



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 03:49 PM UTC

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

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>.

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

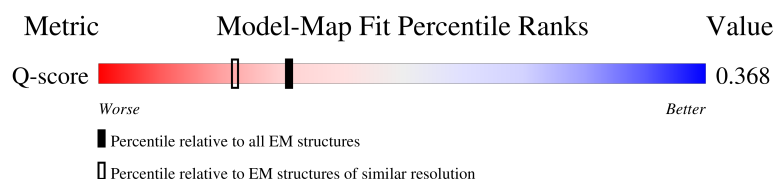
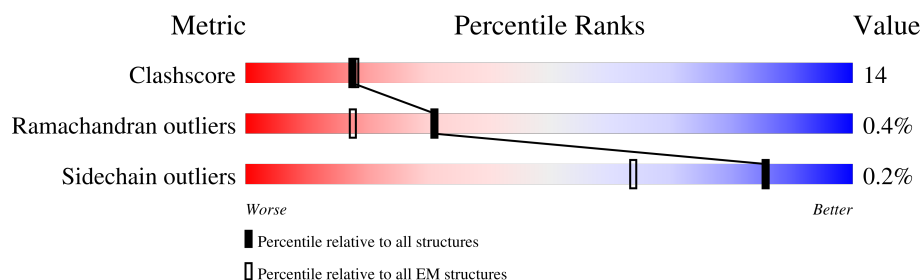
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4646	 5% 78% 19% .
1	B	4646	 72% 25% . .
2	C	638	 57% 38%
2	D	638	 35% 27% 38%

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Mol	Chain	Length	Quality of chain
3	E	492	
3	F	492	
4	G	96	
4	H	96	
5	I	89	
5	J	89	
6	K	113	
6	L	113	

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		

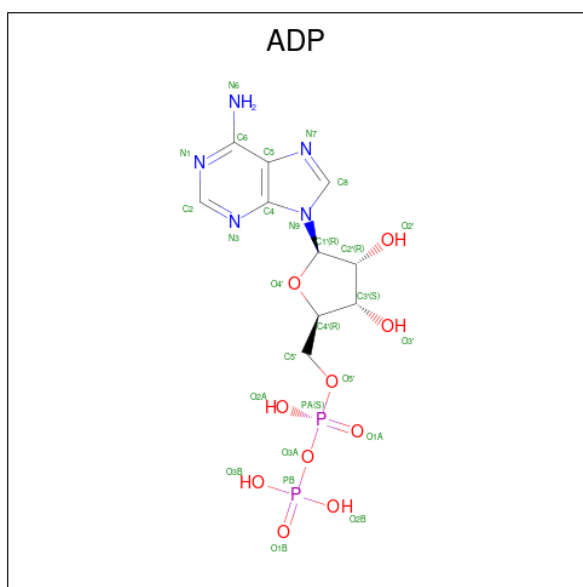
- Molecule 5 is a protein called Dynein light chain 1, cytoplasmic.

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).



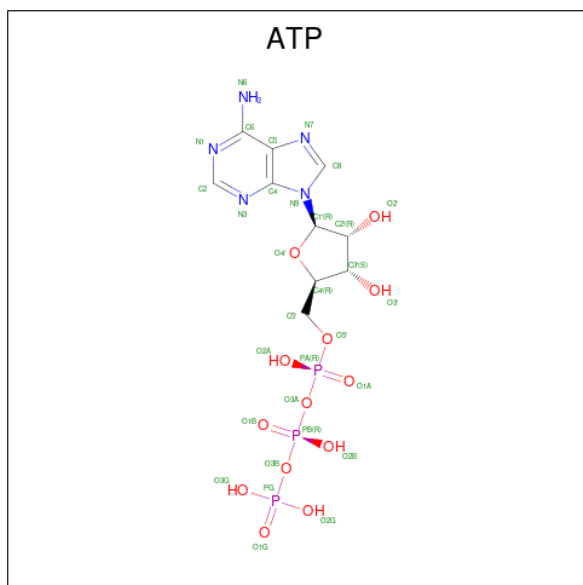
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

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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).



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

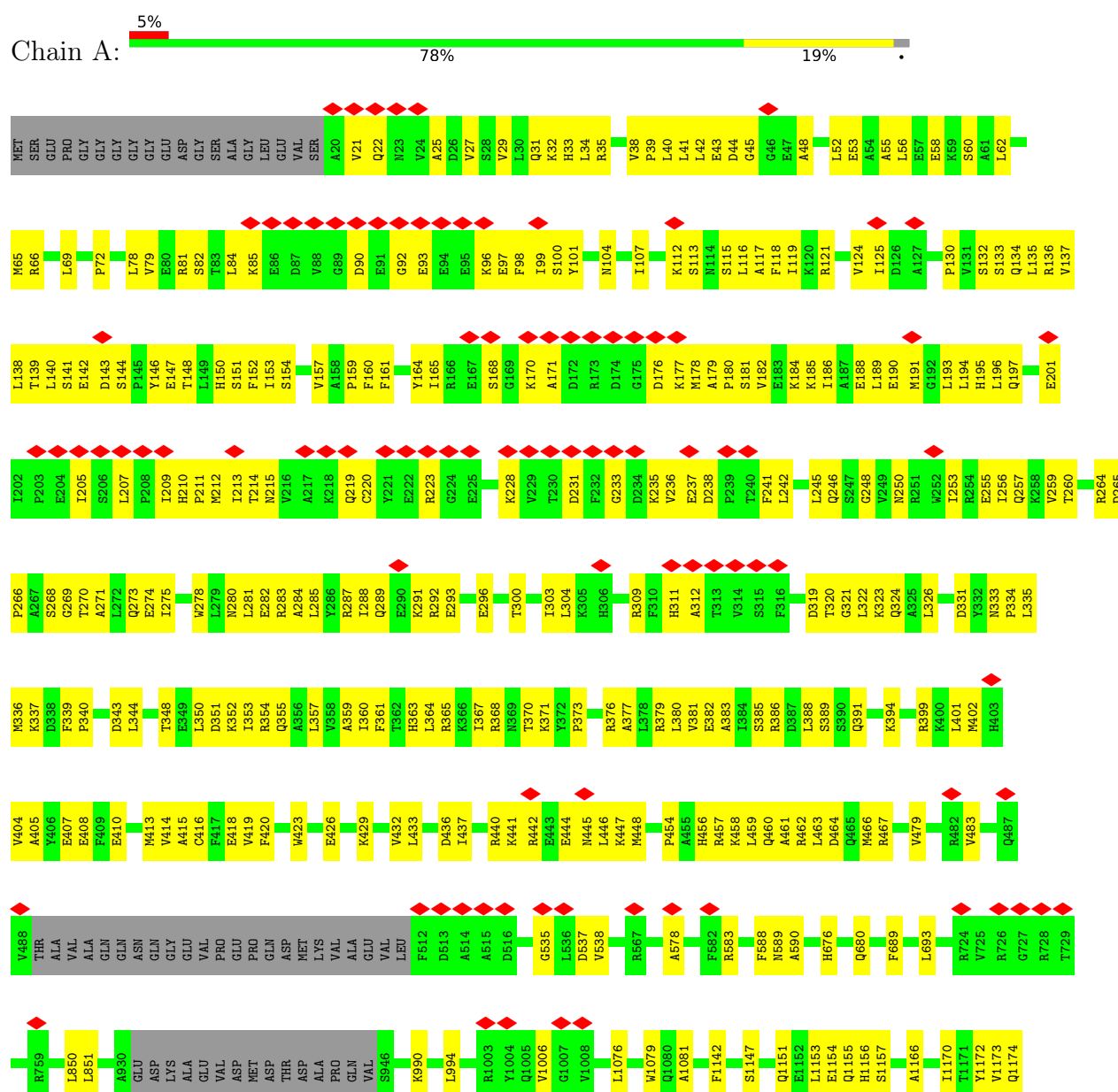
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	A	2	Total	Mg	0
			2	2	
9	B	2	Total	Mg	0
			2	2	

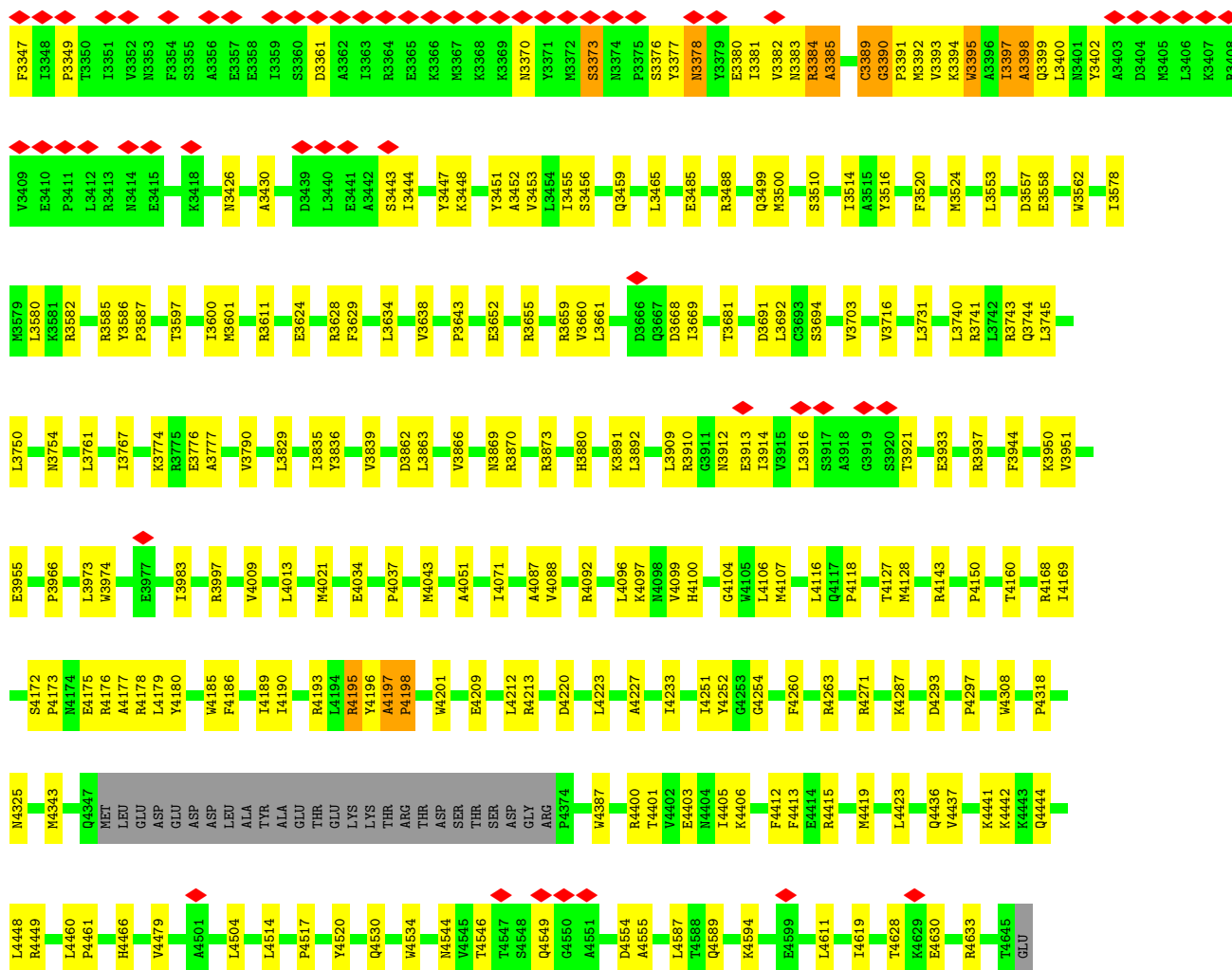
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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

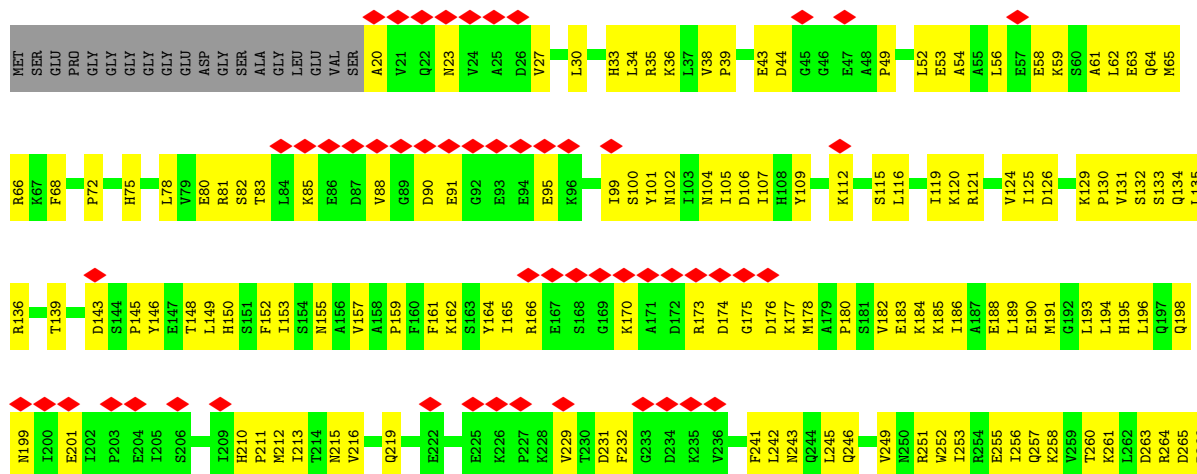


E3269	S3138	R2921	M2755	D2573	ASP	V2907	L2028	R1623	G1455	M1346	S1175
V3270	H3139	Q2930	L2756	R2576	GLU	L2208	L2032	S1624	E1456	K1347	L1176
I3271	R3140	T2961	R2757	T2581	GLU	Y2211	L2039	S1625	M1457	Q1348	K1177
D3272	I3143	K2962	M2773	Y2582	ALA	T2214	R2037	F1629	L1459	Q1349	R1178
K3273	V3148	V2963	E2775	P2590	ALA	M2221	L2039	Y1630	V1351	P1350	K1179
K3274	Q3152	D2973	F2776	L2591	S2410	G2224	Q2047	F1631	V1352	K1181	I1180
M3275	T3153	E2974	F2784	V2592	L2413	P2225	Q2047	G1632	R1467	Q1182	K1181
S3276	L3154	D2975	T2788	L2593	L2422	S2226	Q2047	V1633	V1478	E1184	F1183
V3278	A3157	V2979	Q2789	P2596	V2433	K2230	Q2047	E1635	L1486	K1185	K1185
K3279	R3160	M2994	Q2789	T2604	L2437	K2230	Q2047	L1638	I1487	Y1187	Q1186
K3280	K3163	M2998	H2791	L2612	L2437	L2279	Q2047	V1647	R1488	P1374	Y1187
D3281	T3172	D3001	M2799	L2612	L2443	S2290	Q2079	L1666	W1490	R1378	E1188
D3283	H3175	S3002	W2802	L2620	E2444	E2294	L2080	N1670	H1500	Q1387	L1196
K3284	R3182	R3007	W2803	W2621	H2445	L2295	R2091	K1508	K1508	R1388	L1196
V3285	H3182	R3008	R2804	E2629	L2446	L2295	R2091	Y1512	L1390	L1389	L1197
E3286	H3183	M3008	F2807	L2631	L2449	N2316	K2104	Y1513	K1391	L1390	L1197
V3289	A3184	N3014	F2807	L2631	T2450	S2317	K2104	F1516	G1392	K1199	E1198
I3290	T3194	V3017	W2825	L2638	R2451	V2318	R2107	W1523	Y1393	Q1200	Q1200
A3291	T3211	L3020	D2835	Y2638	L2452	L2319	R2107	W1523	E1402	R1201	R1201
Q3293	E3217	M3030	D2835	L2659	R2453	R2332	E2120	K1697	I1396	F1202	F1202
V3296	R3220	M3043	E2841	D2664	S2457	R2332	E2120	I1698	N1397	Q1203	Q1203
K3297	L3044	M3043	E2841	E2665	M2461	F2343	P2132	K1698	M1398	F1204	F1204
S3298	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	P1205	P1205
I3299	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	W1208	W1208
K3300	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	L1209	L1209
K3301	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	D1212	D1212
R3308	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	N1213	N1213
S3309	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	I1214	I1214
M3310	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	E1215	E1215
A3311	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	G1219	G1219
N3312	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	N1222	N1222
P3313	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	M1225	M1225
P3314	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	R1226	R1226
L3319	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	R1227	R1227
L3328	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	E1426	E1426
G3329	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	S1427	S1427
E3330	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	E1428	E1428
E3331	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	L1429	L1429
T3332	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	T1430	T1430
L3333	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	G1431	G1431
D3334	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	Q1432	Q1432
W3335	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	Q1433	Q1433
K3336	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	W1435	W1435
Q3337	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	D1436	D1436
I3338	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	V1437	V1437
R3339	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	K1441	K1441
I3342	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	A1444	A1444
M3343	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400	V1452	V1452
R3344	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400		
E3345	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400		
N3346	L3044	M3043	E2841	E2665	M2461	F2343	P2132	E1700	I1400		



