



## Full wwPDB EM Validation Report ⓘ

Apr 24, 2025 – 01:37 PM EDT

PDB ID : 9BLY / pdb\_00009bly  
EMDB ID : EMD-44681  
Title : Composite structure of full-length human dynein-1 in phi-particle conformation  
Authors : Chai, P.; Zhang, K.  
Deposited on : 2024-05-02  
Resolution : 3.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42



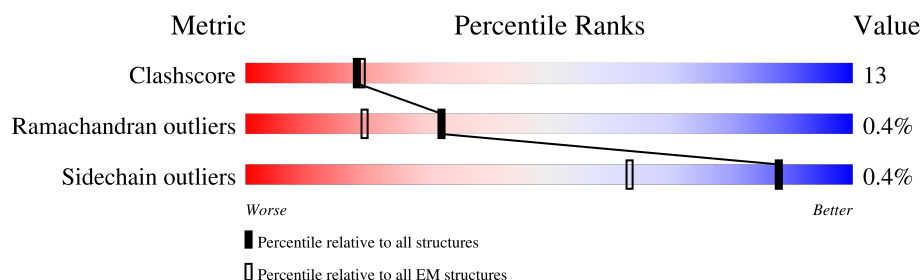
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*




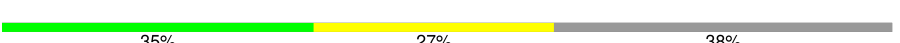

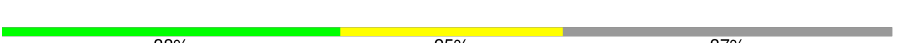



The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415




The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	4646	 79% 18% .
1	B	4646	 73% 24% . .
2	C	638	 57% 5% 38%
2	D	638	 35% 27% 38%
3	E	492	 61% . 37%
3	F	492	 38% 25% 37%
4	G	96	 52% 44% . .
4	H	96	 51% 46% .
5	I	89	 69% 31%

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Mol	Chain	Length	Quality of chain
5	J	89	 53% 44% ..
6	K	113	 84% 16%
6	L	113	 85% 15%



## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 89391 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4542	Total	C	N	O	S	0	0
			36692	23323	6381	6822	166		
1	B	4521	Total	C	N	O	S	0	0
			36527	23221	6349	6791	166		

- Molecule 2 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	394	Total	C	N	O	S	0	0
			3112	1962	541	594	15		
2	D	394	Total	C	N	O	S	0	0
			3112	1962	541	594	15		

- Molecule 3 is a protein called Cytoplasmic dynein 1 light intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	311	Total	C	N	O	S	0	0
			2518	1614	425	468	11		
3	F	311	Total	C	N	O	S	0	0
			2518	1614	425	468	11		

- Molecule 4 is a protein called Dynein light chain roadblock-type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	93	Total	C	N	O	S	0	0
			742	468	128	143	3		
4	H	93	Total	C	N	O	S	0	0
			742	468	128	143	3		

- Molecule 5 is a protein called Dynein light chain 1, cytoplasmic.

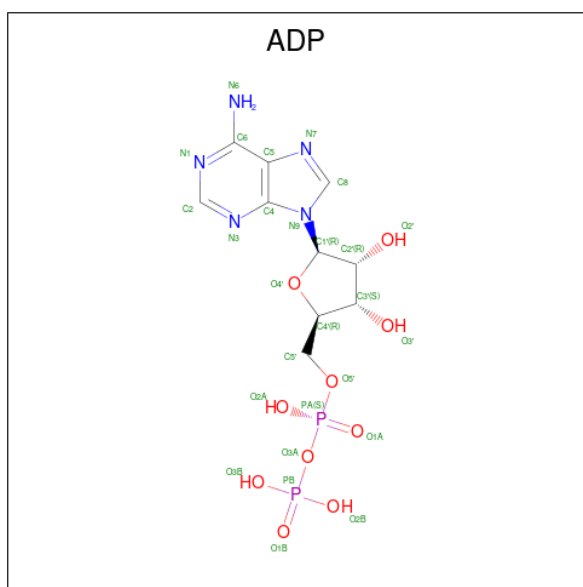


Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
5	J	89	Total	C	N	O	S	0	0
			728	465	122	135	6		

- Molecule 6 is a protein called Dynein light chain Tctex-type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	113	Total	C	N	O	S	0	0
			872	548	142	175	7		
6	L	113	Total	C	N	O	S	0	0
			872	548	142	175	7		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



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

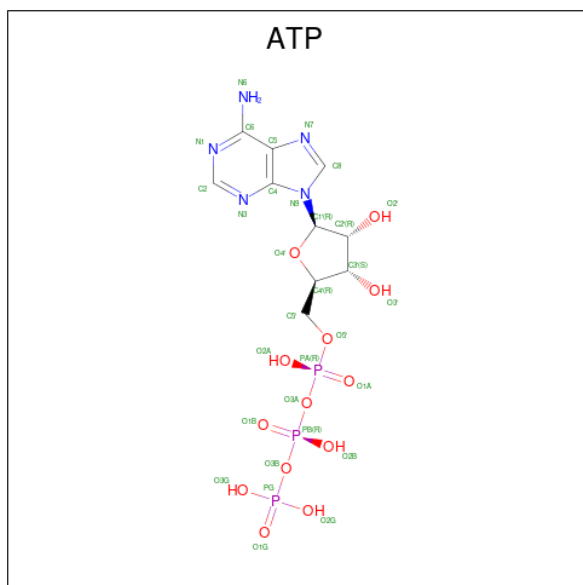
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Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).

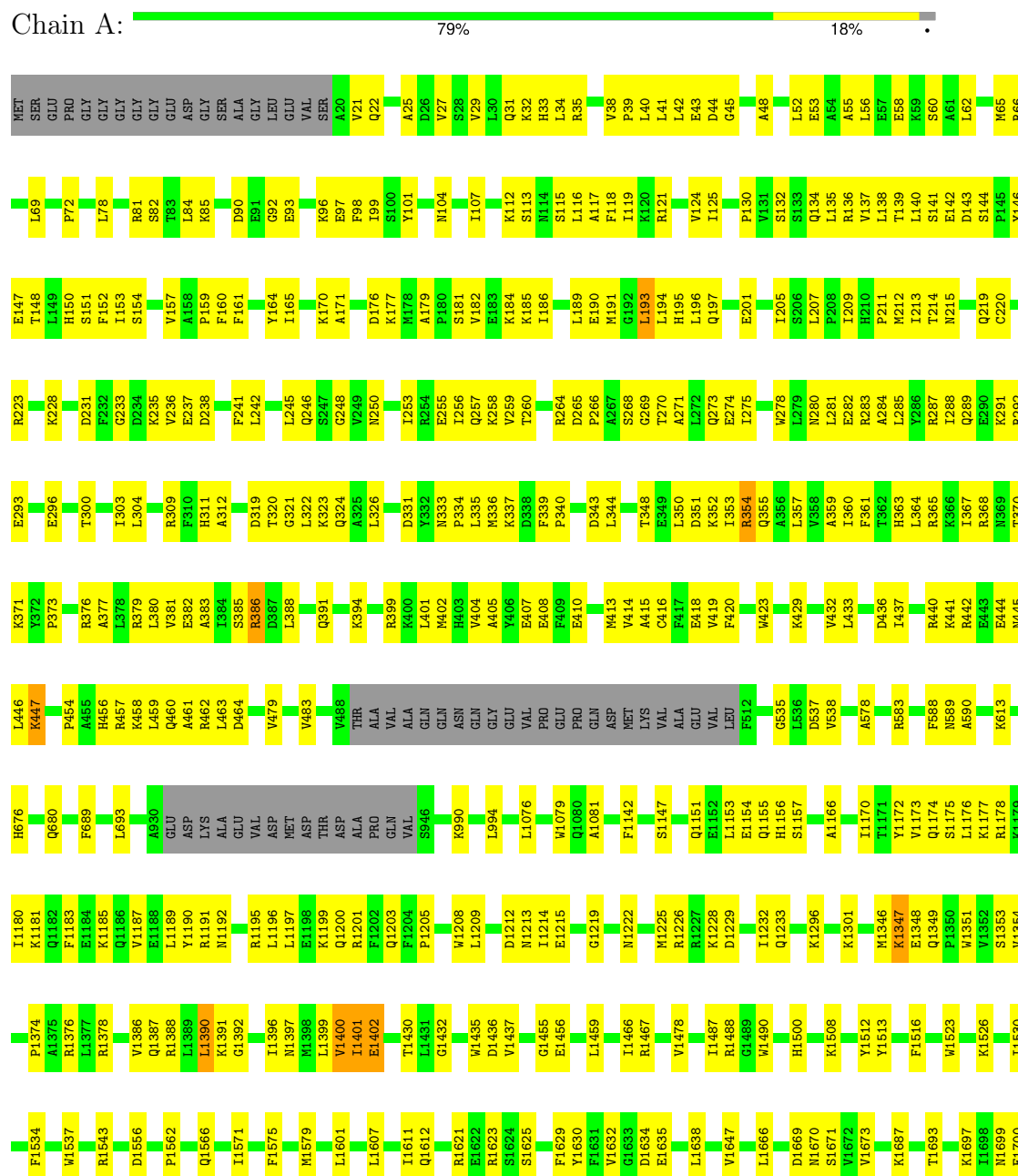




### 3 Residue-property plots

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. 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. 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: Cytoplasmic dynein 1 heavy chain 1









Chain B:  73% 24% ..



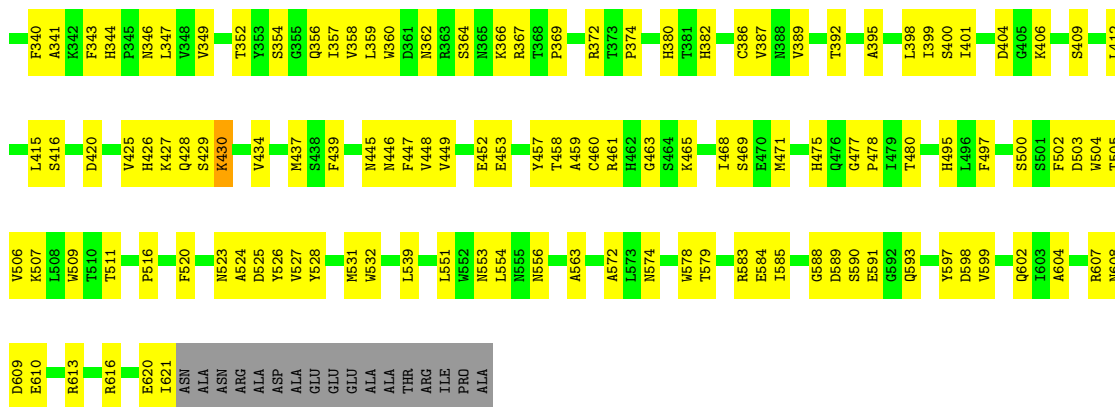


L3750	R3579	A3385	T3153		V2562	V2731	V2562	ARG	D2163	R1983		I1630	F1921	D1159	W1079
N3754	L3580	C3389	L3154	T2961	A2563	F2732	A2563	ARG	V2164	E1984	V1724	F1534	N1222	T1160	L1082
L3761	R3581	G3390	R3160	R2963	A2564	Y2738	V2567	LYS	F2165	H1985	Y1738		D1223	A1161	
I3767	F3583	P3391	K3163	Y2967	D2573	F2751	E2174	LYS	E2175	T1998	K1744	W1537	M1225	T1163	Q1085
	R3585	P3393	T3172	D2973	D2573	K2755	M2175	ASP	T2176	Q2005	Y1745	R1643	R1227	R1087	
E3776	L3588	K3394	H3175	E2974	R2576	L2756	L2756	GLY	R2179		V1751	D1556	K1228	A1166	K1088
A3777	A3396	D2975	R2757	R2757	L2581	R2757	R2757	GLY	D2195	T2017	S1753	I1571	A1231	V1167	A1089
V3790	A3398	V2979	E2775	E2775	Y2582	F2776	Y2582	GLU	D2196		M1761	F1575	Q1234	R1090	
L3829	M2994	M2994	F2784	F2784	P2580		P2580	ALA	Y2211	S2026			Q1234	F1093	
I3835	T2998	N2998			L2591		L2591	ALA	T2214	R2027			I1232	T1171	D1094
Y3836	N2998	N2998			V2592		V2592	L2413	T2214	L2032			E1305	Y1172	N1095
E3624	D3001	D3001			L2593		L2593	L2422	M2221	R2037	L1792	L1601	L1306	V1173	A1096
V3839	S3002	S3002			P2596		P2596	V2433	G2224	S2038	M1832	L1607	R1318	K1177	F1102
D3862	R3220	R3220			T2604		T2604	V2433	P2225	L2039	A1834	K1610	E1348	R1178	G1103
L3863	L3229	L3229			L2612		L2612	L2437	S2226	Q2047	I1611	Q1349	Q1349	P1104	V1105
V3866	K3232	K3232			L2612		L2612	L2437	K2230	Q2047	V1853	Q1612	M1394	K1181	V1106
N3869	A3236	A3236			L2620		L2620	L2443	L2279	F2059	Q1856	R1621	K1395	I1107	
R3870	N3237	N3237			N2621		N2621	H2445	L2279	R2060	Q1856	E1622	K1395	Q1185	
R3873	D3238	D3238			E2629		E2629	L2445	S2290	T2061	Q1860	R1623	M1398	K1189	
H3880	K3239	K3239			L2631		L2631	L2449	E2284	T2069	K1865	S1625	S1624	E1189	
	E3652	E3652			L2631		L2631	L2450	L2295	P2071	K1865	S1625	V1400	Y1190	
	K3241	K3241			L2633		L2633	L2451	L2295	P2071	K1878	V1632	I1401	D1121	
	K3242	K3242			K2633		K2633	L2451	D2308	Q2079	L1879	V1632	E1402	R1191	
	N3243	N3243			Y2638		Y2638	R2453	D2308	L2080	R1887	V1632	T1430	N1192	H1124
	Q3247	Q3247			L2659		L2659	S2457	M2316	Q2079	R1887	V1632	T1430	G1193	K1125
	S3257	S3257			L2659		L2659	S2457	S2317	R2091	A1895	E1635	L1431	Q1194	K1126
	I3260	I3260			D2664		D2664	M2461	V2318	K2104	A1895	L1638	G1455	R1195	V1127
	Q3263	Q3263			E2665		E2665	Q2471	L2319	R2107	R1899	V1647	E1456	L1128	G1127
	E3291	E3291			L2668		L2668	Q2471	R2332	P2132	A1908	L1666	T1466	S1129	K1130
	A3292	A3292			M2666		M2666	R2487	F2343	E2133	E1914	L1666	R1467	K1197	F1131
	L3319	L3319			H2669		H2669	E2487	Q2346	Q2134	E1914	L1666	R1467	L197	K1198
	N3370	N3370			M2669		M2669	R2488	Q2346	E2135	V1929	D1669	T1487	Q1200	G1132
	S3373	S3373			V2667		V2667	Q2491	L2383	L2136	F1930	N1670	I1487	F1203	
	S3376	S3376			H2689		H2689	R2492	L2383	L2137	M1931	S1671	W1490	P1205	N1138
	Y3377	Y3377			R2694		R2694	I2498	C2359	Q2139	D1937	V1673	H1500	P1206	M1139
	R3378	R3378			D2697		D2697	D2505	F2364	T2144	D1958	K1687	K1508	S1207	W1208
	E3379	E3379			Q2698		Q2698	E2513	P2386	M2145	E1959	T1693	K1508	E1141	F1142
	R3380	R3380			A2711		A2711	D2536	E2389	L2149	R1962	K1697	Y1512	I1210	H1143
	A3381	A3381			C2712		C2712	D2536	GLY	L2156	E1965	K1697	Y1513	I1211	S1144
	E3382	E3382			R2720		R2720	D2538	GLU	L2157	R1965	N1699	F1516	D1212	Q1145
	I3381	I3381			R2720		R2720	W2548	ASP	L2160	E1965	E1700	F1516	R1213	G1216
	N3382	N3382			R2729		R2729	W2548	GLU	L2161	E1965	E1700	F1516	E1215	G1216
	R3384	R3384			H2730		H2730	V2557	ALA	L2161	E1965	E1700	F1516	E1217	W1523
								V2557	ARG	S2162	E1980	V1721	K1526	G1219	H1156
														A1220	

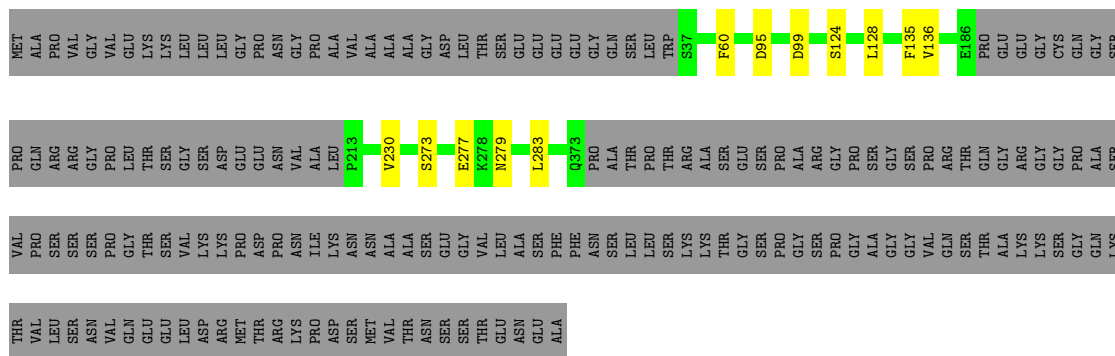




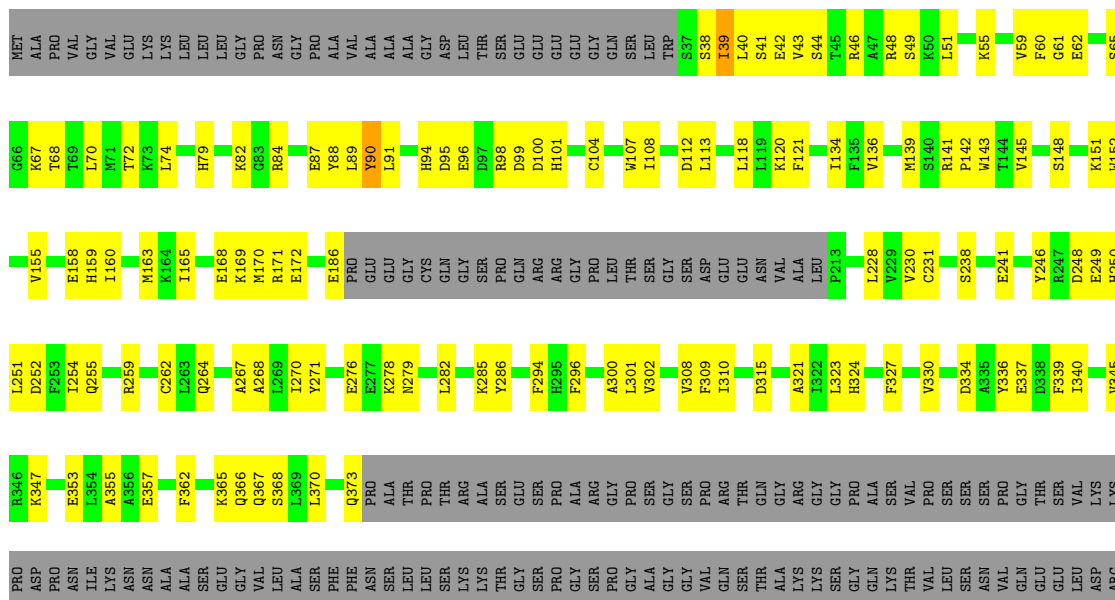




- Molecule 3: Cytoplasmic dynein 1 light intermediate chain 2



- Molecule 3: Cytoplasmic dynein 1 light intermediate chain 2





MET  
THR  
ARG  
LYS  
PRO  
ASP  
SER  
MET  
VAL  
THR  
ASN  
SER  
THR  
GLU  
ASN  
GLU  
ALA

• Molecule 4: Dynein light chain roadblock-type 1

Chain G:  52% 44% . .

MET ALA E3 E6 K9 R10 K14 K15 I20 I21 V22 V23 R24 T25 P29 I30 K31 S32 T33 A43 S44 L45 M46 H47 S48 F49 I50 L51 K52 A53 B54 V57 N64 D65 L66 T67 F68 L69 R70 I71 R72 S73 K74 K75 N76 E77 I78 M79 V80 A81 F87

L88 I89 Q92 N93 P94 T95 GLU

• Molecule 4: Dynein light chain roadblock-type 1

Chain H:  51% 46% .

MET ALA E3 T7 L8 K9 R10 L11 K15 G16 V17 Q18 T21 V22 V23 R24 T25 E26 K31 P37 Q41 Y42 M46 F49 I50 L51 K52 T56 Q63 N64 D65 L66 L69 R70 I71 R72 S73 K74 K75 N76 M79 V80 A81 P82 D83 R84 F87

L88 I89 V90 I91 Q92 N93 P94 T95 GLU

• Molecule 5: Dynein light chain 1, cytoplasmic

Chain I:  69% 31%

H1 I8 M13 S14 M17 Q18 D20 I33 K43 D47 P52 T53 F54 H55 C56 I57 V58 F62 G63 S64 Y65 V66 T67 H68 K71 H72 F73 Y77 A82 I83 L84 S88 G89


• Molecule 5: Dynein light chain 1, cytoplasmic

Chain J:  53% 44% . .

H1 K5 A6 V7 I8 K9 D12 Q18 V22 Y32 N33 I34 E35 K36 D37 I38 A39 A40 K43 D47 Y50 N51 P52 T53 W54 H55 C56 I57 V58 F62 V66 T67 H68 E69 T70 K71 H72 F73 I74 Y75 F76 Y77 L78 A82 I83 L84 L85 F86 K87


S88 G89

• Molecule 6: Dynein light chain Tctex-type 1

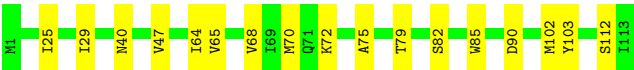
Chain K:  84% 16%

H1 I25 I29 Q35 W42 T43 V47 F61 R62 Y63 V68 I69 N73 L77 H78 T79 M102 L111 S112 I113

• Molecule 6: Dynein light chain Tctex-type 1

Chain L:  85% 15%







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57816	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor



## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.32	0/37420	0.54	5/50628 (0.0%)
1	B	0.32	0/37249	0.54	5/50395 (0.0%)
2	C	0.41	1/3195 (0.0%)	0.54	0/4351
2	D	0.36	0/3195	0.54	0/4351
3	E	0.36	0/2573	0.50	0/3473
3	F	0.36	0/2573	0.52	0/3473
4	G	0.27	0/752	0.51	0/1017
4	H	0.28	0/752	0.56	0/1017
5	I	0.24	0/744	0.49	0/997
5	J	0.36	0/744	0.54	0/997
6	K	0.25	0/888	0.45	0/1203
6	L	0.25	0/888	0.46	0/1203
All	All	0.33	1/90973 (0.0%)	0.54	10/123105 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	6
3	F	0	1
All	All	0	14

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	509	TRP	CB-CG	-5.56	1.40	1.50

All (10) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3242	LYS	O-C-N	-7.56	110.61	122.70
1	A	3242	LYS	O-C-N	-7.55	110.62	122.70
1	B	3402	TYR	CB-CG-CD2	-6.24	117.25	121.00
1	A	3402	TYR	CB-CG-CD2	-6.24	117.26	121.00
1	B	178	MET	CA-CB-CG	5.46	122.59	113.30
1	A	1669	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	1669	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	193	LEU	CA-CB-CG	5.22	127.30	115.30
1	B	2308	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	2308	ASP	CB-CG-OD1	5.10	122.89	118.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1076	LEU	Peptide
1	A	1388	ARG	Sidechain
1	A	2453	ARG	Sidechain
1	A	2729	ARG	Sidechain
1	A	3242	LYS	Mainchain
1	A	3402	TYR	Sidechain
1	A	4195	ARG	Sidechain
1	B	2453	ARG	Sidechain
1	B	2729	ARG	Sidechain
1	B	3242	LYS	Mainchain
1	B	3402	TYR	Sidechain
1	B	4195	ARG	Sidechain
1	B	639	ARG	Sidechain
3	F	90	TYR	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	36692	0	36960	722	0
1	B	36527	0	36807	1027	0
2	C	3112	0	2964	20	0
2	D	3112	0	2964	148	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	2518	0	2525	6	0
3	F	2518	0	2525	113	0
4	G	742	0	768	47	0
4	H	742	0	768	42	0
5	I	728	0	714	28	0
5	J	728	0	714	54	0
6	K	872	0	846	17	0
6	L	872	0	846	17	0
7	A	81	0	36	3	0
7	B	81	0	36	3	0
8	A	31	0	12	3	0
8	B	31	0	12	3	0
9	A	2	0	0	0	0
9	B	2	0	0	0	0
All	All	89391	0	89497	2081	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 13.

