



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:10 PM UTC

PDB ID : 4AKH / pdb_00004akh
Title : Dynein Motor Domain - AMPPNP complex
Authors : Schmidt, H.; Gleave, E.S.; Carter, A.P.
Deposited on : 2012-02-22
Resolution : 3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

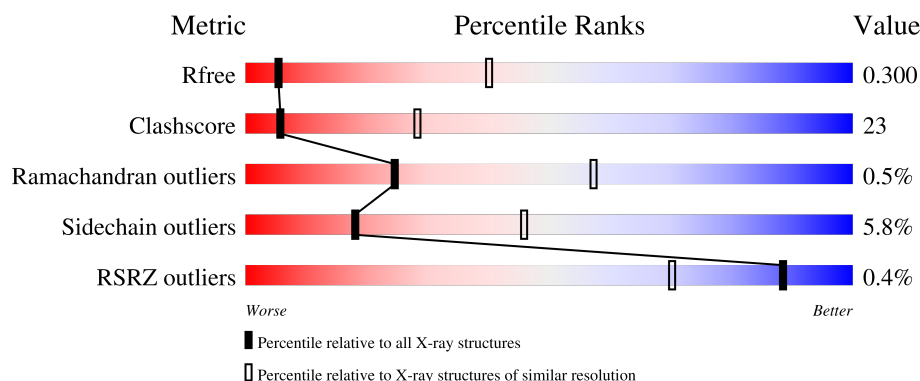
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	2695	 63% 32% ..
1	B	2695	 65% 30% ..

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

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

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 41642 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

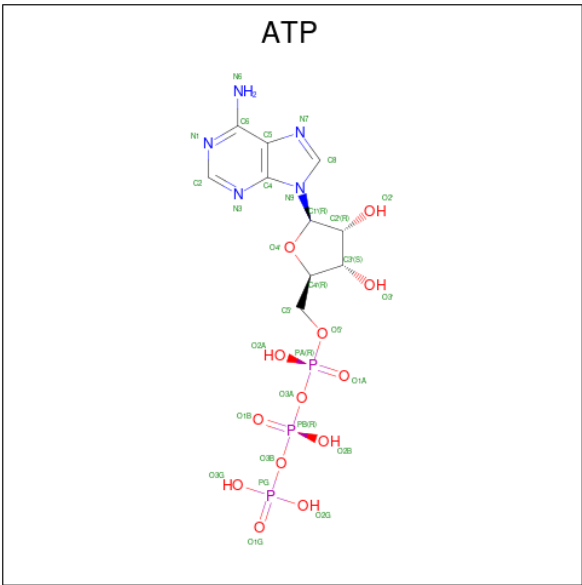
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

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

There are 8 discrepancies between the modelled and reference sequences:

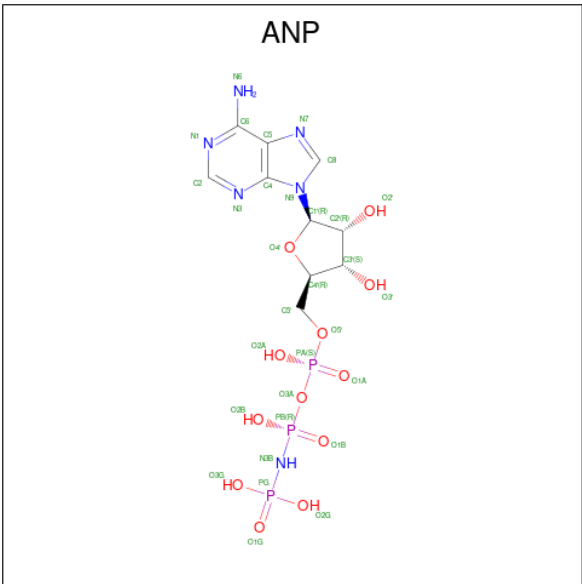
Chain	Residue	Modelled	Actual	Comment	Reference
A	218	SER	-	linker	UNP P36022
A	219	ASP	-	linker	UNP P36022
A	1630	ILE	LEU	conflict	UNP P36022
A	3782	ASP	GLU	conflict	UNP P36022
B	218	SER	-	linker	UNP P36022
B	219	ASP	-	linker	UNP P36022
B	1630	ILE	LEU	conflict	UNP P36022
B	3782	ASP	GLU	conflict	UNP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

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



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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



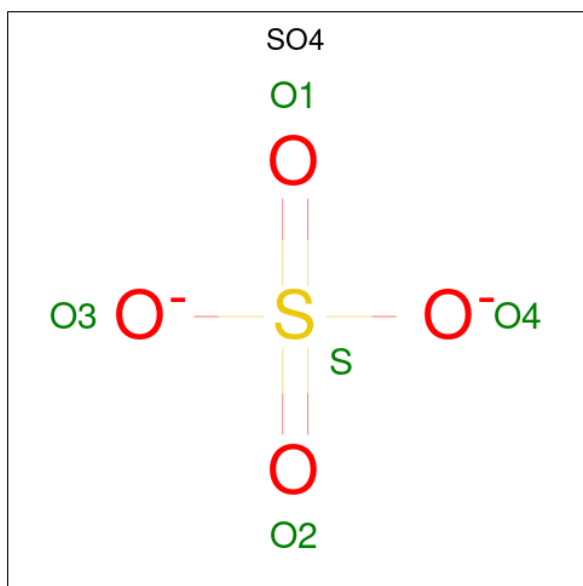
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

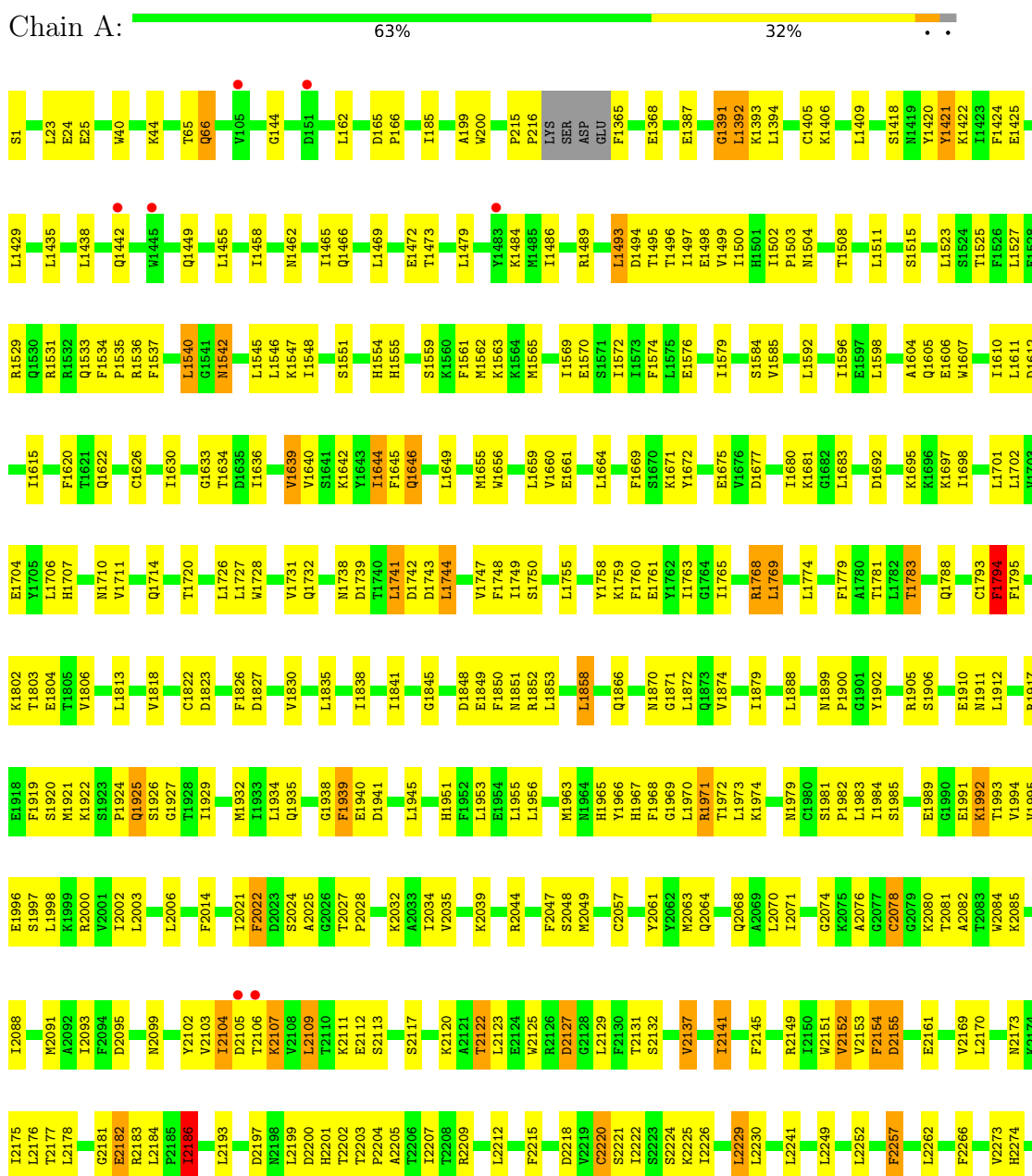
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

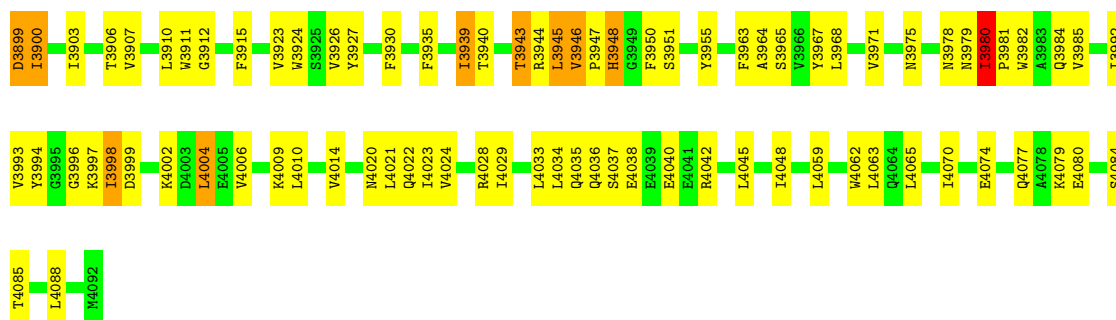
3 Residue-property plots

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

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

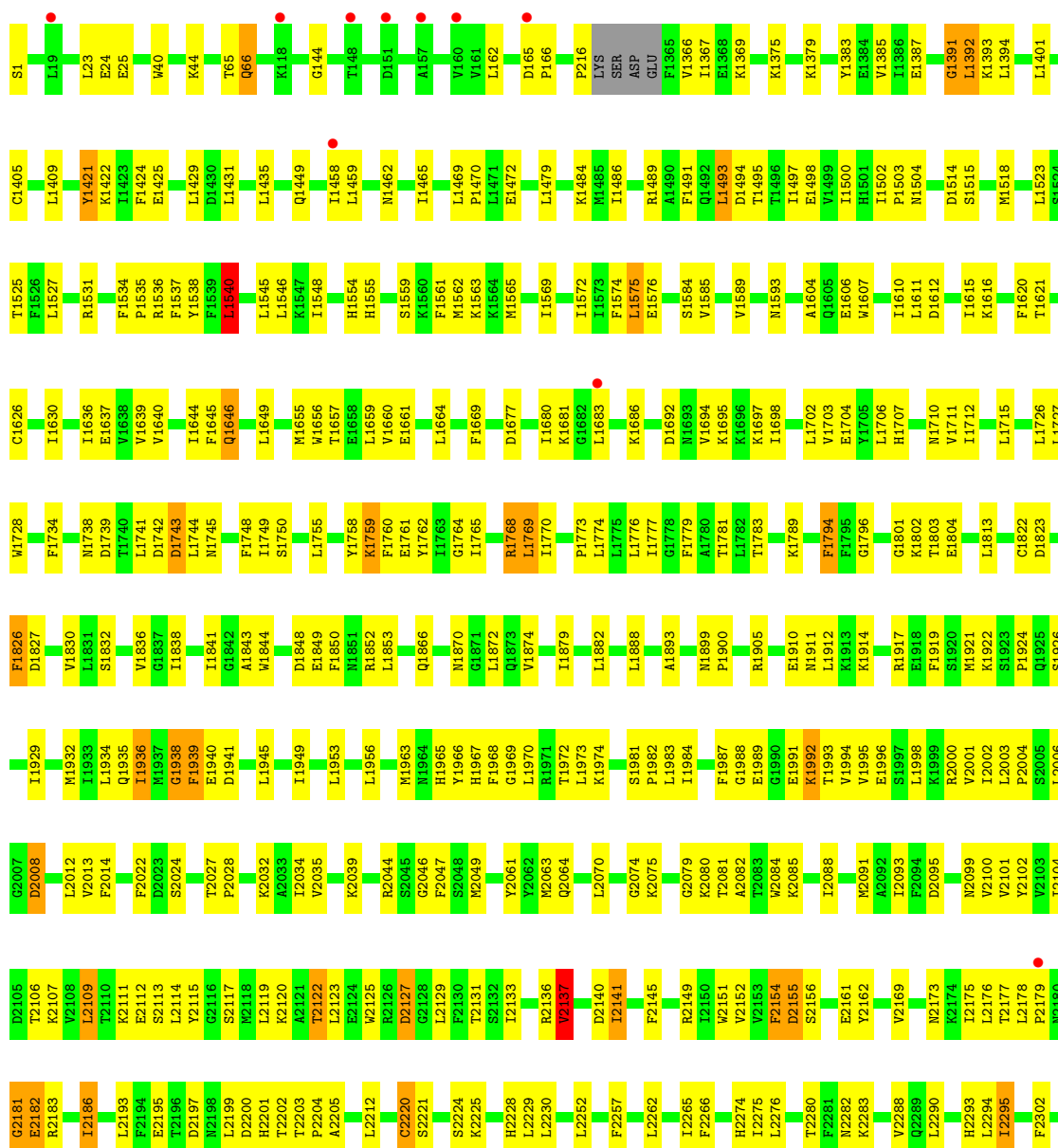






• Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC

Chain B: 65% 30%







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	175.56Å 118.13Å 201.02Å 90.00° 90.29° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 50.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-3.60) 99.2 (50.00-3.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.58Å)	Xtriage
Refinement program	REFMAC 5.7.0019	Depositor
R, R_{free}	0.241 , 0.302 0.236 , 0.300	Depositor DCC
R_{free} test set	4767 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	127.5	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 130.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.074 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	41642	wwPDB-VP
Average B, all atoms (Å ²)	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.72	3/21146 (0.0%)	1.15	72/28618 (0.3%)
1	B	0.63	0/21146	1.07	47/28618 (0.2%)
All	All	0.68	3/42292 (0.0%)	1.11	119/57236 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3980	ILE	CA-C	5.59	1.58	1.52
1	A	3945	LEU	N-CA	-5.34	1.39	1.46
1	A	1741	LEU	N-CA	5.11	1.51	1.45

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2127	ASP	N-CA-C	10.20	121.98	111.07
1	B	2127	ASP	N-CA-C	8.94	121.03	111.28
1	B	3306	TRP	N-CA-C	-8.56	97.43	110.70
1	A	2521	ASN	N-CA-C	8.34	123.49	111.56
1	A	3946	VAL	N-CA-C	-8.28	99.65	109.01
1	A	2479	ILE	N-CA-C	8.00	118.78	110.62
1	B	144	GLY	N-CA-C	7.95	123.13	111.76
1	A	1818	VAL	N-CA-CB	7.79	119.02	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1540	LEU	N-CA-C	7.78	119.40	111.07
1	A	2333	GLU	N-CA-C	-7.62	102.97	111.28
1	B	1794	PHE	N-CA-C	7.56	120.84	108.52
1	A	3772	TRP	N-CA-C	7.28	120.95	110.10
1	B	1540	LEU	N-CA-C	7.27	118.99	111.14
1	B	2333	GLU	N-CA-C	-7.19	103.52	111.36
1	B	2429	ASN	N-CA-C	7.17	118.89	111.14
1	A	2220	CYS	N-CA-C	7.12	120.55	109.52
1	A	1794	PHE	N-CA-C	7.09	120.45	108.90
1	B	2564	GLY	N-CA-C	-7.00	106.53	115.42
1	A	1542	ASN	N-CA-C	6.96	118.52	111.07
1	B	3982	TRP	N-CA-C	6.90	121.31	112.34
1	B	1	SER	CA-C-N	6.85	127.25	119.92
1	B	1	SER	C-N-CA	6.85	127.25	119.92
1	A	2916	TRP	N-CA-C	6.78	119.46	108.41
1	A	3900	ILE	CB-CA-C	-6.78	103.34	110.53
1	B	1939	PHE	N-CA-C	6.73	118.28	111.07
1	B	2101	VAL	N-CA-C	6.69	117.93	108.36
1	B	1575	LEU	N-CA-C	-6.62	104.52	112.59
1	B	2137	VAL	N-CA-C	6.58	117.36	110.72
1	A	3459	ASP	CA-C-N	6.56	126.50	119.28
1	A	3459	ASP	C-N-CA	6.56	126.50	119.28
1	B	2182	GLU	N-CA-C	6.52	118.77	108.79
1	B	1458	ILE	N-CA-C	6.52	116.66	110.53
1	A	2938	MET	N-CA-C	6.47	118.88	110.53
1	A	144	GLY	N-CA-C	6.47	121.38	112.52
1	A	3944	ARG	CA-C-N	-6.44	111.74	122.17
1	A	3944	ARG	C-N-CA	-6.44	111.74	122.17
1	B	2938	MET	N-CA-C	6.40	119.19	110.55
1	B	2392	ILE	N-CA-C	-6.38	101.75	107.56
1	A	2257	PHE	N-CA-C	6.38	118.91	108.52
1	A	3980	ILE	N-CA-C	6.37	122.64	108.88
1	B	1422	LYS	N-CA-C	6.31	117.82	111.07
1	A	1	SER	CA-C-N	6.30	126.66	119.92
1	A	1	SER	C-N-CA	6.30	126.66	119.92
1	B	2375	ILE	N-CA-C	6.24	115.04	107.61
1	A	1939	PHE	N-CA-C	6.17	117.67	111.07
1	B	2257	PHE	N-CA-C	6.12	118.39	108.41
1	A	2471	LEU	CB-CA-C	-6.07	109.59	116.63
1	B	3459	ASP	CA-C-N	6.05	126.49	119.47
1	B	3459	ASP	C-N-CA	6.05	126.49	119.47
1	A	2752	VAL	CB-CA-C	-5.93	104.28	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1793	CYS	CA-C-N	-5.90	114.67	122.99
1	A	1793	CYS	C-N-CA	-5.90	114.67	122.99
1	A	199	ALA	N-CA-C	5.88	118.64	111.82
1	A	2564	GLY	N-CA-C	-5.87	107.84	115.59
1	A	2988	SER	CA-C-N	5.86	127.16	119.84
1	A	2988	SER	C-N-CA	5.86	127.16	119.84
1	A	2984	VAL	N-CA-C	5.86	116.11	107.15
1	A	2186	ILE	N-CA-C	5.85	114.32	107.77
1	A	185	ILE	CA-C-N	5.81	127.10	119.84
1	A	185	ILE	C-N-CA	5.81	127.10	119.84
1	B	2220	CYS	N-CA-C	5.76	118.61	109.50
1	A	2068	GLN	N-CA-C	-5.75	106.81	113.88
1	B	2840	ILE	CA-C-N	5.74	125.21	119.24
1	B	2840	ILE	C-N-CA	5.74	125.21	119.24
1	B	3305	ARG	CA-C-O	-5.74	112.30	120.51
1	A	1458	ILE	N-CA-C	5.72	115.91	110.53
1	B	2418	GLY	CA-C-N	5.71	126.26	120.38
1	B	2418	GLY	C-N-CA	5.71	126.26	120.38
1	A	2120	LYS	N-CA-C	5.71	118.24	111.33
1	A	2182	GLU	N-CA-C	5.70	117.13	108.07
1	A	2942	ASP	N-CA-C	5.64	118.16	111.33
1	B	2916	TRP	N-CA-C	5.63	117.70	108.52
1	B	3980	ILE	N-CA-C	5.63	121.04	108.88
1	A	2373	SER	N-CA-C	5.60	119.57	111.56
1	A	2941	THR	CA-C-N	5.60	128.05	120.38
1	A	2941	THR	C-N-CA	5.60	128.05	120.38
1	A	2027	THR	CA-C-N	5.57	126.81	119.84
1	A	2027	THR	C-N-CA	5.57	126.81	119.84
1	A	2840	ILE	CA-C-N	5.55	125.21	119.05
1	A	2840	ILE	C-N-CA	5.55	125.21	119.05
1	B	3771	GLU	N-CA-C	-5.52	101.88	110.10
1	A	3948	HIS	N-CA-C	-5.51	101.75	109.96
1	A	2752	VAL	N-CA-CB	5.50	116.61	110.51
1	B	3402	ASP	N-CA-C	-5.47	106.37	113.16
1	A	2761	ALA	CB-CA-C	-5.46	110.30	116.63
1	A	2537	PRO	CA-C-N	-5.45	114.40	120.45
1	A	2537	PRO	C-N-CA	-5.45	114.40	120.45
1	A	2900	SER	N-CA-C	-5.45	105.42	111.36
1	A	2025	ALA	N-CA-C	5.43	117.06	108.96
1	A	200	TRP	N-CA-C	5.38	113.07	108.22
1	A	1422	LYS	N-CA-C	5.36	117.13	111.28
1	B	3452	ILE	N-CA-C	5.36	115.30	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3461	ILE	N-CA-C	5.33	116.10	110.72
1	A	2022	PHE	N-CA-C	5.33	118.07	108.48
1	B	3298	SER	N-CA-C	5.31	117.14	111.36
1	A	1747	VAL	CB-CA-C	-5.29	104.35	110.91
1	B	2865	LEU	CA-C-N	-5.29	115.70	123.00
1	B	2865	LEU	C-N-CA	-5.29	115.70	123.00
1	B	2008	ASP	N-CA-C	5.28	117.72	111.33
1	B	2479	ILE	N-CA-C	5.28	117.66	111.05
1	A	1925	GLN	N-CA-C	-5.27	102.24	110.10
1	B	1938	GLY	N-CA-C	-5.24	100.77	113.18
1	A	1906	SER	N-CA-C	5.22	117.06	110.33
1	B	2179	PRO	N-CA-C	-5.21	106.41	113.40
1	A	1971	ARG	N-CA-C	-5.20	105.61	111.28
1	A	3616	GLU	N-CA-C	5.20	117.03	111.36
1	B	2373	SER	N-CA-C	5.18	118.97	111.56
1	A	3943	THR	N-CA-C	5.17	117.58	111.33
1	A	3975	ASN	N-CA-C	5.17	117.74	110.14
1	A	3516	VAL	N-CA-C	5.16	115.41	107.77
1	A	3639	HIS	N-CA-C	5.16	117.83	109.06
1	B	3948	HIS	N-CA-C	-5.15	102.29	109.96
1	A	2152	VAL	N-CA-C	5.13	114.14	106.85
1	B	2120	LYS	N-CA-C	5.12	117.52	111.33
1	A	1902	TYR	CA-C-N	5.11	127.39	120.44
1	A	1902	TYR	C-N-CA	5.11	127.39	120.44
1	B	2761	ALA	CB-CA-C	-5.08	110.32	117.23
1	B	2181	GLY	N-CA-C	5.07	120.76	114.37
1	A	2837	ASN	N-CA-C	-5.05	102.59	110.42