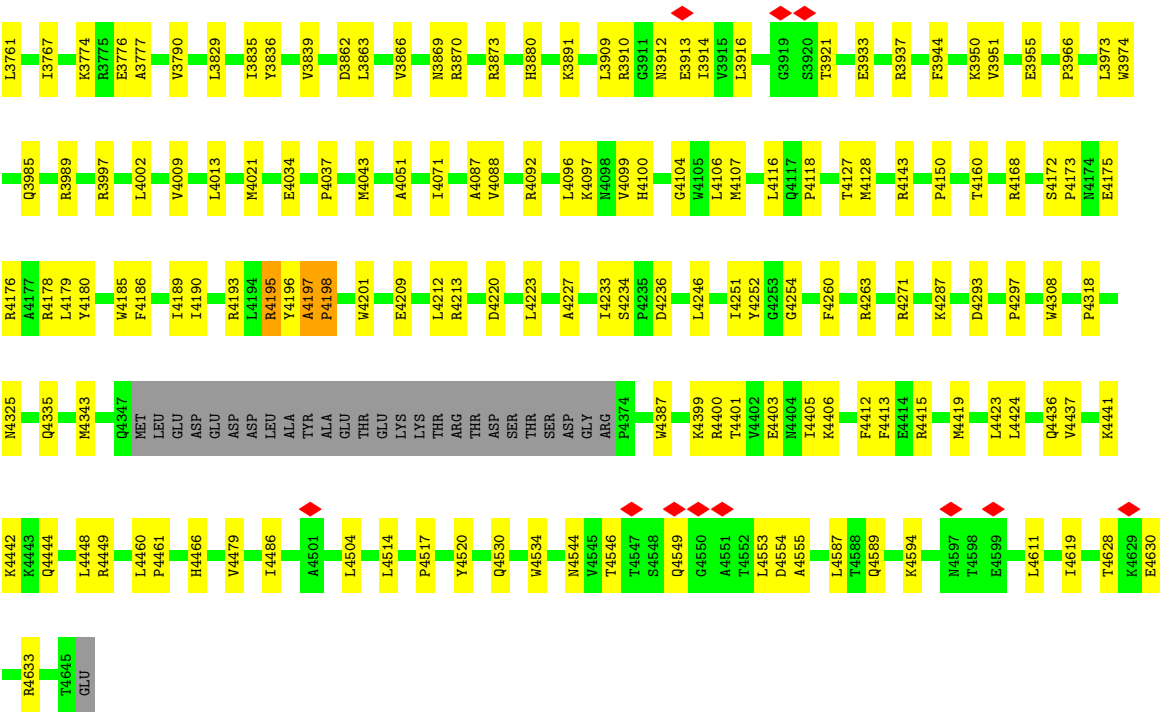
• Molecule 1: Cytoplasmic dynein 1 heavy chain 1

Chain B:

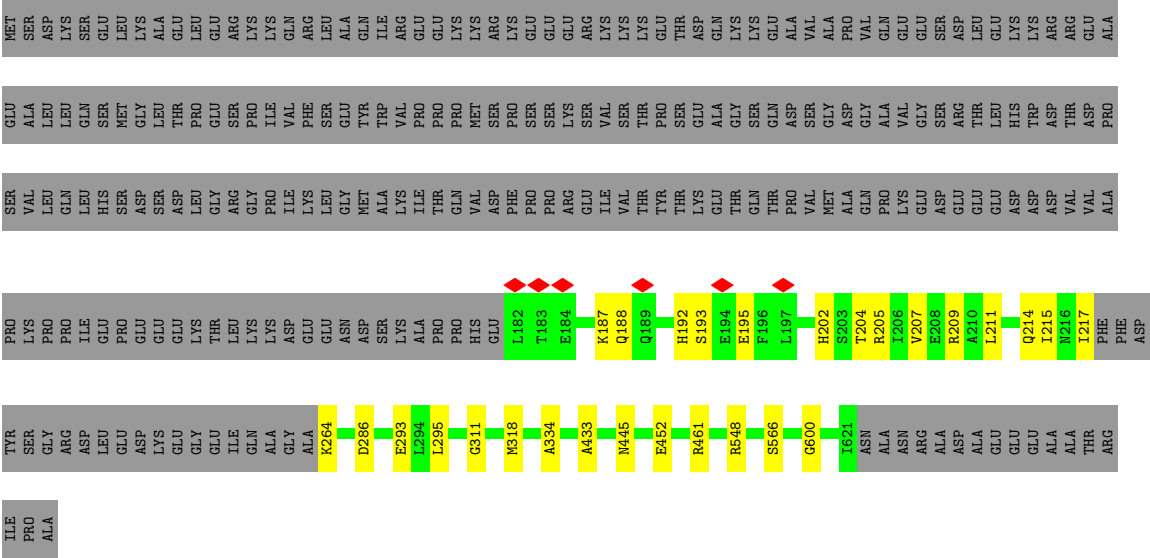


Q1234	T1171	M1095	K1017	PRO	S863	S780	D700	R611	D537	E474	A405	L335	A267
L1304	Y1172	A1096	F1018	GLN	L864	L781	D701	V612	V538	Q475	Y406	M336	S268
E1305	Q1174	K1100	F1019	VAL	E865	W782	W702	K613	S539	E408	E407	D338	G269
L1306	S1175	E1101	R1020	HIS	C867	E783	R704	D614	K540	F409	F409	F339	T270
G1310	L1176	F1102	L1023	LYS	M868	R786	Q707	L619	E541	E410	E410	P340	Q273
L1311	K1177	G1103	T1024	PRO	X869	R790	R716	K622	T543	F417	F417	L341	E274
L1312	R1178	P1104	T1025	GLY	D870	R793	I717	Y627	W546	M413	M413	N342	F277
W1340	V1180	M1026	M1026	GLU	T873	E793	F718	Y627	A549	V414	V414	D343	L279
E1348	K1181	I1107	G1029	P863	F874	R798	I719	Q631	R485	F417	F417	L344	L280
Q1349	Q1113	Q1113	L1033	K956	I877	I801	I720	A632	M550	Q421	Q421	L345	L281
V1352	K1119	K1119	S1036	V959	R880	L804	E721	C633	R552	T422	T422	T348	E282
S1353	L1189	D1121	S1037	H960	V881	W804	W723	M635	Y553	W423	W423	E349	A284
V1354	Y1190	L962	S1038	E961	Q882	V905	R724	S636	E555	D424	D424	L350	L285
R1357	H1124	E963	A1039	R963	D887	G807	W725	R639	R556	D425	D425	K352	Y286
R1388	K1125	M1040	V1040	Q967	L888	L808	R726	D640	I557	E426	E426	R354	R287
L1389	E1126	M1041	I1041	V968	N899	K809	G727	L641	V560	Y427	Y427	R366	T288
L1390	Q1128	G1042	I1043	I969	L890	K810	T728	P642	R563	E428	E428	R367	Q289
L1391	L1128	I1043	I1043	I971	E811	E811	T729	R642	R563	GLN	GLN	R368	E290
K1392	L1129	S1129	V1044	Y970	Y893	V812	G730	S647	R563	GLN	GLN	L357	K291
Y1393	K1130	K1130	S1045	L971	S894	Q813	N731	I648	R567	L430	L430	L360	R292
M1394	F1131	F1131	E1048	E977	N895	A817	V732	I649	L568	Q431	Q431	F361	P295
K1395	G1132	G1132	Q1049	C978	W899	E818	L733	Q653	R569	L432	L432	T362	E296
M1398	L1133	L1133	Y1050	F987	E908	W824	K734	L654	D570	L434	L434	H363	V297
P1400	M1134	M1134	Y1050	F988	E908	W824	L740	I654	Q571	R435	R435	R365	L298
E1401	S1207	S1207	D1062	A988	R914	K928	K735	T659	L572	P436	P436	R366	L299
E1402	W1208	W1208	M1063	W989	R914	K928	V737	T659	L572	I437	I437	T300	L301
L1408	H1143	H1143	N1067	V982	L915	Q916	I743	I744	K576	V438	V438	R367	L301
R1411	Q1145	Q1145	I1068	V993	Q916	Q916	I744	I744	N577	K439	K439	R376	D302
H1412	Y1069	Y1069	Y1069	L994	Q916	Q916	S747	S747	E578	R440	R440	R377	I303
W1413	R1071	R1071	N1070	S995	Q924	R835	E749	E674	N579	K441	K441	P373	I304
V1426	L1072	L1072	L1072	P997	V925	E838	R751	N675	E580	R442	R442	I374	G307
S1427	D1075	D1075	D1075	P998	L926	E838	R751	H676	M581	E443	E443	Q375	K308
E1428	Q1078	Q1078	K1078	Q1000	L927	N842	W755	V677	F582	E444	E444	R378	R309
L1429	W1079	W1079	W1079	GLN	GLY	E845	L756	G679	I584	L446	L446	L379	F310
T1430	L1082	L1082	L1082	ARG	ALA	E845	G757	G679	E521	W450	W450	V381	H311
L1431	Q1085	Q1085	Q1085	TVR	GLU	D848	R759	L682	E522	R451	R451	R386	A312
D1436	I1086	I1086	I1086	GLN	ASP	D848	R759	K683	E522	A461	A461	L387	A312
Q1440	S1162	S1162	S1162	VAL	LYS	D848	R759	K683	E522	Q391	Q391	L388	A312
K1441	R1087	R1087	R1087	VAL	GLU	D848	R759	K683	E522	L322	L322	L389	T313
A1444	H1088	H1088	H1088	HIS	VAL	D848	R759	K683	E522	L322	L322	L390	V314
V1452	K1089	K1089	K1089	ASP	ASP	D848	R759	K683	E522	Q391	Q391	L391	S315
G1455	R1090	R1090	R1090	TVR	MET	D848	R759	K683	E522	Q391	Q391	L392	F316
E1456	R1090	R1090	R1090	ASP	ASP	D848	R759	K683	E522	Q391	Q391	L393	D319
M1457	F1093	F1093	F1093	THR	THR	D848	R759	K683	E522	Q391	Q391	L394	G321
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						D848	R759	K683	E522	Q391	Q391	L396	L326
						D848	R759	K683	E522	Q391	Q391	L397	N330
						D848	R759	K683	E522	Q391	Q391	L398	D331
						D848	R759	K683	E522	Q391	Q391	L399	Y332
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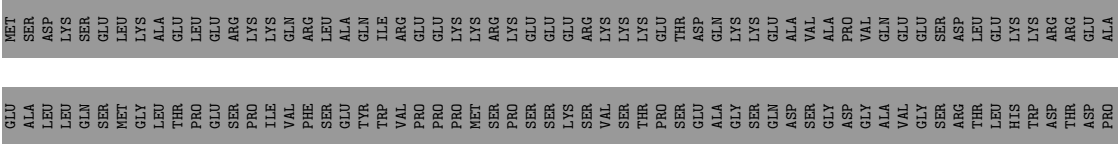
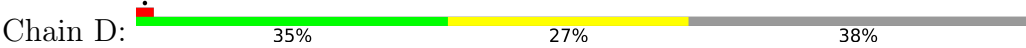
R3585	E3415	N3353	Q3275	V3148	F2767	F2776	P2596	L2422	S2226	K3060	K1865	E1635	L1458
L3588	K3418	F3354	M3276	Q3152	F2784	F2784	T2604	V2433	R2230	T2061	K1878	L1638	L1459
T3597	N3426	S3355	S3277	T3153	T2788	T2788	L2612	L2437	L2279	I2069	L1879	V1647	R1467
L3600	A3430	A3356	V3278	L3154	D2974	D2975	L2612	L2437	S2290	P2071	R1887	L1666	I1487
M3601	A3430	E3357	K3279	A3157	V2979	V2979	L2620	L2443	E2294	Q2079	L1887	L1666	V1490
R3611	D3439	E3280	D3281	R3160	M2994	M2994	N2621	H2446	L2295	L2080	N1670	N1666	W1500
E3624	D3440	S3360	L3282	K3163	N2998	N2998	E2629	L2449	N2316	R2091	R1899	L1666	K1508
R3628	E3441	A3362	D3283	T3172	V2802	V2802	L2630	T2450	S2317	K2104	A1908	V1672	V1673
F3629	A3442	I3363	V3285	H3175	V2803	V2803	L2631	R2451	V2318	R2107	E1914	K1687	Y1512
L3634	I3444	R3364	E3286	H3182	S3002	S3002	L2633	R2453	L2319	R2107	E1914	K1687	Y1513
V3638	Y3447	E3365	V3289	H3183	R3007	R3007	L2638	S2457	R2332	E2120	V1929	T1693	F1516
P3643	K3448	I3290	E3291	A3184	M3008	M3008	T2644	S2457	F2343	P2132	F1930	T1693	F1516
R3651	Y3451	K3368	A3292	L3194	N3014	N3014	G2647	M2461	Q2346	E2133	N1931	K1697	W1593
E3652	L3453	K3369	Q3293	T3211	V3017	V3017	L2659	E2487	Q2346	Q2134	D1937	N1699	K1526
R3655	I3455	N3370	Q3296	E3217	L3020	L3020	L2664	R2488	L2353	L2137	D1958	T1712	I1530
R3659	S3373	Y3371	K3297	R3220	M3030	M3030	E2665	Q2491	T2355	L2138	E1959	V1721	F1534
V3660	N3374	K3372	I3299	R3220	M3043	M3043	L2666	R2492	T2355	Q2139	E1965	V1724	W1537
L3661	P3375	S3376	K3300	L3229	M3043	M3043	L2668	I2498	C2359	T2144	R1966	V1724	W1537
E3685	Y3377	K3301	K3301	K3232	I3059	I3059	L2687	D2505	M2361	M2145	M1967	K1729	R1543
R3688	N3378	R3308	R3308	A3236	F3066	F3066	V2687	M2510	F2364	L2149	E1980	Y1738	D1566
D3666	Y3379	S3309	S3309	N3237	K3076	K3076	H2689	E2513	P2386	L2156	R1983	K1744	E1564
Q3667	K3380	M3310	M3310	D3238	K3076	K3076	R2694	E2513	P2386	L2157	E1984	Y1745	E1564
L3669	I3381	K3311	K3311	K3239	N3092	N3092	D2697	D2537	E2389	L2160	H1985	R1567	R1567
T3681	V3382	A3311	A3311	L3240	D3096	D3096	Q2698	E2538	GLY	L2161	K1992	V1751	I1571
D3691	N3383	P3312	P3312	K3241	W3097	W3097	A2711	W2548	GLU	S2162	T1993	L1752	I1571
L3692	R3384	P3313	P3313	M3243	K3242	K3242	C2712	V2567	ASP	D2163	S1753	S1753	F1575
C3693	A3385	P3314	P3314	Q3247	T3110	T3110	R2720	V2567	ALA	F2165	M1997	M1761	M1579
S3694	C3389	L3319	L3319	Q3248	M3113	M3113	R2720	V2567	ARG	E2174	T1998	G1771	L1601
V3703	G3390	G3328	G3328	E3249	P3114	P3114	R2720	V2567	ARG	M2175	Q2005	G1772	L1601
M3524	M3392	Q3329	Q3329	S3257	L3115	L3115	H2730	A2564	ARG	T2176	G1773	G1773	L1607
L3553	V3393	E3330	E3330	S3257	E3116	E3116	V2731	A2564	LYS	R2179	T2017	D1774	K1610
D3557	K3394	K3331	K3331	I3260	K3117	K3117	P2732	V2567	LYS	S2026	N2027	V1781	I1611
E3558	W3395	T3332	T3332	L3263	L3133	L3133	Y2738	D2573	ASP	D2195	L2028	L1792	Q1612
W3562	I3397	D3334	D3334	H3265	Q3134	Q3134	F2751	R2576	GLY	L2208	L2032	R1621	R1621
L3578	A3402	P3136	P3136	Q3268	Q3135	Q3135	M2755	L2581	GLY	Y2211	R2037	E1622	E1622
M3579	Y3402	F3137	F3137	E3269	R3138	R3138	L2756	Y2582	GLU	T2214	S2037	A1832	R1623
D3404	A3403	K3336	K3336	I3271	H3139	H3139	R2757	Q2930	ALA	R2221	R2037	A1833	S1624
M3405	Q3404	Q3337	Q3337	I3271	K3140	K3140	M2773	P2590	ALA	G2224	L2039	K1834	S1625
L3406	D3404	I3338	I3338	A3272	E3141	E3141	E2774	L2591	S2410	M2221	Q2047	V1853	Y1630
K3407	L3406	R3339	R3339	D3273	A3142	A3142	E2775	L2593	L2413	G2224	Q2047	F1631	F1631
R3408	I3342	M3343	M3343	D3273	I3143	I3143	E2775	L2593	L2413	P2295	F2059	Q1856	V1632
V3409	M3343	R3344	R3344	K3274	T3143	T3143	E2775	L2593	L2413	P2295	F2059	Q1856	V1632
E3410	E3345	F3347	F3347	K3274	T3143	T3143	E2775	L2593	L2413	P2295	F2059	Q1856	V1632
P3411	N3346	N3346	N3346	K3274	T3143	T3143	E2775	L2593	L2413	P2295	F2059	Q1856	V1632
L3412	F3347	F3347	F3347	K3274	T3143	T3143	E2775	L2593	L2413	P2295	F2059	Q1856	V1632
R3413	P3349	P3349	P3349	K3274	T3143	T3143	E2775	L2593	L2413	P2295	F2059	Q1856	V1632
N3414	T3350	T3350	T3350	K3274	T3143	T3143	E2775	L2593	L2413	P2295	F2059	Q1856	V1632
	V3352	V3352	V3352	K3274	T3143	T3143	E2775	L2593	L2413	P2295	F2059	Q1856	V1632