All (2081) 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:B:3381:ILE:CG2	1:B:3390:GLY:HA2	1.30	1.58
1:A:3381:ILE:CG2	1:A:3390:GLY:HA2	1.30	1.57
1:B:3381:ILE:CG2	1:B:3390:GLY:CA	1.94	1.46
1:A:3381:ILE:HG21	1:A:3390:GLY:CA	1.49	1.42
1:A:3381:ILE:CG2	1:A:3390:GLY:CA	1.94	1.41
1:B:3381:ILE:HG21	1:B:3390:GLY:CA	1.49	1.38
1:A:3381:ILE:CD1	1:A:3393:VAL:HG21	1.59	1.32
1:B:3381:ILE:CD1	1:B:3393:VAL:HG21	1.59	1.32
1:A:3455:ILE:CD1	1:B:3455:ILE:HD11	1.65	1.26
1:A:3455:ILE:HD11	1:B:3455:ILE:CD1	1.65	1.26
1:A:3381:ILE:HG23	1:A:3390:GLY:CA	1.72	1.17
1:B:3381:ILE:HG23	1:B:3390:GLY:CA	1.72	1.09
1:A:3381:ILE:HD11	1:A:3393:VAL:CG2	1.85	1.05
1:B:3381:ILE:HD11	1:B:3393:VAL:CG2	1.85	1.05
1:B:1209:LEU:HG	1:B:1214:ILE:HG23	1.40	1.04
1:B:1212:ASP:HA	1:B:1215:GLU:HB2	1.34	1.03
1:B:1214:ILE:O	1:B:1217:GLU:HG2	1.64	0.97
1:A:3380:GLU:HA	1:A:3383:ASN:HD22	1.27	0.96
1:A:3381:ILE:CG2	1:A:3390:GLY:HA3	1.95	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3380:GLU:HA	1:B:3383:ASN:HD22	1.27	0.96
1:B:1348:GLU:O	1:B:1430:THR:HA	1.67	0.95
1:B:3381:ILE:CG2	1:B:3390:GLY:HA3	1.95	0.94
5:J:8:ILE:HG22	5:J:74:ILE:HD11	1.47	0.94
1:A:3459:GLN:NE2	1:B:3456:SER:OG	2.01	0.92
1:A:402:MET:HA	1:A:535:GLY:HA3	1.50	0.91
1:A:3381:ILE:HD11	1:A:3393:VAL:HG21	0.92	0.91
1:A:3456:SER:OG	1:B:3459:GLN:NE2	2.03	0.91
1:B:3381:ILE:HD11	1:B:3393:VAL:HG21	0.92	0.89
1:B:3381:ILE:CG1	1:B:3393:VAL:HG11	2.01	0.89
1:A:3381:ILE:CG1	1:A:3393:VAL:HG11	2.01	0.89
1:B:3381:ILE:HG23	1:B:3390:GLY:N	1.88	0.88
1:A:3381:ILE:HG23	1:A:3390:GLY:N	1.88	0.87
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.55	0.87
1:B:2221:MET:HG2	1:B:2343:PHE:HB2	1.55	0.87
1:A:3459:GLN:CD	1:B:3456:SER:OG	2.14	0.86
1:A:182:VAL:HA	1:A:185:LYS:HG2	1.56	0.86
1:A:115:SER:H	1:A:140:LEU:HB3	1.41	0.86
1:A:3456:SER:OG	1:B:3459:GLN:CD	2.15	0.85
1:A:3455:ILE:HD11	1:B:3455:ILE:HD11	0.90	0.85
1:A:193:LEU:HD13	1:B:182:VAL:HG11	1.57	0.84
5:J:6:ALA:HB2	5:J:78:LEU:HD21	1.57	0.84
1:B:4271:ARG:HD3	1:B:4633:ARG:HH12	1.43	0.84
1:B:530:VAL:HG12	1:B:549:ALA:HB1	1.60	0.84
1:B:162:LYS:HG2	1:B:166:ARG:HE	1.41	0.83
1:B:3381:ILE:CD1	1:B:3393:VAL:CG2	2.52	0.83
1:A:2629:GLU:OE2	1:A:2633:LYS:NZ	2.12	0.83
1:A:1400:VAL:O	1:A:1402:GLU:N	2.11	0.83
3:F:72:THR:HG21	3:F:79:HIS:HA	1.60	0.82
1:A:4271:ARG:HD3	1:A:4633:ARG:HH12	1.43	0.82
1:B:2629:GLU:OE2	1:B:2633:LYS:NZ	2.12	0.82
1:B:1212:ASP:HA	1:B:1215:GLU:CB	2.09	0.82
1:B:516:ASP:HA	1:B:563:ARG:HH12	1.45	0.82
1:B:1203:GLN:HA	5:J:5:LYS:HZ1	1.44	0.81
1:B:3381:ILE:HG13	1:B:3393:VAL:HG11	1.63	0.80
1:B:483:VAL:O	1:B:567:ARG:NH1	2.14	0.80
1:B:3238:ASP:HA	1:B:3241:LYS:HD2	1.63	0.80
1:A:3238:ASP:HA	1:A:3241:LYS:HD2	1.64	0.80
1:A:81:ARG:HD3	1:A:99:ILE:HG13	1.64	0.80
1:B:264:ARG:HD3	1:B:274:GLU:HG2	1.64	0.79
1:B:1399:LEU:O	1:B:1401:ILE:N	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3239:LYS:HB3	1:B:3451:TYR:CZ	2.18	0.79
1:B:3398:ALA:O	1:B:3400:LEU:N	2.14	0.79
4:G:54:ARG:HH12	4:G:65:ASP:HA	1.46	0.79
1:A:3239:LYS:HB3	1:A:3451:TYR:CZ	2.18	0.79
1:A:3381:ILE:HG13	1:A:3393:VAL:HG11	1.63	0.79
1:A:3398:ALA:O	1:A:3400:LEU:N	2.14	0.79
1:B:78:LEU:HD11	1:B:115:SER:HB2	1.65	0.78
1:B:2729:ARG:HD2	1:B:2730:HIS:CE1	2.17	0.78
1:B:1202:PHE:HD2	1:B:1204:PHE:CD2	2.01	0.78
5:J:69:GLU:N	5:J:87:LYS:O	2.14	0.78
1:A:246:GLN:HB2	1:A:309:ARG:HD3	1.64	0.78
1:B:150:HIS:HB2	1:B:193:LEU:HB3	1.66	0.78
1:B:130:PRO:HB2	1:B:133:SER:HB2	1.66	0.78
1:B:399:ARG:NH2	1:B:408:GLU:OE1	2.17	0.78
1:A:2729:ARG:HD2	1:A:2730:HIS:CE1	2.17	0.78
1:B:1212:ASP:CB	1:B:1216:GLY:H	1.97	0.77
1:A:1490:TRP:HH2	1:A:1537:TRP:HD1	1.30	0.77
1:B:1490:TRP:HH2	1:B:1537:TRP:HD1	1.29	0.77
1:B:853:ILE:HG21	1:B:888:LEU:HD21	1.67	0.77
1:A:1571:ILE:HD12	1:A:1611:ILE:HD11	1.67	0.77
1:B:195:HIS:O	1:B:198:GLN:NE2	2.18	0.77
1:A:189:LEU:HG	1:B:189:LEU:HD11	1.67	0.76
1:A:350:LEU:HB3	1:A:419:VAL:HG21	1.67	0.76
1:A:147:GLU:HA	1:A:196:LEU:HD13	1.67	0.76
1:B:1087:ARG:HH21	1:B:1200:GLN:HE22	1.31	0.76
1:B:1210:TYR:HB2	5:J:8:ILE:O	1.84	0.76
1:B:4088:VAL:HG11	1:B:4116:LEU:HD21	1.67	0.76
1:B:365:ARG:NH2	1:B:429:LYS:O	2.18	0.76
1:A:1195:ARG:NH2	3:F:96:GLU:O	2.19	0.76
1:B:1215:GLU:O	1:B:1218:TRP:N	2.19	0.76
2:D:272:PHE:HB2	2:D:593:GLN:HG3	1.68	0.76
1:B:987:PHE:HE2	3:F:87:GLU:HG2	1.49	0.76
1:B:960:HIS:ND1	1:B:978:CYS:SG	2.59	0.76
1:A:2590:PRO:O	1:A:2732:PRO:HD2	1.86	0.75
4:H:79:MET:HB2	4:H:90:VAL:HB	1.66	0.75
1:B:266:PRO:HB3	1:B:376:ARG:HG3	1.69	0.75
2:D:531:MET:HG3	2:D:578:TRP:HD1	1.50	0.75
1:A:113:SER:H	1:A:142:GLU:HG3	1.51	0.75
1:B:1214:ILE:C	1:B:1217:GLU:HG2	2.06	0.75
1:B:1196:LEU:HD23	1:B:1199:LYS:HE2	1.69	0.74
1:B:2590:PRO:O	1:B:2732:PRO:HD2	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3381:ILE:CD1	1:A:3393:VAL:CG2	2.52	0.74
1:B:1214:ILE:HG13	1:B:1215:GLU:H	1.53	0.74
1:B:399:ARG:HH22	1:B:404:VAL:HG11	1.51	0.74
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	1.68	0.74
1:A:4088:VAL:HG11	1:A:4116:LEU:HD21	1.67	0.74
1:B:1349:GLN:C	1:B:1431:LEU:H	1.90	0.74
1:B:2149:LEU:HD11	1:B:2157:LEU:HD13	1.68	0.74
2:D:273:ASP:O	2:D:277:SER:OG	2.06	0.74
1:A:44:ASP:HB2	1:B:130:PRO:HB3	1.68	0.74
1:A:365:ARG:NH2	1:A:429:LYS:O	2.21	0.74
1:B:3381:ILE:HG13	1:B:3393:VAL:CG1	2.18	0.74
1:B:1571:ILE:HD13	1:B:1607:LEU:HB3	1.69	0.73
1:A:2562:VAL:O	1:A:2804:ARG:NH1	2.21	0.73
1:B:386:ARG:NH2	1:B:453:ASN:O	2.21	0.73
1:A:3381:ILE:HG13	1:A:3393:VAL:CG1	2.18	0.73
1:B:2562:VAL:O	1:B:2804:ARG:NH1	2.21	0.73
5:J:68:HIS:HA	5:J:88:SER:HB2	1.71	0.73
1:A:3243:MET:HE3	1:A:3444:ILE:HG23	1.71	0.73
1:B:336:MET:HA	1:B:339:PHE:HE2	1.54	0.73
1:B:669:LEU:HD22	1:B:673:TRP:HB3	1.69	0.73
1:B:1209:LEU:HG	1:B:1214:ILE:CG2	2.16	0.73
1:B:441:LYS:O	1:B:445:ASN:N	2.22	0.73
5:I:57:ILE:HD13	5:J:57:ILE:HD12	1.71	0.73
1:B:530:VAL:N	1:B:553:TYR:OH	2.18	0.72
2:C:445:ASN:O	2:C:461:ARG:N	2.20	0.72
3:F:113:LEU:HD21	3:F:151:LYS:HD2	1.70	0.72
2:D:553:ASN:ND2	2:D:556:ASN:OD1	2.22	0.72
3:F:62:GLU:HG3	3:F:65:SER:HB2	1.71	0.72
1:A:1490:TRP:CH2	1:A:1537:TRP:HD1	2.08	0.72
1:B:4037:PRO:HB2	1:B:4118:PRO:HG2	1.71	0.72
1:A:181:SER:HA	1:A:184:LYS:HD2	1.72	0.72
1:B:869:TYR:HB2	1:B:914:ARG:HH21	1.54	0.72
1:B:1490:TRP:CH2	1:B:1537:TRP:HD1	2.08	0.72
1:B:1348:GLU:O	1:B:1430:THR:CA	2.37	0.71
1:B:170:LYS:NZ	1:B:176:ASP:O	2.23	0.71
1:B:874:PHE:HB3	1:B:996:LEU:HD21	1.72	0.71
1:A:2788:THR:HG22	1:A:2789:GLN:HG2	1.72	0.71
1:B:1399:LEU:O	1:B:1402:GLU:N	2.23	0.71
2:D:358:VAL:HG13	2:D:369:PRO:HB3	1.72	0.71
1:A:2930:GLN:HG3	1:A:3059:ILE:HG23	1.73	0.71
1:A:4190:ILE:HD12	1:A:4201:TRP:HZ2	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:68:HIS:ND1	5:J:69:GLU:O	2.22	0.71
1:B:242:LEU:HB3	1:B:309:ARG:HE	1.54	0.71
1:B:1211:ILE:C	1:B:1213:ASN:N	2.42	0.71
1:B:1170:ILE:O	1:B:1174:GLN:NE2	2.24	0.71
1:B:1173:VAL:HG22	1:B:1177:LYS:HE3	1.71	0.71
1:B:1202:PHE:CE2	1:B:1204:PHE:HA	2.26	0.71
1:B:1212:ASP:HB2	1:B:1216:GLY:H	1.54	0.71
3:F:259:ARG:HH11	3:F:323:LEU:HD22	1.54	0.70
1:A:253:ILE:HD12	1:A:256:ILE:HD11	1.74	0.70
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.71	0.70
1:B:4190:ILE:HD12	1:B:4201:TRP:HZ2	1.56	0.70
1:A:343:ASP:O	1:A:352:LYS:NZ	2.24	0.70
1:A:4549:GLN:HG3	1:A:4587:LEU:HB2	1.73	0.70
1:B:2581:LEU:HD11	1:B:2593:LEU:HD21	1.73	0.70
1:A:93:GLU:HB2	1:A:211:PRO:HB2	1.73	0.70
1:A:266:PRO:HB3	1:A:376:ARG:HG3	1.73	0.70
1:A:201:GLU:HA	1:A:280:ASN:HD21	1.56	0.70
1:B:2930:GLN:HG3	1:B:3059:ILE:HG23	1.72	0.70
1:A:3455:ILE:CG1	1:B:3455:ILE:HD11	2.20	0.70
2:D:332:GLN:OE1	2:D:372:ARG:NH1	2.24	0.70
1:A:207:LEU:HG	1:A:209:ILE:HG12	1.74	0.70
1:A:3455:ILE:HD11	1:B:3455:ILE:CG1	2.22	0.70
1:B:751:ARG:NH2	2:D:452:GLU:OE2	2.24	0.70
1:B:3392:MET:HA	1:B:3395:TRP:HB2	1.74	0.70
1:B:3381:ILE:HG21	1:B:3390:GLY:HA2	0.71	0.70
1:A:3239:LYS:HA	1:A:3242:LYS:HD2	1.74	0.69
1:A:3381:ILE:HG21	1:A:3390:GLY:HA2	0.71	0.69
1:B:251:ARG:NH1	1:B:251:ARG:O	2.25	0.69
1:B:264:ARG:NH1	1:B:265:ASP:O	2.25	0.69
1:B:2788:THR:HG22	1:B:2789:GLN:HG2	1.72	0.69
1:B:354:ARG:NH1	1:B:422:THR:OG1	2.25	0.69
1:B:977:GLU:HA	3:F:90:TYR:OH	1.92	0.69
2:C:188:GLN:O	2:C:192:HIS:ND1	2.24	0.69
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.24	0.69
1:A:3392:MET:HA	1:A:3395:TRP:HB2	1.74	0.69
1:B:2775:GLU:OE1	1:B:2857:HIS:NE2	2.24	0.69
5:I:43:LYS:NZ	5:I:47:ASP:OD2	2.24	0.69
5:J:43:LYS:NZ	5:J:47:ASP:OD2	2.26	0.69
1:B:1214:ILE:HG22	1:B:1217:GLU:OE2	1.92	0.69
1:B:3243:MET:SD	1:B:3451:TYR:HE2	2.16	0.69
1:B:1209:LEU:CG	1:B:1214:ILE:HG23	2.18	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ALA:O	1:A:363:HIS:ND1	2.23	0.69
1:B:3239:LYS:HA	1:B:3242:LYS:HD2	1.74	0.69
4:G:74:LYS:NZ	4:H:65:ASP:OD1	2.25	0.69
5:J:57:ILE:HG22	5:J:84:LEU:HB3	1.73	0.69
1:A:1181:LYS:HG2	1:A:1185:LYS:HZ1	1.58	0.69
1:B:3239:LYS:HB3	1:B:3451:TYR:CE2	2.28	0.69
1:B:4549:GLN:HG3	1:B:4587:LEU:HB2	1.73	0.69
1:B:722:SER:HB3	1:B:731:ASN:HD21	1.58	0.69
1:B:1466:ILE:HG12	1:B:1500:HIS:HD1	1.57	0.69
1:A:119:ILE:HD12	1:B:155:ASN:HB2	1.74	0.68
1:A:2581:LEU:HD11	1:A:2593:LEU:HD21	1.73	0.68
1:A:3381:ILE:HD12	1:A:3393:VAL:HG21	1.72	0.68
1:A:4197:ALA:HB3	1:A:4198:PRO:HD3	1.75	0.68
1:B:266:PRO:HB2	1:B:379:ARG:HB2	1.74	0.68
5:J:18:GLN:HG2	5:J:74:ILE:HD12	1.75	0.68
1:B:582:PHE:CE1	1:B:668:VAL:HG11	2.27	0.68
1:B:1215:GLU:O	1:B:1217:GLU:N	2.26	0.68
1:A:3239:LYS:HB3	1:A:3451:TYR:CE2	2.28	0.68
1:A:3243:MET:SD	1:A:3451:TYR:HE2	2.16	0.68
1:B:4197:ALA:HB3	1:B:4198:PRO:HD3	1.75	0.68
1:A:458:LYS:O	1:A:461:ALA:HB3	1.93	0.68
1:B:121:ARG:NH1	1:B:133:SER:O	2.25	0.68
1:B:1198:GLU:HA	1:B:1204:PHE:HZ	1.57	0.68
1:B:332:TYR:CE2	1:B:336:MET:HB3	2.29	0.68
2:D:357:ILE:HD11	2:D:380:HIS:HD2	1.58	0.68
1:A:1466:ILE:HG12	1:A:1500:HIS:HD1	1.57	0.68
1:A:3373:SER:HB2	1:A:3377:TYR:CE2	2.29	0.68
1:A:4176:ARG:NH1	1:A:4220:ASP:OD2	2.27	0.68
1:B:813:GLN:NE2	3:F:357:GLU:OE1	2.27	0.68
1:A:3661:LEU:HD12	1:A:3668:ASP:HB2	1.76	0.68
1:B:442:ARG:O	1:B:445:ASN:ND2	2.27	0.68
1:B:639:ARG:HH22	2:D:574:ASN:HD21	1.43	0.68
1:B:1181:LYS:HG2	1:B:1185:LYS:HZ1	1.58	0.67
1:B:1211:ILE:O	1:B:1213:ASN:N	2.27	0.67
2:D:607:ARG:NH1	2:D:610:GLU:OE2	2.28	0.67
4:G:49:PHE:HA	4:G:52:LYS:HG2	1.76	0.67
6:K:79:THR:HG22	6:L:68:VAL:HG22	1.75	0.67
1:B:3373:SER:HB2	1:B:3377:TYR:CE2	2.29	0.67
1:B:264:ARG:O	1:B:376:ARG:NH1	2.27	0.67
1:B:3661:LEU:HD12	1:B:3668:ASP:HB2	1.76	0.67
4:H:80:VAL:HA	4:H:88:LEU:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1126:GLU:OE1	1:B:1130:LYS:NZ	2.26	0.67
1:B:4176:ARG:NH1	1:B:4220:ASP:OD2	2.26	0.67
1:B:717:ILE:HA	1:B:824:TRP:HE3	1.60	0.67
2:C:215:ILE:O	2:D:209:ARG:NH1	2.27	0.67
2:D:315:VAL:HB	2:D:327:TYR:HB2	1.77	0.67
1:B:83:THR:O	1:B:112:LYS:NZ	2.26	0.67
1:B:255:GLU:HA	1:B:258:LYS:HE3	1.76	0.67
1:B:649:ILE:O	1:B:653:GLN:HG2	1.95	0.67
2:D:211:LEU:HG	4:H:15:LYS:HE3	1.77	0.67
1:A:385:SER:HB2	1:A:454:PRO:HB3	1.77	0.67
1:B:3243:MET:HE3	1:B:3444:ILE:HG23	1.76	0.67
1:A:1170:ILE:HD11	1:A:1232:ILE:HG12	1.76	0.66
1:A:3239:LYS:O	1:A:3243:MET:HG2	1.95	0.66
1:A:357:LEU:HD21	1:A:388:LEU:HD21	1.77	0.66
4:G:65:ASP:HB3	4:H:74:LYS:HD3	1.76	0.66
5:I:55:HIS:NE2	5:I:88:SER:O	2.24	0.66
1:B:1218:TRP:O	1:B:1222:ASN:ND2	2.28	0.66
1:B:1085:GLN:HE22	3:F:39:ILE:HD12	1.61	0.66
1:B:3292:ALA:HA	1:B:3395:TRP:CZ2	2.30	0.66
1:A:3239:LYS:HB3	1:A:3451:TYR:CE1	2.30	0.66
1:B:2906:ASP:OD2	1:B:3655:ARG:NH1	2.29	0.66
3:F:120:LYS:HA	3:F:159:HIS:HE1	1.59	0.66
1:A:132:SER:O	1:A:136:ARG:NH2	2.28	0.66
4:G:14:GLN:NE2	4:G:92:GLN:OE1	2.29	0.66
4:H:21:ILE:HG12	4:H:89:ILE:HD11	1.76	0.66
1:B:456:HIS:HA	1:B:459:LEU:HB2	1.77	0.66
1:B:3239:LYS:HB3	1:B:3451:TYR:CE1	2.31	0.66
1:B:3239:LYS:O	1:B:3243:MET:HG2	1.95	0.66
4:G:49:PHE:HB3	4:H:52:LYS:HZ2	1.60	0.66
1:B:1191:ARG:O	1:B:1194:GLN:NE2	2.29	0.66
1:A:460:GLN:HA	1:A:463:LEU:HD12	1.78	0.65
1:B:1214:ILE:O	1:B:1217:GLU:N	2.23	0.65
1:A:2906:ASP:OD2	1:A:3655:ARG:NH1	2.29	0.65
1:B:260:THR:HG23	1:B:261:LYS:HD3	1.77	0.65
1:B:1206:PRO:O	1:B:1208:TRP:N	2.29	0.65
1:A:3292:ALA:HA	1:A:3395:TRP:CZ2	2.30	0.65
1:B:1211:ILE:C	1:B:1213:ASN:H	1.98	0.65
1:B:3383:ASN:O	1:B:3384:ARG:HB3	1.97	0.65
1:B:3638:VAL:HG12	1:B:3681:THR:HB	1.79	0.65
1:A:348:THR:O	1:A:399:ARG:NH2	2.28	0.65
1:B:270:THR:HG23	1:B:273:GLN:H	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:ARG:NH2	1:B:451:ARG:O	2.29	0.65
1:B:581:MET:HG2	1:B:611:ARG:HH21	1.61	0.65
1:B:801:ILE:HD11	1:B:850:LEU:HB3	1.79	0.65
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.79	0.65
1:B:961:GLU:OE2	1:B:963:ARG:NH2	2.30	0.65
1:A:270:THR:HG23	1:A:273:GLN:H	1.62	0.65
1:B:4097:LYS:HA	1:B:4127:THR:HB	1.79	0.65
4:G:20:ILE:HD13	4:G:31:LYS:HZ2	1.62	0.65
1:A:3383:ASN:O	1:A:3384:ARG:HB3	1.97	0.64
1:B:3373:SER:HB2	1:B:3377:TYR:HE2	1.61	0.64
5:I:8:ILE:HD13	5:I:18:GLN:HE21	1.61	0.64
1:A:3373:SER:HB2	1:A:3377:TYR:HE2	1.61	0.64
1:A:3381:ILE:HG12	1:A:3393:VAL:HG11	1.80	0.64
1:B:1202:PHE:HB3	1:B:1204:PHE:CE2	2.32	0.64
2:D:287:TRP:CD1	2:D:579:THR:HA	2.32	0.64
1:B:648:ILE:HD11	1:B:698:ILE:HB	1.80	0.64
1:B:2138:ILE:HD12	1:B:2161:LEU:HD22	1.79	0.64
1:A:4097:LYS:HA	1:A:4127:THR:HB	1.79	0.64
4:G:49:PHE:HB3	4:H:52:LYS:NZ	2.12	0.64
1:A:1400:VAL:C	1:A:1402:GLU:N	2.50	0.64
1:B:3319:LEU:HD21	1:B:3377:TYR:HA	1.79	0.64
1:A:365:ARG:HH22	1:A:432:VAL:HB	1.62	0.64
1:A:2138:ILE:HD12	1:A:2161:LEU:HD22	1.79	0.64
1:A:2536:ASP:OD1	1:A:2576:ARG:NH1	2.31	0.64
1:B:58:GLU:HG3	1:B:61:ALA:H	1.62	0.64
1:B:2536:ASP:OD1	1:B:2576:ARG:NH1	2.31	0.64
1:A:336:MET:HB3	1:A:363:HIS:HD2	1.63	0.63
1:B:755:TRP:CG	2:D:453:GLU:HG3	2.33	0.63
2:D:296:VAL:HG12	2:D:315:VAL:HG22	1.79	0.63
1:A:3659:ARG:HD2	1:B:3628:ARG:CD	2.28	0.63
1:B:1487:ILE:HD12	1:B:1537:TRP:NE1	2.14	0.63
5:I:57:ILE:HD12	5:I:84:LEU:HD23	1.79	0.63
1:B:292:ARG:NH2	1:B:316:PHE:O	2.30	0.63
1:B:987:PHE:CE2	3:F:87:GLU:HG2	2.32	0.63
5:J:8:ILE:HA	5:J:76:PHE:HB3	1.80	0.63
1:A:337:LYS:HZ2	1:A:367:ILE:HB	1.63	0.63
1:B:322:LEU:O	1:B:326:LEU:N	2.24	0.63
1:A:441:LYS:NZ	1:A:447:LYS:O	2.32	0.63
1:A:3557:ASP:OD1	1:A:3743:ARG:NH1	2.32	0.63
1:B:798:ARG:HH12	1:B:855:GLU:HB3	1.64	0.63
1:B:1212:ASP:CA	1:B:1215:GLU:HB2	2.19	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:MET:HB3	1:A:363:HIS:CD2	2.33	0.63
1:B:1188:GLU:O	1:B:1191:ARG:HG2	1.99	0.63
3:F:38:SER:O	3:F:40:LEU:N	2.31	0.63
3:F:336:TYR:CZ	3:F:340:ILE:HD11	2.34	0.63
1:A:242:LEU:HB3	1:A:309:ARG:HE	1.63	0.63
1:A:1174:GLN:HA	1:A:1177:LYS:HG2	1.80	0.63
1:A:1201:ARG:NH2	1:B:967:GLN:O	2.31	0.63
1:A:3319:LEU:HD21	1:A:3377:TYR:HA	1.79	0.63
1:B:613:LYS:HE2	1:B:682:LEU:HB2	1.81	0.63
3:F:51:LEU:HB3	3:F:98:ARG:HE	1.62	0.63
1:B:552:ARG:O	1:B:555:GLU:HG2	1.99	0.62
1:A:84:LEU:HB3	1:A:98:PHE:HB3	1.80	0.62
1:A:1487:ILE:HD12	1:A:1537:TRP:NE1	2.14	0.62
1:B:1174:GLN:OE1	1:B:1233:GLN:NE2	2.32	0.62
1:A:264:ARG:HG3	1:A:376:ARG:HH22	1.64	0.62
1:B:1215:GLU:O	1:B:1216:GLY:C	2.37	0.62
1:B:485:ARG:NH1	1:B:486:PRO:O	2.32	0.62
1:B:1908:ALA:HB3	1:B:2353:LEU:HD22	1.81	0.62
1:A:40:LEU:O	1:B:132:SER:OG	2.13	0.62
1:B:3557:ASP:OD1	1:B:3743:ARG:NH1	2.32	0.62
2:D:551:LEU:HB3	2:D:563:ALA:HB3	1.82	0.62
1:A:1229:ASP:O	1:A:1233:GLN:NE2	2.31	0.62
1:A:3628:ARG:CD	1:B:3659:ARG:HD2	2.29	0.62
1:B:482:ARG:O	1:B:487:GLN:NE2	2.31	0.62
2:D:475:HIS:HE2	2:D:503:ASP:HB2	1.64	0.62
6:L:85:TRP:CD1	6:L:90:ASP:HB2	2.34	0.62
1:A:1222:ASN:HA	1:A:1225:MET:HG2	1.80	0.62
1:B:1203:GLN:HA	5:J:5:LYS:NZ	2.14	0.62
1:B:2226:SER:HA	8:B:4702:ATP:O1G	2.00	0.62
1:B:3381:ILE:HG12	1:B:3393:VAL:HG11	1.80	0.62
2:D:268:ASN:OD1	2:D:598:ASP:N	2.27	0.62
6:K:78:HIS:NE2	6:L:40:ASN:OD1	2.32	0.62
2:D:277:SER:HA	2:D:280:ARG:HD2	1.82	0.62
1:A:1908:ALA:HB3	1:A:2353:LEU:HD22	1.81	0.62
1:B:718:PHE:HA	1:B:738:ASN:H	1.65	0.62
1:A:96:LYS:NZ	1:A:97:GLU:O	2.33	0.61
1:B:2080:LEU:O	1:B:4415:ARG:NH1	2.33	0.61
2:D:509:TRP:HB3	2:D:516:PRO:HA	1.80	0.61
1:B:150:HIS:CE1	1:B:194:LEU:HB3	2.35	0.61
1:B:770:GLN:HG2	1:B:773:GLN:HE21	1.64	0.61
1:B:895:ASN:OD1	3:F:353:GLU:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:GLU:OE2	1:A:385:SER:OG	2.17	0.61
1:A:1153:LEU:HD11	1:A:1228:LYS:HG3	1.80	0.61
1:A:1399:LEU:C	1:A:1401:ILE:N	2.53	0.61
2:D:500:SER:OG	2:D:527:VAL:O	2.18	0.61
1:A:2488:ARG:HG3	1:A:2492:ARG:HH12	1.65	0.61
1:B:264:ARG:NH1	1:B:274:GLU:OE2	2.32	0.61
1:B:1214:ILE:O	1:B:1215:GLU:C	2.39	0.61
1:B:264:ARG:NH2	1:B:268:SER:O	2.33	0.61
1:A:2226:SER:HA	8:A:4702:ATP:O1G	2.00	0.61
1:B:721:GLU:OE2	1:B:736:LYS:NZ	2.31	0.61
1:A:2080:LEU:O	1:A:4415:ARG:NH1	2.33	0.61
1:B:88:VAL:HG22	1:B:90:ASP:H	1.65	0.61
5:J:69:GLU:HG3	5:J:88:SER:HA	1.82	0.61
1:B:1043:ILE:HA	1:B:1102:PHE:HE2	1.64	0.61
1:A:3628:ARG:HD2	1:B:3659:ARG:HD2	1.83	0.61
1:B:3319:LEU:CD2	1:B:3377:TYR:HA	2.31	0.61
2:C:214:GLN:HB2	2:D:209:ARG:NH1	2.16	0.61
3:F:59:VAL:HG12	3:F:108:ILE:HA	1.83	0.61
1:A:3659:ARG:HD2	1:B:3628:ARG:HD2	1.82	0.60
1:B:464:ASP:HA	1:B:467:ARG:HG2	1.82	0.60
1:B:666:GLU:OE1	1:B:673:TRP:NE1	2.35	0.60
1:B:870:ASP:HB3	1:B:873:THR:HG22	1.83	0.60
6:L:25:ILE:HG23	6:L:29:ILE:HD12	1.82	0.60
1:B:1210:TYR:H	1:B:1213:ASN:CB	2.15	0.60
1:B:1212:ASP:O	1:B:1213:ASN:C	2.38	0.60
3:F:139:MET:SD	3:F:139:MET:N	2.74	0.60
1:B:466:MET:CE	1:B:470:ARG:HG3	2.32	0.60
1:B:1177:LYS:O	1:B:1180:ILE:HB	2.00	0.60
1:B:1193:GLY:HA2	1:B:1196:LEU:HD12	1.82	0.60
1:A:3381:ILE:HG23	1:A:3390:GLY:H	1.65	0.60
1:A:3761:LEU:HA	1:A:3767:ILE:HD11	1.82	0.60
1:B:761:PRO:HD2	1:B:764:ILE:HD12	1.82	0.60
1:B:1751:VAL:HG21	1:B:1878:LYS:HE3	1.83	0.60
1:B:4436:GLN:HG3	1:B:4441:LYS:HB2	1.84	0.60
2:D:374:PRO:HD3	2:D:416:SER:HA	1.82	0.60
4:G:64:ASN:ND2	4:H:76:ASN:OD1	2.34	0.60
1:B:466:MET:HE2	1:B:470:ARG:HG3	1.83	0.60
1:B:1204:PHE:HB3	1:B:1208:TRP:HE1	1.66	0.60
1:B:1205:PRO:O	1:B:1208:TRP:HD1	1.82	0.60
8:B:4702:ATP:H8	8:B:4702:ATP:H5'1	1.66	0.60
2:D:283:SER:HB2	2:D:298:SER:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:HIS:HB2	1:B:178:MET:HE1	1.82	0.60
1:A:242:LEU:HG	1:A:304:LEU:HA	1.83	0.60
1:A:3319:LEU:CD2	1:A:3377:TYR:HA	2.31	0.60
1:B:242:LEU:HD21	1:B:307:GLY:HA3	1.83	0.60
2:C:187:LYS:HB3	4:G:30:ILE:HG13	1.82	0.60
5:I:13:MET:HE3	5:I:17:MET:HG2	1.83	0.60
5:I:64:SER:H	5:J:36:LYS:HD3	1.67	0.60
1:A:1219:GLY:HA2	1:A:1222:ASN:HD21	1.64	0.60
1:A:2905:LEU:HD11	1:A:3652:GLU:HB3	1.82	0.60
1:B:292:ARG:HH12	1:B:320:THR:HG22	1.67	0.60
1:B:526:ALA:O	1:B:553:TYR:OH	2.12	0.60
2:D:457:TYR:CE1	2:D:471:MET:HG2	2.37	0.60
1:B:391:GLN:O	1:B:394:LYS:HG2	2.02	0.60
1:B:633:CYS:SG	1:B:634:LYS:N	2.75	0.60
1:B:3761:LEU:HA	1:B:3767:ILE:HD11	1.82	0.60
1:A:1490:TRP:HH2	1:A:1537:TRP:CD1	2.17	0.59
1:A:2039:LEU:HD12	1:A:4254:GLY:HA2	1.84	0.59
1:B:1490:TRP:HH2	1:B:1537:TRP:CD1	2.17	0.59
1:B:2488:ARG:HG3	1:B:2492:ARG:HH12	1.65	0.59
3:F:241:GLU:HA	3:F:246:TYR:H	1.67	0.59
1:A:1466:ILE:HG12	1:A:1500:HIS:ND1	2.17	0.59
3:E:95:ASP:O	3:E:99:ASP:N	2.34	0.59
4:G:54:ARG:NH2	4:G:64:ASN:O	2.35	0.59
1:A:296:GLU:OE2	1:A:300:THR:OG1	2.20	0.59
1:A:320:THR:OG1	1:A:323:LYS:NZ	2.23	0.59
1:A:456:HIS:HA	1:A:459:LEU:HD13	1.83	0.59
1:A:3377:TYR:O	1:A:3381:ILE:HG12	2.03	0.59
1:B:174:ASP:HA	1:B:177:LYS:HE3	1.85	0.59
2:D:475:HIS:NE2	2:D:503:ASP:HB2	2.16	0.59
