ASP:HB3	1:A:1852:ARG:O	1.95	0.65
1:A:1392:LEU:HD13	1:A:1392:LEU:C	2.16	0.65
1:A:1922:LYS:HZ1	1:A:4004:LEU:HD12	1.60	0.65
1:A:1489:ARG:HH12	1:A:1503:PRO:HG2	1.61	0.65
1:B:2076:ALA:HA	2:B:5093:ATP:O1G	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3837:GLY:O	1:A:3871:PHE:HD1	1.79	0.65
1:B:3592:LYS:O	1:B:3596:ASN:HB2	1.96	0.65
1:A:2034:ILE:HD12	1:A:2061:TYR:CZ	2.31	0.65
1:A:1983:LEU:HD23	1:A:1993:THR:CG2	2.26	0.65
1:B:2141:ILE:CG2	1:B:2145:PHE:HB2	2.25	0.65
1:B:3839:ILE:HG23	1:B:3873:MET:HG3	1.77	0.65
1:A:3792:ARG:HB2	1:A:3955:TYR:CD2	2.30	0.65
1:A:1622:GLN:HE22	1:A:1644:ILE:H	1.44	0.65
1:A:1536:ARG:HD3	1:A:1841:ILE:HD13	1.77	0.65
1:A:1405:CYS:O	1:A:1409:LEU:HG	1.96	0.65
1:A:3877:CYS:SG	1:A:3884:LEU:HD22	2.37	0.65
1:A:3998:ILE:HG21	1:A:4004:LEU:HG	1.79	0.65
1:A:2394:THR:H	1:A:2397:THR:HB	1.62	0.65
1:A:3737:THR:OG1	1:A:3740:THR:HB	1.97	0.65
1:A:1922:LYS:HE2	1:A:3999:ASP:O	1.97	0.65
1:B:3777:VAL:CG1	1:B:3895:PHE:CE1	2.68	0.65
1:B:1620:PHE:HA	1:B:1760:PHE:HE1	1.61	0.65
1:B:1983:LEU:HD21	1:B:1993:THR:O	1.94	0.65
1:B:3459:ASP:OD2	1:B:3461:ILE:HG12	1.97	0.64
1:B:2563:SER:HB2	1:B:2566:SER:OG	1.97	0.64
1:A:1783:THR:CG2	1:A:1809:PHE:CZ	2.80	0.64
1:B:1540:LEU:HD12	1:B:1548:ILE:CD1	2.27	0.64
1:B:2637:PRO:O	1:B:2639:GLN:NE2	2.30	0.64
1:B:1826:PHE:HZ	1:B:1831:LEU:HB2	1.53	0.64
1:B:3509:LEU:CD1	1:B:3513:VAL:HG21	2.27	0.64
1:B:2655:ILE:HD11	1:B:2747:ARG:HH22	1.62	0.64
1:A:113:ASP:O	1:A:115:GLU:N	2.31	0.64
1:A:1645:PHE:CG	1:A:1765:ILE:HG22	2.31	0.64
1:B:2282:ASN:HB3	1:B:2552:ARG:HG3	1.80	0.64
1:A:2362:ALA:HB3	1:A:2365:LYS:O	1.97	0.64
1:A:2203:THR:HG22	1:A:2205:ALA:H	1.62	0.64
1:A:1425:GLU:OE2	1:A:1429:LEU:CD1	2.45	0.64
1:A:1645:PHE:CD2	1:A:1765:ILE:HG22	2.32	0.64
1:A:2293:HIS:CE1	1:A:2409:ASN:HB3	2.33	0.64
1:A:3797:THR:HG23	1:A:3840:LEU:HD21	1.79	0.64
1:A:2134:LEU:CD1	1:A:2138:ASN:ND2	2.60	0.64
1:B:2574:TYR:HE2	3:B:5094:ADP:C2	2.16	0.64
1:A:2475:PRO:C	1:A:2476:LYS:HD2	2.18	0.64
1:B:2755:HIS:NE2	1:B:2835:LEU:HG	2.13	0.64
1:A:2336:ARG:HD2	1:A:2355:ASP:OD2	1.97	0.64
1:B:2765:GLY:HA2	5:B:5096:SO4:O2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1953:LEU:CD1	1:A:1973:LEU:HB3	2.28	0.64
1:B:2080:LYS:CD	1:B:2195:GLU:HB2	2.25	0.64
1:B:1391:GLY:HA3	1:B:1484:LYS:NZ	2.13	0.64
1:A:1774:LEU:HD21	1:A:1922:LYS:O	1.97	0.64
1:B:2458:LEU:HD11	1:B:2484:LEU:HD11	1.79	0.64
1:B:1495:THR:HG22	1:B:1497:ILE:HG22	1.80	0.64
1:B:1493:LEU:O	1:B:1494:ASP:HB2	1.96	0.64
1:B:1852:ARG:HG3	1:B:1852:ARG:O	1.98	0.63
1:B:2225:LYS:HA	2:B:5093:ATP:N3	2.13	0.63
1:B:3964:ALA:HB2	1:B:3993:VAL:HG11	1.80	0.63
1:A:1871:GLY:HA3	1:A:1879:ILE:HG21	1.79	0.63
1:B:1991:GLU:O	1:B:1995:VAL:HG23	1.98	0.63
1:B:2064:GLN:OE1	1:B:2191:ARG:HD2	1.98	0.63
1:B:2141:ILE:HG22	1:B:2145:PHE:CB	2.26	0.63
1:B:4020:ASN:HB3	1:B:4028:ARG:NH1	2.14	0.63
1:B:2336:ARG:HD3	1:B:2355:ASP:OD2	1.97	0.63
1:B:3851:VAL:HG13	1:B:3855:LEU:HD23	1.80	0.63
1:B:3460:PRO:O	1:B:3463:SER:CB	2.44	0.63
1:B:2111:LYS:HZ2	1:B:2161:GLU:HG2	1.63	0.63
1:A:1425:GLU:OE2	1:A:1429:LEU:HD11	1.98	0.63
1:A:1965:HIS:CD2	1:A:2212:LEU:HD21	2.33	0.63
1:A:2095:ASP:CG	1:A:2149:ARG:NH2	2.51	0.63
1:A:1536:ARG:N	1:A:1841:ILE:HD11	2.13	0.63
1:A:2426:MET:HG3	1:A:2427:ILE:N	2.11	0.63
1:A:2757:MET:CG	1:A:2889:PHE:CD2	2.80	0.63
1:B:1849:GLU:HG2	1:B:1899:ASN:ND2	2.14	0.63
1:A:2266:PHE:HD1	1:A:2326:LEU:HD21	1.64	0.63
1:A:3810:SER:O	1:A:3838:TRP:HB2	1.97	0.63
1:B:3886:ALA:N	1:B:3887:PRO:HD2	2.13	0.63
1:A:1704:GLU:OE2	1:A:1768:ARG:NH1	2.32	0.63
1:A:1706:LEU:HD22	1:A:1935:GLN:HG2	1.81	0.63
1:A:3979:ASN:O	1:A:3981:PRO:HD2	1.99	0.62
1:B:3810:SER:O	1:B:3838:TRP:HB2	1.97	0.62
1:A:2054:LEU:O	1:A:2058:MET:HG2	1.99	0.62
1:A:2620:ARG:NH1	1:A:2910:ASN:ND2	2.47	0.62
1:B:1750:SER:HB2	1:B:1755:LEU:CD2	2.29	0.62
1:B:2788:ARG:HB2	1:B:3459:ASP:HB3	1.80	0.62
1:B:3530:PHE:CE1	1:B:3618:TYR:CD2	2.87	0.62
1:B:2293:HIS:NE2	1:B:2409:ASN:HB3	2.14	0.62
1:A:1540:LEU:HD11	1:A:1548:ILE:HD11	1.82	0.62
1:B:1803:THR:HG21	1:B:1848:ASP:OD1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3641:PHE:HA	1:A:3889:LEU:HD21	1.82	0.62
1:B:2426:MET:HG3	1:B:2427:ILE:H	1.64	0.62
1:A:2578:ILE:HG21	1:A:2630:TYR:HB2	1.79	0.62
1:B:3330:TYR:OH	1:B:3346:LEU:HD22	1.98	0.62
1:B:2741:HIS:HA	1:B:2744:ARG:HD2	1.81	0.62
1:A:2840:ILE:HB	1:A:2843:LEU:HD22	1.81	0.62
1:A:3819:ILE:O	1:A:3823:ASN:HB2	1.99	0.62
1:A:3541:MET:HA	1:A:3544:LYS:HG2	1.81	0.62
1:B:162:LEU:HA	1:B:165:ASP:O	1.98	0.62
1:A:3951:SER:HB2	1:A:4002:LYS:HD2	1.81	0.62
1:A:2163:VAL:HA	1:A:2166:MET:HG2	1.82	0.62
1:B:3912:GLY:O	1:B:3915:PHE:CZ	2.53	0.62
1:B:2362:ALA:HB3	1:B:2365:LYS:O	2.00	0.62
1:B:2003:LEU:HA	1:B:2006:LEU:HD12	1.82	0.62
1:B:2080:LYS:HZ3	2:B:5093:ATP:PG	2.22	0.62
1:A:2940:PHE:HZ	1:A:2943:PHE:HE2	1.48	0.62
1:A:1849:GLU:HG2	1:A:1899:ASN:ND2	2.15	0.62
1:A:2728:LEU:HD12	1:A:2771:ARG:CZ	2.30	0.62
1:A:1646:GLN:NE2	1:A:1761:GLU:O	2.24	0.61
1:A:2536:ASN:HB2	1:A:2543:ARG:HE	1.65	0.61
1:A:1559:SER:HB3	1:A:1572:ILE:HG22	1.81	0.61
1:B:3819:ILE:O	1:B:3823:ASN:HB2	2.01	0.61
1:B:1531:ARG:HG2	1:B:1537:PHE:HB3	1.81	0.61
1:A:3871:PHE:HZ	1:A:3873:MET:HB2	1.64	0.61
1:B:2410:SER:C	1:B:2411:LYS:HG3	2.20	0.61
1:A:1645:PHE:CZ	1:A:1649:LEU:HD22	2.35	0.61
1:B:1534:PHE:CE2	1:B:1536:ARG:HB2	2.35	0.61
1:B:2276:LEU:HD23	1:B:2556:ILE:HG21	1.83	0.61
1:B:3308:ASN:O	1:B:3312:GLN:HB2	2.00	0.61
1:A:3566:LEU:CD2	1:A:3587:LEU:HD11	2.29	0.61
1:A:1540:LEU:CD1	1:A:1548:ILE:CD1	2.78	0.61
1:B:2426:MET:HG3	1:B:2427:ILE:N	2.15	0.61
1:A:2640:THR:HG23	1:A:2643:SER:H	1.66	0.61
1:B:1706:LEU:HD22	1:B:1935:GLN:HG2	1.83	0.61
1:B:1914:LYS:HD3	1:B:3959:CYS:SG	2.40	0.61
1:B:2386:MET:CB	1:B:2627:ARG:CD	2.77	0.61
1:A:1391:GLY:HA3	1:A:1484:LYS:NZ	2.15	0.61
1:B:3912:GLY:O	1:B:3915:PHE:CE2	2.54	0.61
1:A:2378:VAL:HG11	1:A:2392:ILE:HD12	1.81	0.61
1:B:1649:LEU:CD1	1:B:1704:GLU:HG3	2.31	0.61
1:B:2048:SER:H	2:B:5093:ATP:N6	1.97	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1802:LYS:NZ	5:A:5097:SO4:O2	2.34	0.61
1:B:3702:MET:HB3	1:B:3767:PHE:HZ	1.64	0.61
1:B:2707:VAL:CG1	1:B:2712:LEU:HD12	2.31	0.61
1:B:3303:LYS:HA	1:B:3306:TRP:HE1	1.62	0.61
1:A:1563:LYS:HD2	1:A:1570:GLU:HG3	1.82	0.61
1:B:2472:THR:HG21	1:B:2524:VAL:HG22	1.82	0.61
1:A:3737:THR:HB	1:A:3740:THR:CB	2.31	0.61
1:A:1783:THR:CG2	1:A:1809:PHE:CE1	2.83	0.61
1:A:2578:ILE:CG2	1:A:2630:TYR:HB2	2.31	0.61
1:A:3839:ILE:CG2	1:A:3873:MET:HG3	2.30	0.61
1:B:2336:ARG:HA	1:B:2339:ILE:HD12	1.82	0.61
1:B:2293:HIS:CE1	1:B:2409:ASN:HB3	2.36	0.61
1:A:2421:GLY:HA2	3:A:5094:ADP:O5'	2.00	0.61
1:A:2032:LYS:O	1:A:2035:VAL:HG12	2.00	0.61
1:B:2201:HIS:NE2	1:B:2497:TYR:O	2.34	0.61
1:B:2380:LEU:CD2	1:B:2384:GLU:OE1	2.37	0.61
1:A:2064:GLN:CD	1:A:2151:TRP:CH2	2.74	0.61
1:B:2481:ASN:HD21	1:B:2528:ARG:HD3	1.64	0.61
1:A:1900:PRO:HB3	1:A:1905:ARG:HA	1.82	0.61
1:B:2386:MET:HB3	1:B:2627:ARG:HD3	1.82	0.60
1:B:2835:LEU:HD23	1:B:2911:ARG:HB2	1.83	0.60
1:A:3583:LEU:O	1:A:3587:LEU:HG	2.00	0.60
1:A:3964:ALA:HB2	1:A:3993:VAL:HG11	1.84	0.60
1:B:2112:GLU:CB	1:B:2117:SER:HB2	2.20	0.60
1:B:3541:MET:HA	1:B:3544:LYS:HG2	1.82	0.60
1:A:3592:LYS:O	1:A:3596:ASN:HB2	2.01	0.60
1:B:2064:GLN:HE22	1:B:2070:LEU:HG	1.61	0.60
1:A:1911:ASN:OD1	1:A:1912:LEU:HG	2.01	0.60
1:A:2563:SER:CB	1:A:2566:SER:OG	2.49	0.60
1:B:3911:TRP:HH2	1:B:3926:VAL:HG12	1.66	0.60
1:B:1375:LYS:HE3	1:B:1431:LEU:HD13	1.83	0.60
1:B:1940:GLU:HG3	1:B:1941:ASP:N	2.16	0.60
1:B:1748:PHE:CD2	1:B:1755:LEU:HD22	2.37	0.60
1:B:2785:LYS:HD3	1:B:3482:GLY:O	2.01	0.60
1:B:2280:THR:HA	1:B:2283:LYS:HD2	1.84	0.60
1:B:2252:LEU:HD21	1:B:2310:LEU:HD23	1.83	0.60
1:B:1536:ARG:HD2	1:B:1565:MET:O	2.00	0.60
1:A:3683:TYR:O	1:A:3687:SER:HB2	2.02	0.60
1:A:1827:ASP:HB3	1:A:1830:VAL:HG12	1.84	0.60
1:A:2071:ILE:HB	1:A:2212:LEU:HD12	1.84	0.60
1:A:3690:LEU:HD23	1:A:3694:PHE:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3440:LEU:HD23	1:B:3462:ILE:HD12	1.83	0.60
1:B:1416:LYS:CB	1:B:1421:TYR:OH	2.50	0.60
1:B:3737:THR:OG1	1:B:3740:THR:HB	2.01	0.60
1:A:2784:PRO:HG2	1:A:2817:ILE:HD13	1.83	0.60
1:A:4033:LEU:HD12	1:A:4036:GLN:H	1.67	0.59
1:A:3656:VAL:CG1	1:A:3677:LEU:HB3	2.30	0.59
1:A:3850:TRP:NE1	1:A:3854:TYR:HB3	2.17	0.59
1:A:2081:THR:O	1:A:2085:LYS:HB2	2.01	0.59
1:B:3692:LYS:HE3	1:B:3898:GLU:HB3	1.83	0.59
1:A:2795:PHE:CE2	1:A:2799:LEU:HD11	2.37	0.59
1:A:2282:ASN:HB3	1:A:2552:ARG:HG3	1.84	0.59
1:A:2378:VAL:HG11	1:A:2392:ILE:CD1	2.32	0.59
1:A:3530:PHE:CE1	1:A:3618:TYR:CD2	2.90	0.59
1:A:1612:ASP:HA	1:A:1615:ILE:CD1	2.32	0.59
1:B:2833:THR:HG21	1:B:2841:PRO:HD2	1.83	0.59
1:B:1744:LEU:HD22	1:B:1760:PHE:CG	2.38	0.59
1:A:1462:ASN:HB2	1:A:1465:ILE:CG2	2.32	0.59
1:B:2394:THR:H	1:B:2397:THR:HB	1.66	0.59
1:B:2536:ASN:HB2	1:B:2543:ARG:HE	1.67	0.59
1:A:1995:VAL:HG22	1:A:2022:PHE:HE2	1.67	0.59
1:A:1620:PHE:CD1	1:A:1624:ARG:NH1	2.70	0.59
1:A:1826:PHE:HE1	1:A:1853:LEU:HD22	1.68	0.59
1:B:2127:ASP:O	1:B:2131:THR:OG1	2.21	0.59
1:A:3818:SER:O	1:A:3821:ASN:N	2.35	0.59
1:B:1616:LYS:NZ	1:B:1759:LYS:NZ	2.49	0.59
1:A:3813:ILE:HG22	1:A:3840:LEU:HD23	1.83	0.59
1:B:2072:LEU:HD23	1:B:2215:PHE:CE1	2.37	0.59
1:A:2111:LYS:HZ3	1:A:2161:GLU:HG2	1.67	0.59
1:A:1421:TYR:O	1:A:1425:GLU:N	2.36	0.59
1:A:2064:GLN:OE1	1:A:2151:TRP:HH2	1.85	0.59
1:A:3440:LEU:CD2	1:A:3462:ILE:HD12	2.32	0.59
1:A:1626:CYS:SG	1:A:1639:VAL:CG1	2.90	0.59
1:B:1683:LEU:HB3	1:B:1702:LEU:HD21	1.84	0.59
1:A:2620:ARG:HH12	1:A:2910:ASN:ND2	1.99	0.59
1:A:1917:ARG:HD2	1:A:3963:PHE:CE2	2.37	0.59
1:B:1422:LYS:HA	1:B:1425:GLU:HB2	1.85	0.59
1:A:1998:LEU:HD11	1:A:2022:PHE:HZ	1.68	0.59
1:B:2386:MET:HB3	1:B:2627:ARG:NE	2.18	0.59
1:B:1416:LYS:HA	1:B:1421:TYR:OH	2.01	0.59
1:B:2476:LYS:HZ1	1:B:2528:ARG:HD2	1.68	0.58
1:B:3353:LEU:HD23	1:B:3358:VAL:HG11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2293:HIS:NE2	1:A:2409:ASN:HB3	2.18	0.58
1:B:3017:VAL:HG21	1:B:3313:PHE:CE2	2.38	0.58