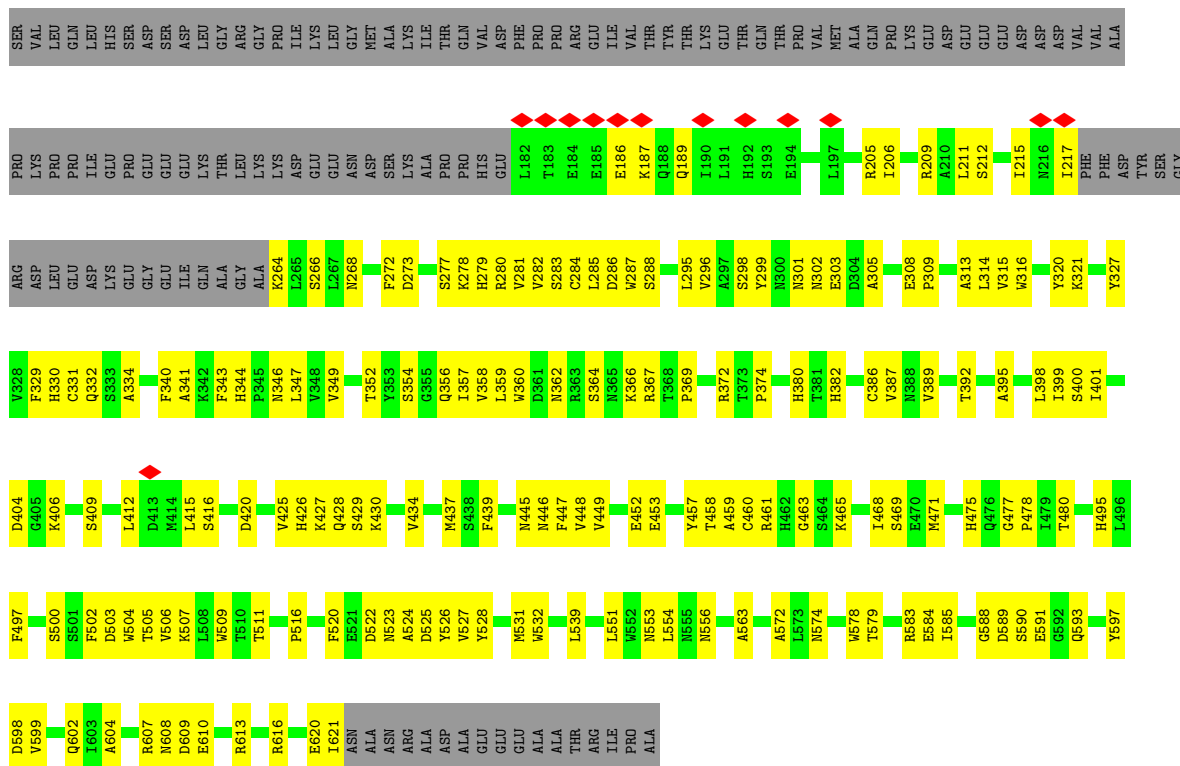


• Molecule 2: Cytoplasmic dynein 1 intermediate chain 2

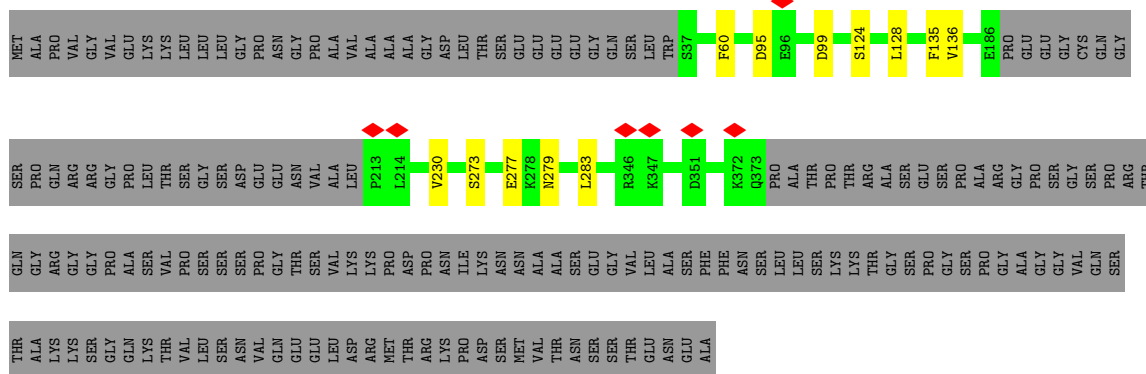


• Molecule 2: Cytoplasmic dynein 1 intermediate chain 2

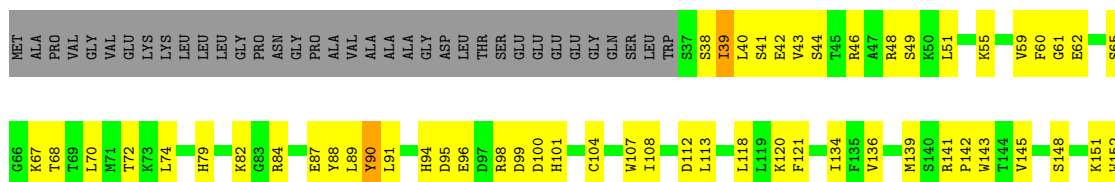


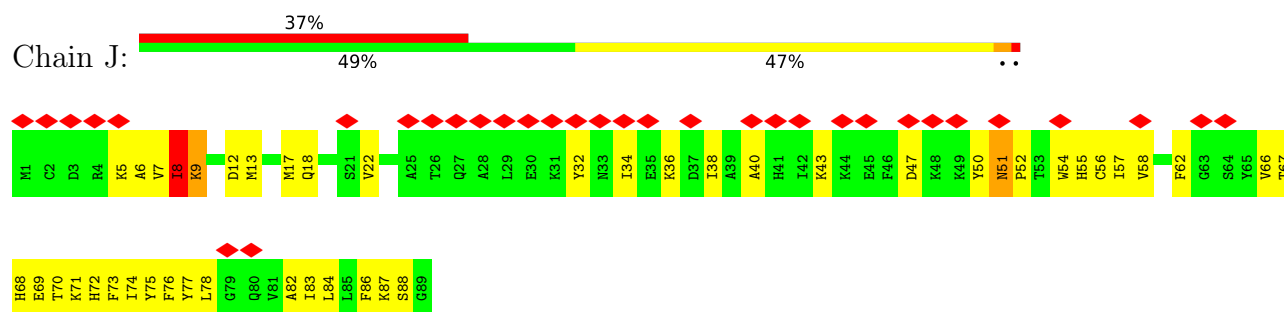


- Molecule 3: Cytoplasmic dynein 1 light intermediate chain 2

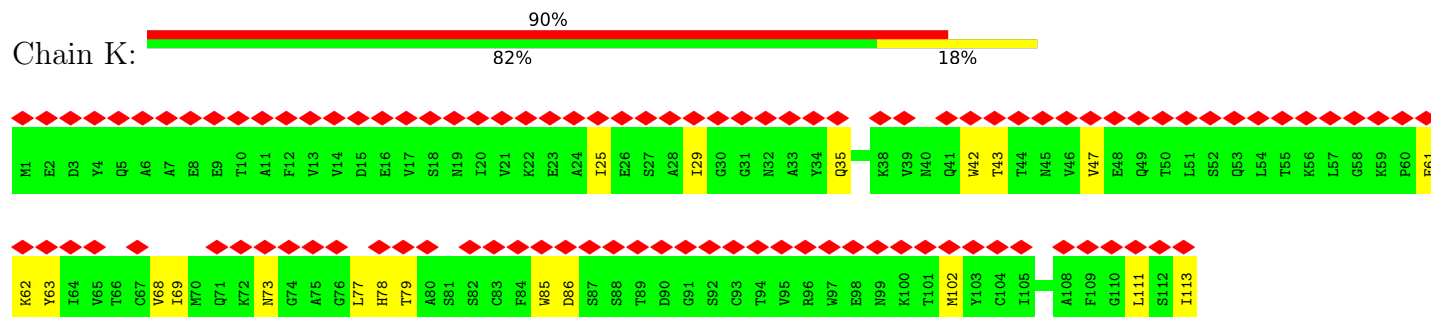


- Molecule 3: Cytoplasmic dynein 1 light intermediate chain 2

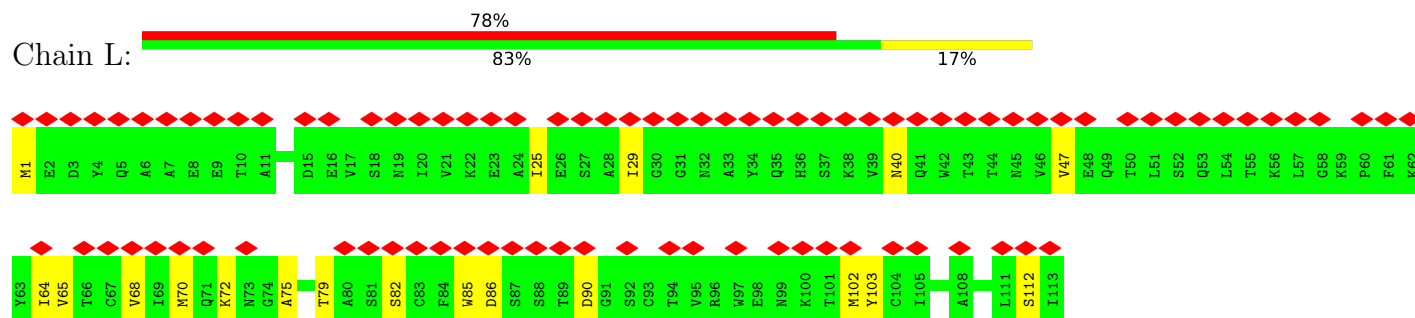




- Molecule 6: Dynein light chain Tctex-type 1



- Molecule 6: Dynein light chain Tctex-type 1



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
Maximum map value	2.250	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	851.968, 851.968, 851.968	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.664, 1.664, 1.664	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.31	1/37420 (0.0%)	0.53	15/50628 (0.0%)
1	B	0.31	1/37249 (0.0%)	0.52	12/50395 (0.0%)
2	C	0.32	0/3195	0.45	0/4351
2	D	0.29	0/3195	0.45	0/4351
3	E	0.28	0/2573	0.40	0/3473
3	F	0.27	0/2573	0.41	0/3473
4	G	0.17	0/752	0.36	0/1017
4	H	0.18	0/752	0.41	0/1017
5	I	0.16	0/744	0.43	0/997
5	J	0.34	0/744	0.56	0/997
6	K	0.12	0/888	0.33	0/1203
6	L	0.13	0/888	0.35	0/1203
All	All	0.30	2/90973 (0.0%)	0.51	27/123105 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3242	LYS	C-O	-6.03	1.16	1.24
1	B	3242	LYS	C-O	-6.03	1.16	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1352	VAL	N-CA-C	-10.62	103.01	113.20
1	B	3242	LYS	O-C-N	-9.93	110.61	122.22
1	A	3242	LYS	O-C-N	-9.92	110.62	122.22
1	A	3361	ASP	CA-CB-CG	-9.67	102.93	112.60
1	B	3361	ASP	CA-CB-CG	-9.66	102.94	112.60
1	A	1350	PRO	N-CA-C	-8.29	103.83	114.03
1	B	3346	ASN	CA-CB-CG	-6.62	105.98	112.60
1	A	3346	ASN	CA-CB-CG	-6.54	106.06	112.60
1	B	3430	ALA	N-CA-C	6.37	117.89	111.07
1	A	3430	ALA	N-CA-C	6.36	117.87	111.07
1	B	1206	PRO	N-CA-C	-6.31	103.56	113.78
1	A	1401	ILE	CA-C-N	6.07	133.13	121.54
1	A	1401	ILE	C-N-CA	6.07	133.13	121.54
1	B	1391	LYS	N-CA-C	-5.99	104.88	111.82
1	B	1389	LEU	N-CA-C	-5.97	105.95	113.18
1	B	530	VAL	CB-CA-C	-5.96	102.13	110.95
1	A	1391	LYS	N-CA-C	-5.54	105.24	111.28
1	A	3347	PHE	CA-CB-CG	-5.44	108.36	113.80
1	B	3347	PHE	CA-CB-CG	-5.44	108.36	113.80
1	B	1390	LEU	N-CA-C	-5.37	105.08	111.69
1	A	1434	ILE	N-CA-C	-5.34	104.53	110.62
1	A	1006	VAL	N-CA-C	-5.29	106.72	112.80
1	A	3342	ILE	N-CA-C	5.10	115.82	110.62
1	B	3342	ILE	N-CA-C	5.08	115.81	110.62
1	A	1389	LEU	N-CA-C	-5.02	105.81	111.28
1	A	3349	PRO	N-CA-C	-5.02	108.26	114.68
1	A	1388	ARG	N-CA-C	-5.01	105.90	111.36

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

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Mol	Chain	Res	Type	Group
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	767	0
1	B	36527	0	36807	1072	0
2	C	3112	0	2964	20	0
2	D	3112	0	2964	152	0
3	E	2518	0	2525	6	0
3	F	2518	0	2525	116	0
4	G	742	0	768	48	0
4	H	742	0	768	41	0
5	I	728	0	714	28	0
5	J	728	0	714	56	0
6	K	872	0	846	17	0
6	L	872	0	846	18	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	2178	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 14.