6:L:72:LYS:HE2	6:L:103:TYR:CZ	2.36	0.59
1:B:1134:MET:N	1:B:1134:MET:SD	2.75	0.59
1:A:236:VAL:HG23	1:A:303:ILE:HB	1.83	0.59
8:A:4702:ATP:C8	8:A:4702:ATP:H5'1	2.38	0.59
1:B:210:HIS:HB3	1:B:213:ILE:HG22	1.83	0.59
1:B:530:VAL:HG13	1:B:553:TYR:CZ	2.37	0.59
5:J:6:ALA:HB2	5:J:78:LEU:CD2	2.32	0.59
1:A:3447:TYR:HB3	1:A:3451:TYR:CZ	2.38	0.59
1:A:4436:GLN:HG3	1:A:4441:LYS:HB2	1.84	0.59
1:B:582:PHE:HE1	1:B:668:VAL:HG11	1.67	0.59
1:B:2039:LEU:HD12	1:B:4254:GLY:HA2	1.84	0.59
2:D:359:LEU:HB2	2:D:415:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3455:ILE:HD12	1:B:3452:ALA:CB	2.32	0.59
1:B:689:PHE:HA	1:B:692:LYS:HE3	1.84	0.59
1:B:3377:TYR:O	1:B:3381:ILE:HG12	2.02	0.59
1:B:3951:VAL:CG2	1:B:3973:LEU:HD21	2.33	0.59
1:A:2422:ILE:HD13	1:A:2487:GLU:HA	1.85	0.59
1:B:85:LYS:HE3	1:B:95:GLU:HB2	1.84	0.59
1:B:2905:LEU:HD11	1:B:3652:GLU:HB3	1.82	0.59
2:D:427:LYS:O	2:D:430:LYS:HG3	2.02	0.59
1:B:343:ASP:O	1:B:352:LYS:NZ	2.36	0.59
1:B:1146:ILE:O	1:B:1150:ARG:HG2	2.03	0.59
1:B:1168:THR:O	1:B:1171:THR:OG1	2.17	0.59
1:B:1212:ASP:HB2	1:B:1216:GLY:N	2.18	0.59
1:B:3381:ILE:HD12	1:B:3393:VAL:HG21	1.72	0.59
1:B:3447:TYR:HB3	1:B:3451:TYR:CZ	2.38	0.59
1:B:4287:LYS:H	1:B:4293:ASP:HB3	1.68	0.59
8:B:4702:ATP:H5'1	8:B:4702:ATP:C8	2.38	0.59
1:A:1623:ARG:HD3	1:A:1630:TYR:HA	1.84	0.59
1:A:1751:VAL:HG21	1:A:1878:LYS:HE3	1.83	0.59
1:A:2841:GLU:OE1	1:A:2844:ARG:NH1	2.36	0.59
1:B:1174:GLN:O	1:B:1178:ARG:NH1	2.35	0.59
1:B:1623:ARG:HD3	1:B:1630:TYR:HA	1.84	0.59
1:B:121:ARG:HB3	1:B:136:ARG:HB2	1.85	0.58
1:B:335:LEU:HD13	1:B:367:ILE:HD12	1.85	0.58
1:B:1210:TYR:H	1:B:1213:ASN:CG	2.06	0.58
1:B:1466:ILE:HG12	1:B:1500:HIS:ND1	2.17	0.58
2:D:215:ILE:HG13	2:D:217:ILE:H	1.68	0.58
2:D:613:ARG:HA	2:D:616:ARG:HG2	1.85	0.58
4:H:72:ARG:NE	4:H:94:PRO:O	2.33	0.58
8:A:4702:ATP:H5'1	8:A:4702:ATP:H8	1.66	0.58
1:B:994:LEU:HD11	1:B:1020:ARG:HA	1.84	0.58
1:B:2841:GLU:OE1	1:B:2844:ARG:NH1	2.36	0.58
2:D:553:ASN:OD1	2:D:554:LEU:N	2.36	0.58
4:G:74:LYS:HG3	4:G:75:LYS:HD2	1.85	0.58
1:A:209:ILE:HA	1:A:248:GLY:HA3	1.84	0.58
1:B:869:TYR:OH	1:B:989:TRP:O	2.20	0.58
1:B:1931:ASN:HD22	1:B:2317:SER:H	1.51	0.58
1:B:2422:ILE:HD13	1:B:2487:GLU:HA	1.85	0.58
3:F:48:ARG:HH11	3:F:49:SER:HB2	1.67	0.58
3:F:139:MET:SD	3:F:231:CYS:HB3	2.42	0.58
5:J:7:VAL:O	5:J:9:LYS:N	2.36	0.58
1:B:120:LYS:HA	1:B:135:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:LYS:HD2	1:B:130:PRO:HD2	1.85	0.58
1:B:229:VAL:HG12	1:B:303:ILE:HG22	1.85	0.58
3:F:48:ARG:HD2	3:F:49:SER:N	2.18	0.58
1:A:3243:MET:SD	1:A:3451:TYR:CE2	2.96	0.58
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.85	0.58
1:B:1131:PHE:HA	1:B:1134:MET:HE1	1.85	0.58
1:B:1161:ALA:HA	1:B:1163:THR:HG23	1.85	0.58
1:B:1205:PRO:HG2	1:B:1207:SER:OG	2.03	0.58
1:B:3243:MET:SD	1:B:3451:TYR:CE2	2.96	0.58
1:A:170:LYS:HG2	1:A:179:ALA:HB3	1.84	0.58
1:A:405:ALA:HB3	1:A:408:GLU:HG2	1.85	0.58
1:A:1191:ARG:NH2	1:A:1215:GLU:OE2	2.36	0.58
1:B:724:ARG:HH11	1:B:726:ARG:HE	1.52	0.58
1:B:3381:ILE:HG23	1:B:3390:GLY:H	1.65	0.58
2:D:607:ARG:HG2	2:D:610:GLU:HG2	1.84	0.58
1:A:321:GLY:O	1:A:324:GLN:NE2	2.36	0.58
1:A:2279:LEU:HA	1:A:2698:GLN:HG3	1.86	0.58
1:A:3452:ALA:HB1	1:B:3455:ILE:HD12	1.86	0.58
1:A:3452:ALA:CB	1:B:3455:ILE:HD12	2.33	0.58
1:A:3951:VAL:CG2	1:A:3973:LEU:HD21	2.33	0.58
1:B:130:PRO:O	1:B:134:GLN:N	2.36	0.58
1:B:2279:LEU:HA	1:B:2698:GLN:HG3	1.86	0.58
1:A:1196:LEU:O	1:A:1200:GLN:N	2.35	0.58
1:A:3455:ILE:HD12	1:B:3452:ALA:HB1	1.86	0.58
1:A:4287:LYS:H	1:A:4293:ASP:HB3	1.68	0.58
3:F:142:PRO:HA	3:F:145:VAL:HG23	1.85	0.58
1:A:1435:TRP:C	1:A:1437:VAL:H	2.06	0.58
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.85	0.58
1:B:908:GLU:HG3	1:B:1025:ARG:HG2	1.85	0.58
1:B:1169:PHE:O	1:B:1172:TYR:HB3	2.04	0.58
2:D:495:HIS:HB2	2:D:511:THR:HG22	1.85	0.58
5:J:72:HIS:HB3	5:J:87:LYS:HB3	1.85	0.58
1:A:22:GLN:HE21	1:A:125:ILE:HA	1.68	0.58
1:A:118:PHE:HB3	1:A:135:LEU:HD21	1.86	0.58
1:A:3655:ARG:HG2	1:A:3660:VAL:HG22	1.86	0.58
1:B:4554:ASP:OD1	1:B:4555:ALA:N	2.37	0.58
1:B:4318:PRO:HG2	1:B:4325:ASN:HA	1.85	0.57
1:A:43:GLU:HG3	1:A:81:ARG:HH22	1.69	0.57
1:A:151:SER:O	1:A:154:SER:OG	2.20	0.57
1:A:3597:THR:HG23	1:A:3634:LEU:HD21	1.86	0.57
1:A:4554:ASP:OD1	1:A:4555:ALA:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ASP:OD1	1:B:232:PHE:N	2.37	0.57
1:B:438:VAL:HA	1:B:441:LYS:HB2	1.86	0.57
1:B:864:LEU:HB2	1:B:877:ILE:HG21	1.85	0.57
1:B:4071:ILE:HD11	1:B:4096:LEU:HB3	1.86	0.57
1:A:189:LEU:O	1:A:193:LEU:HD23	2.04	0.57
1:A:1399:LEU:O	1:A:1401:ILE:N	2.38	0.57
1:A:4071:ILE:HD11	1:A:4096:LEU:HB3	1.86	0.57
1:B:734:LYS:HD3	1:B:736:LYS:HZ2	1.69	0.57
1:B:1455:GLY:HA3	1:B:1512:TYR:CE2	2.39	0.57
1:B:3381:ILE:HD12	1:B:3389:CYS:HB3	1.86	0.57
1:B:3510:SER:HB3	1:B:3553:LEU:HD21	1.84	0.57
4:G:66:LEU:HG	4:H:71:ILE:HD11	1.85	0.57
2:D:352:THR:HG23	2:D:354:SER:H	1.69	0.57
2:D:480:THR:OG1	2:D:500:SER:O	2.19	0.57
1:A:442:ARG:NH2	1:A:445:ASN:OD1	2.37	0.57
1:A:1455:GLY:HA3	1:A:1512:TYR:CE2	2.39	0.57
1:B:315:SER:O	1:B:319:ASP:N	2.25	0.57
1:A:160:PHE:HB2	1:B:107:ILE:HD12	1.86	0.57
1:A:228:LYS:N	1:A:231:ASP:OD2	2.31	0.57
1:A:1386:VAL:O	1:A:1390:LEU:N	2.36	0.57
1:B:808:LEU:O	1:B:811:GLU:HG2	2.05	0.57
1:B:3597:THR:HG23	1:B:3634:LEU:HD21	1.86	0.57
1:A:2592:VAL:HG23	1:A:2731:VAL:HG11	1.86	0.57
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.85	0.57
1:B:88:VAL:HB	1:B:95:GLU:HA	1.86	0.57
1:B:1085:GLN:HA	1:B:1088:LYS:HE3	1.86	0.57
1:B:2107:ARG:NH2	1:B:2139:GLN:OE1	2.38	0.57
2:D:583:ARG:NH1	2:D:599:VAL:O	2.31	0.57
1:A:116:LEU:HD22	1:A:139:THR:HG22	1.87	0.57
1:A:2562:VAL:HG11	1:A:2755:MET:HB2	1.85	0.57
1:B:2562:VAL:HG11	1:B:2755:MET:HB2	1.85	0.57
1:B:3839:VAL:HG21	1:B:3863:LEU:HA	1.85	0.57
1:B:4071:ILE:HG13	1:B:4099:VAL:HG12	1.87	0.57
2:D:349:VAL:HG21	2:D:398:LEU:HD11	1.87	0.57
1:A:1931:ASN:HD22	1:A:2317:SER:H	1.51	0.57
1:A:4168:ARG:NE	1:A:4220:ASP:OD1	2.30	0.57
1:A:4544:ASN:HD22	1:A:4589:GLN:HG3	1.70	0.57
3:F:251:LEU:HA	3:F:254:ILE:HG12	1.87	0.57
5:J:58:VAL:HG22	5:J:83:ILE:HG12	1.86	0.57
1:A:3381:ILE:HG13	1:A:3393:VAL:CB	2.35	0.57
1:A:3381:ILE:HD12	1:A:3389:CYS:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3655:ARG:HG2	1:B:3660:VAL:HG22	1.86	0.57
1:B:4168:ARG:NE	1:B:4220:ASP:OD1	2.30	0.57
2:D:187:LYS:HE3	4:H:24:ASN:H	1.69	0.57
3:F:67:LYS:HB3	3:F:136:VAL:HG21	1.86	0.57
3:F:87:GLU:HB2	3:F:108:ILE:HG23	1.86	0.57
1:A:3459:GLN:OE1	1:B:3456:SER:OG	2.14	0.56
1:B:3951:VAL:HG22	1:B:3973:LEU:HD21	1.87	0.56
2:D:505:THR:HG22	2:D:507:LYS:HG3	1.87	0.56
4:G:25:THR:HA	4:G:87:PHE:HE2	1.70	0.56
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.38	0.56
1:A:3243:MET:HE1	1:A:3447:TYR:HB2	1.86	0.56
1:A:3951:VAL:HG22	1:A:3973:LEU:HD21	1.87	0.56
1:B:1206:PRO:O	1:B:1207:SER:C	2.42	0.56
2:D:448:VAL:HG21	2:D:497:PHE:CZ	2.39	0.56
1:A:2319:LEU:HD13	1:A:2359:CYS:SG	2.45	0.56
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.87	0.56
1:B:1170:ILE:O	1:B:1173:VAL:HG12	2.06	0.56
1:B:1174:GLN:HA	1:B:1177:LYS:HG2	1.87	0.56
1:B:1220:ALA:O	1:B:1224:ILE:HG12	2.05	0.56
1:B:3172:THR:HG21	1:B:3694:SER:HB3	1.87	0.56
1:B:3891:LYS:HD2	1:B:4013:LEU:HD23	1.87	0.56
1:B:4444:GLN:O	1:B:4449:ARG:NH1	2.38	0.56
2:C:202:HIS:NE2	4:G:81:ALA:HB1	2.21	0.56
2:D:268:ASN:HB2	2:D:597:TYR:HA	1.86	0.56
3:E:124:SER:O	3:E:128:LEU:N	2.36	0.56
3:F:365:LYS:O	3:F:368:SER:OG	2.21	0.56
5:J:9:LYS:HB2	5:J:75:TYR:O	2.06	0.56
1:A:3443:SER:HB2	1:A:3447:TYR:CE2	2.40	0.56
1:A:4209:GLU:OE2	1:A:4213:ARG:NE	2.36	0.56
1:B:91:GLU:HA	1:B:243:ASN:HB3	1.88	0.56
1:B:1045:SER:O	1:B:1048:GLU:HG3	2.06	0.56
2:D:266:SER:O	2:D:597:TYR:HB2	2.05	0.56
4:H:22:VAL:H	4:H:31:LYS:HZ3	1.53	0.56
1:A:189:LEU:HD22	1:B:185:LYS:HE2	1.88	0.56
1:A:1174:GLN:O	1:A:1178:ARG:NH1	2.33	0.56
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.87	0.56
1:B:960:HIS:O	1:B:1107:ILE:HA	2.05	0.56
1:B:2319:LEU:HD13	1:B:2359:CYS:SG	2.46	0.56
1:B:2592:VAL:HG23	1:B:2731:VAL:HG11	1.86	0.56
1:B:4544:ASN:HD22	1:B:4589:GLN:HG3	1.70	0.56
1:B:1139:MET:O	1:B:1143:HIS:ND1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:VAL:HG13	1:A:237:GLU:HG2	1.87	0.56
1:A:3891:LYS:HD2	1:A:4013:LEU:HD23	1.87	0.56
1:B:153:ILE:O	1:B:157:VAL:HG12	2.06	0.56
1:B:365:ARG:HH22	1:B:432:VAL:HB	1.71	0.56
1:B:1138:ASN:OD1	1:B:1139:MET:N	2.38	0.56
3:F:255:GLN:HE22	3:F:323:LEU:HD11	1.69	0.56
1:A:1985:HIS:CD2	1:A:1997:ILE:HD13	2.41	0.56
1:B:1998:THR:HG21	1:B:2005:GLN:HB3	1.88	0.56
1:B:3381:ILE:HG13	1:B:3393:VAL:CB	2.35	0.56
5:J:12:ASP:OD2	5:J:68:HIS:HE1	1.89	0.56
1:A:4071:ILE:HG13	1:A:4099:VAL:HG12	1.87	0.56
1:B:3443:SER:HB2	1:B:3447:TYR:CE2	2.40	0.56
1:B:817:ALA:HA	3:F:366:GLN:HE21	1.71	0.56
1:B:819:GLY:HA3	1:B:832:TYR:CZ	2.40	0.56
1:B:1079:TRP:HB3	1:B:1131:PHE:CZ	2.41	0.56
1:B:1537:TRP:CE3	1:B:1601:LEU:HD11	2.41	0.55
1:B:1985:HIS:CD2	1:B:1997:ILE:HD13	2.41	0.55
6:K:73:ASN:HD21	6:L:75:ALA:HB2	1.72	0.55
1:A:3601:MET:HG3	1:A:3611:ARG:NH2	2.21	0.55
1:A:4444:GLN:O	1:A:4449:ARG:NH1	2.38	0.55
1:B:349:GLU:OE1	1:B:349:GLU:N	2.40	0.55
1:B:724:ARG:HD2	1:B:726:ARG:HH21	1.69	0.55
1:B:2433:VAL:HG22	1:B:2498:ILE:HD11	1.87	0.55
2:D:589:ASP:OD1	2:D:590:SER:N	2.38	0.55
1:B:387:ASP:OD1	1:B:388:LEU:N	2.38	0.55
2:D:531:MET:HG3	2:D:578:TRP:CD1	2.36	0.55
1:A:21:VAL:HA	1:A:124:VAL:HB	1.88	0.55
1:A:179:ALA:HA	1:A:182:VAL:HG22	1.87	0.55
1:B:2573:ASP:OD1	1:B:2576:ARG:NH2	2.39	0.55
1:A:55:ALA:HB3	1:A:101:TYR:HD2	1.70	0.55
1:B:1150:ARG:O	1:B:1153:LEU:HG	2.06	0.55
1:B:3601:MET:HG3	1:B:3611:ARG:NH2	2.21	0.55
5:I:58:VAL:HG22	5:I:83:ILE:HG12	1.89	0.55
1:A:1154:GLU:HA	1:A:1156:HIS:CE1	2.42	0.55
1:A:1998:THR:HG21	1:A:2005:GLN:HB3	1.88	0.55
1:B:72:PRO:O	1:B:75:HIS:NE2	2.38	0.55
1:B:246:GLN:HA	1:B:249:VAL:HG12	1.88	0.55
1:B:1131:PHE:O	1:B:1135:LEU:HG	2.06	0.55
1:A:29:VAL:O	1:A:33:HIS:ND1	2.39	0.55
1:A:371:LYS:HE3	1:A:440:ARG:HH21	1.71	0.55
1:A:1435:TRP:C	1:A:1437:VAL:N	2.59	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1537:TRP:CE3	1:A:1601:LEU:HD11	2.41	0.55
1:A:3243:MET:HE1	1:A:3444:ILE:O	2.07	0.55
1:A:1155:GLN:HE22	1:A:1157:SER:HB2	1.71	0.55
1:B:335:LEU:HG	1:B:366:LYS:NZ	2.22	0.55
2:D:448:VAL:HG22	2:D:458:THR:HG23	1.89	0.55
4:H:83:ASP:OD1	4:H:84:LYS:N	2.37	0.55
1:A:3455:ILE:HD12	1:B:3452:ALA:HA	1.87	0.55
1:B:148:THR:HG23	1:B:152:PHE:CE2	2.41	0.55
1:B:613:LYS:HG3	1:B:682:LEU:HD12	1.88	0.55
1:B:1212:ASP:CA	1:B:1216:GLY:H	2.20	0.55
1:A:136:ARG:NE	1:B:139:THR:HG23	2.21	0.54
1:A:354:ARG:NH1	1:A:355:GLN:HG2	2.21	0.54
1:A:2694:ARG:NH1	1:A:2697:ASP:OD2	2.40	0.54
4:H:21:ILE:HD12	4:H:31:LYS:HB2	1.90	0.54
5:J:70:THR:O	5:J:72:HIS:ND1	2.29	0.54
2:D:503:ASP:O	2:D:505:THR:OG1	2.22	0.54
5:J:50:TYR:HB2	5:J:54:TRP:CH2	2.42	0.54
1:A:265:ASP:OD2	1:A:268:SER:OG	2.23	0.54
1:A:479:VAL:O	1:A:483:VAL:N	2.31	0.54
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.89	0.54
1:B:241:PHE:O	1:B:245:LEU:HG	2.08	0.54
1:B:3580:LEU:HD13	1:B:3600:ILE:HD11	1.89	0.54
3:F:88:TYR:HD1	3:F:107:TRP:CD1	2.26	0.54
1:A:264:ARG:O	1:A:376:ARG:NH1	2.18	0.54
1:A:269:GLY:O	1:A:386:ARG:NH2	2.40	0.54
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.39	0.54
1:B:479:VAL:HG11	1:B:590:ALA:HB3	1.90	0.54
1:B:1126:GLU:O	1:B:1129:SER:OG	2.18	0.54
1:B:1198:GLU:O	1:B:1201:ARG:NH1	2.40	0.54
1:B:1832:ASN:HD21	1:B:1834:LYS:HB2	1.72	0.54
2:D:504:TRP:CE3	2:D:523:ASN:HB3	2.43	0.54
5:J:50:TYR:HB2	5:J:54:TRP:CZ2	2.42	0.54
1:A:1196:LEU:HA	1:A:1199:LYS:HG2	1.90	0.54
5:I:55:HIS:ND1	5:J:66:VAL:HB	2.22	0.54
1:A:274:GLU:OE1	1:A:376:ARG:NH2	2.40	0.54
1:B:639:ARG:NH2	2:D:574:ASN:HD21	2.05	0.54
1:B:4209:GLU:OE2	1:B:4213:ARG:NE	2.36	0.54
1:B:2596:PRO:HB2	1:B:2738:TYR:CZ	2.43	0.54
1:A:456:HIS:CE1	1:A:460:GLN:HB2	2.43	0.54
1:B:126:ASP:H	1:B:134:GLN:NE2	2.06	0.54
1:B:1013:THR:OG1	1:B:1014:GLU:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1832:ASN:HD21	1:A:1834:LYS:HB2	1.72	0.54
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.89	0.54
1:B:27:VAL:HG23	1:B:66:ARG:HH11	1.73	0.54
1:B:78:LEU:HB3	1:B:104:ASN:HB2	1.90	0.54
1:B:1141:GLU:O	1:B:1145:GLN:HG2	2.07	0.54
1:B:1212:ASP:HA	1:B:1216:GLY:H	1.72	0.54
2:D:475:HIS:CE1	2:D:477:GLY:H	2.26	0.54
1:A:3182:HIS:NE2	1:A:3582:ARG:O	2.40	0.54
1:B:480:ILE:HG23	1:B:484:LEU:HB2	1.89	0.54
1:B:664:ARG:HG2	1:B:664:ARG:HH11	1.73	0.54
1:B:1100:LYS:NZ	1:B:1102:PHE:HB2	2.23	0.54
1:B:1176:LEU:HD13	1:B:1179:LYS:HD3	1.89	0.54
1:B:1571:ILE:HD12	1:B:1611:ILE:HD11	1.90	0.54
1:A:3452:ALA:HA	1:B:3455:ILE:HD12	1.88	0.53
1:B:862:ARG:HA	1:B:865:GLU:HG3	1.90	0.53
1:B:2665:GLU:HB3	1:B:2668:LEU:HD12	1.90	0.53
1:B:3383:ASN:O	1:B:3384:ARG:CB	2.56	0.53
2:D:578:TRP:HA	2:D:585:ILE:HD12	1.91	0.53
3:F:39:ILE:HA	3:F:42:GLU:HG2	1.90	0.53
4:G:57:VAL:HG11	4:G:66:LEU:HD11	1.88	0.53
5:I:13:MET:HA	5:I:71:LYS:HD2	1.89	0.53
1:A:53:GLU:HA	1:A:56:LEU:HB3	1.90	0.53
1:A:401:LEU:HA	1:A:404:VAL:HB	1.89	0.53
1:A:1467:ARG:HE	1:A:1523:TRP:HZ2	1.56	0.53
1:A:2294:GLU:OE1	1:A:2294:GLU:N	2.39	0.53
1:B:257:GLN:HA	1:B:260:THR:HG22	1.89	0.53
1:B:3243:MET:HE1	1:B:3447:TYR:HB2	1.89	0.53
1:B:3914:ILE:O	1:B:3937:ARG:NH1	2.42	0.53
2:D:445:ASN:OD1	2:D:446:ASN:N	2.36	0.53
1:A:3914:ILE:O	1:A:3937:ARG:NH1	2.42	0.53
1:B:361:PHE:CD1	1:B:426:GLU:HG3	2.43	0.53
1:B:1139:MET:HE3	1:B:1209:LEU:H	1.73	0.53
1:B:1156:HIS:NE2	1:B:1166:ALA:HA	2.24	0.53
1:B:1212:ASP:C	1:B:1214:ILE:N	2.59	0.53
1:B:1467:ARG:HE	1:B:1523:TRP:HZ2	1.57	0.53
1:B:3691:ASP:OD1	1:B:3692:LEU:N	2.42	0.53
1:A:3456:SER:OG	1:B:3459:GLN:OE1	2.14	0.53
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.91	0.53
1:B:631:GLN:HG3	2:D:572:ALA:HB2	1.90	0.53
1:B:2694:ARG:NH1	1:B:2697:ASP:OD2	2.41	0.53
2:D:439:PHE:HB3	2:D:447:PHE:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:46:MET:O	4:H:50:ILE:HG12	2.08	0.53
1:A:148:THR:O	1:A:152:PHE:HD2	1.92	0.53
1:A:189:LEU:HD21	1:B:185:LYS:HB3	1.91	0.53
1:A:368:ARG:NH1	1:A:436:ASP:O	2.42	0.53
1:A:3459:GLN:OE1	1:B:3453:VAL:HA	2.09	0.53
1:B:848:ASP:OD1	1:B:849:ASP:N	2.41	0.53
1:B:2047:GLN:HA	1:B:2070:VAL:HG21	1.89	0.53
1:B:3243:MET:HE3	1:B:3444:ILE:HA	1.89	0.53
2:D:457:TYR:HE1	2:D:471:MET:HG2	1.73	0.53
3:F:59:VAL:HG11	3:F:108:ILE:HG13	1.89	0.53
5:I:77:TYR:CZ	5:I:82:ALA:HB2	2.44	0.53
1:A:241:PHE:O	1:A:245:LEU:HG	2.09	0.53
1:A:1487:ILE:HD12	1:A:1537:TRP:HE1	1.74	0.53
1:B:676:HIS:CD2	1:B:678:GLU:HB2	2.44	0.53
1:B:2835:ASP:HB3	1:B:3092:ASN:HD22	1.74	0.53
1:A:40:LEU:HD23	1:A:45:GLY:HA2	1.90	0.53
1:A:3292:ALA:HA	1:A:3395:TRP:HZ2	1.74	0.53
1:B:1161:ALA:C	1:B:1163:THR:H	2.12	0.53
1:B:3237:ASN:O	1:B:3241:LYS:HG3	2.09	0.53
1:B:3520:PHE:HB3	1:B:3524:MET:HB3	1.91	0.53
6:K:69:ILE:HG23	6:K:102:MET:SD	2.49	0.53
1:A:182:VAL:HB	1:A:185:LYS:HE2	1.90	0.53
1:A:361:PHE:HA	1:A:364:LEU:HD12	1.91	0.53
1:B:1398:MET:O	1:B:1399:LEU:C	2.47	0.53
1:B:3380:GLU:O	1:B:3383:ASN:HB2	2.08	0.53
1:A:2596:PRO:HB2	1:A:2738:TYR:CZ	2.43	0.53
1:A:1887:ARG:HE	1:A:2039:LEU:HD11	1.74	0.53
1:A:3750:LEU:O	1:A:3754:ASN:ND2	2.42	0.53
1:B:116:LEU:HD23	1:B:139:THR:HB	1.91	0.53
1:B:3292:ALA:HA	1:B:3395:TRP:HZ2	1.74	0.53
1:B:3750:LEU:O	1:B:3754:ASN:ND2	2.42	0.53
2:D:475:HIS:CE1	2:D:503:ASP:HB2	2.44	0.53
3:F:48:ARG:HD2	3:F:49:SER:HB2	1.90	0.53
1:A:253:ILE:HA	1:A:256:ILE:HG12	1.91	0.52
1:A:1147:SER:O	1:A:1151:GLN:HG2	2.09	0.52
1:A:2665:GLU:HB3	1:A:2668:LEU:HD12	1.90	0.52
1:B:330:ASN:HA	1:B:333:ASN:HB2	1.90	0.52
1:B:1130:LYS:O	1:B:1133:GLN:HG2	2.09	0.52
1:B:3916:LEU:HD11	1:B:3937:ARG:HG3	1.91	0.52
2:D:344:HIS:CD2	2:D:347:LEU:HD13	2.44	0.52
4:G:68:PHE:HD2	4:H:72:ARG:HB3	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3380:GLU:O	1:A:3383:ASN:HB2	2.08	0.52
1:B:264:ARG:NH1	1:B:267:ALA:O	2.39	0.52
1:B:431:GLN:O	1:B:435:ARG:HG2	2.09	0.52
1:B:530:VAL:HG13	1:B:553:TYR:CE1	2.45	0.52
1:B:1487:ILE:HD12	1:B:1537:TRP:HE1	1.73	0.52
1:B:1887:ARG:HE	1:B:2039:LEU:HD11	1.74	0.52
2:D:445:ASN:HD21	2:D:463:GLY:H	1.58	0.52
2:D:579:THR:HG21	2:D:584:GLU:CD	2.29	0.52
3:F:250:HIS:HD2	3:F:340:ILE:HG22	1.73	0.52
1:A:205:ILE:HD13	1:A:255:GLU:HG2	1.91	0.52
1:A:3382:VAL:O	1:A:3383:ASN:C	2.48	0.52
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.42	0.52
1:B:350:LEU:HA	1:B:353:ILE:HD12	1.91	0.52
1:B:636:SER:HB2	1:B:641:LEU:HB2	1.92	0.52
1:B:642:PRO:HB2	1:B:749:GLU:OE2	2.08	0.52
1:B:867:CYS:SG	1:B:873:THR:OG1	2.60	0.52
1:B:1543:ARG:NH1	1:B:1612:GLN:OE1	2.41	0.52
1:B:1687:LYS:HD3	1:B:1712:THR:HG23	1.91	0.52
2:D:607:ARG:HG3	2:D:609:ASP:HB3	1.92	0.52
3:F:228:LEU:HD21	3:F:286:TYR:CE1	2.44	0.52
3:F:321:ALA:HA	3:F:324:HIS:NE2	2.25	0.52
1:A:78:LEU:HD22	1:A:107:ILE:HA	1.91	0.52
1:B:487:GLN:H	1:B:567:ARG:HH22	1.58	0.52
1:A:242:LEU:HB3	1:A:309:ARG:NE	2.24	0.52
1:B:581:MET:HA	1:B:584:ILE:HD12	1.91	0.52
1:B:1194:GLN:NE2	1:B:1195:ARG:HG3	2.24	0.52
1:B:3243:MET:HE1	1:B:3444:ILE:O	2.08	0.52
2:D:506:VAL:H	2:D:520:PHE:HB3	1.74	0.52
3:F:68:THR:HG21	3:F:82:LYS:HE2	1.92	0.52
1:A:27:VAL:O	1:A:31:GLN:HB2	2.10	0.52
1:A:2835:ASP:HB3	1:A:3092:ASN:HD22	1.74	0.52
1:A:3237:ASN:O	1:A:3241:LYS:HG3	2.09	0.52
1:A:3916:LEU:HD11	1:A:3937:ARG:HG3	1.91	0.52
1:B:439:LYS:O	1:B:442:ARG:NH1	2.43	0.52
1:B:2620:LEU:HD22	1:B:2631:LEU:HD23	1.91	0.52
5:J:50:TYR:C	5:J:54:TRP:HH2	2.13	0.52
6:L:90:ASP:OD1	6:L:112:SER:N	2.26	0.52
1:A:38:VAL:HG21	1:A:52:LEU:HD22	1.91	0.52
1:A:193:LEU:HB2	1:B:178:MET:HE2	1.90	0.52
1:B:569:ARG:NH1	1:B:603:GLU:OE1	2.43	0.52
1:B:580:GLU:HA	1:B:583:ARG:NH2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:804:LEU:HD11	1:B:899:TRP:CD1	2.45	0.52
1:B:1210:TYR:N	1:B:1213:ASN:OD1	2.36	0.52
1:B:3182:HIS:NE2	1:B:3582:ARG:O	2.40	0.52
1:B:3382:VAL:O	1:B:3383:ASN:C	2.48	0.52
1:A:1205:PRO:O	1:A:1208:TRP:HB3	2.09	0.52
1:B:988:ALA:O	1:B:992:VAL:HG23	2.10	0.52
1:B:2621:ASN:OD1	1:B:3014:ASN:ND2	2.42	0.52
3:F:168:GLU:O	3:F:171:ARG:NH2	2.43	0.52
3:F:241:GLU:HA	3:F:246:TYR:HB2	1.91	0.52
1:A:373:PRO:HB2	1:A:376:ARG:HB3	1.91	0.52
1:A:2620:LEU:HD22	1:A:2631:LEU:HD23	1.91	0.52
1:B:464:ASP:OD1	1:B:465:GLN:N	2.43	0.52
1:B:1965:GLU:HG2	1:B:2026:SER:HB3	1.91	0.52
1:B:2294:GLU:OE1	1:B:2294:GLU:N	2.39	0.52
1:B:3381:ILE:CD1	1:B:3389:CYS:HB3	2.40	0.52
2:D:526:TYR:CE1	2:D:528:TYR:HB2	2.45	0.52
3:F:120:LYS:HA	3:F:159:HIS:CE1	2.43	0.52
1:A:195:HIS:CE1	1:A:264:ARG:HE	2.28	0.52
1:A:1543:ARG:NH1	1:A:1612:GLN:OE1	2.41	0.52
1:A:4179:LEU:HD12	1:A:4223:LEU:HD22	1.92	0.52
1:B:476:LEU:HD22	1:B:591:LEU:HD11	1.91	0.52
1:B:755:TRP:CD2	2:D:453:GLU:HG3	2.44	0.52
1:B:1227:ARG:HH21	1:B:1228:LYS:HZ1	1.56	0.52
1:A:146:TYR:OH	1:B:164:TYR:HB3	2.10	0.51
1:A:195:HIS:CE1	1:A:264:ARG:HB2	2.45	0.51
1:A:340:PRO:HB2	1:A:360:ILE:HB	1.91	0.51
1:A:1929:VAL:H	1:A:2332:ARG:HH21	1.59	0.51
1:A:2807:PHE:CE2	1:A:2811:ARG:HD3	2.46	0.51
1:A:2973:ASP:OD2	1:A:3007:ARG:NH2	2.44	0.51
1:B:331:ASP:OD1	1:B:332:TYR:N	2.43	0.51
1:B:1139:MET:HE1	1:B:1208:TRP:HA	1.92	0.51
2:D:480:THR:HB	2:D:528:TYR:CD2	2.45	0.51
1:A:42:LEU:HB3	1:A:81:ARG:HH21	1.75	0.51
1:A:280:ASN:HA	1:A:283:ARG:NE	2.25	0.51
1:A:368:ARG:HH11	1:A:437:ILE:HD13	1.74	0.51
1:A:1687:LYS:HD3	1:A:1712:THR:HG23	1.91	0.51