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20748	0	20206	975	0
1	B	20748	0	20206	940	0
2	A	31	0	12	8	0
2	B	31	0	12	17	0
3	A	31	0	13	7	0
3	B	31	0	13	8	0
4	A	10	0	0	3	0
4	B	10	0	0	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	41642	0	40462	1915	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 (1915) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:PRO:CB	1:A:1365:PHE:CE1	2.05	1.38
1:B:3303:LYS:HD2	1:B:3306:TRP:CD1	1.67	1.28
1:B:1620:PHE:HD1	1:B:1760:PHE:CZ	1.53	1.25
1:A:1368:GLU:HG2	1:A:1424:PHE:CZ	1.69	1.24
1:B:2467:THR:HB	1:B:2473:LEU:CD1	1.66	1.23
1:A:2061:TYR:CE1	1:A:2091:MET:SD	2.35	1.20
1:A:2061:TYR:HE1	1:A:2091:MET:SD	1.65	1.19
1:A:3777:VAL:HG11	1:A:3895:PHE:CE1	1.80	1.16
1:A:1970:LEU:HD13	1:A:1974:LYS:HE3	1.25	1.16
1:A:4033:LEU:CD1	1:A:4035:GLN:HB2	1.76	1.16
1:B:3534:LEU:CD1	1:B:3618:TYR:HE2	1.58	1.16
1:B:2111:LYS:HD3	1:B:2161:GLU:HG3	1.18	1.14
1:B:3023:LYS:CD	1:B:3567:LEU:HD21	1.77	1.14
1:A:2111:LYS:HD3	1:A:2161:GLU:HG3	1.23	1.14
1:B:2141:ILE:HG22	1:B:2145:PHE:HB2	1.27	1.14
1:A:3534:LEU:CD1	1:A:3618:TYR:HE2	1.61	1.13
1:A:215:PRO:CB	1:A:3475:ASN:HD22	1.61	1.13
1:B:2470:GLY:HA3	1:B:2473:LEU:HD21	1.29	1.13
1:A:3303:LYS:HA	1:A:3306:TRP:CD1	1.84	1.12
1:B:1970:LEU:CD2	1:B:1974:LYS:HE2	1.77	1.12
1:B:2404:PHE:CZ	1:B:2428:MET:SD	2.43	1.12
1:B:2107:LYS:HE3	1:B:2495:ASP:OD2	1.49	1.12
1:B:2707:VAL:HB	1:B:2712:LEU:HD11	1.22	1.11
1:A:2707:VAL:HB	1:A:2712:LEU:HD11	1.13	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1421:TYR:O	1:B:1425:GLU:HB2	1.51	1.10
1:A:1620:PHE:HD1	1:A:1760:PHE:CZ	1.68	1.10
1:B:2112:GLU:HB3	1:B:2117:SER:HB2	1.32	1.10
1:B:2488:GLU:HB3	1:B:2491:LEU:HD12	1.13	1.10
1:A:2488:GLU:HB3	1:A:2491:LEU:HD12	1.09	1.09
1:B:3777:VAL:HG11	1:B:3895:PHE:CE1	1.88	1.09
1:A:2988:SER:HB3	1:A:2989:PRO:CD	1.83	1.09
1:A:1421:TYR:O	1:A:1425:GLU:HB2	1.50	1.08
1:B:3525:ILE:HD11	1:B:3646:ILE:HG22	1.28	1.08
1:A:1822:CYS:HB2	1:A:1853:LEU:HD21	1.36	1.08
1:B:1409:LEU:HD21	1:B:1435:LEU:HB3	1.18	1.08
1:B:1992:LYS:HG3	1:B:2024:SER:HB2	1.22	1.08
1:B:3023:LYS:CD	1:B:3567:LEU:CD2	2.31	1.08
1:A:1992:LYS:CG	1:A:2024:SER:HB2	1.83	1.08
1:B:3024:LEU:HD11	1:B:3303:LYS:HG3	1.36	1.08
1:B:3777:VAL:HG11	1:B:3895:PHE:HE1	0.96	1.07
1:A:1645:PHE:HB3	1:A:1765:ILE:HG22	1.37	1.07
1:B:1645:PHE:HB3	1:B:1765:ILE:CG2	1.85	1.07
1:B:2920:TRP:HB2	1:B:2989:PRO:HG3	1.10	1.07
1:B:2988:SER:HB3	1:B:2989:PRO:CD	1.84	1.07
1:A:1645:PHE:HB3	1:A:1765:ILE:CG2	1.85	1.06
1:B:2467:THR:HB	1:B:2473:LEU:HD12	1.32	1.06
1:B:1645:PHE:HB3	1:B:1765:ILE:HG22	1.34	1.06
1:A:2494:LEU:CD1	1:A:2498:GLY:HA2	1.86	1.05
1:B:2467:THR:CB	1:B:2473:LEU:HD12	1.86	1.05
1:B:1620:PHE:CD1	1:B:1760:PHE:CZ	2.43	1.05
1:B:2061:TYR:HE1	1:B:2091:MET:CE	1.70	1.05
1:A:2494:LEU:HD13	1:A:2498:GLY:CA	1.86	1.05
1:A:2707:VAL:CB	1:A:2712:LEU:HD11	1.86	1.05
1:B:2494:LEU:HD13	1:B:2498:GLY:CA	1.86	1.04
1:A:3777:VAL:HG11	1:A:3895:PHE:HE1	0.90	1.04
1:A:1409:LEU:HD21	1:A:1435:LEU:HB3	1.36	1.03
1:B:2494:LEU:CD1	1:B:2498:GLY:HA2	1.88	1.03
1:A:1823:ASP:HB2	1:A:1852:ARG:O	1.58	1.03
1:A:3303:LYS:O	1:A:3306:TRP:HD1	1.41	1.03
1:B:1620:PHE:CD1	1:B:1760:PHE:HZ	1.73	1.03
1:B:2386:MET:HB2	1:B:2627:ARG:HD3	1.35	1.03
1:A:2476:LYS:CD	1:A:2476:LYS:H	1.66	1.02
1:A:3525:ILE:HD11	1:A:3646:ILE:HG22	1.41	1.02
1:B:2779:LEU:HD23	1:B:2812:ARG:O	1.60	1.02
1:B:3023:LYS:HD3	1:B:3567:LEU:HD21	1.37	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2061:TYR:CE1	1:B:2091:MET:SD	2.53	1.02
1:A:2920:TRP:HB2	1:A:2989:PRO:HG3	1.03	1.02
1:B:2386:MET:CB	1:B:2627:ARG:HD3	1.90	1.02
1:B:3303:LYS:HD2	1:B:3306:TRP:HD1	0.87	1.02
1:A:3530:PHE:CD1	1:A:3618:TYR:HD2	1.77	1.01
1:B:2391:VAL:HG23	1:B:2426:MET:SD	2.00	1.01
1:A:1983:LEU:HD21	1:A:2000:ARG:HD2	1.36	1.01
1:A:1992:LYS:HG3	1:A:2024:SER:HB2	1.40	1.01
1:A:2988:SER:CB	1:A:2989:PRO:HD2	1.91	1.01
1:A:2107:LYS:HE3	1:A:2495:ASP:OD2	1.58	1.01
1:A:4033:LEU:HD11	1:A:4035:GLN:HB2	1.43	1.00
1:B:2494:LEU:HD13	1:B:2498:GLY:HA2	1.02	1.00
1:B:1421:TYR:CE2	1:B:1425:GLU:CG	2.45	1.00
1:A:2488:GLU:CB	1:A:2491:LEU:HD12	1.89	1.00
1:B:2988:SER:HB3	1:B:2989:PRO:HD2	1.03	1.00
1:B:1822:CYS:HB2	1:B:1853:LEU:HD21	1.41	1.00
1:B:1866:GLN:OE1	1:B:1911:ASN:HB2	1.61	0.99
1:A:1983:LEU:HD22	1:A:1997:SER:OG	1.63	0.99
1:B:2081:THR:HB	2:B:5093:ATP:O2A	1.60	0.99
1:A:215:PRO:CB	1:A:3475:ASN:ND2	2.24	0.99
1:B:3023:LYS:HD2	1:B:3567:LEU:CD2	1.92	0.99
1:A:1421:TYR:CE2	1:A:1425:GLU:CG	2.46	0.99
1:A:1421:TYR:CE2	1:A:1425:GLU:HG3	1.97	0.99
1:B:3534:LEU:CD1	1:B:3618:TYR:CE2	2.44	0.99
1:B:2707:VAL:CB	1:B:2712:LEU:HD11	1.92	0.99
1:B:1421:TYR:CE2	1:B:1425:GLU:HG3	1.97	0.99
1:A:3777:VAL:CG1	1:A:3895:PHE:HE1	1.75	0.98
1:A:2988:SER:HB3	1:A:2989:PRO:HD2	1.00	0.98
1:B:3645:SER:HB3	1:B:3890:GLN:HE21	1.26	0.97
1:A:3534:LEU:CD1	1:A:3618:TYR:CE2	2.46	0.97
1:B:1970:LEU:HD21	1:B:1974:LYS:HE2	1.46	0.97
1:A:3534:LEU:HD12	1:A:3618:TYR:HE2	1.26	0.97
1:A:3406:PHE:HB2	1:A:3513:VAL:CG1	1.93	0.97
1:B:1645:PHE:CB	1:B:1765:ILE:HG22	1.94	0.97
1:B:2488:GLU:CB	1:B:2491:LEU:HD12	1.94	0.97
1:A:2494:LEU:HD13	1:A:2498:GLY:HA2	0.98	0.97
1:B:1744:LEU:HA	1:B:1760:PHE:CE2	1.99	0.97
1:B:1823:ASP:HB2	1:B:1852:ARG:O	1.64	0.97
1:B:3737:THR:HB	1:B:3740:THR:OG1	1.65	0.97
1:A:2745:ILE:HG23	1:A:2756:MET:HE1	1.46	0.97
1:A:2920:TRP:CB	1:A:2989:PRO:HG3	1.95	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1535:PRO:C	1:B:1841:ILE:HD11	1.90	0.96
1:A:3024:LEU:HD11	1:A:3303:LYS:HG3	1.43	0.96
1:B:2988:SER:CB	1:B:2989:PRO:HD2	1.95	0.96
1:B:3534:LEU:HD12	1:B:3618:TYR:HE2	1.31	0.96
1:A:3946:VAL:HG12	1:A:3950:PHE:O	1.66	0.96
1:B:1992:LYS:CG	1:B:2024:SER:HB2	1.94	0.96
1:A:2488:GLU:HB3	1:A:2491:LEU:CD1	1.95	0.95
1:B:1983:LEU:HG	1:B:1993:THR:HG23	1.45	0.95
1:A:2787:HIS:HA	1:A:3460:PRO:HD2	1.43	0.95
1:B:2787:HIS:HA	1:B:3460:PRO:HD2	1.47	0.95
1:B:3023:LYS:HE2	1:B:3567:LEU:HG	1.49	0.95
1:B:3530:PHE:CD1	1:B:3618:TYR:HD2	1.85	0.94
1:B:2755:HIS:HB2	1:B:2911:ARG:O	1.66	0.94
1:B:3777:VAL:CG1	1:B:3895:PHE:HE1	1.79	0.94
1:B:1956:LEU:HB3	1:B:1968:PHE:HE2	1.32	0.94
1:A:2332:GLY:HA2	1:A:2335:GLN:HB2	1.50	0.93
1:B:2380:LEU:HD12	1:B:2577:ALA:HB1	1.49	0.93
1:B:1630:ILE:HG22	1:B:1655:MET:SD	2.09	0.93
1:A:2380:LEU:HD12	1:A:2577:ALA:CB	1.98	0.93
1:B:2488:GLU:HB3	1:B:2491:LEU:CD1	1.98	0.93
1:B:2745:ILE:HG23	1:B:2756:MET:HE1	1.48	0.93
1:A:1421:TYR:CZ	1:A:1425:GLU:HG3	2.04	0.93
1:B:3946:VAL:HG12	1:B:3950:PHE:O	1.69	0.93
1:B:3023:LYS:HD2	1:B:3567:LEU:HD21	1.51	0.92
1:B:3534:LEU:HD13	1:B:3618:TYR:HE2	1.31	0.92
1:B:2853:LEU:HD21	1:B:2870:GLU:HG3	1.52	0.92
1:A:1535:PRO:C	1:A:1841:ILE:HD11	1.94	0.92
1:B:1939:PHE:CD2	1:B:1940:GLU:O	2.23	0.92
1:A:3656:VAL:HG13	1:A:3677:LEU:HB3	1.52	0.92
1:A:3303:LYS:HD2	1:A:3306:TRP:CD1	2.04	0.92
1:A:3534:LEU:HD12	1:A:3618:TYR:CE2	2.03	0.92
1:A:2787:HIS:HA	1:A:3460:PRO:CD	1.99	0.91
1:B:2061:TYR:HE1	1:B:2091:MET:SD	1.91	0.91
1:B:2332:GLY:HA2	1:B:2335:GLN:HB2	1.52	0.91
1:A:3303:LYS:HA	1:A:3306:TRP:NE1	1.85	0.91
1:A:3303:LYS:O	1:A:3306:TRP:CD1	2.24	0.91
1:B:1956:LEU:HB3	1:B:1968:PHE:CE2	2.06	0.91
1:A:1645:PHE:CB	1:A:1765:ILE:HG22	2.00	0.91
1:B:1421:TYR:CZ	1:B:1425:GLU:HG3	2.05	0.91
1:A:2707:VAL:HB	1:A:2712:LEU:CD1	2.01	0.91
1:A:3737:THR:HB	1:A:3740:THR:OG1	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1983:LEU:HD21	1:A:2000:ARG:CD	2.01	0.90
1:B:2380:LEU:CD1	1:B:2577:ALA:CB	2.49	0.90
1:A:1823:ASP:CB	1:A:1852:ARG:O	2.20	0.90
1:B:2112:GLU:HB3	1:B:2117:SER:CB	2.00	0.90
1:B:2380:LEU:HD12	1:B:2577:ALA:CB	2.01	0.90
1:A:2137:VAL:O	1:A:2141:ILE:HG23	1.72	0.90
1:A:3530:PHE:CD1	1:A:3618:TYR:CD2	2.60	0.90
1:A:1620:PHE:CD1	1:A:1760:PHE:CZ	2.60	0.90
1:B:3303:LYS:CD	1:B:3306:TRP:HD1	1.82	0.90
1:B:1726:LEU:CD1	1:B:3984:GLN:HB3	2.02	0.89
1:B:1774:LEU:HD21	1:B:1922:LYS:O	1.72	0.89
1:B:2404:PHE:HZ	1:B:2428:MET:SD	1.94	0.89
1:B:2131:THR:HG22	1:B:2176:LEU:HD21	1.55	0.89
1:A:2274:HIS:HE1	1:A:2326:LEU:O	1.54	0.89
1:A:2787:HIS:HA	1:A:3460:PRO:CG	2.02	0.89
1:B:1992:LYS:HE2	1:B:2024:SER:O	1.71	0.89
1:A:2476:LYS:H	1:A:2476:LYS:HD3	1.37	0.89
1:B:2111:LYS:HD3	1:B:2161:GLU:CG	2.00	0.89
1:B:2404:PHE:CE1	1:B:2428:MET:SD	2.66	0.89
1:B:2467:THR:HB	1:B:2473:LEU:HD11	1.54	0.89
1:A:1939:PHE:CD2	1:A:1940:GLU:O	2.26	0.89
1:A:2757:MET:CE	1:A:2912:CYS:HB2	2.01	0.89
1:B:3303:LYS:CD	1:B:3306:TRP:CD1	2.54	0.89
1:A:2563:SER:HB3	1:A:2566:SER:H	1.37	0.88
1:B:3406:PHE:HB2	1:B:3513:VAL:CG1	2.04	0.88
1:A:1924:PRO:HB2	1:A:1929:ILE:HD11	1.55	0.88
1:A:1940:GLU:HB2	1:A:1989:GLU:O	1.72	0.88
1:B:1535:PRO:HB2	1:B:1841:ILE:HG13	1.53	0.88
1:A:1535:PRO:HB2	1:A:1841:ILE:HG13	1.53	0.88
1:A:2745:ILE:HG23	1:A:2756:MET:CE	2.04	0.88
1:B:1604:ALA:HA	1:B:1607:TRP:CD1	2.09	0.88
1:A:1979:ASN:O	1:A:1983:LEU:HD13	1.73	0.87
1:B:1409:LEU:HD21	1:B:1435:LEU:CB	2.04	0.87
1:B:2224:SER:O	2:B:5093:ATP:H2	1.57	0.87
1:A:1992:LYS:HE2	1:A:2024:SER:O	1.74	0.87
1:A:3024:LEU:CD1	1:A:3303:LYS:HG3	2.03	0.87
1:A:1744:LEU:HA	1:A:1760:PHE:CE2	2.11	0.86
1:B:2563:SER:HB3	1:B:2566:SER:H	1.38	0.86
1:B:3024:LEU:CD1	1:B:3303:LYS:HG3	2.05	0.86
1:A:2111:LYS:HD3	1:A:2161:GLU:CG	2.04	0.86
1:B:2787:HIS:HA	1:B:3460:PRO:CD	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3534:LEU:HD12	1:B:3618:TYR:CE2	2.10	0.86
1:A:3534:LEU:HD13	1:A:3618:TYR:HE2	1.39	0.86
1:A:2412:ARG:HB2	1:A:2412:ARG:HH11	1.41	0.86
1:A:3525:ILE:CD1	1:A:3646:ILE:HG22	2.06	0.85
1:B:1744:LEU:HA	1:B:1760:PHE:CD2	2.10	0.85
1:B:1926:SER:CB	1:B:1970:LEU:HD12	2.06	0.85
1:A:2757:MET:HE2	1:A:2912:CYS:HB2	1.58	0.85
1:A:3923:VAL:HG23	1:A:4038:GLU:HA	1.58	0.85
1:B:1996:GLU:O	1:B:2000:ARG:HG3	1.76	0.85
1:B:2061:TYR:HE1	1:B:2091:MET:HE1	1.38	0.85
1:B:2787:HIS:HA	1:B:3460:PRO:CG	2.07	0.85
1:A:1368:GLU:HG2	1:A:1424:PHE:HZ	1.36	0.85
1:A:2380:LEU:HD12	1:A:2577:ALA:HB1	1.56	0.85
1:A:2380:LEU:CD1	1:A:2577:ALA:CB	2.54	0.85
1:B:1425:GLU:OE2	1:B:1429:LEU:HG	1.76	0.85
1:A:166:PRO:CB	1:A:3476:ARG:HD3	2.06	0.84
1:B:1726:LEU:HD12	1:B:3984:GLN:HB3	1.57	0.84
1:A:1726:LEU:HD12	1:A:3984:GLN:HB3	1.59	0.84
1:A:1866:GLN:OE1	1:A:1911:ASN:HB2	1.77	0.84
1:A:2446:SER:H	1:A:2449:THR:CG2	1.90	0.84
1:B:2081:THR:HB	2:B:5093:ATP:PA	2.17	0.84
1:A:216:PRO:CB	1:A:1365:PHE:CZ	2.59	0.84
1:A:1620:PHE:HD1	1:A:1760:PHE:HZ	1.22	0.84
1:A:2061:TYR:CE1	1:A:2091:MET:CE	2.60	0.84
1:B:1425:GLU:OE2	1:B:1429:LEU:CG	2.24	0.84
1:A:2920:TRP:HB2	1:A:2989:PRO:CG	1.99	0.84
1:A:1368:GLU:CG	1:A:1424:PHE:CZ	2.58	0.83
1:A:2787:HIS:HA	1:A:3460:PRO:HG2	1.57	0.83
1:A:3303:LYS:CA	1:A:3306:TRP:CD1	2.61	0.83
1:A:3509:LEU:CD1	1:A:3513:VAL:HG21	2.08	0.83
1:B:1983:LEU:HD23	1:B:1993:THR:O	1.78	0.83
1:B:2141:ILE:HG22	1:B:2145:PHE:CB	2.06	0.83
1:B:2623:THR:HG21	3:B:5094:ANP:O3'	1.78	0.83
1:B:3631:MET:HE1	1:B:3698:MET:HG3	1.60	0.83
1:A:2476:LYS:HD3	1:A:2476:LYS:N	1.90	0.83
1:A:1604:ALA:HA	1:A:1607:TRP:CD1	2.13	0.83
1:B:1421:TYR:O	1:B:1425:GLU:CB	2.26	0.83
1:A:2064:GLN:OE1	1:A:2151:TRP:HH2	1.61	0.83
1:B:2274:HIS:HE1	1:B:2326:LEU:O	1.60	0.83
1:A:1387:GLU:HB3	1:A:1393:LYS:HG2	1.58	0.83
1:A:1409:LEU:HD21	1:A:1435:LEU:CB	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1392:LEU:HD13	1:B:1393:LYS:N	1.93	0.83
1:B:1562:MET:HB3	1:B:1569:ILE:HD11	1.61	0.83
1:A:1421:TYR:O	1:A:1425:GLU:CB	2.26	0.83
1:B:2920:TRP:CB	1:B:2989:PRO:HG3	2.04	0.83
1:A:1562:MET:HB3	1:A:1569:ILE:HD11	1.59	0.83
1:A:2386:MET:HB2	1:A:2627:ARG:HD3	1.61	0.83
1:B:2787:HIS:HA	1:B:3460:PRO:HG2	1.59	0.83
1:A:2410:SER:C	1:A:2411:LYS:HG3	2.03	0.83
1:A:3534:LEU:HD11	1:A:3614:LEU:HD23	1.60	0.83
1:A:1604:ALA:HA	1:A:1607:TRP:NE1	1.94	0.82
1:B:1940:GLU:HB2	1:B:1989:GLU:O	1.77	0.82
1:B:2472:THR:CG2	1:B:2524:VAL:HG22	2.08	0.82
1:B:1409:LEU:CD2	1:B:1435:LEU:HB3	2.06	0.82
1:B:4065:LEU:HD11	1:B:4070:ILE:HD11	1.61	0.82
1:B:1421:TYR:CE2	1:B:1425:GLU:HG2	2.13	0.82
1:B:1574:PHE:HB3	1:B:1576:GLU:H	1.45	0.82
1:B:1967:HIS:C	1:B:1968:PHE:HD1	1.88	0.82
1:A:1392:LEU:HD13	1:A:1393:LYS:N	1.95	0.82
1:A:1569:ILE:HA	1:A:1584:SER:HA	1.59	0.82
1:B:2513:GLN:O	1:B:2526:ILE:HG13	1.78	0.82
1:A:1365:PHE:CZ	1:A:1420:TYR:CD1	2.68	0.82
1:B:1802:LYS:HG2	1:B:1921:MET:HG3	1.61	0.82
1:A:1462:ASN:HB2	1:A:1465:ILE:HG22	1.62	0.82
1:B:3534:LEU:HD13	1:B:3618:TYR:CE2	2.10	0.82
1:A:1421:TYR:CE2	1:A:1425:GLU:HG2	2.14	0.81
1:A:2755:HIS:HB2	1:A:2911:ARG:O	1.80	0.81
1:A:2490:ASN:HB3	1:A:2546:MET:HE2	1.60	0.81
1:A:3303:LYS:C	1:A:3306:TRP:HD1	1.87	0.81
1:B:1924:PRO:HB2	1:B:1929:ILE:HD11	1.61	0.81
1:A:1779:PHE:O	1:A:1783:THR:HG22	1.80	0.81
1:B:3645:SER:HB3	1:B:3890:GLN:NE2	1.96	0.81
1:A:2224:SER:O	2:A:5093:ATP:H2	1.63	0.81
1:B:2106:THR:OG1	1:B:2154:PHE:HB3	1.81	0.81
1:A:1630:ILE:HG22	1:A:1655:MET:SD	2.21	0.81
1:A:1970:LEU:HD13	1:A:1974:LYS:CE	2.08	0.81
1:A:4033:LEU:HD13	1:A:4035:GLN:HB2	1.61	0.81
1:A:1645:PHE:CB	1:A:1765:ILE:CG2	2.57	0.80
1:A:2493:LYS:HG3	1:A:2494:LEU:H	1.45	0.80
1:B:1970:LEU:CD2	1:B:1974:LYS:CE	2.59	0.80
1:B:3799:LYS:O	1:B:3803:LEU:HG	1.80	0.80
1:A:2757:MET:HE2	1:A:2912:CYS:CB	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2112:GLU:HB3	1:A:2117:SER:HB2	1.62	0.80
1:B:1823:ASP:CB	1:B:1852:ARG:O	2.29	0.80
1:A:2111:LYS:NZ	1:A:2161:GLU:HG2	1.96	0.80
1:A:2225:LYS:HA	2:A:5093:ATP:C2	2.16	0.80
1:A:2362:ALA:HB3	1:A:2365:LYS:O	1.82	0.80
1:A:3700:MET:HB3	1:A:4085:THR:HG21	1.64	0.80
1:A:1992:LYS:HG2	1:A:2024:SER:HB2	1.62	0.80
1:B:1604:ALA:HA	1:B:1607:TRP:NE1	1.97	0.80
1:A:2745:ILE:HG12	1:A:2756:MET:HE1	1.62	0.79
1:B:3509:LEU:CD1	1:B:3513:VAL:HG21	2.12	0.79
1:A:2061:TYR:CE1	1:A:2091:MET:HE1	2.17	0.79
1:A:3998:ILE:CG2	1:A:4004:LEU:HG	2.12	0.79
1:A:1822:CYS:SG	1:A:1850:PHE:HA	2.22	0.79
1:B:2141:ILE:CG2	1:B:2145:PHE:HB2	2.09	0.79
1:B:3023:LYS:HD2	1:B:3567:LEU:HD23	1.64	0.79
1:A:2386:MET:CB	1:A:2627:ARG:HD3	2.13	0.78
1:A:2513:GLN:O	1:A:2526:ILE:HG13	1.82	0.78
1:B:2111:LYS:NZ	1:B:2161:GLU:HG2	1.99	0.78
1:A:3792:ARG:HB2	1:A:3955:TYR:CD2	2.18	0.78
1:B:1939:PHE:HD2	1:B:1940:GLU:O	1.64	0.78
1:A:2512:LYS:O	1:A:2513:GLN:HB2	1.82	0.78
1:A:4033:LEU:CD1	1:A:4035:GLN:CB	2.61	0.78
1:A:2106:THR:OG1	1:A:2154:PHE:HB3	1.83	0.78
1:A:2631:THR:O	1:A:2635:THR:HG22	1.81	0.78
1:B:3530:PHE:CD1	1:B:3618:TYR:CD2	2.70	0.78
1:B:3656:VAL:HG13	1:B:3677:LEU:HB3	1.64	0.78
1:A:2941:THR:HG22	1:A:2942:ASP:H	1.49	0.78
1:A:2181:GLY:O	1:A:2182:GLU:HG3	1.84	0.78
1:A:2552:ARG:HG2	1:A:2552:ARG:HH11	1.48	0.78
1:A:1970:LEU:HD12	1:A:1971:ARG:N	1.98	0.77
1:B:3024:LEU:HD11	1:B:3303:LYS:CG	2.14	0.77
1:A:1922:LYS:NZ	1:A:4004:LEU:HD12	1.99	0.77
1:A:2175:ILE:HG12	1:A:2183:ARG:HB3	1.64	0.77
1:B:1392:LEU:HD13	1:B:1392:LEU:C	2.10	0.77
1:B:2061:TYR:CE1	1:B:2091:MET:CE	2.63	0.77
1:A:1956:LEU:HB3	1:A:1968:PHE:CE2	2.20	0.77
1:B:3774:ILE:O	1:B:3778:VAL:HG23	1.83	0.77
1:A:1939:PHE:HD2	1:A:1940:GLU:O	1.67	0.77
1:A:2336:ARG:HD3	1:A:2355:ASP:OD2	1.84	0.77
1:A:2446:SER:H	1:A:2449:THR:HG23	1.49	0.77
1:A:2061:TYR:CD1	1:A:2091:MET:SD	2.78	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2107:LYS:HE2	1:B:2499:SER:HB3	1.66	0.77
1:B:3871:PHE:CZ	1:B:3873:MET:HB2	2.20	0.77
1:A:3946:VAL:CG1	1:A:3950:PHE:O	2.32	0.76
1:B:2420:PRO:HD3	1:B:2536:ASN:HD21	1.50	0.76
1:A:2103:VAL:CG1	1:A:2155:ASP:OD1	2.33	0.76
1:B:1645:PHE:CB	1:B:1765:ILE:CG2	2.59	0.76
1:B:3946:VAL:CG1	1:B:3950:PHE:O	2.33	0.76
1:A:1495:THR:HG22	1:A:1497:ILE:HG22	1.67	0.76
1:B:2512:LYS:O	1:B:2513:GLN:HB2	1.84	0.76
1:A:216:PRO:CB	1:A:1365:PHE:CD1	2.69	0.76
1:A:1922:LYS:HZ1	1:A:4004:LEU:HD12	1.49	0.76
1:B:3473:ALA:HB3	1:B:3476:ARG:O	1.85	0.76
1:B:3998:ILE:HG21	1:B:4004:LEU:HG	1.66	0.76
1:A:2766:LYS:HE3	1:A:2892:CYS:SG	2.26	0.76
1:B:2380:LEU:HD11	1:B:2577:ALA:CB	2.15	0.76
1:B:3019:VAL:O	1:B:3023:LYS:HG3	1.86	0.76
1:B:3566:LEU:HA	1:B:3583:LEU:CD2	2.16	0.76
1:A:2061:TYR:CD1	1:A:2091:MET:CE	2.69	0.76
1:A:2787:HIS:CA	1:A:3460:PRO:HD2	2.14	0.76
1:A:1849:GLU:HG2	1:A:1899:ASN:ND2	2.01	0.76
1:A:3406:PHE:HB2	1:A:3513:VAL:HG11	1.65	0.75
1:B:2572:GLU:CD	1:B:2590:GLU:HG3	2.11	0.75
1:A:3774:ILE:O	1:A:3778:VAL:HG23	1.86	0.75
1:B:2467:THR:CB	1:B:2473:LEU:CD1	2.50	0.75
1:B:2707:VAL:HB	1:B:2712:LEU:CD1	2.11	0.75
1:B:3923:VAL:HG23	1:B:4038:GLU:HA	1.68	0.75
1:B:2446:SER:H	1:B:2449:THR:HG23	1.52	0.75
1:B:3998:ILE:CG2	1:B:4004:LEU:HG	2.16	0.75
1:A:2107:LYS:HE2	1:A:2499:SER:HB3	1.66	0.75
1:B:2061:TYR:CE1	1:B:2091:MET:HE1	2.22	0.75
1:A:2003:LEU:HA	1:A:2006:LEU:HD12	1.66	0.75
1:B:1940:GLU:HG3	1:B:1941:ASP:H	1.52	0.75
1:A:2779:LEU:HD23	1:A:2812:ARG:O	1.87	0.75
1:B:1405:CYS:O	1:B:1409:LEU:HG	1.86	0.75
1:B:2707:VAL:CG1	1:B:2712:LEU:CD1	2.64	0.75
1:B:2176:LEU:O	1:B:2183:ARG:HA	1.87	0.74
1:B:2380:LEU:CD1	1:B:2577:ALA:HB1	2.15	0.74
1:A:2220:CYS:SG	1:A:2224:SER:HB2	2.27	0.74
1:A:3618:TYR:CD1	1:A:3618:TYR:N	2.54	0.74
1:B:2175:ILE:HG12	1:B:2183:ARG:HB3	1.68	0.74
1:B:2476:LYS:HZ1	1:B:2528:ARG:HD2	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3023:LYS:HE2	1:B:3567:LEU:CG	2.16	0.74
1:A:2745:ILE:CG2	1:A:2756:MET:HE1	2.17	0.74
1:A:3998:ILE:HG21	1:A:4004:LEU:HG	1.69	0.74
1:B:2081:THR:CB	2:B:5093:ATP:O2A	2.28	0.74
1:B:2517:LYS:HE2	1:B:2520:GLU:OE1	1.88	0.74
1:A:1707:HIS:O	1:A:1711:VAL:HG23	1.88	0.74
1:A:1922:LYS:HE2	1:A:3999:ASP:O	1.87	0.74
1:B:1630:ILE:CG2	1:B:1655:MET:SD	2.74	0.74
1:B:2112:GLU:CB	1:B:2117:SER:HB2	2.15	0.74
1:B:2220:CYS:CB	2:B:5093:ATP:C6	2.71	0.74
1:A:2152:VAL:HG12	1:A:2154:PHE:HE1	1.51	0.74
1:A:1965:HIS:HD2	1:A:2212:LEU:HD21	1.53	0.74
1:B:2380:LEU:CD1	1:B:2577:ALA:HB2	2.18	0.73
1:A:3566:LEU:HA	1:A:3583:LEU:CD2	2.18	0.73
1:B:2203:THR:HG22	1:B:2205:ALA:H	1.51	0.73
1:B:3618:TYR:N	1:B:3618:TYR:CD1	2.51	0.73
1:A:1559:SER:HB3	1:A:1572:ILE:HG22	1.70	0.73
1:A:1938:GLY:O	1:A:1989:GLU:HB3	1.88	0.73
1:A:1392:LEU:HD13	1:A:1392:LEU:C	2.13	0.73
1:A:3530:PHE:HD1	1:A:3618:TYR:HD2	1.36	0.73
1:B:1535:PRO:HB2	1:B:1841:ILE:CG1	2.18	0.73
1:B:2032:LYS:O	1:B:2035:VAL:HG12	1.86	0.73
1:B:3792:ARG:HB2	1:B:3955:TYR:CD2	2.23	0.73
1:B:3919:LYS:NZ	1:B:4038:GLU:CD	2.47	0.73
1:A:3645:SER:HB3	1:A:3890:GLN:NE2	2.04	0.73
1:A:2425:THR:CG2	3:A:5094:ANP:O3G	2.37	0.73
1:A:1493:LEU:HD23	1:A:1498:GLU:HB3	1.70	0.73
1:A:1527:LEU:CD2	1:A:1545:LEU:HD22	2.18	0.72
1:A:3534:LEU:HD13	1:A:3618:TYR:CE2	2.18	0.72
1:B:2476:LYS:HG2	1:B:2478:ASP:O	1.88	0.72
1:B:3566:LEU:HA	1:B:3583:LEU:HD21	1.71	0.72
1:A:2176:LEU:O	1:A:2183:ARG:HA	1.89	0.72
1:A:3877:CYS:SG	1:A:3884:LEU:HD22	2.29	0.72
1:B:3406:PHE:HB2	1:B:3513:VAL:HG12	1.70	0.72
1:A:3509:LEU:HD12	1:A:3513:VAL:CG2	2.20	0.72
1:B:2446:SER:H	1:B:2449:THR:CG2	2.01	0.72
1:B:2620:ARG:HH12	1:B:2910:ASN:CG	1.97	0.72
1:B:3851:VAL:HG13	1:B:3855:LEU:HD23	1.72	0.72
1:A:3330:TYR:OH	1:A:3346:LEU:HD22	1.90	0.72
1:B:1569:ILE:HA	1:B:1584:SER:HA	1.71	0.72
1:A:3777:VAL:CG1	1:A:3895:PHE:CE1	2.60	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2107:LYS:CE	1:A:2495:ASP:OD2	2.36	0.71
1:A:2380:LEU:CD1	1:A:2577:ALA:HB2	2.20	0.71
1:B:1706:LEU:HD22	1:B:1935:GLN:HG2	1.72	0.71
1:B:2476:LYS:NZ	1:B:2528:ARG:HD2	2.04	0.71
1:A:2336:ARG:CD	1:A:2355:ASP:OD2	2.38	0.71
1:A:3979:ASN:C	1:A:3981:PRO:HD2	2.15	0.71
1:B:2448:ASP:HB2	1:B:2829:GLU:OE1	1.91	0.71
1:B:3618:TYR:N	1:B:3618:TYR:HD1	1.87	0.71
1:B:3534:LEU:HD11	1:B:3614:LEU:HD23	1.73	0.71
1:B:3792:ARG:HB2	1:B:3955:TYR:CE2	2.26	0.71
1:A:2293:HIS:CE1	1:A:2409:ASN:HB3	2.25	0.71
1:B:1540:LEU:CD1	1:B:1548:ILE:HD11	2.21	0.71
1:A:2960:THR:HB	1:A:2963:ASP:HB2	1.72	0.71
1:B:1852:ARG:O	1:B:1852:ARG:HG3	1.91	0.71
1:A:1626:CYS:SG	1:A:1639:VAL:HG11	2.31	0.71
1:A:2549:ARG:HE	2:A:5093:ATP:PG	2.13	0.71
1:A:4065:LEU:HD11	1:A:4070:ILE:HD11	1.72	0.71
1:B:1620:PHE:HB2	1:B:1760:PHE:CE1	2.26	0.71
1:B:2111:LYS:CD	1:B:2161:GLU:HG3	2.10	0.71
1:A:2103:VAL:HG13	1:A:2155:ASP:OD1	1.91	0.71
1:A:3566:LEU:O	1:A:3570:LEU:HG	1.91	0.71
1:B:1738:ASN:O	1:B:1739:ASP:OD1	2.09	0.71
1:B:2787:HIS:CA	1:B:3460:PRO:HD2	2.20	0.71
1:A:2222:ILE:HG23	1:A:2284:LEU:HD11	1.73	0.70
1:A:3024:LEU:HD11	1:A:3303:LYS:CG	2.17	0.70
1:A:3473:ALA:HB3	1:A:3476:ARG:O	1.91	0.70
1:B:2420:PRO:HB2	1:B:2620:ARG:NH2	2.06	0.70
1:A:1620:PHE:CZ	1:A:1743:ASP:HB3	2.25	0.70
1:A:4033:LEU:HD13	1:A:4035:GLN:CB	2.22	0.70
1:B:1938:GLY:O	1:B:1989:GLU:HB3	1.92	0.70
1:B:1953:LEU:CD1	1:B:1973:LEU:HB3	2.21	0.70
1:A:2891:ILE:HD11	1:A:2903:ILE:HD11	1.73	0.70
1:B:3737:THR:HB	1:B:3740:THR:HG1	1.53	0.70
1:A:2563:SER:HB2	1:A:2566:SER:OG	1.92	0.70
1:B:2472:THR:HG21	1:B:2524:VAL:HG22	1.74	0.70
1:A:2095:ASP:CG	1:A:2149:ARG:HH22	2.00	0.70
1:A:3459:ASP:OD2	1:A:3461:ILE:HG12	1.92	0.70
1:B:3577:MET:O	1:B:3579:GLU:N	2.24	0.70
1:A:3951:SER:HB2	1:A:4002:LYS:HD2	1.73	0.70
1:B:2064:GLN:OE1	1:B:2151:TRP:HH2	1.74	0.70
1:A:216:PRO:CB	1:A:1365:PHE:HE1	1.99	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2225:LYS:HA	2:A:5093:ATP:N3	2.07	0.70
1:A:3935:PHE:HB2	1:A:4014:VAL:HG11	1.73	0.70
1:B:3631:MET:CE	1:B:3698:MET:HG3	2.21	0.70
1:B:1620:PHE:HD1	1:B:1760:PHE:HZ	0.81	0.69
1:B:3406:PHE:HB2	1:B:3513:VAL:HG11	1.72	0.69
1:B:1698:ILE:O	1:B:1702:LEU:HG	1.92	0.69
1:B:2745:ILE:HG23	1:B:2756:MET:CE	2.22	0.69
1:B:3645:SER:CB	1:B:3890:GLN:HE21	2.03	0.69
1:A:1574:PHE:HB3	1:A:1576:GLU:H	1.57	0.69
1:A:3631:MET:HE1	1:A:3698:MET:HG3	1.74	0.69
1:B:3330:TYR:OH	1:B:3346:LEU:HD22	1.92	0.69
1:A:3566:LEU:HA	1:A:3583:LEU:HD21	1.74	0.69
1:B:2220:CYS:SG	1:B:2224:SER:CB	2.81	0.69
1:A:1540:LEU:CD1	1:A:1548:ILE:CD1	2.71	0.69
1:A:1726:LEU:CD1	1:A:3984:GLN:HB3	2.23	0.69
1:A:3848:LEU:HD21	1:A:3852:LYS:HE3	1.73	0.69
1:A:1405:CYS:O	1:A:1409:LEU:HG	1.92	0.69
1:A:1849:GLU:HG2	1:A:1899:ASN:HD22	1.57	0.69
1:A:2632:ALA:HB3	1:A:2647:LEU:HD21	1.75	0.69
1:B:1387:GLU:HB3	1:B:1393:LYS:HG2	1.73	0.69
1:B:2410:SER:C	1:B:2411:LYS:HG3	2.16	0.69
1:B:2707:VAL:CG1	1:B:2712:LEU:HD11	2.21	0.69
1:B:3871:PHE:HZ	1:B:3873:MET:HB2	1.57	0.69
1:A:3799:LYS:O	1:A:3803:LEU:HG	1.93	0.69
1:B:3837:GLY:O	1:B:3871:PHE:HD1	1.75	0.69
1:A:1802:LYS:NZ	4:A:5095:SO4:O2	2.26	0.69
1:A:1970:LEU:CD1	1:A:1974:LYS:HE3	2.14	0.69
1:A:1562:MET:CB	1:A:1569:ILE:HD11	2.21	0.68
1:B:2061:TYR:CD1	1:B:2091:MET:SD	2.86	0.68
1:A:1368:GLU:HG2	1:A:1424:PHE:CE2	2.25	0.68
1:A:1462:ASN:CB	1:A:1465:ILE:HG22	2.22	0.68
1:A:2109:LEU:HD13	1:A:2129:LEU:HD23	1.75	0.68
1:A:2173:ASN:HB3	1:A:2175:ILE:HG22	1.73	0.68
1:B:1489:ARG:HH12	1:B:1503:PRO:HG2	1.57	0.68
1:B:1540:LEU:CD1	1:B:1548:ILE:CD1	2.71	0.68
1:B:3023:LYS:CD	1:B:3567:LEU:HD23	2.19	0.68
1:A:1394:LEU:HD22	1:A:1449:GLN:HE22	1.57	0.68
1:A:2290:LEU:HD13	1:A:2407:LEU:HD23	1.75	0.68