All (2178) 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
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:193:LEU:HB2	1:B:178:MET:HE2	1.52	0.91
1:A:3456:SER:OG	1:B:3459:GLN:NE2	2.03	0.91
1:A:3459:GLN:CD	1:B:3456:SER:OG	2.14	0.90
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:A:3456:SER:OG	1:B:3459:GLN:CD	2.15	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1203:GLN:HA	5:J:5:LYS:HZ1	1.42	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:466:MET:HE2	1:B:470:ARG:HG3	1.61	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:1214:ILE:C	1:B:1217:GLU:HG2	2.06	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
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:B:3243:MET:HE1	1:B:3444:ILE:HA	1.64	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:1349:GLN:C	1:B:1431:LEU:H	1.90	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:A:3243:MET:HE1	1:A:3444:ILE:HA	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3243:MET:HE3	1:A:3444:ILE:HG23	1.66	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
4:G:69:LEU:H	4:G:79:MET:HE1	1.49	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:413:MET:HE1	1:B:463:LEU:HB3	1.68	0.76
1:B:987:PHE:HE2	3:F:87:GLU:HG2	1.49	0.76
1:B:1211:ILE:C	1:B:1213:ASN:N	2.42	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: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
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:3243:MET:HE3	1:B:3444:ILE:HG23	1.66	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1211:ILE:C	1:B:1213:ASN:H	1.98	0.70
1:B:3381:ILE:HG21	1:B:3390:GLY:HA2	0.71	0.70
4:G:20:ILE:HD13	4:G:31:LYS:HZ2	1.57	0.69
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
4:H:22:VAL:H	4:H:31:LYS:HZ3	1.38	0.69
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:1400:VAL:C	1:A:1402:GLU:N	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:180:PRO:HB2	1:A:184:LYS:HZ1	1.59	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
1:B:1215:GLU:O	1:B:1216:GLY:C	2.37	0.67
4:H:80:VAL:HA	4:H:88:LEU:HB2	1.77	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1399:LEU:C	1:A:1401:ILE:N	2.53	0.66
1:B:1085:GLN:HE22	3:F:39:ILE:HD12	1.61	0.66
1:B:1214:ILE:O	1:B:1215:GLU:C	2.39	0.66
1:B:3292:ALA:HA	1:B:3395:TRP:CZ2	2.30	0.66
1:A:2444:GLU:H	1:A:2510:MET:HE3	1.61	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
1:B:2444:GLU:H	1:B:2510:MET:HE3	1.61	0.66
4:G:14:GLN:NE2	4:G:92:GLN:OE1	2.29	0.66
4:G:49:PHE:HB3	4:H:52:LYS:HZ2	1.61	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
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:A:413:MET:HE1	1:A:464:ASP:HA	1.77	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:B:1212:ASP:O	1:B:1213:ASN:C	2.38	0.65
1:A:3292:ALA:HA	1:A:3395:TRP:CZ2	2.30	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1139:MET:HE3	1:B:1209:LEU:H	1.62	0.65
1:B:4097:LYS:HA	1:B:4127:THR:HB	1.79	0.65
1:A:3383:ASN:O	1:A:3384:ARG:HB3	1.97	0.64
1:B:180:PRO:O	1:B:184:LYS:NZ	2.29	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: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:1210:TYR:H	1:B:1213:ASN:CG	2.06	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:A:337:LYS:HZ2	1:A:367:ILE:HB	1.63	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: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:1435:TRP:C	1:A:1437:VAL:H	2.06	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ARG:NH2	1:B:268:SER:O	2.33	0.61
1:B:1206:PRO:O	1:B:1207:SER:C	2.42	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
3:F:142:PRO:O	3:F:336:TYR:OH	2.18	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:572:LEU:HD11	1:B:581:MET:HE2	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
2:D:504:TRP:CD1	2:D:522:ASP:H	2.19	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
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: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
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
1:B:413:MET:HE2	1:B:467:ARG:HD2	1.83	0.60
2:C:187:LYS:HB3	4:G:30:ILE:HG13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:480:THR:OG1	2:D:500:SER:O	2.19	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:A:178:MET:HE2	1:B:195:HIS:CD2	2.37	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:1435:TRP:C	1:A:1437:VAL:N	2.59	0.59
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:869:TYR:OH	1:B:989:TRP:O	2.20	0.59
1:B:1490:TRP:HH2	1:B:1537:TRP:CD1	2.17	0.59
1:B:2356:VAL:HG13	1:B:2361:MET:HE3	1.84	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
1:A:2356:VAL:HG13	1:A:2361:MET:HE3	1.84	0.59
1:B:734:LYS:HD3	1:B:736:LYS:HZ2	1.67	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:B:3909:LEU:HD21	1:B:4343:MET:HE2	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:3909:LEU:HD21	1:A:4343:MET:HE2	1.84	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: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
5:I:13:MET:HE3	5:I:17:MET:HG2	1.85	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:A:3043:MET:HE1	1:B:1564:GLU:HG3	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:1212:ASP:C	1:B:1214:ILE:N	2.59	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1161:ALA:C	1:B:1163:THR:H	2.12	0.57
1:B:1398:MET:O	1:B:1399:LEU:C	2.47	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: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
1:A:1222:ASN:HA	1:A:1225:MET:HE3	1.86	0.57
2:D:352:THR:HG23	2:D:354:SER:H	1.69	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
2:D:579:THR:HG21	2:D:584:GLU:CD	2.29	0.57
1:A:2592:VAL:HG23	1:A:2731:VAL:HG11	1.86	0.57
1:A:3382:VAL:O	1:A:3383:ASN:C	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
5:J:50:TYR:C	5:J:54:TRP:HH2	2.13	0.57
1:B:3382:VAL:O	1:B:3383:ASN:C	2.48	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:3951:VAL:HG22	1:A:3973:LEU:HD21	1.87	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:196:LEU:H	1:B:178:MET:HE1	1.70	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1215:GLU:C	1:B:1217:GLU:N	2.63	0.55
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:A:441:LYS:HB3	1:A:448:MET:HE2	1.88	0.55
1:B:1150:ARG:O	1:B:1153:LEU:HG	2.06	0.55
1:B:1218:TRP:CD1	1:B:1222:ASN:HD21	2.24	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
5:J:13:MET:HE2	5:J:17:MET:SD	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1537:TRP:CE3	1:A:1601:LEU:HD11	2.41	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
1:A:2144:THR:HG22	1:A:2145:MET:HE2	1.89	0.55
1:B:4104:GLY:HA2	1:B:4107:MET:HE3	1.88	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:A:4104:GLY:HA2	1:A:4107:MET:HE3	1.88	0.54
1:B:241:PHE:O	1:B:245:LEU:HG	2.08	0.54
1:B:1205:PRO:O	1:B:1206:PRO:C	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:3384:ARG:O	1:B:3385:ALA:C	2.51	0.54
2:D:523:ASN:CG	2:D:524:ALA:H	2.15	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:A:3384:ARG:O	1:A:3385:ALA:C	2.51	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: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:A:3243:MET:HE2	1:A:3448:LYS:HB2	1.90	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:1203:GLN:O	1:B:1204:PHE:C	2.50	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:3914:ILE:O	1:B:3937:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1156:HIS:NE2	1:B:1166:ALA:HA	2.24	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
2:D:504:TRP:NE1	2:D:522:ASP:H	2.06	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:2144:THR:HG22	1:B:2145:MET:HE2	1.89	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
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
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:1013:THR:OG1	1:B:1014:GLU:N	2.39	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:3380:GLU:O	1:B:3383:ASN:HB2	2.08	0.53
1:B:4196:TYR:O	1:B:4197:ALA:C	2.52	0.53
1:A:2596:PRO:HB2	1:A:2738:TYR:CZ	2.43	0.53
1:B:530:VAL:H	1:B:553:TYR:HH	1.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:4196:TYR:O	1:A:4197:ALA:C	2.52	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:3243:MET:HE2	1:B:3448:LYS:HB2	1.90	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
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
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: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:210:HIS:CE1	1:A:212:MET:HE2	2.44	0.52
1:A:242:LEU:HB3	1:A:309:ARG:NE	2.24	0.52
1:B:466:MET:HE3	1:B:466:MET:O	2.09	0.52
1:B:581:MET:HA	1:B:584:ILE:HD12	1.91	0.52
1:B:1061:TRP:HB2	1:B:1119:LYS:HZ1	1.75	0.52
1:B:1194:GLN:NE2	1:B:1195:ARG:HG3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:B:804:LEU:HD11	1:B:899:TRP:CD1	2.45	0.52
1:B:1172:TYR:O	1:B:1175:SER:OG	2.21	0.52
1:B:1210:TYR:N	1:B:1213:ASN:OD1	2.36	0.52
1:B:1399:LEU:C	1:B:1401:ILE:N	2.68	0.52
1:B:3182:HIS:NE2	1:B:3582:ARG:O	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:210:HIS:NE2	1:A:212:MET:HE2	2.25	0.51
1:A:442:ARG:HH22	1:A:448:MET:HE1	1.75	0.51
1:A:1172:TYR:O	1:A:1175:SER:OG	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2621:ASN:OD1	1:A:3014:ASN:ND2	2.42	0.51
1:B:467:ARG:O	1:B:471:ARG:HG2	2.11	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
1:A:2061:THR:OG1	1:A:2133:GLU:OE1	2.28	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:68:PHE:O	1:B:120:LYS:NZ	2.37	0.51
1:B:1860:GLN:HG2	1:B:1865:LYS:HG2	1.93	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:3043:MET:HE3	1:B:1567:ARG:HD3	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:581:MET:HE1	1:B:608:LEU:HD12	1.93	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
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:337:LYS:HD2	1:A:363:HIS:C	2.36	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:333:ASN:HB3	1:A:337:LYS:HZ3	1.76	0.50
1:A:2211:TYR:O	1:A:2214:THR:OG1	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:423:TRP:NE1	1:A:457:ARG:HH12	2.10	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
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
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
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
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
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:659:THR:C	1:B:663:LYS:HZ2	2.20	0.49
1:B:1013:THR:O	1:B:1017:LYS:N	2.41	0.49
1:B:2773:MET:HB3	1:B:2799:MET:HE1	1.94	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:2994:MET:HE1	1:A:3008:MET:HG3	1.95	0.49
1:B:441:LYS:HZ2	1:B:450:TRP:HH2	1.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:33:HIS:HA	1:B:36:LYS:HZ2	1.78	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
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
2:D:504:TRP:CD1	2:D:523:ASN:H	2.31	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:2564:ALA:HB3	1:B:2567:VAL:HG23	1.95	0.49
1:B:2773:MET:HE2	1:B:2802:TRP:CG	2.48	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:525:LEU:HA	1:B:528:GLU:CD	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:79:VAL:C	1:A:115:SER:HG	2.20	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:2773:MET:HE2	1:A:2802:TRP:CG	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
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: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
1:B:2994:MET:HE1	1:B:3008:MET:HG3	1.95	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:2061:THR:OG1	1:B:2133:GLU:OE1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:A:2773:MET:HB3	1:A:2799:MET:HE1	1.94	0.48
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:1353:SER:O	1:A:1354:VAL:C	2.56	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:27:VAL:HA	1:B:65:MET:HE1	1.95	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:C:214:GLN:C	2:D:209:ARG:HH12	2.22	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:B:462:ARG:HH22	1:B:535:GLY:C	2.22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:546:TRP:CD1	1:B:550:MET:HE2	2.49	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
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
1:B:1209:LEU:C	1:B:1210:TYR:HD2	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
1:B:3389:CYS:O	1:B:3390:GLY:C	2.57	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:A:2850:ILE:HG22	1:A:2867:MET:HE1	1.95	0.47
1:A:3389:CYS:O	1:A:3390:GLY:C	2.57	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:1914:GLU:HG2	7:B:4701:ADP:O1A	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:2850:ILE:HG22	1:B:2867:MET:HE1	1.95	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:986:MET:HE1	1:B:1037:TYR:CE2	2.50	0.47
1:B:1399:LEU:O	1:B:1400:VAL:C	2.57	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:3030:MET:HE2	1:B:3030:MET:HA	1.97	0.47
1:B:3243:MET:CE	1:B:3444:ILE:HG23	2.41	0.47
1:B:3381:ILE:HG13	1:B:3393:VAL:HB	1.96	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
4:G:79:MET:HE3	4:G:80:VAL:N	2.30	0.47
6:L:47:VAL:HG13	6:L:65:VAL:HB	1.96	0.47
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:A:3030:MET:HA	1:A:3030:MET:HE2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2175:MET:HE3	1:A:2208:LEU:HD22	1.97	0.47
1:A:3966:PRO:HG3	1:A:3997:ARG:HG3	1.97	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:1079:TRP:C	1:A:1081:ALA:H	2.22	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:180:PRO:HA	1:B:183:GLU:CD	2.40	0.46
1:B:361:PHE:HB2	1:B:426:GLU:CD	2.40	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
2:C:193:SER:OG	2:C:195:GLU:OE1	2.31	0.46
3:F:60:PHE:HE2	3:F:148:SER:HB2	1.80	0.46
1:A:1399:LEU:O	1:A:1400:VAL:C	2.58	0.46
1:A:3247:GLN:HG3	1:A:3444:ILE:HD13	1.96	0.46
1:A:3485:GLU:OE2	1:A:3774:LYS:NZ	2.43	0.46
1:B:828:LYS:C	1:B:831:PRO:HD2	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:632:ALA:HA	1:B:635:MET:HE2	1.97	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:121:ARG:HH22	1:B:143:ASP:CG	2.24	0.46
1:A:1203:GLN:CD	3:F:48:ARG:HB3	2.40	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
1:A:2994:MET:HE3	1:A:3066:PHE:HE1	1.81	0.46
1:A:3601:MET:HG3	1:A:3611:ARG:HH21	1.80	0.46
1:B:264:ARG:HH11	1:B:274:GLU:CD	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2994:MET:HE3	1:B:3066:PHE:HE1	1.81	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
2:D:528:TYR:CD2	2:D:528:TYR:C	2.92	0.46
1:A:170:LYS:HZ2	1:A:179:ALA:HB3	1.80	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:277:PHE:O	1:B:281:LEU:HG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1176:LEU:HA	1:B:1179:LYS:HD3	1.97	0.46
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:1211:ILE:O	1:B:1212:ASP:C	2.57	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: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:A:3243:MET:HE1	1:A:3444:ILE:CA	2.43	0.45
1:B:277:PHE:CE2	1:B:281:LEU:HD11	2.51	0.45
1:B:279:LEU:HA	1:B:336:MET:HE1	1.98	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
6:L:1:MET:HE2	6:L:1:MET:HA	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:1210:TYR:N	1:B:1213:ASN:CB	2.78	0.45
1:B:2175:MET:HE3	1:B:2208:LEU:HD22	1.97	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: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
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
1:B:1139:MET:HE1	1:B:1208:TRP:HA	1.98	0.45
1:B:3263:GLN:CD	1:B:3426:ASN:HB3	2.42	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:196:LEU:N	1:B:178:MET:HE1	2.32	0.45
1:A:361:PHE:HB2	1:A:426:GLU:CD	2.42	0.45
1:A:689:PHE:O	1:A:693:LEU:N	2.47	0.45
1:A:1969:SER:O	1:A:1972:SER:OG	2.31	0.45
1:A:2668:LEU:HD21	1:A:2720:ARG:CZ	2.47	0.45
1:A:2851:ASP:HA	1:A:2867:MET:HE3	1.99	0.45
1:B:301:LEU:HD12	1:B:304:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1346:MET:C	1:A:1348:GLU:N	2.72	0.45
1:A:1456:GLU:O	1:A:1516:PHE:HE2	2.00	0.45
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:744:ILE:O	1:B:747:SER:OG	2.27	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:1079:TRP:CZ3	1:B:1134:MET:HE3	2.52	0.44
1:B:2851:ASP:HA	1:B:2867:MET:HE3	1.99	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:334:ALA:O	2:D:352:THR:OG1	2.28	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
6:L:29:ILE:HD13	6:L:102:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:635:MET:HE2	1:B:635:MET:HB3	1.74	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
1:A:1937:ASP:HA	1:A:1967:MET:HG3	1.98	0.44
1:A:3263:GLN:CD	1:A:3426:ASN:HB3	2.42	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:852:ILE:HA	1:B:855:GLU:CD	2.41	0.44
1:B:1179:LYS:O	1:B:1182:GLN:HB2	2.17	0.44
1:B:1304:LEU:C	1:B:1306:LEU:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:578:ALA:C	1:A:583:ARG:H	2.22	0.44
1:A:1567:ARG:HD3	1:B:3043:MET:HE3	2.00	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
1:B:1159:ASP:O	1:B:1160:THR:OG1	2.30	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
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
3:F:94:HIS:HD1	3:F:100:ASP:C	2.26	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:423:TRP:NE1	1:A:457:ARG:HH22	2.15	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: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:1153:LEU:HB3	1:B:1225:MET:HE1	2.00	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
4:G:61:ASP:CG	4:G:64:ASN:HB2	2.43	0.44
1:A:1170:ILE:O	1:A:1174:GLN:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:13:MET:HE1	5:I:21:SER:OG	2.17	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:3456:SER:OG	1:B:3459:GLN:OE1	2.14	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:B:4234:SER:OG	1:B:4236:ASP:OD1	2.31	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
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: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:82:SER:HG	1:A:100:SER:HB2	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1063:MET:HE1	3:F:46:ARG:C	2.44	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
6:K:77:LEU:HD13	6:L:70:MET:CE	2.48	0.43
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
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:1349:GLN:C	1:A:1351:TRP:N	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:697:GLU:H	1:B:697:GLU:CD	2.25	0.43
1:B:959:VAL:HA	1:B:1106:VAL:O	2.18	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
6:L:85:TRP:HD1	6:L:86:ASP:C	2.27	0.43
1:A:118:PHE:HB3	1:A:135:LEU:HD11	2.01	0.43
1:A:1229:ASP:CG	1:A:1233:GLN:HE22	2.27	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:H:22:VAL:H	4:H:31:LYS:NZ	2.13	0.43
1:A:22:GLN:HE22	1:A:134:GLN:CD	2.27	0.42
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:1433:GLN:O	1:A:1434:ILE:C	2.62	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:3910:ARG:HE	1:B:3913:GLU:CD	2.27	0.42
3:F:259:ARG:NE	3:F:315:ASP:OD2	2.52	0.42
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:537:ASP:O	1:B:543:THR:OG1	2.24	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:1457:MET:HE3	1:B:1457:MET:HB3	1.82	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:170:LYS:NZ	1:A:176:ASP:O	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1457:MET:HE3	1:A:1457:MET:HB3	1.82	0.42
1:A:2994:MET:HG3	1:A:2998:ASN:HD22	1.84	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:1218:TRP:NE1	1:B:1222:ASN:HD21	2.17	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:L:72:LYS:HG2	6:L:103:TYR:CE2	2.55	0.42
1:A:215:ASN:C	1:A:215:ASN:HD22	2.25	0.42
1:A:850:LEU:O	1:A:851:LEU:C	2.62	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
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:1209:LEU:CD1	5:J:18:GLN:HE22	2.32	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:164:TYR:O	1:A:168:SER:OG	2.32	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:2221:MET:HE1	1:A:2355:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3910:ARG:HE	1:A:3913:GLU:CD	2.27	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
1:B:3243:MET:CE	1:B:3447:TYR:HB2	2.50	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: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: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
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: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:470:ARG:HH22	1:B:531:LYS:HZ3	1.67	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:1139:MET:CE	1:B:1209:LEU:H	2.30	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:1348:GLU:O	1:B:1430:THR:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1526:LYS:O	1:B:1530:ILE:HG13	2.20	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:808:LEU:HA	1:B:811:GLU:CD	2.45	0.42
1:B:998:ARG:CZ	1:B:1019:TYR:HD1	2.33	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:130:PRO:O	1:A:133:SER:OG	2.24	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:1067:ASN:C	1:B:1067:ASN:HD22	2.27	0.42
1:B:2221:MET:HE1	1:B:2355:THR:HG22	2.02	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
2:D:346:ASN:CG	2:D:362:ASN:HB3	2.45	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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
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:1212:ASP:O	1:B:1214:ILE:C	2.63	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:3113:MET:HE3	1:B:3184:ALA:HA	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1738:TYR:HE2	1:A:1792:LEU:HD21	1.85	0.41
1:A:2612:LEU:HD12	1:A:2612:LEU:HA	1.96	0.41
1:A:3157:ALA:HB1	1:A:3524:MET:HE2	2.03	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: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: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
6:K:102:MET:HE3	6:K:102:MET:HB3	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3157:ALA:HB1	1:B:3524:MET:HE2	2.03	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
5:J:12:ASP:CG	5:J:71:LYS:H	2.29	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
1:A:4534:TRP:CD2	1:A:4594:LYS:HD3	2.56	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:3485:GLU:OE2	1:B:3774:LYS:NZ	2.43	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:916:GLN:HB2	1:B:1026:MET:HE1	2.02	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
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
2:D:503:ASP:C	2:D:505:THR:N	2.79	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:466:MET:O	1:A:467:ARG:C	2.60	0.41
1:A:1183:PHE:O	1:A:1187:VAL:HG23	2.20	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:3113:MET:HE3	1:A:3184:ALA:HA	2.02	0.41
1:A:3243:MET:CE	1:A:3447:TYR:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:406:TYR:O	1:B:410:GLU:HG2	2.21	0.41
1:B:537:ASP:HB3	1:B:542:GLY:C	2.46	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
6:K:85:TRP:HD1	6:K:86:ASP:C	2.29	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:2644:THR:OG1	1:B:2647:GLY:O	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1486:LEU:HD23	1:A:1579:MET:HE2	2.03	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:343:ASP:OD1	1:B:352:LYS:NZ	2.28	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: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:388:LEU:O	1:A:389:SER:C	2.63	0.40
1:A:2590:PRO:HG3	1:A:2687:VAL:CG1	2.51	0.40
1:A:3955:GLU:H	1:A:3955:GLU:CD	2.28	0.40
1:B:199:ASN:CG	1:B:201:GLU:H	2.29	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
1:B:3955:GLU:H	1:B:3955:GLU:CD	2.28	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:185:LYS:HA	1:A:188:GLU:CD	2.46	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
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:2353:LEU:HD23	1:A:2353:LEU:C	2.47	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:2353:LEU:HD23	1:B:2353:LEU:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:250:HIS:CD2	3:F:340:ILE:HG22	2.54	0.40
3:F:368:SER:C	3:F:372:LYS:HZ2	2.30	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 [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	62
1	B	4509/4646 (97%)	4356 (97%)	132 (3%)	21 (0%)	24	57
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%)	18	51
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	23
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%)	31	62