1:A:1996:GLU:O	1:A:2000:ARG:HG3	2.03	0.58
1:B:3671:VAL:O	1:B:3674:ILE:HG22	2.03	0.58
1:A:4024:VAL:HG11	1:A:4062:TRP:CD2	2.37	0.58
1:B:3700:MET:HB3	1:B:4085:THR:HG21	1.83	0.58
1:B:1620:PHE:HA	1:B:1760:PHE:CE1	2.37	0.58
1:B:2766:LYS:HE2	1:B:2890:THR:HB	1.85	0.58
1:A:3303:LYS:C	1:A:3306:TRP:CD1	2.72	0.58
1:B:1939:PHE:O	1:B:1940:GLU:HB3	2.03	0.58
1:B:2708:ASN:O	1:B:2712:LEU:HD13	2.04	0.58
1:B:2274:HIS:CE1	1:B:2326:LEU:O	2.52	0.58
1:A:3350:LYS:HA	1:A:3353:LEU:HD12	1.86	0.58
1:B:2967:ASN:HB3	1:B:3356:PHE:CE2	2.38	0.58
1:A:2107:LYS:CE	1:A:2495:ASP:OD2	2.51	0.58
1:A:3458:PHE:CZ	1:A:3459:ASP:O	2.57	0.58
1:A:1983:LEU:HD23	1:A:1993:THR:HG23	1.84	0.58
1:A:2002:ILE:HG22	1:A:2006:LEU:HD11	1.86	0.58
1:A:3017:VAL:HG21	1:A:3313:PHE:CE2	2.39	0.58
1:A:2336:ARG:HA	1:A:2339:ILE:HD12	1.84	0.58
1:A:1706:LEU:CD2	1:A:1935:GLN:HG2	2.34	0.58
1:A:2225:LYS:HG2	1:A:2229:LEU:HD12	1.85	0.58
1:A:1929:ILE:H	1:A:1929:ILE:HD12	1.69	0.58
1:A:1992:LYS:HG2	1:A:2024:SER:HB2	1.85	0.58
1:A:162:LEU:HA	1:A:165:ASP:O	2.03	0.58
1:A:2741:HIS:HA	1:A:2744:ARG:HD2	1.83	0.58
1:B:23:LEU:O	1:B:24:GLU:CB	2.52	0.58
1:B:3839:ILE:CG2	1:B:3873:MET:HG3	2.32	0.58
1:A:1469:LEU:HB3	1:A:1472:GLU:HB2	1.84	0.58
1:A:3636:GLY:HA2	1:A:3642:TYR:O	2.04	0.58
1:A:2111:LYS:HZ2	1:A:2161:GLU:HG2	1.69	0.58
1:B:2160:PRO:O	1:B:2164:GLU:HG3	2.04	0.58
1:B:2081:THR:HB	2:B:5093:ATP:PA	2.44	0.57
1:A:2295:ILE:HG12	1:A:2314:ILE:HD12	1.85	0.57
1:A:3912:GLY:O	1:A:3915:PHE:CZ	2.57	0.57
1:B:2080:LYS:CG	2:B:5093:ATP:O1B	2.51	0.57
1:B:1926:SER:HA	1:B:1970:LEU:HD12	1.84	0.57
1:B:1953:LEU:HD11	1:B:1973:LEU:HB3	1.84	0.57
1:A:1493:LEU:HD23	1:A:1498:GLU:CB	2.33	0.57
1:A:3728:GLU:HG3	1:A:4079:LYS:HE2	1.85	0.57
1:B:1967:HIS:O	1:B:1968:PHE:HD1	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2386:MET:CB	1:A:2627:ARG:CD	2.82	0.57
1:B:2745:ILE:HG23	1:B:2756:MET:HE3	1.85	0.57
1:A:2047:PHE:HB3	2:A:5093:ATP:N6	2.19	0.57
1:A:2445:PHE:HA	1:A:2449:THR:HG21	1.86	0.57
1:B:2391:VAL:CG2	1:B:2426:MET:HE3	2.34	0.57
1:A:3817:GLY:H	1:A:3821:ASN:HB2	1.69	0.57
1:B:3547:ASP:HA	1:B:3550:LYS:HB3	1.86	0.57
1:A:3851:VAL:HG13	1:A:3855:LEU:HD23	1.86	0.57
1:A:3671:VAL:HA	1:A:3674:ILE:HG22	1.86	0.57
1:B:2856:LEU:HD23	1:B:2873:LEU:HB3	1.86	0.57
1:A:2737:SER:HB2	1:A:2924:THR:HG21	1.87	0.57
1:B:2095:ASP:CG	1:B:2149:ARG:NH2	2.58	0.57
1:B:1421:TYR:O	1:B:1421:TYR:CD1	2.58	0.57
1:B:2571:TYR:HA	1:B:2574:TYR:HB2	1.85	0.57
1:B:1965:HIS:CD2	1:B:2212:LEU:HD21	2.39	0.57
1:A:3877:CYS:SG	1:A:3884:LEU:CD2	2.92	0.57
1:B:3845:GLN:OE1	1:B:3878:HIS:HB2	2.04	0.57
1:A:3945:LEU:O	1:A:3948:HIS:O	2.23	0.57
1:A:2064:GLN:CD	1:A:2151:TRP:HH2	2.08	0.57
1:B:2563:SER:CB	1:B:2566:SER:OG	2.52	0.57
1:A:1779:PHE:O	1:A:1783:THR:HG23	2.04	0.57
1:A:1849:GLU:CG	1:A:1899:ASN:HD22	2.17	0.57
1:A:3725:VAL:HG22	1:A:3731:ASP:HA	1.86	0.57
1:A:2490:ASN:HB3	1:A:2546:MET:CE	2.35	0.57
1:A:2127:ASP:O	1:A:2131:THR:OG1	2.23	0.57
1:B:3979:ASN:C	1:B:3981:PRO:HD2	2.25	0.57
1:B:2707:VAL:HB	1:B:2712:LEU:CD1	2.16	0.57
1:B:1534:PHE:HD2	1:B:1537:PHE:CE1	2.23	0.57
1:A:2368:PHE:O	1:A:2369:SER:OG	2.16	0.57
1:B:1416:LYS:HA	1:B:1421:TYR:CE1	2.34	0.57
1:B:3737:THR:HB	1:B:3740:THR:CB	2.34	0.57
1:B:1612:ASP:HA	1:B:1615:ILE:HD11	1.85	0.57
1:B:2072:LEU:HD23	1:B:2215:PHE:HE1	1.68	0.57
1:A:1794:PHE:CZ	1:A:1805:THR:HG21	2.39	0.57
1:B:1911:ASN:OD1	1:B:1912:LEU:N	2.38	0.57
1:A:1621:THR:CA	1:A:1624:ARG:NH1	2.66	0.57
1:A:2293:HIS:CE1	1:A:2409:ASN:CB	2.88	0.57
1:A:3449:VAL:HG22	1:A:3493:LYS:HB2	1.86	0.57
1:A:2280:THR:HA	1:A:2283:LYS:HD2	1.85	0.57
1:A:2060:PHE:HZ	1:A:2064:GLN:NE2	1.99	0.56
1:B:1469:LEU:HB3	1:B:1472:GLU:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:THR:O	1:A:66:GLN:CB	2.53	0.56
1:A:3530:PHE:HD1	1:A:3618:TYR:CD2	2.14	0.56
1:B:2060:PHE:CZ	1:B:2064:GLN:NE2	2.73	0.56
1:A:1497:ILE:O	1:A:1500:ILE:HG12	2.06	0.56
1:B:3631:MET:HE3	1:B:3698:MET:HG3	1.86	0.56
1:A:2758:LEU:HD23	1:A:2915:ASN:HB3	1.86	0.56
1:B:2320:ARG:NH1	1:B:2406:ASP:OD2	2.33	0.56
1:A:2581:LEU:HD13	1:A:2633:ILE:HG22	1.86	0.56
1:A:2201:HIS:CE1	1:A:2497:TYR:HA	2.39	0.56
1:A:3559:LEU:O	1:A:3563:GLU:HG3	2.06	0.56
1:A:2707:VAL:CG1	1:A:2712:LEU:HD12	2.35	0.56
1:A:1459:LEU:HD22	1:A:1473:THR:CG2	2.35	0.56
1:A:3519:VAL:HG13	1:A:3521:ASN:ND2	2.20	0.56
1:A:2332:GLY:HA2	1:A:2335:GLN:CB	2.34	0.56
1:A:1392:LEU:HD13	1:A:1393:LYS:C	2.26	0.56
1:B:3690:LEU:HD23	1:B:3694:PHE:HB3	1.88	0.56
1:B:3925:SER:HB2	1:B:3972:LEU:HD13	1.86	0.56
1:B:1416:LYS:CA	1:B:1421:TYR:CZ	2.71	0.56
1:A:2755:HIS:HB3	1:A:2912:CYS:SG	2.45	0.56
1:A:1463:LEU:HA	1:A:1466:GLN:CG	2.36	0.56
1:A:1922:LYS:HZ2	1:A:4004:LEU:CD1	2.19	0.56
1:A:3636:GLY:CA	1:A:3642:TYR:O	2.53	0.56
1:A:1794:PHE:HZ	1:A:1805:THR:HG21	1.71	0.56
1:B:1692:ASP:O	1:B:1695:LYS:HB3	2.05	0.56
1:B:2452:GLU:HA	1:B:2455:LEU:HD12	1.86	0.56
1:B:1741:LEU:O	1:B:1742:ASP:HB2	2.05	0.56
1:B:3995:GLY:HA2	1:B:3998:ILE:HD13	1.87	0.56
1:A:2389:ASP:HB3	1:A:2433:ARG:NH1	2.20	0.56
1:B:2707:VAL:HG12	1:B:2712:LEU:CD1	2.36	0.56
1:B:1823:ASP:HB2	1:B:1853:LEU:HD23	1.88	0.56
1:B:2755:HIS:CB	1:B:2911:ARG:O	2.48	0.56
1:B:2489:ILE:HD11	1:B:2506:LEU:HD13	1.87	0.56
1:B:1781:THR:HG21	1:B:1919:PHE:CE1	2.40	0.56
1:B:2838:ALA:HB3	1:B:2878:VAL:HG13	1.86	0.56
1:A:2387:ARG:O	1:A:2390:ILE:HG22	2.06	0.56
1:B:1726:LEU:CD1	1:B:3984:GLN:CB	2.77	0.56
1:A:3537:GLU:OE1	1:A:3618:TYR:OH	2.24	0.56
1:B:1802:LYS:NZ	5:B:5097:SO4:O3	2.39	0.56
1:A:3679:TYR:HB3	1:A:3767:PHE:HE1	1.71	0.56
1:B:1649:LEU:HD11	1:B:1704:GLU:HG3	1.87	0.56
1:A:3566:LEU:CD1	1:A:3570:LEU:HD11	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3481:ILE:O	1:A:3483:ASP:N	2.38	0.56
1:B:1416:LYS:HG2	1:B:1421:TYR:CZ	2.40	0.55
1:A:3303:LYS:CD	1:A:3306:TRP:CD1	2.80	0.55
1:A:1744:LEU:HA	1:A:1760:PHE:CD1	2.41	0.55
1:A:3810:SER:HB3	1:A:3837:GLY:HA2	1.86	0.55
1:B:3322:GLY:HA2	1:B:3325:ILE:HD12	1.88	0.55
1:B:3919:LYS:NZ	1:B:4038:GLU:CG	2.69	0.55
1:B:2391:VAL:HG23	1:B:2426:MET:HE1	1.88	0.55
1:A:2856:LEU:HD23	1:A:2873:LEU:HB3	1.88	0.55
1:A:1963:MET:HB3	1:A:1966:TYR:CD2	2.42	0.55
1:B:2391:VAL:CG2	1:B:2426:MET:CE	2.84	0.55
1:A:1646:GLN:CD	1:A:1763:ILE:HG12	2.27	0.55
1:A:1612:ASP:HA	1:A:1615:ILE:HD11	1.88	0.55
1:A:3569:GLU:O	1:A:3573:SER:OG	2.20	0.55
1:A:2757:MET:CE	1:A:2908:LEU:HB3	2.37	0.55
1:B:1983:LEU:CG	1:B:1993:THR:CG2	2.75	0.55
1:B:3583:LEU:O	1:B:3587:LEU:HG	2.06	0.55
1:A:2339:ILE:HG23	1:A:2353:LEU:HB3	1.88	0.55
1:B:2391:VAL:HG23	1:B:2426:MET:CE	2.36	0.55
1:B:2002:ILE:HB	1:B:2014:PHE:CE2	2.42	0.55
1:A:1559:SER:HB2	1:A:1572:ILE:H	1.71	0.55
1:A:3628:ILE:HG22	1:A:3649:PHE:HE2	1.72	0.55
1:A:2318:ILE:O	1:A:2322:LEU:HB2	2.07	0.55
1:A:1660:VAL:HG13	1:A:1728:TRP:CH2	2.41	0.55
1:B:1744:LEU:HD22	1:B:1760:PHE:CD2	2.41	0.55
1:A:1493:LEU:CD2	1:A:1498:GLU:HB3	2.36	0.55
1:A:2229:LEU:HD11	1:A:2285:GLU:HG3	1.88	0.55
1:B:1396:ARG:HG3	1:B:1397:GLU:H	1.71	0.55
1:A:2152:VAL:HG12	1:A:2154:PHE:CE1	2.35	0.55
1:B:1392:LEU:HD13	1:B:1393:LYS:C	2.27	0.55
1:A:1851:ASN:ND2	1:A:1899:ASN:O	2.39	0.55
1:B:2481:ASN:ND2	1:B:2528:ARG:HD3	2.22	0.55
1:A:2163:VAL:HA	1:A:2166:MET:CG	2.36	0.55
1:B:1394:LEU:HD22	1:B:1449:GLN:NE2	2.21	0.55
1:A:1826:PHE:O	1:A:1826:PHE:CG	2.60	0.55
1:B:3645:SER:CB	1:B:3890:GLN:NE2	2.69	0.55
1:A:2252:LEU:HD21	1:A:2310:LEU:HD23	1.89	0.55
1:A:2095:ASP:CG	1:A:2149:ARG:HH22	2.10	0.55
1:A:2420:PRO:HD3	1:A:2536:ASN:HD21	1.72	0.55
1:B:1826:PHE:HZ	1:B:1831:LEU:CB	2.15	0.55
1:A:3566:LEU:HD13	1:A:3570:LEU:CD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3323:ASN:HD21	1:A:3361:ASP:H	1.54	0.55
1:A:3555:TYR:HE1	1:A:3593:GLU:HG2	1.71	0.55
1:A:3612:ASP:O	1:A:3615:VAL:HG22	2.06	0.55
1:B:2380:LEU:HD13	1:B:2390:ILE:CD1	2.21	0.55
1:B:1575:LEU:O	1:B:1576:GLU:HB3	2.06	0.55
1:B:2391:VAL:HG21	1:B:2426:MET:HE3	1.88	0.55
1:A:1660:VAL:CG1	1:A:1728:TRP:CH2	2.90	0.55
1:A:3911:TRP:HH2	1:A:3926:VAL:CG1	2.20	0.55
1:A:3785:TYR:HE2	1:A:3859:VAL:HG22	1.72	0.55
1:B:2470:GLY:C	1:B:2473:LEU:HD11	2.27	0.54
1:B:3330:TYR:CE1	1:B:3334:PHE:CD2	2.96	0.54
1:B:3440:LEU:CD2	1:B:3462:ILE:HD12	2.36	0.54
1:B:3951:SER:HB2	1:B:4002:LYS:HD2	1.87	0.54
1:B:1707:HIS:O	1:B:1711:VAL:HG23	2.07	0.54
1:A:2786:ILE:HG12	1:A:2821:ASN:HA	1.89	0.54
1:B:2266:PHE:HD1	1:B:2326:LEU:HD21	1.71	0.54
1:B:2173:ASN:HB3	1:B:2175:ILE:HG22	1.89	0.54
1:B:2109:LEU:CD1	1:B:2129:LEU:HD23	2.37	0.54
1:B:1527:LEU:HD21	1:B:1546:LEU:HD21	1.89	0.54
1:B:2786:ILE:O	1:B:3460:PRO:HB2	2.06	0.54
1:B:1995:VAL:HG21	1:B:2024:SER:HB3	1.89	0.54
1:A:2081:THR:OG1	1:A:2195:GLU:OE2	2.26	0.54
1:A:2637:PRO:O	1:A:2639:GLN:NE2	2.40	0.54
1:B:3010:LEU:HD21	1:B:3317:SER:HB3	1.90	0.54
1:A:2475:PRO:O	1:A:2476:LYS:C	2.46	0.54
1:A:2842:ASP:O	1:A:2845:GLN:HG2	2.08	0.54
1:B:3612:ASP:O	1:B:3615:VAL:HG22	2.05	0.54
1:B:1620:PHE:CB	1:B:1760:PHE:CE1	2.91	0.54
1:A:2786:ILE:O	1:A:3460:PRO:HB2	2.07	0.54
1:B:3406:PHE:HB2	1:B:3513:VAL:HG12	1.85	0.54
1:B:3924:TRP:O	1:B:3927:TYR:HB3	2.07	0.54
1:A:1649:LEU:HD13	1:A:1704:GLU:HG3	1.87	0.54
1:B:2472:THR:HG22	1:B:2524:VAL:HG13	1.88	0.54
1:A:3406:PHE:CZ	1:A:3505:ILE:HG21	2.42	0.54
1:A:3912:GLY:O	1:A:3915:PHE:CE2	2.61	0.54
1:B:2787:HIS:HB3	1:B:3461:ILE:HG23	1.90	0.54
1:B:1416:LYS:HA	1:B:1421:TYR:CE2	2.36	0.54
1:A:1649:LEU:HD11	1:A:1704:GLU:HG3	1.87	0.54
1:A:3995:GLY:HA2	1:A:3998:ILE:HD13	1.90	0.54
1:B:1748:PHE:HD2	1:B:1755:LEU:HD22	1.73	0.54
1:A:1540:LEU:CD1	1:A:1548:ILE:HD11	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3930:PHE:HE2	1:B:4029:ILE:HD13	1.71	0.54
1:A:1956:LEU:HB3	1:A:1968:PHE:HE2	1.72	0.54
1:A:1425:GLU:OE2	1:A:1429:LEU:CD2	2.56	0.54
1:B:2447:LYS:HE3	1:B:2493:LYS:HD3	1.90	0.54
1:A:3935:PHE:HB2	1:A:4014:VAL:HG11	1.89	0.54
1:B:2074:GLY:O	1:B:2197:ASP:HA	2.08	0.54
1:B:1813:LEU:HD12	1:B:1844:TRP:HH2	1.73	0.54
1:B:3537:GLU:OE1	1:B:3618:TYR:OH	2.25	0.54
1:A:1698:ILE:O	1:A:1702:LEU:HG	2.08	0.54
1:A:2354:SER:OG	1:A:2357:SER:HB2	2.08	0.54