1:A:2707:VAL:CG1	1:A:2712:LEU:HD11	2.22	0.68
1:B:3819:ILE:O	1:B:3823:ASN:HB2	1.93	0.68
1:A:1995:VAL:HG21	1:A:2024:SER:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2336:ARG:HD3	1:B:2355:ASP:OD2	1.93	0.68
1:B:2181:GLY:O	1:B:2182:GLU:HG3	1.93	0.68
1:A:2476:LYS:NZ	1:A:2528:ARG:HD3	2.09	0.68
1:A:3816:LEU:HD23	1:A:3847:SER:OG	1.93	0.68
1:B:2563:SER:HB2	1:B:2566:SER:OG	1.93	0.68
1:A:2203:THR:HG22	1:A:2205:ALA:H	1.59	0.68
1:B:3459:ASP:OD2	1:B:3461:ILE:HG12	1.93	0.68
1:A:2428:MET:HE2	1:A:2432:LEU:HD12	1.74	0.68
1:A:3837:GLY:O	1:A:3871:PHE:HD1	1.76	0.68
1:B:3777:VAL:CG1	1:B:3895:PHE:CE1	2.64	0.68
1:A:2846:GLY:O	1:A:2849:TYR:HB3	1.92	0.68
1:B:3612:ASP:O	1:B:3615:VAL:HG22	1.93	0.68
1:B:3566:LEU:HD13	1:B:3570:LEU:CD1	2.24	0.67
1:A:2095:ASP:CG	1:A:2149:ARG:NH2	2.53	0.67
1:B:3839:ILE:CG2	1:B:3873:MET:HG3	2.24	0.67
1:A:1645:PHE:CG	1:A:1765:ILE:HG22	2.29	0.67
1:B:1536:ARG:N	1:B:1841:ILE:HD11	2.09	0.67
1:B:1929:ILE:HD13	1:B:1970:LEU:HD11	1.75	0.67
1:B:2293:HIS:CE1	1:B:2409:ASN:HB3	2.29	0.67
1:A:2220:CYS:SG	1:A:2224:SER:CB	2.82	0.67
1:A:3303:LYS:CA	1:A:3306:TRP:HD1	2.03	0.67
1:A:3886:ALA:N	1:A:3887:PRO:HD2	2.10	0.67
1:B:1645:PHE:CG	1:B:1765:ILE:HG22	2.28	0.67
1:B:3566:LEU:O	1:B:3570:LEU:HG	1.94	0.67
1:B:3592:LYS:O	1:B:3596:ASN:HB2	1.94	0.67
1:B:1611:LEU:O	1:B:1615:ILE:HG23	1.95	0.67
1:B:1726:LEU:HD13	1:B:3984:GLN:HB3	1.77	0.67
1:B:3919:LYS:HZ3	1:B:4038:GLU:CD	2.02	0.67
1:A:2707:VAL:CG1	1:A:2712:LEU:CD1	2.72	0.67
1:B:3886:ALA:N	1:B:3887:PRO:HD2	2.09	0.67
1:A:2380:LEU:HD12	1:A:2577:ALA:HB2	1.75	0.67
1:B:1620:PHE:HA	1:B:1760:PHE:HE1	1.59	0.67
1:B:2394:THR:H	1:B:2397:THR:HB	1.59	0.67
1:A:1744:LEU:HA	1:A:1760:PHE:CD2	2.29	0.67
1:A:3530:PHE:HD1	1:A:3618:TYR:CD2	2.09	0.67
1:B:2745:ILE:CG2	1:B:2756:MET:HE1	2.22	0.67
1:B:3816:LEU:HD23	1:B:3847:SER:OG	1.95	0.67
1:A:2080:LYS:HG2	1:A:2215:PHE:CE1	2.29	0.67
1:A:2131:THR:HG22	1:A:2176:LEU:HD21	1.77	0.67
1:A:2224:SER:O	2:A:5093:ATP:C2	2.48	0.67
1:A:2386:MET:HB3	1:A:2627:ARG:NE	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3871:PHE:CZ	1:A:3873:MET:HB2	2.30	0.67
1:B:1612:ASP:HA	1:B:1615:ILE:CD1	2.25	0.67
1:A:1536:ARG:N	1:A:1841:ILE:HD11	2.10	0.66
1:A:1922:LYS:NZ	1:A:4004:LEU:CD1	2.58	0.66
1:B:1649:LEU:CD1	1:B:1704:GLU:HG3	2.25	0.66
1:B:2489:ILE:HG22	1:B:2535:CYS:HB3	1.77	0.66
1:B:1495:THR:HG22	1:B:1497:ILE:HG22	1.77	0.66
1:B:1540:LEU:HD12	1:B:1548:ILE:CD1	2.25	0.66
1:A:1527:LEU:HD23	1:A:1545:LEU:HD22	1.77	0.66
1:A:2112:GLU:HB3	1:A:2117:SER:CB	2.25	0.66
1:B:2936:ILE:HG22	1:B:2962:ARG:HD3	1.78	0.66
1:A:2081:THR:O	1:A:2085:LYS:HB2	1.96	0.66
1:A:1540:LEU:HD11	1:A:1548:ILE:HD11	1.76	0.66
1:A:2425:THR:HG23	3:A:5094:ANP:O3G	1.95	0.66
1:A:1540:LEU:CD1	1:A:1548:ILE:HD11	2.26	0.66
1:A:1466:GLN:CB	1:A:1473:THR:HG21	2.26	0.66
1:B:2745:ILE:HG12	1:B:2756:MET:HE1	1.77	0.66
1:A:1531:ARG:HG2	1:A:1537:PHE:HB3	1.77	0.66
1:A:2495:ASP:O	1:A:2498:GLY:N	2.29	0.66
1:A:3303:LYS:HA	1:A:3306:TRP:HE1	1.59	0.66
1:B:3566:LEU:CD1	1:B:3570:LEU:HD11	2.25	0.66
1:B:2109:LEU:CD1	1:B:2129:LEU:HD23	2.26	0.65
1:B:2302:PHE:HA	1:B:2310:LEU:HD11	1.77	0.65
1:B:3023:LYS:CE	1:B:3567:LEU:HG	2.25	0.65
1:A:3618:TYR:N	1:A:3618:TYR:HD1	1.94	0.65
1:A:1620:PHE:CD1	1:A:1760:PHE:HZ	2.10	0.65
1:A:2302:PHE:HA	1:A:2310:LEU:HD11	1.76	0.65
1:B:2220:CYS:SG	1:B:2224:SER:HB2	2.36	0.65
1:A:1706:LEU:CD2	1:A:1935:GLN:HG2	2.27	0.65
1:B:1849:GLU:OE2	1:B:1899:ASN:ND2	2.30	0.65
1:B:3850:TRP:NE1	1:B:3854:TYR:HB3	2.12	0.65
1:B:2173:ASN:HB3	1:B:2175:ILE:HG22	1.77	0.65
1:A:1649:LEU:CD1	1:A:1704:GLU:HG3	2.27	0.65
1:A:1706:LEU:HD21	1:A:1935:GLN:HG2	1.79	0.65
1:A:1425:GLU:OE2	1:A:1429:LEU:HD11	1.96	0.65
1:A:2032:LYS:O	1:A:2035:VAL:HG12	1.96	0.65
1:A:2111:LYS:HZ2	1:A:2161:GLU:HG2	1.61	0.65
1:A:2766:LYS:CE	1:A:2892:CYS:SG	2.84	0.65
1:B:2508:GLN:HG3	1:B:2512:LYS:HG3	1.77	0.65
1:B:3460:PRO:O	1:B:3463:SER:HB3	1.97	0.65
1:B:1391:GLY:HA3	1:B:1484:LYS:NZ	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2391:VAL:CG2	1:B:2426:MET:SD	2.83	0.65
1:B:2513:GLN:O	1:B:2526:ILE:CG1	2.45	0.65
1:B:1425:GLU:OE2	1:B:1429:LEU:CD2	2.45	0.65
1:B:1748:PHE:CD2	1:B:1755:LEU:HD22	2.32	0.65
1:B:1995:VAL:HG21	1:B:2024:SER:HB3	1.78	0.64
1:B:2941:THR:HG22	1:B:2942:ASP:H	1.62	0.64
1:B:2109:LEU:HD11	1:B:2129:LEU:HD23	1.79	0.64
1:B:2637:PRO:O	1:B:2639:GLN:NE2	2.30	0.64
1:A:1535:PRO:HB2	1:A:1841:ILE:CG1	2.27	0.64
1:A:2039:LYS:HG2	1:A:2049:MET:HG3	1.78	0.64
1:A:3979:ASN:O	1:A:3981:PRO:HD2	1.98	0.64
1:A:2728:LEU:HD12	1:A:2771:ARG:NH2	2.12	0.64
1:B:3911:TRP:HH2	1:B:3926:VAL:HG12	1.62	0.64
1:A:1630:ILE:CG2	1:A:1655:MET:SD	2.86	0.64
1:A:3785:TYR:HE2	1:A:3859:VAL:HG22	1.62	0.64
1:B:1726:LEU:CD1	1:B:3984:GLN:CB	2.75	0.64
1:A:1645:PHE:CD2	1:A:1765:ILE:HG22	2.32	0.64
1:A:3541:MET:HA	1:A:3544:LYS:HG2	1.78	0.64
1:A:1991:GLU:O	1:A:1995:VAL:HG23	1.98	0.64
1:B:1822:CYS:SG	1:B:1849:GLU:O	2.56	0.64
1:B:2003:LEU:HA	1:B:2006:LEU:HD12	1.80	0.64
1:B:2413:GLY:HA3	1:B:2510:MET:HE3	1.80	0.64
1:B:1531:ARG:HG2	1:B:1537:PHE:HB3	1.79	0.64
1:B:2293:HIS:NE2	1:B:2409:ASN:HB3	2.13	0.64
1:A:1365:PHE:CZ	1:A:1420:TYR:CE1	2.86	0.63
1:B:1983:LEU:CD2	1:B:1993:THR:O	2.45	0.63
1:B:3737:THR:OG1	1:B:3740:THR:HB	1.98	0.63
1:A:2401:GLU:HG2	1:A:2431:ALA:HB2	1.81	0.63
1:B:2623:THR:HB	3:B:5094:ANP:O2'	1.99	0.63
1:B:3440:LEU:CD2	1:B:3462:ILE:HD12	2.29	0.63
1:A:1392:LEU:HD13	1:A:1393:LYS:C	2.24	0.63
1:A:2257:PHE:HD1	1:A:2262:LEU:HD11	1.61	0.63
1:B:2728:LEU:HD12	1:B:2771:ARG:CZ	2.28	0.63
1:A:1425:GLU:C	1:A:1425:GLU:OE1	2.42	0.63
1:A:1967:HIS:C	1:A:1968:PHE:HD1	2.06	0.63
1:A:2034:ILE:HD12	1:A:2061:TYR:CZ	2.33	0.63
1:B:2932:MET:HE1	1:B:2993:ILE:HG23	1.79	0.63
1:B:3509:LEU:HD12	1:B:3513:VAL:CG2	2.28	0.63
1:A:1489:ARG:HH12	1:A:1503:PRO:HG2	1.64	0.63
1:A:2552:ARG:HG2	1:A:2552:ARG:NH1	2.14	0.63
1:A:3679:TYR:HB3	1:A:3767:PHE:HE1	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3948:HIS:NE2	1:B:4072:ASN:CG	2.57	0.63
1:B:3979:ASN:C	1:B:3981:PRO:HD2	2.24	0.63
1:A:1900:PRO:HB3	1:A:1905:ARG:HA	1.80	0.63
1:B:1744:LEU:HD22	1:B:1760:PHE:CG	2.34	0.63
1:B:2508:GLN:CG	1:B:2512:LYS:HG3	2.28	0.63
1:B:1421:TYR:O	1:B:1425:GLU:N	2.32	0.63
1:A:1391:GLY:HA3	1:A:1484:LYS:NZ	2.13	0.62
1:A:1965:HIS:HD2	1:A:2212:LEU:CD2	2.11	0.62
1:A:3509:LEU:CD1	1:A:3513:VAL:CG2	2.74	0.62
1:A:3850:TRP:NE1	1:A:3854:TYR:HB3	2.13	0.62
1:B:2220:CYS:SG	2:B:5093:ATP:C6	2.92	0.62
1:B:3925:SER:HB2	1:B:3972:LEU:HD13	1.81	0.62
1:A:3530:PHE:CE1	1:A:3618:TYR:CD2	2.87	0.62
1:B:2109:LEU:HD11	1:B:2129:LEU:CD2	2.29	0.62
1:B:3530:PHE:CE1	1:B:3618:TYR:CD2	2.87	0.62
1:B:3912:GLY:O	1:B:3915:PHE:CZ	2.52	0.62
1:B:1425:GLU:OE2	1:B:1429:LEU:HD21	1.98	0.62
1:B:2224:SER:C	2:B:5093:ATP:H2	2.07	0.62
1:A:3737:THR:OG1	1:A:3740:THR:HB	1.99	0.62
1:B:1706:LEU:HD11	1:B:1936:ILE:HG12	1.80	0.62
1:B:2428:MET:SD	1:B:2532:VAL:HG11	2.39	0.62
1:B:3700:MET:HB3	1:B:4085:THR:HG21	1.81	0.62
1:B:1911:ASN:OD1	1:B:1912:LEU:N	2.33	0.62
1:B:2095:ASP:CG	1:B:2149:ARG:NH2	2.57	0.62
1:B:3839:ILE:HG23	1:B:3873:MET:HG3	1.81	0.62
1:A:3566:LEU:CD1	1:A:3570:LEU:HD11	2.30	0.62
1:B:2280:THR:HA	1:B:2283:LYS:HD2	1.81	0.62
1:B:2467:THR:OG1	1:B:2473:LEU:HD12	1.99	0.62
1:B:2677:VAL:HG11	1:B:2686:LEU:HD21	1.82	0.62
1:A:1664:LEU:HD23	1:A:1669:PHE:HZ	1.63	0.62
1:A:2151:TRP:HE3	1:A:2193:LEU:HD11	1.63	0.62
1:A:2280:THR:HA	1:A:2283:LYS:HD2	1.80	0.62
1:A:2578:ILE:CG2	1:A:2630:TYR:HB2	2.29	0.62
1:A:2709:LYS:O	1:A:2713:VAL:HG23	1.98	0.62
1:B:1726:LEU:HD12	1:B:3984:GLN:CB	2.29	0.62
1:B:3566:LEU:HD13	1:B:3570:LEU:HD11	1.81	0.62
1:A:1536:ARG:HD3	1:A:1841:ILE:HD13	1.82	0.62
1:A:3787:THR:HG22	1:A:3875:MET:HB2	1.81	0.62
1:B:1392:LEU:HD13	1:B:1393:LYS:C	2.25	0.62
1:B:1748:PHE:HD2	1:B:1755:LEU:HD22	1.65	0.61
1:B:1965:HIS:HD2	1:B:2212:LEU:HD21	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2631:THR:O	1:B:2635:THR:HG22	1.99	0.61
1:A:1984:ILE:HG21	1:A:1989:GLU:HG3	1.82	0.61
1:B:3692:LYS:HE3	1:B:3898:GLU:HB3	1.81	0.61
1:A:2578:ILE:HG21	1:A:2630:TYR:HB2	1.82	0.61
1:B:2111:LYS:HZ3	1:B:2161:GLU:HG2	1.63	0.61
1:B:3737:THR:HB	1:B:3740:THR:CB	2.29	0.61
1:A:3813:ILE:HG22	1:A:3840:LEU:HD23	1.83	0.61
1:A:2757:MET:HE3	1:A:2912:CYS:HB2	1.81	0.61
1:B:2063:MET:HB3	1:B:2070:LEU:HD11	1.82	0.61
1:A:1612:ASP:HA	1:A:1615:ILE:CD1	2.30	0.61
1:A:2380:LEU:HD11	1:A:2577:ALA:CB	2.30	0.61
1:B:3023:LYS:HD3	1:B:3567:LEU:CD2	2.10	0.61
1:A:1469:LEU:HD13	1:A:1523:LEU:CD2	2.30	0.61
1:A:1802:LYS:HG2	1:A:1921:MET:HG3	1.83	0.61
1:A:3696:MET:SD	1:A:3760:LEU:HD23	2.41	0.61
1:B:2493:LYS:HG3	1:B:2494:LEU:H	1.66	0.61
1:A:2293:HIS:CE1	1:A:2409:ASN:CB	2.84	0.61
1:A:2745:ILE:CG1	1:A:2756:MET:HE1	2.29	0.61
1:A:3964:ALA:HB2	1:A:3993:VAL:HG11	1.82	0.61
1:A:4021:LEU:HD23	1:A:4023:ILE:HG12	1.82	0.61
1:B:1493:LEU:O	1:B:1494:ASP:HB2	2.00	0.61
1:B:3023:LYS:CE	1:B:3567:LEU:CD2	2.79	0.61
1:A:2394:THR:H	1:A:2397:THR:HB	1.65	0.61
1:A:1826:PHE:CE1	1:A:1853:LEU:HD22	2.36	0.60
1:A:3839:ILE:CG2	1:A:3873:MET:HG3	2.31	0.60
1:B:1849:GLU:HG2	1:B:1899:ASN:ND2	2.16	0.60
1:B:2386:MET:HB3	1:B:2627:ARG:HD3	1.77	0.60
1:B:2707:VAL:CG1	1:B:2712:LEU:HD12	2.31	0.60
1:A:1849:GLU:OE2	1:A:1899:ASN:ND2	2.34	0.60
1:A:3912:GLY:O	1:A:3915:PHE:CZ	2.55	0.60
1:B:1744:LEU:HD22	1:B:1760:PHE:CD2	2.36	0.60
1:B:3912:GLY:O	1:B:3915:PHE:CE2	2.54	0.60
1:B:1706:LEU:HD22	1:B:1935:GLN:CG	2.30	0.60
1:B:1983:LEU:HD21	1:B:1996:GLU:HB2	1.84	0.60
1:B:3525:ILE:HD11	1:B:3646:ILE:CG2	2.18	0.60
1:A:1493:LEU:HD23	1:A:1498:GLU:CB	2.31	0.60
1:A:2111:LYS:HZ3	1:A:2161:GLU:HG2	1.66	0.60
1:A:2230:LEU:HD23	1:A:2288:VAL:HG13	1.83	0.60
1:A:3656:VAL:CG1	1:A:3677:LEU:HB3	2.30	0.60
1:B:1991:GLU:O	1:B:1995:VAL:HG23	2.01	0.60
1:B:3330:TYR:CD1	1:B:3334:PHE:CD2	2.90	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2332:GLY:O	1:A:2336:ARG:HG3	2.01	0.60
1:A:3303:LYS:C	1:A:3306:TRP:CD1	2.72	0.60
1:A:3641:PHE:HA	1:A:3889:LEU:HD21	1.84	0.60
1:A:3566:LEU:HD13	1:A:3570:LEU:CD1	2.32	0.60
1:B:1692:ASP:O	1:B:1695:LYS:HB3	2.01	0.60
1:B:1983:LEU:CG	1:B:1993:THR:HG23	2.25	0.60
1:B:2107:LYS:CE	1:B:2495:ASP:OD2	2.38	0.60
1:B:2476:LYS:H	1:B:2476:LYS:HD2	1.67	0.60
1:A:2125:TRP:CZ2	1:A:2178:LEU:HD13	2.37	0.60
1:B:3728:GLU:HG3	1:B:4079:LYS:HE2	1.82	0.60
1:A:2476:LYS:H	1:A:2476:LYS:HD2	1.64	0.59
1:A:2512:LYS:O	1:A:2513:GLN:CB	2.50	0.59
1:A:3583:LEU:O	1:A:3587:LEU:HG	2.02	0.59
1:A:3819:ILE:O	1:A:3823:ASN:HB2	2.01	0.59
1:A:2446:SER:H	1:A:2449:THR:HG21	1.66	0.59
1:A:3592:LYS:O	1:A:3596:ASN:HB2	2.02	0.59
1:B:2490:ASN:HB3	1:B:2546:MET:HE2	1.83	0.59
1:B:2960:THR:HB	1:B:2963:ASP:HB2	1.84	0.59
1:B:3671:VAL:O	1:B:3674:ILE:HG22	2.02	0.59
1:A:1956:LEU:HB3	1:A:1968:PHE:HE2	1.67	0.59
1:A:3839:ILE:HG23	1:A:3873:MET:HG3	1.84	0.59
1:B:2074:GLY:O	1:B:2197:ASP:HA	2.03	0.59
1:B:2131:THR:HG22	1:B:2176:LEU:CD2	2.32	0.59
1:B:3612:ASP:O	1:B:3615:VAL:CG2	2.50	0.59
1:A:1493:LEU:O	1:A:1494:ASP:HB2	2.01	0.59
1:A:1802:LYS:NZ	4:A:5095:SO4:S	2.75	0.59
1:A:1970:LEU:HD12	1:A:1970:LEU:C	2.27	0.59
1:A:2197:ASP:HB3	1:A:2549:ARG:HD2	1.84	0.59
1:A:3671:VAL:HA	1:A:3674:ILE:HG22	1.83	0.59
1:A:3785:TYR:CE2	1:A:3859:VAL:HG22	2.37	0.59
1:A:1534:PHE:HD2	1:A:1537:PHE:CE1	2.20	0.59
1:B:1536:ARG:HD2	1:B:1565:MET:O	2.01	0.59
1:B:2423:GLY:N	3:B:5094:ANP:O1B	2.29	0.59
1:B:3877:CYS:SG	1:B:3884:LEU:HD22	2.41	0.59
1:A:1391:GLY:HA3	1:A:1484:LYS:HZ3	1.67	0.59
1:B:2293:HIS:CE1	1:B:2409:ASN:CB	2.86	0.59
1:A:1939:PHE:HD1	1:A:1939:PHE:H	1.51	0.59
1:B:3541:MET:HA	1:B:3544:LYS:HG2	1.85	0.59
1:B:2512:LYS:O	1:B:2513:GLN:CB	2.50	0.59
1:B:3995:GLY:HA2	1:B:3998:ILE:HD13	1.84	0.59
1:A:2080:LYS:HG2	1:A:2215:PHE:CD1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2201:HIS:CE1	1:A:2497:TYR:HA	2.38	0.59
1:B:166:PRO:CB	1:B:1369:LYS:HB3	2.32	0.59
1:B:1926:SER:HB2	1:B:1970:LEU:HD12	1.84	0.59
1:B:2266:PHE:HD1	1:B:2326:LEU:HD21	1.67	0.59
1:B:2856:LEU:HD23	1:B:2873:LEU:HB3	1.84	0.59
1:A:1852:ARG:O	1:A:1852:ARG:HG3	2.03	0.59
1:A:1965:HIS:CD2	1:A:2212:LEU:HD21	2.38	0.59
1:A:2786:ILE:O	1:A:3460:PRO:HB2	2.01	0.59
1:A:3460:PRO:O	1:A:3463:SER:HB3	2.03	0.59
1:B:2274:HIS:CE1	1:B:2326:LEU:O	2.51	0.59
1:B:2503:VAL:HA	1:B:2506:LEU:HD12	1.83	0.59
1:B:3525:ILE:CD1	1:B:3646:ILE:HG22	2.19	0.59
1:A:2425:THR:HG21	3:A:5094:ANP:O3G	2.02	0.58
1:A:3350:LYS:HA	1:A:3353:LEU:HD12	1.84	0.58
1:A:3737:THR:HB	1:A:3740:THR:CB	2.32	0.58
1:B:1620:PHE:HA	1:B:1760:PHE:CE1	2.37	0.58
1:B:3807:SER:O	1:B:3808:LYS:HB2	2.03	0.58
1:A:2102:TYR:HB2	1:A:2152:VAL:HG22	1.84	0.58
1:B:1683:LEU:HB3	1:B:1702:LEU:HD21	1.84	0.58
1:A:1823:ASP:HB2	1:A:1853:LEU:HD23	1.83	0.58
1:B:1649:LEU:HD11	1:B:1704:GLU:HG3	1.82	0.58
1:A:1368:GLU:CG	1:A:1424:PHE:CE2	2.86	0.58
1:B:2517:LYS:CE	1:B:2520:GLU:OE1	2.50	0.58
1:A:1683:LEU:HD22	1:A:1698:ILE:HG23	1.85	0.58
1:A:2293:HIS:NE2	1:A:2409:ASN:HB3	2.18	0.58
1:A:2842:ASP:O	1:A:2845:GLN:HG2	2.04	0.58
1:B:2655:ILE:HD11	1:B:2747:ARG:HH22	1.68	0.58
1:B:2766:LYS:HE2	1:B:2890:THR:HB	1.85	0.58
1:A:1774:LEU:HD21	1:A:1922:LYS:O	2.03	0.58
1:A:2563:SER:CB	1:A:2566:SER:OG	2.51	0.58
1:A:3409:ASP:HB3	1:A:3518:PHE:HB2	1.85	0.58
1:B:1703:VAL:HG13	1:B:1770:ILE:HD13	1.85	0.58
1:B:2332:GLY:HA2	1:B:2335:GLN:CB	2.30	0.58
1:B:3946:VAL:HA	1:B:3947:PRO:C	2.28	0.58
1:A:1421:TYR:O	1:A:1425:GLU:N	2.36	0.58
1:B:1929:ILE:HD13	1:B:1970:LEU:CD1	2.34	0.58
1:B:2127:ASP:O	1:B:2131:THR:OG1	2.22	0.58
1:B:3530:PHE:HD1	1:B:3618:TYR:HD2	1.49	0.58
1:B:3612:ASP:C	1:B:3615:VAL:HG22	2.29	0.58
1:A:2755:HIS:O	1:A:2913:ILE:HG13	2.03	0.58
1:A:3792:ARG:HB2	1:A:3955:TYR:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1534:PHE:CE2	1:B:1536:ARG:HB2	2.39	0.58
1:B:2846:GLY:O	1:B:2849:TYR:HB3	2.02	0.58
1:A:1559:SER:CB	1:A:1572:ILE:HG22	2.34	0.58
1:A:2420:PRO:HD3	1:A:2536:ASN:HD21	1.69	0.58
1:A:3569:GLU:O	1:A:3573:SER:OG	2.22	0.58
1:B:1391:GLY:HA3	1:B:1484:LYS:HZ1	1.68	0.58
1:B:1707:HIS:O	1:B:1711:VAL:HG23	2.04	0.58
1:B:1940:GLU:HG3	1:B:1941:ASP:N	2.19	0.58
1:B:2786:ILE:O	1:B:3460:PRO:HB2	2.04	0.58
1:A:1409:LEU:CD2	1:A:1435:LEU:HB3	2.24	0.57
1:A:1620:PHE:HA	1:A:1760:PHE:CE1	2.39	0.57
1:A:1953:LEU:CD1	1:A:1973:LEU:HB3	2.33	0.57
1:A:3449:VAL:HG22	1:A:3493:LYS:HB2	1.85	0.57
1:A:2064:GLN:OE1	1:A:2151:TRP:CH2	2.51	0.57
1:A:3912:GLY:O	1:A:3915:PHE:CE2	2.57	0.57
1:B:1984:ILE:HG21	1:B:1989:GLU:HG3	1.86	0.57
1:B:4020:ASN:HB3	1:B:4028:ARG:HH11	1.68	0.57
1:A:2266:PHE:HD1	1:A:2326:LEU:HD21	1.69	0.57
1:A:2382:ALA:O	1:A:2385:VAL:HG12	2.04	0.57
1:A:3810:SER:O	1:A:3838:TRP:HB2	2.03	0.57
1:A:1493:LEU:CD2	1:A:1498:GLU:HB3	2.33	0.57
1:A:1611:LEU:O	1:A:1615:ILE:HG23	2.05	0.57
1:A:1612:ASP:HA	1:A:1615:ILE:HD11	1.86	0.57
1:B:2428:MET:HE2	1:B:2485:PHE:CD1	2.39	0.57
1:A:1738:ASN:O	1:A:1739:ASP:OD1	2.23	0.57
1:A:1945:LEU:HD13	1:A:1994:VAL:HG21	1.86	0.57
1:A:2932:MET:HE1	1:A:2993:ILE:HG23	1.87	0.57
1:B:1940:GLU:CB	1:B:1989:GLU:O	2.52	0.57
1:B:2755:HIS:NE2	1:B:2835:LEU:HG	2.20	0.57
1:B:3350:LYS:HA	1:B:3353:LEU:HD12	1.87	0.57
1:A:1698:ILE:O	1:A:1702:LEU:HG	2.05	0.57
1:A:2225:LYS:HG2	1:A:2229:LEU:HD12	1.87	0.57
1:A:3566:LEU:HD13	1:A:3570:LEU:HD11	1.87	0.57
1:A:4021:LEU:HD23	1:A:4023:ILE:CG1	2.34	0.57
1:B:1953:LEU:HD11	1:B:1973:LEU:HB3	1.86	0.57
1:A:1469:LEU:HB3	1:A:1472:GLU:HB2	1.86	0.57
1:A:2274:HIS:CE1	1:A:2326:LEU:O	2.47	0.57
1:B:2788:ARG:HB2	1:B:3459:ASP:HB3	1.87	0.57
1:B:1620:PHE:CB	1:B:1760:PHE:CE1	2.87	0.57
1:B:2084:TRP:HE3	1:B:2088:ILE:HD12	1.70	0.57
1:B:2563:SER:CB	1:B:2566:SER:OG	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2620:ARG:O	1:B:2623:THR:HG22	2.04	0.57
1:A:2127:ASP:O	1:A:2131:THR:OG1	2.23	0.57
1:A:2437:LEU:H	1:A:2437:LEU:HD12	1.70	0.57
1:A:2637:PRO:O	1:A:2639:GLN:NE2	2.38	0.57
1:A:4020:ASN:ND2	1:A:4028:ARG:HD3	2.20	0.57
1:B:2034:ILE:HD12	1:B:2061:TYR:CZ	2.39	0.57
1:B:3353:LEU:HD23	1:B:3358:VAL:HG11	1.85	0.57
1:A:2047:PHE:CE2	1:A:2082:ALA:HB1	2.40	0.57
1:A:2137:VAL:O	1:A:2141:ILE:CG2	2.51	0.57
1:B:1527:LEU:CD2	1:B:1545:LEU:HD22	2.35	0.57
1:B:1744:LEU:HA	1:B:1760:PHE:HE2	1.66	0.57
1:B:2536:ASN:HB2	1:B:2543:ARG:HE	1.70	0.57
1:A:1535:PRO:O	1:A:1841:ILE:HD11	2.05	0.56
1:A:1794:PHE:HD1	1:A:1802:LYS:HB3	1.69	0.56
1:A:2290:LEU:HD23	1:A:2321:SER:HA	1.86	0.56
1:B:1823:ASP:HB2	1:B:1853:LEU:HD23	1.86	0.56
1:B:2755:HIS:CB	1:B:2911:ARG:O	2.47	0.56
1:B:3017:VAL:HG21	1:B:3313:PHE:CE2	2.40	0.56
1:B:3330:TYR:CE1	1:B:3334:PHE:CD2	2.93	0.56
1:B:3810:SER:O	1:B:3838:TRP:HB2	2.04	0.56
1:A:2517:LYS:HG2	1:A:2520:GLU:HB2	1.87	0.56
1:A:3618:TYR:O	1:A:3622:GLY:N	2.37	0.56
1:B:2448:ASP:HB2	1:B:2829:GLU:CD	2.31	0.56
1:B:3583:LEU:O	1:B:3587:LEU:HG	2.05	0.56
1:A:1394:LEU:HD22	1:A:1449:GLN:NE2	2.20	0.56
1:A:1645:PHE:HZ	1:A:1768:ARG:HD2	1.69	0.56
1:B:1394:LEU:HD22	1:B:1449:GLN:NE2	2.20	0.56
1:B:1612:ASP:HA	1:B:1615:ILE:HD11	1.86	0.56
1:B:1813:LEU:HD12	1:B:1844:TRP:HH2	1.71	0.56
1:B:3519:VAL:HG13	1:B:3521:ASN:ND2	2.20	0.56
1:A:1704:GLU:OE2	1:A:1768:ARG:NH1	2.39	0.56
1:A:1963:MET:HB3	1:A:1966:TYR:CD2	2.41	0.56
1:A:2581:LEU:HD13	1:A:2633:ILE:HG22	1.87	0.56
1:B:1469:LEU:HB3	1:B:1472:GLU:HB2	1.87	0.56
1:B:1781:THR:HG21	1:B:1919:PHE:CE1	2.40	0.56
1:B:1803:THR:HG21	1:B:1848:ASP:OD1	2.05	0.56
1:B:2842:ASP:O	1:B:2845:GLN:HG2	2.05	0.56
1:B:1998:LEU:HD11	1:B:2022:PHE:HZ	1.71	0.56
1:B:2225:LYS:HA	2:B:5093:ATP:N3	2.21	0.56
1:B:3919:LYS:NZ	1:B:4038:GLU:CG	2.69	0.56
1:A:1462:ASN:HB2	1:A:1465:ILE:CG2	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1967:HIS:O	1:A:1968:PHE:HD1	1.88	0.56
1:A:2356:TYR:CE1	1:A:2395:ILE:HG22	2.41	0.56
1:A:2386:MET:CB	1:A:2627:ARG:CD	2.84	0.56
1:A:2445:PHE:HA	1:A:2449:THR:HG21	1.88	0.56
1:A:3566:LEU:HD23	1:A:3587:LEU:HD11	1.87	0.56
1:B:3440:LEU:HD23	1:B:3462:ILE:HD12	1.87	0.56
1:A:2513:GLN:O	1:A:2526:ILE:CG1	2.50	0.56
1:A:3519:VAL:HG13	1:A:3521:ASN:ND2	2.20	0.56
1:A:1418:SER:HB2	1:A:3446:PHE:HB3	1.87	0.56
1:A:2741:HIS:HA	1:A:2744:ARG:HD2	1.87	0.56
1:B:1981:SER:HB3	1:B:1982:PRO:HD3	1.87	0.56
1:A:3612:ASP:O	1:A:3615:VAL:HG22	2.06	0.56
1:B:3919:LYS:NZ	1:B:4038:GLU:HG3	2.21	0.56
1:A:3481:ILE:O	1:A:3483:ASP:N	2.35	0.56
1:B:3845:GLN:OE1	1:B:3878:HIS:HB2	2.06	0.56
1:A:1394:LEU:CD2	1:A:1449:GLN:HE22	2.19	0.55
1:A:2380:LEU:CD1	1:A:2577:ALA:HB1	2.30	0.55
1:A:3871:PHE:HZ	1:A:3873:MET:HB2	1.71	0.55
1:B:216:PRO:CB	1:B:1424:PHE:CG	2.89	0.55
1:B:2623:THR:HG21	3:B:5094:ANP:HO3'	1.67	0.55
1:B:3537:GLU:OE1	1:B:3618:TYR:OH	2.24	0.55
1:B:3930:PHE:HE2	1:B:4029:ILE:HD13	1.71	0.55
1:A:2048:SER:H	2:A:5093:ATP:HN62	1.54	0.55
1:A:2339:ILE:HG12	1:A:2353:LEU:HD23	1.87	0.55
1:B:1527:LEU:HD22	1:B:1545:LEU:HD22	1.88	0.55
1:B:2225:LYS:HA	2:B:5093:ATP:C2	2.40	0.55
1:B:2362:ALA:HB3	1:B:2365:LYS:O	2.07	0.55
1:B:2728:LEU:HD12	1:B:2771:ARG:NH2	2.21	0.55
1:B:3566:LEU:CA	1:B:3583:LEU:HD21	2.36	0.55
1:A:1604:ALA:HA	1:A:1607:TRP:HE1	1.71	0.55
1:B:2386:MET:CB	1:B:2627:ARG:CD	2.77	0.55
1:A:2320:ARG:NH1	1:A:2406:ASP:OD2	2.30	0.55
1:B:2201:HIS:CE1	1:B:2497:TYR:HA	2.41	0.55
1:B:2472:THR:CB	1:B:2524:VAL:HG22	2.37	0.55
1:A:1365:PHE:CE2	1:A:1420:TYR:CE2	2.94	0.55
1:A:1922:LYS:HZ2	1:A:4004:LEU:CD1	2.18	0.55
1:A:2795:PHE:CE2	1:A:2799:LEU:HD11	2.42	0.55
1:A:3810:SER:HB3	1:A:3837:GLY:HA2	1.87	0.55
1:A:3998:ILE:HG22	1:A:4004:LEU:HG	1.89	0.55
1:A:1851:ASN:HD21	1:A:1899:ASN:HB2	1.71	0.55
1:A:1911:ASN:OD1	1:A:1912:LEU:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2488:GLU:CD	1:A:2491:LEU:HD11	2.32	0.55
1:A:2563:SER:C	1:A:2565:LYS:H	2.15	0.55
1:A:2762:SER:O	1:A:2763:ARG:HB2	2.06	0.55
1:B:1939:PHE:O	1:B:1940:GLU:HB3	2.06	0.55
1:B:1970:LEU:HD23	1:B:1974:LYS:CE	2.35	0.55
1:B:2220:CYS:SG	2:B:5093:ATP:N1	2.79	0.55
1:B:2252:LEU:HD21	1:B:2310:LEU:HD23	1.87	0.55
1:A:1781:THR:HG21	1:A:1919:PHE:CD1	2.42	0.55
1:A:2984:VAL:C	1:A:2986:PRO:HD3	2.30	0.55
1:A:3631:MET:CE	1:A:3698:MET:HG3	2.37	0.55
1:B:1534:PHE:HD2	1:B:1537:PHE:CE1	2.25	0.55
1:B:1620:PHE:CA	1:B:1760:PHE:CE1	2.90	0.55
1:B:2420:PRO:HB2	1:B:2620:ARG:HH21	1.69	0.55
1:B:2495:ASP:O	1:B:2498:GLY:N	2.39	0.55
1:B:2787:HIS:CA	1:B:3460:PRO:HG2	2.35	0.55
1:A:1365:PHE:CD1	1:A:1365:PHE:N	2.74	0.55
1:A:2339:ILE:HG23	1:A:2353:LEU:HB3	1.89	0.55
1:A:2354:SER:OG	1:A:2357:SER:HB2	2.07	0.55
1:A:2825:THR:O	1:A:2829:GLU:HG2	2.06	0.55
1:A:3911:TRP:HH2	1:A:3926:VAL:CG1	2.20	0.55
1:B:2151:TRP:HE3	1:B:2193:LEU:HD11	1.72	0.55
1:B:2201:HIS:NE2	1:B:2497:TYR:O	2.40	0.55
1:B:2336:ARG:HA	1:B:2339:ILE:HD12	1.88	0.55
1:B:3323:ASN:HD21	1:B:3361:ASP:H	1.55	0.55
1:A:1940:GLU:CB	1:A:1989:GLU:O	2.51	0.55
1:A:3509:LEU:HD11	1:A:3513:VAL:HG21	1.89	0.55
1:B:1970:LEU:HD23	1:B:1974:LYS:HE2	1.78	0.55
1:B:2780:LYS:HD3	1:B:2813:THR:HG22	1.88	0.55
1:B:2891:ILE:HG21	1:B:2902:MET:HG3	1.89	0.55
1:B:3656:VAL:CG1	1:B:3677:LEU:HB3	2.35	0.55
1:B:4065:LEU:HD11	1:B:4070:ILE:CD1	2.34	0.55
1:A:1802:LYS:NZ	4:A:5095:SO4:O1	2.40	0.55
1:A:2257:PHE:CD1	1:A:2262:LEU:HD11	2.41	0.55
1:A:2728:LEU:HD12	1:A:2771:ARG:CZ	2.37	0.55
1:A:3945:LEU:O	1:A:3948:HIS:O	2.24	0.55
1:A:3978:ASN:O	1:A:3981:PRO:CD	2.54	0.55
1:B:1462:ASN:HB2	1:B:1465:ILE:HG22	1.89	0.55
1:B:1562:MET:CB	1:B:1569:ILE:HD11	2.36	0.55
1:B:2620:ARG:NH1	1:B:2910:ASN:CG	2.65	0.55
1:A:1660:VAL:HG13	1:A:1728:TRP:CH2	2.42	0.54
1:A:3460:PRO:O	1:A:3463:SER:CB	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3817:GLY:H	1:A:3821:ASN:HB2	1.72	0.54
1:A:3851:VAL:HG13	1:A:3855:LEU:HD23	1.88	0.54
1:B:1802:LYS:NZ	4:B:5096:SO4:O4	2.40	0.54
1:A:1540:LEU:HD12	1:A:1548:ILE:CD1	2.37	0.54
1:A:3303:LYS:HD2	1:A:3306:TRP:HD1	1.66	0.54
1:A:3537:GLU:OE1	1:A:3618:TYR:OH	2.24	0.54
1:B:1750:SER:HB2	1:B:1755:LEU:CD2	2.37	0.54
1:B:3023:LYS:HE2	1:B:3567:LEU:CD2	2.37	0.54
1:B:3509:LEU:HD12	1:B:3513:VAL:HG21	1.86	0.54
1:A:1741:LEU:O	1:A:1742:ASP:HB2	2.07	0.54
1:A:3541:MET:HB2	1:A:3607:PHE:HE1	1.72	0.54
1:B:3303:LYS:O	1:B:3306:TRP:CD1	2.60	0.54
1:B:3461:ILE:C	1:B:3463:SER:H	2.15	0.54
1:A:1826:PHE:HE1	1:A:1853:LEU:HD22	1.72	0.54
1:A:1969:GLY:O	1:A:1972:THR:HB	2.07	0.54
1:A:1649:LEU:HD11	1:A:1704:GLU:HG3	1.88	0.54
1:A:3461:ILE:C	1:A:3463:SER:H	2.15	0.54
1:A:4084:SER:O	1:A:4088:LEU:HG	2.07	0.54
1:B:2081:THR:O	1:B:2085:LYS:HB2	2.06	0.54
1:B:2424:LYS:HE2	1:B:2534:ALA:HB1	1.88	0.54
1:B:3645:SER:CB	1:B:3890:GLN:NE2	2.65	0.54
1:A:1996:GLU:O	1:A:2000:ARG:HG3	2.07	0.54
1:A:2386:MET:HB3	1:A:2627:ARG:CD	2.38	0.54
1:A:3797:THR:HG23	1:A:3840:LEU:HD21	1.90	0.54
1:A:1497:ILE:O	1:A:1500:ILE:HG12	2.07	0.54
1:A:2064:GLN:HE22	1:A:2091:MET:HG3	1.73	0.54
1:A:2448:ASP:HB2	1:A:2829:GLU:OE2	2.08	0.54