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
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%)	4034 (100%)	10 (0%)	87	85
1	B	4028/4125 (98%)	4015 (100%)	13 (0%)	86	83
2	C	344/557 (62%)	344 (100%)	0	100	100
2	D	344/557 (62%)	344 (100%)	0	100	100
3	E	279/422 (66%)	279 (100%)	0	100	100
3	F	279/422 (66%)	279 (100%)	0	100	100
4	G	87/89 (98%)	87 (100%)	0	100	100
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%)	61	72
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%)	9818 (100%)	24 (0%)	85	85

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	219	GLN
1	A	1390	LEU
1	A	1397	ASN
1	A	1430	THR
1	A	1452	VAL
1	A	2729	ARG
1	A	3373	SER
1	A	3378	ASN
1	A	3395	TRP
1	A	3397	ILE
1	B	1203	GLN
1	B	1204	PHE
1	B	1213	ASN
1	B	1214	ILE

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Mol	Chain	Res	Type
1	B	1354	VAL
1	B	1394	MET
1	B	1395	LYS
1	B	1452	VAL
1	B	2729	ARG
1	B	3373	SER
1	B	3378	ASN
1	B	3395	TRP
1	B	3397	ILE
5	J	8	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	102	ASN
1	A	195	HIS
1	A	280	ASN
1	A	421	GLN
1	A	456	HIS
1	A	460	GLN
1	A	1186	GLN
1	A	1222	ASN
1	A	1233	GLN
1	A	1569	GLN
1	A	1643	ASN
1	A	1646	ASN
1	A	1670	ASN
1	A	1855	GLN
1	A	1894	GLN
1	A	1931	ASN
1	A	1976	GLN
1	A	2067	ASN
1	A	2171	HIS
1	A	2296	GLN
1	A	2463	HIS
1	A	2464	GLN
1	A	2471	GLN
1	A	2475	ASN
1	A	2554	GLN
1	A	2685	GLN
1	A	2713	ASN

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Mol	Chain	Res	Type
1	A	2725	HIS
1	A	2930	GLN
1	A	3069	ASN
1	A	3092	ASN
1	A	3200	HIS
1	A	3214	GLN
1	A	3378	ASN
1	A	3383	ASN
1	A	3523	GLN
1	A	3526	GLN
1	A	3602	ASN
1	A	3636	GLN
1	A	3735	GLN
1	A	3744	GLN
1	A	3754	ASN
1	A	3877	HIS
1	A	3878	GLN
1	A	3956	GLN
1	A	4054	HIS
1	A	4335	GLN
1	A	4425	GLN
1	A	4429	GLN
1	A	4453	ASN
1	A	4532	ASN
1	A	4566	GLN
1	B	150	HIS
1	B	195	HIS
1	B	330	ASN
1	B	421	GLN
1	B	607	GLN
1	B	680	GLN
1	B	731	ASN
1	B	773	GLN
1	B	871	HIS
1	B	882	GLN
1	B	1056	GLN
1	B	1151	GLN
1	B	1200	GLN
1	B	1222	ASN
1	B	1569	GLN
1	B	1643	ASN
1	B	1646	ASN

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Mol	Chain	Res	Type
1	B	1670	ASN
1	B	1855	GLN
1	B	1856	GLN
1	B	1894	GLN
1	B	1931	ASN
1	B	1974	GLN
1	B	1976	GLN
1	B	2067	ASN
1	B	2171	HIS
1	B	2296	GLN
1	B	2463	HIS
1	B	2464	GLN
1	B	2471	GLN
1	B	2475	ASN
1	B	2554	GLN
1	B	2685	GLN
1	B	2713	ASN
1	B	2725	HIS
1	B	2930	GLN
1	B	3069	ASN
1	B	3092	ASN
1	B	3200	HIS
1	B	3214	GLN
1	B	3378	ASN
1	B	3383	ASN
1	B	3523	GLN
1	B	3526	GLN
1	B	3602	ASN
1	B	3636	GLN
1	B	3735	GLN
1	B	3744	GLN
1	B	3754	ASN
1	B	3877	HIS
1	B	3878	GLN
1	B	3956	GLN
1	B	4054	HIS
1	B	4098	ASN
1	B	4335	GLN
1	B	4425	GLN
1	B	4453	ASN
1	B	4532	ASN
1	B	4566	GLN

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Mol	Chain	Res	Type
2	D	290	GLN
2	D	330	HIS
2	D	344	HIS
2	D	356	GLN
2	D	380	HIS
2	D	462	HIS
3	F	159	HIS
3	F	295	HIS
5	I	51	ASN
5	I	80	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	4703	-	28,29,29	0.47	0	43,45,45	0.47	0
7	ADP	A	4704	-	28,29,29	0.46	0	43,45,45	0.47	0
7	ADP	B	4704	-	28,29,29	0.46	0	43,45,45	0.47	0
8	ATP	B	4702	9	32,33,33	0.55	0	48,52,52	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ADP	B	4703	-	28,29,29	0.47	0	43,45,45	0.47	0
8	ATP	A	4702	9	32,33,33	0.55	0	48,52,52	0.58	0
7	ADP	A	4701	9	28,29,29	0.46	0	43,45,45	0.49	0
7	ADP	B	4701	9	28,29,29	0.45	0	43,45,45	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ADP	A	4703	-	-	0/16/32/32	0/3/3/3
7	ADP	A	4704	-	-	2/16/32/32	0/3/3/3
7	ADP	B	4704	-	-	2/16/32/32	0/3/3/3
8	ATP	B	4702	9	-	2/22/38/38	0/3/3/3
7	ADP	B	4703	-	-	0/16/32/32	0/3/3/3
8	ATP	A	4702	9	-	2/22/38/38	0/3/3/3
7	ADP	A	4701	9	-	0/16/32/32	0/3/3/3
7	ADP	B	4701	9	-	0/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

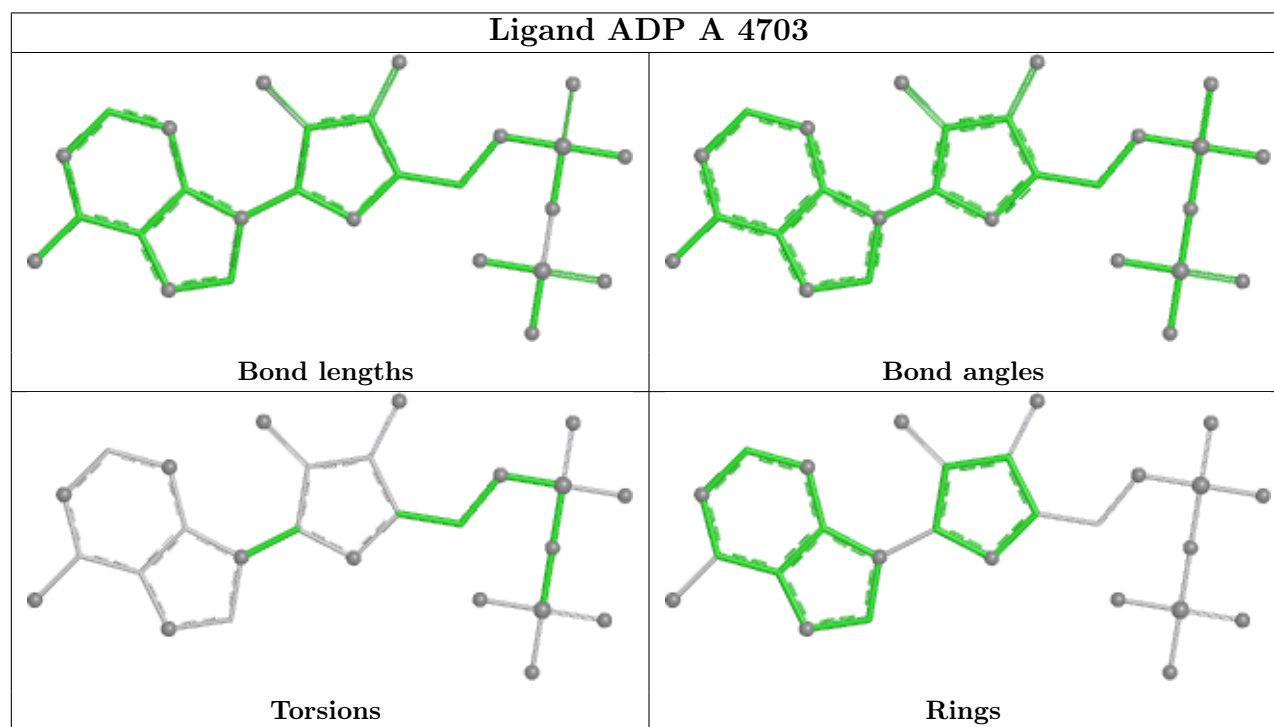
Mol	Chain	Res	Type	Atoms
7	A	4704	ADP	PA-O3A-PB-O2B
7	B	4704	ADP	PA-O3A-PB-O2B
8	A	4702	ATP	O4'-C4'-C5'-O5'
8	B	4702	ATP	O4'-C4'-C5'-O5'
7	A	4704	ADP	PA-O3A-PB-O1B
7	B	4704	ADP	PA-O3A-PB-O1B
8	A	4702	ATP	C3'-C4'-C5'-O5'
8	B	4702	ATP	C3'-C4'-C5'-O5'