1:A:3757:ILE:HD11	1:A:4074:GLU:HG2	1.90	0.54
1:B:3935:PHE:HB2	1:B:4014:VAL:HG11	1.90	0.54
1:B:2728:LEU:HD12	1:B:2771:ARG:CZ	2.37	0.53
1:A:2513:GLN:O	1:A:2526:ILE:HG13	2.09	0.53
1:B:2737:SER:HB2	1:B:2924:THR:HG21	1.90	0.53
1:A:1743:ASP:HA	1:A:1746:SER:HB3	1.90	0.53
1:B:2755:HIS:CE1	1:B:2835:LEU:HG	2.43	0.53
1:A:4074:GLU:HA	1:A:4077:GLN:HE21	1.73	0.53
1:B:2758:LEU:HD23	1:B:2915:ASN:HB3	1.89	0.53
1:A:1939:PHE:HD1	1:A:1939:PHE:H	1.56	0.53
1:A:1911:ASN:OD1	1:A:1912:LEU:N	2.41	0.53
1:B:2131:THR:HG22	1:B:2176:LEU:CD2	2.38	0.53
1:B:1540:LEU:HD11	1:B:1561:PHE:HB3	1.91	0.53
1:A:2451:THR:O	1:A:2455:LEU:HD12	2.08	0.53
1:A:2437:LEU:H	1:A:2437:LEU:HD12	1.73	0.53
1:B:1421:TYR:CD1	1:B:1421:TYR:C	2.82	0.53
1:A:3845:GLN:OE1	1:A:3878:HIS:HB2	2.08	0.53
1:A:1783:THR:HG23	1:A:1809:PHE:CE1	2.44	0.53
1:B:2842:ASP:O	1:B:2845:GLN:HG2	2.08	0.53
1:B:3566:LEU:CA	1:B:3583:LEU:HD21	2.36	0.53
1:A:2177:THR:HG22	1:A:2183:ARG:HG2	1.89	0.53
1:A:1922:LYS:NZ	1:A:4004:LEU:CD1	2.71	0.53
1:A:2336:ARG:CD	1:A:2355:ASP:OD2	2.57	0.53
1:A:2358:THR:HG22	1:A:2359:ILE:N	2.22	0.53
1:B:2047:PHE:CE2	1:B:2082:ALA:HB1	2.44	0.53
1:A:2222:ILE:HG23	1:A:2284:LEU:HD11	1.90	0.53
1:B:1620:PHE:CA	1:B:1760:PHE:CE1	2.91	0.53
1:B:3303:LYS:C	1:B:3306:TRP:CD1	2.74	0.53
1:B:2220:CYS:SG	1:B:2224:SER:HB3	2.49	0.53
1:A:1394:LEU:HD22	1:A:1449:GLN:NE2	2.23	0.53
1:B:2437:LEU:H	1:B:2437:LEU:HD12	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2780:LYS:HD3	1:B:2813:THR:HG22	1.90	0.53
1:B:3525:ILE:HD11	1:B:3646:ILE:CG2	2.26	0.53
1:A:1748:PHE:CD2	1:A:1755:LEU:HD22	2.44	0.53
1:A:1970:LEU:HD12	1:A:1973:LEU:CD1	2.38	0.53
1:B:3534:LEU:HD11	1:B:3614:LEU:HD23	1.90	0.53
1:A:1620:PHE:CE2	1:A:1743:ASP:HB3	2.43	0.53
1:B:1926:SER:CA	1:B:1970:LEU:HD12	2.39	0.53
1:B:1612:ASP:HA	1:B:1615:ILE:HG12	1.91	0.53
1:B:3785:TYR:CE2	1:B:3859:VAL:HG22	2.43	0.53
1:B:1396:ARG:HG3	1:B:1397:GLU:N	2.24	0.53
1:A:2655:ILE:HD11	1:A:2747:ARG:HH22	1.74	0.53
1:A:1367:ILE:H	1:A:1367:ILE:HD12	1.73	0.53
1:A:2060:PHE:HZ	1:A:2064:GLN:HE21	1.51	0.52
1:A:2137:VAL:O	1:A:2141:ILE:CG2	2.55	0.52
1:A:1387:GLU:HA	1:A:1393:LYS:HA	1.91	0.52
1:A:2967:ASN:HB3	1:A:3356:PHE:CE2	2.44	0.52
1:A:1967:HIS:C	1:A:1968:PHE:HD1	2.13	0.52
1:B:2111:LYS:HZ3	1:B:2161:GLU:HG2	1.75	0.52
1:A:2084:TRP:HE3	1:A:2088:ILE:HD12	1.74	0.52
1:A:2463:ASN:CB	1:A:2477:SER:HA	2.39	0.52
1:B:2620:ARG:NH1	1:B:2910:ASN:ND2	2.56	0.52
1:B:3429:LEU:HD21	1:B:3439:ARG:HB3	1.90	0.52
1:A:3547:ASP:HA	1:A:3550:LYS:HB3	1.90	0.52
1:A:2494:LEU:HD12	1:A:2495:ASP:O	2.08	0.52
1:B:2386:MET:HB3	1:B:2627:ARG:CD	2.37	0.52
1:B:2081:THR:O	1:B:2085:LYS:HB2	2.09	0.52
1:B:2276:LEU:HD21	1:B:2415:ILE:HG21	1.91	0.52
1:A:2421:GLY:N	3:A:5094:ADP:O2B	2.35	0.52
1:B:2034:ILE:HD12	1:B:2061:TYR:CZ	2.45	0.52
1:B:2788:ARG:HG3	1:B:3459:ASP:HA	1.90	0.52
1:B:1422:LYS:O	1:B:1425:GLU:CB	2.48	0.52
1:B:1531:ARG:HG2	1:B:1537:PHE:CB	2.39	0.52
1:A:2441:VAL:HG21	1:A:2482:LEU:HD21	1.91	0.52
1:B:3306:TRP:HH2	1:B:3594:ALA:HB1	1.73	0.52
1:A:2151:TRP:HE3	1:A:2193:LEU:HD11	1.75	0.52
1:B:2332:GLY:HA2	1:B:2335:GLN:CB	2.35	0.52
1:B:3919:LYS:NZ	1:B:4038:GLU:HG3	2.25	0.52
1:B:3330:TYR:CD1	1:B:3334:PHE:CD2	2.98	0.52
1:B:1616:LYS:HZ1	1:B:1759:LYS:NZ	2.07	0.52
1:B:1965:HIS:HD2	1:B:2212:LEU:CD2	2.21	0.52
1:B:3736:LEU:HD11	1:B:3745:ARG:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1635:ASP:HB2	1:B:1638:VAL:HG23	1.91	0.52
1:B:1563:LYS:HE2	1:B:1585:VAL:HG12	1.90	0.52
1:A:2476:LYS:H	1:A:2476:LYS:HD2	1.64	0.52
1:A:1535:PRO:HB2	1:A:1841:ILE:CG1	2.33	0.52
1:B:2293:HIS:CE1	1:B:2409:ASN:CB	2.92	0.52
1:B:1706:LEU:CD1	1:B:1936:ILE:HG12	2.40	0.52
1:B:1703:VAL:HG13	1:B:1770:ILE:HD13	1.91	0.52
1:A:2382:ALA:O	1:A:2385:VAL:HG12	2.10	0.52
1:B:2476:LYS:HZ2	1:B:2528:ARG:HD2	1.72	0.52
1:A:3978:ASN:O	1:A:3981:PRO:CD	2.57	0.52
1:B:1493:LEU:HD23	1:B:1498:GLU:CB	2.39	0.52
1:A:2448:ASP:O	1:A:2829:GLU:OE2	2.27	0.52
1:B:1900:PRO:HB3	1:B:1905:ARG:HA	1.92	0.52
1:A:2489:ILE:HD11	1:A:2506:LEU:HD13	1.92	0.52
1:A:3303:LYS:HA	1:A:3306:TRP:HE1	1.68	0.52
1:A:1991:GLU:O	1:A:1994:VAL:HB	2.10	0.52
1:B:1926:SER:HB2	1:B:1970:LEU:HD12	1.92	0.52
1:B:2941:THR:HG22	1:B:2942:ASP:N	2.24	0.52
1:B:2640:THR:HG23	1:B:2643:SER:H	1.75	0.52
1:B:1448:VAL:HG22	1:B:1513:ILE:HB	1.92	0.52
1:B:2846:GLY:O	1:B:2849:TYR:HB3	2.10	0.52
1:A:2320:ARG:NH1	1:A:2406:ASP:OD2	2.32	0.52
1:B:1970:LEU:HD23	1:B:1974:LYS:HE3	1.92	0.52
1:B:2305:LEU:HB3	1:B:2310:LEU:HD12	1.92	0.52
1:A:3737:THR:CB	1:A:3740:THR:CB	2.87	0.51
1:A:2181:GLY:O	1:A:2182:GLU:CG	2.58	0.51
1:A:1502:ILE:HG23	1:A:1503:PRO:HD2	1.91	0.51
1:B:1493:LEU:HD23	1:B:1498:GLU:HB2	1.91	0.51
1:A:1559:SER:CB	1:A:1572:ILE:HG22	2.39	0.51
1:B:3372:THR:HG23	1:B:3375:GLU:HB2	1.91	0.51
1:A:1995:VAL:CG1	1:A:2018:LEU:HD21	2.40	0.51
1:B:2228:HIS:HB3	2:B:5093:ATP:C2	2.44	0.51
1:A:1493:LEU:O	1:A:1494:ASP:HB2	2.10	0.51
1:B:1771:TYR:HA	1:B:1775:LEU:HD13	1.92	0.51
1:B:1983:LEU:HD21	1:B:1996:GLU:HB2	1.92	0.51
1:B:2494:LEU:HB2	1:B:2499:SER:N	2.25	0.51
1:A:3737:THR:CB	1:A:3740:THR:HB	2.40	0.51
1:A:1983:LEU:HD23	1:A:1993:THR:HG22	1.92	0.51
1:A:2078:CYS:N	2:A:5093:ATP:O2B	2.41	0.51
1:A:3330:TYR:CE2	1:A:3346:LEU:HD13	2.45	0.51
1:A:3911:TRP:HH2	1:A:3926:VAL:HG12	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2792:LEU:HD13	1:B:2826:ALA:HB3	1.92	0.51
1:A:3458:PHE:CD1	1:A:3459:ASP:O	2.63	0.51
1:A:3509:LEU:HD11	1:A:3513:VAL:HG21	1.89	0.51
1:B:2225:LYS:HA	2:B:5093:ATP:H2	1.71	0.51
1:A:1536:ARG:HD3	1:A:1841:ILE:CD1	2.40	0.51
1:A:1771:TYR:HA	1:A:1775:LEU:HD13	1.92	0.51
1:A:2494:LEU:O	1:A:2495:ASP:O	2.29	0.51
1:A:3566:LEU:CA	1:A:3583:LEU:HD21	2.39	0.51
1:A:2386:MET:HB3	1:A:2627:ARG:CD	2.40	0.51
1:B:3923:VAL:CG2	1:B:4038:GLU:HA	2.39	0.51
1:A:3541:MET:HB2	1:A:3607:PHE:HE1	1.74	0.51
1:B:2276:LEU:HD23	1:B:2556:ILE:CG2	2.41	0.51
1:A:2965:VAL:HG13	1:A:3325:ILE:HD11	1.92	0.51
1:A:1574:PHE:HB3	1:A:1576:GLU:H	1.75	0.51
1:A:2055:LYS:HE3	1:A:2056:LYS:HE2	1.93	0.51
1:A:1394:LEU:CD2	1:A:1449:GLN:HE22	2.22	0.51
1:A:1849:GLU:CD	1:A:1899:ASN:HD22	2.14	0.51
1:A:3728:GLU:CG	1:A:4079:LYS:HE2	2.40	0.51
1:A:1650:LEU:O	1:A:1654:VAL:HG23	2.11	0.51
1:B:2064:GLN:NE2	1:B:2070:LEU:CG	2.67	0.51
1:A:3998:ILE:HG22	1:A:4004:LEU:HG	1.92	0.51
1:B:4024:VAL:HG11	1:B:4062:TRP:CD2	2.46	0.51
1:B:1917:ARG:HD2	1:B:3963:PHE:CE2	2.46	0.51
1:A:2378:VAL:HG21	1:A:2380:LEU:HD13	1.89	0.51
1:A:2102:TYR:HB2	1:A:2152:VAL:HG22	1.93	0.51
1:A:1744:LEU:HD22	1:A:1760:PHE:CD1	2.45	0.51
1:A:1940:GLU:HG3	1:A:1941:ASP:H	1.76	0.51
1:A:1826:PHE:O	1:A:1826:PHE:CD1	2.63	0.51
1:B:1514:ASP:O	1:B:1518:MET:HG2	2.11	0.51
1:B:1826:PHE:HZ	1:B:1831:LEU:CA	2.24	0.51
1:A:3737:THR:OG1	1:A:3740:THR:CB	2.58	0.51
1:B:3530:PHE:CE1	1:B:3618:TYR:HD2	2.26	0.50
1:A:2446:SER:H	1:A:2449:THR:HG21	1.76	0.50
1:A:3817:GLY:H	1:A:3821:ASN:CB	2.24	0.50
1:A:1703:VAL:HG13	1:A:1770:ILE:HD13	1.91	0.50
1:A:2425:THR:HG22	1:A:2485:PHE:HE2	1.77	0.50
1:A:2039:LYS:HG2	1:A:2049:MET:HG3	1.93	0.50
1:B:2378:VAL:HG22	1:B:2380:LEU:HG	1.92	0.50
1:B:2578:ILE:CG2	1:B:2630:TYR:HB2	2.41	0.50
1:A:3924:TRP:O	1:A:3927:TYR:HB3	2.11	0.50
1:A:2762:SER:O	1:A:2763:ARG:CB	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2517:LYS:HG2	1:B:2520:GLU:HB2	1.93	0.50
1:B:2262:LEU:HA	1:B:2265:ILE:HD12	1.93	0.50
1:B:1606:GLU:O	1:B:1610:ILE:HG12	2.11	0.50
1:B:1998:LEU:HD11	1:B:2022:PHE:HZ	1.76	0.50
1:A:1425:GLU:OE2	1:A:1429:LEU:HD21	2.12	0.50
1:B:1849:GLU:CD	1:B:1899:ASN:HD22	2.15	0.50
1:B:1803:THR:HG21	1:B:1848:ASP:CG	2.32	0.50
1:A:4059:LEU:HA	1:A:4063:LEU:HD13	1.94	0.50
1:B:1469:LEU:HD13	1:B:1523:LEU:CD2	2.41	0.50
1:B:2860:THR:HG22	1:B:2865:LEU:O	2.11	0.50
1:B:2382:ALA:O	1:B:2385:VAL:HG12	2.11	0.50
1:A:2488:GLU:CG	1:A:2491:LEU:HD12	2.42	0.50
1:B:2493:LYS:HG3	1:B:2494:LEU:H	1.76	0.50
1:A:3010:LEU:HD22	1:A:3320:LEU:HD12	1.94	0.50
1:B:1750:SER:HB2	1:B:1755:LEU:HD23	1.93	0.50
1:A:2257:PHE:HD1	1:A:2262:LEU:HD11	1.77	0.50
1:A:3429:LEU:HD21	1:A:3439:ARG:HB3	1.93	0.50
1:A:2380:LEU:HD23	1:A:2384:GLU:HB3	1.94	0.50
1:B:3461:ILE:C	1:B:3463:SER:H	2.14	0.50
1:A:1645:PHE:HB3	1:A:1765:ILE:HG21	1.90	0.50
1:A:3509:LEU:CD1	1:A:3513:VAL:CG2	2.76	0.50
1:B:1910:GLU:HB2	1:B:3846:MET:CB	2.42	0.50
1:B:3612:ASP:O	1:B:3615:VAL:CG2	2.60	0.50
1:B:3338:ASN:HD22	1:B:3341:GLU:HG2	1.76	0.50
1:B:1744:LEU:HA	1:B:1760:PHE:HE2	1.68	0.50
1:B:1849:GLU:HG2	1:B:1899:ASN:HD22	1.76	0.50
1:B:1646:GLN:NE2	1:B:1758:TYR:OH	2.45	0.50
1:A:1826:PHE:CE1	1:A:1853:LEU:CD2	2.94	0.50
1:A:2755:HIS:CE1	1:A:2835:LEU:HG	2.47	0.50
1:B:1981:SER:HB3	1:B:1982:PRO:HD3	1.93	0.50
1:B:3459:ASP:OD2	1:B:3461:ILE:CG1	2.60	0.50
1:A:1995:VAL:HG22	1:A:2022:PHE:CD2	2.47	0.50
1:A:4023:ILE:HD11	1:A:4029:ILE:HD12	1.93	0.50
1:A:2228:HIS:HB3	2:A:5093:ATP:C2	2.47	0.50
1:A:4065:LEU:HD12	1:A:4065:LEU:C	2.32	0.50
1:B:2448:ASP:HB2	1:B:2829:GLU:CD	2.32	0.50
1:B:2428:MET:SD	1:B:2428:MET:C	2.90	0.50
1:A:1969:GLY:O	1:A:1972:THR:HB	2.11	0.50
1:B:3330:TYR:CE1	1:B:3334:PHE:CE2	2.99	0.50
1:A:2201:HIS:NE2	1:A:2497:TYR:O	2.45	0.50
1:A:3628:ILE:HG22	1:A:3649:PHE:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3848:LEU:HD21	1:A:3852:LYS:HE3	1.93	0.50
1:A:2788:ARG:HB2	1:A:3459:ASP:HB3	1.94	0.50
1:B:2761:ALA:O	1:B:2892:CYS:SG	2.70	0.50
1:A:2654:ARG:NH1	1:A:2658:ASP:OD1	2.44	0.50
1:B:2960:THR:HB	1:B:2963:ASP:HB2	1.93	0.50
1:B:2786:ILE:HG12	1:B:2821:ASN:HA	1.94	0.49
1:B:2002:ILE:HG22	1:B:2006:LEU:HD11	1.94	0.49
1:B:2252:LEU:HD22	1:B:2314:ILE:HG13	1.94	0.49
1:B:3787:THR:HG22	1:B:3875:MET:HB2	1.94	0.49
1:A:1604:ALA:HA	1:A:1607:TRP:HE1	1.75	0.49
1:A:2339:ILE:HG12	1:A:2353:LEU:HD23	1.94	0.49
1:A:3818:SER:O	1:A:3820:GLU:N	2.45	0.49
1:A:2109:LEU:HB3	1:A:2113:SER:HB2	1.94	0.49
1:B:3323:ASN:HD21	1:B:3361:ASP:H	1.60	0.49
1:B:2467:THR:CB	1:B:2473:LEU:HD22	2.40	0.49
1:B:1929:ILE:HD12	1:B:1929:ILE:H	1.77	0.49
1:A:3566:LEU:HD13	1:A:3570:LEU:HD11	1.94	0.49