1:A:3671:VAL:O	1:A:3674:ILE:HG22	2.07	0.54
1:B:1965:HIS:HD2	1:B:2212:LEU:CD2	2.21	0.54
1:B:2421:GLY:C	3:B:5094:ANP:O1B	2.51	0.54
1:A:2566:SER:O	1:A:2570:ILE:HD12	2.08	0.54
1:B:3330:TYR:CE1	1:B:3334:PHE:CE2	2.95	0.54
1:B:3945:LEU:O	1:B:3948:HIS:O	2.25	0.54
1:A:1826:PHE:CG	1:A:1826:PHE:O	2.61	0.54
1:B:1493:LEU:HD23	1:B:1498:GLU:CB	2.38	0.54
1:B:1620:PHE:CZ	1:B:1743:ASP:HB3	2.42	0.54
1:B:1900:PRO:HB3	1:B:1905:ARG:HA	1.90	0.54
1:B:1926:SER:HB3	1:B:1970:LEU:HD12	1.86	0.54
1:B:2708:ASN:O	1:B:2712:LEU:HD13	2.08	0.54
1:B:3964:ALA:HB2	1:B:3993:VAL:HG11	1.90	0.54
1:A:2412:ARG:HH11	1:A:2412:ARG:CB	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3010:LEU:HD22	1:A:3320:LEU:HD12	1.90	0.54
1:B:2385:VAL:O	1:B:2574:TYR:HE1	1.91	0.54
1:B:2412:ARG:HH11	1:B:2412:ARG:HB2	1.73	0.54
1:B:2420:PRO:CB	1:B:2620:ARG:NH2	2.71	0.54
1:B:3785:TYR:CE2	1:B:3859:VAL:HG22	2.42	0.54
1:A:1692:ASP:O	1:A:1695:LYS:HB3	2.07	0.53
1:A:1803:THR:HG21	1:A:1848:ASP:CG	2.33	0.53
1:A:4020:ASN:HB3	1:A:4028:ARG:HH11	1.73	0.53
1:B:1769:LEU:HD11	1:B:1804:GLU:HB3	1.90	0.53
1:B:1965:HIS:CD2	1:B:2212:LEU:HD21	2.42	0.53
1:B:2425:THR:HG23	1:B:2485:PHE:HE2	1.71	0.53
1:B:2514:GLY:HA3	1:B:2525:THR:HA	1.90	0.53
1:B:3429:LEU:HD21	1:B:3439:ARG:HB3	1.89	0.53
1:B:3702:MET:HB3	1:B:3767:PHE:HZ	1.71	0.53
1:A:2112:GLU:CB	1:A:2117:SER:HB2	2.37	0.53
1:B:3509:LEU:HD11	1:B:3513:VAL:HG21	1.90	0.53
1:B:4060:SER:HB3	1:B:4070:ILE:HG13	1.90	0.53
1:B:3855:LEU:HD12	1:B:3859:VAL:HG23	1.90	0.53
1:A:2336:ARG:HA	1:A:2339:ILE:HD12	1.91	0.53
1:A:2391:VAL:HG23	1:A:2426:MET:SD	2.47	0.53
1:A:3406:PHE:HB2	1:A:3513:VAL:HG12	1.83	0.53
1:A:2154:PHE:N	1:A:2154:PHE:HD1	2.05	0.53
1:A:2252:LEU:HD21	1:A:2310:LEU:HD23	1.89	0.53
1:A:4024:VAL:HG11	1:A:4062:TRP:CD2	2.44	0.53
1:B:2808:LEU:HD21	1:B:2856:LEU:HD12	1.91	0.53
1:A:1911:ASN:OD1	1:A:1912:LEU:HG	2.09	0.53
1:A:2410:SER:O	1:A:2411:LYS:CG	2.57	0.53
1:A:2640:THR:HG23	1:A:2643:SER:H	1.74	0.53
1:A:3323:ASN:HD21	1:A:3361:ASP:H	1.55	0.53
1:B:1645:PHE:CD2	1:B:1765:ILE:HG22	2.44	0.53
1:B:3530:PHE:HD1	1:B:3618:TYR:CD2	2.24	0.53
1:B:3683:TYR:O	1:B:3687:SER:HB2	2.09	0.53
1:B:3911:TRP:HH2	1:B:3926:VAL:CG1	2.21	0.53
1:A:1365:PHE:CE2	1:A:1420:TYR:CZ	2.97	0.53
1:A:2151:TRP:CE3	1:A:2193:LEU:HD11	2.44	0.53
1:A:2154:PHE:N	1:A:2154:PHE:CD1	2.74	0.53
1:A:2410:SER:O	1:A:2411:LYS:HG3	2.08	0.53
1:B:1425:GLU:OE2	1:B:1429:LEU:CD1	2.57	0.53
1:B:2122:THR:O	1:B:2123:LEU:C	2.52	0.53
1:B:2467:THR:O	1:B:2471:LEU:N	2.42	0.53
1:A:1991:GLU:O	1:A:1994:VAL:HB	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1995:VAL:HG22	1:A:2022:PHE:CE2	2.44	0.53
1:A:2175:ILE:HG13	1:A:2184:LEU:C	2.34	0.53
1:A:2424:LYS:HE2	3:A:5094:ANP:O1G	2.08	0.53
1:A:3965:SER:HA	1:A:3968:LEU:HD12	1.91	0.53
1:B:1759:LYS:HE3	1:B:1761:GLU:OE2	2.09	0.53
1:B:1879:ILE:HG12	1:B:1888:LEU:HB2	1.89	0.53
1:B:1914:LYS:HD3	1:B:3959:CYS:SG	2.48	0.53
1:B:3978:ASN:O	1:B:3981:PRO:CD	2.57	0.53
1:A:1849:GLU:CG	1:A:1899:ASN:HD22	2.20	0.53
1:A:2220:CYS:SG	1:A:2221:SER:N	2.82	0.53
1:A:2332:GLY:HA2	1:A:2335:GLN:CB	2.30	0.53
1:A:2490:ASN:HB3	1:A:2546:MET:CE	2.37	0.53
1:A:2492:PRO:CB	1:A:2502:VAL:HG11	2.39	0.53
1:A:2536:ASN:HB2	1:A:2543:ARG:HE	1.73	0.53
1:A:3555:TYR:HE1	1:A:3593:GLU:HG2	1.72	0.53
1:A:1827:ASP:HB3	1:A:1830:VAL:HG12	1.90	0.53
1:A:1929:ILE:H	1:A:1929:ILE:HD12	1.74	0.53
1:A:3807:SER:O	1:A:3808:LYS:HB2	2.09	0.53
1:B:2224:SER:O	2:B:5093:ATP:C2	2.53	0.53
1:B:4021:LEU:HD23	1:B:4023:ILE:HG12	1.91	0.53
1:A:3924:TRP:O	1:A:3927:TYR:HB3	2.09	0.52
1:B:2428:MET:HE2	1:B:2485:PHE:HD1	1.74	0.52
1:B:2472:THR:HG21	1:B:2524:VAL:CG2	2.39	0.52
1:B:3923:VAL:CG2	1:B:4038:GLU:HA	2.37	0.52
1:B:1803:THR:HG21	1:B:1848:ASP:CG	2.34	0.52
1:B:2354:SER:OG	1:B:2357:SER:HB2	2.10	0.52
1:B:3459:ASP:OD2	1:B:3461:ILE:CG1	2.57	0.52
1:B:3924:TRP:O	1:B:3927:TYR:HB3	2.09	0.52
1:A:1981:SER:HB3	1:A:1982:PRO:HD3	1.91	0.52
1:A:2673:LEU:O	1:A:2677:VAL:HG23	2.10	0.52
1:B:1527:LEU:HD21	1:B:1546:LEU:HD21	1.91	0.52
1:B:1963:MET:HB3	1:B:1966:TYR:CD2	2.44	0.52
1:B:3785:TYR:HE2	1:B:3859:VAL:HG22	1.74	0.52
1:A:1983:LEU:HD21	1:A:2000:ARG:NE	2.24	0.52
1:A:3772:TRP:HZ3	1:A:3780:ASN:HD22	1.57	0.52
1:B:2064:GLN:NE2	1:B:2091:MET:HE2	2.25	0.52
1:A:1531:ARG:HG2	1:A:1537:PHE:CB	2.39	0.52
1:A:1849:GLU:CG	1:A:1899:ASN:ND2	2.70	0.52
1:A:1995:VAL:HG22	1:A:2022:PHE:CD2	2.44	0.52
1:A:2780:LYS:HD3	1:A:2813:THR:HG22	1.92	0.52
1:B:1612:ASP:HA	1:B:1615:ILE:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3010:LEU:HD21	1:A:3317:SER:HB3	1.90	0.52
1:A:3845:GLN:OE1	1:A:3878:HIS:HB2	2.09	0.52
1:B:2458:LEU:HD11	1:B:2484:LEU:HD11	1.91	0.52
1:B:3632:LEU:HD13	1:B:3644:ILE:HD13	1.92	0.52
1:B:3951:SER:HB2	1:B:4002:LYS:HD2	1.91	0.52
1:A:1535:PRO:O	1:A:1841:ILE:CD1	2.58	0.52
1:A:2386:MET:HB3	1:A:2627:ARG:HD3	1.89	0.52
1:B:1502:ILE:HG23	1:B:1503:PRO:HD2	1.91	0.52
1:B:1531:ARG:HG2	1:B:1537:PHE:CB	2.39	0.52
1:B:1606:GLU:O	1:B:1610:ILE:HG12	2.10	0.52
1:B:1781:THR:HG21	1:B:1919:PHE:CD1	2.45	0.52
1:B:2476:LYS:H	1:B:2476:LYS:CD	2.23	0.52
1:B:3737:THR:CB	1:B:3740:THR:CB	2.87	0.52
1:A:1392:LEU:C	1:A:1392:LEU:CD1	2.83	0.52
1:B:1844:TRP:CD1	1:B:1893:ALA:HB3	2.44	0.52
1:B:3460:PRO:O	1:B:3463:SER:CB	2.58	0.52
1:A:1559:SER:HB3	1:A:1572:ILE:CG2	2.40	0.52
1:A:1748:PHE:CE2	1:A:1755:LEU:HD22	2.44	0.52
1:A:1870:ASN:O	1:A:1874:VAL:HG23	2.09	0.52
1:A:2494:LEU:HD12	1:A:2494:LEU:O	2.10	0.52
1:A:2834:LEU:HD21	1:A:2885:LEU:HD21	1.92	0.52
1:B:2111:LYS:CD	1:B:2161:GLU:CG	2.82	0.52
1:A:65:THR:O	1:A:66:GLN:CB	2.57	0.52
1:A:1531:ARG:HD3	1:A:1537:PHE:O	2.10	0.52
1:A:2122:THR:O	1:A:2123:LEU:C	2.53	0.52
1:A:2181:GLY:O	1:A:2182:GLU:CG	2.56	0.52
1:B:3618:TYR:O	1:B:3622:GLY:N	2.38	0.52
1:A:1822:CYS:SG	1:A:1849:GLU:C	2.93	0.51
1:A:2580:LYS:HG2	1:A:2586:ARG:HH22	1.74	0.51
1:A:3330:TYR:CE1	1:A:3334:PHE:CD2	2.98	0.51
1:A:3330:TYR:CD1	1:A:3334:PHE:CD2	2.99	0.51
1:A:3566:LEU:CD2	1:A:3587:LEU:HD11	2.41	0.51
1:B:1826:PHE:CE1	1:B:1853:LEU:HD22	2.45	0.51
1:B:1910:GLU:HB2	1:B:3846:MET:CB	2.39	0.51
1:B:2220:CYS:HB2	2:B:5093:ATP:C6	2.45	0.51
1:B:2867:LEU:HB3	1:B:2872:GLU:HB3	1.92	0.51
1:B:3810:SER:HB3	1:B:3837:GLY:HA2	1.92	0.51
1:A:2201:HIS:NE2	1:A:2497:TYR:O	2.43	0.51
1:A:2849:TYR:O	1:A:2853:LEU:HB2	2.11	0.51
1:B:1563:LYS:HE2	1:B:1585:VAL:HG12	1.91	0.51
1:A:1992:LYS:HG2	1:A:2024:SER:CB	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:THR:O	1:B:66:GLN:CB	2.58	0.51
1:B:3854:TYR:O	1:B:3858:HIS:HB2	2.10	0.51
1:B:3939:ILE:HG23	1:B:3950:PHE:HE2	1.75	0.51
1:A:2002:ILE:HG22	1:A:2006:LEU:HD11	1.92	0.51
1:A:2177:THR:HG22	1:A:2183:ARG:HG2	1.93	0.51
1:A:3566:LEU:CA	1:A:3583:LEU:HD21	2.38	0.51
1:B:1822:CYS:SG	1:B:1849:GLU:C	2.94	0.51
1:B:1968:PHE:HD1	1:B:1968:PHE:N	2.08	0.51
1:B:2154:PHE:N	1:B:2154:PHE:CD1	2.78	0.51
1:B:2425:THR:HG23	1:B:2485:PHE:CE2	2.45	0.51
1:B:2470:GLY:CA	1:B:2473:LEU:HD21	2.20	0.51
1:A:2385:VAL:O	1:A:2574:TYR:HE1	1.93	0.51
1:A:2655:ILE:HD11	1:A:2747:ARG:HH22	1.76	0.51
1:B:1826:PHE:HE1	1:B:1853:LEU:HD22	1.76	0.51
1:B:1917:ARG:HD2	1:B:3963:PHE:CE2	2.46	0.51
1:B:2084:TRP:CZ3	1:B:2085:LYS:HG3	2.45	0.51
1:B:2494:LEU:HB2	1:B:2499:SER:N	2.25	0.51
1:B:2741:HIS:HA	1:B:2744:ARG:HD2	1.91	0.51
1:B:3509:LEU:CD1	1:B:3513:VAL:CG2	2.83	0.51
1:B:3919:LYS:HZ2	1:B:4038:GLU:CD	2.18	0.51
1:B:1469:LEU:HD13	1:B:1523:LEU:CD2	2.40	0.51
1:B:2707:VAL:HG12	1:B:2712:LEU:CD1	2.41	0.51
1:B:2788:ARG:HG3	1:B:3459:ASP:HA	1.91	0.51
1:B:3737:THR:CB	1:B:3740:THR:HB	2.41	0.51
1:A:3737:THR:CB	1:A:3740:THR:CB	2.88	0.51
1:A:3869:GLU:O	1:A:3870:LYS:C	2.54	0.51
1:B:1540:LEU:HD11	1:B:1561:PHE:HB3	1.93	0.51
1:B:2368:PHE:CD1	1:B:2368:PHE:N	2.77	0.51
1:B:3308:ASN:O	1:B:3312:GLN:HB2	2.11	0.51
1:B:3353:LEU:HD23	1:B:3358:VAL:CG1	2.41	0.51
1:B:3817:GLY:H	1:B:3821:ASN:HB2	1.76	0.51
1:A:3461:ILE:C	1:A:3463:SER:N	2.67	0.51
1:A:3725:VAL:HG22	1:A:3731:ASP:HA	1.93	0.51
1:B:1646:GLN:NE2	1:B:1758:TYR:OH	2.43	0.51
1:B:2382:ALA:O	1:B:2385:VAL:HG12	2.11	0.51
1:B:2620:ARG:NH1	1:B:2910:ASN:ND2	2.58	0.51
1:A:2061:TYR:CD1	1:A:2091:MET:HE1	2.43	0.51
1:A:2084:TRP:HE3	1:A:2088:ILE:HD12	1.76	0.51
1:A:2141:ILE:HG22	1:A:2145:PHE:HB2	1.91	0.51
1:B:1744:LEU:CD2	1:B:1760:PHE:CD2	2.94	0.51
1:B:2125:TRP:CZ2	1:B:2178:LEU:HD13	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3023:LYS:CE	1:B:3567:LEU:HD23	2.41	0.51
1:B:3330:TYR:CE2	1:B:3346:LEU:HD13	2.44	0.51
1:B:2002:ILE:HB	1:B:2014:PHE:CE2	2.46	0.51
1:B:2472:THR:HB	1:B:2524:VAL:HG22	1.92	0.51
1:B:3869:GLU:O	1:B:3870:LYS:C	2.52	0.51
1:B:4024:VAL:HG11	1:B:4062:TRP:CD2	2.46	0.51
1:A:3414:MET:HE3	1:A:3518:PHE:CD1	2.46	0.50
1:B:1462:ASN:CB	1:B:1465:ILE:HG22	2.42	0.50
1:B:3461:ILE:C	1:B:3463:SER:N	2.68	0.50
1:A:2201:HIS:CE1	1:A:2497:TYR:CA	2.94	0.50
1:A:3017:VAL:HG21	1:A:3313:PHE:CE2	2.46	0.50
1:A:2336:ARG:HG2	1:A:2355:ASP:OD1	2.11	0.50
1:B:1929:ILE:H	1:B:1929:ILE:HD12	1.75	0.50
1:B:2312:ASP:HB3	1:B:2351:GLN:HG3	1.93	0.50
1:B:2336:ARG:CD	1:B:2355:ASP:OD2	2.59	0.50
1:B:2563:SER:C	1:B:2565:LYS:H	2.18	0.50
1:A:1749:ILE:O	1:A:1755:LEU:HA	2.12	0.50
1:A:215:PRO:C	1:A:3475:ASN:ND2	2.69	0.50
1:A:1660:VAL:CG1	1:A:1728:TRP:CH2	2.95	0.50
1:A:1714:GLN:HB3	1:A:1727:LEU:HD11	1.92	0.50
1:A:1822:CYS:SG	1:A:1849:GLU:O	2.69	0.50
1:A:2109:LEU:CD1	1:A:2129:LEU:HD23	2.41	0.50
1:A:3547:ASP:HA	1:A:3550:LYS:HB3	1.93	0.50
1:A:3737:THR:OG1	1:A:3740:THR:CB	2.59	0.50
1:A:3757:ILE:HD11	1:A:4074:GLU:HG2	1.91	0.50
1:A:3979:ASN:C	1:A:3981:PRO:CD	2.84	0.50
1:A:1534:PHE:CE2	1:A:1536:ARG:HB2	2.47	0.50
1:A:2048:SER:H	2:A:5093:ATP:N6	2.08	0.50
1:A:2410:SER:O	1:A:2411:LYS:CB	2.57	0.50
1:A:2514:GLY:HA3	1:A:2525:THR:HA	1.93	0.50
1:A:3939:ILE:HG13	1:A:4010:LEU:CD2	2.41	0.50
1:B:1939:PHE:H	1:B:1939:PHE:HD1	1.58	0.50
1:B:1968:PHE:N	1:B:1968:PHE:CD1	2.79	0.50
1:B:2220:CYS:SG	1:B:2224:SER:HB3	2.51	0.50
1:B:2941:THR:HG22	1:B:2942:ASP:N	2.25	0.50
1:B:2960:THR:HG22	1:B:2961:ILE:N	2.27	0.50
1:A:162:LEU:HA	1:A:165:ASP:O	2.11	0.50
1:A:1622:GLN:HE22	1:A:1644:ILE:H	1.59	0.50
1:A:1822:CYS:SG	1:A:1850:PHE:CA	2.97	0.50
1:A:2839:ASP:O	1:A:2841:PRO:HD3	2.12	0.50
1:B:1998:LEU:CD1	1:B:2022:PHE:HZ	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1611:LEU:O	1:A:1615:ILE:HG12	2.12	0.50
1:A:2201:HIS:CE1	1:A:2497:TYR:HB3	2.47	0.50
1:A:2787:HIS:CA	1:A:3460:PRO:HG2	2.35	0.50
1:B:1392:LEU:C	1:B:1392:LEU:CD1	2.81	0.50
1:B:2833:THR:HG21	1:B:2841:PRO:HD2	1.94	0.50
1:B:3767:PHE:HB3	1:B:3769:VAL:HG23	1.94	0.50
1:A:1646:GLN:NE2	1:A:1758:TYR:OH	2.45	0.50
1:A:2489:ILE:HG22	1:A:2535:CYS:HB3	1.93	0.50
1:A:4065:LEU:HD12	1:A:4065:LEU:C	2.37	0.50
1:B:2262:LEU:HA	1:B:2265:ILE:HD12	1.93	0.50
1:B:4006:VAL:HA	1:B:4009:LYS:HG2	1.93	0.50
1:A:1387:GLU:HA	1:A:1393:LYS:HA	1.94	0.49
1:B:1394:LEU:CD2	1:B:1449:GLN:HE22	2.25	0.49
1:B:1611:LEU:O	1:B:1615:ILE:HG12	2.11	0.49
1:B:2620:ARG:HH12	1:B:2910:ASN:ND2	2.10	0.49
1:B:3566:LEU:HD11	1:B:3570:LEU:HD11	1.93	0.49
1:A:1748:PHE:CD2	1:A:1755:LEU:HD22	2.47	0.49
1:A:1749:ILE:HD13	1:A:1813:LEU:HD22	1.93	0.49
1:A:2003:LEU:HD23	1:A:2006:LEU:HD12	1.93	0.49
1:A:2492:PRO:HB2	1:A:2502:VAL:HG11	1.93	0.49
1:A:3817:GLY:H	1:A:3821:ASN:CB	2.25	0.49
1:A:3848:LEU:CD2	1:A:3852:LYS:HE3	2.41	0.49
1:A:4022:GLN:O	1:A:4023:ILE:C	2.56	0.49
1:B:1425:GLU:OE2	1:B:1429:LEU:HD11	2.13	0.49
1:B:1536:ARG:HE	1:B:1841:ILE:HD13	1.77	0.49
1:B:1822:CYS:HB2	1:B:1853:LEU:CD2	2.29	0.49
1:B:1926:SER:CA	1:B:1970:LEU:HD12	2.42	0.49
1:A:1731:VAL:HG12	1:A:1732:GLN:N	2.27	0.49
1:A:2249:LEU:HD21	1:A:2302:PHE:HD2	1.77	0.49
1:A:2708:ASN:O	1:A:2712:LEU:HD13	2.12	0.49
1:A:3737:THR:CB	1:A:3740:THR:HB	2.43	0.49
1:B:3023:LYS:HZ3	1:B:3571:ASN:HD21	1.58	0.49
1:B:3979:ASN:O	1:B:3981:PRO:HD2	2.11	0.49
1:A:2141:ILE:HG22	1:A:2145:PHE:CB	2.42	0.49
1:A:2318:ILE:O	1:A:2322:LEU:HB2	2.12	0.49
1:A:3683:TYR:O	1:A:3687:SER:HB2	2.12	0.49
1:B:1983:LEU:HD11	1:B:2000:ARG:HH21	1.76	0.49
1:B:2640:THR:HG23	1:B:2643:SER:H	1.77	0.49
1:B:2908:LEU:O	1:B:2912:CYS:HB2	2.12	0.49
1:B:4059:LEU:HA	1:B:4063:LEU:HD13	1.93	0.49
1:A:1917:ARG:HD2	1:A:3963:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2853:LEU:HD21	1:A:2870:GLU:HG3	1.94	0.49
1:A:2941:THR:HG22	1:A:2942:ASP:N	2.24	0.49
1:B:2380:LEU:HD11	1:B:2577:ALA:HB2	1.88	0.49
1:A:2099:ASN:HA	1:A:2149:ARG:O	2.12	0.49
1:A:2784:PRO:HG2	1:A:2817:ILE:HD13	1.94	0.49
1:A:2808:LEU:HD21	1:A:2856:LEU:HD12	1.95	0.49
1:A:2936:ILE:HG22	1:A:2962:ARG:HD3	1.95	0.49
1:B:2835:LEU:HD23	1:B:2911:ARG:HB2	1.95	0.49
1:B:4084:SER:O	1:B:4088:LEU:HG	2.13	0.49
1:A:1502:ILE:HG23	1:A:1503:PRO:HD2	1.94	0.49
1:A:4074:GLU:HA	1:A:4077:GLN:HE21	1.78	0.49
1:B:1655:MET:HE3	1:B:1659:LEU:HD12	1.94	0.49
1:B:3303:LYS:HA	1:B:3306:TRP:CD1	2.47	0.49
1:A:1849:GLU:CD	1:A:1899:ASN:HD22	2.20	0.49
1:A:1967:HIS:C	1:A:1968:PHE:CD1	2.87	0.49
1:A:2080:LYS:O	1:A:2084:TRP:CD1	2.65	0.49
1:A:2819:GLU:HB3	1:A:2891:ILE:HG22	1.95	0.49
1:B:2136:ARG:O	1:B:2140:ASP:O	2.30	0.49
1:B:2154:PHE:N	1:B:2154:PHE:HD1	2.10	0.49
1:A:2833:THR:HG21	1:A:2841:PRO:HD2	1.94	0.49
1:A:2988:SER:CB	1:A:2989:PRO:CD	2.66	0.49
1:A:3429:LEU:HD21	1:A:3439:ARG:HB3	1.95	0.49
1:A:3693:LYS:HE3	1:A:4080:GLU:HB3	1.94	0.49
1:B:162:LEU:HA	1:B:165:ASP:O	2.12	0.49
1:B:1375:LYS:HE3	1:B:1431:LEU:HD13	1.94	0.49
1:B:3409:ASP:HB3	1:B:3518:PHE:HB2	1.95	0.49
1:A:2152:VAL:HG12	1:A:2154:PHE:CE1	2.39	0.48
1:A:2407:LEU:HB2	1:A:2414:ILE:HD11	1.94	0.48
1:A:2878:VAL:HA	1:A:2881:ILE:HD12	1.95	0.48
1:A:3440:LEU:CD2	1:A:3462:ILE:HD12	2.42	0.48
1:B:1801:GLY:N	4:B:5096:SO4:O4	2.46	0.48
1:B:2339:ILE:HG23	1:B:2353:LEU:HB3	1.94	0.48
1:A:1630:ILE:HA	1:A:1634:THR:HG22	1.95	0.48
1:B:2177:THR:HG22	1:B:2183:ARG:HG2	1.94	0.48
1:A:1953:LEU:HD11	1:A:1973:LEU:HB3	1.94	0.48
1:A:2034:ILE:CD1	1:A:2061:TYR:CE2	2.95	0.48
1:A:2226:ILE:HG23	1:A:2288:VAL:HG21	1.95	0.48
1:A:2305:LEU:HD11	1:A:2368:PHE:CG	2.48	0.48
1:A:2856:LEU:HD23	1:A:2873:LEU:HB3	1.95	0.48
1:A:3855:LEU:HD11	1:A:3873:MET:HE1	1.94	0.48
1:B:1802:LYS:NZ	4:B:5096:SO4:S	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1911:ASN:OD1	1:B:1912:LEU:HG	2.13	0.48
1:B:2441:VAL:HB	1:B:2484:LEU:HD23	1.95	0.48
1:B:3848:LEU:HD21	1:B:3852:LYS:HE3	1.95	0.48
1:B:2046:GLY:O	1:B:2228:HIS:HB2	2.13	0.48
1:B:2838:ALA:HB3	1:B:2878:VAL:HG13	1.94	0.48
1:A:2109:LEU:CD1	1:A:2129:LEU:CD2	2.92	0.48
1:A:2822:ILE:O	1:A:2822:ILE:HG13	2.14	0.48
1:B:1497:ILE:O	1:B:1500:ILE:HG12	2.14	0.48
1:B:1926:SER:HA	1:B:1970:LEU:HD12	1.94	0.48
1:B:2489:ILE:HD11	1:B:2506:LEU:HD13	1.94	0.48
1:B:2984:VAL:C	1:B:2986:PRO:HD3	2.39	0.48
1:B:4024:VAL:HG23	1:B:4027:VAL:H	1.78	0.48
1:A:1645:PHE:CB	1:A:1765:ILE:HG21	2.41	0.48
1:A:2074:GLY:O	1:A:2197:ASP:HA	2.13	0.48
1:A:4033:LEU:HD12	1:A:4036:GLN:H	1.79	0.48
1:B:2100:VAL:HG12	1:B:2102:TYR:CE2	2.48	0.48
1:B:2623:THR:CB	3:B:5094:ANP:O2'	2.61	0.48
1:B:2833:THR:CG2	1:B:2841:PRO:HD2	2.43	0.48
1:B:3023:LYS:NZ	1:B:3571:ASN:HD21	2.11	0.48
1:B:3848:LEU:O	1:B:3849:SER:C	2.57	0.48
1:A:1826:PHE:O	1:A:1826:PHE:CD1	2.67	0.48
1:A:1939:PHE:O	1:A:1940:GLU:HB3	2.13	0.48
1:A:2071:ILE:HB	1:A:2212:LEU:HD12	1.96	0.48
1:A:2314:ILE:HG22	1:A:2318:ILE:HD12	1.96	0.48
1:A:2387:ARG:O	1:A:2390:ILE:HG22	2.13	0.48
1:B:1493:LEU:HD23	1:B:1498:GLU:HB2	1.94	0.48
1:B:1995:VAL:HG22	1:B:2022:PHE:CE2	2.47	0.48
1:B:2102:TYR:HB2	1:B:2152:VAL:HG22	1.95	0.48
1:B:2252:LEU:HD22	1:B:2314:ILE:HG13	1.96	0.48
1:B:2473:LEU:CD2	1:B:2525:THR:HB	2.43	0.48
1:B:3406:PHE:CZ	1:B:3505:ILE:HG21	2.49	0.48
1:A:1409:LEU:CD2	1:A:1435:LEU:CB	2.86	0.48
1:A:2425:THR:OG1	3:A:5094:ANP:O2A	2.31	0.48
1:B:2111:LYS:HZ2	1:B:2161:GLU:HG2	1.73	0.48
1:B:2290:LEU:HD23	1:B:2321:SER:HA	1.96	0.48
1:B:2755:HIS:CE1	1:B:2835:LEU:HG	2.49	0.48
1:B:2780:LYS:HB3	1:B:2813:THR:HG22	1.94	0.48
1:B:3348:ILE:HA	1:B:3351:ARG:HG2	1.95	0.48
1:B:4065:LEU:C	1:B:4065:LEU:HD12	2.39	0.48
1:B:1604:ALA:HA	1:B:1607:TRP:HE1	1.75	0.48
1:B:2445:PHE:HA	1:B:2449:THR:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2488:GLU:CG	1:A:2491:LEU:HD12	2.41	0.48
1:A:2745:ILE:HG23	1:A:2756:MET:HE2	1.91	0.48
1:B:23:LEU:O	1:B:25:GLU:N	2.47	0.48
1:B:2745:ILE:CG1	1:B:2756:MET:HE1	2.43	0.48
1:B:4022:GLN:O	1:B:4022:GLN:HG2	2.14	0.48
1:A:2294:LEU:HB3	1:A:2317:LEU:HD22	1.94	0.47
1:A:4059:LEU:HA	1:A:4063:LEU:HD13	1.96	0.47
1:B:2305:LEU:HB3	1:B:2310:LEU:HD12	1.95	0.47
1:B:3566:LEU:HD13	1:B:3570:LEU:HD12	1.96	0.47
1:A:1466:GLN:HB3	1:A:1473:THR:HG21	1.95	0.47
1:A:1534:PHE:CD2	1:A:1537:PHE:CE1	3.02	0.47
1:A:1649:LEU:HD13	1:A:1704:GLU:HG3	1.96	0.47
1:A:2354:SER:OG	1:A:2357:SER:CB	2.62	0.47
1:A:2582:VAL:O	1:A:2582:VAL:HG23	2.14	0.47
1:B:1822:CYS:SG	1:B:1850:PHE:HA	2.54	0.47
1:B:2224:SER:C	2:B:5093:ATP:C2	2.92	0.47
1:B:3671:VAL:HA	1:B:3674:ILE:HG22	1.95	0.47
1:A:2707:VAL:CG1	1:A:2712:LEU:HD12	2.45	0.47
1:B:2099:ASN:HA	1:B:2149:ARG:O	2.14	0.47
1:B:3787:THR:HG22	1:B:3875:MET:HB2	1.96	0.47
1:B:3978:ASN:O	1:B:3981:PRO:HD2	2.14	0.47
1:A:1421:TYR:CD2	1:A:1425:GLU:CG	2.97	0.47
1:A:1645:PHE:HB2	1:A:1697:LYS:HG3	1.95	0.47
1:A:2375:ILE:HG22	1:A:2376:PRO:O	2.14	0.47
1:A:3443:ALA:HB1	1:A:3450:VAL:HG21	1.96	0.47
1:A:3728:GLU:HG3	1:A:4079:LYS:HE2	1.95	0.47
1:A:3812:LYS:HB2	1:A:3839:ILE:HD12	1.97	0.47
1:A:3911:TRP:HH2	1:A:3926:VAL:HG13	1.79	0.47
1:B:40:TRP:O	1:B:44:LYS:N	2.48	0.47
1:B:1469:LEU:HD13	1:B:1523:LEU:HD21	1.96	0.47
1:B:2002:ILE:HG22	1:B:2006:LEU:HD11	1.96	0.47
1:B:2420:PRO:HD3	1:B:2536:ASN:ND2	2.25	0.47
1:B:2563:SER:CB	1:B:2566:SER:H	2.16	0.47
1:B:3772:TRP:HZ3	1:B:3780:ASN:HD22	1.62	0.47
1:A:1495:THR:CG2	1:A:1497:ILE:HG22	2.41	0.47
1:A:1527:LEU:HD21	1:A:1546:LEU:HD23	1.96	0.47
1:A:2677:VAL:HG11	1:A:2686:LEU:HD21	1.95	0.47
1:A:3728:GLU:CG	1:A:4079:LYS:HE2	2.44	0.47
1:B:1967:HIS:O	1:B:1968:PHE:HD1	1.97	0.47
1:A:1951:HIS:O	1:A:1955:LEU:HB2	2.14	0.47
1:A:2169:VAL:HG13	1:A:2186:ILE:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2463:ASN:O	1:A:2475:PRO:HD2	2.15	0.47
1:A:3854:TYR:O	1:A:3858:HIS:HB2	2.15	0.47
1:B:2282:ASN:HB3	1:B:2552:ARG:HG3	1.97	0.47
1:B:3737:THR:OG1	1:B:3740:THR:CB	2.62	0.47
1:B:3979:ASN:C	1:B:3981:PRO:CD	2.86	0.47
1:A:1365:PHE:HE2	1:A:1420:TYR:CZ	2.33	0.47
1:A:2860:THR:HG22	1:A:2865:LEU:O	2.15	0.47
1:A:3365:ARG:HD2	1:A:3368:ASP:OD2	2.15	0.47
1:B:1387:GLU:HA	1:B:1393:LYS:HA	1.97	0.47
1:B:1657:THR:HG21	1:B:1734:PHE:O	2.15	0.47
1:B:2437:LEU:H	1:B:2437:LEU:HD12	1.79	0.47
1:B:2760:GLY:O	1:B:2761:ALA:HB3	2.14	0.47
1:B:2795:PHE:CE2	1:B:2799:LEU:HD11	2.49	0.47
1:A:2839:ASP:HB3	1:A:2878:VAL:HG22	1.97	0.47
1:B:2061:TYR:O	1:B:2064:GLN:HG2	2.14	0.47
1:B:2785:LYS:HD3	1:B:3482:GLY:O	2.15	0.47
1:B:2967:ASN:HB3	1:B:3356:PHE:CE2	2.49	0.47
1:A:1656:TRP:O	1:A:1660:VAL:HG12	2.15	0.47
1:A:2745:ILE:CB	1:A:2756:MET:HE1	2.45	0.47
1:A:3570:LEU:HD23	1:A:3580:ASN:CG	2.40	0.47
1:B:1849:GLU:CD	1:B:1899:ASN:HD22	2.23	0.47
1:B:2472:THR:CG2	1:B:2524:VAL:CG2	2.86	0.47
1:A:1750:SER:HA	1:A:1755:LEU:HD23	1.96	0.47
1:A:2422:SER:N	3:A:5094:ANP:O1B	2.47	0.47
1:A:2761:ALA:O	1:A:2892:CYS:HB3	2.15	0.47
1:A:3307:LEU:HA	1:A:3310:THR:HB	1.97	0.47
1:A:3466:ILE:HD13	1:A:3509:LEU:HD13	1.97	0.47
1:B:23:LEU:C	1:B:25:GLU:N	2.73	0.47
1:B:2276:LEU:CD2	1:B:2415:ILE:HG21	2.45	0.47
1:B:2472:THR:HG22	1:B:2524:VAL:HG13	1.96	0.47
1:B:4020:ASN:ND2	1:B:4028:ARG:HD3	2.30	0.47
1:A:2034:ILE:CD1	1:A:2061:TYR:CZ	2.98	0.46
1:A:3304:GLU:C	1:A:3306:TRP:H	2.23	0.46
1:A:3632:LEU:HD13	1:A:3644:ILE:HD13	1.96	0.46
1:A:3844:ILE:HG12	1:A:3851:VAL:HG21	1.96	0.46
1:B:1656:TRP:HE1	1:B:1712:ILE:HD11	1.81	0.46
1:B:2155:ASP:O	1:B:2549:ARG:NH1	2.46	0.46
1:B:2318:ILE:O	1:B:2322:LEU:HB2	2.14	0.46
1:B:2441:VAL:HG21	1:B:2482:LEU:HD21	1.96	0.46
1:B:2758:LEU:HD23	1:B:2915:ASN:HB3	1.96	0.46
1:B:3307:LEU:HA	1:B:3310:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1592:LEU:CD1	1:A:1596:ILE:HD12	2.45	0.46
1:A:2178:LEU:HD12	1:A:2182:GLU:HB2	1.97	0.46
1:A:2516:TRP:CZ3	1:A:2523:TRP:HB2	2.51	0.46
1:A:2758:LEU:HD23	1:A:2915:ASN:HB3	1.96	0.46
1:B:2354:SER:OG	1:B:2357:SER:CB	2.63	0.46
1:B:2860:THR:HG22	1:B:2865:LEU:O	2.15	0.46
1:B:2938:MET:SD	1:B:3321:ILE:HG21	2.55	0.46
1:B:3547:ASP:HA	1:B:3550:LYS:HB3	1.97	0.46
1:A:1871:GLY:HA3	1:A:1879:ILE:HG21	1.98	0.46
1:A:2358:THR:HG22	1:A:2359:ILE:N	2.29	0.46
1:A:2761:ALA:O	1:A:2892:CYS:CB	2.63	0.46
1:B:1636:ILE:O	1:B:1640:VAL:HG23	2.16	0.46
1:B:2464:TYR:CE1	1:B:2524:VAL:HG11	2.49	0.46
1:B:3372:THR:HG23	1:B:3375:GLU:HB2	1.97	0.46
1:A:1479:LEU:HD11	1:A:1515:SER:HB3	1.97	0.46
1:A:1527:LEU:HD21	1:A:1546:LEU:CD2	2.45	0.46
1:A:1606:GLU:O	1:A:1610:ILE:HG12	2.16	0.46
1:A:1727:LEU:O	1:A:1731:VAL:HG23	2.15	0.46
1:A:2225:LYS:HD2	1:A:2281:PHE:CZ	2.51	0.46
1:B:1367:ILE:H	1:B:1367:ILE:HD12	1.80	0.46
1:B:1593:ASN:HD21	1:B:1621:THR:CB	2.29	0.46
1:B:2220:CYS:HG	1:B:2224:SER:HB3	1.80	0.46
1:B:2761:ALA:O	1:B:2892:CYS:SG	2.73	0.46
1:B:3641:PHE:HA	1:B:3889:LEU:HD21	1.96	0.46
1:A:1540:LEU:HD11	1:A:1561:PHE:HB3	1.97	0.46
1:A:1744:LEU:HA	1:A:1760:PHE:HE2	1.75	0.46
1:A:3911:TRP:CH2	1:A:3926:VAL:HG13	2.50	0.46
1:B:1612:ASP:HA	1:B:1615:ILE:CG1	2.46	0.46
1:B:1983:LEU:HD13	1:B:2000:ARG:HE	1.80	0.46
1:B:2137:VAL:O	1:B:2141:ILE:HG23	2.16	0.46
1:A:3470:PHE:CE1	1:A:3488:VAL:HG21	2.51	0.46
1:B:1421:TYR:O	1:B:1425:GLU:CA	2.63	0.46
1:B:2107:LYS:CE	1:B:2499:SER:HB3	2.43	0.46
1:B:2112:GLU:HB3	1:B:2117:SER:OG	2.14	0.46
1:B:2464:TYR:HE1	1:B:2524:VAL:HG11	1.80	0.46
1:B:2493:LYS:HG3	1:B:2494:LEU:N	2.30	0.46
1:B:2737:SER:HB2	1:B:2924:THR:HG21	1.97	0.46
1:A:2084:TRP:CH2	1:A:2153:VAL:HG21	2.50	0.46
1:B:1392:LEU:HD13	1:B:1393:LYS:CA	2.45	0.46
1:B:1514:ASP:O	1:B:1518:MET:HG2	2.15	0.46
1:B:1681:LYS:HE2	1:B:1939:PHE:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2080:LYS:O	1:B:2081:THR:C	2.59	0.46
1:B:2169:VAL:HG13	1:B:2186:ILE:HG12	1.98	0.46
1:B:4022:GLN:O	1:B:4023:ILE:C	2.58	0.46
1:A:1626:CYS:SG	1:A:1639:VAL:CG1	3.01	0.46
1:A:1910:GLU:HB2	1:A:3846:MET:HA	1.97	0.46
1:A:2063:MET:HB3	1:A:2070:LEU:HD11	1.98	0.46
1:A:2305:LEU:CD1	1:A:2368:PHE:CD1	2.98	0.46
1:A:3319:GLU:HA	1:A:3359:LYS:O	2.15	0.46
1:A:3473:ALA:HB3	1:A:3476:ARG:HG3	1.97	0.46
1:A:3889:LEU:HG	1:A:3894:ARG:HD3	1.97	0.46
1:A:4033:LEU:HD13	1:A:4035:GLN:CG	2.46	0.46
1:B:1620:PHE:HB2	1:B:1760:PHE:CZ	2.50	0.46
1:B:2181:GLY:C	1:B:2182:GLU:HG3	2.40	0.46
1:B:4017:GLY:HA3	1:B:4021:LEU:HD12	1.97	0.46
1:B:1969:GLY:O	1:B:1972:THR:HB	2.15	0.46
1:B:3889:LEU:HG	1:B:3894:ARG:HD3	1.97	0.46
1:B:3924:TRP:CD1	1:B:3924:TRP:C	2.94	0.46