1:A:1965:GLU:HG2	1:A:2026:SER:HB3	1.91	0.51
2:D:278:LYS:O	2:D:280:ARG:HG3	2.11	0.51
5:I:8:ILE:HD13	5:I:18:GLN:NE2	2.25	0.51
1:A:136:ARG:HG3	1:B:152:PHE:CE2	2.44	0.51
1:A:1392:GLY:O	1:A:1396:ILE:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3453:VAL:HA	1:B:3459:GLN:OE1	2.11	0.51
1:A:3624:GLU:HG3	1:A:3669:ILE:HD13	1.93	0.51
1:B:694:ASN:ND2	1:B:697:GLU:OE1	2.43	0.51
1:B:2973:ASP:OD2	1:B:3007:ARG:NH2	2.44	0.51
1:B:4413:PHE:HD2	1:B:4504:LEU:HD13	1.75	0.51
1:A:1671:SER:HB2	1:A:1693:THR:HG23	1.92	0.51
1:A:2729:ARG:HD2	1:A:2730:HIS:NE2	2.25	0.51
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	1.93	0.51
1:B:81:ARG:HE	1:B:99:ILE:HG21	1.74	0.51
1:B:286:TYR:O	1:B:290:GLU:HG2	2.11	0.51
1:B:1037:TYR:HB3	3:F:121:PHE:CZ	2.45	0.51
1:B:1093:PHE:CZ	1:B:1113:GLN:HG3	2.46	0.51
1:B:4178:ARG:NH2	1:B:4297:PRO:O	2.43	0.51
1:B:4179:LEU:HD12	1:B:4223:LEU:HD22	1.92	0.51
4:H:26:GLU:HA	4:H:87:PHE:HE2	1.75	0.51
1:A:4517:PRO:HG3	1:A:4611:LEU:HD13	1.93	0.51
1:B:365:ARG:NH2	1:B:432:VAL:HB	2.26	0.51
1:B:717:ILE:HG13	1:B:822:LEU:HB2	1.93	0.51
1:B:755:TRP:CE2	2:D:453:GLU:HA	2.45	0.51
1:B:2807:PHE:CE2	1:B:2811:ARG:HD3	2.45	0.51
1:B:3624:GLU:HG3	1:B:3669:ILE:HD13	1.93	0.51
2:D:429:SER:O	2:D:429:SER:OG	2.28	0.51
1:A:195:HIS:HE1	1:A:264:ARG:HE	1.57	0.51
1:A:3378:ASN:HD22	1:A:3378:ASN:H	1.59	0.51
1:B:106:ASP:OD1	1:B:107:ILE:N	2.38	0.51
1:B:363:HIS:O	1:B:366:LYS:HG2	2.10	0.51
2:D:264:LYS:HG2	2:D:602:GLN:HE22	1.74	0.51
2:D:426:HIS:HD2	2:D:468:ILE:HG21	1.75	0.51
1:A:29:VAL:HA	1:A:32:LYS:HE2	1.92	0.51
1:A:1929:VAL:H	1:A:2332:ARG:NH2	2.09	0.51
1:A:3381:ILE:CD1	1:A:3389:CYS:HB3	2.40	0.51
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.43	0.51
1:B:296:GLU:O	1:B:300:THR:HG23	2.10	0.51
1:B:1033:LEU:O	1:B:1036:SER:OG	2.11	0.51
1:B:1213:ASN:N	5:J:9:LYS:O	2.44	0.51
1:B:1671:SER:HB2	1:B:1693:THR:HG23	1.92	0.51
1:B:1929:VAL:H	1:B:2332:ARG:HH21	1.59	0.51
1:B:2729:ARG:HD2	1:B:2730:HIS:NE2	2.24	0.51
2:D:584:GLU:HA	2:D:598:ASP:HA	1.91	0.51
1:A:193:LEU:HB2	1:B:178:MET:CE	2.41	0.51
1:A:2621:ASN:OD1	1:A:3014:ASN:ND2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:ARG:O	1:B:471:ARG:HG2	2.11	0.51
1:B:1215:GLU:C	1:B:1217:GLU:N	2.63	0.51
1:B:2638:TYR:HB3	1:B:2659:LEU:HD11	1.93	0.51
5:I:68:HIS:CD2	5:I:73:PHE:HB2	2.46	0.51
6:K:77:LEU:HD13	6:L:70:MET:HE3	1.92	0.51
1:B:572:LEU:HD11	1:B:581:MET:HE2	1.92	0.51
1:B:1210:TYR:CG	5:J:8:ILE:HG13	2.46	0.51
1:B:4460:LEU:HD12	1:B:4461:PRO:HD2	1.93	0.51
1:B:4517:PRO:HG3	1:B:4611:LEU:HD13	1.93	0.51
2:D:526:TYR:CZ	2:D:528:TYR:HB2	2.45	0.51
3:F:276:GLU:HG3	3:F:278:LYS:HG3	1.93	0.51
1:A:3211:THR:HG23	1:A:3761:LEU:HD11	1.93	0.51
1:B:59:LYS:HZ1	1:B:63:GLU:HB2	1.74	0.51
1:B:1860:GLN:HG2	1:B:1865:LYS:HG2	1.93	0.51
1:B:3243:MET:CE	1:B:3444:ILE:HG23	2.41	0.51
1:A:21:VAL:HG13	1:A:124:VAL:HG21	1.93	0.50
1:A:117:ALA:HB3	1:A:138:LEU:HB2	1.93	0.50
1:A:385:SER:O	1:A:388:LEU:HB2	2.11	0.50
1:A:3238:ASP:O	1:A:3242:LYS:HG3	2.11	0.50
1:A:4413:PHE:HD2	1:A:4504:LEU:HD13	1.75	0.50
1:B:361:PHE:CG	1:B:426:GLU:HG3	2.46	0.50
1:B:717:ILE:HG22	1:B:718:PHE:CD2	2.46	0.50
3:F:118:LEU:O	3:F:121:PHE:HB3	2.11	0.50
1:A:253:ILE:HG12	1:A:319:ASP:HB3	1.92	0.50
1:A:3194:LEU:HD23	1:A:3500:MET:SD	2.51	0.50
1:A:3383:ASN:O	1:A:3384:ARG:CB	2.56	0.50
1:B:253:ILE:HA	1:B:256:ILE:HG12	1.93	0.50
1:B:368:ARG:NH1	1:B:437:ILE:HD13	2.27	0.50
1:B:526:ALA:O	1:B:553:TYR:CZ	2.64	0.50
1:B:1061:TRP:HB2	1:B:1119:LYS:NZ	2.26	0.50
1:B:1159:ASP:O	1:B:1160:THR:OG1	2.30	0.50
1:B:1199:LYS:HA	1:B:1201:ARG:CZ	2.41	0.50
1:B:2224:GLY:O	1:B:2346:GLN:HA	2.12	0.50
1:B:3750:LEU:HG	1:B:3754:ASN:HD21	1.76	0.50
1:A:85:LYS:HB2	1:A:112:LYS:HE3	1.94	0.50
1:A:150:HIS:CE1	1:A:190:GLU:HA	2.46	0.50
1:A:152:PHE:HZ	1:B:121:ARG:HA	1.77	0.50
1:B:351:ASP:OD2	1:B:352:LYS:N	2.43	0.50
1:B:1929:VAL:H	1:B:2332:ARG:NH2	2.09	0.50
1:B:2487:GLU:O	1:B:2491:GLN:HG3	2.12	0.50
1:B:4009:VAL:HG13	1:B:4013:LEU:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:228:LEU:HD23	3:F:268:ALA:HB3	1.93	0.50
1:A:3750:LEU:HG	1:A:3754:ASN:HD21	1.76	0.50
1:B:68:PHE:HZ	1:B:135:LEU:HD11	1.76	0.50
1:B:1075:ASP:HB3	1:B:1078:LYS:HB3	1.93	0.50
1:B:3378:ASN:H	1:B:3378:ASN:HD22	1.59	0.50
4:G:70:ARG:NH2	4:G:72:ARG:HH21	2.08	0.50
1:A:1435:TRP:O	1:A:1437:VAL:N	2.45	0.50
1:B:378:LEU:HG	1:B:379:ARG:HH21	1.76	0.50
1:B:622:LYS:NZ	2:D:525:ASP:OD2	2.35	0.50
1:B:3194:LEU:HD23	1:B:3500:MET:SD	2.51	0.50
1:B:3211:THR:HG23	1:B:3761:LEU:HD11	1.93	0.50
2:D:409:SER:HB2	2:D:420:ASP:HB3	1.93	0.50
1:A:2917:ASP:OD2	1:A:2921:ARG:NH2	2.45	0.50
1:B:333:ASN:HA	1:B:336:MET:HG2	1.94	0.50
1:B:401:LEU:HB2	1:B:409:PHE:CE1	2.47	0.50
1:B:3319:LEU:HD21	1:B:3377:TYR:CA	2.42	0.50
1:A:1201:ARG:CZ	1:B:968:VAL:HG22	2.42	0.50
1:A:3319:LEU:HD21	1:A:3377:TYR:CA	2.42	0.50
1:B:126:ASP:H	1:B:134:GLN:HE22	1.58	0.50
1:B:213:ILE:HD13	1:B:300:THR:HG22	1.93	0.50
1:B:335:LEU:HD23	1:B:339:PHE:HZ	1.77	0.50
1:B:3238:ASP:O	1:B:3242:LYS:HG3	2.11	0.50
2:C:548:ARG:HA	2:C:566:SER:HA	1.92	0.50
4:G:6:GLU:O	4:G:9:LYS:HG3	2.11	0.50
1:A:146:TYR:OH	1:B:165:ILE:HG23	2.12	0.50
1:A:256:ILE:HA	1:A:259:VAL:HG12	1.94	0.50
1:A:2224:GLY:O	1:A:2346:GLN:HA	2.12	0.50
1:B:526:ALA:O	1:B:529:ASN:N	2.42	0.50
1:B:716:ARG:HG2	3:F:370:LEU:HD11	1.94	0.50
2:D:299:TYR:OH	2:D:302:ASN:HA	2.12	0.50
2:D:343:PHE:HD2	2:D:412:LEU:HD23	1.76	0.50
1:A:235:LYS:HA	1:A:238:ASP:HB2	1.93	0.50
1:A:1860:GLN:HG2	1:A:1865:LYS:HG2	1.93	0.50
1:A:2487:GLU:O	1:A:2491:GLN:HG3	2.12	0.50
1:A:141:SER:OG	1:A:143:ASP:OD1	2.28	0.49
1:A:159:PRO:HD2	1:B:107:ILE:HD11	1.93	0.49
1:A:2174:GLU:OE1	1:A:2176:THR:OG1	2.30	0.49
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.93	0.49
1:B:1205:PRO:O	1:B:1206:PRO:C	2.49	0.49
2:D:478:PRO:HD2	2:D:502:PHE:HB2	1.93	0.49
3:F:262:CYS:HB2	3:F:267:ALA:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:46:MET:HA	4:G:49:PHE:CE2	2.47	0.49
5:J:34:ILE:O	5:J:38:ILE:HG12	2.12	0.49
3:F:142:PRO:O	3:F:336:TYR:OH	2.18	0.49
4:H:17:VAL:HA	4:H:92:GLN:HE22	1.77	0.49
1:A:65:MET:O	1:A:69:LEU:HG	2.12	0.49
1:A:121:ARG:HD2	1:A:136:ARG:HG2	1.93	0.49
1:A:2638:TYR:HB3	1:A:2659:LEU:HD11	1.93	0.49
1:B:161:PHE:O	1:B:165:ILE:HG12	2.12	0.49
1:B:340:PRO:HG2	1:B:360:ILE:HB	1.94	0.49
1:B:3384:ARG:O	1:B:3385:ALA:C	2.51	0.49
2:D:296:VAL:HG13	2:D:340:PHE:CZ	2.47	0.49
2:D:459:ALA:HB2	2:D:468:ILE:HD13	1.94	0.49
2:D:523:ASN:CG	2:D:524:ALA:H	2.15	0.49
1:A:78:LEU:HB3	1:A:104:ASN:HB2	1.95	0.49
1:A:233:GLY:O	1:A:236:VAL:HG12	2.12	0.49
1:A:1929:VAL:HG13	1:A:1958:ASP:OD2	2.12	0.49
1:B:43:GLU:OE2	1:B:81:ARG:NH2	2.38	0.49
1:B:1013:THR:O	1:B:1017:LYS:N	2.41	0.49
1:B:4387:TRP:CD1	1:B:4479:VAL:HG11	2.48	0.49
2:D:288:SER:HB2	2:D:340:PHE:CE1	2.47	0.49
2:D:313:ALA:HB3	2:D:329:PHE:HB3	1.95	0.49
1:A:3384:ARG:O	1:A:3385:ALA:C	2.51	0.49
1:B:701:ASP:OD1	1:B:704:ARG:NH2	2.46	0.49
1:B:2174:GLU:OE1	1:B:2176:THR:OG1	2.30	0.49
2:D:277:SER:CA	2:D:280:ARG:HD2	2.42	0.49
1:A:331:ASP:N	1:A:331:ASP:OD1	2.43	0.49
1:A:4387:TRP:CD1	1:A:4479:VAL:HG11	2.48	0.49
1:B:180:PRO:O	1:B:184:LYS:NZ	2.29	0.49
1:B:980:TYR:HB2	3:F:88:TYR:CE2	2.48	0.49
1:B:1175:SER:HA	1:B:1178:ARG:NH2	2.28	0.49
1:B:2538:GLU:HB3	1:B:2548:TRP:CE2	2.48	0.49
2:D:425:VAL:HG11	2:D:429:SER:HA	1.94	0.49
2:D:504:TRP:CD2	2:D:523:ASN:HB3	2.47	0.49
4:G:70:ARG:HH21	4:G:72:ARG:HH21	1.59	0.49
1:A:1176:LEU:O	1:A:1180:ILE:HG13	2.12	0.49
1:A:3377:TYR:HD1	1:A:3397:ILE:HG12	1.78	0.49
1:A:4180:TYR:OH	1:A:4220:ASP:OD1	2.30	0.49
1:B:23:ASN:O	1:B:126:ASP:HA	2.13	0.49
1:B:35:ARG:NH2	1:B:53:GLU:OE2	2.46	0.49
1:B:354:ARG:O	1:B:357:LEU:HB3	2.12	0.49
1:B:409:PHE:CD2	1:B:470:ARG:HD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:903:LEU:O	1:B:907:ILE:HG12	2.13	0.49
1:B:1211:ILE:HG13	1:B:1212:ASP:OD1	2.12	0.49
1:B:1556:ASP:OD2	1:B:1621:ARG:NH2	2.43	0.49
2:D:320:TYR:CE2	2:D:321:LYS:HG2	2.48	0.49
4:G:69:LEU:HD11	4:H:69:LEU:HD11	1.93	0.49
1:A:1197:LEU:HA	1:A:1200:GLN:HB2	1.95	0.49
1:A:4043:MET:HB3	1:A:4051:ALA:HB3	1.95	0.49
1:B:195:HIS:CE1	1:B:198:GLN:HE21	2.30	0.49
1:B:592:PHE:HA	1:B:597:ILE:HD11	1.94	0.49
1:B:1929:VAL:HG13	1:B:1958:ASP:OD2	2.12	0.49
1:B:2211:TYR:O	1:B:2214:THR:OG1	2.29	0.49
2:D:301:ASN:OD1	2:D:302:ASN:N	2.46	0.49
1:A:4403:GLU:HA	1:A:4406:LYS:HE2	1.95	0.49
1:A:4436:GLN:HG2	1:A:4442:LYS:HG2	1.95	0.49
1:B:185:LYS:O	1:B:189:LEU:HG	2.13	0.49
1:B:1203:GLN:O	1:B:1204:PHE:C	2.50	0.49
1:B:2564:ALA:HB3	1:B:2567:VAL:HG23	1.95	0.49
1:B:2869:ARG:NE	1:B:2869:ARG:HA	2.28	0.49
4:G:23:VAL:HA	4:G:29:PRO:HA	1.94	0.49
1:A:165:ILE:HG23	1:A:170:LYS:HB3	1.94	0.49
1:A:1374:PRO:O	1:A:1378:ARG:N	2.41	0.49
1:A:2869:ARG:NE	1:A:2869:ARG:HA	2.28	0.49
1:B:242:LEU:HB3	1:B:309:ARG:NE	2.27	0.49
1:B:413:MET:HE1	1:B:463:LEU:HB3	1.95	0.49
1:B:4180:TYR:OH	1:B:4220:ASP:OD1	2.30	0.49
1:B:4436:GLN:HG2	1:B:4442:LYS:HG2	1.95	0.49
1:A:423:TRP:HE1	1:A:457:ARG:HH12	1.61	0.48
1:A:578:ALA:O	1:A:583:ARG:N	2.37	0.48
1:A:588:PHE:O	1:A:590:ALA:N	2.46	0.48
1:A:1166:ALA:O	1:A:1170:ILE:HG12	2.13	0.48
1:A:1219:GLY:HA2	1:A:1222:ASN:ND2	2.28	0.48
1:A:2564:ALA:HB3	1:A:2567:VAL:HG23	1.94	0.48
1:B:399:ARG:O	1:B:399:ARG:NH1	2.41	0.48
1:B:1959:GLU:HB3	1:B:1962:ARG:HG3	1.95	0.48
4:H:18:GLN:HB2	4:H:91:ILE:HG23	1.94	0.48
5:I:55:HIS:HE1	5:J:67:THR:O	1.95	0.48
5:J:77:TYR:CE2	5:J:82:ALA:HB2	2.47	0.48
1:A:146:TYR:CZ	1:B:164:TYR:HD2	2.31	0.48
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.48	0.48
1:A:3950:LYS:HB3	1:A:3973:LEU:CD1	2.43	0.48
1:A:4400:ARG:HE	1:A:4405:ILE:HD11	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ARG:HE	1:B:136:ARG:NH2	2.10	0.48
1:B:406:TYR:CD2	1:B:474:GLU:HG2	2.48	0.48
1:B:810:LYS:HE2	3:F:357:GLU:HB3	1.95	0.48
1:B:842:ASN:O	1:B:845:GLU:HG3	2.12	0.48
1:B:1182:GLN:HA	1:B:1185:LYS:HZ2	1.78	0.48
1:B:4400:ARG:HE	1:B:4405:ILE:HD11	1.78	0.48
2:D:352:THR:HG22	2:D:356:GLN:H	1.77	0.48
2:D:620:GLU:HG3	2:D:621:ILE:HG12	1.95	0.48
5:I:17:MET:HA	5:I:20:ASP:HB2	1.95	0.48
1:A:333:ASN:HB3	1:A:337:LYS:HZ3	1.78	0.48
1:A:446:LEU:HD23	1:A:446:LEU:H	1.79	0.48
1:A:462:ARG:NH1	1:A:537:ASP:O	2.46	0.48
1:A:1142:PHE:HA	1:A:1183:PHE:HE1	1.78	0.48
1:A:1647:VAL:HG21	1:A:1670:ASN:HB3	1.95	0.48
1:B:82:SER:O	1:B:100:SER:N	2.41	0.48
1:B:557:ILE:HA	1:B:560:VAL:HG22	1.96	0.48
1:B:1575:PHE:O	1:B:1579:MET:HG2	2.12	0.48
3:F:252:ASP:HB3	3:F:327:PHE:HE1	1.79	0.48
4:G:68:PHE:O	4:H:71:ILE:HG13	2.13	0.48
1:A:143:ASP:OD1	1:A:144:SER:N	2.39	0.48
1:A:364:LEU:O	1:A:367:ILE:HG22	2.13	0.48
1:B:581:MET:HE3	1:B:608:LEU:HD12	1.94	0.48
1:B:2061:THR:OG1	1:B:2133:GLU:OE1	2.28	0.48
1:A:1575:PHE:O	1:A:1579:MET:HG2	2.12	0.48
1:B:35:ARG:HD2	1:B:56:LEU:HD11	1.95	0.48
1:B:1128:LEU:HD21	1:B:1200:GLN:HG3	1.94	0.48
1:B:3377:TYR:HD1	1:B:3397:ILE:HG12	1.78	0.48
1:B:4043:MET:HB3	1:B:4051:ALA:HB3	1.95	0.48
1:A:1172:TYR:O	1:A:1175:SER:OG	2.23	0.48
1:A:3243:MET:SD	1:A:3447:TYR:HB2	2.54	0.48
1:B:80:GLU:HB3	1:B:102:ASN:HB2	1.94	0.48
1:B:388:LEU:O	1:B:391:GLN:HG3	2.14	0.48
1:B:2917:ASP:OD2	1:B:2921:ARG:NH2	2.45	0.48
1:B:4196:TYR:O	1:B:4197:ALA:C	2.52	0.48
1:B:4251:ILE:HG22	1:B:4252:TYR:CD2	2.49	0.48
3:F:230:VAL:HA	3:F:270:ILE:O	2.14	0.48
4:G:53:ALA:HB2	4:H:49:PHE:CE1	2.49	0.48
5:J:54:TRP:NE1	5:J:87:LYS:HB2	2.28	0.48
1:A:130:PRO:HB3	1:B:44:ASP:HB2	1.96	0.48
1:A:1346:MET:O	1:A:1348:GLU:N	2.46	0.48
1:A:1914:GLU:HG2	7:A:4701:ADP:O1A	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:639:ARG:NH1	2:D:528:TYR:CE2	2.80	0.48
1:A:31:GLN:HE21	1:A:56:LEU:HG	1.78	0.48
1:A:266:PRO:HB2	1:A:379:ARG:HB2	1.94	0.48
1:A:2069:ILE:HB	1:A:2137:LEU:HD21	1.96	0.48
1:A:3944:PHE:CE1	1:A:3974:TRP:HB3	2.48	0.48
1:B:185:LYS:O	1:B:188:GLU:HG3	2.14	0.48
1:B:4403:GLU:HA	1:B:4406:LYS:HE2	1.95	0.48
2:D:382:HIS:CG	2:D:404:ASP:HB2	2.49	0.48
1:A:82:SER:HA	1:A:113:SER:HB2	1.95	0.48
1:A:1347:LYS:HA	1:A:1432:GLY:N	2.29	0.48
1:A:4196:TYR:O	1:A:4197:ALA:C	2.52	0.48
1:B:810:LYS:HA	1:B:810:LYS:HD3	1.66	0.48
1:B:1085:GLN:NE2	3:F:39:ILE:HD12	2.29	0.48
1:B:1090:ARG:HH21	1:B:1121:ASP:HA	1.78	0.48
1:B:3243:MET:SD	1:B:3447:TYR:HB2	2.54	0.48
2:D:599:VAL:HG23	2:D:604:ALA:HB2	1.95	0.48
3:F:43:VAL:O	3:F:46:ARG:HG2	2.13	0.48
4:G:69:LEU:H	4:G:79:MET:HE3	1.77	0.48
1:A:171:ALA:HA	1:A:177:LYS:NZ	2.29	0.48
1:A:365:ARG:HD3	1:A:433:LEU:HD13	1.96	0.48
1:A:3452:ALA:CA	1:B:3455:ILE:HD12	2.44	0.48
1:B:365:ARG:HD3	1:B:433:LEU:HD22	1.96	0.48
1:B:1192:ASN:O	1:B:1195:ARG:HB2	2.13	0.48
1:B:1202:PHE:CD2	1:B:1204:PHE:N	2.82	0.48
1:B:3835:ILE:HG12	1:B:3870:ARG:HD2	1.95	0.48
2:D:445:ASN:OD1	2:D:461:ARG:N	2.45	0.48
3:F:59:VAL:HA	3:F:134:ILE:O	2.14	0.48
5:J:6:ALA:HB2	5:J:22:VAL:HG13	1.96	0.48
1:A:3455:ILE:HD12	1:B:3452:ALA:CA	2.43	0.47
1:B:180:PRO:O	1:B:184:LYS:HG2	2.14	0.47
1:B:1647:VAL:HG21	1:B:1670:ASN:HB3	1.95	0.47
1:B:3944:PHE:CE1	1:B:3974:TRP:HB3	2.48	0.47
2:C:433:ALA:O	2:C:452:GLU:N	2.32	0.47
3:F:186:GLU:OE2	3:F:300:ALA:N	2.47	0.47
1:A:309:ARG:HG3	1:A:311:HIS:CE1	2.49	0.47
1:A:4251:ILE:HG22	1:A:4252:TYR:CD2	2.49	0.47
1:B:146:TYR:CE1	1:B:196:LEU:HD22	2.50	0.47
1:A:78:LEU:HD13	1:A:107:ILE:HG22	1.97	0.47
1:A:1931:ASN:HD21	1:A:2316:ASN:HB2	1.79	0.47
1:A:3381:ILE:HG13	1:A:3393:VAL:HB	1.95	0.47
1:A:3731:LEU:HD11	1:A:3790:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:HIS:O	1:B:119:ILE:HA	2.14	0.47
1:B:1042:GLY:O	1:B:1045:SER:OG	2.22	0.47
2:D:279:HIS:NE2	2:D:303:GLU:OE2	2.35	0.47
2:D:401:ILE:HD12	2:D:406:LYS:O	2.14	0.47
6:K:73:ASN:ND2	6:L:75:ALA:HB2	2.30	0.47
1:B:131:VAL:HA	1:B:134:GLN:HB3	1.96	0.47
1:B:717:ILE:HG22	1:B:718:PHE:HD2	1.80	0.47
1:B:1931:ASN:HD21	1:B:2316:ASN:HB2	1.79	0.47
4:H:17:VAL:HA	4:H:92:GLN:NE2	2.28	0.47
1:A:195:HIS:HE1	1:A:264:ARG:HB2	1.80	0.47
1:A:351:ASP:OD1	1:A:352:LYS:N	2.45	0.47
1:A:2138:ILE:HD11	1:A:2165:PHE:CG	2.50	0.47
1:B:487:GLN:H	1:B:567:ARG:NH2	2.12	0.47
1:B:817:ALA:HA	3:F:366:GLN:NE2	2.29	0.47
1:B:969:ILE:CG1	1:B:1058:GLN:HB3	2.44	0.47
1:B:1166:ALA:O	1:B:1170:ILE:HG12	2.15	0.47
1:B:1399:LEU:C	1:B:1401:ILE:N	2.68	0.47
1:B:1914:GLU:HG2	7:B:4701:ADP:O1A	2.13	0.47
1:B:3175:HIS:HB3	1:B:3516:TYR:CE1	2.50	0.47
1:B:4415:ARG:HE	1:B:4415:ARG:HB3	1.54	0.47
2:C:214:GLN:O	2:D:209:ARG:NH2	2.34	0.47
1:B:484:LEU:HD11	1:B:563:ARG:NH1	2.30	0.47
1:B:2751:PHE:HB3	1:B:2803:VAL:HG11	1.96	0.47
2:D:314:LEU:CD2	2:D:316:TRP:HB2	2.45	0.47
5:J:54:TRP:CD1	5:J:87:LYS:HB2	2.50	0.47
1:A:42:LEU:HB3	1:A:81:ARG:NH2	2.29	0.47
1:A:456:HIS:CE1	1:A:460:GLN:HE21	2.32	0.47
1:A:1959:GLU:HB3	1:A:1962:ARG:HG3	1.96	0.47
1:A:3175:HIS:HB3	1:A:3516:TYR:CE1	2.50	0.47
1:A:3835:ILE:HG12	1:A:3870:ARG:HD2	1.95	0.47
1:B:54:ALA:O	1:B:58:GLU:N	2.47	0.47
1:B:720:ILE:HG23	3:F:367:GLN:HG2	1.97	0.47
1:B:2069:ILE:HB	1:B:2137:LEU:HD21	1.96	0.47
1:B:2134:GLN:O	1:B:2138:ILE:HG12	2.15	0.47
1:B:2138:ILE:HD11	1:B:2165:PHE:CG	2.50	0.47
1:B:2179:ARG:NH2	1:B:2195:ASP:OD1	2.43	0.47
1:B:3381:ILE:HG13	1:B:3393:VAL:HB	1.96	0.47
2:D:480:THR:OG1	2:D:528:TYR:O	2.33	0.47
3:F:231:CYS:HB2	3:F:271:TYR:CD1	2.50	0.47
3:F:285:LYS:HB3	3:F:296:PHE:HE1	1.80	0.47
6:L:47:VAL:HG13	6:L:65:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ILE:O	1:A:157:VAL:HG22	2.15	0.47
1:A:365:ARG:HD3	1:A:433:LEU:HD22	1.97	0.47
1:A:676:HIS:O	1:A:680:GLN:N	2.45	0.47
1:B:212:MET:HA	1:B:215:ASN:HD21	1.80	0.47
1:B:382:GLU:O	1:B:386:ARG:HG2	2.15	0.47
1:B:627:TYR:O	1:B:633:CYS:HB3	2.15	0.47
1:B:1205:PRO:O	1:B:1208:TRP:CD1	2.66	0.47
1:B:1227:ARG:HE	1:B:1228:LYS:NZ	2.13	0.47
1:B:3247:GLN:HG3	1:B:3444:ILE:HD13	1.96	0.47
1:B:3950:LYS:HB3	1:B:3973:LEU:CD1	2.44	0.47
1:B:4628:THR:OG1	1:B:4630:GLU:HG2	2.15	0.47
2:D:305:ALA:HB3	2:D:308:GLU:HG2	1.96	0.47
3:F:357:GLU:OE1	3:F:362:PHE:HB2	2.15	0.47
1:A:136:ARG:HE	1:B:139:THR:HG23	1.77	0.47
1:A:152:PHE:CZ	1:B:121:ARG:HA	2.50	0.47
1:A:1181:LYS:HG2	1:A:1185:LYS:NZ	2.28	0.47
1:A:3966:PRO:HG3	1:A:3997:ARG:HG3	1.97	0.47
1:B:347:ALA:HB2	1:B:352:LYS:HZ2	1.80	0.47
1:B:476:LEU:HD13	1:B:591:LEU:HG	1.96	0.47
1:B:779:ILE:HA	1:B:782:ILE:HG22	1.95	0.47
1:B:3175:HIS:CD2	1:B:3585:ARG:HH22	2.32	0.47
3:E:273:SER:O	3:E:277:GLU:N	2.48	0.47
1:A:85:LYS:HE2	1:A:112:LYS:HE3	1.97	0.47
1:A:1761:ASN:HB3	1:A:1781:VAL:HG22	1.96	0.47
1:A:2443:LEU:HD21	1:A:2513:GLU:OE1	2.14	0.47
1:A:3239:LYS:HB3	1:A:3451:TYR:CD2	2.50	0.47
1:B:368:ARG:HH11	1:B:437:ILE:HD13	1.80	0.47
1:B:2386:PRO:HG3	1:B:2413:LEU:HD13	1.97	0.47
1:B:3731:LEU:HD11	1:B:3790:VAL:HG12	1.97	0.47
1:B:3966:PRO:HG3	1:B:3997:ARG:HG3	1.97	0.47
1:A:55:ALA:HB3	1:A:101:TYR:CD2	2.48	0.46
1:A:139:THR:OG1	1:B:136:ARG:HD3	2.15	0.46
1:A:256:ILE:O	1:A:260:THR:OG1	2.11	0.46
1:A:377:ALA:O	1:A:381:VAL:HG23	2.14	0.46
1:A:456:HIS:O	1:A:459:LEU:HB2	2.14	0.46
1:A:2386:PRO:HG3	1:A:2413:LEU:HD13	1.97	0.46
1:A:3553:LEU:HB2	1:A:3578:ILE:HD13	1.97	0.46
1:A:3703:VAL:HG21	1:A:3829:LEU:HD22	1.97	0.46
1:B:424:ASP:O	1:B:428:GLU:HG2	2.15	0.46
1:B:444:GLU:HB3	1:B:446:LEU:HD22	1.96	0.46
1:B:1196:LEU:O	1:B:1200:GLN:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:60:PHE:HE2	3:F:148:SER:HB2	1.80	0.46
1:A:3247:GLN:HG3	1:A:3444:ILE:HD13	1.96	0.46
1:B:915:LEU:HD12	1:B:993:VAL:HB	1.96	0.46
1:B:2443:LEU:HD21	1:B:2513:GLU:OE1	2.14	0.46
3:F:345:VAL:HG22	3:F:347:LYS:H	1.80	0.46
4:G:21:ILE:HG23	4:G:89:ILE:HG13	1.96	0.46
1:A:415:ALA:O	1:A:418:GLU:HG3	2.15	0.46
1:A:4175:GLU:OE1	1:A:4175:GLU:N	2.48	0.46
1:B:49:PRO:HD2	1:B:52:LEU:HD13	1.96	0.46
1:B:581:MET:HG2	1:B:611:ARG:NH2	2.30	0.46
1:B:4423:LEU:HD13	1:B:4466:HIS:ND1	2.31	0.46
2:D:590:SER:OG	2:D:591:GLU:OE1	2.34	0.46
1:A:255:GLU:OE2	1:A:258:LYS:NZ	2.37	0.46
1:A:3236:ALA:O	1:A:3240:LEU:HG	2.16	0.46
1:A:3452:ALA:HA	1:B:3455:ILE:CD1	2.46	0.46
1:B:373:PRO:HB2	1:B:376:ARG:HB3	1.96	0.46
1:B:977:GLU:HG2	3:F:90:TYR:OH	2.15	0.46
1:B:1163:THR:O	1:B:1166:ALA:HB3	2.15	0.46
1:B:1202:PHE:HE2	1:B:1204:PHE:HA	1.79	0.46
1:B:1623:ARG:NH1	1:B:1632:VAL:O	2.48	0.46
1:B:1761:ASN:HB3	1:B:1781:VAL:HG22	1.96	0.46
1:B:3239:LYS:HB3	1:B:3451:TYR:CD2	2.50	0.46
2:D:427:LYS:HG3	2:D:428:GLN:OE1	2.15	0.46
1:A:2091:ARG:NH1	7:A:4701:ADP:H5'2	2.31	0.46
1:A:3455:ILE:CD1	1:B:3452:ALA:HA	2.46	0.46
1:A:4423:LEU:HD13	1:A:4466:HIS:ND1	2.31	0.46
1:B:35:ARG:NH1	1:B:52:LEU:HB3	2.30	0.46
1:B:52:LEU:O	1:B:56:LEU:HG	2.15	0.46
1:B:2091:ARG:NH1	7:B:4701:ADP:H5'2	2.31	0.46
2:D:359:LEU:HD22	2:D:415:LEU:HD13	1.96	0.46
2:D:531:MET:SD	2:D:532:TRP:N	2.89	0.46
5:I:53:THR:HB	5:I:89:GLY:HA3	1.98	0.46
1:A:1879:LEU:HD22	7:A:4701:ADP:C4	2.51	0.46
1:A:2751:PHE:HB3	1:A:2803:VAL:HG11	1.96	0.46
1:A:4628:THR:OG1	1:A:4630:GLU:HG2	2.15	0.46
1:B:434:LEU:HD23	1:B:435:ARG:HH12	1.81	0.46
1:B:543:THR:O	1:B:546:TRP:HB3	2.16	0.46
4:H:9:LYS:HE2	4:H:9:LYS:HA	1.97	0.46
5:J:77:TYR:CZ	5:J:82:ALA:HB2	2.51	0.46
1:A:323:LYS:HG3	1:A:324:GLN:H	1.79	0.46
1:A:1931:ASN:ND2	1:A:2316:ASN:HB2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3601:MET:HG3	1:A:3611:ARG:HH21	1.80	0.46
1:B:591:LEU:HB3	1:B:594:ARG:HB3	1.98	0.46
1:B:786:ARG:NH1	1:B:790:ARG:HH12	2.14	0.46
1:B:1071:ARG:CZ	3:F:43:VAL:HG12	2.46	0.46
1:B:1937:ASP:HA	1:B:1967:MET:HG3	1.98	0.46