1:B:3854:TYR:O	1:B:3858:HIS:HB2	2.11	0.49
1:A:2758:LEU:HD22	1:A:2917:MET:SD	2.52	0.49
1:B:1394:LEU:CD2	1:B:1449:GLN:HE22	2.25	0.49
1:B:2822:ILE:O	1:B:2822:ILE:CG1	2.38	0.49
1:A:1645:PHE:HZ	1:A:1768:ARG:HD2	1.76	0.49
1:B:1616:LYS:HZ2	1:B:1759:LYS:CE	2.19	0.49
1:B:2476:LYS:N	1:B:2476:LYS:CD	2.74	0.49
1:B:2574:TYR:CE2	3:B:5094:ADP:C2	2.98	0.49
1:B:3737:THR:CB	1:B:3740:THR:CB	2.90	0.49
1:A:1940:GLU:CB	1:A:1989:GLU:O	2.53	0.49
1:A:3930:PHE:HE2	1:A:4029:ILE:CD1	2.26	0.49
1:B:1540:LEU:HD11	1:B:1548:ILE:HD11	1.95	0.49
1:A:23:LEU:O	1:A:25:GLU:N	2.45	0.49
1:B:2181:GLY:O	1:B:2182:GLU:HG3	2.12	0.49
1:A:2575:TYR:HD1	1:A:2578:ILE:HD11	1.78	0.49
1:A:3844:ILE:HG12	1:A:3851:VAL:HG21	1.93	0.49
1:B:1620:PHE:CZ	1:B:1743:ASP:HB3	2.48	0.49
3:B:5094:ADP:N3	3:B:5094:ADP:H2'	2.27	0.49
1:A:2476:LYS:O	1:A:2476:LYS:HD3	2.11	0.49
1:B:2080:LYS:CE	2:B:5093:ATP:O3G	2.60	0.49
1:B:3785:TYR:HE2	1:B:3859:VAL:HG22	1.77	0.49
1:A:3671:VAL:O	1:A:3674:ILE:HG22	2.12	0.49
1:A:3785:TYR:CE2	1:A:3859:VAL:HG22	2.46	0.49
1:A:1448:VAL:HG22	1:A:1513:ILE:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3579:GLU:O	1:B:3582:GLU:N	2.44	0.49
1:B:3409:ASP:HB3	1:B:3518:PHE:HB2	1.93	0.49
1:B:3897:TYR:CZ	1:B:3899:ASP:HB3	2.48	0.49
1:A:2582:VAL:O	1:A:2582:VAL:HG23	2.13	0.49
2:B:5093:ATP:O3G	2:B:5093:ATP:O1B	2.30	0.49
1:A:2076:ALA:HB2	1:A:2549:ARG:HG2	1.94	0.49
1:A:1459:LEU:HD22	1:A:1473:THR:HG22	1.95	0.49
1:A:2960:THR:HB	1:A:2963:ASP:HB2	1.94	0.49
1:A:4034:LEU:O	1:A:4036:GLN:HG3	2.13	0.49
1:A:2084:TRP:CH2	1:A:2153:VAL:HG21	2.48	0.49
1:B:2339:ILE:HG23	1:B:2353:LEU:HB3	1.94	0.49
1:B:1422:LYS:CA	1:B:1425:GLU:HB2	2.43	0.49
1:B:2495:ASP:O	1:B:2498:GLY:N	2.46	0.49
1:B:2107:LYS:CE	1:B:2499:SER:HB3	2.42	0.49
1:B:1822:CYS:SG	1:B:1849:GLU:C	2.91	0.49
1:B:3509:LEU:HD12	1:B:3513:VAL:CG2	2.42	0.49
1:B:4065:LEU:HD11	1:B:4070:ILE:CD1	2.39	0.49
1:B:1749:ILE:HD13	1:B:1813:LEU:HD22	1.94	0.49
1:B:1963:MET:HB3	1:B:1966:TYR:CD2	2.48	0.49
1:A:2920:TRP:CG	1:A:2989:PRO:HG3	2.47	0.48
1:A:1823:ASP:CG	1:A:1823:ASP:O	2.51	0.48
1:A:2134:LEU:HD12	1:A:2138:ASN:ND2	2.28	0.48
1:A:1714:GLN:HB3	1:A:1727:LEU:HD11	1.95	0.48
1:B:2290:LEU:HD23	1:B:2321:SER:HA	1.94	0.48
1:B:3656:VAL:CG1	1:B:3677:LEU:HB3	2.36	0.48
1:A:2034:ILE:HD12	1:A:2061:TYR:CE2	2.48	0.48
1:B:3979:ASN:O	1:B:3981:PRO:HD2	2.13	0.48
1:A:4022:GLN:HA	1:A:4027:VAL:O	2.12	0.48
1:B:1425:GLU:OE2	1:B:1429:LEU:CD1	2.60	0.48
1:B:2080:LYS:HE2	2:B:5093:ATP:O3G	2.13	0.48
1:A:1466:GLN:HB2	1:A:1473:THR:HG21	1.95	0.48
1:B:2476:LYS:HE3	1:B:2528:ARG:HB3	1.95	0.48
1:B:2763:ARG:HA	5:B:5096:SO4:O3	2.13	0.48
1:B:1394:LEU:HD22	1:B:1449:GLN:HE22	1.78	0.48
1:A:3409:ASP:HB3	1:A:3518:PHE:HB2	1.94	0.48
1:B:3519:VAL:HG13	1:B:3521:ASN:ND2	2.29	0.48
1:B:3618:TYR:O	1:B:3622:GLY:N	2.42	0.48
1:A:2475:PRO:O	1:A:2476:LYS:O	2.30	0.48
1:A:2154:PHE:HD1	1:A:2154:PHE:N	2.10	0.48
1:A:3461:ILE:C	1:A:3463:SER:H	2.15	0.48
1:B:2467:THR:HG22	1:B:2468:SER:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3737:THR:CB	1:B:3740:THR:HB	2.44	0.48
1:B:1956:LEU:CB	1:B:1968:PHE:CE2	2.92	0.48
1:A:2627:ARG:NH1	1:A:2630:TYR:CE2	2.81	0.48
1:A:2175:ILE:HG13	1:A:2184:LEU:C	2.34	0.48
1:B:2109:LEU:HD13	1:B:2129:LEU:HD23	1.96	0.48
1:A:3618:TYR:O	1:A:3622:GLY:N	2.38	0.48
1:A:3365:ARG:HD2	1:A:3368:ASP:OD2	2.14	0.48
1:A:1677:ASP:HA	1:A:1680:ILE:HD12	1.95	0.48
1:A:3462:ILE:N	1:A:3462:ILE:HD13	2.28	0.48
1:B:2467:THR:HB	1:B:2473:LEU:CD2	2.42	0.48
1:B:2084:TRP:HE3	1:B:2088:ILE:HD12	1.79	0.48
1:A:2942:ASP:HB3	1:A:3357:ALA:HB1	1.95	0.48
1:A:2109:LEU:CD1	1:A:2129:LEU:HD23	2.42	0.48
1:B:65:THR:O	1:B:66:GLN:CB	2.61	0.48
1:B:1645:PHE:CD2	1:B:1765:ILE:HG22	2.48	0.48
1:A:2494:LEU:O	1:A:2494:LEU:HD12	2.14	0.48
1:A:2154:PHE:CD1	1:A:2154:PHE:N	2.79	0.48
1:B:1750:SER:CB	1:B:1755:LEU:HD23	2.44	0.48
1:B:2109:LEU:HD11	1:B:2129:LEU:CD2	2.43	0.48
1:B:4074:GLU:HA	1:B:4077:GLN:HE21	1.79	0.48
1:A:1692:ASP:O	1:A:1695:LYS:HB3	2.13	0.48
1:B:1423:ILE:C	1:B:1425:GLU:N	2.66	0.48
1:A:1620:PHE:HD2	1:A:1760:PHE:HZ	1.49	0.48
1:B:3406:PHE:CZ	1:B:3505:ILE:HG21	2.49	0.48
1:A:2099:ASN:HA	1:A:2149:ARG:O	2.14	0.48
1:B:1773:PRO:HA	1:B:1776:LEU:HD12	1.96	0.48
1:B:3459:ASP:HB2	1:B:3460:PRO:HD2	1.96	0.48
1:A:3934:TRP:CG	1:A:4023:ILE:HD12	2.49	0.48
1:B:1392:LEU:HD23	1:B:1484:LYS:HA	1.96	0.48
1:A:1531:ARG:HG2	1:A:1537:PHE:CB	2.40	0.48
1:B:1844:TRP:CD1	1:B:1893:ALA:HB3	2.48	0.48
1:A:2354:SER:OG	1:A:2357:SER:CB	2.61	0.48
1:A:2105:ASP:OD2	1:A:2508:GLN:HB2	2.13	0.48
1:A:1531:ARG:HD3	1:A:1537:PHE:O	2.14	0.48
1:A:2426:MET:HG3	1:A:2427:ILE:H	1.79	0.48
1:B:3538:ASN:HB3	1:B:3541:MET:HG2	1.95	0.48
1:B:3817:GLY:H	1:B:3821:ASN:HB2	1.79	0.48
1:A:3307:LEU:O	1:A:3311:LYS:HB3	2.14	0.48
1:B:3628:ILE:HD11	1:B:3679:TYR:CZ	2.49	0.48
1:A:1421:TYR:CD2	1:A:1425:GLU:CG	2.97	0.47
1:A:2565:LYS:O	1:A:2569:GLN:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1466:GLN:HB3	1:A:1473:THR:HG21	1.94	0.47
1:A:2473:LEU:HD23	1:A:2525:THR:HB	1.96	0.47
1:B:4024:VAL:HG23	1:B:4027:VAL:H	1.79	0.47
1:A:2257:PHE:CD1	1:A:2262:LEU:HD11	2.49	0.47
1:B:3530:PHE:HD1	1:B:3618:TYR:CD2	2.29	0.47
1:A:2707:VAL:HG12	1:A:2712:LEU:CD1	2.44	0.47
1:A:2493:LYS:HG3	1:A:2494:LEU:N	2.16	0.47
1:A:2385:VAL:O	1:A:2574:TYR:HE1	1.96	0.47
1:A:2034:ILE:CD1	1:A:2061:TYR:CE2	2.96	0.47
1:B:3869:GLU:O	1:B:3870:LYS:C	2.52	0.47
1:B:2491:LEU:HD23	1:B:2491:LEU:HA	1.71	0.47
1:A:3978:ASN:O	1:A:3981:PRO:HD3	2.14	0.47
1:A:3979:ASN:C	1:A:3981:PRO:CD	2.83	0.47
1:A:2134:LEU:HD11	1:A:2138:ASN:HD21	1.79	0.47
1:B:2653:TRP:HB3	1:B:2654:ARG:NH1	2.30	0.47
1:B:3461:ILE:C	1:B:3463:SER:N	2.67	0.47
1:B:1645:PHE:HB2	1:B:1697:LYS:HG3	1.95	0.47
1:B:2060:PHE:CE1	1:B:2064:GLN:NE2	2.81	0.47
1:A:2441:VAL:CG2	1:A:2482:LEU:HD21	2.43	0.47
1:A:3772:TRP:HZ3	1:A:3780:ASN:HD22	1.62	0.47
1:A:1636:ILE:O	1:A:1640:VAL:HG23	2.14	0.47
1:A:2378:VAL:CG1	1:A:2392:ILE:HD12	2.44	0.47
1:A:1645:PHE:CB	1:A:1765:ILE:HG21	2.41	0.47
1:A:2563:SER:C	1:A:2565:LYS:H	2.17	0.47
1:A:2127:ASP:HB3	1:A:2132:SER:HB3	1.96	0.47
1:A:4020:ASN:ND2	1:A:4028:ARG:HD3	2.29	0.47
1:A:2761:ALA:O	1:A:2892:CYS:HB3	2.15	0.47
1:B:1744:LEU:CD2	1:B:1760:PHE:CD2	2.98	0.47
1:B:2755:HIS:HB3	1:B:2912:CYS:SG	2.55	0.47
1:B:1968:PHE:CD1	1:B:1968:PHE:N	2.83	0.47
1:B:3566:LEU:HD11	1:B:3570:LEU:HD11	1.95	0.47
1:B:1387:GLU:HA	1:B:1393:LYS:HA	1.96	0.47
1:A:2760:GLY:HA2	1:A:2917:MET:HB2	1.96	0.47
1:A:1646:GLN:OE1	1:A:1763:ILE:N	2.42	0.47
1:A:2354:SER:H	1:A:2357:SER:HB2	1.80	0.47
1:B:2780:LYS:HB3	1:B:2813:THR:HG22	1.96	0.47
1:A:3471:ASN:HB2	1:A:3478:THR:HG23	1.97	0.47
1:B:2318:ILE:O	1:B:2322:LEU:HB2	2.14	0.47
1:B:1789:LYS:HD3	1:B:1872:LEU:O	2.14	0.47
1:B:3813:ILE:HG22	1:B:3840:LEU:HD23	1.97	0.47
1:B:2470:GLY:O	1:B:2471:LEU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2473:LEU:HD12	1:B:2473:LEU:N	2.28	0.47
1:B:4060:SER:HB3	1:B:4070:ILE:HG13	1.96	0.47
1:A:2252:LEU:HD22	1:A:2314:ILE:HG13	1.96	0.47
1:B:1612:ASP:HA	1:B:1615:ILE:CG1	2.45	0.47
1:A:2967:ASN:HB3	1:A:3356:PHE:CZ	2.49	0.47
1:A:2383:HIS:CE1	1:A:2384:GLU:HG3	2.50	0.47
1:B:3855:LEU:HD12	1:B:3859:VAL:HG23	1.97	0.47
1:A:1540:LEU:HD23	1:A:1540:LEU:HA	1.66	0.47
1:A:2358:THR:CG2	1:A:2359:ILE:N	2.78	0.47
1:A:2109:LEU:HD11	1:A:2129:LEU:CD2	2.44	0.47
1:B:3367:ILE:O	1:B:3371:VAL:HG22	2.15	0.47
1:B:1715:LEU:HG	1:B:1727:LEU:HD22	1.96	0.47
1:B:1934:LEU:HD22	1:B:1945:LEU:HD12	1.97	0.47
1:A:1744:LEU:HD22	1:A:1760:PHE:CG	2.50	0.47
1:A:2112:GLU:CB	1:A:2117:SER:HB2	2.39	0.47
1:B:2446:SER:H	1:B:2449:THR:HG21	1.79	0.47
1:A:1802:LYS:NZ	5:A:5097:SO4:S	2.88	0.47
1:B:2761:ALA:O	1:B:2892:CYS:CB	2.63	0.47
1:B:2125:TRP:CZ2	1:B:2178:LEU:HD13	2.51	0.47
1:A:2241:LEU:HD13	1:A:2299:ARG:HH11	1.80	0.47
1:B:2787:HIS:CA	1:B:3460:PRO:HG2	2.44	0.46
1:B:2920:TRP:CG	1:B:2989:PRO:HG3	2.50	0.46
1:B:3737:THR:OG1	1:B:3740:THR:CB	2.62	0.46
1:B:3641:PHE:HA	1:B:3889:LEU:HD21	1.97	0.46
1:B:2421:GLY:N	3:B:5094:ADP:O2B	2.39	0.46
1:A:2111:LYS:CD	1:A:2161:GLU:HG3	2.17	0.46
1:A:3927:TYR:HE1	1:A:4029:ILE:HG22	1.80	0.46
1:B:2709:LYS:O	1:B:2713:VAL:HG23	2.15	0.46
1:B:1949:ILE:HD11	1:B:1994:VAL:HG11	1.96	0.46
1:A:2517:LYS:NZ	1:A:2520:GLU:OE1	2.46	0.46
1:A:2063:MET:HB3	1:A:2070:LEU:HD11	1.97	0.46
1:B:1826:PHE:CE1	1:B:1830:VAL:HG13	2.51	0.46
1:B:1938:GLY:O	1:B:1989:GLU:HB3	2.15	0.46
1:A:1563:LYS:HA	1:A:1569:ILE:O	2.15	0.46
1:B:2225:LYS:HG3	2:B:5093:ATP:H1'	1.96	0.46
1:A:1781:THR:HG21	1:A:1919:PHE:CE1	2.50	0.46
1:B:2503:VAL:HA	1:B:2506:LEU:HD12	1.97	0.46
1:B:2761:ALA:O	1:B:2892:CYS:HB3	2.15	0.46
1:B:1714:GLN:HB3	1:B:1727:LEU:HD11	1.98	0.46
1:B:1657:THR:HG21	1:B:1734:PHE:O	2.15	0.46
1:A:2507:ARG:HG3	1:A:2550:PHE:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1953:LEU:HA	1:A:1956:LEU:HD12	1.98	0.46
1:A:2411:LYS:HG2	1:A:2530:HIS:CE1	2.42	0.46
1:A:3818:SER:O	1:A:3819:ILE:C	2.54	0.46
1:B:2620:ARG:HH11	1:B:2910:ASN:ND2	2.13	0.46
1:B:4059:LEU:HA	1:B:4063:LEU:HD13	1.96	0.46
1:A:3692:LYS:HE3	1:A:3898:GLU:HB3	1.97	0.46
1:B:1626:CYS:SG	1:B:1639:VAL:HG11	2.56	0.46
1:A:1835:LEU:O	1:A:1838:ILE:HG22	2.15	0.46
1:B:1422:LYS:C	1:B:1425:GLU:HB3	2.33	0.46
1:A:3431:PHE:CZ	1:A:3458:PHE:HD1	2.33	0.46
1:A:2141:ILE:HG22	1:A:2145:PHE:HB2	1.97	0.46
1:B:1604:ALA:HA	1:B:1607:TRP:HE1	1.78	0.46
1:B:1497:ILE:O	1:B:1500:ILE:HG12	2.16	0.46
1:A:1559:SER:HB3	1:A:1572:ILE:CG2	2.44	0.46
1:B:3978:ASN:O	1:B:3981:PRO:CD	2.62	0.46
1:B:203:GLN:O	1:B:204:GLY:C	2.54	0.46
1:A:2151:TRP:CE3	1:A:2193:LEU:HD11	2.51	0.46
1:B:1911:ASN:OD1	1:B:1912:LEU:HG	2.16	0.46
1:B:2305:LEU:HB3	1:B:2310:LEU:CD1	2.45	0.46
1:A:2905:SER:HA	1:A:2906:PRO:HD2	1.70	0.46
1:B:2795:PHE:CE2	1:B:2799:LEU:HD11	2.51	0.46
1:B:1939:PHE:HD1	1:B:1939:PHE:H	1.61	0.46
1:A:3461:ILE:C	1:A:3463:SER:N	2.67	0.46
1:B:3462:ILE:O	1:B:3465:LEU:N	2.49	0.46
1:B:3845:GLN:NE2	1:B:3882:ASP:O	2.49	0.46
1:A:2654:ARG:HH22	1:A:2691:SER:HB2	1.80	0.46
1:A:1981:SER:HB3	1:A:1982:PRO:HD3	1.97	0.46