1:A:215:PRO:C	1:A:3475:ASN:HD21	2.24	0.46
1:A:3509:LEU:HD12	1:A:3513:VAL:HG23	1.94	0.46
1:B:1706:LEU:CD1	1:B:1936:ILE:HG12	2.45	0.46
1:B:1956:LEU:CB	1:B:1968:PHE:CE2	2.90	0.46
1:B:3815:PRO:O	1:B:3821:ASN:HB3	2.16	0.46
1:B:3935:PHE:HB2	1:B:4014:VAL:HG11	1.97	0.46
1:A:1529:ARG:O	1:A:1533:GLN:HG2	2.16	0.45
1:A:1802:LYS:O	1:A:1806:VAL:HG23	2.16	0.45
1:A:2755:HIS:HB3	1:A:2912:CYS:SG	2.56	0.45
1:A:3612:ASP:C	1:A:3615:VAL:HG22	2.40	0.45
1:B:1827:ASP:HB3	1:B:1830:VAL:HG12	1.98	0.45
1:B:2488:GLU:CG	1:B:2491:LEU:HD12	2.45	0.45
1:B:2761:ALA:O	1:B:2892:CYS:CB	2.64	0.45
1:A:2241:LEU:HD13	1:A:2299:ARG:HH11	1.80	0.45
1:A:2788:ARG:HG3	1:A:3459:ASP:HA	1.96	0.45
1:A:3308:ASN:O	1:A:3312:GLN:HB2	2.15	0.45
1:A:3322:GLY:HA2	1:A:3325:ILE:HD12	1.98	0.45
1:A:3692:LYS:HE3	1:A:3898:GLU:HB3	1.98	0.45
1:B:1392:LEU:HD22	1:B:1393:LYS:H	1.82	0.45
1:B:1813:LEU:HD12	1:B:1844:TRP:CH2	2.50	0.45
1:B:2109:LEU:HD13	1:B:2129:LEU:HD23	1.97	0.45
1:B:2380:LEU:HD12	1:B:2577:ALA:HB2	1.85	0.45
1:B:2420:PRO:CB	1:B:2620:ARG:HH21	2.29	0.45
1:B:2571:TYR:HA	1:B:2574:TYR:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3338:ASN:HD22	1:B:3341:GLU:HG2	1.81	0.45
1:A:1365:PHE:CZ	1:A:1420:TYR:CG	3.05	0.45
1:A:1706:LEU:HD22	1:A:1935:GLN:HG2	1.98	0.45
1:A:1710:ASN:HB2	1:A:1932:MET:HE1	1.98	0.45
1:A:2476:LYS:HZ1	1:A:2528:ARG:HD3	1.82	0.45
1:A:2563:SER:CB	1:A:2566:SER:H	2.19	0.45
1:A:2757:MET:CE	1:A:2912:CYS:CB	2.77	0.45
1:A:2757:MET:HE2	1:A:2912:CYS:SG	2.56	0.45
1:B:1626:CYS:SG	1:B:1639:VAL:HG11	2.56	0.45
1:B:2488:GLU:CD	1:B:2491:LEU:HD11	2.41	0.45
1:B:3538:ASN:HB3	1:B:3541:MET:HG2	1.98	0.45
1:A:1365:PHE:HZ	1:A:1420:TYR:CE1	2.31	0.45
1:A:1563:LYS:HA	1:A:1569:ILE:O	2.17	0.45
1:A:1563:LYS:HE2	1:A:1585:VAL:HG12	1.98	0.45
1:A:2081:THR:HG22	1:A:2085:LYS:HD2	1.98	0.45
1:A:3592:LYS:O	1:A:3596:ASN:N	2.49	0.45
1:A:3721:THR:O	1:A:3725:VAL:HG23	2.16	0.45
1:A:3832:SER:O	1:A:3836:GLY:N	2.43	0.45
1:A:3848:LEU:O	1:A:3849:SER:C	2.57	0.45
1:B:1535:PRO:C	1:B:1841:ILE:CD1	2.77	0.45
1:B:1554:HIS:O	1:B:1555:HIS:HB2	2.17	0.45
1:B:1704:GLU:OE2	1:B:1768:ARG:NH1	2.49	0.45
1:B:2471:LEU:O	1:B:2473:LEU:HG	2.16	0.45
1:B:3965:SER:HA	1:B:3968:LEU:HD12	1.98	0.45
1:A:23:LEU:O	1:A:25:GLU:N	2.50	0.45
1:A:1570:GLU:HB2	1:A:1585:VAL:HA	1.99	0.45
1:A:2204:PRO:HA	1:A:2207:ILE:HD12	1.97	0.45
1:A:2419:PRO:O	1:A:2424:LYS:NZ	2.50	0.45
1:A:3342:ARG:NH2	1:A:3393:ASN:OD1	2.47	0.45
1:A:3926:VAL:HG11	1:A:4042:ARG:HG2	1.97	0.45
1:B:23:LEU:C	1:B:25:GLU:H	2.25	0.45
1:B:1749:ILE:HD13	1:B:1813:LEU:HD22	1.99	0.45
1:B:2201:HIS:CE1	1:B:2497:TYR:HB3	2.52	0.45
1:B:2494:LEU:HD12	1:B:2494:LEU:O	2.17	0.45
1:B:2839:ASP:O	1:B:2841:PRO:HD3	2.17	0.45
1:A:1677:ASP:HA	1:A:1680:ILE:HD12	1.98	0.45
1:A:1919:PHE:CD1	1:A:3996:GLY:HA2	2.51	0.45
1:A:2412:ARG:HD3	1:A:2555:ALA:HB2	1.99	0.45
1:A:2938:MET:SD	1:A:3321:ILE:HG21	2.57	0.45
1:A:4033:LEU:HD12	1:A:4035:GLN:N	2.32	0.45
1:B:1495:THR:HB	1:B:1498:GLU:CG	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1940:GLU:CG	1:B:1941:ASP:H	2.18	0.45
1:A:2493:LYS:HG3	1:A:2494:LEU:N	2.22	0.45
1:B:1383:TYR:CE2	1:B:1401:LEU:HD13	2.52	0.45
1:B:1531:ARG:CD	1:B:1538:TYR:HA	2.47	0.45
1:B:3946:VAL:HB	1:B:3947:PRO:HA	1.98	0.45
1:A:1750:SER:HB2	1:A:1755:LEU:CD2	2.47	0.45
1:A:1803:THR:HG21	1:A:1848:ASP:OD1	2.17	0.45
1:A:1934:LEU:HD22	1:A:1945:LEU:HD12	1.98	0.45
1:A:1984:ILE:CG2	1:A:1989:GLU:HG3	2.46	0.45
1:A:2385:VAL:HG23	1:A:2574:TYR:HD1	1.82	0.45
1:A:2755:HIS:O	1:A:2913:ILE:N	2.48	0.45
1:A:3353:LEU:HD23	1:A:3358:VAL:HG11	1.98	0.45
1:A:3509:LEU:CG	1:A:3513:VAL:HG21	2.46	0.45
1:A:3628:ILE:HG22	1:A:3649:PHE:HE2	1.82	0.45
1:A:3903:ILE:O	1:A:3907:VAL:HG23	2.17	0.45
1:A:3994:TYR:O	1:A:3998:ILE:HD12	2.16	0.45
1:B:1743:ASP:C	1:B:1745:ASN:N	2.74	0.45
1:B:2155:ASP:OD1	1:B:2195:GLU:OE2	2.34	0.45
1:B:2225:LYS:HG3	2:B:5093:ATP:H1'	1.99	0.45
1:B:2354:SER:H	1:B:2357:SER:HB2	1.81	0.45
1:B:2386:MET:HB3	1:B:2627:ARG:CD	2.45	0.45
1:B:2474:LEU:HB3	1:B:2526:ILE:HG22	1.99	0.45
1:A:1392:LEU:HD13	1:A:1393:LYS:CA	2.46	0.45
1:A:1469:LEU:HD13	1:A:1523:LEU:HD21	1.99	0.45
1:A:1998:LEU:HD11	1:A:2022:PHE:HZ	1.82	0.45
1:A:2002:ILE:HB	1:A:2014:PHE:CE2	2.52	0.45
1:A:2084:TRP:CZ3	1:A:2085:LYS:HG3	2.52	0.45
1:A:4034:LEU:HD23	1:A:4034:LEU:C	2.42	0.45
1:B:1849:GLU:HG2	1:B:1899:ASN:HD22	1.82	0.45
1:B:2106:THR:HG1	1:B:2154:PHE:HB3	1.80	0.45
1:B:3897:TYR:CZ	1:B:3899:ASP:HB3	2.52	0.45
1:A:1365:PHE:CE2	1:A:1420:TYR:CD2	3.04	0.45
1:A:1535:PRO:C	1:A:1841:ILE:CD1	2.79	0.45
1:A:1970:LEU:HD12	1:A:1971:ARG:CA	2.47	0.45
1:A:3330:TYR:CE1	1:A:3334:PHE:CE2	3.04	0.45
1:B:1677:ASP:HA	1:B:1680:ILE:HD12	1.99	0.45
1:B:2047:PHE:CE2	1:B:2082:ALA:HB1	2.52	0.45
1:B:2104:ILE:O	1:B:2154:PHE:HA	2.16	0.45
1:B:2203:THR:HG23	1:B:2204:PRO:HD2	1.99	0.45
1:B:2294:LEU:HB3	1:B:2317:LEU:HD22	1.98	0.45
1:B:2447:LYS:HE3	1:B:2493:LYS:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2508:GLN:HG2	1:B:2512:LYS:HG3	1.97	0.45
1:B:2755:HIS:HD2	1:B:2911:ARG:HB3	1.82	0.45
1:B:3862:THR:HB	1:B:3865:ALA:HB2	1.99	0.45
1:A:1940:GLU:HG3	1:A:1941:ASP:H	1.82	0.44
1:A:2199:LEU:O	1:A:2200:ASP:C	2.59	0.44
1:A:2654:ARG:NH1	1:A:2658:ASP:OD1	2.50	0.44
1:A:3330:TYR:CE2	1:A:3346:LEU:HD13	2.51	0.44
1:B:1421:TYR:CD2	1:B:1425:GLU:CG	2.98	0.44
1:B:2654:ARG:HH22	1:B:2691:SER:HB2	1.81	0.44
1:A:1527:LEU:HD22	1:A:1545:LEU:HD22	1.97	0.44
1:A:2424:LYS:HA	1:A:2559:LEU:HD12	1.99	0.44
1:A:2428:MET:HE1	1:A:2440:VAL:CG1	2.47	0.44
1:A:3372:THR:HG23	1:A:3375:GLU:HB2	2.00	0.44
1:B:1392:LEU:HD23	1:B:1484:LYS:HA	1.99	0.44
1:B:1612:ASP:CA	1:B:1615:ILE:HG12	2.47	0.44
1:B:2109:LEU:HB3	1:B:2113:SER:HB2	2.00	0.44
1:B:3481:ILE:O	1:B:3483:ASP:N	2.46	0.44
1:B:3570:LEU:HD23	1:B:3580:ASN:CG	2.42	0.44
1:B:3817:GLY:H	1:B:3821:ASN:CB	2.29	0.44
1:B:3845:GLN:NE2	1:B:3882:ASP:O	2.50	0.44
1:A:2356:TYR:CE1	1:A:2399:LYS:HD2	2.52	0.44
1:A:3505:ILE:O	1:A:3510:ARG:NH1	2.51	0.44
1:B:1995:VAL:HG22	1:B:2022:PHE:CD2	2.52	0.44
1:A:3968:LEU:HA	1:A:3971:VAL:HG12	2.00	0.44
1:B:2745:ILE:HG12	1:B:2756:MET:CE	2.46	0.44
1:B:3010:LEU:HD22	1:B:3320:LEU:HD12	1.99	0.44
1:A:1536:ARG:HD3	1:A:1841:ILE:CD1	2.47	0.44
1:A:1982:PRO:O	1:A:1985:SER:HB2	2.18	0.44
1:A:2960:THR:HG22	1:A:2961:ILE:N	2.32	0.44
1:A:3671:VAL:HA	1:A:3674:ILE:CG2	2.46	0.44
1:B:2707:VAL:HG12	1:B:2712:LEU:HD12	1.99	0.44
1:B:3636:GLY:CA	1:B:3642:TYR:O	2.66	0.44
1:B:1531:ARG:HD3	1:B:1537:PHE:O	2.17	0.44
1:B:1715:LEU:HG	1:B:1727:LEU:HD22	2.00	0.44
1:B:1779:PHE:O	1:B:1783:THR:HG22	2.18	0.44
1:B:3330:TYR:OH	1:B:3346:LEU:HD13	2.17	0.44
1:B:3998:ILE:HG22	1:B:4004:LEU:HG	1.97	0.44
1:A:2982:VAL:HG12	1:A:2983:GLY:N	2.32	0.44
1:A:3833:LYS:NZ	1:A:3862:THR:HG21	2.33	0.44
1:B:2421:GLY:CA	3:B:5094:ANP:O1B	2.66	0.44
1:B:2783:GLN:HG2	1:B:2816:ILE:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3330:TYR:CZ	1:B:3346:LEU:HD13	2.53	0.44
1:A:1706:LEU:HD21	1:A:1935:GLN:CG	2.47	0.44
1:A:2044:ARG:HH21	1:A:2093:ILE:HD11	1.82	0.44
1:A:2105:ASP:OD2	1:A:2508:GLN:HB2	2.17	0.44
1:A:2423:GLY:N	3:A:5094:ANP:O1B	2.39	0.44
1:A:2757:MET:HE1	1:A:2909:PHE:HA	2.00	0.44
1:A:2838:ALA:HB3	1:A:2878:VAL:HG13	2.00	0.44
1:A:3671:VAL:C	1:A:3674:ILE:HG22	2.43	0.44
1:A:3798:PHE:HA	1:A:3801:ILE:HG12	2.00	0.44
1:B:1385:VAL:HG21	1:B:1491:PHE:CD1	2.53	0.44
1:A:1540:LEU:HD23	1:A:1540:LEU:HA	1.71	0.44
1:A:1646:GLN:OE1	1:A:1763:ILE:HG12	2.18	0.44
1:A:1983:LEU:HB3	1:A:1993:THR:HG23	2.00	0.44
1:A:2127:ASP:HB3	1:A:2132:SER:HB3	2.00	0.44
1:A:2494:LEU:HD12	1:A:2494:LEU:C	2.42	0.44
1:A:3473:ALA:CB	1:A:3476:ARG:HG3	2.48	0.44
1:A:3930:PHE:HE2	1:A:4029:ILE:CD1	2.31	0.44
1:B:1375:LYS:O	1:B:1379:LYS:HG2	2.18	0.44
1:B:2389:ASP:HB3	1:B:2433:ARG:HH11	1.83	0.44
1:B:2572:GLU:CG	1:B:2590:GLU:HG3	2.47	0.44
1:B:2755:HIS:HB3	1:B:2912:CYS:SG	2.58	0.44
1:A:1636:ILE:O	1:A:1640:VAL:HG23	2.18	0.43
1:A:2088:ILE:HG12	1:A:2151:TRP:CZ2	2.53	0.43
1:A:2383:HIS:CE1	1:A:2384:GLU:HG3	2.53	0.43
1:A:2941:THR:CG2	1:A:2942:ASP:H	2.25	0.43
1:A:4045:LEU:O	1:A:4048:ILE:HG22	2.18	0.43
1:B:1495:THR:CG2	1:B:1497:ILE:HG22	2.48	0.43
1:B:1645:PHE:HB2	1:B:1697:LYS:HG3	2.00	0.43
1:B:3671:VAL:C	1:B:3674:ILE:HG22	2.43	0.43
1:B:3911:TRP:CH2	1:B:3926:VAL:CG1	3.01	0.43
1:B:4020:ASN:HB3	1:B:4028:ARG:NH1	2.33	0.43
1:A:1744:LEU:HD22	1:A:1760:PHE:CD2	2.53	0.43
1:A:2201:HIS:CE1	1:A:2497:TYR:O	2.71	0.43
1:A:2565:LYS:O	1:A:2569:GLN:HG3	2.19	0.43
1:A:3845:GLN:NE2	1:A:3882:ASP:O	2.51	0.43
1:A:1759:LYS:HE3	1:A:1761:GLU:OE2	2.18	0.43
1:A:2034:ILE:HD12	1:A:2061:TYR:CE2	2.52	0.43
1:A:2099:ASN:HB3	1:A:2151:TRP:HE1	1.83	0.43
1:A:2203:THR:HG23	1:A:2204:PRO:HD2	1.99	0.43
1:A:2760:GLY:O	1:A:2761:ALA:HB3	2.18	0.43
1:A:3471:ASN:HB2	1:A:3478:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3978:ASN:O	1:A:3981:PRO:HD3	2.17	0.43
1:B:1394:LEU:HD22	1:B:1449:GLN:HE22	1.83	0.43
1:B:1540:LEU:HD23	1:B:1540:LEU:HA	1.72	0.43
1:B:2762:SER:C	1:B:2764:THR:H	2.27	0.43
1:B:3592:LYS:O	1:B:3596:ASN:N	2.51	0.43
1:B:3832:SER:O	1:B:3836:GLY:N	2.46	0.43
1:A:1536:ARG:CD	1:A:1841:ILE:HD13	2.48	0.43
1:A:1849:GLU:CD	1:A:1899:ASN:ND2	2.76	0.43
1:A:2104:ILE:O	1:A:2154:PHE:HA	2.18	0.43
1:A:4033:LEU:CD1	1:A:4035:GLN:H	2.31	0.43
1:B:1535:PRO:O	1:B:1841:ILE:CD1	2.65	0.43
1:B:2152:VAL:HG12	1:B:2154:PHE:HE1	1.83	0.43
1:B:2201:HIS:CE1	1:B:2497:TYR:CA	3.01	0.43
1:B:2494:LEU:HD12	1:B:2494:LEU:C	2.43	0.43
1:B:3555:TYR:HE1	1:B:3593:GLU:HG2	1.83	0.43
1:B:3886:ALA:N	1:B:3887:PRO:CD	2.78	0.43
1:A:1421:TYR:O	1:A:1425:GLU:CA	2.65	0.43
1:A:1655:MET:HE3	1:A:1659:LEU:HD12	2.00	0.43
1:A:1934:LEU:HD13	1:A:1945:LEU:HB2	2.01	0.43
1:A:3544:LYS:O	1:A:3548:LEU:HB2	2.19	0.43
1:A:3800:LEU:HA	1:A:3803:LEU:HD12	1.99	0.43
1:A:3967:TYR:HE2	1:A:3985:VAL:HA	1.83	0.43
1:A:4034:LEU:O	1:A:4036:GLN:HG3	2.19	0.43
1:B:1794:PHE:HB3	1:B:1919:PHE:HB3	2.01	0.43
1:B:3544:LYS:O	1:B:3548:LEU:HB2	2.18	0.43
1:A:2141:ILE:CG2	1:A:2145:PHE:HB2	2.49	0.43
1:A:2787:HIS:HB3	1:A:3461:ILE:HG23	2.00	0.43
1:B:1826:PHE:O	1:B:1826:PHE:CG	2.71	0.43
1:B:2517:LYS:HD2	1:B:2524:VAL:CG2	2.49	0.43
1:B:3462:ILE:O	1:B:3465:LEU:N	2.51	0.43
1:A:1835:LEU:O	1:A:1838:ILE:HG22	2.18	0.43
1:A:1872:LEU:HG	1:A:1888:LEU:HD21	2.00	0.43
1:A:3459:ASP:OD2	1:A:3461:ILE:CG1	2.65	0.43
1:A:3566:LEU:HD11	1:A:3570:LEU:HD11	1.99	0.43
1:A:3690:LEU:HD23	1:A:3694:PHE:HB3	2.01	0.43
1:A:3785:TYR:CE2	1:A:3859:VAL:HG13	2.54	0.43
1:A:4021:LEU:CD2	1:A:4023:ILE:HG12	2.49	0.43
1:B:1741:LEU:O	1:B:1742:ASP:HB2	2.18	0.43
1:B:2425:THR:CG2	1:B:2485:PHE:HE2	2.32	0.43
1:B:2754:GLY:HA3	1:B:2886:HIS:HD1	1.83	0.43
1:B:2761:ALA:O	1:B:2892:CYS:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2252:LEU:HD22	1:A:2314:ILE:HG13	2.01	0.43
1:A:2788:ARG:HB2	1:A:3459:ASP:HB3	2.01	0.43
1:A:3788:MET:O	1:A:3788:MET:HG3	2.19	0.43
1:B:2220:CYS:SG	1:B:2221:SER:N	2.92	0.43
1:B:2510:MET:O	1:B:2513:GLN:NE2	2.52	0.43
1:B:3930:PHE:CE2	1:B:4029:ILE:HD13	2.51	0.43
1:A:1794:PHE:CD1	1:A:1802:LYS:HB3	2.51	0.43
1:A:1953:LEU:HA	1:A:1956:LEU:HD12	2.01	0.43
1:A:2141:ILE:HG22	1:A:2145:PHE:CG	2.54	0.43
1:B:1789:LYS:HD3	1:B:1872:LEU:O	2.19	0.43
1:B:2129:LEU:O	1:B:2133:ILE:HG12	2.19	0.43
1:B:2152:VAL:HG12	1:B:2154:PHE:CE1	2.54	0.43
1:B:2446:SER:H	1:B:2449:THR:HG21	1.80	0.43
1:B:3505:ILE:O	1:B:3510:ARG:NH1	2.52	0.43
1:A:1438:LEU:O	1:A:1442:GLN:HB2	2.19	0.43
1:A:2061:TYR:O	1:A:2064:GLN:HG2	2.19	0.43
1:A:3924:TRP:CD1	1:A:3924:TRP:C	2.96	0.43
1:B:1409:LEU:CD2	1:B:1435:LEU:CB	2.80	0.43
1:B:1536:ARG:HD3	1:B:1536:ARG:HA	1.67	0.43
1:B:2034:ILE:CD1	1:B:2061:TYR:CE2	3.02	0.43
1:B:2368:PHE:O	1:B:2369:SER:OG	2.25	0.43
1:A:23:LEU:C	1:A:25:GLU:N	2.77	0.42
1:A:1469:LEU:CD1	1:A:1523:LEU:CD2	2.97	0.42
1:A:1645:PHE:CZ	1:A:1768:ARG:HD2	2.52	0.42
1:A:2170:LEU:HB3	1:A:2209:ARG:HD3	2.01	0.42
1:A:2220:CYS:SG	1:A:2224:SER:HB3	2.59	0.42
1:A:4023:ILE:HG13	1:A:4029:ILE:HD12	2.01	0.42
1:B:1616:LYS:HE3	1:B:1761:GLU:HG3	2.01	0.42
1:B:3304:GLU:C	1:B:3306:TRP:H	2.27	0.42
1:A:1702:LEU:HD23	1:A:1702:LEU:HA	1.85	0.42
1:A:1744:LEU:HD22	1:A:1760:PHE:CG	2.54	0.42
1:A:3326:ILE:HG22	1:A:3330:TYR:CE2	2.54	0.42
1:A:3629:PHE:O	1:A:3633:GLU:HB2	2.20	0.42
1:A:3930:PHE:HE2	1:A:4029:ILE:HD13	1.83	0.42
1:B:1612:ASP:C	1:B:1615:ILE:HG12	2.43	0.42
1:B:2001:VAL:O	1:B:2004:PRO:HD2	2.19	0.42
1:B:2027:THR:HA	1:B:2028:PRO:HD3	1.55	0.42
1:B:2151:TRP:CE3	1:B:2193:LEU:HD11	2.54	0.42
1:B:2220:CYS:SG	2:B:5093:ATP:N6	2.93	0.42
1:B:2220:CYS:HB2	2:B:5093:ATP:N6	2.33	0.42
1:B:2707:VAL:HG11	1:B:2712:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2742:ILE:HG23	1:A:2773:VAL:HG22	2.00	0.42
1:A:3409:ASP:HA	1:A:3410:PRO:HD3	1.93	0.42
1:A:3897:TYR:CZ	1:A:3899:ASP:HB3	2.54	0.42
1:B:1630:ILE:HG21	1:B:1655:MET:SD	2.57	0.42
1:B:1870:ASN:O	1:B:1874:VAL:HG23	2.19	0.42
1:B:3930:PHE:HE2	1:B:4029:ILE:CD1	2.31	0.42
1:A:1392:LEU:HD23	1:A:1484:LYS:HA	2.01	0.42
1:A:1554:HIS:O	1:A:1555:HIS:HB2	2.19	0.42
1:A:1822:CYS:HB2	1:A:1853:LEU:CD2	2.27	0.42
1:A:3844:ILE:O	1:A:3845:GLN:C	2.63	0.42
1:A:4022:GLN:O	1:A:4022:GLN:HG2	2.19	0.42
1:B:1535:PRO:O	1:B:1841:ILE:HD11	2.13	0.42
1:B:2747:ARG:O	1:B:2751:GLN:HG2	2.19	0.42
1:B:2980:MET:HE3	1:B:3337:LEU:HD13	2.02	0.42
1:B:3431:PHE:CZ	1:B:3458:PHE:HD1	2.38	0.42
1:B:3459:ASP:HB2	1:B:3460:PRO:HD2	2.01	0.42
1:A:1365:PHE:N	1:A:1365:PHE:HD1	2.17	0.42
1:A:2109:LEU:HD11	1:A:2129:LEU:CD2	2.50	0.42
1:A:2378:VAL:HG11	1:A:2392:ILE:HD12	2.00	0.42
1:A:2707:VAL:HG12	1:A:2708:ASN:N	2.35	0.42
1:A:3854:TYR:CD1	1:A:3854:TYR:C	2.98	0.42
1:A:4006:VAL:HG13	1:A:4009:LYS:HE2	2.01	0.42
1:A:4037:SER:HB3	1:A:4040:GLU:HB3	2.01	0.42
1:B:2745:ILE:CB	1:B:2756:MET:HE1	2.49	0.42
1:B:3919:LYS:HZ3	1:B:4038:GLU:CG	2.30	0.42
1:B:4033:LEU:HD23	1:B:4033:LEU:HA	1.84	0.42
1:A:1536:ARG:HD2	1:A:1565:MET:O	2.19	0.42
1:A:3784:ASN:ND2	1:A:3865:ALA:O	2.52	0.42
1:B:1656:TRP:O	1:B:1660:VAL:HG12	2.18	0.42
1:B:3813:ILE:HG22	1:B:3840:LEU:HD23	2.01	0.42
1:A:1672:TYR:O	1:A:1675:GLU:HB3	2.19	0.42
1:A:2653:TRP:HB3	1:A:2654:ARG:NH1	2.34	0.42
1:A:2737:SER:HB2	1:A:2924:THR:HG21	2.01	0.42
1:A:3645:SER:CB	1:A:3890:GLN:NE2	2.80	0.42
1:B:1459:LEU:HD23	1:B:1465:ILE:HG13	2.02	0.42
1:B:1743:ASP:C	1:B:1745:ASN:H	2.28	0.42
1:B:1762:TYR:CZ	1:B:1764:GLY:HA2	2.55	0.42
1:B:2467:THR:HG22	1:B:2468:SER:N	2.34	0.42
1:B:3848:LEU:O	1:B:3851:VAL:N	2.53	0.42
1:A:1706:LEU:HD23	1:A:1706:LEU:HA	1.90	0.42
1:A:3628:ILE:HD11	1:A:3679:TYR:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4022:GLN:HA	1:A:4028:ARG:HA	2.01	0.42
1:B:1531:ARG:HD2	1:B:1538:TYR:HA	2.01	0.42
1:B:1660:VAL:CG1	1:B:1728:TRP:CH2	3.02	0.42
1:B:2114:LEU:HA	1:B:2129:LEU:HB3	2.02	0.42
1:A:1769:LEU:HD11	1:A:1804:GLU:HB3	2.01	0.42
1:A:2354:SER:H	1:A:2357:SER:HB2	1.85	0.42
1:A:2799:LEU:HD13	1:A:2840:ILE:CD1	2.49	0.42
1:A:3462:ILE:O	1:A:3465:LEU:N	2.48	0.42
1:A:3509:LEU:HG	1:A:3513:VAL:HG21	2.02	0.42
1:A:3845:GLN:O	1:A:3848:LEU:HB2	2.20	0.42
1:A:4033:LEU:CD1	1:A:4035:GLN:N	2.83	0.42
1:B:1750:SER:CB	1:B:1755:LEU:HD23	2.50	0.42
1:B:1838:ILE:HG13	1:B:1843:ALA:HB3	2.02	0.42
1:B:2106:THR:H	1:B:2156:SER:HB2	1.83	0.42
1:B:3808:LYS:O	1:B:3809:GLU:C	2.63	0.42
1:B:3855:LEU:HD11	1:B:3873:MET:HE1	2.02	0.42
1:A:1645:PHE:CZ	1:A:1649:LEU:HD22	2.55	0.42
1:A:3600:LYS:HA	1:A:3603:GLU:HG2	2.01	0.42
1:A:3671:VAL:CA	1:A:3674:ILE:HG22	2.49	0.42
1:B:1593:ASN:ND2	1:B:1621:THR:OG1	2.47	0.42
1:B:2095:ASP:CG	1:B:2149:ARG:HH21	2.28	0.42
1:B:2336:ARG:HG2	1:B:2355:ASP:OD1	2.19	0.42
1:A:40:TRP:O	1:A:44:LYS:N	2.53	0.41
1:A:3725:VAL:HA	1:A:3730:SER:O	2.19	0.41
1:A:3886:ALA:N	1:A:3887:PRO:CD	2.80	0.41
1:B:1575:LEU:O	1:B:1576:GLU:HB3	2.19	0.41
1:B:1983:LEU:CD1	1:B:2000:ARG:HH21	2.33	0.41
1:B:1992:LYS:CG	1:B:2024:SER:CB	2.83	0.41
1:B:2707:VAL:CB	1:B:2712:LEU:CD1	2.76	0.41
1:B:2754:GLY:HA3	1:B:2886:HIS:CE1	2.55	0.41
1:B:2965:VAL:HA	1:B:2968:ILE:HD12	2.01	0.41
1:B:3002:LEU:HD21	1:B:3370:LEU:HD11	2.02	0.41
1:B:3303:LYS:O	1:B:3306:TRP:HD1	2.03	0.41
1:B:3319:GLU:HA	1:B:3359:LYS:O	2.19	0.41
1:A:1823:ASP:HB3	1:A:1852:ARG:O	2.15	0.41
1:A:2034:ILE:HG13	1:A:2061:TYR:CE2	2.55	0.41
1:A:2226:ILE:HG23	1:A:2288:VAL:CG2	2.49	0.41
1:A:2755:HIS:NE2	1:A:2835:LEU:HG	2.35	0.41
1:A:2828:LEU:HD13	1:A:2902:MET:SD	2.60	0.41
1:A:3373:LEU:HD13	1:A:3557:LEU:HD13	2.02	0.41
1:A:3979:ASN:OD1	1:A:3979:ASN:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1479:LEU:HD11	1:B:1515:SER:HB3	2.02	0.41
1:B:3901:PRO:HG2	1:B:3906:THR:HG23	2.01	0.41
1:A:1542:ASN:O	1:A:1546:LEU:HG	2.20	0.41
1:A:1671:LYS:HA	1:A:1671:LYS:HD3	1.96	0.41
1:A:1681:LYS:HE2	1:A:1939:PHE:CZ	2.55	0.41
1:A:2109:LEU:HB3	1:A:2113:SER:HB2	2.02	0.41
1:A:3406:PHE:CZ	1:A:3505:ILE:HG21	2.56	0.41
1:A:3538:ASN:HB3	1:A:3541:MET:HG2	2.02	0.41
1:A:3946:VAL:HB	1:A:3947:PRO:HA	2.02	0.41
1:B:1934:LEU:HD22	1:B:1945:LEU:HD12	2.01	0.41
1:B:1939:PHE:CD1	1:B:1939:PHE:N	2.88	0.41
1:A:1697:LYS:O	1:A:1701:LEU:HG	2.20	0.41
1:A:2078:CYS:N	2:A:5093:ATP:O2B	2.49	0.41
1:A:2279:ARG:HH11	1:A:2279:ARG:HD2	1.66	0.41
1:A:2336:ARG:HG2	1:A:2355:ASP:CG	2.45	0.41
1:A:2428:MET:SD	1:A:2428:MET:C	3.03	0.41
1:B:1536:ARG:NE	1:B:1841:ILE:HD13	2.35	0.41
1:B:2661:VAL:HG12	1:B:2916:TRP:CD2	2.55	0.41
1:B:2938:MET:SD	1:B:3321:ILE:CG2	3.09	0.41
1:A:1940:GLU:HG3	1:A:1941:ASP:N	2.35	0.41
1:A:2099:ASN:HB3	1:A:2151:TRP:NE1	2.34	0.41
1:A:2282:ASN:HB3	1:A:2552:ARG:HG3	2.02	0.41
1:A:2494:LEU:HD12	1:A:2495:ASP:O	2.20	0.41
1:B:2748:ALA:O	1:B:2751:GLN:HG3	2.19	0.41
1:A:23:LEU:C	1:A:25:GLU:H	2.28	0.41
1:A:1392:LEU:N	1:A:1484:LYS:HE2	2.36	0.41
1:A:2761:ALA:O	1:A:2892:CYS:SG	2.78	0.41
1:A:3024:LEU:HD13	1:A:3303:LYS:HG3	1.92	0.41
1:A:3367:ILE:O	1:A:3371:VAL:HG22	2.21	0.41
1:A:3930:PHE:CE2	1:A:4029:ILE:HD13	2.55	0.41
1:B:1774:LEU:HA	1:B:1777:ILE:HD12	2.02	0.41
1:B:1832:SER:HB3	1:B:1882:LEU:HD22	2.03	0.41
1:B:3305:ARG:C	1:B:3307:LEU:H	2.28	0.41
1:B:3584:MET:HA	1:B:3587:LEU:HD12	2.03	0.41
1:A:1496:THR:O	1:A:1499:VAL:HG23	2.21	0.41
1:A:1866:GLN:O	1:A:1870:ASN:HB2	2.21	0.41
1:A:2021:ILE:HG22	1:A:2022:PHE:HD1	1.85	0.41
1:A:2762:SER:O	1:A:2763:ARG:CB	2.69	0.41
1:B:1392:LEU:N	1:B:1484:LYS:HE2	2.35	0.41
1:B:1949:ILE:HD11	1:B:1994:VAL:HG11	2.03	0.41
1:B:2034:ILE:CD1	1:B:2061:TYR:CZ	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2290:LEU:HD13	1:B:2407:LEU:HD23	2.02	0.41
1:B:2464:TYR:CZ	1:B:2474:LEU:HD12	2.55	0.41
1:B:4034:LEU:HD23	1:B:4034:LEU:C	2.45	0.41
1:A:1406:LYS:HE2	1:A:1406:LYS:HB3	1.95	0.41
1:A:1547:LYS:O	1:A:1551:SER:HB3	2.20	0.41
1:A:1795:PHE:CE1	1:A:1920:SER:HB3	2.55	0.41
1:A:2076:ALA:HB2	1:A:2549:ARG:HG2	2.02	0.41
1:A:2316:LEU:HD13	1:A:2351:GLN:HB3	2.01	0.41
1:A:2571:TYR:HA	1:A:2574:TYR:HB2	2.03	0.41
1:B:1826:PHE:CE1	1:B:1853:LEU:CD2	3.04	0.41
1:B:2044:ARG:HH21	1:B:2093:ILE:HD11	1.85	0.41
1:B:2079:GLY:HA2	2:B:5093:ATP:H5'2	2.02	0.41
1:B:2230:LEU:HD23	1:B:2288:VAL:HG13	2.03	0.41
1:B:2428:MET:HG2	1:B:2485:PHE:CE1	2.55	0.41
1:A:2938:MET:HG2	1:A:3321:ILE:HG12	2.03	0.41
1:A:3430:SER:HB2	1:A:3453:GLN:HB3	2.02	0.41
1:A:3772:TRP:HZ3	1:A:3780:ASN:ND2	2.19	0.41
1:B:1559:SER:HB3	1:B:1572:ILE:HG22	2.02	0.41
1:B:1702:LEU:O	1:B:1706:LEU:HG	2.21	0.41
1:B:2000:ARG:O	1:B:2004:PRO:HG2	2.21	0.41
1:B:2199:LEU:O	1:B:2200:ASP:C	2.64	0.41
1:B:2295:ILE:HG12	1:B:2314:ILE:HD12	2.02	0.41
1:B:2422:SER:N	3:B:5094:ANP:O1B	2.54	0.41
1:B:2491:LEU:HD23	1:B:2491:LEU:HA	1.78	0.41
1:B:2572:GLU:HG3	1:B:2590:GLU:HG3	2.02	0.41
1:B:2578:ILE:CG2	1:B:2630:TYR:HB2	2.50	0.41
1:B:2707:VAL:HG11	1:B:2712:LEU:CD1	2.46	0.41
1:B:2787:HIS:HB3	1:B:3461:ILE:HG23	2.02	0.41
1:B:3462:ILE:O	1:B:3465:LEU:HB3	2.21	0.41
1:B:3551:LEU:HA	1:B:3554:GLU:HB3	2.02	0.41
1:B:3846:MET:HG3	1:B:3847:SER:N	2.35	0.41
1:A:1620:PHE:CE1	1:A:1743:ASP:HB3	2.55	0.41
1:A:1968:PHE:CD1	1:A:1968:PHE:N	2.88	0.41
1:A:2320:ARG:O	1:A:2323:LEU:HB3	2.20	0.41
1:A:3642:TYR:N	1:A:3642:TYR:CD1	2.87	0.41
1:B:1637:GLU:HG2	1:B:1686:LYS:HG3	2.03	0.41
1:B:2336:ARG:HG2	1:B:2355:ASP:CG	2.45	0.41
1:B:3330:TYR:HH	1:B:3346:LEU:HD22	1.82	0.41
1:B:3414:MET:HE3	1:B:3518:PHE:CD1	2.56	0.41
1:A:1704:GLU:O	1:A:1707:HIS:HB3	2.21	0.40
1:A:1838:ILE:HD11	1:A:1845:GLY:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1853:LEU:HB2	1:A:1858:LEU:HD12	2.03	0.40
1:A:2415:ILE:O	1:A:2556:ILE:HA	2.21	0.40
1:A:3862:THR:HB	1:A:3865:ALA:HB2	2.03	0.40
1:A:4065:LEU:HD12	1:A:4065:LEU:O	2.21	0.40
1:B:1710:ASN:HB2	1:B:1932:MET:HE1	2.03	0.40
1:B:2039:LYS:HG2	1:B:2049:MET:HG3	2.02	0.40
1:B:2115:TYR:OH	1:B:2162:TYR:O	2.28	0.40
1:B:2178:LEU:HB2	1:B:2182:GLU:H	1.86	0.40
1:B:2476:LYS:CD	1:B:2476:LYS:N	2.84	0.40
1:A:1579:ILE:HG13	1:A:1598:LEU:HD11	2.03	0.40
1:A:1592:LEU:HD13	1:A:1596:ILE:CD1	2.50	0.40
1:A:1620:PHE:HA	1:A:1760:PHE:HE1	1.86	0.40
1:A:2510:MET:O	1:A:2513:GLN:NE2	2.53	0.40
1:A:2627:ARG:NH1	1:A:2630:TYR:CE2	2.89	0.40
1:A:2797:MET:HE2	1:A:2797:MET:HB3	1.91	0.40
1:A:3978:ASN:O	1:A:3981:PRO:HD2	2.19	0.40
1:B:1664:LEU:HD23	1:B:1669:PHE:HZ	1.86	0.40
1:B:1987:PHE:HB3	1:B:1988:GLY:H	1.73	0.40
1:B:2752:VAL:HG13	1:B:2883:LYS:CB	2.50	0.40
1:B:3784:ASN:ND2	1:B:3865:ALA:O	2.54	0.40
1:A:1926:SER:O	1:A:1927:GLY:C	2.63	0.40
1:A:1939:PHE:CD1	1:A:1939:PHE:N	2.81	0.40
1:A:2125:TRP:CE2	1:A:2178:LEU:HD13	2.56	0.40
1:A:3534:LEU:HD12	1:A:3618:TYR:CZ	2.54	0.40
1:A:4033:LEU:HD13	1:A:4035:GLN:H	1.87	0.40
1:B:1734:PHE:CD2	1:B:1749:ILE:HG12	2.56	0.40
1:B:2012:LEU:HD12	1:B:2013:VAL:N	2.36	0.40
1:B:2820:SER:O	1:B:2823:LEU:HD12	2.21	0.40
1:A:2071:ILE:HB	1:A:2212:LEU:CD1	2.51	0.40
1:A:3443:ALA:HB1	1:A:3450:VAL:CG2	2.50	0.40
1:A:3564:LYS:O	1:A:3568:GLU:HG2	2.21	0.40
1:B:1750:SER:HB2	1:B:1755:LEU:HD23	2.03	0.40
1:B:1826:PHE:O	1:B:1826:PHE:CD1	2.75	0.40
1:B:2759:ILE:HG21	1:B:2916:TRP:CZ2	2.56	0.40
1:A:2378:VAL:HG11	1:A:2392:ILE:CD1	2.51	0.40
1:A:2980:MET:HE3	1:A:3337:LEU:HD13	2.03	0.40
1:A:3566:LEU:HD13	1:A:3570:LEU:HD12	2.02	0.40
1:A:3939:ILE:CG1	1:A:4010:LEU:CD2	2.99	0.40
1:A:4033:LEU:HD12	1:A:4033:LEU:C	2.47	0.40
1:B:1773:PRO:HA	1:B:1776:LEU:HD12	2.03	0.40
1:B:1796:GLY:O	1:B:1900:PRO:HD3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1832:SER:O	1:B:1836:VAL:HG23	2.21	0.40
1:B:2463:ASN:O	1:B:2475:PRO:HD2	2.21	0.40
1:B:2653:TRP:HB3	1:B:2654:ARG:NH1	2.35	0.40
1:B:3566:LEU:HA	1:B:3583:LEU:HD23	1.96	0.40
1:B:3773:ASN:O	1:B:3774:ILE:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2640/2695 (98%)	2518 (95%)	110 (4%)	12 (0%)	24	57
1	B	2640/2695 (98%)	2515 (95%)	111 (4%)	14 (0%)	24	57
All	All	5280/5390 (98%)	5033 (95%)	221 (4%)	26 (0%)	24	57