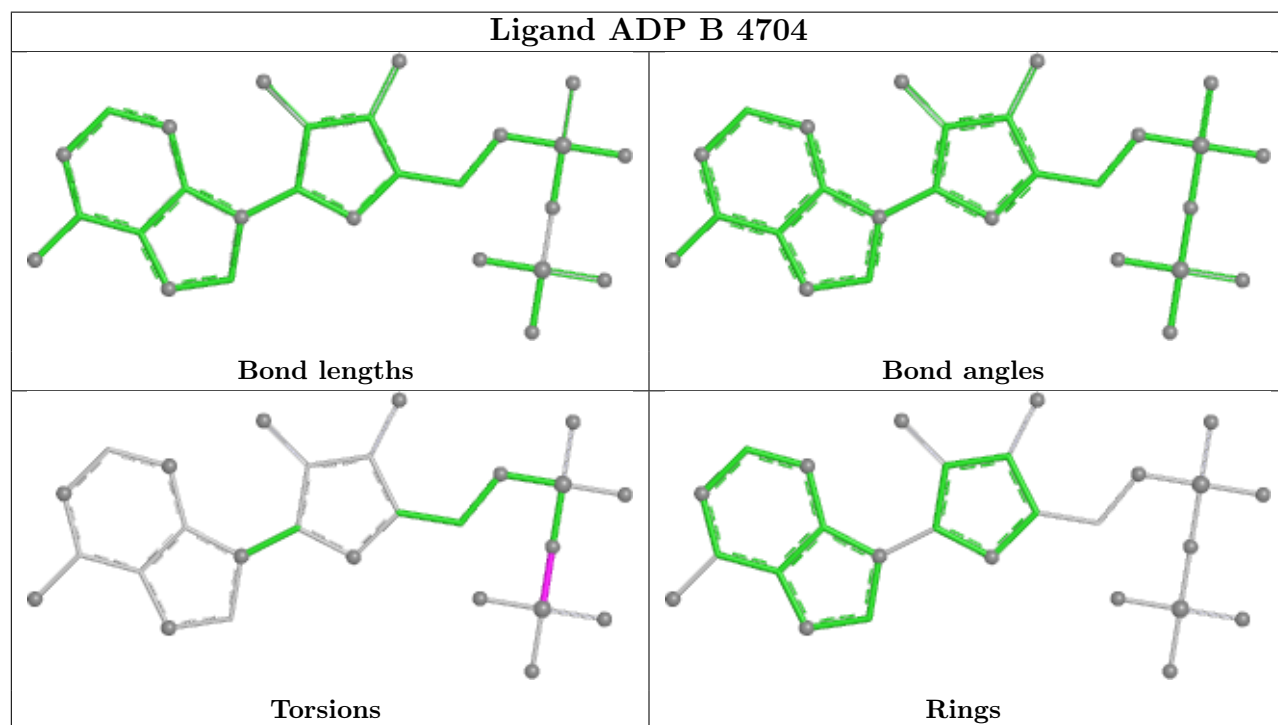
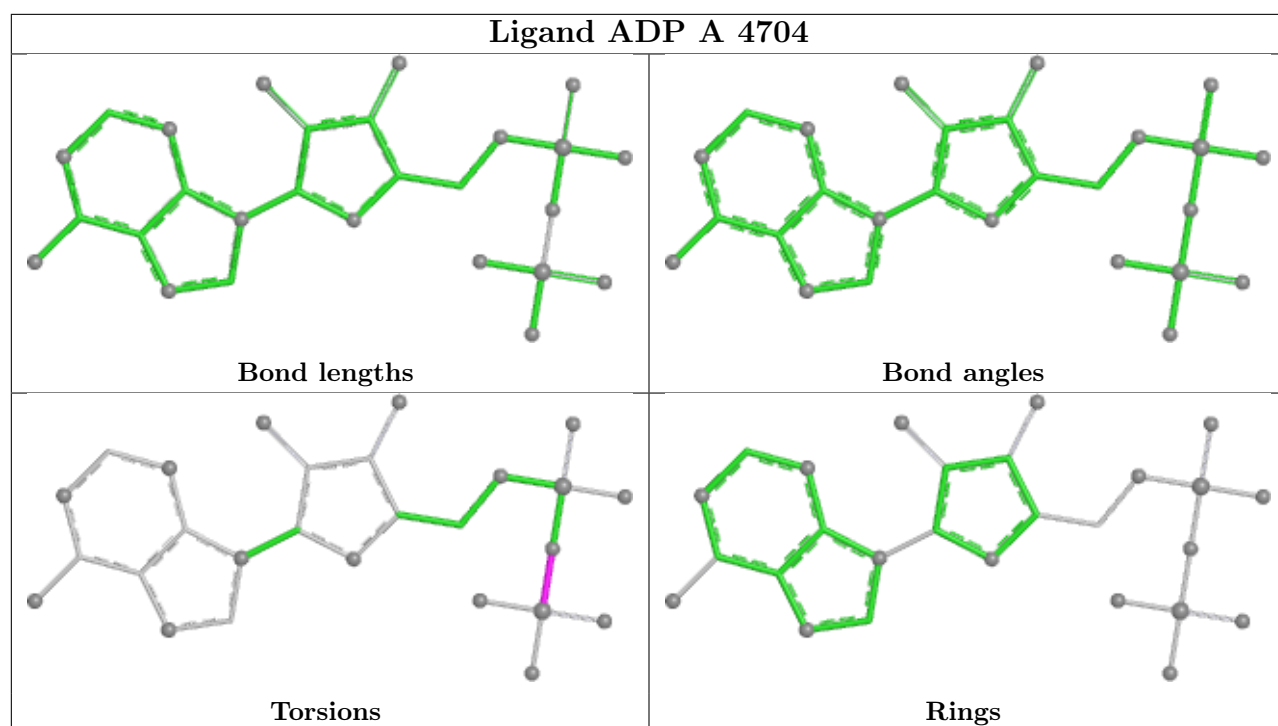
There are no ring outliers.

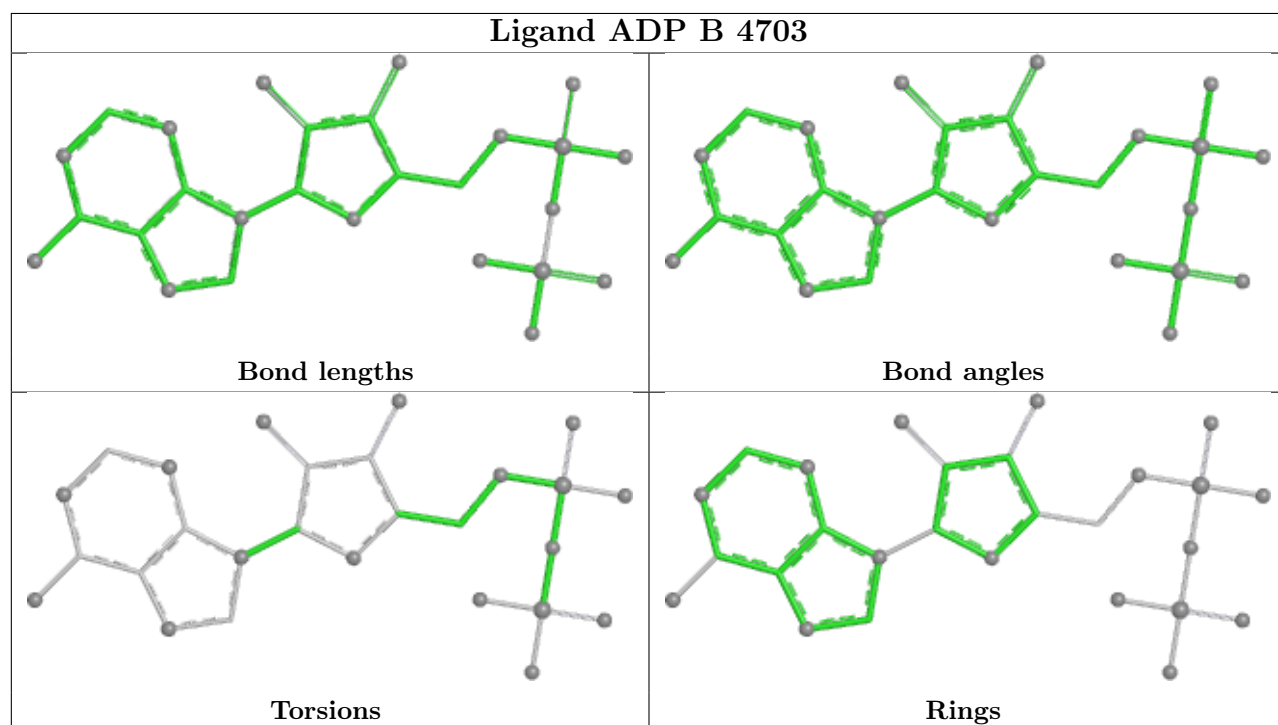
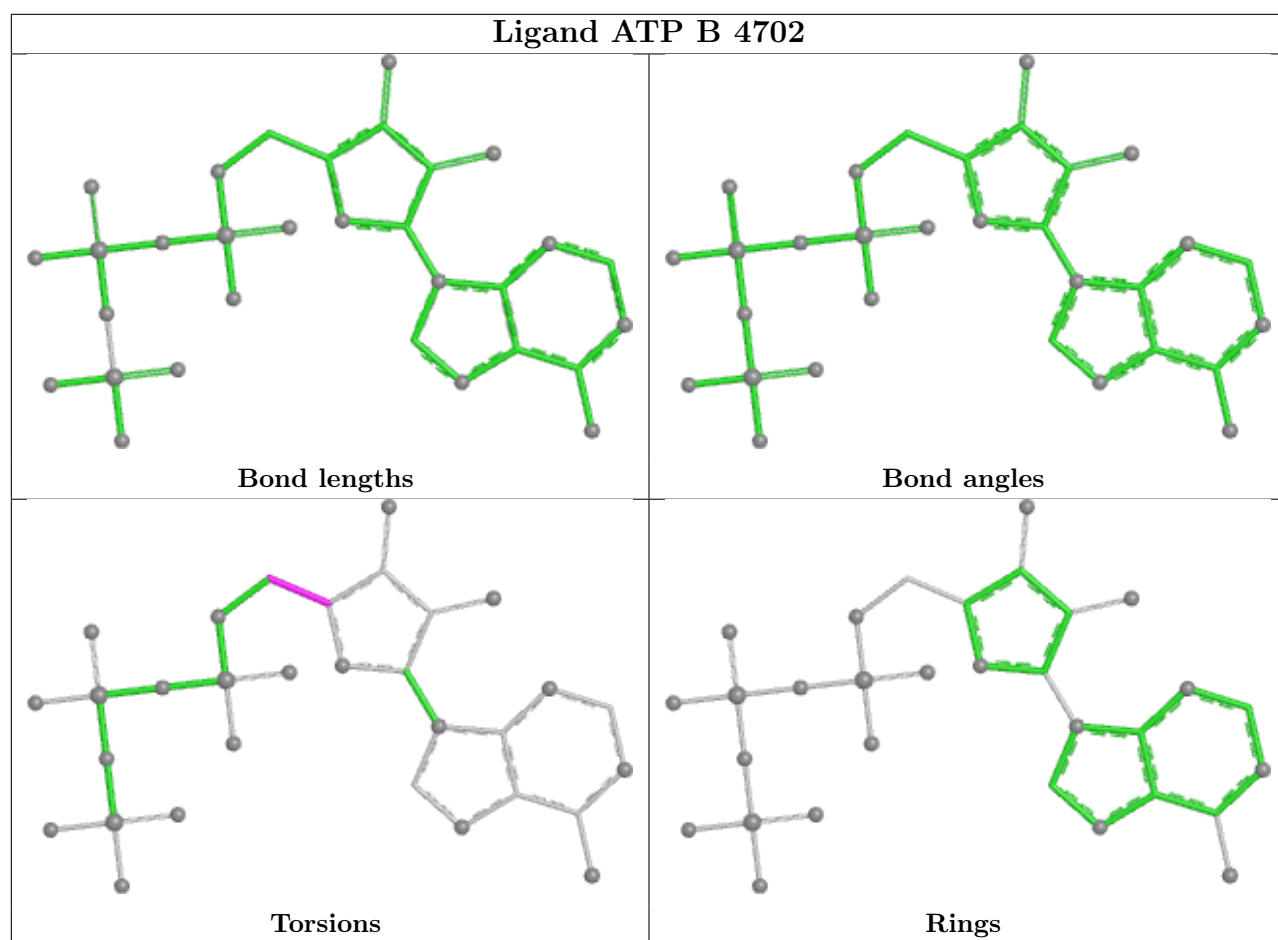
4 monomers are involved in 12 short contacts:

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

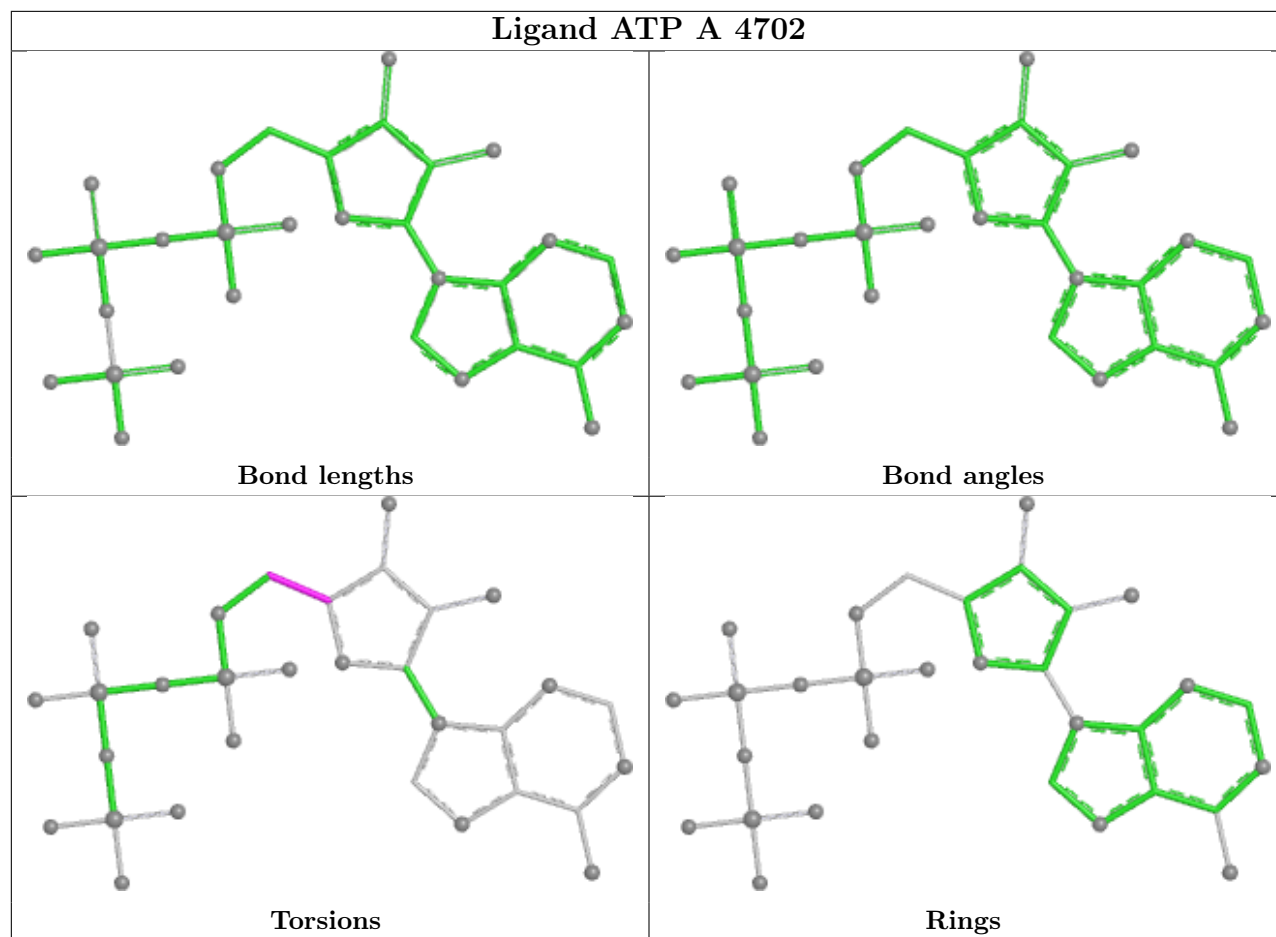
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