1:B:3236:ALA:O	1:B:3240:LEU:HG	2.16	0.46
1:B:3703:VAL:HG21	1:B:3829:LEU:HD22	1.97	0.46
2:D:437:MET:HB3	2:D:449:VAL:HG12	1.97	0.46
6:K:111:LEU:HD11	6:L:64:ILE:HD11	1.97	0.46
1:A:293:GLU:N	1:A:293:GLU:OE1	2.48	0.46
1:A:331:ASP:HB3	1:A:370:THR:HB	1.96	0.46
1:A:354:ARG:HB3	1:A:419:VAL:HG13	1.98	0.46
1:A:1172:TYR:CE2	1:A:1176:LEU:HD11	2.51	0.46
1:A:1556:ASP:OD2	1:A:1621:ARG:NH2	2.43	0.46
1:A:3243:MET:CE	1:A:3444:ILE:HG23	2.41	0.46
1:B:186:ILE:O	1:B:190:GLU:HG2	2.16	0.46
1:B:399:ARG:HE	1:B:412:VAL:HG11	1.81	0.46
1:B:439:LYS:O	1:B:442:ARG:HD3	2.15	0.46
1:B:1931:ASN:ND2	1:B:2316:ASN:HB2	2.31	0.46
1:B:2445:HIS:HB3	1:B:2505:ASP:OD2	2.15	0.46
1:B:3921:THR:HG21	1:B:3933:GLU:HG2	1.98	0.46
2:D:392:THR:HG22	2:D:395:ALA:HB3	1.96	0.46
2:D:465:LYS:HB3	2:D:465:LYS:HE3	1.79	0.46
1:A:1229:ASP:OD2	1:A:1233:GLN:NE2	2.47	0.46
1:A:2790:PRO:HB3	1:A:3076:LYS:HG2	1.98	0.46
1:A:3175:HIS:CD2	1:A:3585:ARG:HH22	2.32	0.46
1:A:3239:LYS:HB3	1:A:3451:TYR:CD1	2.51	0.46
1:A:3921:THR:HG21	1:A:3933:GLU:HG2	1.98	0.46
1:B:146:TYR:CZ	1:B:196:LEU:HD22	2.51	0.46
1:B:1209:LEU:CB	1:B:1214:ILE:HG23	2.45	0.46
2:D:329:PHE:CE2	2:D:360:TRP:HB2	2.51	0.46
2:D:401:ILE:HG12	2:D:434:VAL:HG11	1.98	0.46
2:D:504:TRP:CZ3	2:D:523:ASN:HB3	2.51	0.46
4:H:66:LEU:HD21	4:H:69:LEU:HB2	1.97	0.46
5:I:65:TYR:CD2	5:J:40:ALA:HA	2.51	0.46
1:A:191:MET:HA	1:A:194:LEU:HD21	1.97	0.46
1:A:257:GLN:NE2	1:A:320:THR:O	2.37	0.46
1:B:30:LEU:O	1:B:34:LEU:HG	2.16	0.46
1:B:33:HIS:HA	1:B:36:LYS:HZ2	1.81	0.46
1:B:277:PHE:O	1:B:281:LEU:HG	2.16	0.46
1:B:1176:LEU:HA	1:B:1179:LYS:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3553:LEU:HB2	1:B:3578:ILE:HD13	1.97	0.46
2:D:286:ASP:OD1	2:D:287:TRP:N	2.48	0.46
2:D:458:THR:O	2:D:469:SER:OG	2.21	0.46
5:I:63:GLY:HA2	5:J:36:LYS:HE2	1.98	0.46
1:A:282:GLU:O	1:A:285:LEU:HG	2.16	0.45
1:A:288:ILE:HD11	1:A:322:LEU:HD22	1.97	0.45
1:A:2290:SER:HB2	1:A:2295:LEU:HG	1.99	0.45
1:A:2445:HIS:HB3	1:A:2505:ASP:OD2	2.15	0.45
1:B:1071:ARG:HH11	3:F:46:ARG:HD2	1.80	0.45
1:B:2290:SER:HB2	1:B:2295:LEU:HG	1.99	0.45
1:B:3110:THR:O	1:B:3140:ARG:NH1	2.49	0.45
3:F:88:TYR:O	3:F:89:LEU:HD12	2.16	0.45
1:A:223:ARG:HH12	1:A:228:LYS:NZ	2.14	0.45
1:A:337:LYS:HD2	1:A:363:HIS:C	2.36	0.45
1:A:3117:LYS:HE2	1:A:3139:HIS:CD2	2.51	0.45
1:B:186:ILE:HA	1:B:189:LEU:HD12	1.98	0.45
1:B:338:ASP:OD1	1:B:339:PHE:N	2.49	0.45
1:B:516:ASP:HA	1:B:563:ARG:NH1	2.22	0.45
1:B:1069:TYR:CE1	1:B:1130:LYS:HG2	2.52	0.45
1:B:4034:GLU:OE1	1:B:4143:ARG:NH1	2.41	0.45
1:B:4160:THR:HG23	1:B:4212:LEU:HD21	1.99	0.45
3:F:55:LYS:HB2	3:F:104:CYS:SG	2.56	0.45
1:A:22:GLN:NE2	1:A:134:GLN:OE1	2.49	0.45
1:A:2134:GLN:O	1:A:2138:ILE:HG12	2.15	0.45
1:A:3110:THR:O	1:A:3140:ARG:NH1	2.49	0.45
1:B:277:PHE:CE2	1:B:281:LEU:HD11	2.51	0.45
1:B:635:MET:HB3	1:B:635:MET:HE2	1.70	0.45
1:B:1212:ASP:O	1:B:1214:ILE:N	2.49	0.45
1:B:1721:VAL:HA	1:B:1724:VAL:HG12	1.98	0.45
1:B:4517:PRO:HG2	1:B:4619:ILE:HD12	1.98	0.45
2:D:357:ILE:H	2:D:357:ILE:HD12	1.82	0.45
4:G:76:ASN:HA	4:G:94:PRO:HD3	1.97	0.45
4:G:78:ILE:HD11	4:G:89:ILE:HB	1.97	0.45
1:A:335:LEU:HB3	1:A:339:PHE:CZ	2.50	0.45
1:B:641:LEU:HD23	1:B:641:LEU:HA	1.79	0.45
1:B:770:GLN:HG2	1:B:773:GLN:NE2	2.29	0.45
1:B:1879:LEU:HD22	7:B:4701:ADP:C4	2.51	0.45
2:C:264:LYS:O	2:C:600:GLY:N	2.50	0.45
4:G:45:LEU:HD21	4:H:56:THR:HA	1.99	0.45
6:K:43:THR:HG23	6:K:69:ILE:HD12	1.98	0.45
1:A:350:LEU:HA	1:A:353:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1071:ARG:NH1	3:F:43:VAL:HA	2.32	0.45
1:B:1198:GLU:HA	1:B:1204:PHE:CZ	2.45	0.45
1:B:1204:PHE:HD2	1:B:1208:TRP:HZ2	1.63	0.45
1:A:322:LEU:O	1:A:326:LEU:N	2.47	0.45
1:A:382:GLU:O	1:A:385:SER:OG	2.35	0.45
1:B:518:ASN:O	1:B:521:GLU:HG2	2.16	0.45
1:B:1135:LEU:O	1:B:1139:MET:HG3	2.17	0.45
1:B:1139:MET:CE	1:B:1209:LEU:H	2.30	0.45
1:B:1210:TYR:N	1:B:1213:ASN:CB	2.78	0.45
1:B:2961:ILE:HD11	1:B:2998:ASN:HB3	1.98	0.45
1:B:3117:LYS:HE2	1:B:3139:HIS:CD2	2.51	0.45
1:B:3601:MET:HG3	1:B:3611:ARG:HH21	1.80	0.45
1:B:4175:GLU:N	1:B:4175:GLU:OE1	2.48	0.45
2:D:284:CYS:SG	2:D:285:LEU:N	2.90	0.45
3:F:62:GLU:OE2	3:F:141:ARG:NH2	2.45	0.45
1:A:177:LYS:HD3	1:A:177:LYS:HA	1.69	0.45
1:A:1635:GLU:HA	1:A:1638:LEU:HD12	1.98	0.45
1:A:3243:MET:HE3	1:A:3444:ILE:HA	1.99	0.45
1:A:4100:HIS:HB3	1:A:4128:MET:HB2	1.99	0.45
1:B:213:ILE:HG13	1:B:232:PHE:CE1	2.52	0.45
1:B:440:ARG:NH1	1:B:444:GLU:HB2	2.31	0.45
1:B:1078:LYS:O	1:B:1082:LEU:HD23	2.16	0.45
1:B:3239:LYS:HB3	1:B:3451:TYR:CD1	2.51	0.45
2:D:446:ASN:HA	2:D:460:CYS:HA	1.98	0.45
4:H:22:VAL:H	4:H:31:LYS:NZ	2.13	0.45
1:A:339:PHE:HB2	1:A:340:PRO:HD3	1.98	0.45
1:B:283:ARG:HG3	1:B:287:ARG:HH12	1.81	0.45
1:B:363:HIS:HA	1:B:366:LYS:HD3	1.99	0.45
1:B:780:SER:O	1:B:783:GLU:HG3	2.17	0.45
3:F:165:ILE:HD13	3:F:170:MET:HB2	1.99	0.45
1:A:27:VAL:HG22	1:A:65:MET:SD	2.57	0.45
1:A:152:PHE:HE1	1:B:119:ILE:O	2.00	0.45
1:A:689:PHE:O	1:A:693:LEU:N	2.47	0.45
1:A:2668:LEU:HD21	1:A:2720:ARG:CZ	2.47	0.45
1:B:301:LEU:HD12	1:B:304:LEU:HD11	1.99	0.45
1:B:391:GLN:HB2	1:B:394:LYS:HE3	1.99	0.45
1:B:1224:ILE:HG23	1:B:1228:LYS:NZ	2.32	0.45
1:B:1997:ILE:H	1:B:1997:ILE:HD12	1.82	0.45
1:B:3217:GLU:HB2	1:B:3220:ARG:HH21	1.82	0.45
2:D:282:VAL:HG11	2:D:588:GLY:HA3	1.98	0.45
1:A:1456:GLU:O	1:A:1516:PHE:HE2	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.98	0.45
1:A:2028:LEU:HG	1:A:2032:LEU:HD23	1.99	0.45
1:A:2963:VAL:HG23	1:A:3643:PRO:HB2	1.99	0.45
1:A:3239:LYS:HD3	1:A:3451:TYR:CE1	2.52	0.45
1:B:161:PHE:HE2	1:B:183:GLU:HG3	1.81	0.45
1:B:659:THR:C	1:B:663:LYS:HZ2	2.20	0.45
1:B:760:VAL:HG23	1:B:765:VAL:HG22	1.99	0.45
1:B:1037:TYR:O	1:B:1040:VAL:HB	2.16	0.45
1:B:2028:LEU:HG	1:B:2032:LEU:HD23	1.99	0.45
1:B:2668:LEU:HD21	1:B:2720:ARG:CZ	2.47	0.45
1:B:3239:LYS:HD3	1:B:3451:TYR:CE1	2.52	0.45
1:B:4401:THR:O	1:B:4405:ILE:HG12	2.17	0.45
2:D:308:GLU:HB2	2:D:309:PRO:HD2	1.99	0.45
2:D:331:CYS:SG	2:D:358:VAL:HG11	2.57	0.45
4:G:71:ILE:HB	4:G:78:ILE:HG23	1.99	0.45
6:K:25:ILE:HG23	6:K:29:ILE:HD12	2.00	0.45
1:A:157:VAL:O	1:A:161:PHE:N	2.30	0.44
1:A:164:TYR:HD2	1:B:109:TYR:CZ	2.36	0.44
1:A:990:LYS:O	1:A:994:LEU:N	2.50	0.44
1:A:3257:SER:HA	1:A:3260:ILE:HD12	1.99	0.44
1:B:251:ARG:NH2	1:B:255:GLU:HB2	2.31	0.44
1:B:1026:MET:HG2	1:B:1029:GLY:O	2.18	0.44
1:B:4189:ILE:O	1:B:4193:ARG:HG3	2.17	0.44
1:B:4412:PHE:HZ	1:B:4514:LEU:HD13	1.82	0.44
2:D:364:SER:HB2	2:D:366:LYS:HE3	2.00	0.44
3:E:279:ASN:O	3:E:283:LEU:N	2.42	0.44
4:G:71:ILE:HD13	4:H:69:LEU:HD13	1.98	0.44
5:J:9:LYS:HG2	5:J:76:PHE:HA	1.97	0.44
1:A:1623:ARG:NH1	1:A:1632:VAL:O	2.48	0.44
1:A:2912:PHE:CE2	1:A:2914:GLU:HB2	2.52	0.44
1:A:3659:ARG:HG3	1:B:3629:PHE:HZ	1.82	0.44
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.99	0.44
1:A:4517:PRO:HG2	1:A:4619:ILE:HD12	1.98	0.44
1:B:182:VAL:HA	1:B:185:LYS:HD3	1.98	0.44
1:B:459:LEU:O	1:B:463:LEU:HG	2.17	0.44
1:B:485:ARG:O	1:B:487:GLN:NE2	2.50	0.44
1:B:3096:ASP:OD1	1:B:3097:TRP:N	2.50	0.44
1:B:3160:ARG:O	1:B:3163:LYS:HG2	2.17	0.44
2:D:212:SER:HA	2:D:320:TYR:OH	2.17	0.44
3:F:152:TRP:O	3:F:155:VAL:HB	2.16	0.44
4:H:37:PRO:O	4:H:41:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LYS:HZ2	1:A:179:ALA:HB3	1.82	0.44
1:A:1937:ASP:HA	1:A:1967:MET:HG3	1.98	0.44
1:A:4189:ILE:O	1:A:4193:ARG:HG3	2.17	0.44
1:B:64:GLN:HB3	1:B:105:ILE:HD11	1.99	0.44
1:B:193:LEU:O	1:B:196:LEU:HB2	2.17	0.44
1:B:414:VAL:HG22	1:B:467:ARG:HH22	1.82	0.44
1:B:439:LYS:HG2	1:B:442:ARG:CZ	2.47	0.44
1:B:462:ARG:HE	1:B:537:ASP:HB2	1.81	0.44
1:B:674:GLU:HB2	1:B:683:LYS:HD3	1.98	0.44
1:B:1179:LYS:O	1:B:1182:GLN:HB2	2.17	0.44
1:B:2548:TRP:CD1	1:B:2576:ARG:HG2	2.53	0.44
1:B:2790:PRO:HB3	1:B:3076:LYS:HG2	1.98	0.44
1:B:4172:SER:HB2	1:B:4173:PRO:HD3	1.98	0.44
4:G:23:VAL:HG11	4:G:43:ALA:HB1	2.00	0.44
4:H:7:THR:O	4:H:11:LEU:HD23	2.17	0.44
1:A:1697:LYS:HB3	1:A:1700:GLU:OE1	2.18	0.44
1:A:1997:ILE:H	1:A:1997:ILE:HD12	1.82	0.44
1:A:2206:LYS:HD3	1:A:2206:LYS:HA	1.86	0.44
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.98	0.44
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.98	0.44
1:A:4087:ALA:HA	1:A:4092:ARG:HB3	1.98	0.44
1:B:967:GLN:HG2	1:B:1061:TRP:CD2	2.53	0.44
1:B:1060:LEU:HD22	1:B:1119:LYS:HE2	2.00	0.44
1:B:1090:ARG:HH22	1:B:1124:HIS:HB3	1.81	0.44
1:B:1697:LYS:HB3	1:B:1700:GLU:OE1	2.18	0.44
1:B:2437:LEU:HD21	1:B:2451:ARG:HG3	1.98	0.44
1:B:2912:PHE:CE2	1:B:2914:GLU:HB2	2.52	0.44
2:C:205:ARG:NH2	2:C:209:ARG:HH21	2.15	0.44
2:C:207:VAL:O	2:C:211:LEU:HG	2.18	0.44
1:A:52:LEU:HD12	1:A:101:TYR:CD1	2.52	0.44
1:A:365:ARG:NH1	1:A:436:ASP:OD2	2.51	0.44
1:A:2061:THR:OG1	1:A:2133:GLU:OE1	2.28	0.44
1:A:2975:ASP:O	1:A:2979:VAL:HG23	2.18	0.44
1:A:4412:PHE:HZ	1:A:4514:LEU:HD13	1.82	0.44
1:B:435:ARG:HH21	1:B:438:VAL:HG21	1.82	0.44
1:B:1068:ILE:O	1:B:1072:LEU:HG	2.17	0.44
4:G:3:GLU:HG3	4:G:6:GLU:H	1.82	0.44
6:K:68:VAL:HG22	6:L:79:THR:HG22	2.00	0.44
1:A:195:HIS:HE1	1:A:264:ARG:NE	2.14	0.44
1:A:1571:ILE:HD13	1:A:1607:LEU:HB3	1.99	0.44
1:A:2548:TRP:CD1	1:A:2576:ARG:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2776:PHE:HZ	1:A:2846:THR:HG23	1.83	0.44
1:A:4185:TRP:O	1:A:4189:ILE:HG12	2.17	0.44
1:B:1124:HIS:NE2	1:B:1128:LEU:HD11	2.33	0.44
1:B:1197:LEU:HD23	1:B:1208:TRP:CH2	2.52	0.44
1:B:4100:HIS:HB3	1:B:4128:MET:HB2	1.99	0.44
2:D:386:CYS:SG	2:D:437:MET:HG3	2.58	0.44
5:J:75:TYR:CE1	5:J:82:ALA:HB1	2.53	0.44
1:A:41:LEU:HA	1:B:132:SER:HB2	1.98	0.44
1:A:213:ILE:HB	1:A:241:PHE:CZ	2.53	0.44
1:A:213:ILE:HD12	1:A:303:ILE:HD11	1.99	0.44
1:A:1724:VAL:HG11	1:A:1753:SER:HB3	2.00	0.44
1:B:333:ASN:O	1:B:336:MET:HG2	2.18	0.44
1:B:389:SER:O	1:B:393:LEU:HG	2.18	0.44
1:B:441:LYS:HZ2	1:B:450:TRP:HH2	1.64	0.44
1:B:525:LEU:HA	1:B:528:GLU:CD	2.38	0.44
1:B:1060:LEU:HD22	1:B:1119:LYS:HG2	2.00	0.44
1:B:1095:ASN:OD1	1:B:1096:ALA:N	2.48	0.44
1:B:1231:ALA:HA	1:B:1234:GLN:OE1	2.17	0.44
1:B:1456:GLU:O	1:B:1516:PHE:HE2	2.00	0.44
1:B:3485:GLU:HG3	1:B:3488:ARG:HH22	1.83	0.44
1:B:3880:HIS:ND1	1:B:4021:MET:HG3	2.33	0.44
3:F:38:SER:OG	3:F:39:ILE:N	2.50	0.44
1:A:1170:ILE:O	1:A:1174:GLN:HG2	2.18	0.44
1:A:1625:SER:HB2	1:A:1699:ASN:ND2	2.33	0.44
1:B:479:VAL:HG22	1:B:483:VAL:HG21	1.99	0.44
1:B:969:ILE:HG12	1:B:1058:GLN:HB3	1.99	0.44
1:B:1190:TYR:O	1:B:1194:GLN:HG3	2.18	0.44
1:B:1635:GLU:HA	1:B:1638:LEU:HD12	1.98	0.44
1:B:4087:ALA:HA	1:B:4092:ARG:HB3	1.98	0.44
2:D:539:LEU:HD21	2:D:551:LEU:HD11	2.00	0.44
5:I:52:PRO:HA	5:I:53:THR:HA	1.80	0.44
5:J:9:LYS:HE3	5:J:77:TYR:CD1	2.53	0.44
1:A:3217:GLU:HB2	1:A:3220:ARG:HH21	1.82	0.44
1:A:3485:GLU:HG3	1:A:3488:ARG:HH22	1.83	0.44
1:A:4186:PHE:O	1:A:4190:ILE:HG12	2.18	0.44
1:A:4190:ILE:HD12	1:A:4201:TRP:CZ2	2.45	0.44
1:B:1170:ILE:HG22	1:B:1174:GLN:HE22	1.83	0.44
1:B:1625:SER:HB2	1:B:1699:ASN:ND2	2.33	0.44
1:B:2776:PHE:HZ	1:B:2846:THR:HG23	1.83	0.44
1:A:1346:MET:O	1:A:1349:GLN:N	2.50	0.43
1:A:1980:GLU:OE2	1:A:1983:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4401:THR:O	1:A:4405:ILE:HG12	2.17	0.43
1:B:956:LYS:N	1:B:985:GLU:OE2	2.39	0.43
1:B:2961:ILE:HG13	1:B:2963:VAL:HG13	2.00	0.43
1:B:2963:VAL:HG23	1:B:3643:PRO:HB2	1.99	0.43
2:C:214:GLN:C	2:D:209:ARG:HH12	2.22	0.43
2:D:480:THR:HB	2:D:528:TYR:CE2	2.52	0.43
1:A:344:LEU:HD21	1:A:388:LEU:HD23	2.00	0.43
1:A:3160:ARG:O	1:A:3163:LYS:HG2	2.17	0.43
1:A:3370:ASN:OD1	1:A:3377:TYR:CZ	2.72	0.43
1:B:522:GLU:O	1:B:525:LEU:HG	2.18	0.43
1:B:717:ILE:HA	1:B:824:TRP:CE3	2.46	0.43
1:B:921:ALA:O	1:B:924:GLN:HG3	2.18	0.43
1:B:926:LEU:HD13	1:B:1104:PRO:HG3	2.00	0.43
1:B:2557:VAL:O	1:B:2757:ARG:NH2	2.52	0.43
1:B:3232:LYS:HA	1:B:3232:LYS:HD3	1.76	0.43
3:F:366:GLN:OE1	3:F:366:GLN:HA	2.18	0.43
5:J:32:TYR:HB2	5:J:38:ILE:HD13	2.01	0.43
1:A:182:VAL:O	1:A:186:ILE:HG13	2.18	0.43
1:A:3194:LEU:HD21	1:A:3499:GLN:HB2	2.01	0.43
1:A:3629:PHE:HZ	1:B:3659:ARG:HG3	1.83	0.43
1:B:252:TRP:O	1:B:256:ILE:HG23	2.18	0.43
1:B:255:GLU:O	1:B:258:LYS:HG2	2.19	0.43
1:B:287:ARG:HA	1:B:290:GLU:HG2	1.99	0.43
1:B:368:ARG:NH2	1:B:436:ASP:O	2.51	0.43
1:B:572:LEU:HD23	1:B:604:TYR:HD2	1.83	0.43
1:B:860:GLU:OE2	1:B:880:ARG:HB2	2.18	0.43
1:B:882:GLN:HE22	1:B:999:ILE:HA	1.83	0.43
1:B:1490:TRP:HZ3	1:B:1534:PHE:HB3	1.83	0.43
1:B:2457:SER:O	1:B:2461:MET:HG3	2.18	0.43
1:B:4437:VAL:HG21	1:B:4448:LEU:HD13	2.00	0.43
2:C:204:THR:HA	4:G:10:ARG:NH1	2.33	0.43
2:D:387:VAL:HG12	2:D:400:SER:HB2	2.01	0.43
4:H:70:ARG:HB3	4:H:79:MET:SD	2.59	0.43
5:I:13:MET:HE2	5:I:18:GLN:HA	2.00	0.43
1:A:170:LYS:HE2	1:A:176:ASP:HB3	2.00	0.43
1:A:235:LYS:HB3	1:A:241:PHE:CG	2.54	0.43
1:A:270:THR:H	1:A:273:GLN:HB2	1.83	0.43
1:A:285:LEU:HB2	1:A:322:LEU:HD21	2.00	0.43
1:A:388:LEU:O	1:A:391:GLN:HG3	2.18	0.43
1:A:1189:LEU:O	1:A:1192:ASN:HB3	2.18	0.43
1:A:3148:VAL:O	1:A:3152:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3514:ILE:HD11	1:A:3553:LEU:HD13	2.00	0.43
1:B:157:VAL:O	1:B:161:PHE:HB3	2.18	0.43
1:B:330:ASN:O	1:B:334:PRO:HD3	2.18	0.43
1:B:347:ALA:HA	1:B:352:LYS:HD3	1.99	0.43
1:B:468:LYS:HE3	1:B:468:LYS:HB3	1.88	0.43
1:B:718:PHE:CE1	1:B:820:ILE:HD13	2.53	0.43
1:B:860:GLU:HG2	1:B:877:ILE:HG23	2.00	0.43
1:B:1071:ARG:NH1	3:F:46:ARG:HD2	2.33	0.43
1:B:4297:PRO:HB3	1:B:4308:TRP:CD1	2.54	0.43
3:F:41:SER:O	3:F:44:SER:OG	2.24	0.43
3:F:95:ASP:HB2	3:F:294:PHE:CZ	2.53	0.43
1:A:31:GLN:HB3	1:A:35:ARG:HH21	1.83	0.43
1:A:118:PHE:CE1	1:A:137:VAL:HG23	2.53	0.43
1:A:146:TYR:OH	1:B:161:PHE:O	2.36	0.43
1:A:185:LYS:CE	1:B:189:LEU:HA	2.48	0.43
1:A:1353:SER:O	1:A:1354:VAL:C	2.56	0.43
1:A:1666:LEU:HD23	1:A:1673:VAL:HA	2.00	0.43
1:A:4172:SER:HB2	1:A:4173:PRO:HD3	1.98	0.43
1:B:410:GLU:HB3	1:B:471:ARG:NH2	2.33	0.43
1:B:433:LEU:O	1:B:437:ILE:HG12	2.17	0.43
1:B:1050:TYR:CD1	1:B:1100:LYS:HD2	2.52	0.43
1:B:1177:LYS:HA	1:B:1180:ILE:HD12	2.01	0.43
1:B:1182:GLN:O	1:B:1185:LYS:HG2	2.19	0.43
1:B:1724:VAL:HG11	1:B:1753:SER:HB3	2.00	0.43
4:H:3:GLU:OE2	4:H:10:ARG:NH2	2.35	0.43
4:H:22:VAL:HB	4:H:31:LYS:HZ2	1.83	0.43
5:J:56:CYS:HA	5:J:84:LEU:O	2.19	0.43
1:A:2079:GLN:HB2	1:A:2160:LEU:HD11	2.00	0.43
1:A:2538:GLU:HB3	1:A:2548:TRP:CZ2	2.54	0.43
1:A:2557:VAL:O	1:A:2757:ARG:NH2	2.52	0.43
1:B:58:GLU:OE2	1:B:60:SER:OG	2.31	0.43
1:B:146:TYR:CG	1:B:196:LEU:HB3	2.54	0.43
1:B:377:ALA:O	1:B:381:VAL:HG23	2.19	0.43
1:B:456:HIS:CE1	1:B:460:GLN:HB2	2.53	0.43
1:B:462:ARG:HH22	1:B:535:GLY:C	2.22	0.43
1:B:1156:HIS:CE1	1:B:1166:ALA:HA	2.53	0.43
1:B:3154:LEU:HG	1:B:3516:TYR:CD1	2.54	0.43
1:B:4415:ARG:O	1:B:4419:MET:HG2	2.18	0.43
3:F:70:LEU:O	3:F:74:LEU:HD23	2.18	0.43
4:G:64:ASN:HA	4:H:75:LYS:HD3	2.00	0.43
6:K:35:GLN:H	6:K:42:TRP:HZ3	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:TYR:HA	1:B:109:TYR:CD2	2.53	0.43
1:A:284:ALA:O	1:A:287:ARG:HG2	2.18	0.43
1:A:1195:ARG:NH2	3:F:99:ASP:HB2	2.34	0.43
1:A:3291:GLU:O	1:A:3395:TRP:NE1	2.52	0.43
1:B:35:ARG:HH22	1:B:53:GLU:HG2	1.84	0.43
1:B:336:MET:HA	1:B:339:PHE:CE2	2.43	0.43
1:B:525:LEU:HA	1:B:528:GLU:OE2	2.19	0.43
1:B:598:ARG:O	1:B:601:ILE:HG22	2.19	0.43
1:B:997:PRO:HA	1:B:1018:PHE:HA	2.00	0.43
1:B:1090:ARG:HH22	1:B:1124:HIS:CB	2.32	0.43
1:B:2230:LYS:HG2	1:B:2364:PHE:CG	2.54	0.43
1:B:4185:TRP:O	1:B:4189:ILE:HG12	2.18	0.43
3:F:321:ALA:HA	3:F:324:HIS:CD2	2.53	0.43
4:G:21:ILE:HB	4:G:33:THR:OG1	2.19	0.43
5:I:67:THR:O	5:J:55:HIS:HE1	2.01	0.43
6:K:29:ILE:HD13	6:K:102:MET:HE1	2.00	0.43
1:A:288:ILE:HA	1:A:291:LYS:HB3	2.01	0.43
1:A:391:GLN:HA	1:A:394:LYS:HE2	2.00	0.43
1:A:1834:LYS:HA	1:A:1834:LYS:HD3	1.88	0.43
1:A:2457:SER:O	1:A:2461:MET:HG3	2.18	0.43
1:A:3880:HIS:ND1	1:A:4021:MET:HG3	2.33	0.43
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	2.01	0.43
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	2.00	0.43
1:B:101:TYR:CG	1:B:102:ASN:N	2.86	0.43
1:B:211:PRO:O	1:B:215:ASN:ND2	2.51	0.43
1:B:580:GLU:O	1:B:584:ILE:HG13	2.19	0.43
1:B:959:VAL:HA	1:B:1106:VAL:O	2.18	0.43
1:B:2144:THR:HG22	1:B:2145:MET:HE2	2.01	0.43
1:B:2975:ASP:O	1:B:2979:VAL:HG23	2.18	0.43
1:B:4227:ALA:HB2	1:B:4233:ILE:HD12	2.00	0.43
1:B:4246:LEU:HD23	1:B:4246:LEU:HA	1.90	0.43
3:F:337:GLU:OE1	3:F:337:GLU:N	2.49	0.43
5:I:53:THR:HG21	5:J:67:THR:HB	2.00	0.43
5:J:9:LYS:H	5:J:76:PHE:HA	1.83	0.43
6:L:72:LYS:HE2	6:L:103:TYR:CE1	2.53	0.43
1:A:118:PHE:HB3	1:A:135:LEU:HD11	2.01	0.43
1:A:1459:LEU:H	1:A:1459:LEU:HD12	1.83	0.43
1:A:2230:LYS:HG2	1:A:2364:PHE:CG	2.54	0.43
1:A:2457:SER:HB2	1:A:2732:PRO:HB3	2.01	0.43
1:B:462:ARG:HH21	1:B:537:ASP:HB2	1.84	0.43
1:B:908:GLU:HB2	1:B:1019:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1899:ARG:N	1:B:1899:ARG:HD2	2.34	0.43
1:B:3291:GLU:O	1:B:3395:TRP:NE1	2.52	0.43
1:B:3514:ILE:HD11	1:B:3553:LEU:HD13	2.00	0.43
1:B:4186:PHE:O	1:B:4190:ILE:HG12	2.18	0.43
3:F:238:SER:O	3:F:241:GLU:HB3	2.19	0.43
1:A:39:PRO:HG3	1:A:48:ALA:H	1.84	0.43
1:A:107:ILE:HD11	1:B:159:PRO:HD2	2.01	0.43
1:A:1899:ARG:N	1:A:1899:ARG:HD2	2.34	0.43
1:A:3485:GLU:OE2	1:A:3774:LYS:NZ	2.43	0.43
1:B:304:LEU:HD13	1:B:309:ARG:HB3	2.00	0.43
1:B:368:ARG:HD2	1:B:368:ARG:HA	1.82	0.43
1:B:530:VAL:HG22	1:B:553:TYR:CE2	2.53	0.43
1:B:579:ASN:O	1:B:583:ARG:HG3	2.19	0.43
1:B:774:LEU:HD12	1:B:774:LEU:HA	1.84	0.43
1:B:1023:LEU:HD12	1:B:1033:LEU:HD22	2.01	0.43
1:B:1163:THR:HA	1:B:1166:ALA:HB3	2.01	0.43
1:B:1209:LEU:C	1:B:1210:TYR:HD2	2.22	0.43
1:B:1213:ASN:CA	5:J:9:LYS:O	2.67	0.43
1:B:1980:GLU:OE2	1:B:1983:ARG:NH1	2.51	0.43
1:B:2079:GLN:HB2	1:B:2160:LEU:HD11	2.00	0.43
1:B:2784:PHE:HB3	1:B:2792:TYR:CD2	2.54	0.43
1:B:2882:ILE:HB	1:B:2883:PRO:HD2	2.01	0.43
1:B:3381:ILE:CG1	1:B:3393:VAL:CG1	2.82	0.43
1:B:4173:PRO:HD2	1:B:4176:ARG:HH21	1.84	0.43
1:B:4611:LEU:HB2	1:B:4619:ILE:HD11	2.00	0.43
2:D:287:TRP:CZ2	2:D:295:LEU:HD12	2.54	0.43
1:A:55:ALA:HA	1:A:58:GLU:HB2	2.01	0.42
1:A:189:LEU:CD2	1:B:185:LYS:HB3	2.48	0.42
1:A:278:TRP:O	1:A:281:LEU:HG	2.19	0.42
1:A:2882:ILE:HB	1:A:2883:PRO:HD2	2.01	0.42
1:A:3745:LEU:HD13	1:A:3777:ALA:HA	2.01	0.42
1:A:4297:PRO:HB3	1:A:4308:TRP:CD1	2.54	0.42
1:A:4423:LEU:HD22	1:A:4466:HIS:HB2	2.01	0.42
1:B:191:MET:O	1:B:194:LEU:HG	2.19	0.42
1:B:309:ARG:HG2	1:B:312:ALA:HB3	2.00	0.42
1:B:902:LYS:HB2	1:B:902:LYS:HE3	1.71	0.42
1:B:1135:LEU:HD22	1:B:1190:TYR:CD1	2.53	0.42
1:B:2967:TYR:OH	1:B:2975:ASP:OD2	2.34	0.42
1:B:3194:LEU:HD21	1:B:3499:GLN:HB2	2.01	0.42
1:B:3389:CYS:O	1:B:3390:GLY:C	2.57	0.42
3:F:259:ARG:NE	3:F:315:ASP:OD2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:62:PHE:HB2	5:J:57:ILE:HD11	2.01	0.42
1:A:90:ASP:N	1:A:90:ASP:OD1	2.50	0.42
1:A:283:ARG:HG3	1:A:287:ARG:HH21	1.84	0.42
1:A:324:GLN:OE1	1:A:324:GLN:N	2.51	0.42
1:A:1347:LYS:HA	1:A:1432:GLY:H	1.85	0.42
1:A:1853:VAL:HA	1:A:1856:GLN:HG3	2.01	0.42
1:A:4415:ARG:O	1:A:4419:MET:HG2	2.18	0.42
1:B:410:GLU:O	1:B:414:VAL:HG23	2.19	0.42
1:B:722:SER:HA	1:B:733:LEU:HD23	2.02	0.42
1:B:1125:LYS:HA	1:B:1128:LEU:HD12	2.01	0.42
1:B:3110:THR:O	1:B:3113:MET:HB2	2.19	0.42
1:B:3257:SER:HA	1:B:3260:ILE:HD12	1.99	0.42
4:H:42:TYR:O	4:H:46:MET:HG2	2.19	0.42
1:A:25:ALA:O	1:A:66:ARG:NH1	2.40	0.42
1:A:186:ILE:O	1:A:190:GLU:HG2	2.19	0.42
1:A:289:GLN:HA	1:A:292:ARG:CZ	2.48	0.42
1:A:354:ARG:HA	1:A:357:LEU:HB2	2.02	0.42