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1391	GLY
1	B	1391	GLY
1	B	3578	LEU
1	A	24	GLU
1	A	1633	GLY
1	A	2513	GLN
1	A	3482	GLY
1	B	24	GLU
1	B	2513	GLN
1	B	2990	GLY
1	B	3482	GLY
1	A	2990	GLY
1	A	66	GLN

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Mol	Chain	Res	Type
1	A	1744	LEU
1	A	2519	PRO
1	B	66	GLN
1	B	3914	GLN
1	B	2519	PRO
1	B	2562	PRO
1	B	3809	GLU
1	A	3980	ILE
1	B	3305	ARG
1	A	2028	PRO
1	B	3980	ILE
1	A	2562	PRO
1	B	1470	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2218/2453 (90%)	2084 (94%)	134 (6%)	17	45
1	B	2218/2453 (90%)	2094 (94%)	124 (6%)	19	47
All	All	4436/4906 (90%)	4178 (94%)	258 (6%)	18	46

All (258) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1392	LEU
1	A	1421	TYR
1	A	1455	LEU
1	A	1486	ILE
1	A	1493	LEU
1	A	1504	ASN
1	A	1508	THR
1	A	1511	LEU
1	A	1525	THR
1	A	1605	GLN

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Mol	Chain	Res	Type
1	A	1639	VAL
1	A	1642	LYS
1	A	1644	ILE
1	A	1646	GLN
1	A	1661	GLU
1	A	1720	THR
1	A	1768	ARG
1	A	1769	LEU
1	A	1783	THR
1	A	1788	GLN
1	A	1794	PHE
1	A	1858	LEU
1	A	1925	GLN
1	A	1992	LYS
1	A	2057	CYS
1	A	2078	CYS
1	A	2104	ILE
1	A	2107	LYS
1	A	2109	LEU
1	A	2122	THR
1	A	2137	VAL
1	A	2141	ILE
1	A	2154	PHE
1	A	2155	ASP
1	A	2186	ILE
1	A	2202	THR
1	A	2218	ASP
1	A	2229	LEU
1	A	2273	VAL
1	A	2295	ILE
1	A	2310	LEU
1	A	2318	ILE
1	A	2351	GLN
1	A	2352	GLU
1	A	2357	SER
1	A	2361	ILE
1	A	2395	ILE
1	A	2397	THR
1	A	2411	LYS
1	A	2412	ARG
1	A	2472	THR
1	A	2476	LYS