1:A:2749:LEU:HD12	1:A:2773:VAL:HG12	1.97	0.46
1:B:3555:TYR:HE1	1:B:3593:GLU:HG2	1.80	0.46
1:B:2752:VAL:HG13	1:B:2883:LYS:CB	2.46	0.46
1:B:1462:ASN:HB2	1:B:1465:ILE:HG22	1.98	0.46
1:B:4022:GLN:HG2	1:B:4022:GLN:O	2.15	0.46
1:B:1967:HIS:C	1:B:1968:PHE:CD1	2.85	0.46
1:B:2336:ARG:CD	1:B:2355:ASP:OD2	2.62	0.46
1:B:2099:ASN:HA	1:B:2149:ARG:O	2.16	0.46
1:A:1977:LEU:O	1:A:1980:CYS:HB3	2.16	0.46
1:B:2170:LEU:HB3	1:B:2209:ARG:HD3	1.98	0.46
1:A:2860:THR:HG21	1:A:2867:LEU:HD12	1.97	0.46
1:A:1672:TYR:O	1:A:1675:GLU:HB3	2.15	0.46
1:B:1762:TYR:CZ	1:B:1764:GLY:HA2	2.51	0.46
1:A:2104:ILE:O	1:A:2154:PHE:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2787:HIS:HB3	1:A:3461:ILE:HG23	1.96	0.46
1:B:2563:SER:C	1:B:2565:LYS:H	2.19	0.46
1:A:2385:VAL:HG23	1:A:2574:TYR:HD1	1.81	0.46
1:A:2228:HIS:HD2	2:A:5093:ATP:O2'	1.99	0.46
1:B:1611:LEU:O	1:B:1615:ILE:HG12	2.15	0.46
1:B:3807:SER:O	1:B:3808:LYS:HB2	2.16	0.46
1:B:2204:PRO:HA	1:B:2207:ILE:HD12	1.97	0.46
1:A:2475:PRO:HB3	1:A:2527:GLU:HB2	1.98	0.46
1:A:3509:LEU:HD12	1:A:3513:VAL:HG23	1.97	0.46
1:A:1848:ASP:O	1:A:1849:GLU:HB2	2.16	0.46
1:A:2849:TYR:O	1:A:2853:LEU:HB2	2.16	0.46
1:B:3687:SER:HA	1:B:3698:MET:HE1	1.98	0.46
1:A:3854:TYR:O	1:A:3858:HIS:HB2	2.16	0.46
1:A:23:LEU:O	1:A:24:GLU:C	2.50	0.46
1:B:2707:VAL:HG12	1:B:2712:LEU:HD12	1.97	0.45
1:A:1645:PHE:HB2	1:A:1697:LYS:HG3	1.97	0.45
1:A:1621:THR:HA	1:A:1624:ARG:CZ	2.44	0.45
1:A:3505:ILE:O	1:A:3510:ARG:NH1	2.49	0.45
1:A:1940:GLU:HG3	1:A:1941:ASP:N	2.31	0.45
1:B:1536:ARG:HD3	1:B:1536:ARG:HA	1.66	0.45
1:A:3816:LEU:HD21	1:A:3850:TRP:HZ3	1.81	0.45
1:A:3721:THR:O	1:A:3725:VAL:HG23	2.16	0.45
1:A:1656:TRP:O	1:A:1660:VAL:HG12	2.17	0.45
1:A:2129:LEU:O	1:A:2133:ILE:HG12	2.16	0.45
1:B:2385:VAL:O	1:B:2574:TYR:HE1	1.99	0.45
1:A:1694:VAL:HG23	1:A:1697:LYS:HE2	1.98	0.45
1:B:3017:VAL:HG21	1:B:3313:PHE:HE2	1.81	0.45
1:A:1702:LEU:HD23	1:A:1702:LEU:HA	1.81	0.45
1:A:1927:GLY:HA2	1:A:1950:VAL:HG21	1.97	0.45
1:B:3500:ASP:HA	1:B:3501:PRO:HD3	1.88	0.45
1:B:1620:PHE:HB2	1:B:1760:PHE:CZ	2.51	0.45
1:B:1995:VAL:HG22	1:B:2022:PHE:CE2	2.51	0.45
1:B:1392:LEU:C	1:B:1392:LEU:CD1	2.84	0.45
1:A:3629:PHE:O	1:A:3633:GLU:HB2	2.17	0.45
1:B:3330:TYR:CE2	1:B:3346:LEU:HD13	2.51	0.45
1:B:2201:HIS:CE1	1:B:2497:TYR:HA	2.51	0.45
1:B:1781:THR:HG21	1:B:1919:PHE:CD1	2.51	0.45
1:A:3785:TYR:CE2	1:A:3859:VAL:HG13	2.51	0.45
1:A:2567:LEU:HD22	1:A:2622:LEU:HD13	1.98	0.45
1:A:1527:LEU:CD2	1:A:1545:LEU:HD22	2.46	0.45
1:A:1967:HIS:C	1:A:1968:PHE:CD1	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2464:TYR:HE1	1:B:2524:VAL:HG11	1.81	0.45
1:A:1852:ARG:O	1:A:1852:ARG:HG3	2.17	0.45
1:A:2163:VAL:O	1:A:2166:MET:HG3	2.16	0.45
1:A:2316:LEU:HD13	1:A:2351:GLN:HB3	1.98	0.45
1:A:1575:LEU:HD12	1:A:1575:LEU:HA	1.87	0.45
1:A:1967:HIS:O	1:A:1968:PHE:HD1	1.98	0.45
1:B:1646:GLN:OE1	1:B:1763:ILE:HG12	2.16	0.45
1:A:2112:GLU:HB3	1:A:2117:SER:OG	2.15	0.45
1:A:3799:LYS:HG3	1:A:3803:LEU:HD11	1.98	0.45
1:B:3612:ASP:C	1:B:3615:VAL:HG22	2.37	0.45
1:A:2425:THR:HG22	1:A:2485:PHE:CE2	2.51	0.45
1:A:2761:ALA:O	1:A:2892:CYS:CB	2.64	0.45
1:A:3891:ARG:HA	1:A:3891:ARG:HD2	1.79	0.45
1:B:2491:LEU:HD21	1:B:2543:ARG:CZ	2.47	0.45
1:A:2088:ILE:HG12	1:A:2151:TRP:CZ2	2.52	0.45
1:A:2727:GLU:O	1:A:2728:LEU:C	2.55	0.45
1:B:2276:LEU:CD2	1:B:2556:ILE:HG21	2.45	0.45
1:B:2037:CYS:SG	1:B:2094:PHE:HB2	2.56	0.45
1:A:1657:THR:HG21	1:A:1734:PHE:O	2.17	0.45
1:A:1998:LEU:CD1	1:A:2022:PHE:HZ	2.28	0.45
1:A:1409:LEU:CD2	1:A:1435:LEU:HB3	2.39	0.45
1:A:2134:LEU:CD1	1:A:2138:ASN:HD21	2.28	0.45
1:B:3330:TYR:OH	1:B:3346:LEU:HD13	2.16	0.45
1:B:1375:LYS:O	1:B:1379:LYS:HG2	2.16	0.45
1:A:2115:TYR:O	1:A:2131:THR:CG2	2.65	0.45
1:A:1946:ALA:O	1:A:1950:VAL:HG23	2.17	0.45
1:B:1941:ASP:O	1:B:1945:LEU:HG	2.17	0.45
1:B:3939:ILE:HG23	1:B:3950:PHE:HE2	1.80	0.45
1:B:2563:SER:CB	1:B:2566:SER:H	2.20	0.45
1:B:1391:GLY:HA3	1:B:1484:LYS:HZ3	1.81	0.45
1:A:2891:ILE:CD1	1:A:2903:ILE:HD11	2.43	0.45
1:A:1640:VAL:CG1	1:A:1686:LYS:NZ	2.79	0.45
1:B:1459:LEU:HD23	1:B:1465:ILE:HG13	1.99	0.45
1:A:4033:LEU:HD12	1:A:4035:GLN:N	2.32	0.45
1:A:3304:GLU:C	1:A:3306:TRP:H	2.21	0.45
1:A:2474:LEU:N	1:A:2475:PRO:HD3	2.32	0.45
1:A:2788:ARG:HG3	1:A:3459:ASP:HA	1.98	0.45
1:B:2467:THR:O	1:B:2471:LEU:N	2.50	0.45
1:A:2632:ALA:HB3	1:A:2647:LEU:HD21	1.99	0.45
1:B:1753:GLY:HA3	1:B:3970:ASN:HD21	1.81	0.45
1:A:2412:ARG:HH11	1:A:2412:ARG:HG3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3645:SER:CB	1:A:3890:GLN:NE2	2.78	0.44
1:A:3812:LYS:HB2	1:A:3839:ILE:HD12	1.99	0.44
1:A:2100:VAL:N	1:A:2149:ARG:O	2.48	0.44
1:B:2960:THR:HG22	1:B:2961:ILE:N	2.32	0.44
1:B:2752:VAL:HG13	1:B:2883:LYS:HB3	1.98	0.44
1:B:2580:LYS:HG2	1:B:2586:ARG:HH22	1.82	0.44
1:B:2867:LEU:HB3	1:B:2872:GLU:HB3	1.98	0.44
1:A:2941:THR:CG2	1:A:2942:ASP:H	2.20	0.44
1:A:2169:VAL:HG13	1:A:2186:ILE:HG12	1.98	0.44
1:A:2021:ILE:HG22	1:A:2022:PHE:HD1	1.82	0.44
1:A:2755:HIS:CB	1:A:2912:CYS:HA	2.47	0.44
1:B:1392:LEU:HD22	1:B:1393:LYS:H	1.82	0.44
1:A:2220:CYS:SG	1:A:2221:SER:N	2.91	0.44
1:A:2356:TYR:CE1	1:A:2395:ILE:HG22	2.53	0.44
1:B:3600:LYS:HA	1:B:3603:GLU:HG2	1.99	0.44
1:B:1367:ILE:HD12	1:B:1367:ILE:H	1.83	0.44
1:B:2988:SER:CB	1:B:2989:PRO:CD	2.62	0.44
1:A:2386:MET:HB2	1:A:2627:ARG:CD	2.39	0.44
1:B:3810:SER:HB3	1:B:3838:TRP:H	1.83	0.44
1:B:2091:MET:CE	1:B:2149:ARG:NH1	2.80	0.44
1:B:1469:LEU:HD13	1:B:1523:LEU:HD21	1.98	0.44
1:B:2982:VAL:HG12	1:B:2983:GLY:N	2.32	0.44
1:B:3319:GLU:HA	1:B:3359:LYS:O	2.16	0.44
1:B:1851:ASN:HD21	1:B:1899:ASN:HB2	1.81	0.44
1:A:3440:LEU:HD22	1:A:3462:ILE:HD12	1.98	0.44
1:A:3459:ASP:HB2	1:A:3460:PRO:HD2	1.98	0.44
1:B:3509:LEU:CD1	1:B:3513:VAL:CG2	2.95	0.44
1:B:3509:LEU:O	1:B:3513:VAL:HG23	2.17	0.44
1:A:3792:ARG:HB2	1:A:3955:TYR:CE2	2.53	0.44
1:A:3889:LEU:HG	1:A:3894:ARG:HD3	1.99	0.44
1:B:3911:TRP:HH2	1:B:3926:VAL:CG1	2.28	0.44
1:A:3845:GLN:O	1:A:3848:LEU:HB2	2.18	0.44
1:B:2178:LEU:HD12	1:B:2182:GLU:HB2	1.99	0.44
1:A:4020:ASN:HB3	1:A:4028:ARG:HH11	1.81	0.44
1:A:3965:SER:HA	1:A:3968:LEU:HD12	1.99	0.44
1:A:3897:TYR:CZ	1:A:3899:ASP:HB3	2.53	0.44
1:A:3464:ARG:O	1:A:3467:SER:O	2.35	0.44
1:B:1385:VAL:HG21	1:B:1491:PHE:CD1	2.53	0.44
1:B:3737:THR:HB	1:B:3740:THR:HG1	1.78	0.44
1:A:2755:HIS:CB	1:A:2911:ARG:O	2.58	0.44
1:A:3330:TYR:CD1	1:A:3334:PHE:CD2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2673:LEU:O	1:A:2677:VAL:HG23	2.17	0.44
1:A:1706:LEU:HD23	1:A:1706:LEU:HA	1.85	0.44
1:A:1646:GLN:CG	1:A:1763:ILE:HG12	2.47	0.44
1:B:3462:ILE:O	1:B:3465:LEU:HB3	2.17	0.44
1:B:1527:LEU:HD22	1:B:1545:LEU:HD22	1.98	0.44
1:B:4006:VAL:HA	1:B:4009:LYS:HG2	2.00	0.44
1:A:2424:LYS:HB2	1:A:2424:LYS:HZ3	1.82	0.44
1:A:3372:THR:HG23	1:A:3375:GLU:HB2	2.00	0.44
1:B:2387:ARG:O	1:B:2390:ILE:HG22	2.18	0.44
1:B:2084:TRP:CZ3	1:B:2085:LYS:HG3	2.53	0.44
1:A:1983:LEU:HD21	1:A:1993:THR:O	2.16	0.44
1:B:1536:ARG:HE	1:B:1841:ILE:HD13	1.82	0.44
1:A:2141:ILE:HG22	1:A:2145:PHE:CB	2.48	0.44
1:B:1970:LEU:CD2	1:B:1974:LYS:HE3	2.47	0.44
1:B:2276:LEU:HD13	1:B:2417:CYS:SG	2.58	0.44
1:B:2967:ASN:HB3	1:B:3356:PHE:HE2	1.80	0.44
1:A:2428:MET:SD	1:A:2428:MET:C	2.96	0.44
1:A:1664:LEU:O	1:A:1721:LYS:HE3	2.18	0.44
1:A:3788:MET:HG3	1:A:3788:MET:O	2.18	0.44
1:B:2464:TYR:CZ	1:B:2474:LEU:HD12	2.53	0.44
1:A:2940:PHE:CE1	1:A:2941:THR:O	2.71	0.44
1:A:2571:TYR:HA	1:A:2574:TYR:HB2	2.00	0.44
1:A:2446:SER:N	1:A:2449:THR:CG2	2.75	0.44
1:B:1910:GLU:HB2	1:B:3846:MET:HB3	2.00	0.44
1:A:2095:ASP:OD1	1:A:2149:ARG:NH2	2.50	0.44
1:B:3373:LEU:HD13	1:B:3557:LEU:CD1	2.48	0.44
1:A:2141:ILE:CG2	1:A:2145:PHE:HB2	2.48	0.44
1:B:1540:LEU:HA	1:B:1540:LEU:HD23	1.70	0.44
1:A:2125:TRP:CZ2	1:A:2178:LEU:HD13	2.53	0.44
1:A:1749:ILE:O	1:A:1755:LEU:HA	2.17	0.44
1:B:2169:VAL:HG13	1:B:2186:ILE:HG12	1.99	0.44
1:A:1438:LEU:O	1:A:1442:GLN:HB2	2.18	0.44
1:B:1554:HIS:O	1:B:1555:HIS:HB2	2.18	0.44
1:A:3319:GLU:HA	1:A:3359:LYS:O	2.17	0.44
1:B:2420:PRO:HA	3:B:5094:ADP:O2B	2.17	0.43
1:A:1968:PHE:CD1	1:A:1968:PHE:N	2.85	0.43
1:B:1849:GLU:CG	1:B:1899:ASN:ND2	2.81	0.43
1:B:2578:ILE:HG21	1:B:2630:TYR:HB2	1.99	0.43
1:A:1535:PRO:O	1:A:1841:ILE:HD11	2.18	0.43
1:B:2137:VAL:O	1:B:2141:ILE:CG2	2.62	0.43
1:B:2445:PHE:HA	1:B:2449:THR:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3815:PRO:O	1:B:3821:ASN:HB3	2.17	0.43
1:A:2361:ILE:HG22	1:A:2367:SER:O	2.18	0.43
1:B:1512:THR:HG22	1:B:1516:LEU:HD12	1.98	0.43
1:A:2120:LYS:H	1:A:2120:LYS:HG3	1.64	0.43
1:B:3024:LEU:HD13	1:B:3303:LYS:HG3	1.96	0.43
1:A:2228:HIS:CD2	2:A:5093:ATP:O2'	2.71	0.43
1:A:2410:SER:O	1:A:2411:LYS:HB2	2.18	0.43
1:A:3886:ALA:N	1:A:3887:PRO:CD	2.79	0.43
1:A:2042:GLY:HA3	1:A:2049:MET:CE	2.48	0.43
1:B:3817:GLY:H	1:B:3821:ASN:CB	2.31	0.43
1:A:2904:SER:O	1:A:2905:SER:C	2.56	0.43
1:B:2112:GLU:HB3	1:B:2117:SER:OG	2.16	0.43
1:A:1983:LEU:CD2	1:A:1993:THR:CG2	2.88	0.43
1:A:2755:HIS:O	1:A:2913:ILE:N	2.49	0.43
1:B:1612:ASP:CA	1:B:1615:ILE:HG12	2.48	0.43
1:A:1622:GLN:NE2	1:A:1644:ILE:H	2.15	0.43
1:B:1813:LEU:HD12	1:B:1844:TRP:CH2	2.52	0.43
1:A:2708:ASN:ND2	1:A:2710:THR:OG1	2.52	0.43
1:B:1849:GLU:CG	1:B:1899:ASN:HD22	2.31	0.43
1:A:2391:VAL:CG2	1:A:2430:ASN:OD1	2.65	0.43
1:B:3767:PHE:HB3	1:B:3769:VAL:HG23	1.99	0.43
1:B:3544:LYS:O	1:B:3548:LEU:HB2	2.18	0.43
1:B:2833:THR:HG21	1:B:2841:PRO:CD	2.49	0.43
1:A:2418:GLY:CA	1:A:2424:LYS:HE3	2.47	0.43
1:A:1529:ARG:O	1:A:1533:GLN:HG2	2.17	0.43
1:B:3772:TRP:HZ3	1:B:3780:ASN:HD22	1.64	0.43
1:B:2935:VAL:C	1:B:2937:PRO:HD3	2.39	0.43
1:B:1422:LYS:C	1:B:1425:GLU:CB	2.87	0.43
1:A:1970:LEU:CD1	1:A:1973:LEU:HD11	2.48	0.43
1:A:2064:GLN:OE1	1:A:2091:MET:SD	2.77	0.43
1:A:1392:LEU:CD1	1:A:1393:LYS:O	2.67	0.43
1:B:1392:LEU:N	1:B:1484:LYS:HE2	2.33	0.43
1:A:2047:PHE:CE2	1:A:2082:ALA:HB1	2.52	0.43
1:B:3930:PHE:CE2	1:B:4029:ILE:HD13	2.52	0.43
1:B:2100:VAL:HG12	1:B:2102:TYR:CE2	2.53	0.43
1:A:1620:PHE:HA	1:A:1760:PHE:CE2	2.53	0.43