1:A:2994:MET:HG3	1:A:2998:ASN:HD22	1.84	0.42
1:A:3389:CYS:O	1:A:3390:GLY:C	2.57	0.42
1:B:38:VAL:N	1:B:39:PRO:HD2	2.34	0.42
1:B:121:ARG:HD3	1:B:133:SER:O	2.19	0.42
1:B:149:LEU:O	1:B:153:ILE:HG12	2.19	0.42
1:B:1226:ARG:HA	1:B:1226:ARG:NE	2.34	0.42
1:B:1853:VAL:HA	1:B:1856:GLN:HG3	2.01	0.42
1:B:3370:ASN:OD1	1:B:3377:TYR:CZ	2.72	0.42
1:B:3381:ILE:HD12	1:B:3390:GLY:N	2.35	0.42
1:B:3745:LEU:HD13	1:B:3777:ALA:HA	2.01	0.42
2:C:311:GLY:HA3	2:C:334:ALA:HA	2.01	0.42
3:F:169:LYS:O	3:F:172:GLU:HG3	2.19	0.42
3:F:370:LEU:HA	3:F:373:GLN:HG2	2.01	0.42
5:J:7:VAL:HB	5:J:9:LYS:HE2	2.01	0.42
6:K:77:LEU:HD13	6:L:70:MET:CE	2.48	0.42
6:L:72:LYS:HG2	6:L:103:TYR:CE2	2.55	0.42
1:A:1190:TYR:HE1	1:A:1208:TRP:HH2	1.66	0.42
1:A:1562:PRO:O	1:A:1566:GLN:HG2	2.20	0.42
1:A:2825:TRP:CZ3	1:A:2854:ALA:HB2	2.55	0.42
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.50	0.42
1:A:3110:THR:O	1:A:3113:MET:HB2	2.20	0.42
1:A:3115:LEU:HD13	1:A:3143:ILE:HG21	2.01	0.42
1:A:3154:LEU:HG	1:A:3516:TYR:CD1	2.54	0.42
1:A:4196:TYR:CZ	1:A:4318:PRO:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:MET:O	1:B:182:VAL:HG13	2.20	0.42
1:B:578:ALA:HB1	1:B:582:PHE:HE2	1.84	0.42
1:B:627:TYR:CD2	1:B:647:SER:HB3	2.55	0.42
1:B:835:ARG:O	1:B:838:GLU:HG3	2.19	0.42
1:B:1165:ASP:O	1:B:1168:THR:HB	2.19	0.42
1:B:1174:GLN:HA	1:B:1177:LYS:HZ2	1.84	0.42
1:B:1209:LEU:CD1	5:J:18:GLN:HE22	2.32	0.42
1:B:1399:LEU:O	1:B:1400:VAL:C	2.57	0.42
1:B:2538:GLU:HB3	1:B:2548:TRP:CZ2	2.54	0.42
1:B:4423:LEU:HD22	1:B:4466:HIS:HB2	2.01	0.42
3:F:94:HIS:ND1	3:F:100:ASP:O	2.50	0.42
5:J:68:HIS:CG	5:J:73:PHE:HB2	2.55	0.42
1:A:201:GLU:HA	1:A:280:ASN:ND2	2.30	0.42
1:A:257:GLN:NE2	1:A:319:ASP:O	2.52	0.42
1:A:1209:LEU:HD23	1:A:1209:LEU:H	1.84	0.42
1:A:2784:PHE:HB3	1:A:2792:TYR:CD2	2.54	0.42
1:A:3239:LYS:HD3	1:A:3451:TYR:CD1	2.54	0.42
1:A:4437:VAL:HG21	1:A:4448:LEU:HD13	2.00	0.42
1:B:639:ARG:NH1	2:D:528:TYR:CZ	2.88	0.42
1:B:1203:GLN:O	1:B:1205:PRO:N	2.53	0.42
1:B:1459:LEU:H	1:B:1459:LEU:HD12	1.83	0.42
1:B:2825:TRP:CZ3	1:B:2854:ALA:HB2	2.55	0.42
1:B:3115:LEU:HD13	1:B:3143:ILE:HG21	2.01	0.42
2:D:287:TRP:CE2	2:D:295:LEU:HD12	2.54	0.42
3:F:48:ARG:NH1	3:F:49:SER:HB2	2.34	0.42
1:A:58:GLU:HG2	1:A:60:SER:H	1.83	0.42
1:A:150:HIS:CG	1:A:196:LEU:HD21	2.54	0.42
1:A:1209:LEU:HD12	1:A:1214:ILE:HG13	2.02	0.42
1:A:2211:TYR:O	1:A:2214:THR:OG1	2.29	0.42
1:A:3558:GLU:HG2	1:A:3562:TRP:CE2	2.54	0.42
1:B:33:HIS:HA	1:B:36:LYS:NZ	2.34	0.42
1:B:68:PHE:O	1:B:120:LYS:NZ	2.37	0.42
1:B:145:PRO:O	1:B:149:LEU:HG	2.19	0.42
1:B:213:ILE:HD12	1:B:303:ILE:HD11	2.02	0.42
1:B:282:GLU:O	1:B:285:LEU:HG	2.20	0.42
1:B:399:ARG:NH2	1:B:404:VAL:HG11	2.28	0.42
1:B:440:ARG:O	1:B:443:GLU:HB3	2.19	0.42
1:B:539:SER:O	1:B:542:GLY:N	2.49	0.42
1:B:699:PHE:CE2	1:B:758:PHE:HB3	2.55	0.42
1:B:703:ALA:O	1:B:707:GLN:HG3	2.19	0.42
1:B:810:LYS:HE2	3:F:357:GLU:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3148:VAL:O	1:B:3152:GLN:HG3	2.19	0.42
2:D:500:SER:OG	2:D:527:VAL:HG13	2.19	0.42
3:F:59:VAL:HG23	3:F:134:ILE:HG23	2.00	0.42
4:G:47:HIS:HA	4:G:50:ILE:HG12	2.02	0.42
1:A:285:LEU:HA	1:A:288:ILE:HG12	2.01	0.42
1:A:1526:LYS:O	1:A:1530:ILE:HG13	2.20	0.42
1:A:3243:MET:CE	1:A:3444:ILE:HA	2.49	0.42
1:A:3659:ARG:HG3	1:B:3629:PHE:CZ	2.54	0.42
1:B:295:PRO:HA	1:B:298:LEU:HD12	2.01	0.42
1:B:602:ARG:HA	1:B:605:GLN:HB2	2.02	0.42
1:B:610:GLN:NE2	1:B:614:ASP:OD1	2.52	0.42
1:B:1160:THR:O	1:B:1162:SER:N	2.53	0.42
1:B:1212:ASP:N	1:B:1215:GLU:OE1	2.53	0.42
1:B:1526:LYS:O	1:B:1530:ILE:HG13	2.20	0.42
1:B:3243:MET:CE	1:B:3447:TYR:HB2	2.50	0.42
1:B:4628:THR:HG1	1:B:4630:GLU:HG2	1.84	0.42
4:G:70:ARG:HB2	4:H:70:ARG:HG2	2.01	0.42
1:A:420:PHE:CE2	1:A:460:GLN:HG2	2.55	0.42
1:A:462:ARG:NH1	1:A:538:VAL:HA	2.34	0.42
1:A:1744:LYS:HD3	1:A:1745:TYR:CE2	2.55	0.42
1:A:3373:SER:O	1:A:3377:TYR:HD2	2.03	0.42
1:B:332:TYR:CE1	1:B:335:LEU:HD22	2.54	0.42
1:B:361:PHE:HB2	1:B:426:GLU:CD	2.40	0.42
1:B:998:ARG:CZ	1:B:1019:TYR:HD1	2.33	0.42
1:B:1172:TYR:O	1:B:1175:SER:OG	2.21	0.42
1:B:1666:LEU:HD23	1:B:1673:VAL:HA	2.01	0.42
1:B:2445:HIS:NE2	1:B:2449:LEU:HD22	2.34	0.42
2:C:293:GLU:O	2:C:318:MET:N	2.53	0.42
2:D:206:ILE:O	2:D:209:ARG:HB3	2.20	0.42
3:F:168:GLU:HG2	3:F:169:LYS:N	2.34	0.42
4:G:3:GLU:HB3	4:G:6:GLU:HB2	2.02	0.42
4:H:8:LEU:HD12	4:H:9:LYS:N	2.34	0.42
1:A:185:LYS:HE3	1:B:189:LEU:HD23	2.01	0.42
1:A:1490:TRP:HZ3	1:A:1534:PHE:HB3	1.83	0.42
1:A:2059:PHE:CZ	1:A:2104:LYS:HD3	2.55	0.42
1:A:4034:GLU:OE1	1:A:4143:ARG:NH1	2.41	0.42
1:B:619:LEU:HD21	1:B:654:ILE:HG23	2.01	0.42
1:B:2488:ARG:CG	1:B:2492:ARG:HH12	2.32	0.42
1:B:2667:ASN:OD1	1:B:2712:CYS:HB2	2.20	0.42
1:B:3558:GLU:HG2	1:B:3562:TRP:CE2	2.54	0.42
1:B:4196:TYR:CZ	1:B:4318:PRO:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:334:ALA:O	2:D:352:THR:OG1	2.28	0.42
5:I:38:ILE:HG22	5:I:58:VAL:HG21	2.01	0.42
1:A:119:ILE:O	1:A:135:LEU:HG	2.20	0.42
1:A:333:ASN:N	1:A:334:PRO:HD2	2.35	0.42
1:A:413:MET:CE	1:A:464:ASP:HA	2.50	0.42
1:A:1399:LEU:O	1:A:1400:VAL:C	2.58	0.42
1:A:2445:HIS:NE2	1:A:2449:LEU:HD22	2.34	0.42
1:A:3716:VAL:HB	1:A:3836:TYR:OH	2.20	0.42
1:A:3740:LEU:O	1:A:3744:GLN:HG3	2.20	0.42
1:A:4099:VAL:HG23	1:A:4106:LEU:HD11	2.02	0.42
1:A:4173:PRO:HD2	1:A:4176:ARG:HH21	1.84	0.42
1:B:828:LYS:C	1:B:831:PRO:HD2	2.40	0.42
1:B:1210:TYR:N	1:B:1210:TYR:CD2	2.88	0.42
1:B:1744:LYS:HD3	1:B:1745:TYR:CE2	2.55	0.42
1:B:2994:MET:HG3	1:B:2998:ASN:HD22	1.84	0.42
1:B:3951:VAL:HG23	1:B:3973:LEU:HD21	2.01	0.42
1:A:121:ARG:CD	1:A:136:ARG:HG2	2.50	0.41
1:A:271:ALA:O	1:A:275:ILE:HG23	2.19	0.41
1:A:410:GLU:O	1:A:414:VAL:HG23	2.19	0.41
1:A:2132:PRO:HB2	1:A:2135:GLU:HB3	2.02	0.41
1:A:2667:ASN:OD1	1:A:2712:CYS:HB2	2.20	0.41
1:A:2688:GLU:OE1	1:A:2689:HIS:CE1	2.72	0.41
1:B:263:ASP:HA	1:B:277:PHE:HE2	1.85	0.41
1:B:476:LEU:O	1:B:479:VAL:HG12	2.20	0.41
1:B:887:ASP:O	1:B:890:LEU:HG	2.20	0.41
1:B:1181:LYS:HG2	1:B:1185:LYS:NZ	2.30	0.41
1:B:1895:ALA:HB2	1:B:2037:ARG:HB2	2.02	0.41
1:B:3243:MET:CE	1:B:3444:ILE:HA	2.49	0.41
1:B:4099:VAL:HG23	1:B:4106:LEU:HD11	2.02	0.41
1:B:4412:PHE:CZ	1:B:4520:TYR:HB2	2.55	0.41
3:F:155:VAL:O	3:F:158:GLU:HG3	2.20	0.41
6:K:61:PHE:HB2	6:K:63:TYR:CZ	2.54	0.41
6:L:29:ILE:HG21	6:L:102:MET:HE1	2.00	0.41
1:A:115:SER:N	1:A:140:LEU:HB3	2.22	0.41
1:A:220:CYS:O	1:A:223:ARG:NE	2.51	0.41
1:A:246:GLN:HG2	1:A:312:ALA:HB2	2.02	0.41
1:A:1623:ARG:NH1	1:A:1629:PHE:O	2.47	0.41
1:A:2631:LEU:HD13	1:A:2686:MET:HE1	2.02	0.41
1:A:3232:LYS:HD3	1:A:3232:LYS:HA	1.76	0.41
1:A:3381:ILE:HD12	1:A:3390:GLY:N	2.35	0.41
1:A:3629:PHE:CZ	1:B:3659:ARG:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4071:ILE:HD13	1:A:4071:ILE:HA	1.87	0.41
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.55	0.41
1:A:4415:ARG:HE	1:A:4415:ARG:HB3	1.54	0.41
1:B:320:THR:OG1	1:B:323:LYS:NZ	2.53	0.41
1:B:806:ALA:HB1	3:F:355:ALA:O	2.20	0.41
1:B:1124:HIS:CE1	1:B:1128:LEU:HD11	2.54	0.41
1:B:2446:ILE:HD12	1:B:2446:ILE:HA	1.92	0.41
1:B:2688:GLU:OE1	1:B:2689:HIS:CE1	2.73	0.41
1:B:3239:LYS:HD3	1:B:3451:TYR:CD1	2.54	0.41
1:B:3392:MET:CA	1:B:3395:TRP:HB2	2.48	0.41
1:B:4534:TRP:CD2	1:B:4594:LYS:HD3	2.56	0.41
1:B:4553:LEU:HD23	1:B:4553:LEU:HA	1.87	0.41
3:F:330:VAL:HG11	3:F:339:PHE:CD1	2.55	0.41
4:G:22:VAL:O	4:G:30:ILE:N	2.53	0.41
4:H:69:LEU:HB3	4:H:80:VAL:HG13	2.00	0.41
5:J:68:HIS:HB3	5:J:86:PHE:HB2	2.01	0.41
1:A:31:GLN:O	1:A:34:LEU:HG	2.19	0.41
1:A:121:ARG:HH22	1:B:143:ASP:CG	2.24	0.41
1:A:197:GLN:HG2	1:B:170:LYS:HE3	2.03	0.41
1:A:407:GLU:HA	1:A:410:GLU:OE1	2.21	0.41
1:A:429:LYS:HB3	1:A:429:LYS:HE3	1.87	0.41
1:A:1203:GLN:CD	3:F:48:ARG:HB3	2.40	0.41
1:A:1229:ASP:O	1:A:1232:ILE:HG22	2.20	0.41
1:A:2581:LEU:HD12	1:A:2604:THR:HG22	2.02	0.41
1:A:2961:ILE:HG13	1:A:2963:VAL:HG13	2.00	0.41
1:A:3377:TYR:CD1	1:A:3397:ILE:HG12	2.55	0.41
1:A:3392:MET:CA	1:A:3395:TRP:HB2	2.48	0.41
1:B:441:LYS:HD3	1:B:446:LEU:HD21	2.03	0.41
1:B:456:HIS:ND1	1:B:456:HIS:O	2.53	0.41
1:B:1020:ARG:HH22	3:F:84:ARG:N	2.19	0.41
1:B:2457:SER:HB2	1:B:2732:PRO:HB3	2.01	0.41
1:B:3373:SER:O	1:B:3377:TYR:HD2	2.03	0.41
1:B:3588:LEU:HD21	1:B:3638:VAL:HG11	2.02	0.41
1:B:3740:LEU:O	1:B:3744:GLN:HG3	2.20	0.41
1:B:4546:THR:HG21	1:B:4589:GLN:HE21	1.84	0.41
2:C:217:ILE:HG13	2:D:205:ARG:HH11	1.85	0.41
2:D:591:GLU:OE1	2:D:591:GLU:N	2.53	0.41
3:F:228:LEU:CD2	3:F:268:ALA:HB3	2.50	0.41
1:A:35:ARG:O	1:A:39:PRO:HD3	2.21	0.41
1:A:1079:TRP:C	1:A:1081:ALA:H	2.22	0.41
1:A:1738:TYR:HE2	1:A:1792:LEU:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2612:LEU:HD12	1:A:2612:LEU:HA	1.96	0.41
1:A:3586:TYR:HA	1:A:3587:PRO:HD3	1.92	0.41
1:A:3659:ARG:CD	1:B:3628:ARG:HD3	2.50	0.41
1:B:120:LYS:HE2	1:B:125:ILE:HG12	2.01	0.41
1:B:282:GLU:OE2	1:B:333:ASN:ND2	2.53	0.41
1:B:375:GLN:O	1:B:379:ARG:HG2	2.20	0.41
1:B:469:PHE:HZ	1:B:553:TYR:HB2	1.85	0.41
1:B:470:ARG:HH22	1:B:531:LYS:HZ3	1.68	0.41
1:B:484:LEU:HD21	1:B:519:ALA:HB3	2.03	0.41
1:B:3017:VAL:HB	1:B:3020:LEU:HB2	2.03	0.41
2:C:193:SER:OG	2:C:195:GLU:OE1	2.31	0.41
2:D:288:SER:HB2	2:D:340:PHE:CZ	2.55	0.41
2:D:608:ASN:OD1	2:D:608:ASN:N	2.52	0.41
3:E:136:VAL:HA	3:E:230:VAL:O	2.21	0.41
3:F:168:GLU:HB2	3:F:171:ARG:HH21	1.85	0.41
3:F:334:ASP:OD2	3:F:339:PHE:HB2	2.20	0.41
4:G:15:LYS:O	4:G:92:GLN:HG3	2.20	0.41
1:A:40:LEU:HD11	1:B:36:LYS:HD2	2.02	0.41
1:A:72:PRO:HB3	1:A:124:VAL:HG23	2.03	0.41
1:A:241:PHE:CE2	1:A:245:LEU:HD21	2.56	0.41
1:A:288:ILE:HG13	1:A:292:ARG:NH2	2.35	0.41
1:A:1173:VAL:HA	1:A:1176:LEU:HD12	2.01	0.41
1:A:1508:LYS:HG2	1:A:1513:TYR:CZ	2.56	0.41
1:A:2163:ASP:OD1	1:A:4530:GLN:NE2	2.53	0.41
1:A:4546:THR:HG21	1:A:4589:GLN:HE21	1.85	0.41
1:B:740:LEU:O	1:B:743:ILE:HG22	2.20	0.41
1:B:1038:SER:O	1:B:1041:MET:HG2	2.21	0.41
1:B:2912:PHE:HE2	1:B:2914:GLU:HB2	1.86	0.41
1:B:3447:TYR:HB3	1:B:3451:TYR:OH	2.21	0.41
1:B:4399:LYS:HE2	1:B:4399:LYS:HB3	1.95	0.41
2:D:341:ALA:HA	2:D:389:VAL:HG21	2.02	0.41
3:E:60:PHE:O	3:E:135:PHE:HA	2.21	0.41
4:H:80:VAL:HG22	4:H:82:PRO:HD3	2.02	0.41
5:I:14:SER:HB3	5:I:71:LYS:HZ1	1.86	0.41
1:A:160:PHE:CE1	1:B:109:TYR:HA	2.56	0.41
1:A:250:ASN:O	1:A:253:ILE:HG22	2.20	0.41
1:A:350:LEU:HD13	1:A:416:CYS:HA	2.01	0.41
1:A:365:ARG:NH2	1:A:432:VAL:HB	2.31	0.41
1:A:2179:ARG:NH2	1:A:2195:ASP:OD1	2.43	0.41
1:A:2912:PHE:HE2	1:A:2914:GLU:HB2	1.86	0.41
1:A:3741:ARG:NH2	1:A:3776:GLU:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4534:TRP:CD2	1:A:4594:LYS:HD3	2.56	0.41
1:B:180:PRO:HA	1:B:183:GLU:CD	2.40	0.41
1:B:567:ARG:O	1:B:571:GLN:HG3	2.20	0.41
1:B:1188:GLU:HA	1:B:1191:ARG:NE	2.36	0.41
1:B:1304:LEU:O	1:B:1306:LEU:N	2.54	0.41
1:B:2163:ASP:OD1	1:B:4530:GLN:NE2	2.53	0.41
1:B:3001:ASP:OD1	1:B:3002:SER:N	2.54	0.41
1:B:4424:LEU:HD13	1:B:4486:ILE:HG13	2.03	0.41
2:D:215:ILE:HD11	2:D:217:ILE:HG22	2.02	0.41
2:D:528:TYR:CD2	2:D:528:TYR:C	2.92	0.41
3:F:38:SER:HG	3:F:39:ILE:N	2.19	0.41
3:F:91:LEU:HB2	3:F:104:CYS:HB3	2.01	0.41
3:F:141:ARG:HB3	3:F:143:TRP:NE1	2.34	0.41
1:A:65:MET:SD	1:A:66:ARG:HD2	2.61	0.41
1:A:136:ARG:HG3	1:B:152:PHE:CZ	2.56	0.41
1:A:289:GLN:HG3	1:A:292:ARG:HH22	1.86	0.41
1:A:4260:PHE:HD1	1:A:4263:ARG:NH2	2.19	0.41
1:B:59:LYS:HZ3	1:B:62:LEU:HB3	1.86	0.41
1:B:323:LYS:HA	1:B:326:LEU:HB3	2.03	0.41
1:B:417:PHE:O	1:B:421:GLN:HG2	2.20	0.41
1:B:441:LYS:HD3	1:B:446:LEU:CD2	2.50	0.41
1:B:603:GLU:HG2	1:B:604:TYR:CD1	2.55	0.41
1:B:673:TRP:O	1:B:679:GLY:HA3	2.21	0.41
1:B:718:PHE:HB2	1:B:737:VAL:HA	2.03	0.41
1:B:755:TRP:CZ2	2:D:453:GLU:HA	2.55	0.41
1:B:851:LEU:O	1:B:855:GLU:OE1	2.38	0.41
1:B:1018:PHE:CZ	1:B:1020:ARG:HD2	2.55	0.41
1:B:2290:SER:HA	1:B:2294:GLU:OE1	2.21	0.41
2:C:286:ASP:O	2:C:295:LEU:HA	2.20	0.41
1:A:152:PHE:CE1	1:B:136:ARG:HB3	2.56	0.41
1:A:189:LEU:HA	1:B:185:LYS:HE2	2.03	0.41
1:A:214:THR:HA	1:A:296:GLU:OE1	2.21	0.41
1:A:383:ALA:HA	1:A:386:ARG:NE	2.35	0.41
1:A:1153:LEU:HD12	1:A:1153:LEU:HA	1.84	0.41
1:A:2107:ARG:HD2	1:A:2136:ILE:HG12	2.02	0.41
1:A:3001:ASP:OD1	1:A:3002:SER:N	2.54	0.41
1:A:3862:ASP:OD1	1:A:3866:VAL:HG23	2.20	0.41
1:B:20:ALA:N	1:B:124:VAL:HA	2.36	0.41
1:B:311:HIS:HA	1:B:314:VAL:HG22	2.03	0.41
1:B:1610:LYS:HA	1:B:1610:LYS:HD3	1.96	0.41
1:B:1738:TYR:HE2	1:B:1792:LEU:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2905:LEU:HD12	1:B:2905:LEU:HA	1.93	0.41
1:B:4260:PHE:HD1	1:B:4263:ARG:NH2	2.19	0.41
2:D:186:GLU:HA	2:D:189:GLN:HG2	2.03	0.41
2:D:305:ALA:O	2:D:308:GLU:HG3	2.20	0.41
2:D:426:HIS:CD2	2:D:468:ILE:HG21	2.56	0.41
2:D:457:TYR:HB3	2:D:468:ILE:HD12	2.03	0.41
4:H:26:GLU:HA	4:H:87:PHE:CE2	2.56	0.41
1:A:161:PHE:CE2	1:A:165:ILE:HD11	2.56	0.41
1:A:283:ARG:HB2	1:A:287:ARG:NH2	2.35	0.41
1:A:376:ARG:O	1:A:380:LEU:HG	2.21	0.41
1:A:1183:PHE:O	1:A:1187:VAL:HG23	2.20	0.41
1:A:1346:MET:C	1:A:1348:GLU:N	2.72	0.41
1:A:1623:ARG:NH2	1:A:1634:ASP:OD1	2.54	0.41
1:A:2664:ASP:HA	1:A:2711:ALA:HB3	2.03	0.41
1:A:3017:VAL:HB	1:A:3020:LEU:HB2	2.03	0.41
1:A:3243:MET:CE	1:A:3447:TYR:HB2	2.50	0.41
1:A:3291:GLU:OE2	1:A:3394:LYS:HE2	2.21	0.41
1:A:4197:ALA:HB3	1:A:4198:PRO:CD	2.49	0.41
1:B:263:ASP:HA	1:B:277:PHE:CE2	2.56	0.41
1:B:264:ARG:HH11	1:B:274:GLU:CD	2.24	0.41
1:B:406:TYR:O	1:B:410:GLU:HG2	2.21	0.41
1:B:809:LYS:HG2	1:B:813:GLN:OE1	2.21	0.41
1:B:852:ILE:HG13	1:B:853:ILE:N	2.36	0.41
1:B:962:LEU:HD23	1:B:971:LEU:HG	2.03	0.41
1:B:970:TYR:HE1	3:F:101:HIS:CE1	2.39	0.41
1:B:1167:VAL:HA	1:B:1170:ILE:HB	2.02	0.41
1:B:3985:GLN:HB3	1:B:3989:ARG:NH1	2.36	0.41
2:D:399:ILE:HG21	2:D:447:PHE:CZ	2.56	0.41
2:D:589:ASP:OD2	2:D:591:GLU:HB2	2.21	0.41
3:F:60:PHE:CG	3:F:61:GLY:N	2.89	0.41
3:F:279:ASN:O	3:F:282:LEU:HG	2.21	0.41
1:A:92:GLY:O	1:A:212:MET:HA	2.21	0.41
1:A:351:ASP:O	1:A:354:ARG:HD3	2.21	0.41
1:A:1212:ASP:OD1	1:A:1213:ASN:N	2.53	0.41
1:A:2905:LEU:HD12	1:A:2905:LEU:HA	1.93	0.41
1:B:756:LEU:HD23	1:B:756:LEU:HA	1.92	0.41
1:B:1212:ASP:HB2	1:B:1216:GLY:CA	2.50	0.41
1:B:1508:LYS:HG2	1:B:1513:TYR:CZ	2.56	0.41
1:B:2581:LEU:HD12	1:B:2604:THR:HG22	2.02	0.41
1:B:2664:ASP:HA	1:B:2711:ALA:HB3	2.03	0.41
1:B:3135:GLN:O	1:B:3137:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3716:VAL:HB	1:B:3836:TYR:OH	2.21	0.41
1:B:3912:ASN:O	1:B:3937:ARG:NH1	2.54	0.41
2:C:204:THR:HA	4:G:10:ARG:HH12	1.85	0.41
2:D:346:ASN:ND2	2:D:362:ASN:HB3	2.36	0.41
3:F:51:LEU:HB3	3:F:98:ARG:NE	2.32	0.41
3:F:254:ILE:HG22	3:F:340:ILE:HD13	2.03	0.41
3:F:301:LEU:HB3	3:F:309:PHE:HB3	2.03	0.41
3:F:302:VAL:HA	3:F:308:VAL:HG13	2.03	0.41
5:I:77:TYR:CE2	5:I:82:ALA:HB2	2.55	0.41
5:J:62:PHE:CE2	5:J:82:ALA:HB3	2.56	0.41
1:A:323:LYS:O	1:A:326:LEU:HB3	2.20	0.40
1:A:1197:LEU:O	1:A:1201:ARG:N	2.54	0.40
1:A:1222:ASN:O	1:A:1226:ARG:HG3	2.21	0.40
1:A:1478:VAL:CG2	1:A:1488:ARG:HH21	2.34	0.40
1:A:2446:ILE:HD12	1:A:2446:ILE:HA	1.92	0.40
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.21	0.40
1:A:3229:LEU:HD12	1:A:3465:LEU:HD13	2.04	0.40
1:A:3447:TYR:HB3	1:A:3451:TYR:OH	2.21	0.40
1:B:173:ARG:CZ	1:B:175:GLY:HA3	2.51	0.40
1:B:216:VAL:O	1:B:219:GLN:HG2	2.20	0.40
1:B:289:GLN:HE22	1:B:326:LEU:HD13	1.86	0.40
1:B:576:LYS:O	1:B:611:ARG:HD2	2.22	0.40
1:B:790:ARG:O	1:B:793:GLU:HG2	2.21	0.40
1:B:2590:PRO:HG3	1:B:2687:VAL:CG1	2.51	0.40
1:B:2631:LEU:HD13	1:B:2686:MET:HE1	2.03	0.40
1:B:3319:LEU:HD21	1:B:3377:TYR:H	1.86	0.40
4:G:75:LYS:HE2	4:H:63:GLN:HE22	1.86	0.40
5:I:55:HIS:CD2	5:I:88:SER:HB3	2.56	0.40
6:K:62:LYS:HG3	6:K:113:ILE:HG12	2.02	0.40
1:A:2590:PRO:HG3	1:A:2687:VAL:CG1	2.51	0.40
1:B:342:ASN:OD1	1:B:342:ASN:N	2.54	0.40
1:B:2070:VAL:HB	1:B:2071:PRO:HD3	2.02	0.40
1:B:2582:TYR:CE2	1:B:2612:LEU:HD13	2.56	0.40
1:B:3584:ASN:O	1:B:3651:ARG:NH2	2.53	0.40
1:B:3741:ARG:NH2	1:B:3776:GLU:OE1	2.53	0.40
2:D:330:HIS:HB3	2:D:367:ARG:HG3	2.03	0.40
4:G:21:ILE:HG13	4:G:31:LYS:O	2.21	0.40
5:I:88:SER:HG	5:J:55:HIS:CE1	2.33	0.40
1:A:62:LEU:O	1:A:66:ARG:HG2	2.21	0.40
1:A:280:ASN:O	1:A:283:ARG:HG2	2.21	0.40
1:A:283:ARG:HB2	1:A:287:ARG:HH21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ARG:NH2	1:A:440:ARG:HB2	2.36	0.40
1:A:1170:ILE:HD13	1:A:1170:ILE:HA	1.91	0.40
1:A:3319:LEU:HD21	1:A:3377:TYR:H	1.86	0.40
1:A:3869:ASN:O	1:A:3873:ARG:HG2	2.22	0.40
1:B:285:LEU:HB2	1:B:322:LEU:HD11	2.03	0.40
1:B:1202:PHE:CD2	1:B:1204:PHE:CD2	2.93	0.40
1:B:4002:LEU:HD11	1:B:4335:GLN:HB3	2.04	0.40
1:B:4150:PRO:O	1:B:4195:ARG:NH2	2.53	0.40
3:F:139:MET:O	3:F:142:PRO:HD3	2.21	0.40
3:F:248:ASP:OD1	3:F:249:GLU:N	2.55	0.40
5:J:51:ASN:HA	5:J:52:PRO:HD3	1.88	0.40
1:A:182:VAL:HG21	1:B:196:LEU:HD11	2.03	0.40
1:A:420:PHE:HE1	1:A:457:ARG:CZ	2.34	0.40
1:A:1203:GLN:HG2	3:F:46:ARG:HH12	1.85	0.40
1:A:1387:GLN:O	1:A:1391:LYS:N	2.54	0.40
1:A:1895:ALA:HB2	1:A:2037:ARG:HB2	2.02	0.40
1:A:2582:TYR:CE2	1:A:2612:LEU:HD13	2.56	0.40
1:B:296:GLU:OE2	1:B:297:VAL:HG23	2.21	0.40
1:B:365:ARG:CZ	1:B:433:LEU:HB2	2.52	0.40
1:B:388:LEU:O	1:B:392:LEU:HG	2.22	0.40
1:B:850:LEU:HD21	1:B:893:TYR:CE2	2.57	0.40
1:B:980:TYR:HB2	3:F:88:TYR:HE2	1.86	0.40
1:B:2059:PHE:CZ	1:B:2104:LYS:HD3	2.55	0.40
1:B:3133:LEU:HD11	1:B:3141:GLU:HB3	2.03	0.40
1:B:3862:ASP:OD1	1:B:3866:VAL:HG23	2.20	0.40
3:F:308:VAL:HG12	3:F:310:ILE:HD11	2.03	0.40
4:G:68:PHE:HD1	4:G:79:MET:HE1	1.87	0.40
6:K:47:VAL:HG11	6:L:82:SER:H	1.85	0.40
1:A:40:LEU:HA	1:A:45:GLY:N	2.37	0.40
1:A:440:ARG:NH1	1:A:444:GLU:OE2	2.54	0.40
1:A:3243:MET:HE2	1:A:3448:LYS:HB2	2.04	0.40
1:A:3892:LEU:HD13	1:A:3983:ILE:HG21	2.03	0.40
1:A:3912:ASN:O	1:A:3937:ARG:NH1	2.54	0.40
1:A:4106:LEU:HD23	1:A:4106:LEU:HA	1.93	0.40
1:A:4150:PRO:O	1:A:4195:ARG:NH2	2.53	0.40
1:A:4169:ILE:HG23	1:A:4177:ALA:HA	2.03	0.40
1:B:569:ARG:NH2	1:B:600:ALA:HB2	2.37	0.40
1:B:850:LEU:HD23	1:B:850:LEU:HA	1.89	0.40
1:B:1212:ASP:HA	1:B:1216:GLY:N	2.37	0.40
1:B:1958:ASP:HA	1:B:2017:THR:OG1	2.22	0.40
1:B:2132:PRO:HB2	1:B:2135:GLU:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2156:LEU:HD23	1:B:4405:ILE:HG23	2.04	0.40
1:B:3229:LEU:HD12	1:B:3465:LEU:HD13	2.04	0.40
1:B:3263:GLN:CD	1:B:3426:ASN:HB3	2.42	0.40
1:B:3291:GLU:OE2	1:B:3394:LYS:HE2	2.21	0.40
1:B:3869:ASN:O	1:B:3873:ARG:HG2	2.22	0.40
2:D:281:VAL:HG13	2:D:590:SER:HA	2.02	0.40
2:D:327:TYR:HB3	2:D:360:TRP:HH2	1.85	0.40
2:D:554:LEU:HD13	2:D:554:LEU:HA	1.93	0.40
3:F:160:ILE:HA	3:F:163:MET:HG3	2.03	0.40
3:F:250:HIS:CD2	3:F:340:ILE:HG22	2.54	0.40
4:G:46:MET:O	4:G:50:ILE:HG23	2.21	0.40
6:K:35:GLN:HB2	6:K:42:TRP:CH2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4532/4646 (98%)	4352 (96%)	163 (4%)	17 (0%)	30	64
1	B	4509/4646 (97%)	4356 (97%)	132 (3%)	21 (0%)	25	59
2	C	390/638 (61%)	354 (91%)	36 (9%)	0	100	100
2	D	390/638 (61%)	359 (92%)	31 (8%)	0	100	100
3	E	307/492 (62%)	287 (94%)	20 (6%)	0	100	100
3	F	307/492 (62%)	286 (93%)	19 (6%)	2 (1%)	19	53
4	G	91/96 (95%)	84 (92%)	7 (8%)	0	100	100
4	H	91/96 (95%)	83 (91%)	8 (9%)	0	100	100
5	I	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
5	J	87/89 (98%)	80 (92%)	4 (5%)	3 (3%)	3	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	K	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
6	L	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
All	All	11013/12148 (91%)	10541 (96%)	429 (4%)	43 (0%)	32	64