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Mol	Chain	Res	Type
1	A	2482	LEU
1	A	2496	LYS
1	A	2510	MET
1	A	2526	ILE
1	A	2544	ILE
1	A	2548	GLU
1	A	2566	SER
1	A	2570	ILE
1	A	2576	LYS
1	A	2623	THR
1	A	2626	VAL
1	A	2679	LYS
1	A	2681	LEU
1	A	2689	ILE
1	A	2694	LEU
1	A	2732	MET
1	A	2751	GLN
1	A	2785	LYS
1	A	2822	ILE
1	A	2823	LEU
1	A	2833	THR
1	A	2843	LEU
1	A	2853	LEU
1	A	2856	LEU
1	A	2866	LEU
1	A	2936	ILE
1	A	2967	ASN
1	A	2999	LEU
1	A	3002	LEU
1	A	3329	ILE
1	A	3332	THR
1	A	3340	ARG
1	A	3371	VAL
1	A	3372	THR
1	A	3391	LEU
1	A	3400	SER
1	A	3418	ILE
1	A	3456	GLU
1	A	3466	ILE
1	A	3485	GLU
1	A	3496	ILE
1	A	3512	ARG

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Mol	Chain	Res	Type
1	A	3532	ILE
1	A	3534	LEU
1	A	3536	GLU
1	A	3538	ASN
1	A	3548	LEU
1	A	3557	LEU
1	A	3559	LEU
1	A	3566	LEU
1	A	3567	LEU
1	A	3578	LEU
1	A	3601	LEU
1	A	3618	TYR
1	A	3634	LYS
1	A	3646	ILE
1	A	3673	GLU
1	A	3677	LEU
1	A	3697	ILE
1	A	3729	SER
1	A	3737	THR
1	A	3788	MET
1	A	3805	LYS
1	A	3811	LEU
1	A	3823	ASN
1	A	3831	LYS
1	A	3862	THR
1	A	3876	THR
1	A	3884	LEU
1	A	3899	ASP
1	A	3900	ILE
1	A	3906	THR
1	A	3910	LEU
1	A	3939	ILE
1	A	3940	THR
1	A	3943	THR
1	A	3980	ILE
1	A	3982	TRP
1	A	3992	ILE
1	A	3997	LYS
1	A	3998	ILE
1	A	4004	LEU
1	B	1366	VAL
1	B	1392	LEU

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Mol	Chain	Res	Type
1	B	1421	TYR
1	B	1486	ILE
1	B	1493	LEU
1	B	1504	ASN
1	B	1525	THR
1	B	1540	LEU
1	B	1589	VAL
1	B	1644	ILE
1	B	1646	GLN
1	B	1661	GLU
1	B	1694	VAL
1	B	1743	ASP
1	B	1759	LYS
1	B	1768	ARG
1	B	1769	LEU
1	B	1826	PHE
1	B	1936	ILE
1	B	1992	LYS
1	B	2008	ASP
1	B	2075	LYS
1	B	2109	LEU
1	B	2122	THR
1	B	2137	VAL
1	B	2141	ILE
1	B	2154	PHE
1	B	2155	ASP
1	B	2186	ILE
1	B	2202	THR
1	B	2229	LEU
1	B	2275	ILE
1	B	2295	ILE
1	B	2307	ASP
1	B	2310	LEU
1	B	2318	ILE
1	B	2351	GLN
1	B	2361	ILE
1	B	2368	PHE
1	B	2381	GLU
1	B	2390	ILE
1	B	2395	ILE
1	B	2397	THR
1	B	2412	ARG

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Mol	Chain	Res	Type
1	B	2425	THR
1	B	2476	LYS
1	B	2479	ILE
1	B	2496	LYS
1	B	2526	ILE
1	B	2544	ILE
1	B	2566	SER
1	B	2576	LYS
1	B	2616	LEU
1	B	2681	LEU
1	B	2689	ILE
1	B	2694	LEU
1	B	2721	LYS
1	B	2732	MET
1	B	2742	ILE
1	B	2751	GLN
1	B	2764	THR
1	B	2769	LEU
1	B	2822	ILE
1	B	2829	GLU
1	B	2833	THR
1	B	2835	LEU
1	B	2843	LEU
1	B	2853	LEU
1	B	2856	LEU
1	B	2936	ILE
1	B	2967	ASN
1	B	2969	LEU
1	B	3012	GLU
1	B	3305	ARG
1	B	3329	ILE
1	B	3348	ILE
1	B	3371	VAL
1	B	3372	THR
1	B	3380	LEU
1	B	3391	LEU
1	B	3400	SER
1	B	3418	ILE
1	B	3456	GLU
1	B	3461	ILE
1	B	3502	SER
1	B	3534	LEU

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Mol	Chain	Res	Type
1	B	3536	GLU
1	B	3538	ASN
1	B	3548	LEU
1	B	3559	LEU
1	B	3566	LEU
1	B	3567	LEU
1	B	3598	GLU
1	B	3605	GLU
1	B	3618	TYR
1	B	3677	LEU
1	B	3717	GLU
1	B	3729	SER
1	B	3737	THR
1	B	3744	LEU
1	B	3771	GLU
1	B	3805	LYS
1	B	3811	LEU
1	B	3839	ILE
1	B	3844	ILE
1	B	3862	THR
1	B	3884	LEU
1	B	3899	ASP
1	B	3906	THR
1	B	3917	THR
1	B	3940	THR
1	B	3943	THR
1	B	3966	VAL
1	B	3982	TRP
1	B	3992	ILE
1	B	3998	ILE
1	B	4003	ASP
1	B	4016	CYS
1	B	4021	LEU
1	B	4024	VAL
1	B	4040	GLU
1	B	4053	ILE
1	B	4068	GLU
1	B	4087	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1533	GLN
1	A	1605	GLN
1	A	1622	GLN
1	A	1629	GLN
1	A	1646	GLN
1	A	1668	GLN
1	A	1717	ASN
1	A	1745	ASN
1	A	1851	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	2231	ASN
1	A	2239	ASN
1	A	2264	ASN
1	A	2270	ASN
1	A	2274	HIS
1	A	2282	ASN
1	A	2293	HIS
1	A	2335	GLN
1	A	2351	GLN
1	A	2383	HIS
1	A	2409	ASN
1	A	2500	GLN
1	A	2536	ASN
1	A	2601	ASN
1	A	2634	ASN
1	A	2683	ASN
1	A	2688	ASN
1	A	2837	ASN
1	A	2896	ASN
1	A	2927	GLN
1	A	3008	GLN
1	A	3025	ASN
1	A	3323	ASN
1	A	3336	HIS
1	A	3363	ASN
1	A	3413	HIS
1	A	3475	ASN
1	A	3497	HIS

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Mol	Chain	Res	Type
1	A	3521	ASN
1	A	3588	ASN
1	A	3624	HIS
1	A	3637	GLN
1	A	3780	ASN
1	A	3842	GLN
1	A	3890	GLN
1	A	3962	GLN
1	A	3970	ASN
1	A	4020	ASN
1	A	4036	GLN
1	A	4051	ASN
1	A	4077	GLN
1	B	1501	HIS
1	B	1622	GLN
1	B	1646	GLN
1	B	1667	ASN
1	B	1717	ASN
1	B	1736	GLN
1	B	1757	GLN
1	B	1787	HIS
1	B	1811	GLN
1	B	1873	GLN
1	B	1899	ASN
1	B	1965	HIS
1	B	2068	GLN
1	B	2270	ASN
1	B	2282	ASN
1	B	2293	HIS
1	B	2335	GLN
1	B	2383	HIS
1	B	2409	ASN
1	B	2513	GLN
1	B	2536	ASN
1	B	2598	HIS
1	B	2634	ASN
1	B	2667	ASN
1	B	2683	ASN
1	B	2688	ASN
1	B	2753	GLN
1	B	2755	HIS
1	B	2777	ASN