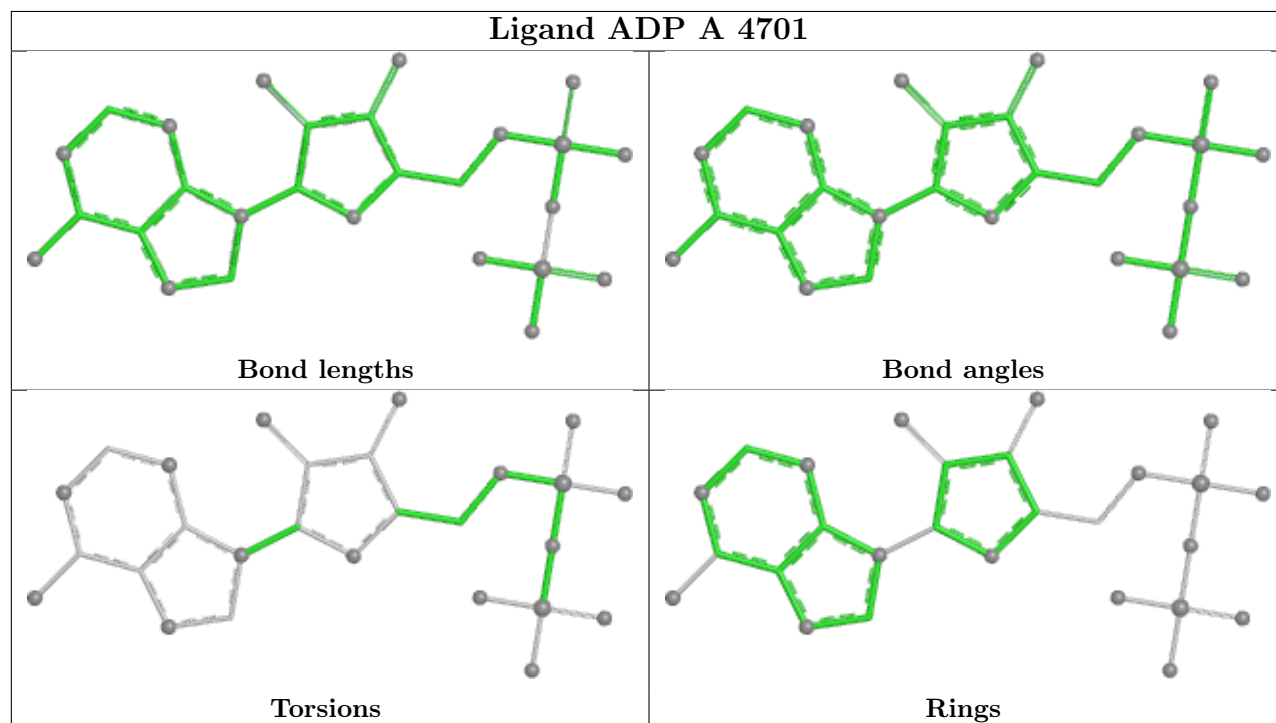


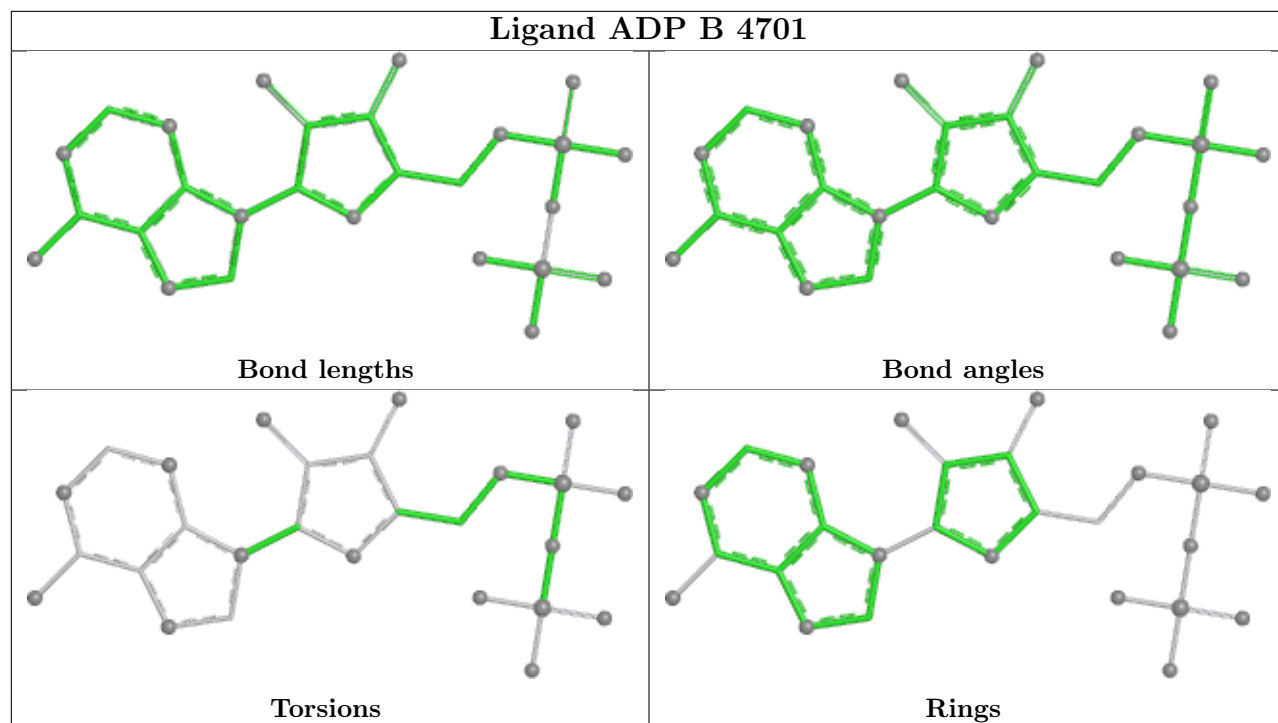


Ligand ATP A 4702



Ligand ADP A 4701





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.

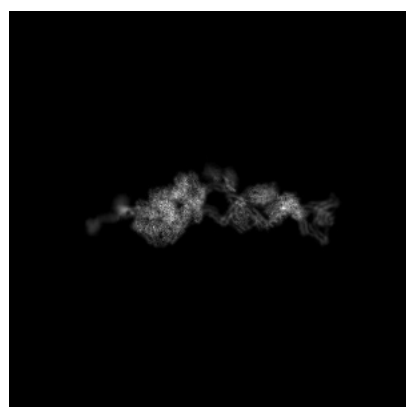
6 Map visualisation [i](#)

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.

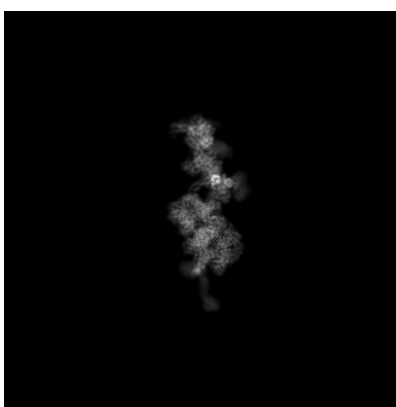
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

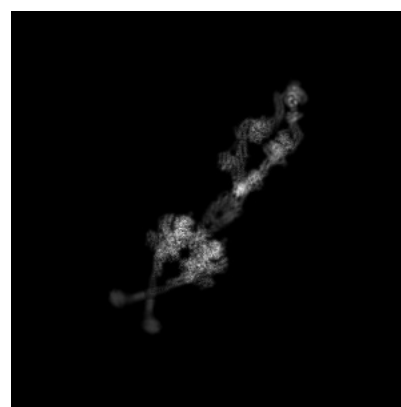
6.1.1 Primary map



X



Y



Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

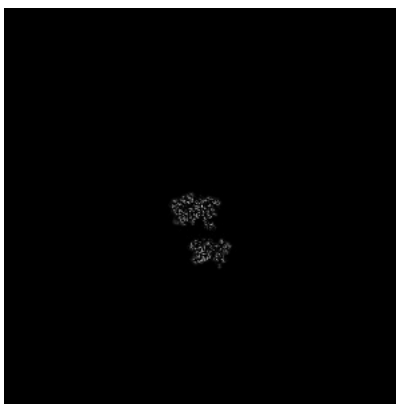
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 228



Y Index: 204

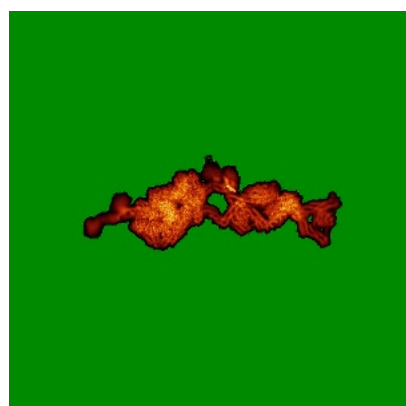


Z Index: 258

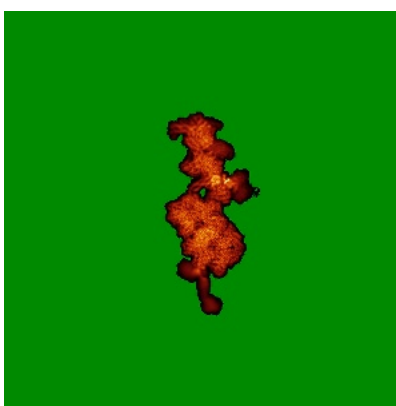
The images above show the largest variance slices of the map in three orthogonal directions.

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

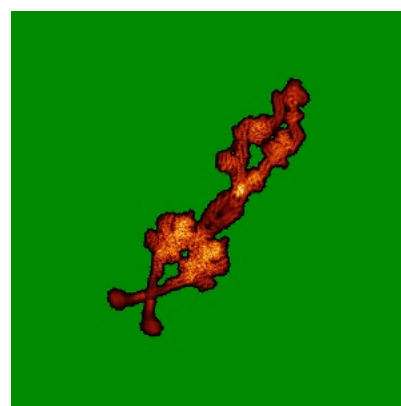
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

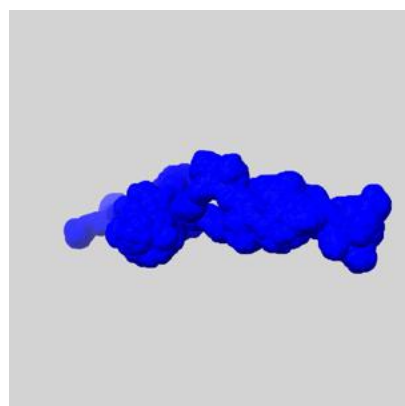
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

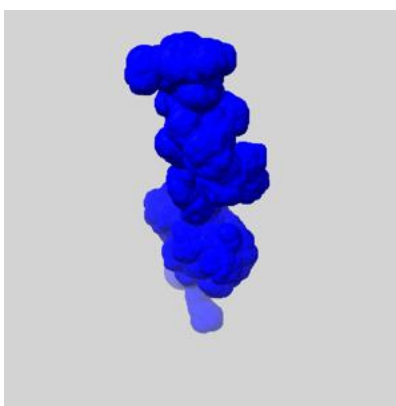
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

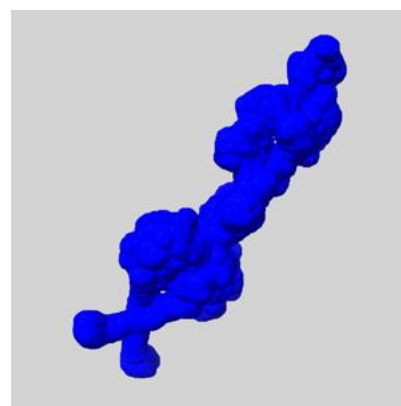
6.6.1 emd_44681_msk_1.map [i](#)



X



Y

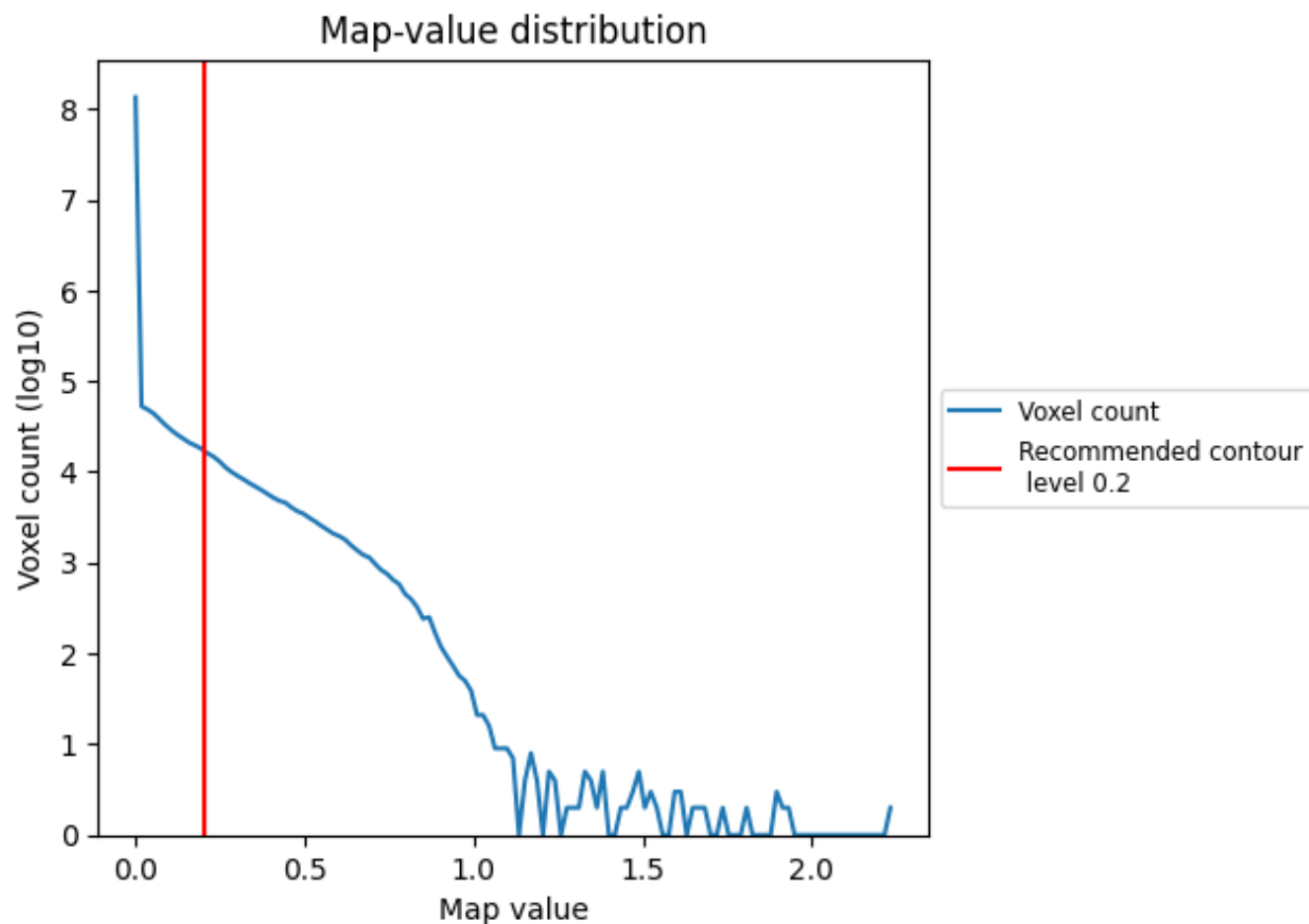


Z

7 Map analysis [i](#)

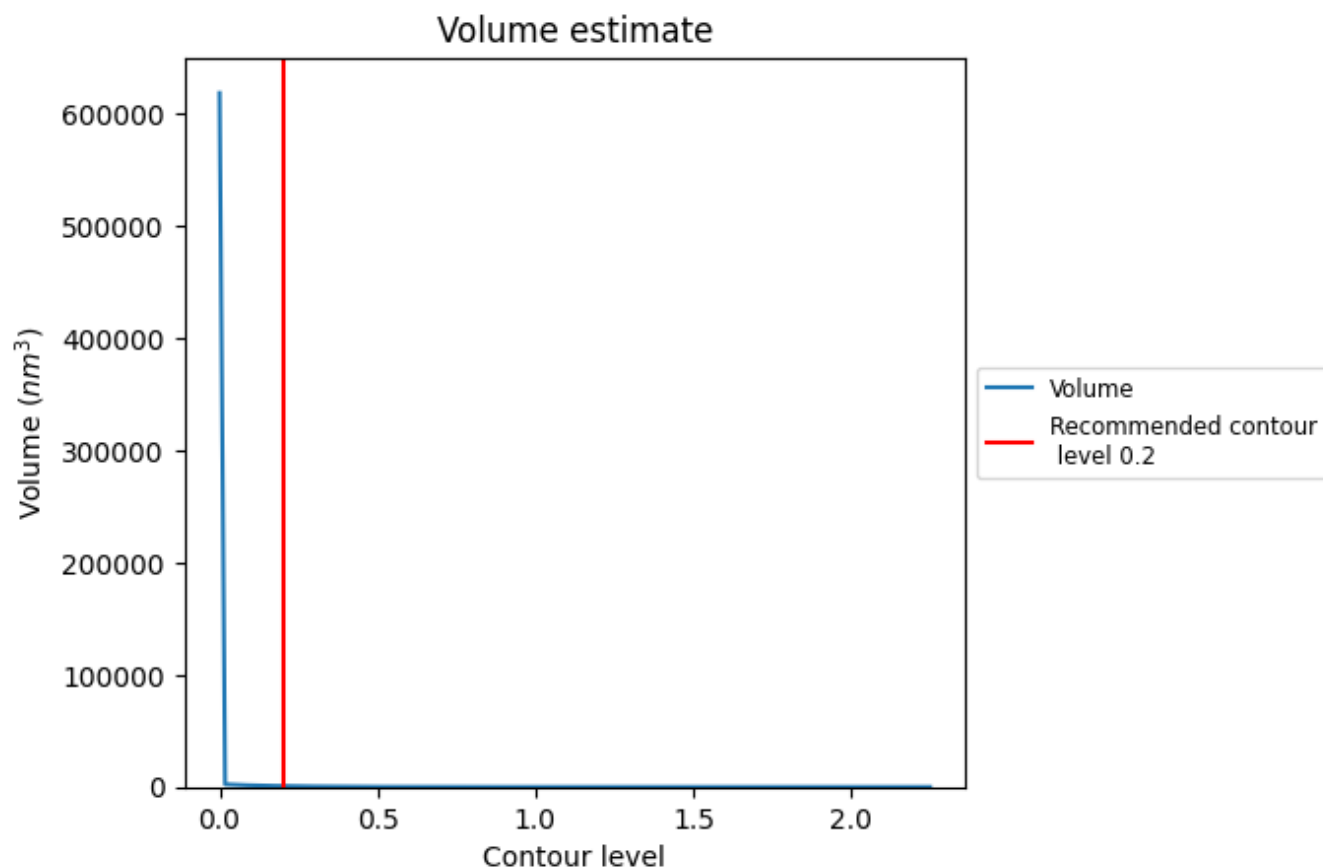
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