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	589	ASN
1	A	1400	VAL
1	A	1401	ILE
1	A	3384	ARG
1	B	540	LYS
1	B	1207	SER
1	B	1211	ILE
1	B	1215	GLU
1	B	1400	VAL
1	B	3384	ARG
5	J	8	ILE
1	A	1402	GLU
1	A	3390	GLY
1	A	3398	ALA
1	B	1161	ALA
1	B	1212	ASP
1	B	1216	GLY
1	B	1398	MET
1	B	1399	LEU
1	B	3390	GLY
1	B	3398	ALA
5	J	9	LYS
1	A	1436	ASP
1	A	3389	CYS
1	A	3399	GLN
1	B	3389	CYS
1	B	3399	GLN
3	F	39	ILE
1	A	1347	LYS
1	A	3376	SER
1	B	3376	SER
1	A	4197	ALA
1	B	1213	ASN
1	B	4197	ALA

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Mol	Chain	Res	Type
3	F	112	ASP
1	A	1351	TRP
1	A	3385	ALA
1	B	3385	ALA
5	J	51	ASN
1	A	3391	PRO
1	B	3391	PRO
1	A	4198	PRO
1	B	4198	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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	4044/4125 (98%)	4026 (100%)	18 (0%)	89	95
1	B	4028/4125 (98%)	4010 (100%)	18 (0%)	89	95
2	C	344/557 (62%)	342 (99%)	2 (1%)	84	91
2	D	344/557 (62%)	342 (99%)	2 (1%)	84	91
3	E	279/422 (66%)	279 (100%)	0	100	100
3	F	279/422 (66%)	278 (100%)	1 (0%)	89	95
4	G	87/89 (98%)	86 (99%)	1 (1%)	70	83
4	H	87/89 (98%)	87 (100%)	0	100	100
5	I	78/78 (100%)	78 (100%)	0	100	100
5	J	78/78 (100%)	77 (99%)	1 (1%)	65	81
6	K	97/97 (100%)	97 (100%)	0	100	100
6	L	97/97 (100%)	97 (100%)	0	100	100
All	All	9842/10736 (92%)	9799 (100%)	43 (0%)	88	95