1:A:2526:ILE:O	1:A:2526:ILE:HG13	2.18	0.43
1:A:3948:HIS:NE2	1:A:4072:ASN:CG	2.71	0.43
1:B:3979:ASN:C	1:B:3981:PRO:CD	2.86	0.43
1:B:2027:THR:HA	1:B:2028:PRO:HD3	1.55	0.43
1:B:1677:ASP:HA	1:B:1680:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2708:ASN:O	1:A:2712:LEU:HD13	2.18	0.43
1:B:1984:ILE:HG21	1:B:1989:GLU:HG3	2.00	0.43
1:A:3436:PHE:HE2	1:A:3462:ILE:HD11	1.82	0.43
1:B:3946:VAL:HA	1:B:3947:PRO:C	2.38	0.43
1:B:2745:ILE:HA	1:B:2756:MET:SD	2.58	0.43
1:B:2785:LYS:HE2	1:B:3480:GLU:OE1	2.18	0.43
1:A:2109:LEU:HD11	1:A:2129:LEU:HD23	1.99	0.43
1:B:3307:LEU:HA	1:B:3310:THR:HB	2.00	0.43
1:B:2463:ASN:O	1:B:2475:PRO:HD2	2.18	0.43
1:A:3443:ALA:HB1	1:A:3450:VAL:HG21	2.00	0.43
1:A:1409:LEU:CD2	1:A:1435:LEU:CB	2.93	0.43
1:A:2266:PHE:CD1	1:A:2326:LEU:HD21	2.48	0.43
1:B:2106:THR:H	1:B:2156:SER:HB2	1.83	0.43
1:A:1794:PHE:HZ	1:A:1805:THR:CG2	2.31	0.43
1:B:1527:LEU:HD21	1:B:1546:LEU:CD2	2.48	0.43
1:A:2960:THR:HG22	1:A:2961:ILE:N	2.33	0.43
1:B:2361:ILE:HG22	1:B:2367:SER:O	2.19	0.43
1:A:1870:ASN:O	1:A:1874:VAL:HG23	2.18	0.43
1:B:2420:PRO:HD3	1:B:2536:ASN:ND2	2.28	0.43
1:A:2197:ASP:CB	1:A:2549:ARG:HD2	2.45	0.43
1:B:1495:THR:CG2	1:B:1497:ILE:HG22	2.48	0.43
1:B:1706:LEU:HD22	1:B:1935:GLN:CG	2.48	0.43
1:A:3352:LEU:O	1:A:3356:PHE:HD1	2.02	0.43
1:B:1664:LEU:HD23	1:B:1669:PHE:HZ	1.84	0.43
1:A:4033:LEU:HD13	1:A:4035:GLN:CG	2.48	0.43
1:A:2074:GLY:O	1:A:2197:ASP:HA	2.19	0.43
1:A:1463:LEU:O	1:A:1467:ASN:HB2	2.19	0.43
1:B:2748:ALA:O	1:B:2751:GLN:HG3	2.19	0.43
1:A:2839:ASP:O	1:A:2841:PRO:HD3	2.18	0.43
1:A:3500:ASP:HA	1:A:3501:PRO:HD3	1.82	0.43
1:B:1416:LYS:CA	1:B:1421:TYR:OH	2.65	0.42
1:B:2494:LEU:HD12	1:B:2494:LEU:O	2.19	0.42
1:B:3525:ILE:CD1	1:B:3646:ILE:HG22	2.29	0.42
1:A:3592:LYS:O	1:A:3596:ASN:N	2.52	0.42
1:A:1542:ASN:O	1:A:1546:LEU:HG	2.19	0.42
1:A:2783:GLN:HG2	1:A:2816:ILE:HB	2.00	0.42
1:A:1926:SER:HA	1:A:1929:ILE:CD1	2.49	0.42
1:B:1976:VAL:HG11	1:B:1998:LEU:HD23	2.01	0.42
1:B:2747:ARG:O	1:B:2751:GLN:HG2	2.19	0.42
1:B:3979:ASN:OD1	1:B:3979:ASN:N	2.52	0.42
1:A:2418:GLY:N	1:A:2424:LYS:HE3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1383:TYR:CE2	1:B:1401:LEU:HD13	2.54	0.42
1:B:4054:GLU:HA	1:B:4055:PRO:HD3	1.90	0.42
1:A:1547:LYS:O	1:A:1551:SER:HB3	2.19	0.42
1:A:4084:SER:O	1:A:4088:LEU:HG	2.19	0.42
1:B:2707:VAL:HG11	1:B:2712:LEU:HD12	1.99	0.42
1:A:2178:LEU:HD12	1:A:2182:GLU:HB2	2.01	0.42
1:B:1910:GLU:CB	1:B:3846:MET:HB3	2.49	0.42
1:A:2808:LEU:HD21	1:A:2856:LEU:HD12	2.01	0.42
1:B:3010:LEU:HD22	1:B:3320:LEU:HD12	2.01	0.42
1:A:2395:ILE:H	1:A:2395:ILE:HD12	1.83	0.42
1:B:2788:ARG:H	1:B:3459:ASP:CB	2.32	0.42
1:B:2383:HIS:CE1	1:B:2384:GLU:HG3	2.53	0.42
1:A:3466:ILE:HD13	1:A:3509:LEU:HD13	2.01	0.42
1:B:3848:LEU:O	1:B:3851:VAL:N	2.52	0.42
1:A:1660:VAL:HG11	1:A:1728:TRP:CH2	2.54	0.42
1:B:2109:LEU:HD11	1:B:2129:LEU:HD23	2.00	0.42
1:B:1527:LEU:CD2	1:B:1545:LEU:HD22	2.49	0.42
1:A:2262:LEU:HA	1:A:2265:ILE:HD12	2.02	0.42
1:B:2488:GLU:CG	1:B:2491:LEU:HD12	2.48	0.42
1:B:2380:LEU:HD11	1:B:2390:ILE:HD11	1.97	0.42
1:B:1704:GLU:OE2	1:B:1768:ARG:NH1	2.53	0.42
1:A:3436:PHE:CE2	1:A:3462:ILE:HD11	2.54	0.42
1:B:1759:LYS:CD	1:B:1761:GLU:OE2	2.67	0.42
1:B:2080:LYS:HG2	2:B:5093:ATP:PB	2.60	0.42
1:A:1540:LEU:CD1	1:A:1548:ILE:HD12	2.50	0.42
1:A:1748:PHE:CE2	1:A:1755:LEU:HD22	2.54	0.42
1:B:2428:MET:SD	1:B:2429:ASN:N	2.93	0.42
1:A:3832:SER:O	1:A:3836:GLY:N	2.46	0.42
1:B:1656:TRP:HE1	1:B:1712:ILE:HD11	1.85	0.42
1:B:1827:ASP:HB3	1:B:1830:VAL:HG12	2.02	0.42
1:A:3946:VAL:HA	1:A:3947:PRO:C	2.39	0.42
1:B:2048:SER:N	2:B:5093:ATP:HN62	2.08	0.42
1:A:2385:VAL:HG13	1:A:2386:MET:N	2.33	0.42
1:B:3846:MET:HG3	1:B:3847:SER:N	2.34	0.42
1:A:3945:LEU:HD21	1:A:4059:LEU:HD22	2.02	0.42
1:A:2354:SER:OG	1:A:2357:SER:CA	2.68	0.42
1:B:2866:LEU:HD12	1:B:2867:LEU:H	1.85	0.42
1:A:2416:LEU:HB3	1:A:2424:LYS:CD	2.50	0.42
1:B:2151:TRP:HE3	1:B:2193:LEU:HD11	1.85	0.42
1:B:1940:GLU:CG	1:B:1941:ASP:H	2.19	0.42
1:B:2549:ARG:HG2	2:B:5093:ATP:O1G	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4023:ILE:HD11	1:A:4029:ILE:CD1	2.50	0.42
1:A:1626:CYS:HB2	1:A:1643:TYR:CD2	2.55	0.42
1:B:3631:MET:HE1	1:B:3698:MET:HG3	2.00	0.42
1:B:1742:ASP:HB3	1:B:1745:ASN:HD22	1.85	0.42
1:B:2437:LEU:HA	1:B:2480:LYS:HD3	2.02	0.42
1:A:1527:LEU:HD21	1:A:1546:LEU:CD2	2.50	0.42
1:A:2312:ASP:HB3	1:A:2351:GLN:HG3	2.01	0.42
1:B:2368:PHE:O	1:B:2368:PHE:CD1	2.72	0.42
1:A:1627:LEU:HD11	1:A:1631:LYS:HE3	2.01	0.42
1:A:1873:GLN:HE22	1:A:1915:SER:HA	1.84	0.42
1:A:3997:LYS:H	1:A:3997:LYS:HG3	1.53	0.42
1:A:1945:LEU:HD13	1:A:1994:VAL:HG21	2.02	0.42
1:A:4021:LEU:CD2	1:A:4023:ILE:HG12	2.41	0.42
1:A:1606:GLU:O	1:A:1610:ILE:HG12	2.20	0.42
1:A:2984:VAL:C	1:A:2986:PRO:HD3	2.40	0.42
1:B:1769:LEU:HD11	1:B:1804:GLU:HB3	2.01	0.42
1:A:2324:TYR:CD1	1:A:2403:ILE:HG12	2.55	0.42
1:A:1406:LYS:HB3	1:A:1406:LYS:HE2	1.84	0.42
1:B:2756:MET:O	1:B:2888:VAL:HA	2.20	0.42
1:A:2224:SER:O	2:A:5093:ATP:H2	2.03	0.42
1:A:2389:ASP:OD1	1:A:2389:ASP:O	2.37	0.42
1:B:2129:LEU:O	1:B:2133:ILE:HG12	2.20	0.42
1:B:1946:ALA:O	1:B:1950:VAL:HG23	2.20	0.42
1:A:1579:ILE:HG13	1:A:1598:LEU:HD11	2.00	0.42
1:A:2044:ARG:HH21	1:A:2093:ILE:HD11	1.85	0.42
1:B:2965:VAL:HA	1:B:2968:ILE:HD12	2.01	0.42
1:B:2107:LYS:HE3	1:B:2495:ASP:OD2	2.19	0.42
1:A:2153:VAL:C	1:A:2154:PHE:HD1	2.24	0.42
1:B:2512:LYS:O	1:B:2513:GLN:CB	2.55	0.42
1:B:2081:THR:OG1	2:B:5093:ATP:O2A	2.37	0.42
1:A:2386:MET:HB3	1:A:2627:ARG:HD3	1.98	0.42
1:B:1801:GLY:N	5:B:5097:SO4:O3	2.52	0.42
1:B:1392:LEU:HD13	1:B:1393:LYS:CA	2.50	0.42
1:B:2104:ILE:O	1:B:2154:PHE:HA	2.20	0.42
1:A:2134:LEU:HD11	1:A:2138:ASN:ND2	2.34	0.42
1:B:2278:VAL:O	1:B:2283:LYS:HE2	2.19	0.42
1:A:2278:VAL:O	1:A:2283:LYS:HE2	2.19	0.42
1:A:1749:ILE:HD13	1:A:1813:LEU:HD22	2.02	0.42
1:A:3939:ILE:HG13	1:A:4010:LEU:CD2	2.50	0.42
1:A:3669:THR:HA	1:A:3672:ASP:HB2	2.00	0.42
1:A:1635:ASP:HB2	1:A:1638:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3965:SER:HA	1:B:3968:LEU:HD12	2.02	0.42
1:A:3888:LEU:O	1:A:3892:THR:HG22	2.19	0.42
1:A:4033:LEU:CD1	1:A:4035:GLN:N	2.83	0.41
1:A:2707:VAL:HG12	1:A:2708:ASN:N	2.35	0.41
1:A:1586:GLU:HG3	1:A:1765:ILE:H	1.84	0.41
1:B:2627:ARG:NH1	1:B:2630:TYR:CE2	2.87	0.41
1:B:1758:TYR:CD1	1:B:1759:LYS:O	2.73	0.41
1:B:2155:ASP:O	1:B:2549:ARG:NH1	2.53	0.41
1:A:1391:GLY:HA3	1:A:1484:LYS:HZ3	1.84	0.41
1:B:3702:MET:CB	1:B:3767:PHE:HZ	2.32	0.41
1:A:3628:ILE:HD11	1:A:3679:TYR:CZ	2.54	0.41
1:A:3411:SER:O	1:A:3413:HIS:N	2.50	0.41
1:A:1910:GLU:HB2	1:A:3846:MET:HA	2.01	0.41
1:B:1645:PHE:CZ	1:B:1649:LEU:HD22	2.55	0.41
1:B:2908:LEU:O	1:B:2912:CYS:HB2	2.20	0.41
1:B:3505:ILE:O	1:B:3510:ARG:NH1	2.54	0.41
1:A:3570:LEU:HD23	1:A:3580:ASN:CG	2.41	0.41
1:A:1392:LEU:HD23	1:A:1484:LYS:HA	2.02	0.41
1:A:2571:TYR:HD1	1:A:2626:VAL:HG21	1.85	0.41
1:A:2401:GLU:HG2	1:A:2431:ALA:HB2	2.02	0.41
1:B:2464:TYR:CE1	1:B:2524:VAL:HG11	2.55	0.41
1:A:1391:GLY:HA3	1:A:1484:LYS:HZ1	1.85	0.41
1:A:1830:VAL:O	1:A:1834:LEU:HG	2.20	0.41
1:A:2503:VAL:HA	1:A:2506:LEU:HD12	2.02	0.41
1:B:1479:LEU:HD11	1:B:1515:SER:HB3	2.03	0.41
1:A:3967:TYR:HE2	1:A:3985:VAL:HA	1.85	0.41
1:A:1659:LEU:O	1:A:1663:CYS:HB2	2.20	0.41
1:A:4033:LEU:CD1	1:A:4035:GLN:H	2.33	0.41
1:A:2412:ARG:HG3	1:A:2412:ARG:NH1	2.34	0.41
1:A:1926:SER:HA	1:A:1929:ILE:HD13	2.02	0.41
1:A:1422:LYS:O	1:A:1425:GLU:HB3	2.21	0.41
1:B:1802:LYS:O	1:B:1806:VAL:HG23	2.20	0.41
1:A:1495:THR:HB	1:A:1498:GLU:CG	2.51	0.41
1:B:2783:GLN:HG2	1:B:2816:ILE:HB	2.02	0.41
1:B:2786:ILE:H	1:B:2786:ILE:HG13	1.68	0.41
1:B:2491:LEU:HD21	1:B:2543:ARG:NH1	2.35	0.41
1:A:2757:MET:HG2	1:A:2889:PHE:HD2	1.78	0.41
1:B:1998:LEU:CD1	1:B:2022:PHE:HZ	2.34	0.41
1:B:3353:LEU:HD23	1:B:3358:VAL:CG1	2.50	0.41
1:A:2397:THR:HG22	1:A:2398:ILE:HD13	2.03	0.41
1:A:2098:ALA:O	1:A:2149:ARG:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2225:LYS:HD2	1:A:2281:PHE:CZ	2.55	0.41
1:A:1748:PHE:HD2	1:A:1755:LEU:HD22	1.85	0.41
1:A:2375:ILE:HG22	1:A:2376:PRO:O	2.20	0.41
1:A:3308:ASN:O	1:A:3312:GLN:HB2	2.21	0.41
1:A:1979:ASN:OD1	1:A:2066:THR:HG21	2.20	0.41
1:B:3431:PHE:CE1	1:B:3458:PHE:HD1	2.37	0.41
1:B:3303:LYS:HD2	1:B:3306:TRP:HD1	1.76	0.41
1:B:1970:LEU:HD23	1:B:1974:LYS:CE	2.46	0.41
1:A:4085:THR:O	1:A:4089:LEU:HG	2.21	0.41
1:A:2415:ILE:O	1:A:2556:ILE:HA	2.21	0.41
1:A:3642:TYR:CD1	1:A:3642:TYR:N	2.87	0.41
1:A:2428:MET:SD	1:A:2429:ASN:N	2.94	0.41
1:B:2632:ALA:HB3	1:B:2647:LEU:HD21	2.01	0.41
1:A:40:TRP:O	1:A:44:LYS:N	2.53	0.41
1:B:2757:MET:HB2	1:B:2889:PHE:HB2	2.01	0.41
1:A:2707:VAL:HG12	1:A:2712:LEU:HD12	2.02	0.41
1:A:1765:ILE:HD13	1:A:1765:ILE:HG21	1.72	0.41
1:B:2464:TYR:CE1	1:B:2474:LEU:HD12	2.56	0.41
1:A:2761:ALA:O	1:A:2892:CYS:SG	2.78	0.41
1:B:2784:PRO:HG2	1:B:2817:ILE:HD13	2.01	0.41
1:B:2824:GLU:HG2	1:B:2825:THR:H	1.86	0.41
1:B:3901:PRO:HB2	1:B:3906:THR:HG23	2.02	0.41
1:A:2475:PRO:HB3	1:A:2527:GLU:CB	2.50	0.41
1:B:1535:PRO:O	1:B:1841:ILE:CD1	2.69	0.41
1:A:2046:GLY:O	1:A:2228:HIS:HB2	2.20	0.41
1:B:3850:TRP:NE1	1:B:3854:TYR:CB	2.82	0.41
1:B:3330:TYR:CZ	1:B:3346:LEU:HD13	2.55	0.41
1:A:2039:LYS:O	1:A:2043:GLN:HG2	2.21	0.41
1:A:2609:THR:HA	1:A:2612:GLN:O	2.20	0.41
1:A:2765:GLY:HA2	1:A:2768:ILE:HG22	2.02	0.41
1:B:216:PRO:C	1:B:1365:PHE:CA	2.82	0.41
1:B:2788:ARG:H	1:B:3459:ASP:HB2	1.86	0.41
1:B:1409:LEU:CD2	1:B:1435:LEU:CB	2.82	0.41
1:B:1945:LEU:HD21	1:B:1991:GLU:HB3	2.03	0.41
1:A:2835:LEU:HD23	1:A:2911:ARG:HB2	2.03	0.41
1:A:1462:ASN:HB3	1:A:1465:ILE:HG22	2.00	0.41
1:B:2481:ASN:ND2	1:B:2528:ARG:HB3	2.36	0.41
1:B:2391:VAL:CG2	1:B:2426:MET:HE1	2.49	0.41
1:B:3978:ASN:O	1:B:3981:PRO:HD2	2.21	0.41
1:A:2201:HIS:CE1	1:A:2497:TYR:CA	3.04	0.41
1:A:3628:ILE:HG13	1:A:3705:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2455:LEU:HD21	1:A:2515:PHE:CE2	2.56	0.41
1:B:2760:GLY:O	1:B:2761:ALA:HB3	2.21	0.41
1:A:4022:GLN:HA	1:A:4028:ARG:HA	2.03	0.41