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Mol	Chain	Res	Type
1	B	2789	HIS
1	B	2837	ASN
1	B	2896	ASN
1	B	2910	ASN
1	B	2927	GLN
1	B	3008	GLN
1	B	3025	ASN
1	B	3323	ASN
1	B	3338	ASN
1	B	3363	ASN
1	B	3521	ASN
1	B	3542	GLN
1	B	3552	ASN
1	B	3561	ASN
1	B	3571	ASN
1	B	3624	HIS
1	B	3780	ASN
1	B	3890	GLN
1	B	3962	GLN
1	B	3970	ASN
1	B	3984	GLN
1	B	4020	ASN
1	B	4036	GLN
1	B	4077	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	5093	5	32,33,33	1.52	7 (21%)	48,52,52	1.77	10 (20%)
2	ATP	A	5093	5	32,33,33	1.48	5 (15%)	48,52,52	1.79	9 (18%)
3	ANP	B	5094	-	33,33,33	2.59	8 (24%)	45,52,52	1.86	9 (20%)
4	SO4	B	5095	-	4,4,4	0.42	0	6,6,6	0.45	0
4	SO4	B	5096	-	4,4,4	0.45	0	6,6,6	0.20	0
3	ANP	A	5094	-	33,33,33	2.58	9 (27%)	45,52,52	1.89	11 (24%)
4	SO4	A	5096	-	4,4,4	0.54	0	6,6,6	0.23	0
4	SO4	A	5095	-	4,4,4	0.60	0	6,6,6	0.71	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	5	-	5/22/38/38	0/3/3/3
3	ANP	B	5094	-	-	6/18/38/38	0/3/3/3
3	ANP	A	5094	-	-	7/18/38/38	0/3/3/3
2	ATP	B	5093	5	-	6/22/38/38	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5094	ANP	PG-O1G	10.13	1.61	1.46
3	A	5094	ANP	PG-O1G	9.93	1.61	1.46
2	A	5093	ATP	C5-C4	5.08	1.48	1.39
2	B	5093	ATP	C5-C4	4.92	1.47	1.39
3	B	5094	ANP	C5-C4	4.78	1.47	1.39
3	B	5094	ANP	PG-N3B	4.66	1.75	1.63
3	A	5094	ANP	PG-N3B	4.66	1.75	1.63
3	A	5094	ANP	C5-C4	4.63	1.47	1.39
3	B	5094	ANP	PB-N3B	4.60	1.75	1.63
3	A	5094	ANP	PB-N3B	4.34	1.74	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5094	ANP	PG-O3G	-3.15	1.48	1.56
3	A	5094	ANP	PG-O3G	-3.10	1.48	1.56
2	A	5093	ATP	PB-O3B	3.02	1.62	1.59
3	B	5094	ANP	C5-C6	2.75	1.48	1.41
3	A	5094	ANP	PA-O3A	2.70	1.62	1.59
3	A	5094	ANP	C5-C6	2.68	1.48	1.41
2	A	5093	ATP	C5-C6	2.60	1.48	1.41
2	B	5093	ATP	PB-O3B	2.55	1.62	1.59
2	B	5093	ATP	C5-C6	2.53	1.48	1.41
3	A	5094	ANP	C8-N7	2.44	1.36	1.31
2	A	5093	ATP	C5-N7	-2.42	1.34	1.39
2	B	5093	ATP	C5-N7	-2.42	1.34	1.39
2	B	5093	ATP	C8-N7	2.41	1.36	1.31
2	B	5093	ATP	PB-O3A	2.37	1.62	1.59
3	B	5094	ANP	C8-N7	2.34	1.36	1.31
2	B	5093	ATP	PA-O3A	2.28	1.62	1.59
3	A	5094	ANP	C5-N7	-2.28	1.34	1.39
3	B	5094	ANP	C5-N7	-2.20	1.35	1.39
2	A	5093	ATP	C8-N7	2.08	1.35	1.31

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5094	ANP	C5-C4-N3	-5.92	118.57	126.72
3	B	5094	ANP	C5-C4-N3	-5.85	118.66	126.72
2	A	5093	ATP	C5-C4-N3	-5.66	118.92	126.72
2	B	5093	ATP	C5-C4-N3	-5.61	118.99	126.72
2	A	5093	ATP	N3-C4-N9	4.63	135.05	127.17
3	B	5094	ANP	N3-C4-N9	4.63	135.04	127.17
2	B	5093	ATP	N3-C4-N9	4.53	134.87	127.17
3	A	5094	ANP	N3-C4-N9	4.49	134.80	127.17
3	A	5094	ANP	C2-N3-C4	3.72	120.91	111.83
3	B	5094	ANP	C2-N3-C4	3.70	120.86	111.83
2	A	5093	ATP	C2-N3-C4	3.63	120.70	111.83
3	A	5094	ANP	C4-C5-N7	-3.61	106.46	110.58
2	B	5093	ATP	C2-N3-C4	3.56	120.53	111.83
3	B	5094	ANP	C4-C5-N7	-3.51	106.57	110.58
2	B	5093	ATP	C4-C5-N7	-3.48	106.60	110.58
2	A	5093	ATP	C4-C5-N7	-3.43	106.66	110.58
3	A	5094	ANP	N3-C2-N1	-3.41	123.42	128.58
3	B	5094	ANP	N3-C2-N1	-3.19	123.75	128.58
2	A	5093	ATP	N3-C2-N1	-3.18	123.77	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5093	ATP	N3-C2-N1	-3.10	123.89	128.58
2	A	5093	ATP	C3'-C2'-C1'	2.91	106.96	101.46
2	B	5093	ATP	C4-N9-C8	2.80	108.68	105.74
2	B	5093	ATP	C5-N7-C8	2.74	107.76	103.45
2	B	5093	ATP	C3'-C2'-C1'	2.74	106.65	101.46
3	A	5094	ANP	C2'-C3'-C4'	2.74	107.90	102.61
2	A	5093	ATP	C5-N7-C8	2.66	107.63	103.45
2	A	5093	ATP	C4-N9-C8	2.63	108.50	105.74
3	B	5094	ANP	C4-N9-C8	2.62	108.49	105.74
3	B	5094	ANP	C3'-C2'-C1'	2.57	106.32	101.46
3	B	5094	ANP	C5-N7-C8	2.55	107.47	103.45
3	A	5094	ANP	C5-N7-C8	2.49	107.37	103.45
3	A	5094	ANP	C4-N9-C8	2.42	108.28	105.74
2	B	5093	ATP	C6-C5-N7	2.22	136.37	132.09
2	B	5093	ATP	N9-C8-N7	-2.20	110.82	113.94
2	A	5093	ATP	C6-C5-N7	2.19	136.31	132.09
3	A	5094	ANP	O2A-PA-O1A	2.18	122.58	112.44
3	B	5094	ANP	C6-C5-N7	2.09	136.13	132.09
3	A	5094	ANP	O3G-PG-O1G	-2.08	108.23	113.45
3	A	5094	ANP	C6-C5-N7	2.06	136.06	132.09

There are no chirality outliers.

All (24) torsion outliers are listed below:

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

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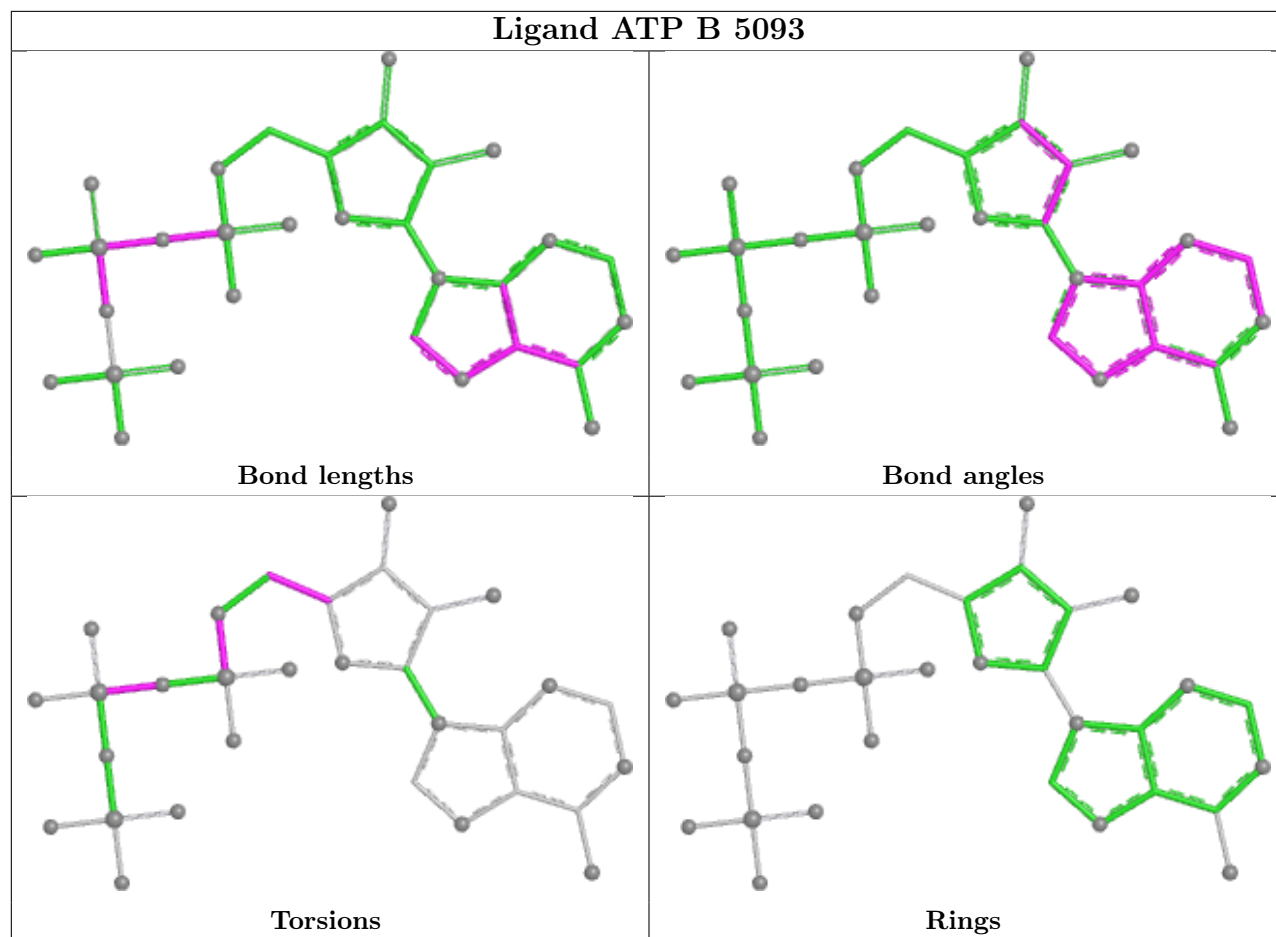
Mol	Chain	Res	Type	Atoms
2	B	5093	ATP	C5'-O5'-PA-O3A
3	A	5094	ANP	C5'-O5'-PA-O1A
3	A	5094	ANP	O4'-C4'-C5'-O5'
3	A	5094	ANP	PB-O3A-PA-O2A
2	A	5093	ATP	PA-O3A-PB-O1B
2	B	5093	ATP	PA-O3A-PB-O2B
2	A	5093	ATP	PA-O3A-PB-O2B

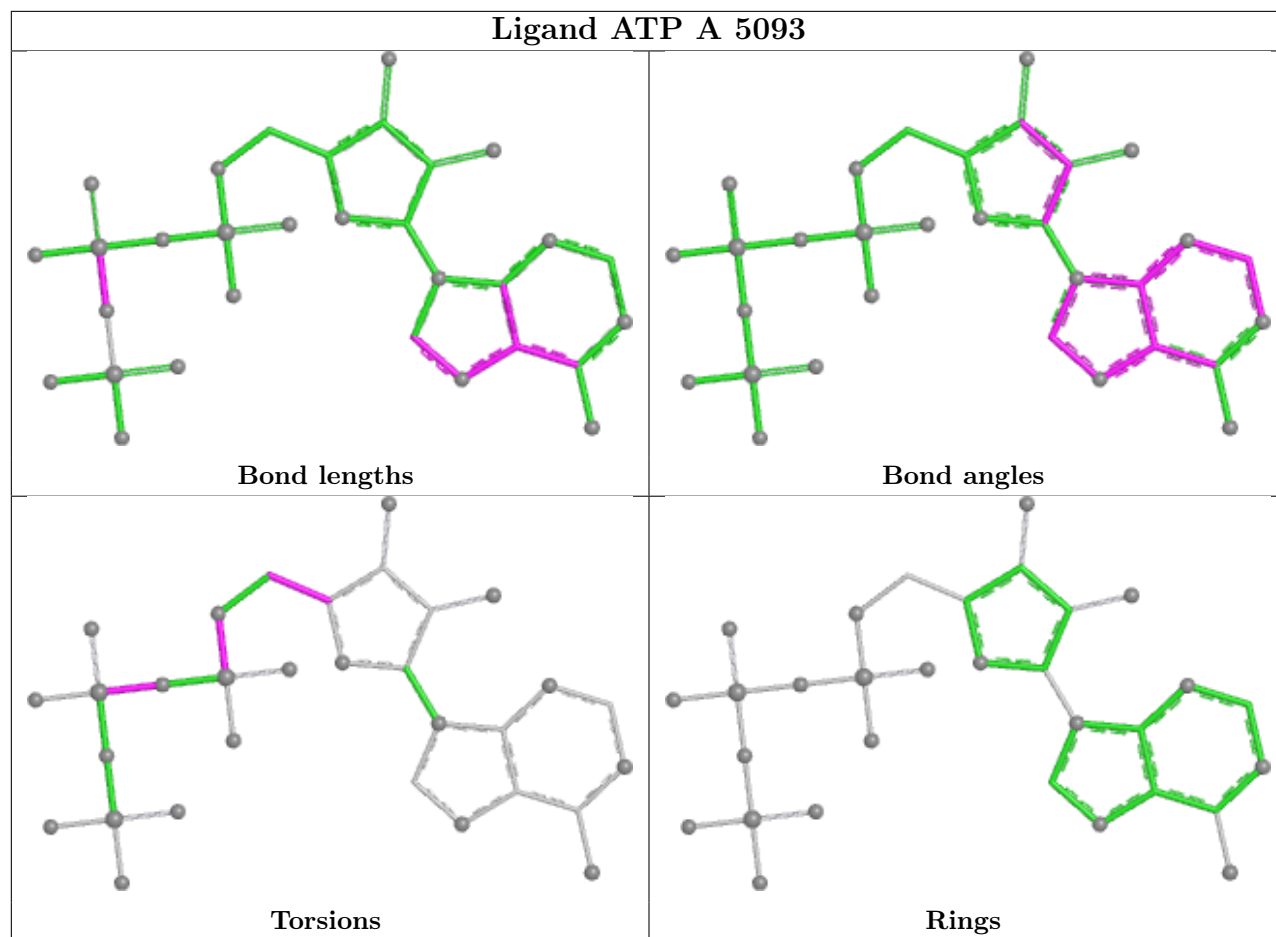
There are no ring outliers.

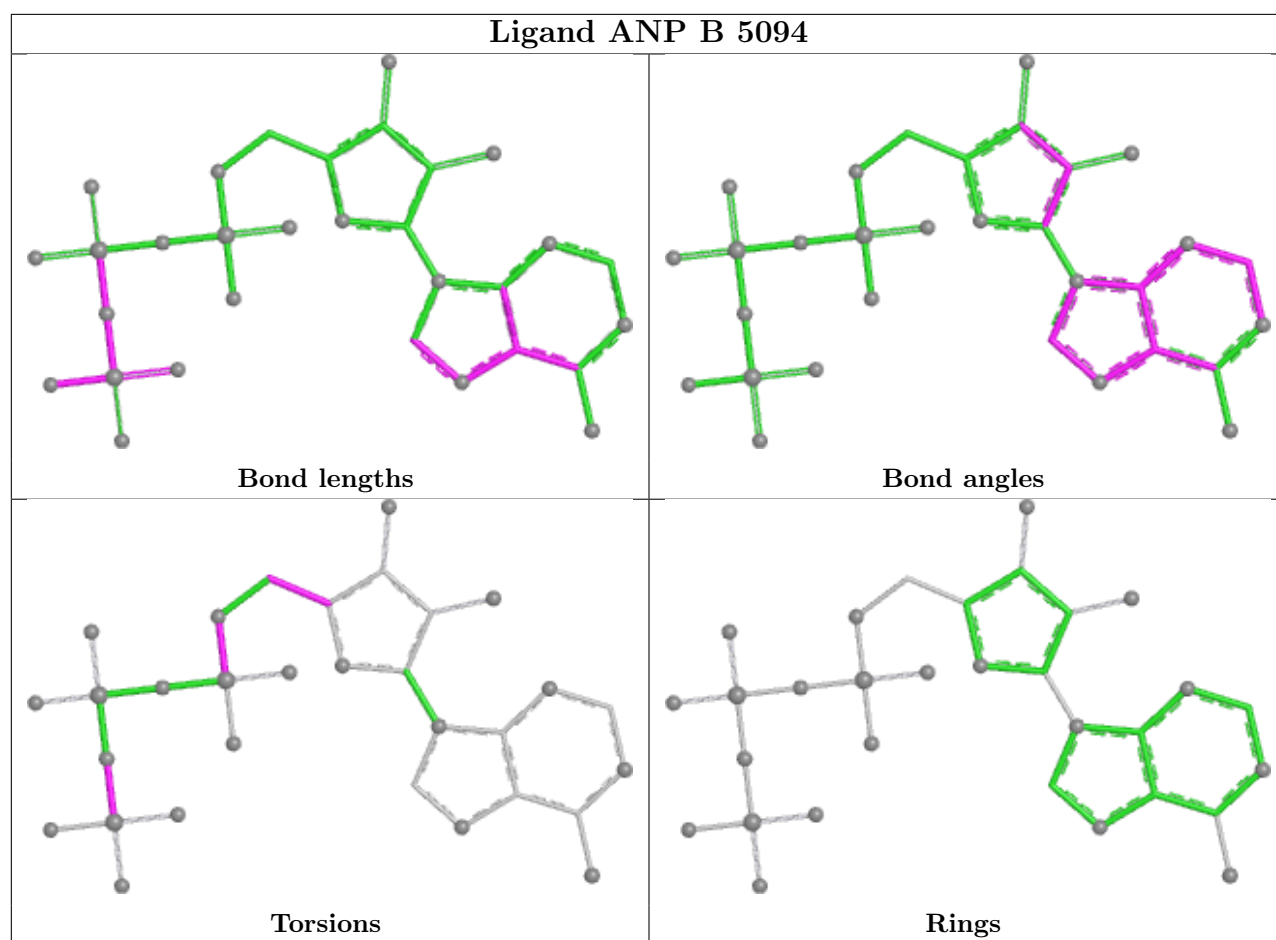
6 monomers are involved in 46 short contacts:

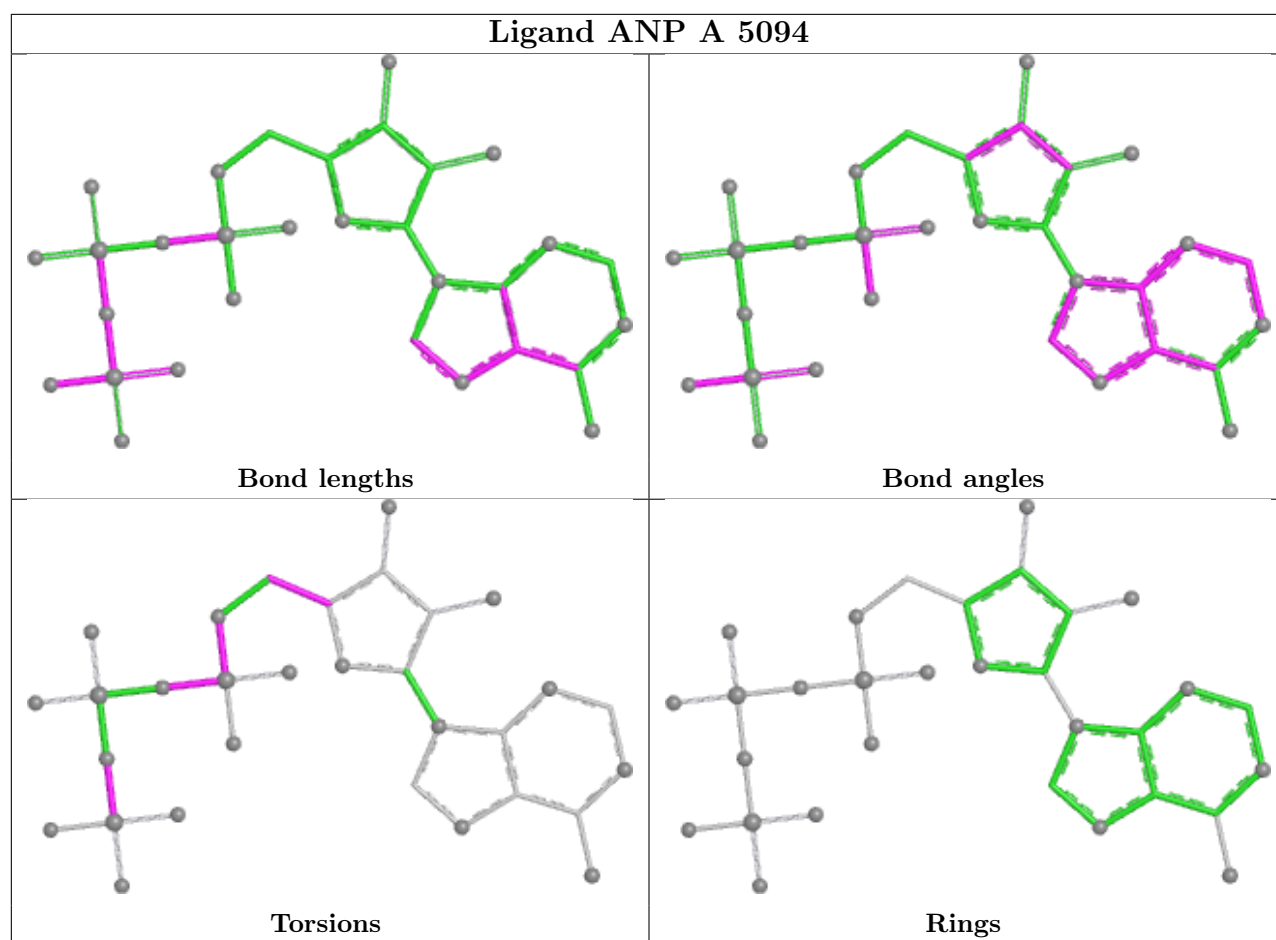
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5093	ATP	17	0
2	A	5093	ATP	8	0
3	B	5094	ANP	8	0
4	B	5096	SO4	3	0
3	A	5094	ANP	7	0
4	A	5095	SO4	3	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	2650/2695 (98%)	-0.44	9 (0%)	90 75	69, 151, 281, 423	0
1	B	2650/2695 (98%)	-0.33	13 (0%)	87 66	92, 193, 357, 500	0
All	All	5300/5390 (98%)	-0.38	22 (0%)	88 70	69, 172, 321, 500	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1483	TYR	4.9
1	B	157	ALA	4.5
1	A	105	VAL	3.8
1	A	3895	PHE	3.1
1	B	165	ASP	2.9
1	B	1683	LEU	2.7
1	B	160	VAL	2.7
1	A	2106	THR	2.7
1	A	151	ASP	2.6
1	B	148	THR	2.6
1	B	1458	ILE	2.6
1	A	2105	ASP	2.6
1	B	151	ASP	2.6
1	B	118	LYS	2.4
1	B	2428	MET	2.3
1	B	19	LEU	2.2
1	B	3393	ASN	2.1
1	A	2623	THR	2.1
1	B	3437	VAL	2.1
1	A	1445	TRP	2.1
1	A	1442	GLN	2.1
1	B	2179	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

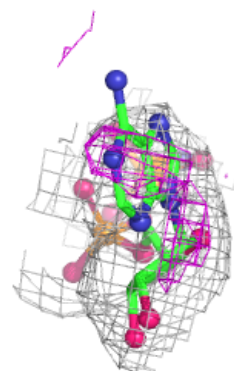
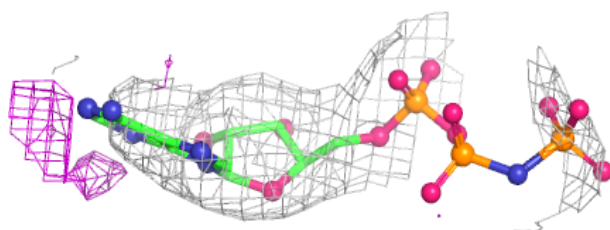
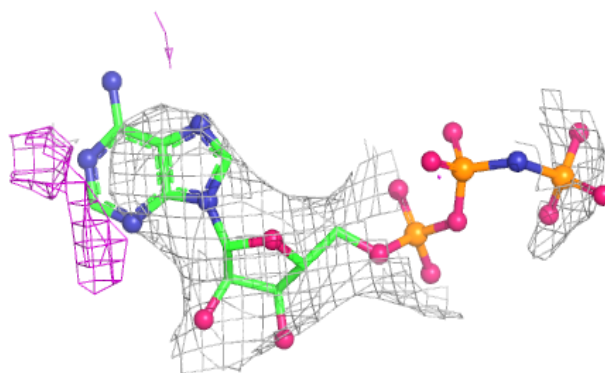
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	5095	5/5	0.90	0.06	152,154,166,167	0
3	ANP	B	5094	31/31	0.94	0.09	112,145,237,257	0
2	ATP	B	5093	31/31	0.94	0.08	99,141,184,200	0
4	SO4	B	5096	5/5	0.95	0.06	155,168,174,176	0
3	ANP	A	5094	31/31	0.96	0.09	111,140,238,248	0
2	ATP	A	5093	31/31	0.97	0.09	88,123,185,204	0
4	SO4	A	5095	5/5	0.97	0.04	84,98,104,105	0
4	SO4	A	5096	5/5	0.98	0.04	115,130,143,145	0
5	MG	A	5097	1/1	0.98	0.04	62,62,62,62	0
5	MG	B	5097	1/1	0.99	0.07	66,66,66,66	0

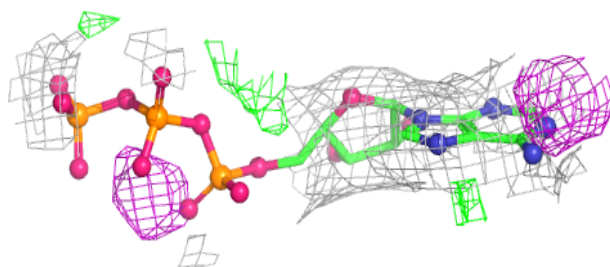
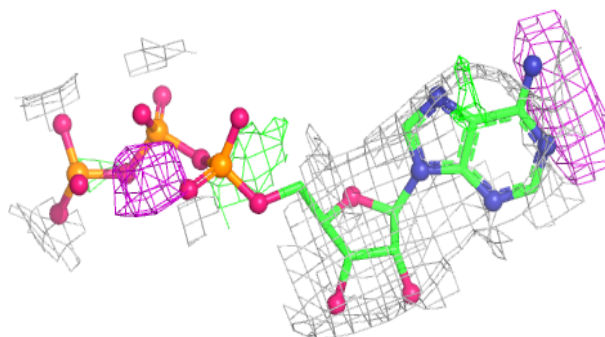
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP B 5094:

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

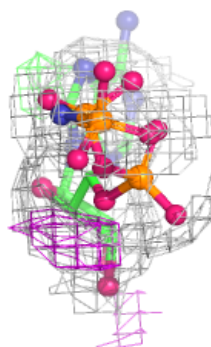
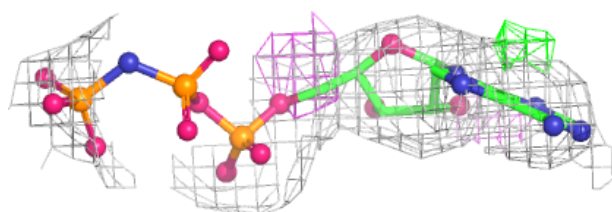
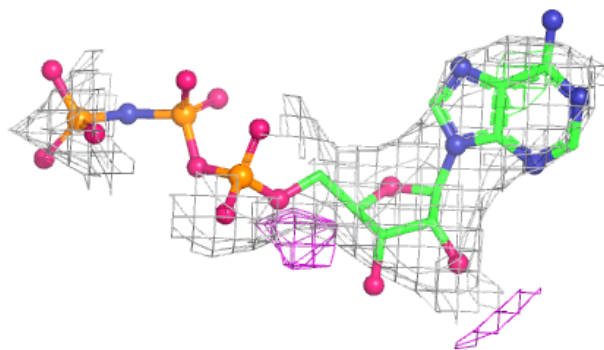
**Electron density around ATP B 5093:**

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

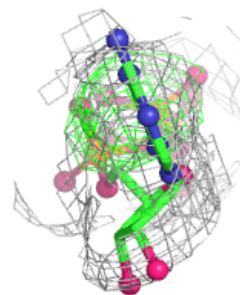
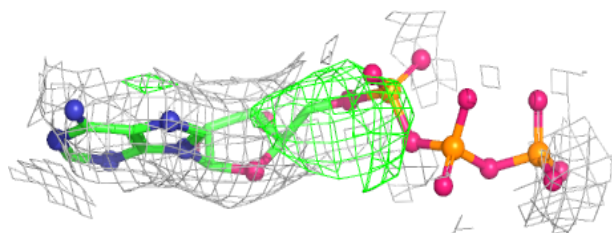
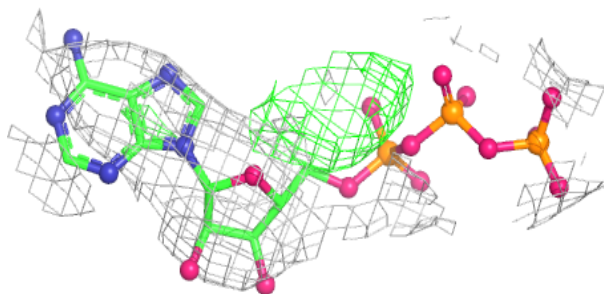


Electron density around ANP A 5094:

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

**Electron density around ATP A 5093:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.