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	ASN

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Mol	Chain	Res	Type
1	A	219	GLN
1	A	354	ARG
1	A	386	ARG
1	A	447	LYS
1	A	613	LYS
1	A	1296	LYS
1	A	1301	LYS
1	A	1376	ARG
1	A	1390	LEU
1	A	1397	ASN
1	A	1430	THR
1	A	2471	GLN
1	A	2729	ARG
1	A	3373	SER
1	A	3378	ASN
1	A	3395	TRP
1	A	3397	ILE
1	B	440	ARG
1	B	442	ARG
1	B	485	ARG
1	B	709	ARG
1	B	1067	ASN
1	B	1203	GLN
1	B	1204	PHE
1	B	1208	TRP
1	B	1213	ASN
1	B	1318	ARG
1	B	1394	MET
1	B	1395	LYS
1	B	2471	GLN
1	B	2729	ARG
1	B	3373	SER
1	B	3378	ASN
1	B	3395	TRP
1	B	3397	ILE
2	C	319	LYS
2	C	427	LYS
2	D	275	ARG
2	D	430	LYS
3	F	264	GLN
4	G	9	LYS
5	J	8	ILE



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	195	HIS
1	A	280	ASN
1	A	456	HIS
1	A	460	GLN
1	A	1233	GLN
1	A	1643	ASN
1	A	1931	ASN
1	A	2554	GLN
1	A	2713	ASN
1	A	3092	ASN
1	A	3200	HIS
1	A	3378	ASN
1	A	3383	ASN
1	A	3602	ASN
1	A	3735	GLN
1	A	3754	ASN
1	A	4335	GLN
1	B	150	HIS
1	B	195	HIS
1	B	773	GLN
1	B	882	GLN
1	B	1151	GLN
1	B	1200	GLN
1	B	1222	ASN
1	B	1643	ASN
1	B	1931	ASN
1	B	2554	GLN
1	B	2713	ASN
1	B	3092	ASN
1	B	3200	HIS
1	B	3378	ASN
1	B	3383	ASN
1	B	3602	ASN
1	B	3735	GLN
1	B	3754	ASN
1	B	4335	GLN
2	D	330	HIS
2	D	344	HIS
2	D	380	HIS
3	F	159	HIS



### 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 12 ligands modelled in this entry, 4 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	$\# Z  > 2$
7	ADP	A	4704	-	24,29,29	0.74	0	29,45,45	0.74	1 (3%)
7	ADP	B	4701	9	24,29,29	0.73	0	29,45,45	0.73	1 (3%)
8	ATP	A	4702	9	28,33,33	0.76	0	34,52,52	0.79	1 (2%)
8	ATP	B	4702	9	28,33,33	0.76	0	34,52,52	0.79	1 (2%)
7	ADP	A	4703	-	24,29,29	0.74	0	29,45,45	0.72	1 (3%)
7	ADP	B	4703	-	24,29,29	0.75	0	29,45,45	0.73	1 (3%)
7	ADP	B	4704	-	24,29,29	0.73	0	29,45,45	0.74	1 (3%)
7	ADP	A	4701	9	24,29,29	0.74	0	29,45,45	0.73	1 (3%)

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ADP	A	4704	-	-	2/12/32/32	0/3/3/3
7	ADP	B	4701	9	-	0/12/32/32	0/3/3/3
8	ATP	A	4702	9	-	2/18/38/38	0/3/3/3
8	ATP	B	4702	9	-	2/18/38/38	0/3/3/3
7	ADP	A	4703	-	-	0/12/32/32	0/3/3/3
7	ADP	B	4703	-	-	0/12/32/32	0/3/3/3
7	ADP	B	4704	-	-	2/12/32/32	0/3/3/3
7	ADP	A	4701	9	-	0/12/32/32	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	4704	ADP	C5-C6-N6	2.34	123.87	120.31
7	A	4704	ADP	C5-C6-N6	2.32	123.85	120.31
8	B	4702	ATP	C5-C6-N6	2.27	123.77	120.31
7	B	4701	ADP	C5-C6-N6	2.26	123.76	120.31
8	A	4702	ATP	C5-C6-N6	2.26	123.75	120.31
7	A	4701	ADP	C5-C6-N6	2.26	123.75	120.31
7	B	4703	ADP	C5-C6-N6	2.24	123.73	120.31
7	A	4703	ADP	C5-C6-N6	2.24	123.72	120.31

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	4704	ADP	PA-O3A-PB-O2B
7	B	4704	ADP	PA-O3A-PB-O2B
8	A	4702	ATP	O4'-C4'-C5'-O5'
8	B	4702	ATP	O4'-C4'-C5'-O5'
7	A	4704	ADP	PA-O3A-PB-O1B
7	B	4704	ADP	PA-O3A-PB-O1B
8	A	4702	ATP	C3'-C4'-C5'-O5'
8	B	4702	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	4701	ADP	3	0
8	A	4702	ATP	3	0

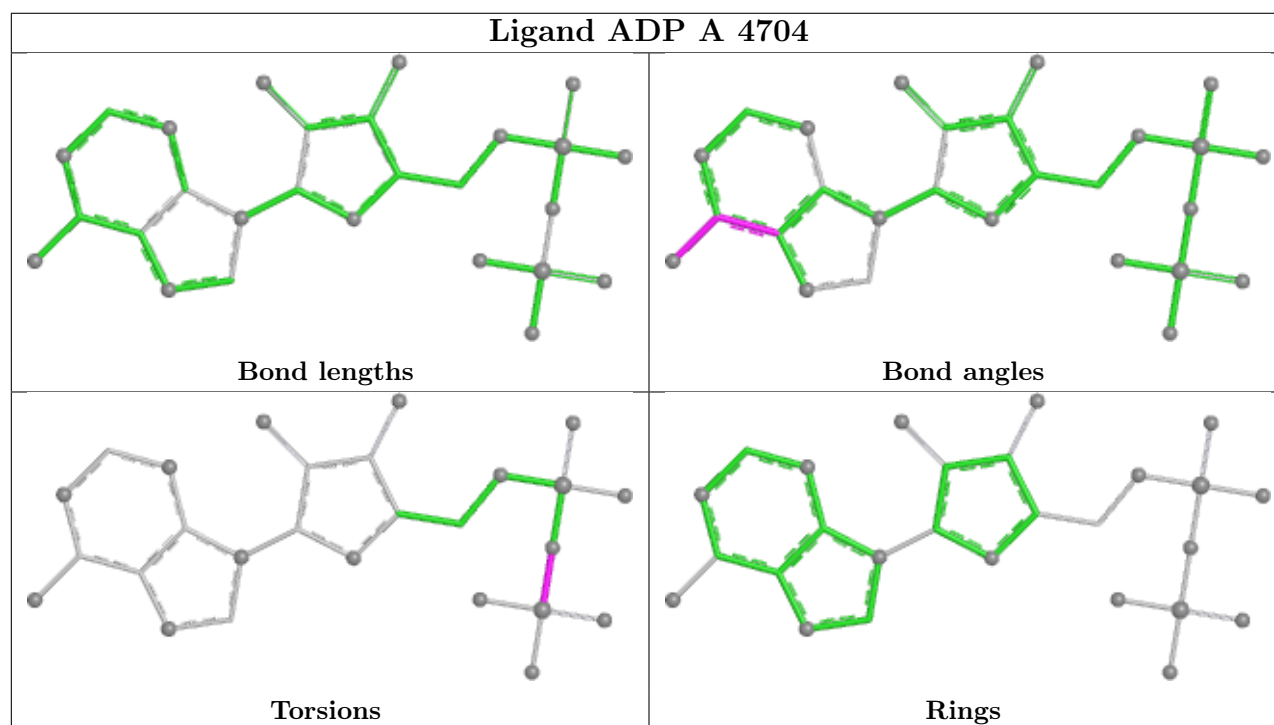
*Continued on next page...*



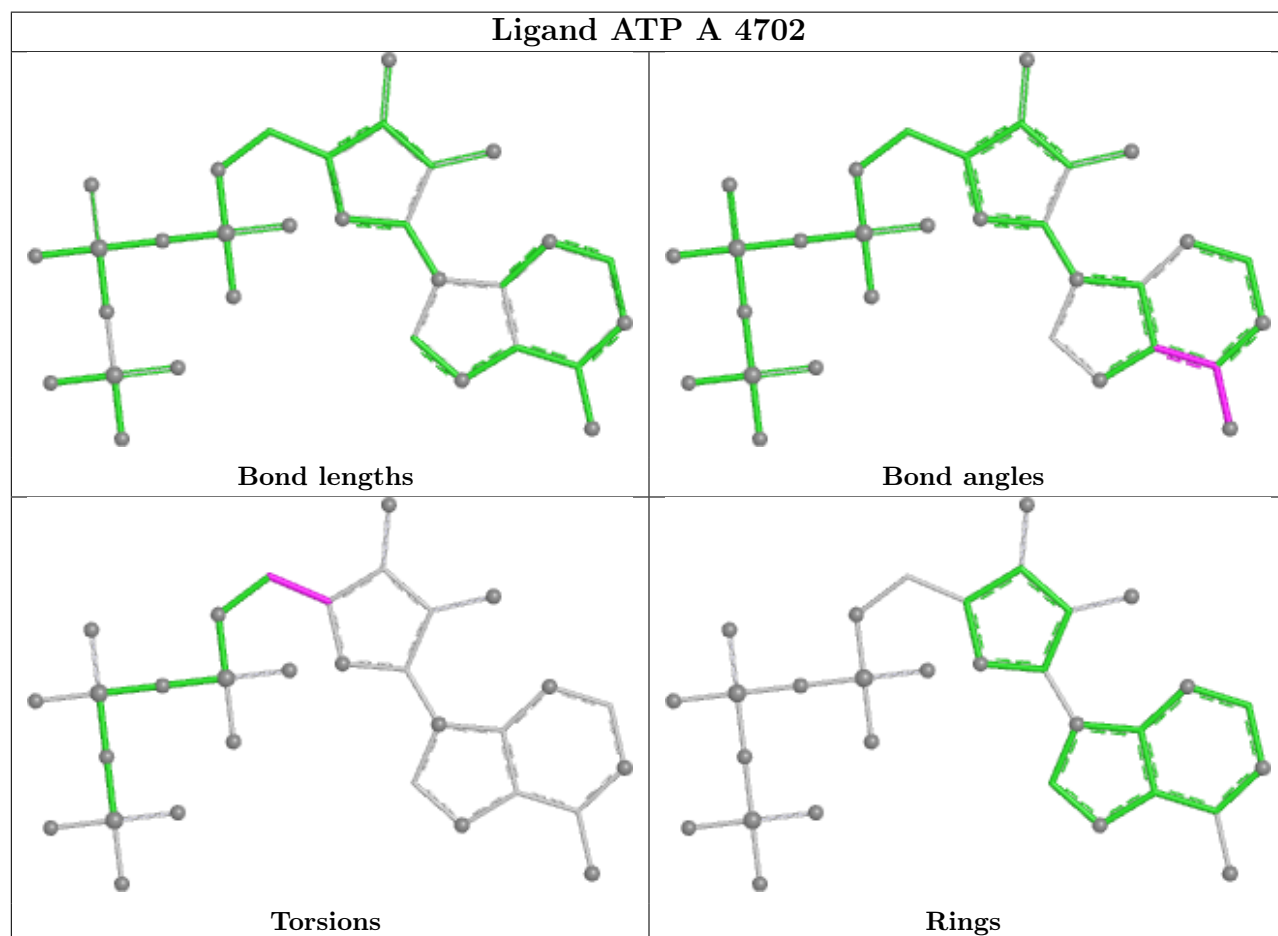
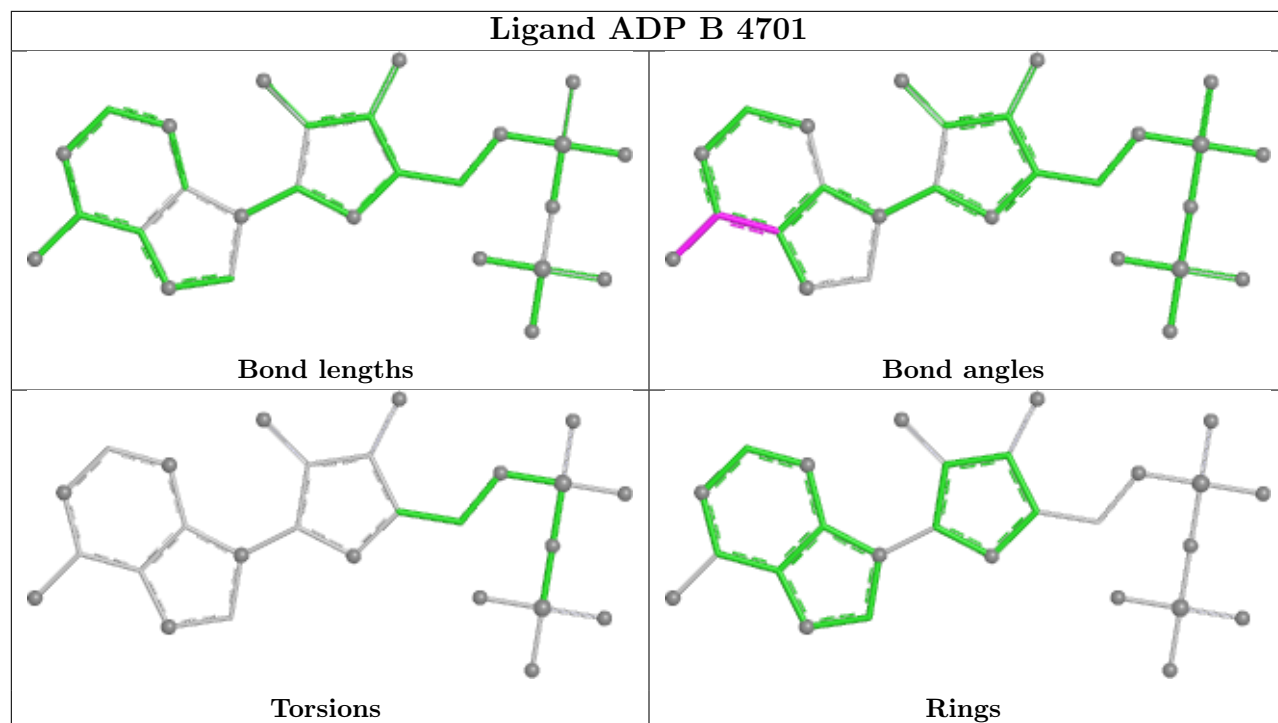
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	4702	ATP	3	0
7	A	4701	ADP	3	0

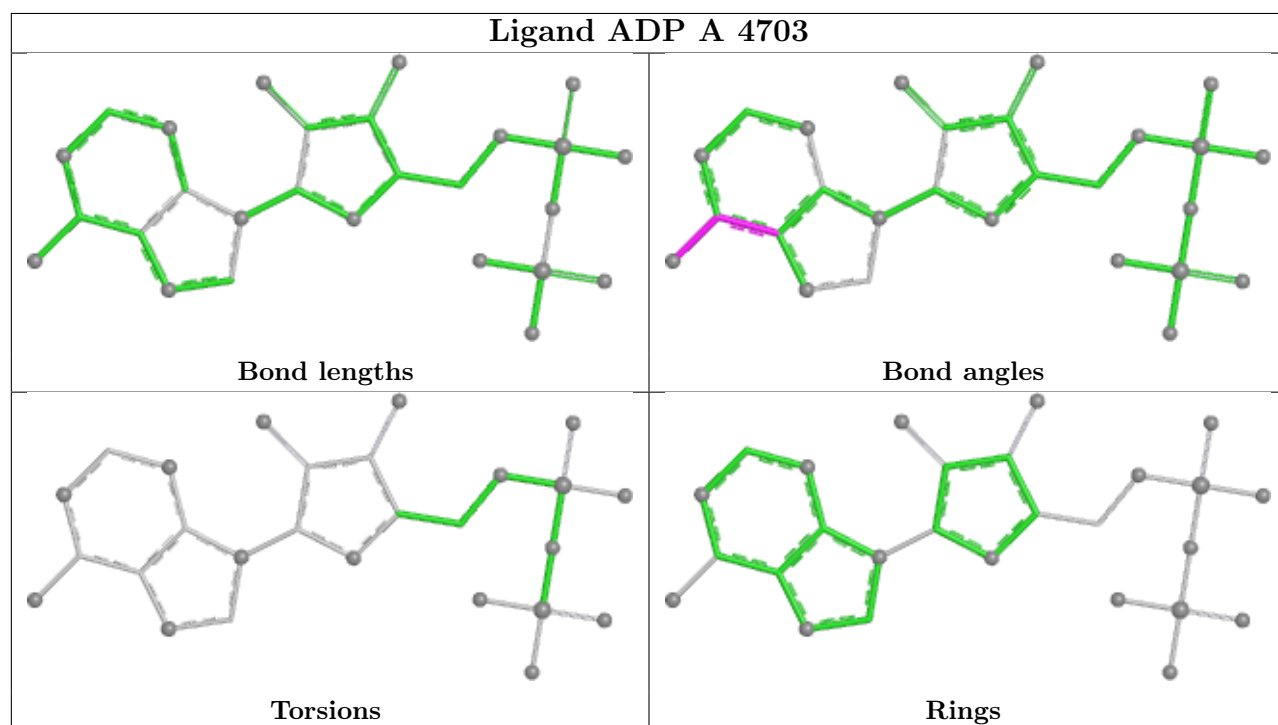
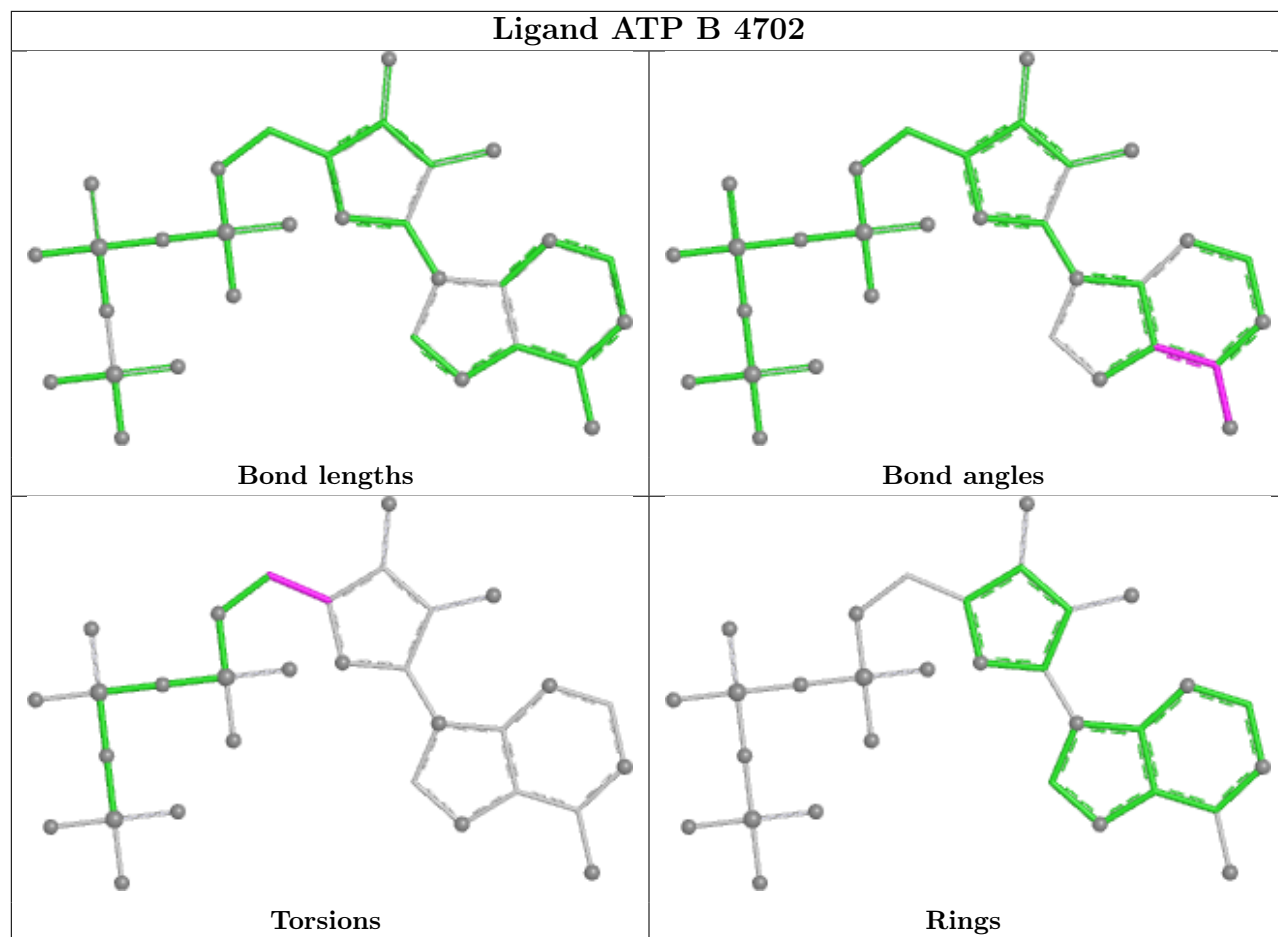
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



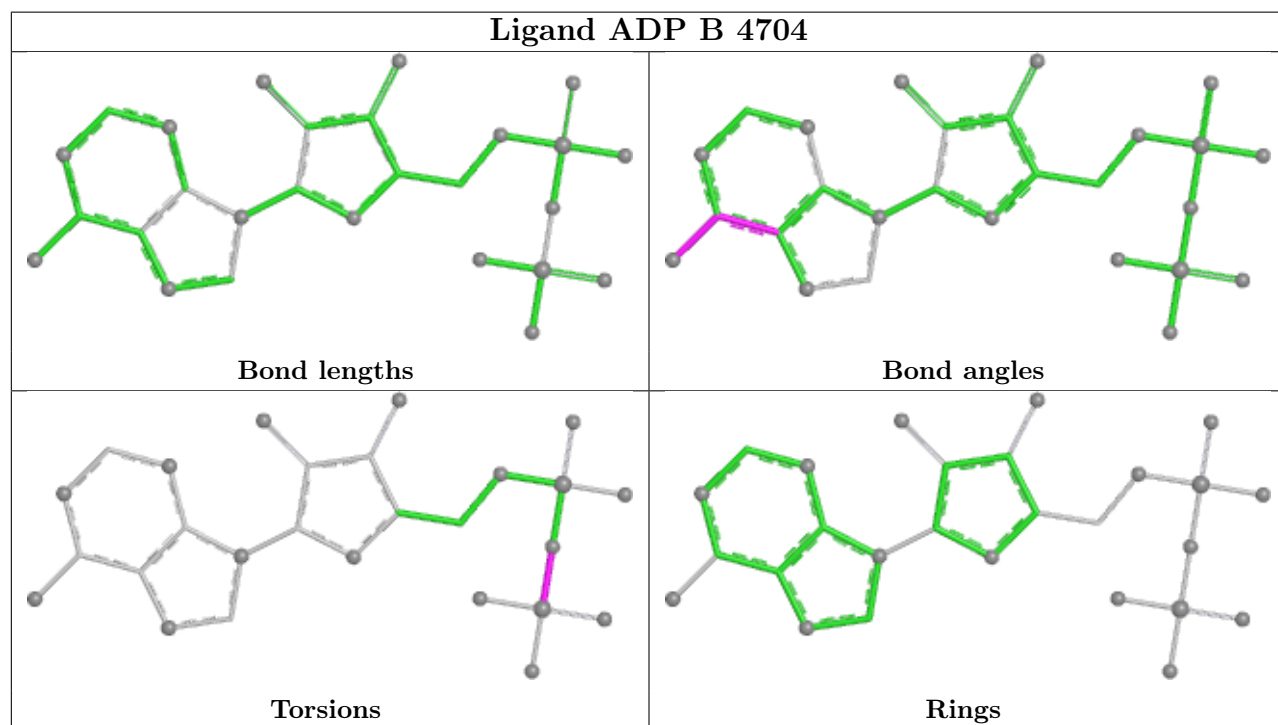
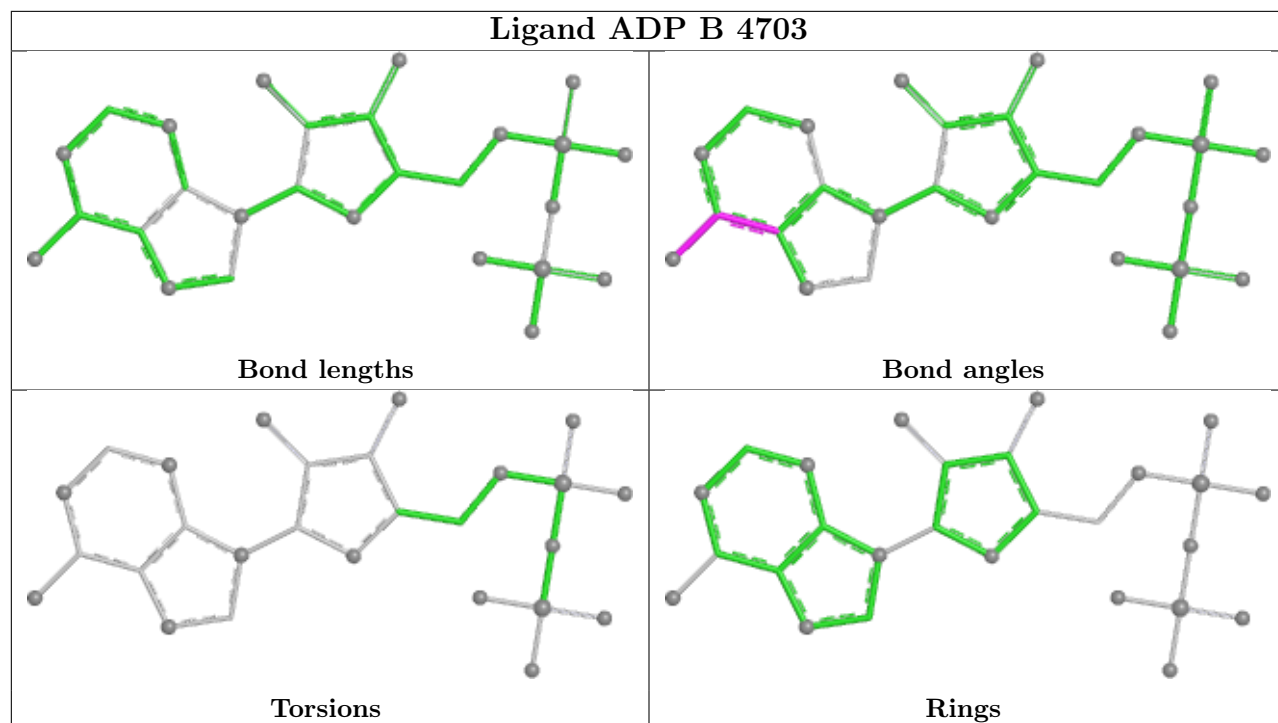




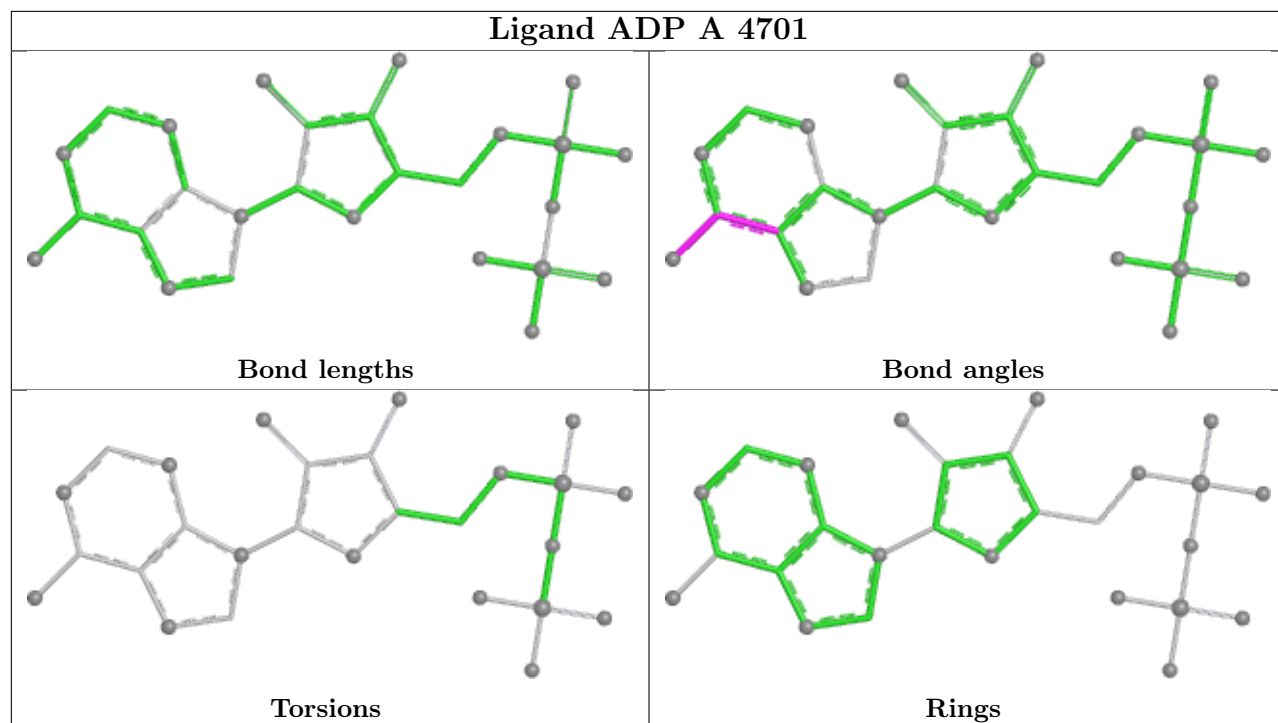












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44681. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

This section was not generated.

### 6.2 Central slices [i](#)

This section was not generated.

### 6.3 Largest variance slices [i](#)

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

This section was not generated.

### 6.5 Orthogonal surface views [i](#)

This section was not generated.

### 6.6 Mask visualisation [i](#)

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



## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.



## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit

This section was not generated.