1:B:2654:ARG:HH22	1:B:2691:SER:HB2	1.84	0.41
1:A:3331:GLU:HA	1:A:3396:ILE:HG12	2.03	0.41
1:B:3413:HIS:O	1:B:3417:VAL:HG23	2.21	0.41
1:A:2780:LYS:HB3	1:A:2813:THR:HG22	2.02	0.41
1:A:3632:LEU:HD13	1:A:3644:ILE:HD13	2.02	0.41
1:A:4034:LEU:C	1:A:4034:LEU:HD23	2.41	0.41
1:B:2354:SER:OG	1:B:2357:SER:CA	2.68	0.41
1:A:2412:ARG:HD2	1:A:2412:ARG:HA	1.86	0.41
1:B:2494:LEU:HD12	1:B:2494:LEU:C	2.41	0.41
1:B:1391:GLY:HA3	1:B:1484:LYS:HZ1	1.86	0.41
1:A:2426:MET:CG	1:A:2427:ILE:N	2.81	0.41
1:B:2808:LEU:HD21	1:B:2856:LEU:HD12	2.03	0.41
1:A:1838:ILE:HG21	1:A:1838:ILE:HD13	1.81	0.41
1:A:2492:PRO:CB	1:A:2502:VAL:HG11	2.50	0.41
1:A:2502:VAL:O	1:A:2505:PHE:HB3	2.20	0.41
1:A:2707:VAL:HG11	1:A:2712:LEU:CD1	2.49	0.40
1:B:2637:PRO:HD3	1:B:2703:ASP:HB3	2.03	0.40
1:A:2416:LEU:O	1:A:2534:ALA:HA	2.22	0.40
1:B:2368:PHE:O	1:B:2369:SER:OG	2.28	0.40
1:A:2407:LEU:HB2	1:A:2414:ILE:HD11	2.03	0.40
1:B:1547:LYS:O	1:B:1551:SER:HB3	2.21	0.40
1:A:1817:VAL:HG22	1:A:1844:TRP:CB	2.51	0.40
1:A:2290:LEU:HD23	1:A:2321:SER:HA	2.02	0.40
1:A:2060:PHE:CZ	1:A:2193:LEU:HD21	2.57	0.40
1:B:1822:CYS:SG	1:B:1850:PHE:HA	2.61	0.40
1:A:2141:ILE:HG22	1:A:2145:PHE:CG	2.55	0.40
1:B:2302:PHE:HA	1:B:2310:LEU:HD11	2.02	0.40
1:A:3848:LEU:O	1:A:3849:SER:C	2.59	0.40
1:A:2653:TRP:HB3	1:A:2654:ARG:NH1	2.35	0.40
1:B:3877:CYS:SG	1:B:3884:LEU:HD22	2.61	0.40
1:B:2507:ARG:HG3	1:B:2550:PHE:HA	2.03	0.40
1:A:2488:GLU:O	1:A:2491:LEU:HB2	2.21	0.40
1:A:2787:HIS:CA	1:A:3460:PRO:HG2	2.40	0.40
1:A:1939:PHE:O	1:A:1940:GLU:HB3	2.22	0.40
1:B:1534:PHE:CD2	1:B:1537:PHE:CE1	3.05	0.40
1:A:3566:LEU:HD13	1:A:3570:LEU:HD12	2.03	0.40
1:B:2745:ILE:CG1	1:B:2756:MET:HE3	2.43	0.40
1:A:1531:ARG:HD3	1:A:1538:TYR:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3848:LEU:O	1:B:3849:SER:C	2.59	0.40
1:A:2514:GLY:HA3	1:A:2525:THR:HA	2.03	0.40
1:A:3968:LEU:HA	1:A:3971:VAL:HG12	2.02	0.40
1:A:3508:PHE:O	1:A:3512:ARG:HG2	2.21	0.40
1:A:1375:LYS:O	1:A:1379:LYS:HG2	2.21	0.40
1:A:3379:TRP:CD2	1:A:3394:MET:HG3	2.56	0.40
1:B:1826:PHE:CZ	1:B:1831:LEU:CA	3.04	0.40
1:B:1409:LEU:O	1:B:1413:VAL:HG23	2.22	0.40
1:A:1421:TYR:O	1:A:1425:GLU:CA	2.69	0.40
1:B:2474:LEU:HB3	1:B:2526:ILE:HG22	2.02	0.40
1:B:1531:ARG:HD3	1:B:1537:PHE:O	2.20	0.40
1:B:2160:PRO:HA	1:B:2163:VAL:HG22	2.04	0.40
1:B:1794:PHE:HB3	1:B:1919:PHE:HB3	2.03	0.40
1:A:23:LEU:C	1:A:25:GLU:N	2.74	0.40
1:A:2516:TRP:CZ3	1:A:2523:TRP:HB2	2.56	0.40
1:B:3908:LYS:HG2	1:B:4049:LEU:HD13	2.03	0.40
1:B:1529:ARG:O	1:B:1533:GLN:HG2	2.21	0.40
1:A:1857:VAL:O	1:A:1861:VAL:HG23	2.21	0.40
1:B:2008:ASP:HA	1:B:2011:GLU:HB2	2.03	0.40
1:A:1421:TYR:CD2	1:A:1425:GLU:HG2	2.55	0.40
1:A:1392:LEU:CD1	1:A:1392:LEU:C	2.86	0.40
1:A:1392:LEU:HD13	1:A:1393:LYS:CA	2.51	0.40
1:A:3671:VAL:HA	1:A:3674:ILE:CG2	2.49	0.40
1:B:3924:TRP:CD1	1:B:3924:TRP:O	2.75	0.40
1:B:3930:PHE:HE2	1:B:4029:ILE:CD1	2.33	0.40
1:A:1727:LEU:O	1:A:1731:VAL:HG23	2.22	0.40
1:B:2582:VAL:O	1:B:2582:VAL:HG23	2.21	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%)	2511 (95%)	118 (4%)	11 (0%)	39	76
1	B	2640/2695 (98%)	2525 (96%)	107 (4%)	8 (0%)	46	81
All	All	5280/5390 (98%)	5036 (95%)	225 (4%)	19 (0%)	39	76

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1391	GLY
1	A	2495	ASP
1	B	1391	GLY
1	A	2476	LYS
1	A	2728	LEU
1	B	66	GLN
1	A	2519	PRO
1	B	2519	PRO
1	B	2990	GLY
1	B	3914	GLN
1	A	66	GLN
1	A	2990	GLY
1	A	3980	ILE
1	A	2562	PRO
1	B	2562	PRO
1	B	3980	ILE
1	A	3462	ILE
1	B	1470	PRO
1	A	2028	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	2115 (95%)	103 (5%)	33	71
1	B	2218/2453 (90%)	2145 (97%)	73 (3%)	45	78
All	All	4436/4906 (90%)	4260 (96%)	176 (4%)	38	74

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1421	TYR
1	A	1455	LEU
1	A	1486	ILE
1	A	1493	LEU
1	A	1641	SER
1	A	1719	SER
1	A	1793	CYS
1	A	1794	PHE
1	A	1852	ARG
1	A	1891	HIS
1	A	1923	SER
1	A	1964	ASN
1	A	2081	THR
1	A	2109	LEU
1	A	2141	ILE
1	A	2154	PHE
1	A	2155	ASP
1	A	2202	THR
1	A	2228	HIS
1	A	2229	LEU
1	A	2273	VAL
1	A	2320	ARG
1	A	2351	GLN
1	A	2357	SER
1	A	2387	ARG
1	A	2390	ILE
1	A	2397	THR
1	A	2425	THR
1	A	2428	MET
1	A	2430	ASN
1	A	2472	THR
1	A	2476	LYS
1	A	2482	LEU
1	A	2510	MET
1	A	2522	LYS
1	A	2526	ILE
1	A	2535	CYS
1	A	2547	SER
1	A	2548	GLU
1	A	2563	SER
1	A	2566	SER
1	A	2574	TYR

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Mol	Chain	Res	Type
1	A	2576	LYS
1	A	2613	SER
1	A	2623	THR
1	A	2689	ILE
1	A	2738	MET
1	A	2769	LEU
1	A	2785	LYS
1	A	2822	ILE
1	A	2823	LEU
1	A	2833	THR
1	A	2843	LEU
1	A	2856	LEU
1	A	2863	LEU
1	A	2911	ARG
1	A	2967	ASN
1	A	2979	LYS
1	A	3012	GLU
1	A	3019	VAL
1	A	3301	PHE
1	A	3329	ILE
1	A	3372	THR
1	A	3391	LEU
1	A	3400	SER
1	A	3401	GLN
1	A	3512	ARG
1	A	3543	ARG
1	A	3548	LEU
1	A	3560	LYS
1	A	3567	LEU
1	A	3578	LEU
1	A	3595	MET
1	A	3598	GLU
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	3812	LYS
1	A	3823	ASN

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Mol	Chain	Res	Type
1	A	3831	LYS
1	A	3862	THR
1	A	3871	PHE
1	A	3876	THR
1	A	3884	LEU
1	A	3899	ASP
1	A	3905	ASP
1	A	3906	THR
1	A	3943	THR
1	A	3952	LYS
1	A	3958	ASP
1	A	3960	ASP
1	A	3982	TRP
1	A	3992	ILE
1	A	3997	LYS
1	A	4016	CYS
1	A	4040	GLU
1	A	4042	ARG
1	A	4046	THR
1	B	1383	TYR
1	B	1421	TYR
1	B	1422	LYS
1	B	1426	GLN
1	B	1486	ILE
1	B	1504	ASN
1	B	1646	GLN
1	B	1694	VAL
1	B	1767	GLU
1	B	1794	PHE
1	B	1936	ILE
1	B	2027	THR
1	B	2068	GLN
1	B	2141	ILE
1	B	2285	GLU
1	B	2295	ILE
1	B	2307	ASP
1	B	2351	GLN
1	B	2381	GLU
1	B	2386	MET
1	B	2390	ILE
1	B	2395	ILE
1	B	2428	MET

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Mol	Chain	Res	Type
1	B	2430	ASN
1	B	2474	LEU
1	B	2476	LYS
1	B	2510	MET
1	B	2566	SER
1	B	2574	TYR
1	B	2613	SER
1	B	2616	LEU
1	B	2623	THR
1	B	2681	LEU
1	B	2689	ILE
1	B	2747	ARG
1	B	2829	GLU
1	B	2835	LEU
1	B	2853	LEU
1	B	2856	LEU
1	B	2920	TRP
1	B	2967	ASN
1	B	2969	LEU
1	B	3329	ILE
1	B	3360	TYR
1	B	3372	THR
1	B	3391	LEU
1	B	3400	SER
1	B	3502	SER
1	B	3538	ASN
1	B	3548	LEU
1	B	3559	LEU
1	B	3565	ARG
1	B	3567	LEU
1	B	3581	ASP
1	B	3598	GLU
1	B	3605	GLU
1	B	3618	TYR
1	B	3677	LEU
1	B	3729	SER
1	B	3737	THR
1	B	3844	ILE
1	B	3860	GLU
1	B	3871	PHE
1	B	3899	ASP
1	B	3905	ASP

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Mol	Chain	Res	Type
1	B	3906	THR
1	B	3917	THR
1	B	3943	THR
1	B	3960	ASP
1	B	3982	TRP
1	B	4016	CYS
1	B	4024	VAL
1	B	4087	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1605	GLN
1	A	1622	GLN
1	A	1745	ASN
1	A	1864	ASN
1	A	1873	GLN
1	A	1899	ASN
1	A	1965	HIS
1	A	2064	GLN
1	A	2068	GLN
1	A	2099	ASN
1	A	2138	ASN
1	A	2228	HIS
1	A	2274	HIS
1	A	2282	ASN
1	A	2293	HIS
1	A	2383	HIS
1	A	2409	ASN
1	A	2459	HIS
1	A	2481	ASN
1	A	2530	HIS
1	A	2536	ASN
1	A	2634	ASN
1	A	2688	ASN
1	A	2896	ASN
1	A	2910	ASN
1	A	2927	GLN
1	A	3323	ASN
1	A	3497	HIS
1	A	3521	ASN
1	A	3624	HIS

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Mol	Chain	Res	Type
1	A	3780	ASN
1	A	3842	GLN
1	A	3890	GLN
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	1745	ASN
1	B	1851	ASN
1	B	1864	ASN
1	B	1873	GLN
1	B	1899	ASN
1	B	1951	HIS
1	B	2068	GLN
1	B	2228	HIS
1	B	2274	HIS
1	B	2282	ASN
1	B	2293	HIS
1	B	2335	GLN
1	B	2351	GLN
1	B	2383	HIS
1	B	2409	ASN
1	B	2481	ASN
1	B	2536	ASN
1	B	2753	GLN
1	B	2910	ASN
1	B	3308	ASN
1	B	3338	ASN
1	B	3471	ASN
1	B	3497	HIS
1	B	3521	ASN
1	B	3542	GLN
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

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Mol	Chain	Res	Type
1	B	4020	ASN
1	B	4031	GLN
1	B	4077	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	A	5093	4	24,33,33	0.98	1 (4%)	31,52,52	1.99	5 (16%)
3	ADP	A	5094	-	22,29,29	1.26	1 (4%)	27,45,45	2.36	5 (18%)
5	SO4	A	5096	-	4,4,4	1.48	1 (25%)	6,6,6	1.34	1 (16%)
5	SO4	A	5097	-	4,4,4	0.61	0	6,6,6	0.58	0
2	ATP	B	5093	4	24,33,33	1.08	1 (4%)	31,52,52	1.91	6 (19%)
3	ADP	B	5094	-	22,29,29	1.31	3 (13%)	27,45,45	2.46	8 (29%)
5	SO4	B	5096	-	4,4,4	1.25	1 (25%)	6,6,6	1.94	1 (16%)
5	SO4	B	5097	-	4,4,4	0.46	0	6,6,6	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	5093	4	-	0/18/38/38	0/3/3/3
3	ADP	A	5094	-	-	0/12/32/32	0/3/3/3
5	SO4	A	5096	-	-	0/0/0/0	0/0/0/0
5	SO4	A	5097	-	-	0/0/0/0	0/0/0/0
2	ATP	B	5093	4	-	0/18/38/38	0/3/3/3
3	ADP	B	5094	-	-	0/12/32/32	0/3/3/3
5	SO4	B	5096	-	-	0/0/0/0	0/0/0/0
5	SO4	B	5097	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5094	ADP	PB-O3B	-2.10	1.47	1.54
5	B	5096	SO4	O2-S	2.05	1.54	1.47
3	B	5094	ADP	C4-N3	2.55	1.39	1.35
5	A	5096	SO4	O1-S	2.89	1.57	1.47
2	A	5093	ATP	C5-C4	3.13	1.47	1.40
2	B	5093	ATP	C5-C4	3.41	1.48	1.40
3	A	5094	ADP	C5-C4	3.65	1.48	1.40
3	B	5094	ADP	C5-C4	3.66	1.48	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5094	ADP	N3-C2-N1	-10.12	121.14	128.89
3	B	5094	ADP	N3-C2-N1	-9.35	121.73	128.89
2	A	5093	ATP	N3-C2-N1	-6.70	123.77	128.89
2	B	5093	ATP	N3-C2-N1	-5.61	124.60	128.89
2	B	5093	ATP	PA-O3A-PB	-4.38	120.43	132.73
3	B	5094	ADP	C2'-C1'-N9	-4.37	107.61	114.29
2	A	5093	ATP	PA-O3A-PB	-4.35	120.51	132.73
2	B	5093	ATP	C4-C5-N7	-3.66	106.11	109.48
2	B	5093	ATP	PB-O3B-PG	-3.64	120.47	132.67
2	A	5093	ATP	PB-O3B-PG	-3.62	120.53	132.67
2	A	5093	ATP	C4-C5-N7	-3.13	106.60	109.48
3	A	5094	ADP	PA-O3A-PB	-3.11	122.24	132.67
2	A	5093	ATP	C2'-C1'-N9	-3.02	109.68	114.29
2	B	5093	ATP	C2'-C1'-N9	-2.99	109.72	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5094	ADP	PA-O3A-PB	-2.96	122.74	132.67
3	B	5094	ADP	C5'-C4'-C3'	-2.51	105.26	115.21
3	B	5094	ADP	O3A-PA-O5'	-2.14	97.27	102.94
3	B	5094	ADP	C4-C5-N7	-2.08	107.57	109.48
2	B	5093	ATP	C4'-O4'-C1'	2.02	111.94	109.72
3	A	5094	ADP	O3B-PB-O2B	2.06	115.23	107.38
5	A	5096	SO4	O2-S-O1	2.23	116.57	109.50
3	B	5094	ADP	C2-N1-C6	2.26	122.80	118.77
3	A	5094	ADP	C2'-C3'-C4'	2.47	107.69	102.61
3	B	5094	ADP	C4'-O4'-C1'	2.63	112.61	109.72
3	A	5094	ADP	C2-N1-C6	2.88	123.91	118.77
5	B	5096	SO4	O2-S-O1	4.41	123.48	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5093	ATP	10	0