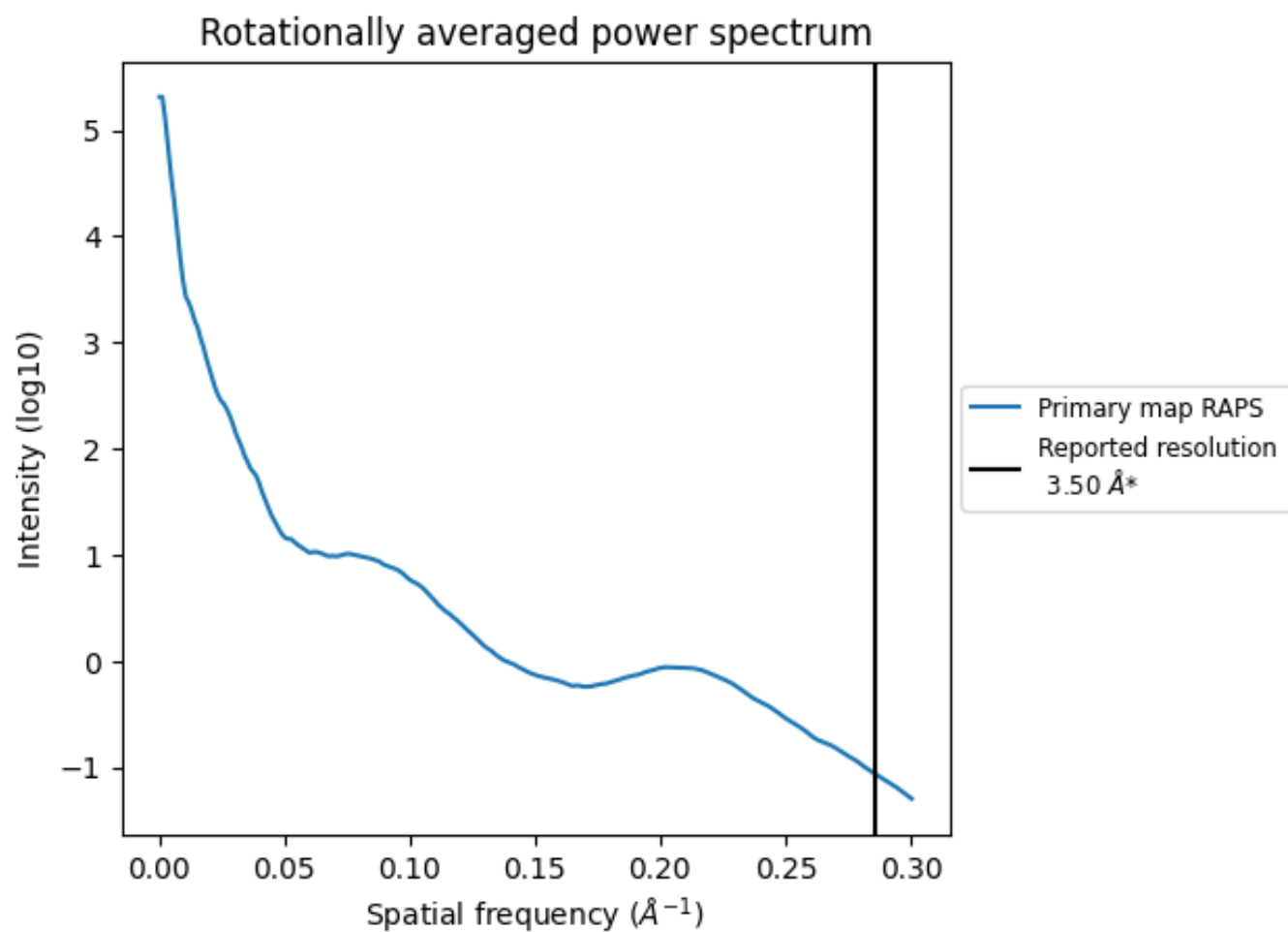
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 810 nm^3 ; this corresponds to an approximate mass of 731 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

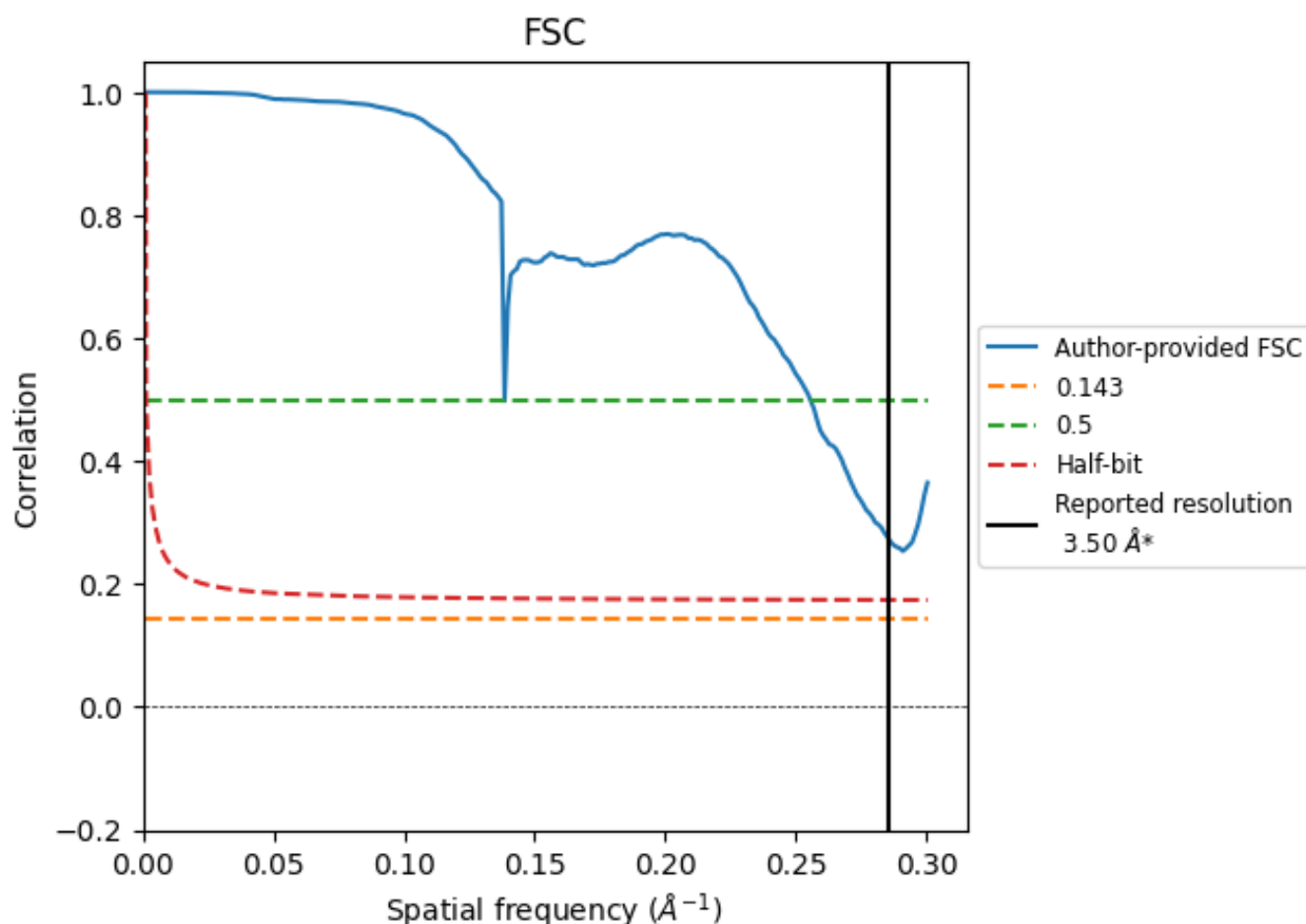


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

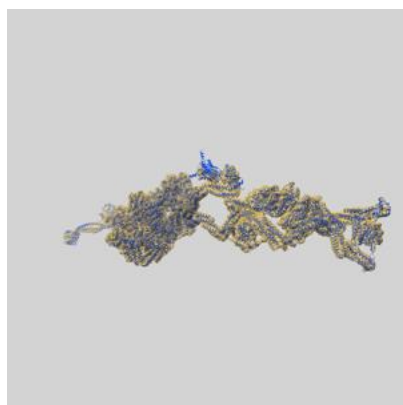
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	7.22	-
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

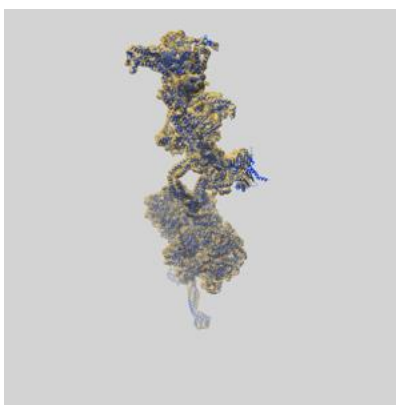
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44681 and PDB model 9BLY. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

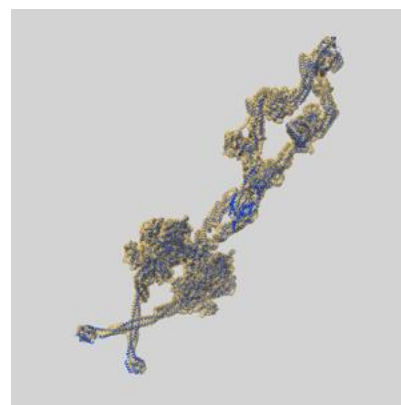
9.1 Map-model overlay [i](#)



X



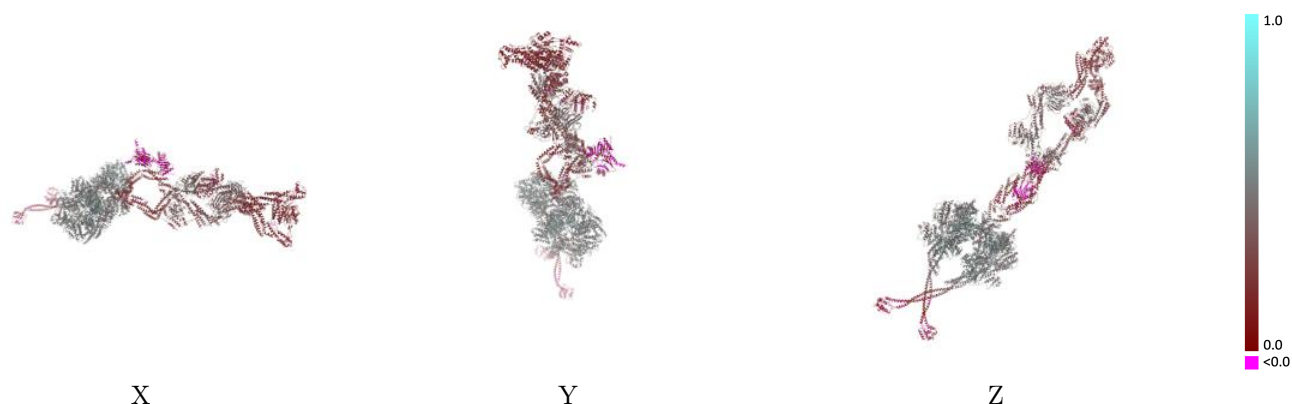
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)

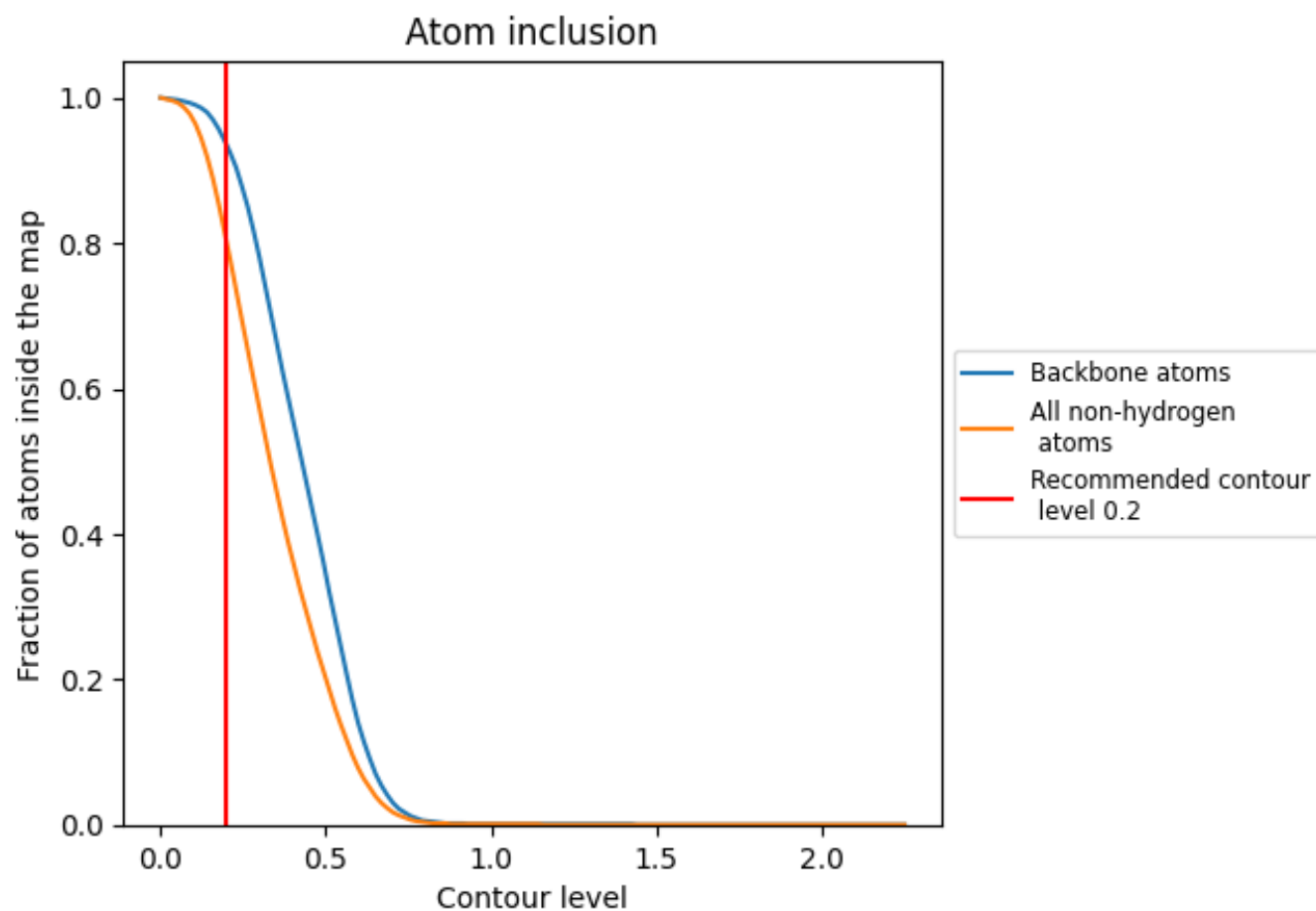


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8020	<div></div> 0.3680
A	<div></div> 0.8120	<div></div> 0.3890
B	<div></div> 0.8190	<div></div> 0.3860
C	<div></div> 0.8850	<div></div> 0.3810
D	<div></div> 0.8570	<div></div> 0.3470
E	<div></div> 0.8340	<div></div> 0.3510
F	<div></div> 0.8580	<div></div> 0.3310
G	<div></div> 0.6840	<div></div> 0.1860
H	<div></div> 0.7400	<div></div> 0.1990
I	<div></div> 0.5190	<div></div> 0.0560
J	<div></div> 0.5850	<div></div> 0.0370
K	<div></div> 0.1050	<div></div> 0.0280
L	<div></div> 0.1960	<div></div> 0.0710