3	A	5094	ADP	2	0
5	A	5097	SO4	2	0
2	B	5093	ATP	24	0
3	B	5094	ADP	6	0
5	B	5096	SO4	2	0
5	B	5097	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	2650/2695 (98%)	0.21	147 (5%)	29 23	62, 134, 265, 480	1 (0%)
1	B	2650/2695 (98%)	0.70	336 (12%)	5 4	83, 185, 334, 500	1 (0%)
All	All	5300/5390 (98%)	0.46	483 (9%)	11 9	62, 158, 303, 500	2 (0%)

All (483) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	SER	19.7
1	B	59	ASP	17.7
1	B	69	ALA	17.3
1	B	31	LEU	16.5
1	B	60	GLY	15.3
1	B	46	GLU	15.2
1	B	70	ILE	15.0
1	B	52	PRO	14.6
1	B	1572	ILE	14.3
1	B	94	LEU	13.9
1	B	18	LEU	13.8
1	B	1549	ILE	13.6
1	B	61	ASP	13.4
1	B	58	ILE	12.1
1	B	1550	GLY	12.1
1	B	47	LEU	11.7
1	B	87	GLU	11.4
1	B	71	ILE	10.9
1	B	95	GLU	10.4
1	A	2	PRO	10.3
1	A	147	VAL	10.3
1	A	20	LEU	10.2
1	B	30	HIS	9.9
1	B	1581	GLY	9.8

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Mol	Chain	Res	Type	RSRZ
1	B	1592	LEU	9.1
1	B	2	PRO	9.0
1	B	1582	VAL	8.9
1	A	63	LYS	8.8
1	B	8	LYS	8.7
1	B	1459	LEU	8.7
1	B	19	LEU	8.5
1	B	1546	LEU	8.3
1	B	199	ALA	8.3
1	B	1596	ILE	8.2
1	B	27	TYR	8.2
1	B	1680	ILE	8.1
1	A	148	THR	8.1
1	A	216	PRO	8.1
1	B	1669	PHE	8.1
1	B	149	HIS	8.0
1	B	1452	TRP	8.0
1	B	1683	LEU	8.0
1	B	17	ARG	7.9
1	B	184	ALA	7.9
1	B	63	LYS	7.6
1	B	3915	PHE	7.6
1	B	186	PRO	7.6
1	B	148	THR	7.5
1	B	155	TYR	7.4
1	B	1845	GLY	7.3
1	B	45	PHE	7.0
1	B	1394	LEU	7.0
1	B	1602	ILE	6.9
1	B	1483	TYR	6.9
1	B	86	LYS	6.9
1	B	55	PRO	6.9
1	A	71	ILE	6.9
1	A	76	ASP	6.9
1	A	1	SER	6.8
1	B	49	LEU	6.7
1	B	151	ASP	6.7
1	B	79	ASN	6.7
1	B	1684	LEU	6.6
1	A	74	ILE	6.6
1	B	16	THR	6.6
1	A	1483	TYR	6.6

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Mol	Chain	Res	Type	RSRZ
1	B	1601	SER	6.6
1	A	84	CYS	6.5
1	B	193	LYS	6.5
1	B	73	TYR	6.5
1	B	1574	PHE	6.4
1	B	88	ARG	6.3
1	A	54	LEU	6.3
1	A	27	TYR	6.3
1	B	1647	ALA	6.2
1	A	135	ARG	6.2
1	B	62	VAL	6.1
1	B	202	LEU	6.1
1	B	44	LYS	6.1
1	B	1603	GLN	6.1
1	B	3919	LYS	6.1
1	B	72	ARG	5.9
1	B	187	GLN	5.9
1	B	96	GLY	5.9
1	A	59	ASP	5.9
1	B	78	HIS	5.9
1	B	1579	ILE	5.9
1	A	73	TYR	5.8
1	B	93	MET	5.8
1	B	1456	TYR	5.7
1	B	3580	ASN	5.7
1	B	1460	GLY	5.6
1	B	7	TRP	5.5
1	B	91	ILE	5.4
1	B	134	ASP	5.4
1	B	84	CYS	5.4
1	B	1545	LEU	5.4
1	B	92	SER	5.4
1	B	85	PRO	5.2
1	B	67	SER	5.1
1	B	43	LYS	5.1
1	B	1573	ILE	5.1
1	B	1644	ILE	5.1
1	B	1760	PHE	5.1
1	B	1730	LYS	5.1
1	B	161	VAL	5.0
1	B	42	ASN	5.0
1	B	143	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	26	LYS	5.0
1	A	3575	GLY	4.9
1	B	1590	LEU	4.9
1	B	1476	PHE	4.9
1	B	3916	PHE	4.9
1	B	80	MET	4.9
1	B	1937	MET	4.9
1	B	54	LEU	4.9
1	A	48	GLY	4.9
1	B	1551	SER	4.9
1	A	23	LEU	4.9
1	B	1894	VAL	4.9
1	B	28	GLU	4.8
1	B	1767	GLU	4.8
1	A	61	ASP	4.8
1	B	1606	GLU	4.8
1	B	1679	LYS	4.8
1	B	1458	ILE	4.8
1	B	3555	TYR	4.8
1	B	1580	THR	4.7
1	B	1497	ILE	4.7
1	B	2353	LEU	4.7
1	B	216	PRO	4.7
1	B	3566	LEU	4.7
1	B	3304	GLU	4.7
1	B	89	ALA	4.7
1	B	1492	GLN	4.6
1	A	62	VAL	4.5
1	B	64	LEU	4.5
1	B	210	GLY	4.5
1	B	3588	ASN	4.5
1	A	3566	LEU	4.4
1	B	32	TYR	4.4
1	B	1605	GLN	4.4
1	A	3567	LEU	4.4
1	B	1505	PHE	4.4
1	A	83	GLY	4.4
1	B	74	ILE	4.4
1	A	77	LYS	4.3
1	B	25	GLU	4.3
1	B	20	LEU	4.3
1	B	150	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	183	GLU	4.3
1	B	3572	ASN	4.2
1	B	1506	ASP	4.2
1	B	198	ILE	4.2
1	A	81	LEU	4.1
1	A	3568	GLU	4.1
1	A	143	ASN	4.1
1	A	19	LEU	4.1
1	A	151	ASP	4.1
1	B	1682	GLY	4.1
1	B	1445	TRP	4.1
1	A	88	ARG	4.0
1	B	2938	MET	4.0
1	B	1675	GLU	4.0
1	B	3734	PRO	4.0
1	B	2363	ASN	4.0
1	A	25	GLU	4.0
1	B	1792	GLY	4.0
1	B	1486	ILE	4.0
1	B	66	GLN	4.0
1	A	142	LEU	3.9
1	B	1465	ILE	3.9
1	B	48	GLY	3.9
1	B	75	ALA	3.9
1	A	184	ALA	3.9
1	B	3571	ASN	3.9
1	B	215	PRO	3.9
1	A	2364	ASP	3.9
1	B	1594	GLU	3.8
1	B	138	HIS	3.8
1	B	3585	VAL	3.8
1	B	192	LEU	3.8
1	B	1395	VAL	3.8
1	B	3934	TRP	3.8
1	B	68	MET	3.8
1	A	85	PRO	3.7
1	A	75	ALA	3.7
1	B	2121	ALA	3.7
1	A	91	ILE	3.7
1	A	3580	ASN	3.7
1	B	50	GLU	3.7
1	B	152	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	24	GLU	3.7
1	B	1893	ALA	3.7
1	B	200	TRP	3.7
1	A	3555	TYR	3.6
1	A	80	MET	3.6
1	B	1595	LYS	3.6
1	B	1604	ALA	3.6
1	B	5	GLY	3.6
1	B	1676	VAL	3.5
1	B	53	ASN	3.5
1	B	1835	LEU	3.5
1	B	1566	PHE	3.5
1	B	1994	VAL	3.5
1	B	6	TYR	3.5
1	A	132	PHE	3.5
1	B	133	GLU	3.5
1	B	1532	ARG	3.5
1	B	1711	VAL	3.5
1	A	18	LEU	3.5
1	B	51	PHE	3.4
1	A	3564	LYS	3.4
1	B	1472	GLU	3.4
1	B	1737	LYS	3.4
1	A	67	SER	3.4
1	B	1423	ILE	3.4
1	B	1562	MET	3.4
1	B	209	PHE	3.4
1	B	201	PRO	3.4
1	B	1732	GLN	3.3
1	B	3020	GLY	3.3
1	A	35	ASP	3.3
1	A	82	GLY	3.3
1	B	1489	ARG	3.3
1	A	2029	LEU	3.3
1	B	3920	ILE	3.3
1	B	3811	LEU	3.2
1	B	3024	LEU	3.2
1	A	2676	THR	3.2
1	B	189	ASP	3.2
1	B	162	LEU	3.2
1	B	1828	TYR	3.2
1	B	1591	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	2863	LEU	3.1
1	A	1458	ILE	3.1
1	B	3301	PHE	3.1
1	A	3865	ALA	3.1
1	A	55	PRO	3.1
1	B	1608	LEU	3.1
1	B	2364	ASP	3.1
1	A	3583	LEU	3.1
1	B	2058	MET	3.1
1	A	2470	GLY	3.1
1	A	68	MET	3.1
1	B	1487	THR	3.1
1	A	22	TYR	3.0
1	B	1705	TYR	3.0
1	A	1445	TRP	3.0
1	B	2179	PRO	3.0
1	A	3418	ILE	3.0
1	B	194	SER	3.0
1	A	52	PRO	3.0
1	B	15	PRO	3.0
1	A	138	HIS	3.0
1	B	159	ASP	3.0
1	A	3	ILE	3.0
1	A	2940	PHE	3.0
1	B	3694	PHE	3.0
1	A	2361	ILE	3.0
1	B	1490	ALA	3.0
1	B	1734	PHE	3.0
1	A	2302	PHE	3.0
1	A	26	LYS	2.9
1	A	146	HIS	2.9
1	B	2856	LEU	2.9
1	B	1762	TYR	2.9
1	B	76	ASP	2.9
1	B	135	ARG	2.9
1	A	145	ASP	2.9
1	B	1552	GLY	2.9
1	B	1424	PHE	2.9
1	B	3300	THR	2.9
1	A	2757	MET	2.9
1	B	2064	GLN	2.9
1	A	3300	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	83	GLY	2.9
1	B	35	ASP	2.9
1	B	1768	ARG	2.9
1	A	130	LYS	2.9
1	B	211	GLY	2.9
1	A	3301	PHE	2.9
1	B	1479	LEU	2.9
1	B	1739	ASP	2.9
1	B	164	MET	2.9
1	B	1583	ARG	2.9
1	B	3590	LEU	2.9
1	B	3726	LEU	2.9
1	B	2844	PHE	2.9
1	A	58	ILE	2.8
1	A	34	ARG	2.8
1	B	170	ASP	2.8
1	B	1421	TYR	2.8
1	B	1401	LEU	2.8
1	A	3923	VAL	2.8
1	B	56	TYR	2.8
1	B	2025	ALA	2.8
1	B	1593	ASN	2.8
1	B	1672	TYR	2.8
1	B	40	TRP	2.8
1	B	145	ASP	2.8
1	B	3866	GLU	2.8
1	A	37	GLY	2.8
1	B	190	LYS	2.8
1	A	1597	GLU	2.8
1	A	1382	GLN	2.8
1	B	204	GLY	2.8
1	A	2064	GLN	2.8
1	B	2370	SER	2.7
1	B	2241	LEU	2.7
1	B	3618	TYR	2.7
1	A	3021	LEU	2.7
1	B	4023	ILE	2.7
1	B	3846	MET	2.7
1	A	3617	GLU	2.7
1	A	9	ILE	2.7
1	B	3768	PHE	2.7
1	A	1719	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	207	ALA	2.7
1	A	21	GLU	2.7
1	B	1740	THR	2.7
1	B	3591	LYS	2.7
1	A	141	TYR	2.7
1	B	1715	LEU	2.7
1	A	38	ASP	2.7
1	A	30	HIS	2.7
1	B	1493	LEU	2.7
1	B	41	ARG	2.7
1	B	1991	GLU	2.6
1	B	206	GLN	2.6
1	A	3561	ASN	2.6
1	B	3735	LYS	2.6
1	B	1383	TYR	2.6
1	A	3025	ASN	2.6
1	B	3586	THR	2.6
1	A	3582	GLU	2.6
1	A	3589	ASN	2.6
1	B	3654	LYS	2.6
1	A	87	GLU	2.6
1	A	4034	LEU	2.6
1	B	3573	SER	2.6
1	B	3656	VAL	2.6
1	B	1482	GLU	2.6
1	B	203	GLN	2.6
1	A	2310	LEU	2.6
1	B	4088	LEU	2.6
1	B	1771	TYR	2.6
1	B	81	LEU	2.6
1	A	16	THR	2.6
1	B	3533	THR	2.6
1	B	185	ILE	2.5
1	B	3451	ILE	2.5
1	A	3020	GLY	2.5
1	B	3589	ASN	2.5
1	B	3845	GLN	2.5
1	B	3356	PHE	2.5
1	A	3563	GLU	2.5
1	A	1459	LEU	2.5
1	B	1547	LYS	2.5
1	A	3581	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1650	LEU	2.5
1	B	1881	LEU	2.5
1	A	3586	THR	2.5
1	B	23	LEU	2.5
1	B	3980	ILE	2.5
1	A	2363	ASN	2.5
1	B	9	ILE	2.5
1	A	2941	THR	2.5
1	A	2942	ASP	2.5
1	A	70	ILE	2.5
1	B	3856	HIS	2.5
1	B	2022	PHE	2.5
1	B	2669	PHE	2.4
1	B	65	THR	2.4
1	B	4092	MET	2.4
1	B	160	VAL	2.4
1	A	134	ASP	2.4
1	A	42	ASN	2.4
1	A	3584	MET	2.4
1	A	3305	ARG	2.4
1	B	3994	TYR	2.4
1	A	1598	LEU	2.4
1	B	1509	LEU	2.4
1	A	157	ALA	2.4
1	B	3945	LEU	2.4
1	B	3865	ALA	2.4
1	B	1420	TYR	2.4
1	B	1513	ILE	2.4
1	A	1452	TRP	2.3
1	B	1933	ILE	2.3
1	B	1649	LEU	2.3
1	B	2125	TRP	2.3
1	B	3706	TYR	2.3
1	A	1465	ILE	2.3
1	B	1415	MET	2.3
1	A	5	GLY	2.3
1	B	1548	ILE	2.3
1	B	1426	GLN	2.3
1	B	2684	GLN	2.3
1	A	3870	LYS	2.3
1	B	2808	LEU	2.3
1	A	36	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1945	LEU	2.3
1	B	1827	ASP	2.3
1	B	3565	ARG	2.3
1	B	1673	TRP	2.3
1	B	3841	LEU	2.3
1	A	24	GLU	2.3
1	A	1389	SER	2.3
1	A	1548	ILE	2.3
1	B	1558	VAL	2.3
1	B	1686	LYS	2.3
1	A	164	MET	2.3
1	B	1905	ARG	2.3
1	A	3593	GLU	2.3
1	B	33	GLU	2.2
1	B	2030	ASN	2.2
1	A	40	TRP	2.2
1	B	90	GLU	2.2
1	B	10	LYS	2.2
1	A	3915	PHE	2.2
1	B	4	LEU	2.2
1	B	1882	LEU	2.2
1	A	1395	VAL	2.2
1	A	3019	VAL	2.2
1	B	3985	VAL	2.2
1	A	136	LEU	2.2
1	B	3597	ILE	2.2
1	A	3026	GLU	2.2
1	B	137	CYS	2.2
1	B	2024	SER	2.2
1	B	1588	GLU	2.2
1	A	1394	LEU	2.2
1	B	3494	LEU	2.2
1	B	3923	VAL	2.2
1	A	3299	LEU	2.2
1	B	4029	ILE	2.2
1	A	2852	LEU	2.2
1	B	29	GLU	2.2
1	A	2024	SER	2.2
1	A	3588	ASN	2.2
1	B	1698	ILE	2.2
1	A	3027	SER	2.1
1	B	1455	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	3369	TYR	2.1
1	A	3419	SER	2.1
1	B	1671	LYS	2.1
1	B	3874	PHE	2.1
1	B	14	GLN	2.1
1	A	3579	GLU	2.1
1	A	53	ASN	2.1
1	B	1504	ASN	2.1
1	B	1664	LEU	2.1
1	B	3958	ASP	2.1
1	B	98	VAL	2.1
1	B	3010	LEU	2.1
1	A	199	ALA	2.1
1	A	2916	TRP	2.1
1	B	57	TYR	2.1
1	A	3784	ASN	2.1
1	B	2000	ARG	2.1
1	A	2732	MET	2.1
1	B	214	HIS	2.1
1	B	1864	ASN	2.1
1	A	3591	LYS	2.1
1	B	3834	ILE	2.1
1	A	3016	PHE	2.1
1	B	1503	PRO	2.1
1	A	3921	SER	2.0
1	A	3576	ASN	2.0
1	B	2940	PHE	2.0
1	B	1712	ILE	2.0
1	A	3919	LYS	2.0
1	B	1569	ILE	2.0
1	A	3934	TRP	2.0
1	B	2764	THR	2.0
1	B	182	ILE	2.0
1	B	1388	HIS	2.0
1	A	1385	VAL	2.0
1	B	2021	ILE	2.0
1	B	181	ARG	2.0
1	B	2172	ASP	2.0
1	B	2355	ASP	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	SO4	A	5096	5/5	0.91	0.45	6.98	77,106,130,132	0
4	MG	A	5095	1/1	0.89	0.40	5.42	76,76,76,76	0
5	SO4	B	5096	5/5	0.87	0.53	3.27	86,103,146,179	0
4	MG	B	5095	1/1	0.97	0.34	2.52	86,86,86,86	0
5	SO4	A	5097	5/5	0.97	0.21	1.25	82,93,104,115	0
2	ATP	A	5093	31/31	0.93	0.28	1.24	78,92,129,144	0
2	ATP	B	5093	31/31	0.92	0.26	0.57	93,138,174,217	0
5	SO4	B	5097	5/5	0.97	0.17	0.44	157,162,176,183	0
3	ADP	B	5094	27/27	0.90	0.27	0.26	81,114,155,168	0
3	ADP	A	5094	27/27	0.94	0.25	-0.12	91,101,113,131	0

6.5 Other polymers [i](#)

There are no such residues in this entry.